



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:23 PM UTC

PDB ID : 6R5R / pdb_00006r5r
Title : The crystal structure of Glycoside Hydrolase BglX inactive mutant D286N from *P. aeruginosa* in complex with cellobiose
Authors : Batuecas, M.T.; Hermoso, J.A.
Deposited on : 2019-03-25
Resolution : 1.65 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

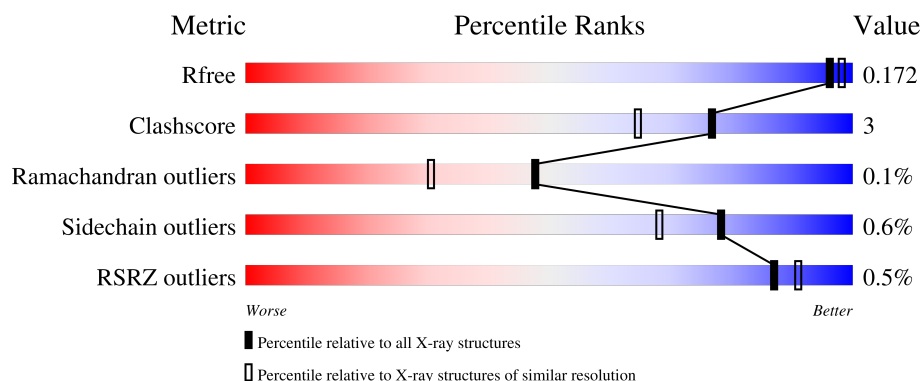
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	B	733	
2	A	734	
3	C	2	
3	D	2	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12943 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 Periplasmic beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	733	Total	C	N	O	S	5	16	0
			5707	3597	1022	1068	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	286	ASN	ASP	engineered mutation	UNP Q9I311

- Molecule 2 is a protein called Periplasmic beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	732	Total	C	N	O	S	5	20	0
			5716	3607	1022	1066	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ASN	ASP	engineered mutation	UNP Q9I311
A	?	-	ASP	deletion	UNP Q9I311
A	621	ASP	-	insertion	UNP Q9I311

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



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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
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
			8	5	3		
5	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		

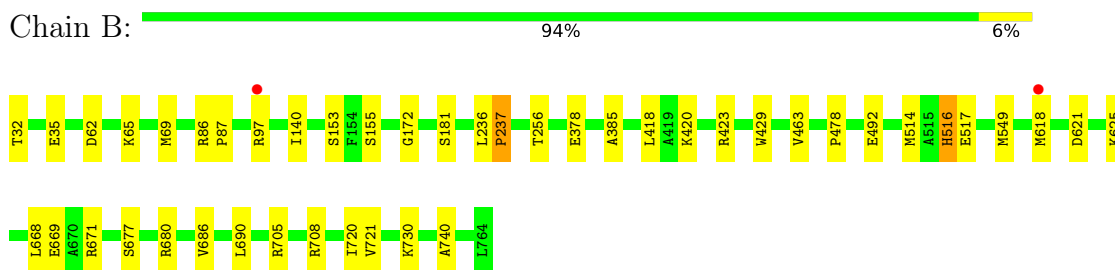
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	746	Total	O	0	0
			746	746		
7	A	663	Total	O	0	0
			663	663		

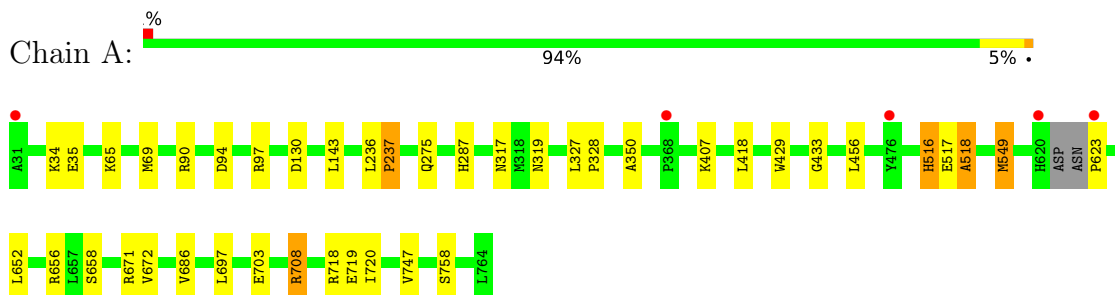
3 Residue-property plots

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: Periplasmic beta-glucosidase



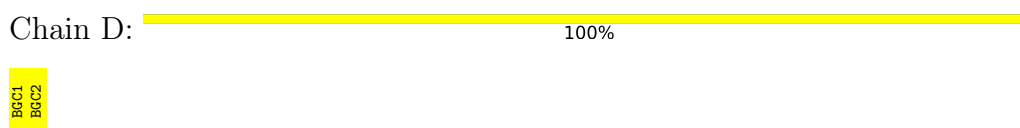
- Molecule 2: Periplasmic beta-glucosidase



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.00Å 73.58Å 81.36Å 65.60° 73.67° 69.70°	Depositor
Resolution (Å)	45.37 – 1.65 45.37 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.3 (45.37-1.65) 96.3 (45.37-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.135 , 0.161 0.148 , 0.172	Depositor DCC
R_{free} test set	8064 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.8	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	0.97	EDS
Total number of atoms	12943	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: MG, BGC, PEG, PGE

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	B	1.05	4/5867 (0.1%)	1.12	4/7952 (0.1%)
2	A	1.03	2/5887 (0.0%)	1.13	6/7974 (0.1%)
All	All	1.04	6/11754 (0.1%)	1.13	10/15926 (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
2	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	433	GLY	C-O	5.79	1.29	1.23
1	B	181	SER	CA-CB	-5.61	1.44	1.53
2	A	287	HIS	CE1-NE2	5.54	1.38	1.32
1	B	478	PRO	C-O	-5.38	1.17	1.24
1	B	256	THR	C-O	5.26	1.30	1.23
1	B	172	GLY	C-O	5.25	1.28	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	35	GLU	CB-CG-CD	7.16	124.78	112.60
1	B	378	GLU	CB-CA-C	6.73	121.96	110.79
2	A	549	MET	CG-SD-CE	-6.72	86.11	100.90
1	B	35	GLU	CB-CG-CD	6.44	123.54	112.60
1	B	237	PRO	N-CA-C	6.23	118.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	GLU	N-CA-CB	-5.95	101.38	110.12
2	A	708	ARG	CG-CD-NE	-5.43	100.05	112.00
2	A	317	ASN	CA-CB-CG	5.39	117.99	112.60
2	A	237	PRO	N-CA-C	5.38	117.27	110.70
2	A	90	ARG	CG-CD-NE	-5.20	100.56	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	518	ALA	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5707	0	5750	33	1
2	A	5716	0	5780	33	0
3	C	23	0	21	0	0
3	D	23	0	21	0	0
4	A	21	0	30	1	0
4	B	28	0	40	2	0
5	B	14	0	14	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	663	0	0	15	5
7	B	746	0	0	12	6
All	All	12943	0	11656	67	8

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 (67) 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:97:ARG:NH1	7:B:903:HOH:O	1.72	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:CZ	7:B:903:HOH:O	1.91	1.17
1:B:492:GLU:OE1	7:B:902:HOH:O	1.65	1.11
1:B:621:ASP:OD1	7:B:904:HOH:O	1.74	1.05
1:B:492:GLU:HG2	7:B:1552:HOH:O	1.71	0.91
2:A:130:ASP:OD2	7:A:901:HOH:O	1.92	0.85
2:A:429:TRP:CE2	2:A:516[B]:HIS:HE1	1.95	0.83
1:B:420:LYS:NZ	7:B:906:HOH:O	2.12	0.78
1:B:669:GLU:OE1	1:B:671:ARG:NH1	2.18	0.77
2:A:516[A]:HIS:CD2	7:A:950:HOH:O	2.37	0.77
1:B:516[A]:HIS:CE1	7:A:905:HOH:O	2.40	0.75
2:A:516[B]:HIS:NE2	7:A:904:HOH:O	2.14	0.72
2:A:652:LEU:HD22	2:A:672[B]:VAL:HG11	1.71	0.71
2:A:94:ASP:HB3	2:A:97:ARG:HH22	1.56	0.70
1:B:618:MET:HB3	7:B:1390:HOH:O	1.90	0.70
2:A:518:ALA:O	7:A:902:HOH:O	2.09	0.69
2:A:623:PRO:N	7:A:906:HOH:O	2.26	0.67
2:A:703:GLU:OE2	7:A:903:HOH:O	2.12	0.67
1:B:621:ASP:CG	7:B:904:HOH:O	2.31	0.65
2:A:516[B]:HIS:CG	2:A:517:GLU:H	2.15	0.63
2:A:516[B]:HIS:CE1	7:A:945:HOH:O	2.50	0.63
2:A:516[B]:HIS:CG	2:A:517:GLU:N	2.67	0.62
2:A:429:TRP:NE1	2:A:516[B]:HIS:HE1	1.97	0.62
1:B:97:ARG:NH2	7:B:903:HOH:O	2.18	0.61
1:B:97:ARG:HD2	7:B:966:HOH:O	2.01	0.61
1:B:625:LYS:HE3	7:A:916:HOH:O	2.00	0.61
2:A:429:TRP:NE1	2:A:516[B]:HIS:CE1	2.71	0.58
1:B:516[B]:HIS:CG	1:B:517:GLU:N	2.71	0.58
1:B:680:ARG:HH12	4:B:803:PEG:H42	1.69	0.56
1:B:680:ARG:HH12	4:B:803:PEG:C4	2.19	0.56
1:B:423:ARG:NH2	7:B:912:HOH:O	2.27	0.55
2:A:652:LEU:HD22	2:A:672[B]:VAL:CG1	2.37	0.55
1:B:463[B]:VAL:CG1	1:B:514:MET:HE3	2.37	0.54
4:A:802:PEG:H12	7:A:1330:HOH:O	2.08	0.54
2:A:34:LYS:HE3	2:A:350:ALA:HB1	1.91	0.52
1:B:65:LYS:O	1:B:69:MET:HG2	2.09	0.52
1:B:516[B]:HIS:CG	1:B:517:GLU:H	2.28	0.50
2:A:65:LYS:O	2:A:69:MET:HG2	2.11	0.50
2:A:656:ARG:HG2	7:A:1551:HOH:O	2.11	0.50
2:A:275:GLN:HG2	7:A:1443:HOH:O	2.12	0.50
2:A:456:LEU:N	2:A:456:LEU:HD12	2.26	0.50
1:B:429:TRP:CE2	1:B:516[B]:HIS:HE1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:708:ARG:HG3	2:A:720:ILE:HG23	1.96	0.48
2:A:429:TRP:CE2	2:A:516[B]:HIS:CE1	2.87	0.47
1:B:516[A]:HIS:HE1	7:A:905:HOH:O	1.88	0.47
2:A:747:VAL:O	2:A:758[A]:SER:HA	2.16	0.46
1:B:730:LYS:HG2	1:B:740:ALA:HB2	1.97	0.46
1:B:690:LEU:HD12	1:B:705:ARG:HG3	1.98	0.45
1:B:625:LYS:NZ	7:B:905:HOH:O	2.11	0.45
2:A:407:LYS:HE3	7:A:1450:HOH:O	2.17	0.45
2:A:143:LEU:HD12	7:A:1042:HOH:O	2.17	0.44
1:B:418[A]:LEU:HD13	1:B:549:MET:HB2	2.00	0.44
2:A:686:VAL:HG21	2:A:720:ILE:CD1	2.47	0.44
2:A:418[A]:LEU:HD13	2:A:549:MET:HB2	2.00	0.44
1:B:463[B]:VAL:CG1	1:B:514:MET:CE	2.96	0.43
2:A:658:SER:HB3	2:A:671[B]:ARG:HH22	1.83	0.43
1:B:708:ARG:NH2	1:B:721:VAL:O	2.52	0.43
1:B:686:VAL:HG21	1:B:720:ILE:CD1	2.49	0.42
2:A:671[A]:ARG:NH2	2:A:719:GLU:OE1	2.53	0.42
2:A:747:VAL:O	2:A:758[B]:SER:HA	2.19	0.42
2:A:236:LEU:N	2:A:237:PRO:CD	2.84	0.41
2:A:94:ASP:HB3	2:A:97:ARG:NH2	2.29	0.41
1:B:153:SER:HG	1:B:155[A]:SER:HB3	1.86	0.40
1:B:236:LEU:N	1:B:237:PRO:CD	2.84	0.40
2:A:327:LEU:N	2:A:328:PRO:CD	2.85	0.40
1:B:86:ARG:HB3	1:B:87:PRO:HD3	2.02	0.40
1:B:140[A]:ILE:CD1	1:B:385:ALA:CB	3.00	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:904:HOH:O	7:B:1297:HOH:O[1_455]	1.58	0.62
7:A:930:HOH:O	7:A:1293:HOH:O[1_565]	1.75	0.45
7:B:1461:HOH:O	7:B:1561:HOH:O[1_655]	1.82	0.38
1:B:97:ARG:NH1	1:B:677:SER:O[1_655]	1.90	0.30
7:B:1618:HOH:O	7:A:1452:HOH:O[1_645]	2.06	0.14
7:B:1441:HOH:O	7:A:1448:HOH:O[1_546]	2.08	0.12
7:B:1533:HOH:O	7:A:1457:HOH:O[1_645]	2.10	0.10
7:B:902:HOH:O	7:A:1304:HOH:O[1_545]	2.17	0.03

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	B	747/733 (102%)	723 (97%)	24 (3%)	0	100	100
2	A	748/734 (102%)	722 (96%)	24 (3%)	2 (0%)	36	21
All	All	1495/1467 (102%)	1445 (97%)	48 (3%)	2 (0%)	48	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	319[A]	ASN
2	A	319[B]	ASN

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	B	602/586 (103%)	597 (99%)	5 (1%)	73	60
2	A	604/586 (103%)	600 (99%)	4 (1%)	76	64
All	All	1206/1172 (103%)	1197 (99%)	9 (1%)	78	64

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	32	THR
1	B	62	ASP
1	B	516[A]	HIS
1	B	516[B]	HIS

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Mol	Chain	Res	Type
1	B	668	LEU
2	A	516[A]	HIS
2	A	516[B]	HIS
2	A	697	LEU
2	A	718	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	735	GLN
2	A	98	HIS
2	A	443	GLN
2	A	447	ASN
2	A	578	ASN
2	A	588	HIS
2	A	620	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 ⓘ

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	$\# Z > 2$
3	BGC	C	1	3	12,12,12	0.74	0	17,17,17	1.50	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	C	2	3	11,11,12	0.84	0	15,15,17	1.25	1 (6%)
3	BGC	D	1	3	12,12,12	0.86	0	17,17,17	1.16	1 (5%)
3	BGC	D	2	3	11,11,12	0.66	0	15,15,17	1.54	3 (20%)

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
3	BGC	C	1	3	-	0/2/22/22	0/1/1/1
3	BGC	C	2	3	-	0/2/19/22	0/1/1/1
3	BGC	D	1	3	-	0/2/22/22	0/1/1/1
3	BGC	D	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	BGC	C4-C3-C2	-4.00	103.80	110.83
3	D	1	BGC	C4-C3-C2	-3.49	104.71	110.83
3	D	2	BGC	C1-O5-C5	-3.29	107.77	112.19
3	C	2	BGC	C1-O5-C5	-2.83	108.39	112.19
3	D	2	BGC	O3-C3-C2	-2.25	105.46	110.05
3	D	2	BGC	O6-C6-C5	-2.16	103.99	111.33

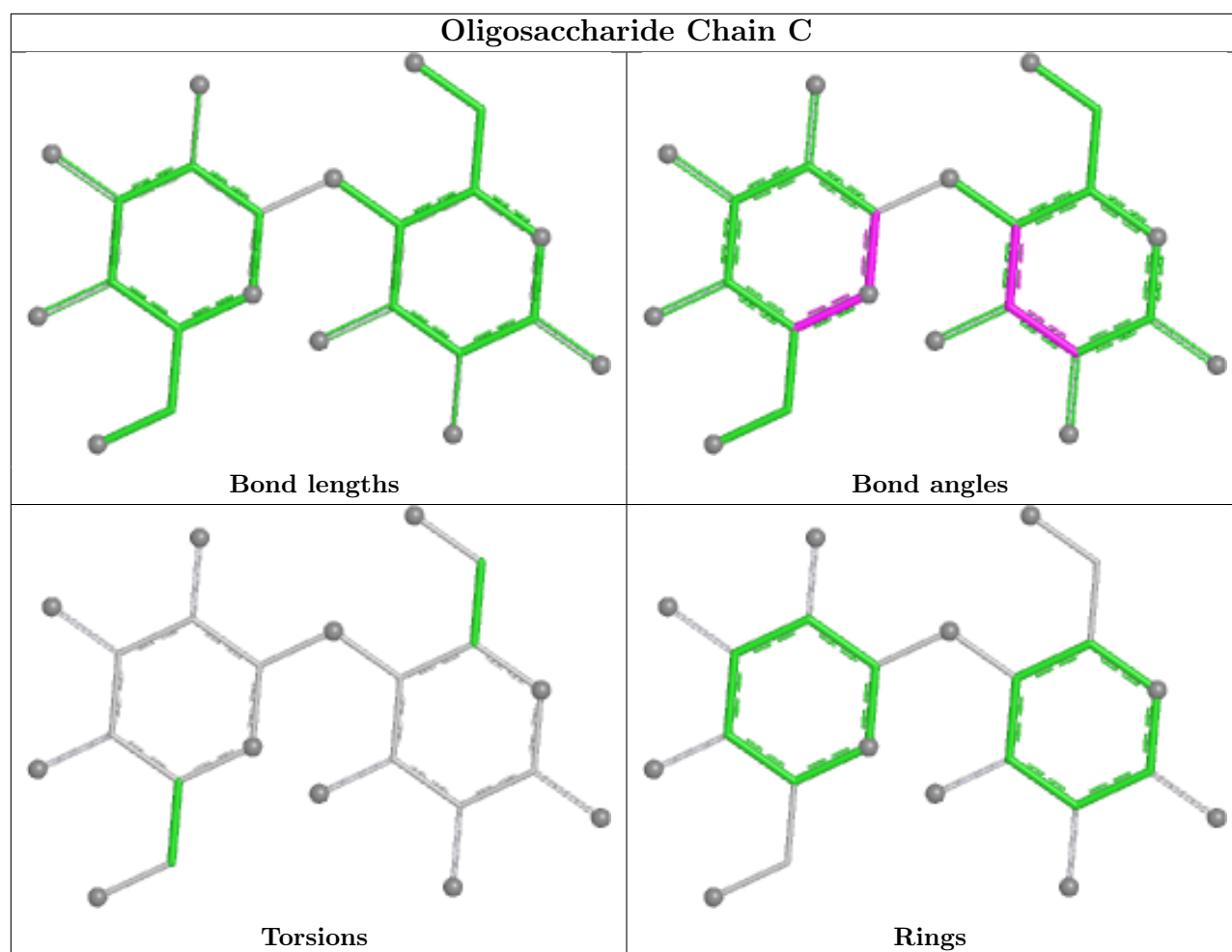
There are no chirality outliers.

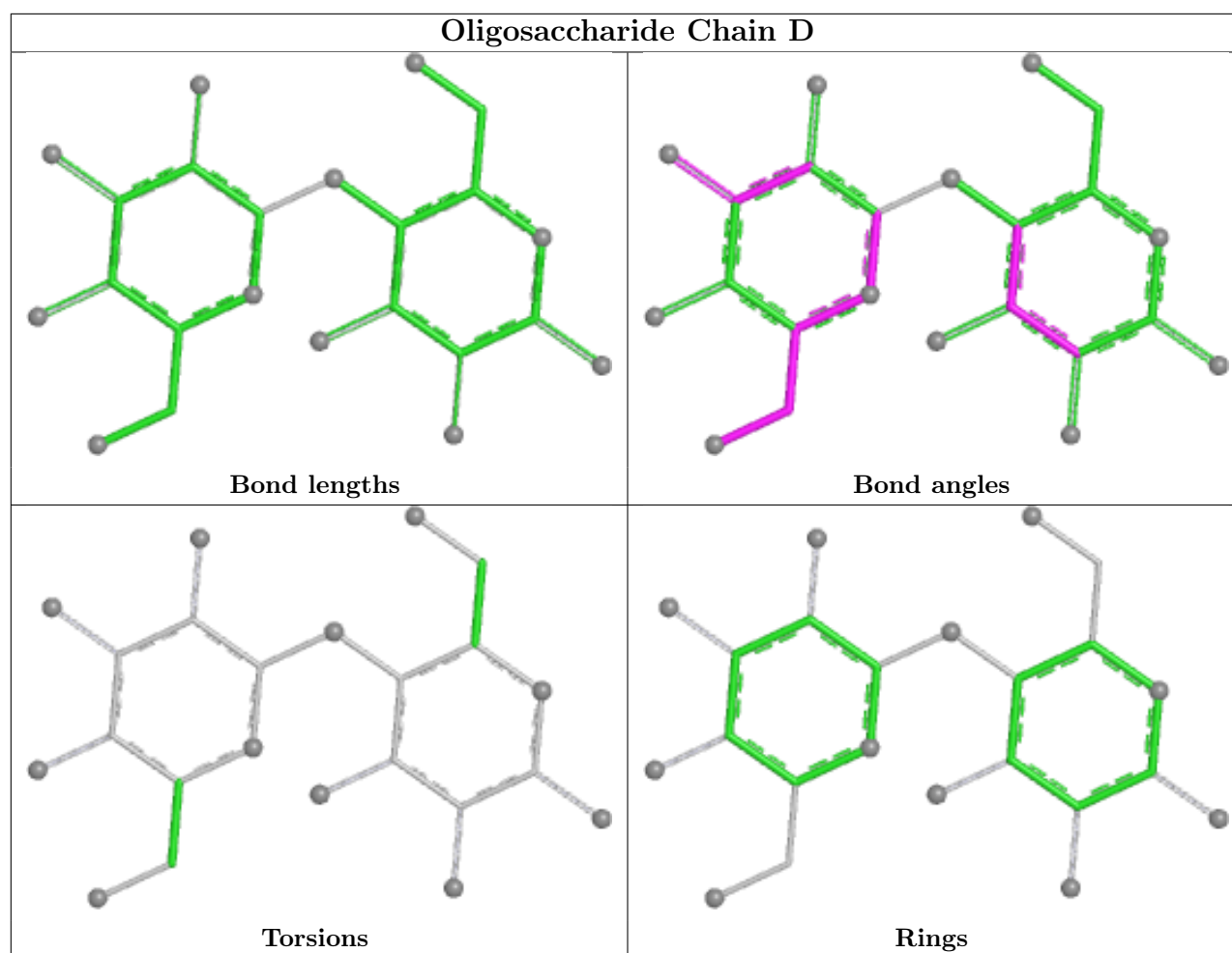
There are no torsion outliers.

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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
4	PEG	A	803	-	6,6,6	0.25	0	5,5,5	0.34	0
4	PEG	A	801	-	6,6,6	0.42	0	5,5,5	0.50	0
4	PEG	A	802	-	6,6,6	0.20	0	5,5,5	0.53	0
4	PEG	B	801	-	6,6,6	0.45	0	5,5,5	0.40	0
5	PGE	B	805	-	6,6,9	0.33	0	4,4,8	0.38	0
4	PEG	B	803	-	6,6,6	0.16	0	5,5,5	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	B	804	-	6,6,6	0.20	0	5,5,5	0.56	0
4	PEG	B	802	-	6,6,6	0.38	0	5,5,5	0.68	0
5	PGE	B	806	-	5,5,9	0.27	0	4,4,8	0.55	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	803	-	-	1/4/4/4	-
4	PEG	A	801	-	-	2/4/4/4	-
4	PEG	A	802	-	-	3/4/4/4	-
4	PEG	B	801	-	-	1/4/4/4	-
5	PGE	B	805	-	-	1/3/3/7	-
4	PEG	B	803	-	-	2/4/4/4	-
4	PEG	B	804	-	-	1/4/4/4	-
4	PEG	B	802	-	-	3/4/4/4	-
5	PGE	B	806	-	-	2/3/3/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803	PEG	O1-C1-C2-O2
4	B	802	PEG	O1-C1-C2-O2
4	A	801	PEG	O2-C3-C4-O4
4	B	803	PEG	O2-C3-C4-O4
4	A	802	PEG	O1-C1-C2-O2
4	A	802	PEG	O2-C3-C4-O4
4	B	804	PEG	O2-C3-C4-O4
4	B	801	PEG	O2-C3-C4-O4
5	B	806	PGE	C3-C4-O3-C5
5	B	806	PGE	O3-C5-C6-O4
4	A	802	PEG	C1-C2-O2-C3
4	B	802	PEG	C1-C2-O2-C3
4	A	801	PEG	C1-C2-O2-C3
5	B	805	PGE	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	A	803	PEG	C1-C2-O2-C3
4	B	802	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	PEG	1	0
4	B	803	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	B	733/733 (100%)	-0.41	2 (0%) 90 93	7, 16, 34, 60	16 (2%)
2	A	732/734 (99%)	-0.33	5 (0%) 84 89	8, 17, 37, 77	20 (2%)
All	All	1465/1467 (99%)	-0.37	7 (0%) 87 91	7, 17, 36, 77	36 (2%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	620	HIS	3.8
2	A	623	PRO	3.5
2	A	368	PRO	3.0
2	A	31	ALA	2.5
1	B	618	MET	2.3
1	B	97	ARG	2.3
2	A	476	TYR	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.

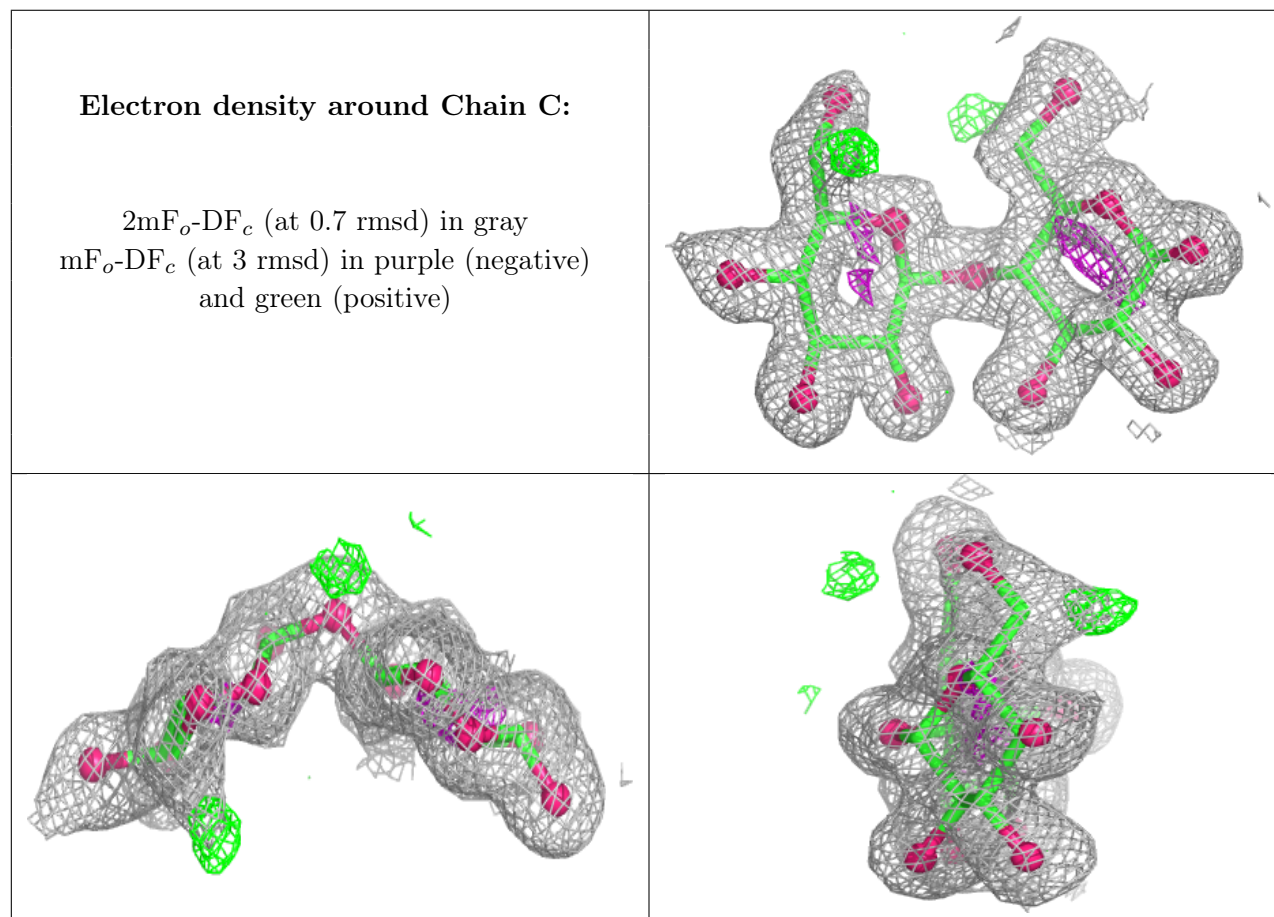
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BGC	C	2	11/12	0.93	0.07	21,26,28,35	0
3	BGC	C	1	12/12	0.95	0.06	16,19,21,21	0

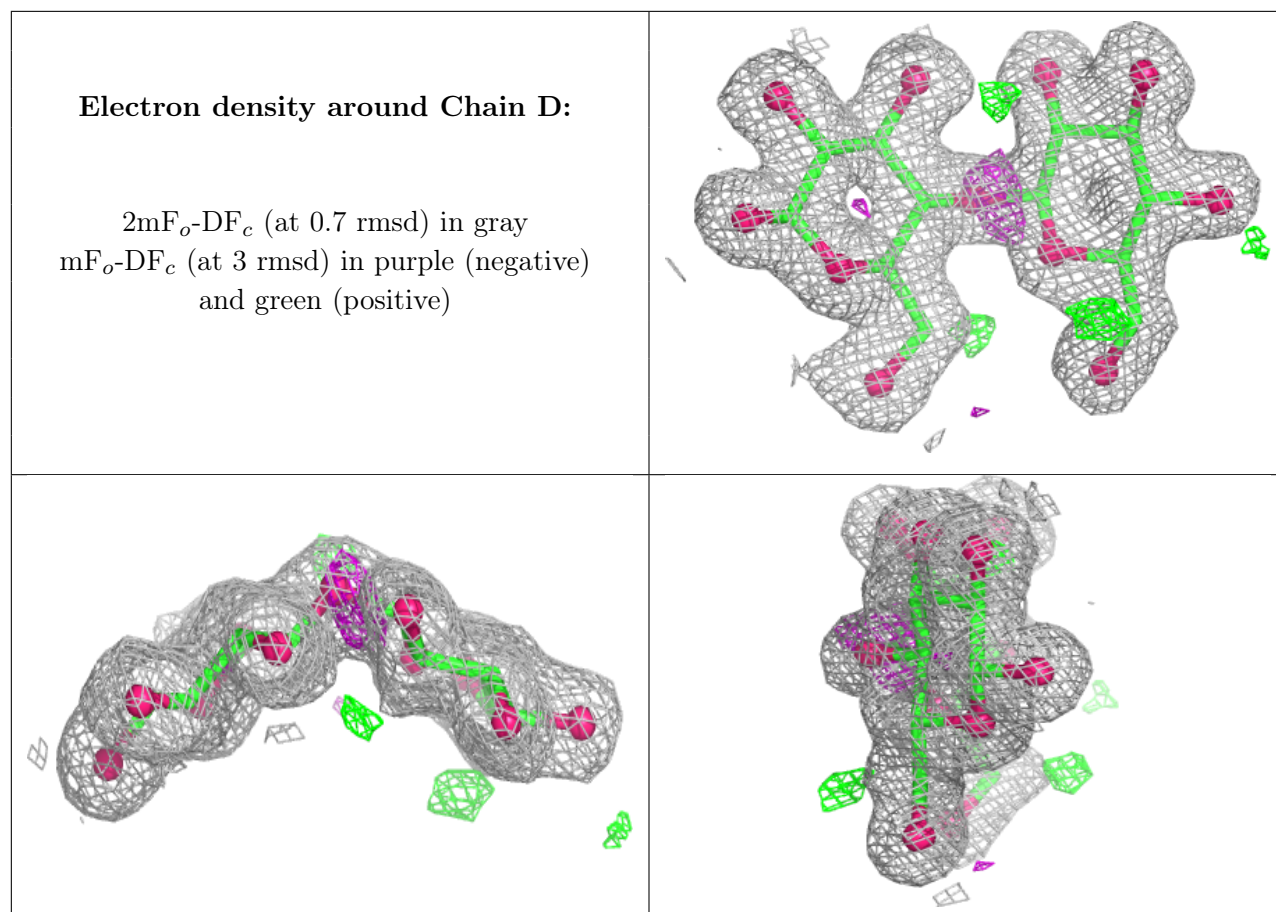
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGC	D	2	11/12	0.95	0.06	20,23,27,29	0
3	BGC	D	1	12/12	0.96	0.05	15,16,20,20	0

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($\text{\AA}^2$)	Q<0.9
5	PGE	B	805	8/10	0.70	0.17	27,35,43,50	0
4	PEG	B	801	7/7	0.77	0.16	40,46,55,56	0
5	PGE	B	806	6/10	0.78	0.13	28,33,36,42	0
4	PEG	B	802	7/7	0.80	0.13	33,40,43,44	0
4	PEG	A	801	7/7	0.81	0.15	48,49,50,54	0
4	PEG	A	802	7/7	0.84	0.13	41,45,51,58	0
4	PEG	B	804	7/7	0.87	0.11	36,38,44,47	0
4	PEG	A	803	7/7	0.89	0.11	39,40,46,50	0
4	PEG	B	803	7/7	0.93	0.09	39,42,45,50	0
6	MG	B	807	1/1	0.98	0.03	17,17,17,17	0
6	MG	A	804	1/1	0.99	0.02	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.