



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2023 – 04:29 pm BST

PDB ID : 8CQF
Title : Crystal Structure of a Chimeric Alpha-Amylase from Pseudoalteromonas Haloplanktis Complexed with Rearranged Acarbose
Authors : Skagseth, S.; Griese, J.J.; Lund, B.A.; van der Ent, F.; Aqvist, J.
Deposited on : 2023-03-06
Resolution : 2.05 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.33

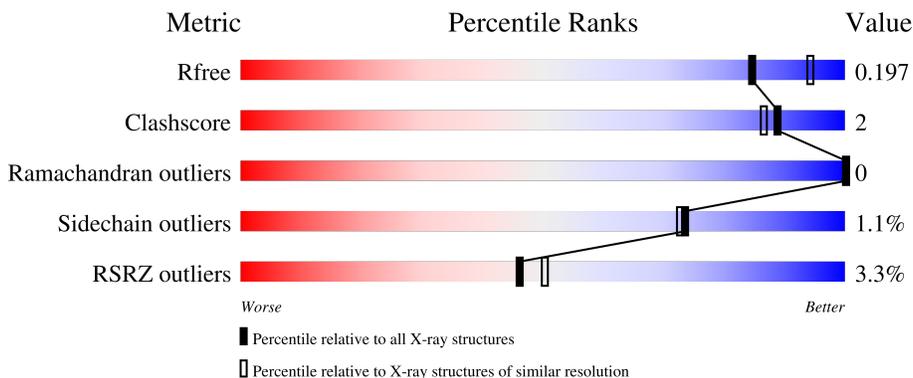
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	450	 3% 93% 6%
2	C	3	 100%
2	D	3	 67% 33%
3	B	2	 100%
4	E	4	 75% 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7369 atoms, of which 3404 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 Alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	448	6718	2181	3232	604	684	17	0	6	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP P29957
A	77	VAL	ALA	engineered mutation	UNP P29957
A	204	LEU	GLN	engineered mutation	UNP P29957
A	209	ILE	-	linker	UNP P29957
A	210	LYS	-	linker	UNP P29957
A	211	SER	-	linker	UNP P29957
A	226	GLY	SER	engineered mutation	UNP P29957
A	227	ALA	THR	engineered mutation	UNP P29957
A	228	LYS	GLU	engineered mutation	UNP P29957
A	231	THR	ASN	engineered mutation	UNP P29957
A	232	VAL	THR	engineered mutation	UNP P29957
A	271	ALA	-	linker	UNP P29957
A	272	GLY	-	linker	UNP P29957
A	273	GLY	-	linker	UNP P29957
A	274	SER	-	linker	UNP P29957
A	275	SER	-	linker	UNP P29957
A	276	ILE	-	linker	UNP P29957
A	277	LEU	-	linker	UNP P29957
A	301	ARG	LYS	engineered mutation	UNP P29957
A	311	ASN	ASP	engineered mutation	UNP P29957
A	312	ASP	THR	engineered mutation	UNP P29957
A	313	TRP	ASP	engineered mutation	UNP P29957
A	449	GLY	-	expression tag	UNP P29957
A	450	ALA	-	expression tag	UNP P29957

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino]-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranos

e-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	D	3	Total	C	H	N	O	0	0	0
			85	25	41	1	18			
2	C	3	Total	C	H	N	O	0	0	0
			85	25	41	1	18			

- Molecule 3 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino]-alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	B	2	Total	C	H	N	O	0	0	0
			63	19	31	1	12			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino]-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	E	4	Total	C	H	N	O	0	0	0
			108	31	53	1	23			

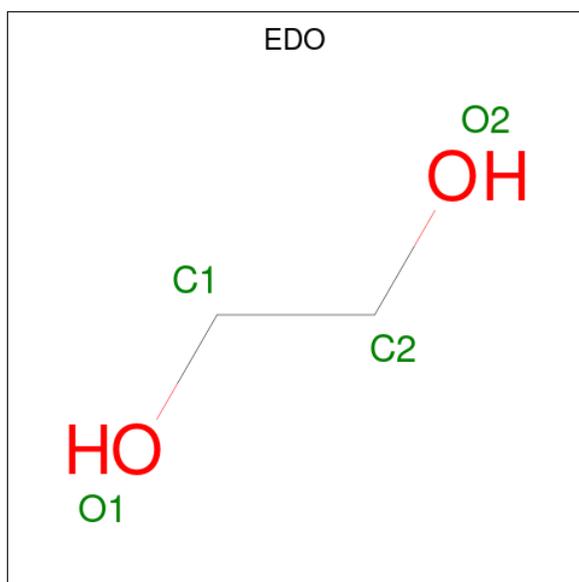
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	10	2	6	2	0	0

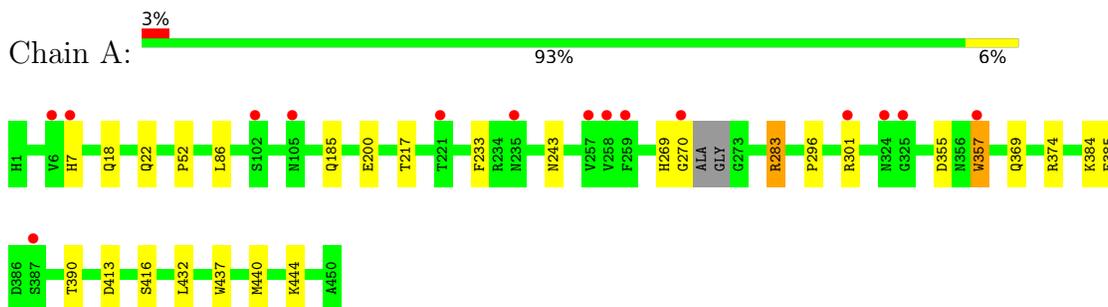
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	297	297	297	0	0

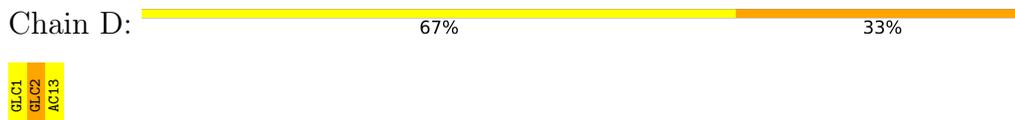
3 Residue-property plots [i](#)

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.

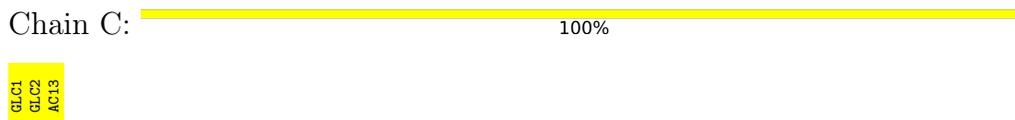
- Molecule 1: Alpha-amylase



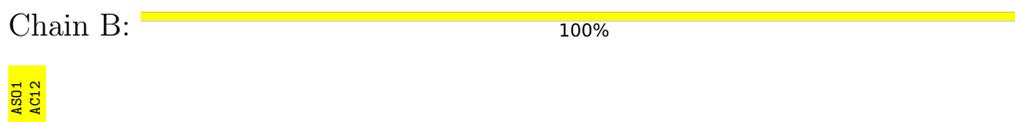
- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ -alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ -alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ -alpha-D-glucopyranose-(1-4)-1,5-anhydro-D-glucitol



- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ -alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.60Å 81.07Å 129.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.69 – 2.05 38.69 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.69-2.05) 97.0 (38.69-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.05Å)	Xtrriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.169 , 0.198 0.169 , 0.197	Depositor DCC
R_{free} test set	1109 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7369	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: AC1, EDO, CA, CL, ASO, GLC

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	0.54	0/3597	0.69	0/4892

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	ARG	Sidechain
1	A	374	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	3486	3232	3218	13	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	41	30	0	0
2	D	44	41	30	1	0
3	B	32	31	21	0	0
4	E	55	53	39	1	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
7	A	4	6	6	0	0
8	A	297	0	0	1	0
All	All	3965	3404	3344	13	1

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 2.

All (13) 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:296:PRO:HB2	1:A:357:TRP:CD1	2.42	0.55
1:A:283:ARG:HD2	1:A:437:TRP:O	2.11	0.50
1:A:269:HIS:O	1:A:270:GLY:C	2.55	0.45
1:A:355:ASP:OD2	1:A:444:LYS:NZ	2.39	0.45
1:A:369:GLN:HG3	1:A:385:GLU:HG3	1.98	0.45
1:A:233:PHE:O	1:A:384:LYS:NZ	2.48	0.45
1:A:357:TRP:CD1	2:D:2:GLC:H2	2.54	0.43
1:A:200:GLU:OE1	4:E:2:AC1:HCB1	2.19	0.43
1:A:18:GLN:O	1:A:22:GLN:HG3	2.20	0.42
1:A:52:PRO:HG3	1:A:86:LEU:HG	2.03	0.41
1:A:185:GLN:NE2	8:A:604:HOH:O	2.37	0.41
1:A:390:THR:HA	1:A:432:LEU:O	2.20	0.41
1:A:7:HIS:HB2	1:A:301:ARG:HD2	2.02	0.40

All (1) 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)
1:A:243[A]:ASN:HD21	1:A:416:SER:OG[3_545]	1.57	0.03

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	450/450 (100%)	433 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	370/365 (101%)	366 (99%)	4 (1%)	73	73

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	THR
1	A	357	TRP
1	A	413	ASP
1	A	440	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 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	ASO	B	1	3	11,11,11	0.34	0	15,15,15	1.35	1 (6%)
3	AC1	B	2	3	21,22,23	0.79	0	22,32,34	1.14	1 (4%)
2	GLC	C	1	2	12,12,12	0.23	0	17,17,17	1.31	2 (11%)
2	GLC	C	2	2	11,11,12	0.32	0	15,15,17	1.96	4 (26%)
2	AC1	C	3	2	21,22,23	1.51	3 (14%)	22,32,34	2.10	8 (36%)
2	GLC	D	1	2	12,12,12	0.22	0	17,17,17	1.29	3 (17%)
2	GLC	D	2	2	11,11,12	0.49	0	15,15,17	1.64	4 (26%)
2	AC1	D	3	2	21,22,23	0.73	0	22,32,34	1.08	2 (9%)
4	GLC	E	1	4	12,12,12	0.89	0	17,17,17	1.50	3 (17%)
4	AC1	E	2	4	21,22,23	2.63	7 (33%)	22,32,34	1.95	6 (27%)
4	GLC	E	3	4	11,11,12	1.69	2 (18%)	15,15,17	1.81	3 (20%)
4	GLC	E	4	4	11,11,12	1.03	0	15,15,17	1.98	5 (33%)

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	ASO	B	1	3	-	0/2/19/19	0/1/1/1
3	AC1	B	2	3	-	1/6/43/46	0/2/2/2
2	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	AC1	C	3	2	-	2/6/43/46	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	1	2	-	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	AC1	D	3	2	-	1/6/43/46	0/2/2/2
4	GLC	E	1	4	-	2/2/22/22	0/1/1/1
4	AC1	E	2	4	-	2/6/43/46	0/2/2/2
4	GLC	E	3	4	-	0/2/19/22	0/1/1/1
4	GLC	E	4	4	-	1/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	AC1	C4A-C5B	7.94	1.57	1.51
4	E	2	AC1	C1B-N4A	4.45	1.55	1.47
4	E	2	AC1	C7B-C5B	4.14	1.38	1.32
2	C	3	AC1	O5-C1	-3.92	1.37	1.43
4	E	2	AC1	C1B-C7B	3.82	1.55	1.50
2	C	3	AC1	C1-C2	3.68	1.60	1.52
4	E	3	GLC	C2-C3	3.35	1.57	1.52
4	E	3	GLC	C1-C2	3.23	1.59	1.52
4	E	2	AC1	C3B-C4A	2.54	1.56	1.53
4	E	2	AC1	C4-N4A	2.27	1.51	1.47
2	C	3	AC1	O2-C2	-2.18	1.38	1.43
4	E	2	AC1	C2-C3	2.12	1.55	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	AC1	C1-C2-C3	-6.01	102.28	109.67
4	E	2	AC1	C7B-C1B-N4A	5.94	119.60	110.68
2	C	2	GLC	O4-C4-C3	-5.09	98.58	110.35
4	E	4	GLC	C1-C2-C3	5.08	115.91	109.67
4	E	3	GLC	C1-C2-C3	4.81	115.58	109.67
4	E	1	GLC	C1-O5-C5	3.59	120.43	113.66
2	C	3	AC1	C7B-C1B-N4A	-3.38	105.61	110.68
4	E	4	GLC	C1-O5-C5	3.23	116.57	112.19
4	E	2	AC1	C4A-C5B-C7B	-3.10	117.13	122.23
2	D	2	GLC	C1-C2-C3	-2.81	106.21	109.67
4	E	4	GLC	C3-C4-C5	2.78	115.19	110.24
2	C	2	GLC	O2-C2-C3	-2.71	104.70	110.14
4	E	2	AC1	O4-C4A-C5B	-2.69	105.63	110.82
4	E	1	GLC	O3-C3-C4	-2.69	104.14	110.35
2	D	2	GLC	C2-C3-C4	-2.68	106.25	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	AC1	O3-C3-C2	-2.68	104.86	109.99
2	C	3	AC1	C2-C3-C4	-2.60	108.33	110.63
2	C	2	GLC	O4-C4-C5	-2.57	102.93	109.30
4	E	3	GLC	C1-O5-C5	2.52	115.61	112.19
4	E	3	GLC	O2-C2-C1	2.52	114.31	109.15
2	C	3	AC1	O6B-C6B-C5B	-2.44	106.66	112.50
2	C	3	AC1	O3-C3-C4	2.42	114.54	109.66
2	D	3	AC1	O4-C4A-C3B	-2.41	105.56	110.53
2	D	2	GLC	O4-C4-C5	-2.39	103.35	109.30
3	B	2	AC1	C1-O5-C5	2.37	118.14	112.78
4	E	4	GLC	C2-C3-C4	2.29	114.86	110.89
3	B	1	ASO	O5-C5-C6	-2.29	103.62	107.20
2	C	1	GLC	O4-C4-C3	-2.23	105.20	110.35
2	C	3	AC1	O3B-C3B-C2B	-2.21	105.25	110.35
4	E	1	GLC	O1-C1-C2	2.18	115.17	109.03
4	E	2	AC1	C2-C3-C4	2.17	112.54	110.63
2	C	1	GLC	O2-C2-C3	-2.17	105.34	110.35
2	D	1	GLC	O2-C2-C3	-2.15	105.39	110.35
2	C	3	AC1	O2B-C2B-C1B	-2.13	104.84	109.12
2	C	2	GLC	C1-C2-C3	-2.12	107.06	109.67
2	C	3	AC1	O2-C2-C1	2.12	113.48	109.15
2	D	3	AC1	O4-C4A-C5B	2.09	114.85	110.82
4	E	2	AC1	C1-O5-C5	2.09	117.50	112.78
2	D	1	GLC	O4-C4-C3	-2.06	105.60	110.35
2	D	2	GLC	O5-C5-C6	-2.05	103.99	107.20
4	E	4	GLC	O5-C5-C6	-2.04	104.01	107.20
2	D	1	GLC	C3-C4-C5	-2.03	106.61	110.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

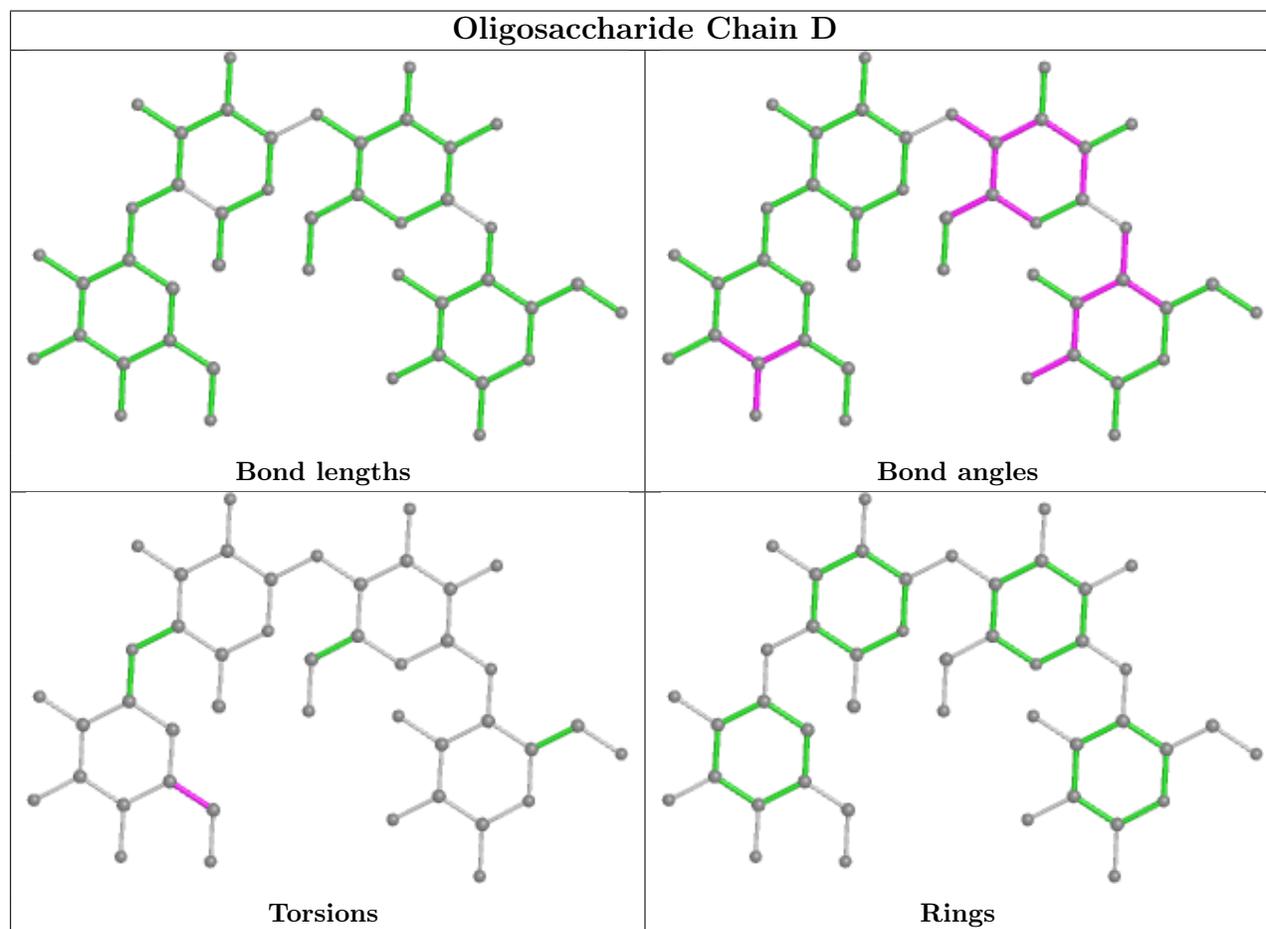
Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C7B-C5B-C6B-O6B
4	E	2	AC1	C7B-C1B-N4A-C4
4	E	2	AC1	C7B-C5B-C6B-O6B
4	E	1	GLC	C4-C5-C6-O6
4	E	1	GLC	O5-C5-C6-O6
2	C	3	AC1	C2B-C1B-N4A-C4
2	C	3	AC1	C5-C4-N4A-C1B
3	B	2	AC1	C7B-C1B-N4A-C4
4	E	4	GLC	O5-C5-C6-O6

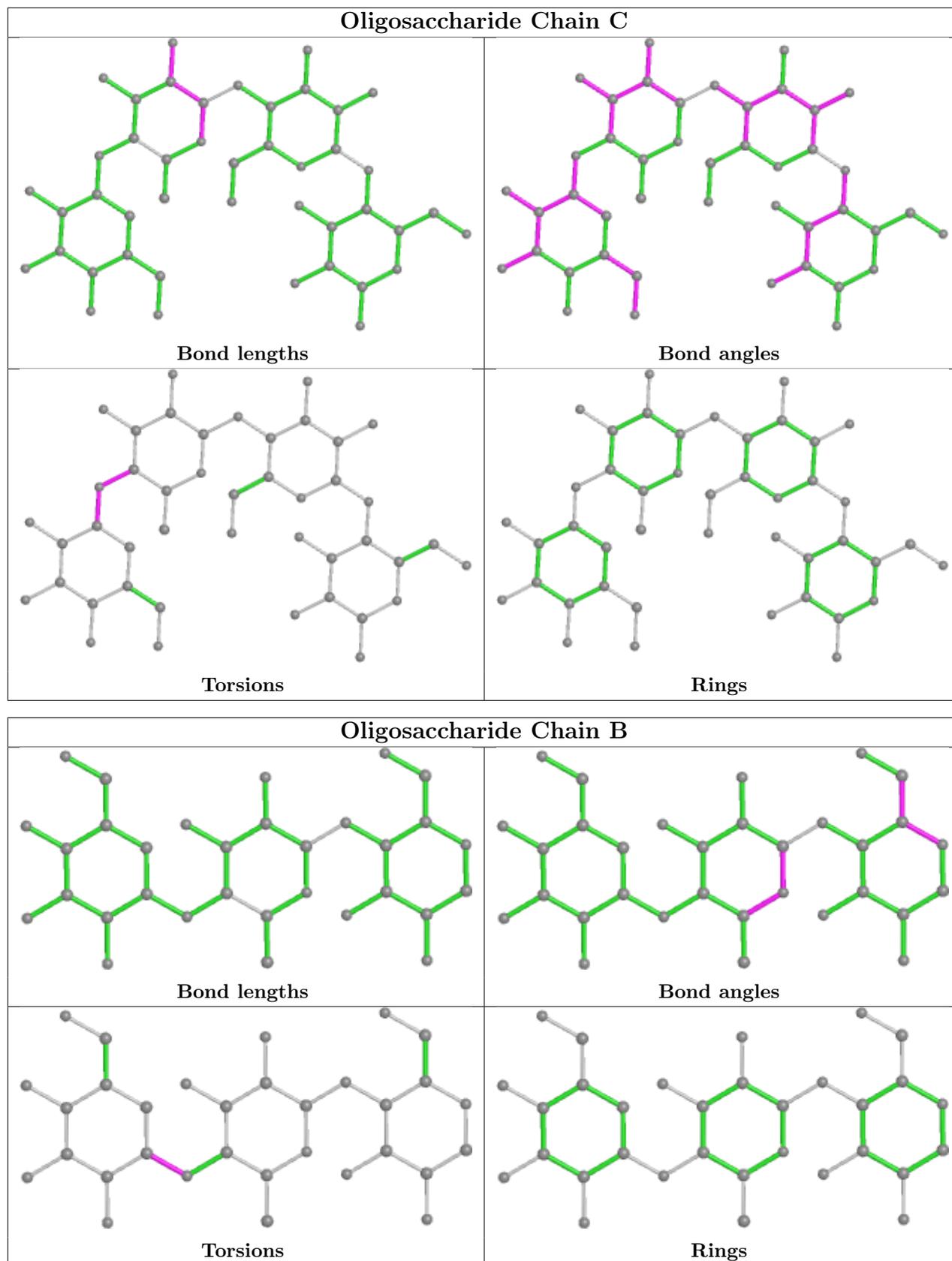
There are no ring outliers.

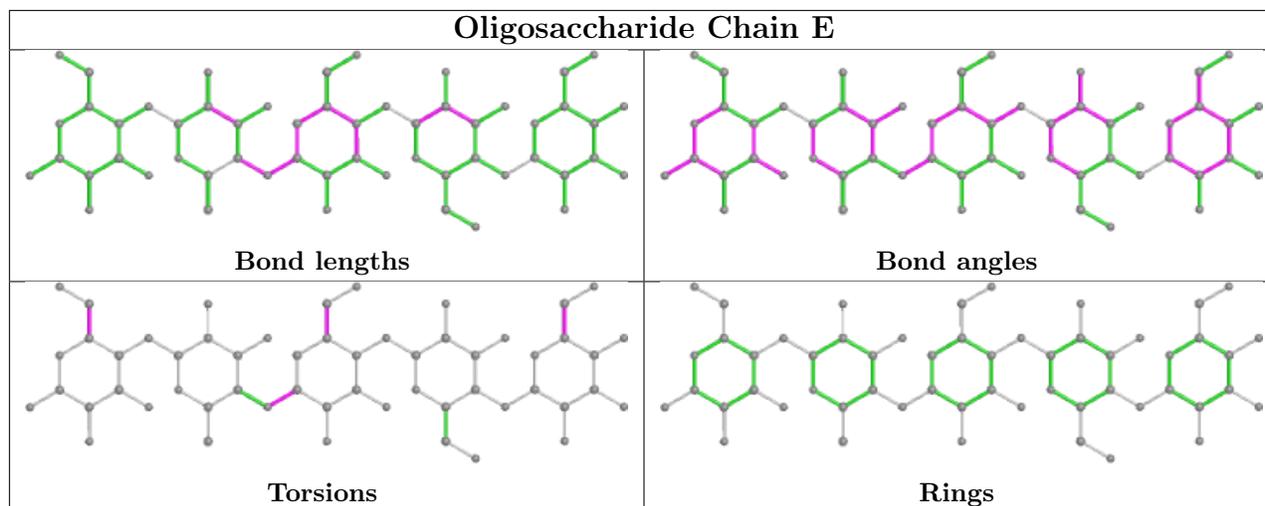
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	1	0
4	E	2	AC1	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
7	EDO	A	504	-	3,3,3	0.31	0	2,2,2	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
7	EDO	A	504	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	504	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	448/450 (99%)	0.17	15 (3%) 46 50	26, 35, 51, 88	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	PHE	3.3
1	A	324	ASN	3.1
1	A	270	GLY	2.7
1	A	105	ASN	2.6
1	A	387	SER	2.4
1	A	235	ASN	2.4
1	A	257	VAL	2.4
1	A	357	TRP	2.4
1	A	221	THR	2.3
1	A	102	SER	2.1
1	A	325	GLY	2.1
1	A	301	ARG	2.1
1	A	6	VAL	2.1
1	A	7	HIS	2.0
1	A	258	VAL	2.0

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

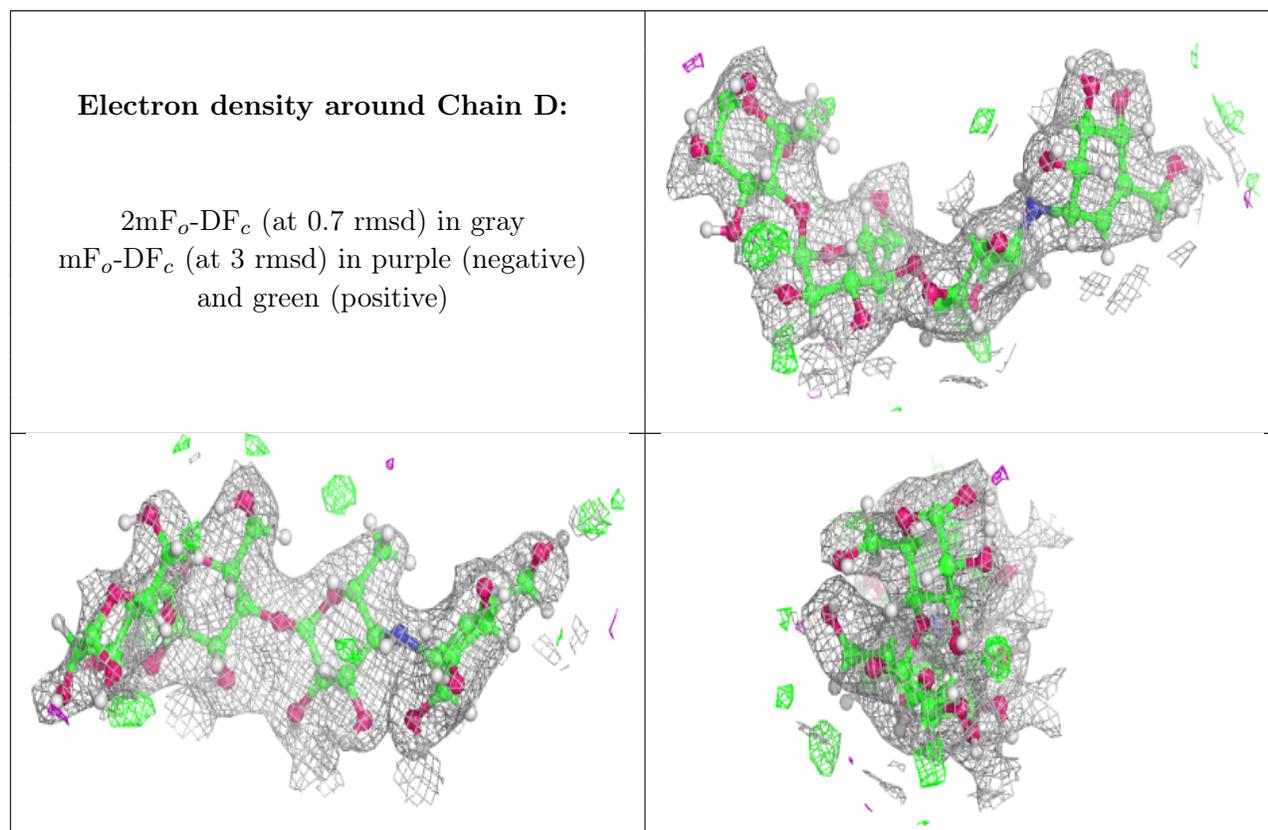
There are no non-standard protein/DNA/RNA residues in this entry.

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.

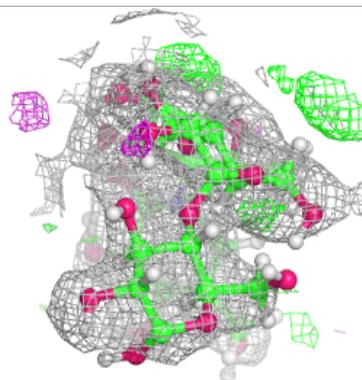
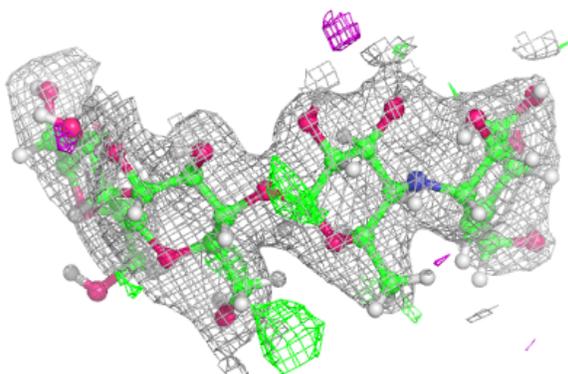
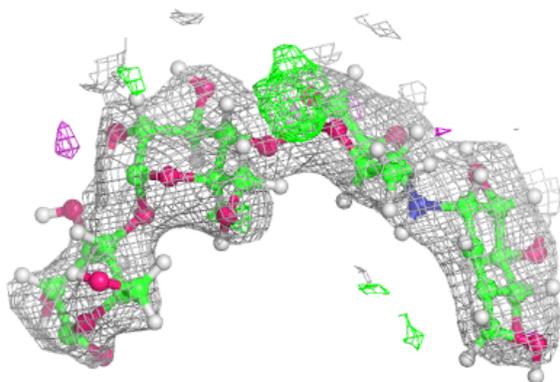
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	C	1	12/12	0.75	0.38	82,107,128,128	0
3	ASO	B	1	11/11	0.77	0.38	68,82,100,103	0
2	GLC	D	1	12/12	0.79	0.32	77,103,122,123	0
4	GLC	E	3	11/12	0.83	0.26	40,63,81,84	0
4	GLC	E	4	11/12	0.83	0.34	62,86,111,114	0
2	GLC	C	2	11/12	0.85	0.15	49,71,91,98	0
2	GLC	D	2	11/12	0.91	0.13	37,61,73,73	0
4	GLC	E	1	12/12	0.93	0.10	33,49,62,82	0
3	AC1	B	2	21/22	0.94	0.26	47,61,80,90	0
2	AC1	C	3	21/22	0.94	0.13	39,52,67,76	0
4	AC1	E	2	21/22	0.95	0.13	33,41,48,50	0
2	AC1	D	3	21/22	0.96	0.10	34,48,60,72	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.

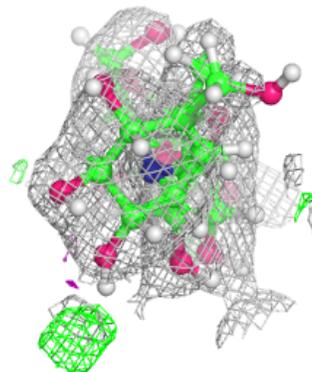
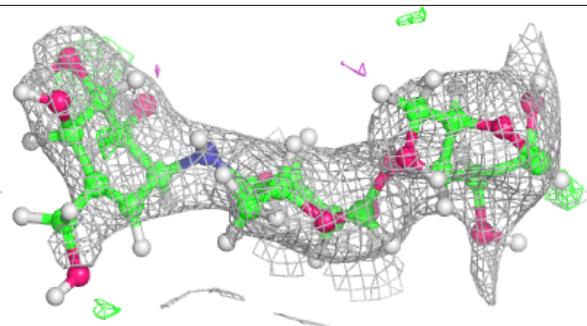
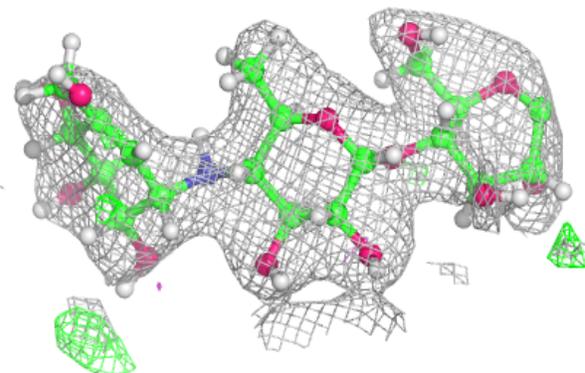


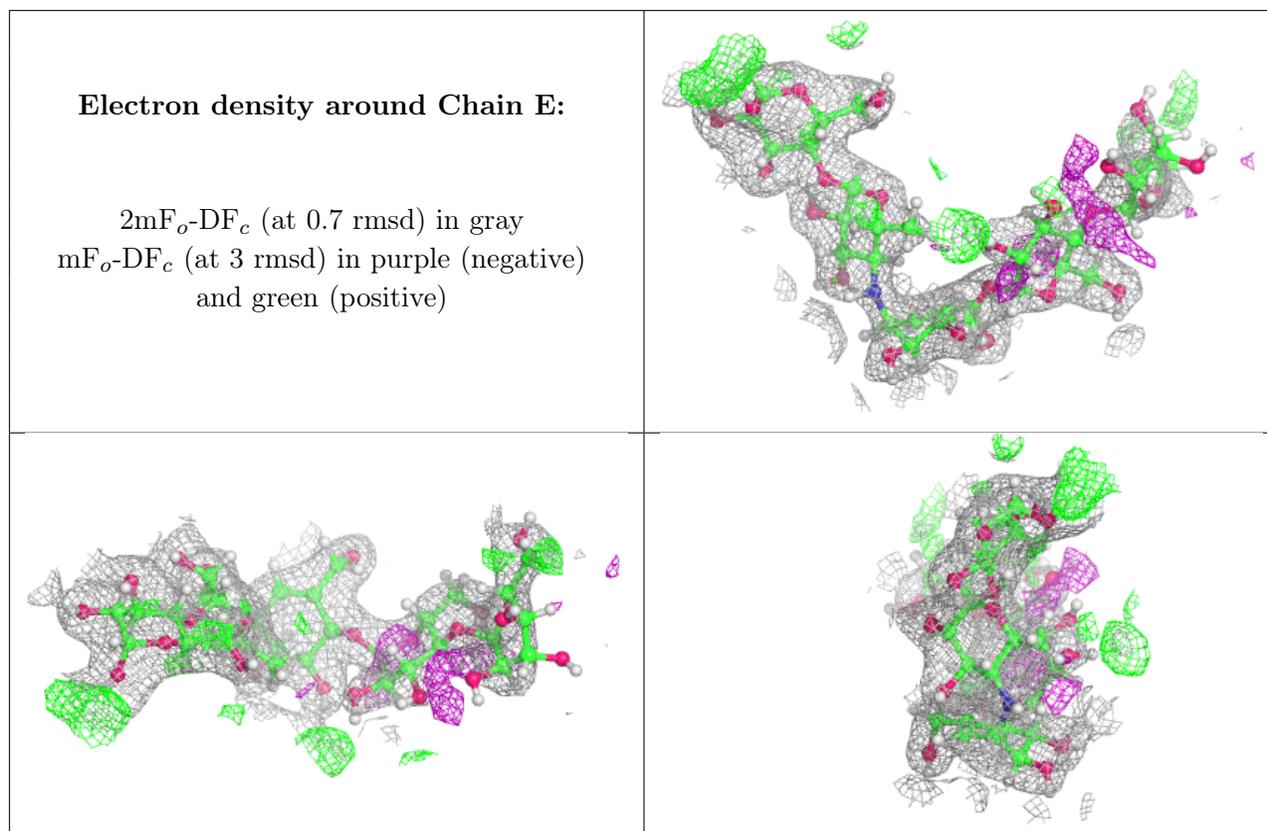
Electron density around Chain C:

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

**Electron density around Chain B:**

$2mF_o-DF_c$ (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
7	EDO	A	504	4/4	0.95	0.29	45,54,63,71	0
5	CL	A	502	1/1	0.99	0.08	42,42,42,42	0
6	CA	A	503	1/1	1.00	0.08	30,30,30,30	0
5	CL	A	501	1/1	1.00	0.26	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.