Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2021 – 06:09 pm BST

PDB ID	:	7P01
Title	:	Structure of the maltase BaAG2 from Blastobotrys adeninivorans in complex with acarbose
Authors	:	Ernits, K.; Visnapuu, T.; Persson, K.
Deposited on	:	2021-06-29
Resolution	:	2.12 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 following versions of software and data (see references ⓘ) were used in the production of this report:

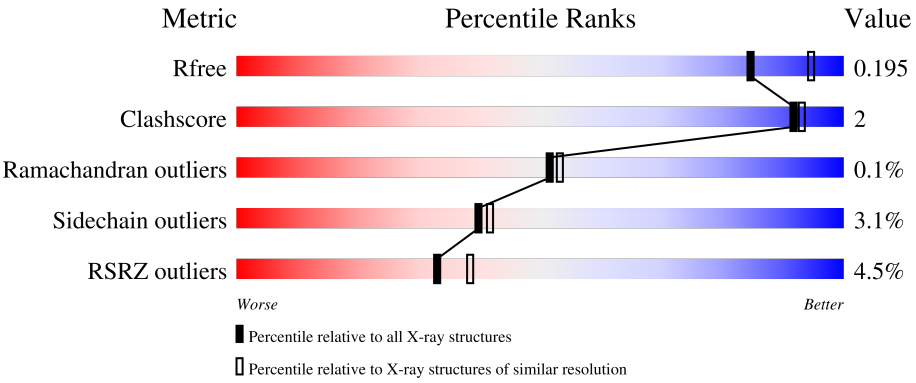
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 <=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	585	2% 94%
1	B	585	7% 89% 9%
2	D	3	33% 67%
2	E	3	100%
2	F	3	67% 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19262 atoms, of which 9085 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.

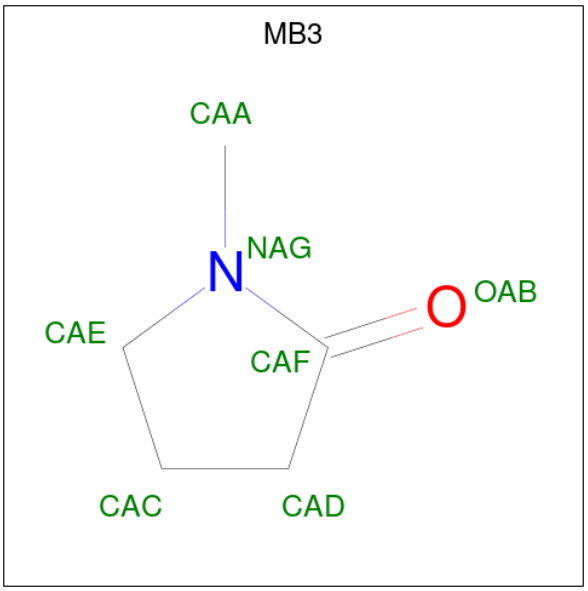
- Molecule 1 is a protein called BaAG2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	572	Total	C	H	N	O	S	0	1	0
			9143	2978	4466	792	895	12			
1	B	571	Total	C	H	N	O	S	0	0	0
			9131	2973	4463	790	893	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	3	Total	C	H	N	O	0	0	0
			87	25	43	1	18			
2	E	3	Total	C	H	N	O	0	0	0
			87	25	43	1	18			
2	F	3	Total	C	H	N	O	0	0	0
			87	25	43	1	18			

- Molecule 3 is 1-methylpyrrolidin-2-one (three-letter code: MB3) (formula: C_5H_9NO).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O 16 5 9 1 1	0	0
3	A	1	Total C H N O 16 5 9 1 1	0	0
3	B	1	Total C H N O 16 5 9 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is water.

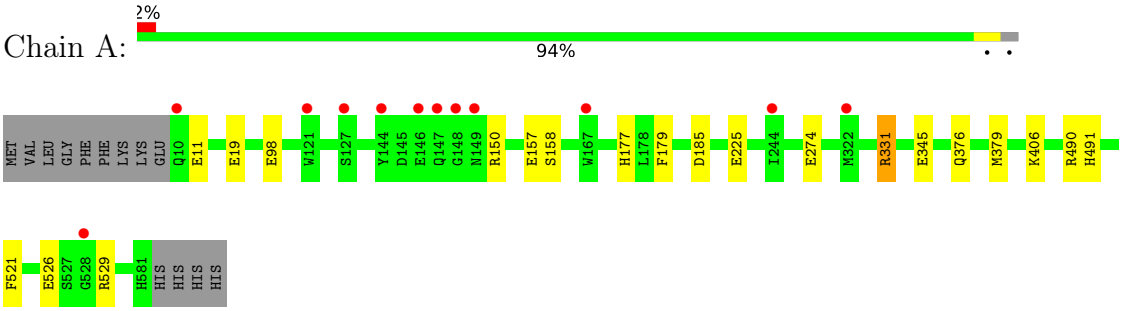
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	443	Total O 443 443	0	0
5	B	234	Total O 234 234	0	0

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.

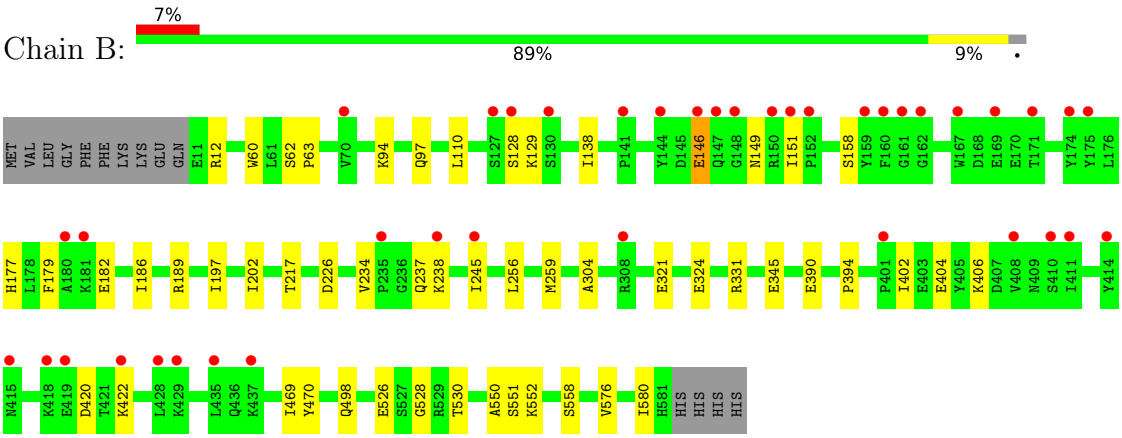
• Molecule 1: BaAG2

Chain A:



• Molecule 1: BaAG2

Chain B:

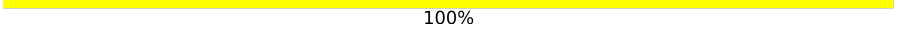


• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:

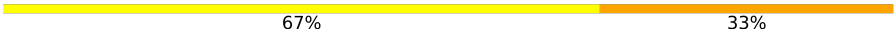
• Molecule 2: 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:



• Molecule 2: 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-(1-4)-alpha-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.03Å 78.08Å 121.93Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	46.32 – 2.12 48.14 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.32-2.12) 100.0 (48.14-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.184 , 0.195 0.184 , 0.195	Depositor DCC
R_{free} test set	2027 reflections (2.80%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19262	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MB3, AC1, GLC, CA

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	0.93	7/4812 (0.1%)	0.85	3/6529 (0.0%)
1	B	0.82	3/4798 (0.1%)	0.85	1/6510 (0.0%)
All	All	0.88	10/9610 (0.1%)	0.85	4/13039 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CD-OE1	-6.52	1.18	1.25
1	A	98	GLU	CD-OE2	-5.66	1.19	1.25
1	A	274	GLU	CD-OE2	-5.48	1.19	1.25
1	A	345	GLU	CD-OE1	-5.47	1.19	1.25
1	A	19	GLU	CD-OE1	-5.25	1.19	1.25
1	B	345	GLU	CD-OE2	-5.23	1.19	1.25
1	B	390	GLU	CD-OE1	-5.15	1.20	1.25
1	A	157	GLU	CD-OE2	-5.15	1.20	1.25
1	A	345	GLU	CD-OE2	-5.08	1.20	1.25
1	B	345	GLU	CD-OE1	-5.02	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	PHE	CB-CA-C	6.17	122.75	110.40
1	B	179	PHE	CB-CA-C	5.72	121.84	110.40
1	A	331	ARG	CB-CA-C	-5.59	99.22	110.40
1	A	490	ARG	NE-CZ-NH2	-5.29	117.66	120.30

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	4677	4466	4465	3	1
1	B	4668	4463	4462	24	1
2	D	44	43	30	1	0
2	E	44	43	29	0	0
2	F	44	43	30	2	0
3	A	14	18	18	0	0
3	B	7	9	9	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	443	0	0	0	0
5	B	234	0	0	0	0
All	All	10177	9085	9043	29	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 (29) 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:256:LEU:HD23	1:B:259:MET:CE	2.19	0.72
1:B:256:LEU:HD23	1:B:259:MET:HE1	1.70	0.72
1:B:146:GLU:OE2	1:B:146:GLU:HA	1.94	0.68
1:B:256:LEU:CD2	1:B:259:MET:HE1	2.27	0.64
1:B:182:GLU:N	1:B:182:GLU:OE1	2.32	0.63
1:B:138:ILE:O	1:B:138:ILE:HG22	2.01	0.59
1:B:234:VAL:HG12	1:B:234:VAL:O	2.03	0.58
1:B:151:ILE:HD12	1:B:151:ILE:O	2.07	0.55
1:B:151:ILE:HD12	1:B:151:ILE:C	2.29	0.53
1:B:321:GLU:OE2	1:B:321:GLU:HA	2.09	0.52
1:B:404:GLU:HA	1:B:404:GLU:OE1	2.10	0.51
2:D:1:GLC:H61	2:D:2:GLC:O5	2.10	0.51
1:A:526:GLU:HA	1:A:526:GLU:OE1	2.11	0.51
1:B:217:THR:O	1:B:217:THR:OG1	2.25	0.51
1:B:402:ILE:HG13	1:B:402:ILE:O	2.11	0.50
1:A:379:MET:CE	1:A:521:PHE:CZ	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ALA:HB2	2:F:1:GLC:H62	1.94	0.49
1:B:420:ASP:N	1:B:420:ASP:OD1	2.47	0.47
1:B:177:HIS:O	1:B:177:HIS:CG	2.68	0.47
1:B:558:SER:HB2	1:B:576:VAL:HG12	1.98	0.45
1:B:189:ARG:HH11	1:B:189:ARG:HG2	1.81	0.44
1:B:60:TRP:C	1:B:60:TRP:CD1	2.90	0.44
1:A:177:HIS:O	1:A:177:HIS:CG	2.71	0.44
1:B:110:LEU:HD21	1:B:202:ILE:HD11	2.00	0.43
1:B:550:ALA:HB1	1:B:580:ILE:HG23	2.01	0.43
1:B:528:GLY:O	1:B:530:THR:HG23	2.19	0.43
1:B:226:ASP:OD1	1:B:226:ASP:N	2.42	0.41
1:B:186:ILE:HD12	1:B:197:ILE:HD11	2.02	0.41
2:F:1:GLC:H1	2:F:1:GLC:O6	2.21	0.41

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:150:ARG:HE	1:B:149:ASN:HD22[2_454]	1.18	0.42

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	571/585 (98%)	556 (97%)	15 (3%)	0	100	100
1	B	569/585 (97%)	541 (95%)	27 (5%)	1 (0%)	47	48
All	All	1140/1170 (97%)	1097 (96%)	42 (4%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	12	ARG

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	508/520 (98%)	499 (98%)	9 (2%)	59	63
1	B	507/520 (98%)	485 (96%)	22 (4%)	29	28
All	All	1015/1040 (98%)	984 (97%)	31 (3%)	40	42

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	158	SER
1	A	185	ASP
1	A	225	GLU
1	A	331	ARG
1	A	376	GLN
1	A	406	LYS
1	A	491	HIS
1	A	529	ARG
1	B	62	SER
1	B	63	PRO
1	B	94	LYS
1	B	97	GLN
1	B	128	SER
1	B	129	LYS
1	B	146	GLU
1	B	158	SER
1	B	237	GLN
1	B	238	LYS
1	B	245	ILE
1	B	324	GLU
1	B	331	ARG
1	B	394	PRO

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Mol	Chain	Res	Type
1	B	406	LYS
1	B	422	LYS
1	B	469	ILE
1	B	470	TYR
1	B	498	GLN
1	B	526	GLU
1	B	551	SER
1	B	552	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	149	ASN

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)

9 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	D	1	2	12,12,12	1.05	0	17,17,17	1.10	1 (5%)
2	GLC	D	2	2	11,11,12	1.32	2 (18%)	15,15,17	1.90	4 (26%)
2	AC1	D	3	2	21,22,23	1.50	4 (19%)	22,32,34	2.10	7 (31%)
2	GLC	E	1	2	12,12,12	1.11	0	17,17,17	2.32	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	E	2	2	11,11,12	1.31	2 (18%)	15,15,17	1.06	1 (6%)
2	AC1	E	3	2	21,22,23	6.41	9 (42%)	22,32,34	1.53	5 (22%)
2	GLC	F	1	2	12,12,12	0.74	0	17,17,17	1.37	3 (17%)
2	GLC	F	2	2	11,11,12	1.08	1 (9%)	15,15,17	1.47	2 (13%)
2	AC1	F	3	2	21,22,23	1.38	2 (9%)	22,32,34	1.83	6 (27%)

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	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
2	GLC	E	1	2	-	1/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	AC1	E	3	2	-	4/6/43/46	0/2/2/2
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLC	F	2	2	-	0/2/19/22	0/1/1/1
2	AC1	F	3	2	-	1/6/43/46	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	AC1	C7B-C5B	22.16	1.63	1.32
2	E	3	AC1	C4A-C5B	-10.85	1.42	1.51
2	E	3	AC1	C2B-C1B	9.20	1.65	1.52
2	E	3	AC1	C3B-C4A	7.89	1.64	1.53
2	E	3	AC1	C3B-C2B	-6.36	1.36	1.52
2	E	3	AC1	C1B-C7B	-6.35	1.41	1.50
2	F	3	AC1	C4A-C5B	-4.13	1.48	1.51
2	E	3	AC1	C3-C4	-3.01	1.47	1.53
2	D	3	AC1	O5-C1	-2.86	1.39	1.43
2	F	2	GLC	O5-C1	-2.76	1.39	1.43
2	E	2	GLC	O5-C1	2.59	1.47	1.43
2	E	2	GLC	C2-C3	-2.45	1.48	1.52
2	D	2	GLC	O5-C1	-2.44	1.39	1.43
2	D	2	GLC	C2-C3	-2.24	1.49	1.52
2	D	3	AC1	C4A-C5B	-2.21	1.49	1.51
2	D	3	AC1	O2B-C2B	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	AC1	O3B-C3B	-2.10	1.38	1.43
2	E	3	AC1	C2-C3	-2.05	1.49	1.52
2	E	3	AC1	C6-C5	-2.01	1.46	1.51
2	F	3	AC1	C4-N4A	-2.01	1.44	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	GLC	O5-C1-C2	5.19	119.55	110.28
2	D	3	AC1	C2B-C3B-C4A	-4.73	102.67	110.18
2	D	3	AC1	C2-C3-C4	-4.55	106.62	110.63
2	D	2	GLC	O5-C1-C2	-4.55	103.75	110.77
2	E	1	GLC	O5-C5-C4	4.23	117.38	109.69
2	F	3	AC1	O6B-C6B-C5B	-4.19	102.48	112.50
2	D	3	AC1	O5-C1-C2	-3.53	105.32	110.77
2	F	3	AC1	C1-C2-C3	3.52	113.99	109.67
2	F	2	GLC	C1-C2-C3	3.36	113.80	109.67
2	E	3	AC1	O5-C1-C2	-3.36	105.58	110.77
2	F	3	AC1	C2-C3-C4	-3.21	107.80	110.63
2	F	1	GLC	O2-C2-C1	3.05	116.24	109.16
2	D	3	AC1	O2B-C2B-C1B	3.04	115.22	109.12
2	D	2	GLC	O4-C4-C3	2.80	116.83	110.35
2	D	3	AC1	O2B-C2B-C3B	2.80	116.81	110.35
2	D	2	GLC	C1-O5-C5	2.66	115.79	112.19
2	E	3	AC1	O3-C3-C2	2.64	115.06	109.99
2	E	1	GLC	O4-C4-C5	-2.59	102.86	109.30
2	E	1	GLC	C3-C4-C5	2.55	114.78	110.24
2	F	3	AC1	C2B-C3B-C4A	-2.54	106.14	110.18
2	F	3	AC1	C7B-C1B-N4A	2.54	114.49	110.68
2	E	1	GLC	C6-C5-C4	-2.43	107.32	113.00
2	E	1	GLC	O6-C6-C5	-2.41	103.01	111.29
2	F	1	GLC	O1-C1-C2	2.41	115.81	109.03
2	D	2	GLC	O3-C3-C2	-2.37	105.45	109.99
2	F	1	GLC	O2-C2-C3	-2.36	104.89	110.35
2	F	2	GLC	O3-C3-C4	-2.30	105.04	110.35
2	E	3	AC1	C1-C2-C3	2.27	112.45	109.67
2	E	2	GLC	C1-C2-C3	2.26	112.44	109.67
2	D	3	AC1	O6B-C6B-C5B	-2.24	107.13	112.50
2	E	1	GLC	C1-C2-C3	2.21	114.89	110.31
2	E	3	AC1	O3-C3-C4	-2.20	105.22	109.66
2	D	1	GLC	C6-C5-C4	-2.17	107.91	113.00
2	D	3	AC1	O3B-C3B-C4A	-2.16	105.56	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	AC1	C3-C4-N4A	-2.15	105.32	111.49
2	F	3	AC1	O2B-C2B-C1B	2.12	113.37	109.12
2	E	1	GLC	C1-O5-C5	2.05	117.54	113.66

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C7B-C1B-N4A-C4
2	E	3	AC1	C7B-C5B-C6B-O6B
2	F	3	AC1	C7B-C1B-N4A-C4
2	E	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	E	3	AC1	C5-C4-N4A-C1B
2	E	2	GLC	O5-C5-C6-O6
2	E	3	AC1	C7B-C1B-N4A-C4
2	E	3	AC1	C4A-C5B-C6B-O6B

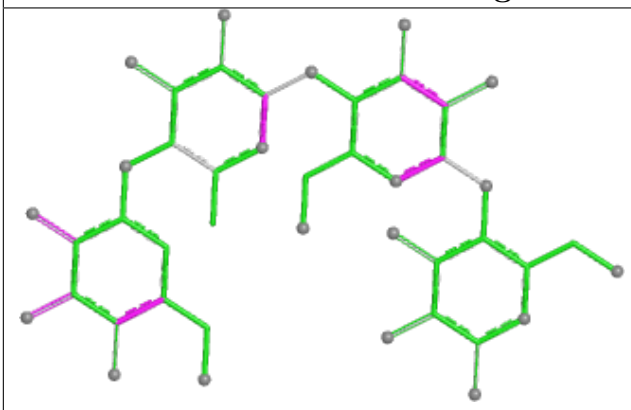
There are no ring outliers.

3 monomers are involved in 3 short contacts:

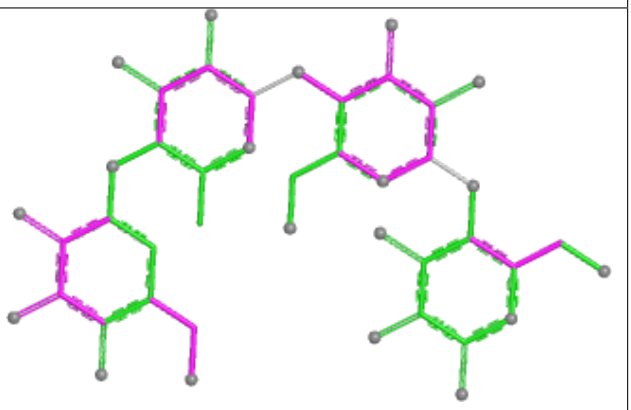
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	GLC	2	0
2	D	2	GLC	1	0
2	D	1	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

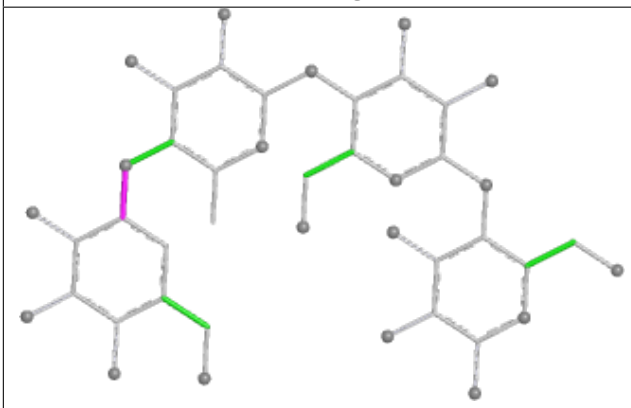
Oligosaccharide Chain D



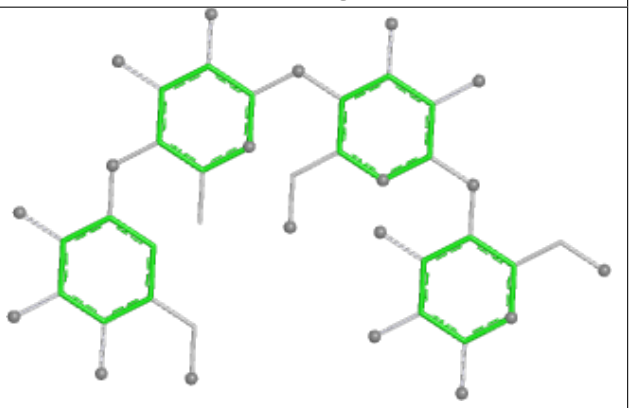
Bond lengths



Bond angles

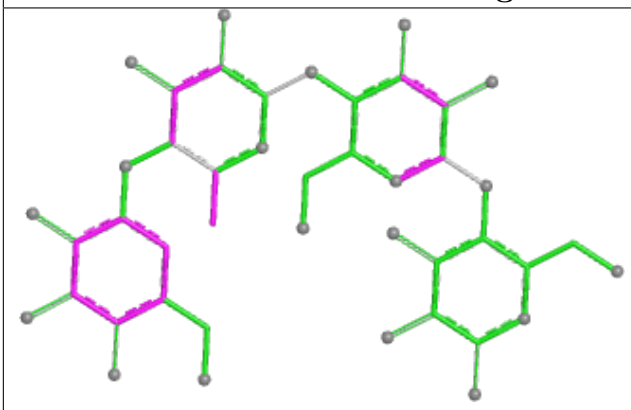


Torsions

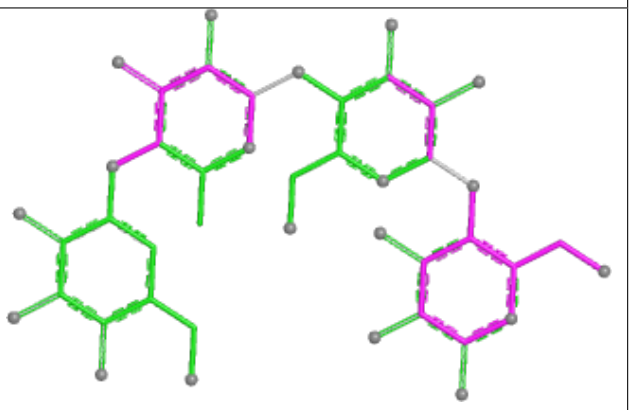


Rings

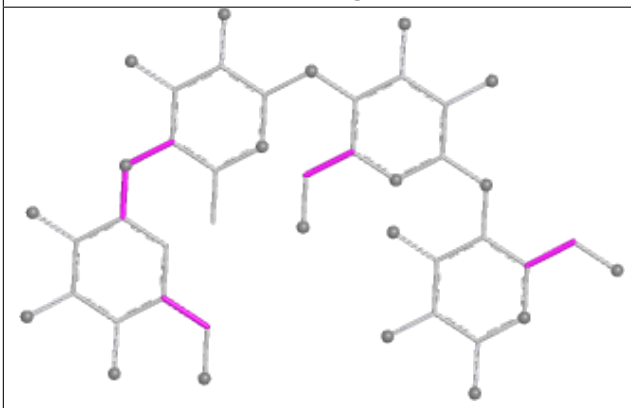
Oligosaccharide Chain E



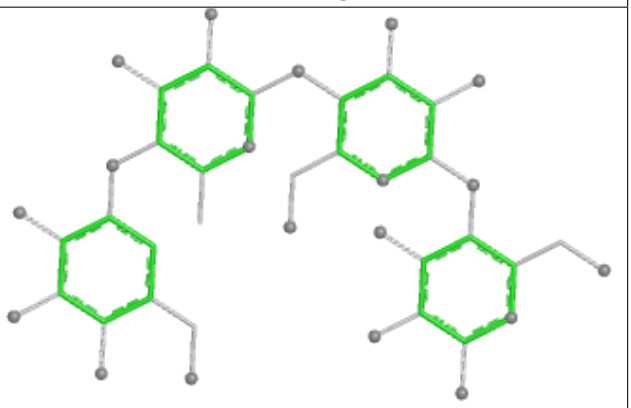
Bond lengths



Bond angles

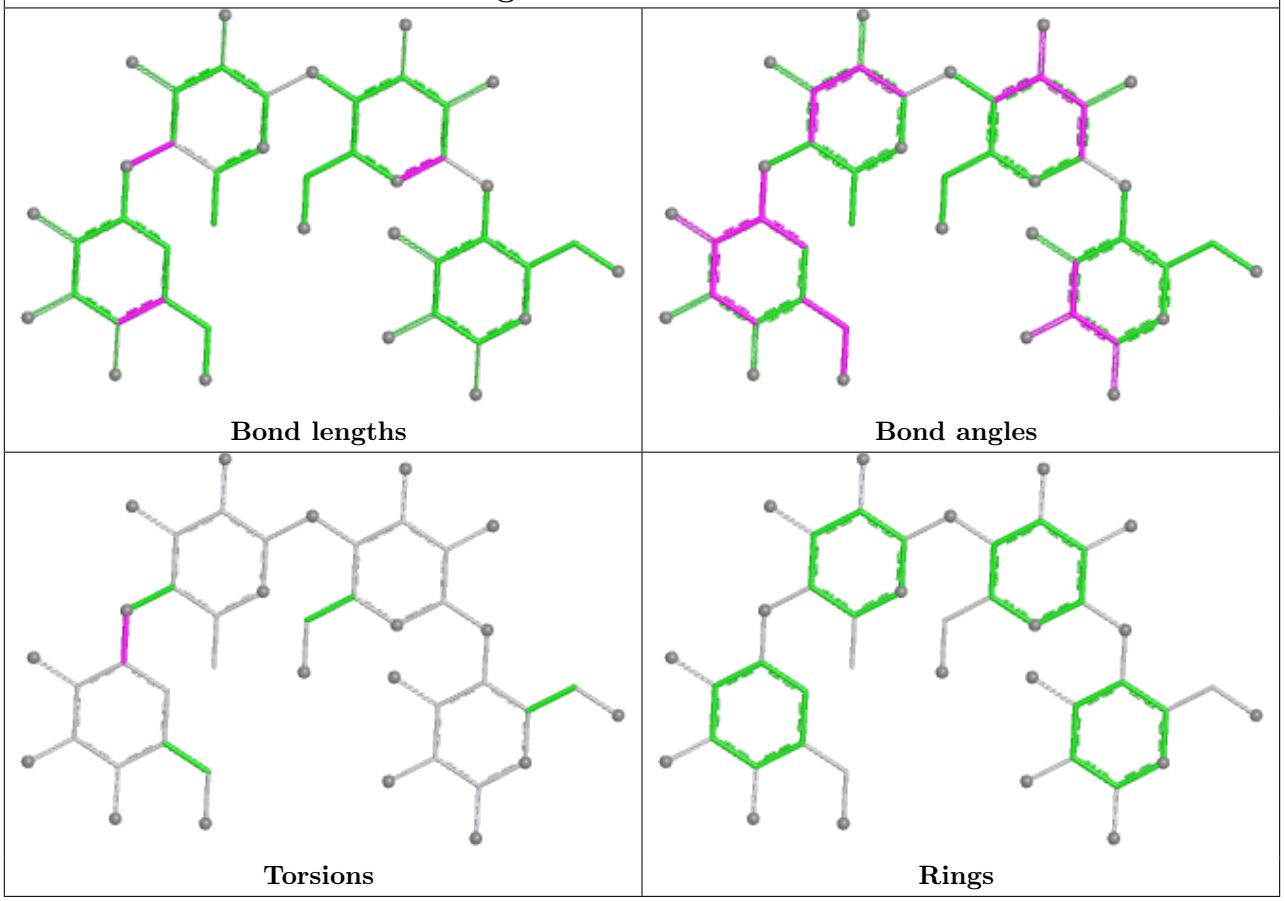


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	MB3	A	901	-	7,7,7	2.59	4 (57%)	9,9,9	1.24	1 (11%)
3	MB3	B	701	-	7,7,7	2.26	4 (57%)	9,9,9	2.04	3 (33%)
3	MB3	A	902	-	7,7,7	2.24	3 (42%)	9,9,9	1.28	1 (11%)

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	MB3	A	901	-	-	-	0/1/1/1
3	MB3	B	701	-	-	-	0/1/1/1
3	MB3	A	902	-	-	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	MB3	OAB-CAF	-4.37	1.13	1.23
3	A	902	MB3	CAC-CAE	3.83	1.65	1.51
3	B	701	MB3	OAB-CAF	-3.34	1.15	1.23
3	A	901	MB3	CAC-CAE	3.32	1.63	1.51
3	A	902	MB3	CAF-NAG	3.27	1.51	1.31
3	B	701	MB3	CAC-CAE	2.93	1.62	1.51
3	B	701	MB3	CAF-NAG	2.89	1.49	1.31
3	A	901	MB3	CAF-NAG	2.75	1.48	1.31
3	A	901	MB3	CAD-CAF	-2.61	1.43	1.51
3	B	701	MB3	CAD-CAF	-2.43	1.43	1.51
3	A	902	MB3	OAB-CAF	-2.20	1.18	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	701	MB3	CAE-CAC-CAD	-3.36	95.43	105.97
3	B	701	MB3	CAC-CAE-NAG	-3.34	90.94	103.07
3	B	701	MB3	CAC-CAD-CAF	-3.03	95.73	104.48
3	A	902	MB3	CAE-CAC-CAD	-2.52	98.04	105.97
3	A	901	MB3	CAE-CAC-CAD	-2.12	99.32	105.97

There are no chirality outliers.

There are no torsion outliers.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	572/585 (97%)	0.19	12 (2%)	63	68	22, 34, 57, 114	0
1	B	571/585 (97%)	0.53	40 (7%)	16	20	28, 49, 86, 129	0
All	All	1143/1170 (97%)	0.36	52 (4%)	33	38	22, 41, 75, 129	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	GLY	4.7
1	A	144	TYR	4.3
1	A	149	ASN	4.0
1	B	160	PHE	3.9
1	B	414	TYR	3.9
1	B	167	TRP	3.8
1	B	422	LYS	3.8
1	A	146	GLU	3.6
1	B	428	LEU	3.5
1	B	127	SER	3.3
1	B	174	TYR	3.3
1	B	151	ILE	3.3
1	B	128	SER	3.3
1	B	147	GLN	3.3
1	B	429	LYS	3.2
1	B	180	ALA	3.0
1	B	308	ARG	2.9
1	B	175	TYR	2.9
1	B	148	GLY	2.8
1	B	235	PRO	2.7
1	B	245	ILE	2.7
1	A	10	GLN	2.6
1	B	411	ILE	2.6
1	A	528	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	435	LEU	2.6
1	B	408	VAL	2.5
1	A	244	ILE	2.5
1	B	144	TYR	2.5
1	B	159	TYR	2.4
1	B	418	LYS	2.4
1	B	410	SER	2.4
1	B	415	ASN	2.4
1	B	146	GLU	2.3
1	B	152	PRO	2.3
1	B	150	ARG	2.3
1	B	171	THR	2.3
1	A	167	TRP	2.3
1	B	419	GLU	2.3
1	B	130	SER	2.3
1	B	169	GLU	2.3
1	B	437	LYS	2.2
1	B	162	GLY	2.2
1	A	147	GLN	2.2
1	B	70	VAL	2.2
1	B	238	LYS	2.1
1	A	127	SER	2.1
1	B	161	GLY	2.0
1	A	322	MET	2.0
1	B	141	PRO	2.0
1	B	401	PRO	2.0
1	A	121	TRP	2.0
1	B	181	LYS	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)

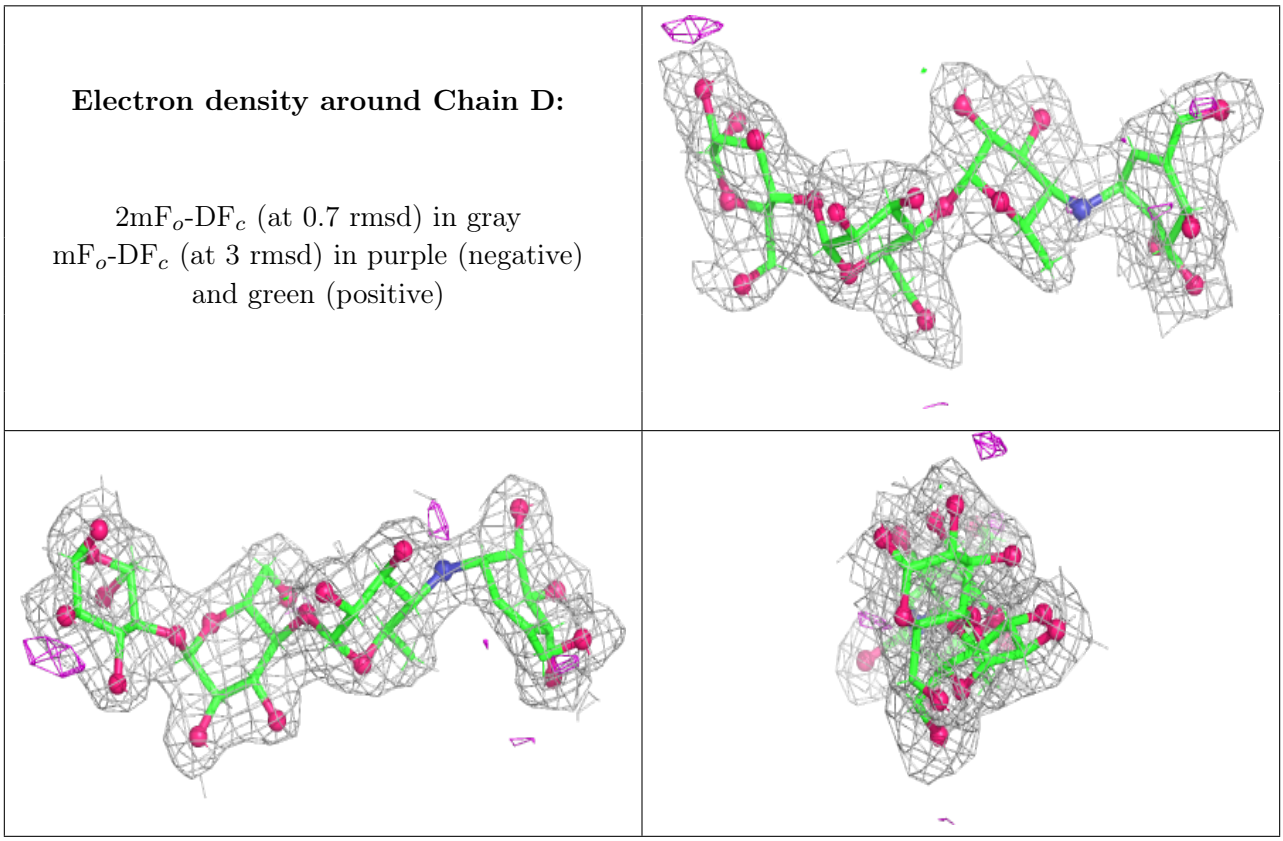
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	F	1	12/12	0.79	0.15	61,68,82,83	0
2	AC1	E	3	21/22	0.87	0.15	36,57,77,78	0
2	GLC	D	1	12/12	0.87	0.15	43,48,58,60	0
2	AC1	F	3	21/22	0.88	0.15	40,45,52,54	0
2	GLC	E	2	11/12	0.89	0.11	31,34,40,43	0
2	GLC	D	2	11/12	0.89	0.14	36,41,49,50	0
2	GLC	F	2	11/12	0.90	0.12	48,55,65,68	0
2	GLC	E	1	12/12	0.94	0.14	29,35,44,47	0
2	AC1	D	3	21/22	0.94	0.13	25,34,43,45	0

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

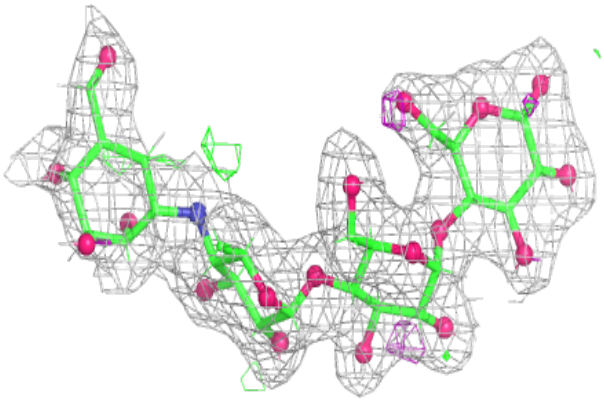
Electron density around Chain D:

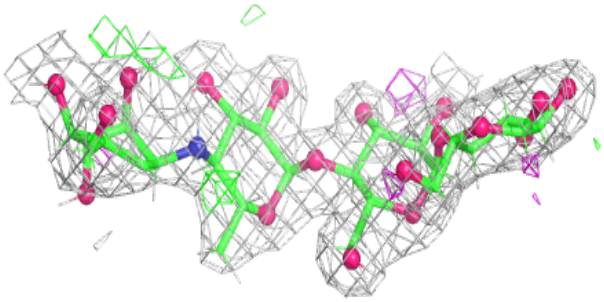
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

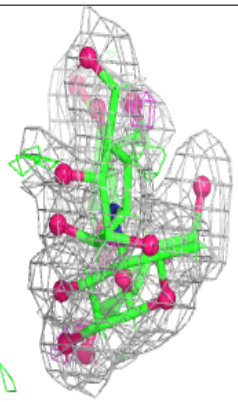


Electron density around Chain E:

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

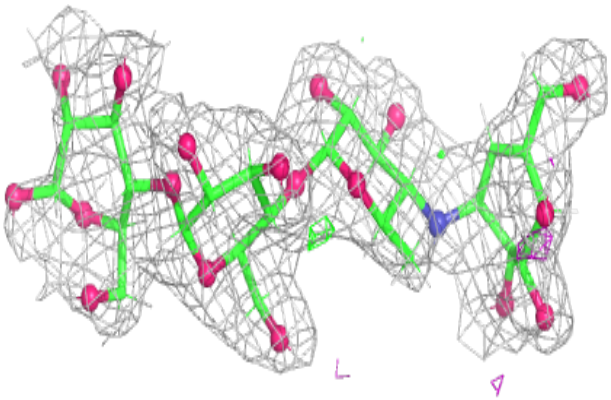


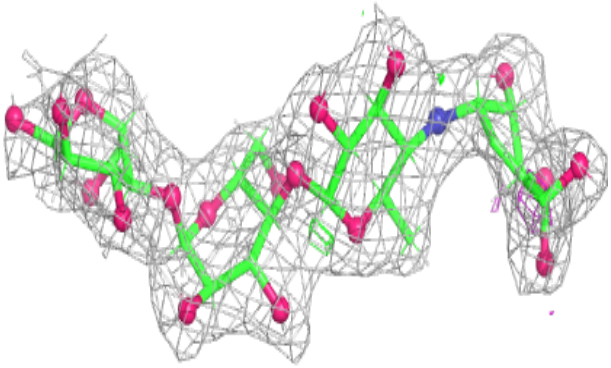


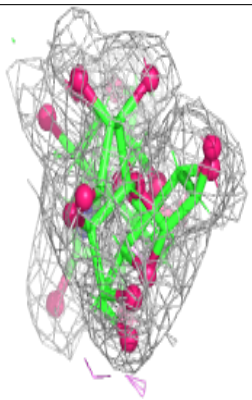


Electron density around Chain F:

$2mF_o$-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, 95^{th} 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	MB3	A	902	7/7	0.76	0.16	71,86,86,86	0
3	MB3	A	901	7/7	0.85	0.28	44,55,60,60	0
3	MB3	B	701	7/7	0.91	0.19	59,72,73,73	0
4	CA	B	702	1/1	0.96	0.11	44,44,44,44	0
4	CA	A	903	1/1	0.98	0.14	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.