WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 06:50 pm GMT

PDB ID : 1UMZ

Title : Xyloglucan endotransglycosylase in complex with the xyloglucan nonasaccharide XLLG.

Authors : Johansson, P.; Brumer, H.; Kallas, A.M.; Henriksson, H.; Denman, S.E.; Teeri, T.T.; Jones, T.A.

Deposited on : 2003-09-03

Resolution : 1.80 Å(reported)

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

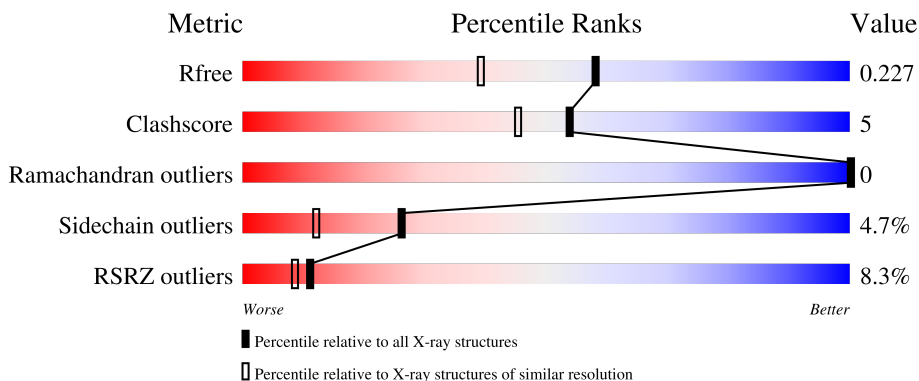|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.80 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.
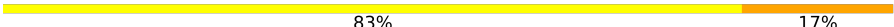
Metric	Percentile Ranks	Value
Rfree		0.227
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		4.7%
RSRZ outliers		8.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	278	11% · 82% · 13% · ·
1	B	278	5% · 81% · 12% · 5%
2	C	3	33% · 33% · 33%
2	E	3	67% · 33%
3	D	6	17% · 50% · 33%

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| Mol	Chain	Length	Quality of chain
3	F	6	83% 17%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4873 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 XYLOGLUCAN ENDOTRANSGLYCOSYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	15	0	0
			2220	1432	373	404	11			
1	B	264	Total	C	N	O	S	8	1	0
			2206	1426	371	398	11			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
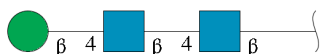
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1-2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.
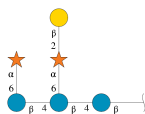
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	6	Total	C	O	0	0	0
			62	34	28			
3	F	6	Total	C	O	0	0	0
			62	34	28			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	111	Total O 111 111	0	0
4	B	134	Total O 134 134	0	0

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: gr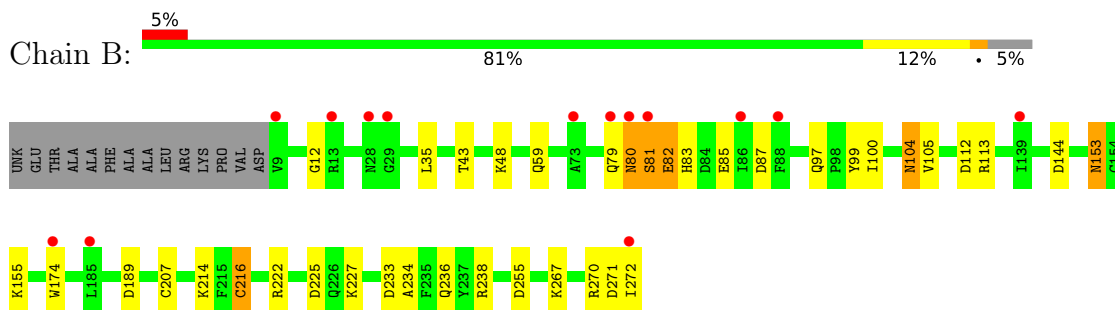een = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: XYLOGLUCAN ENDOTRANSGLYCOSYLASE
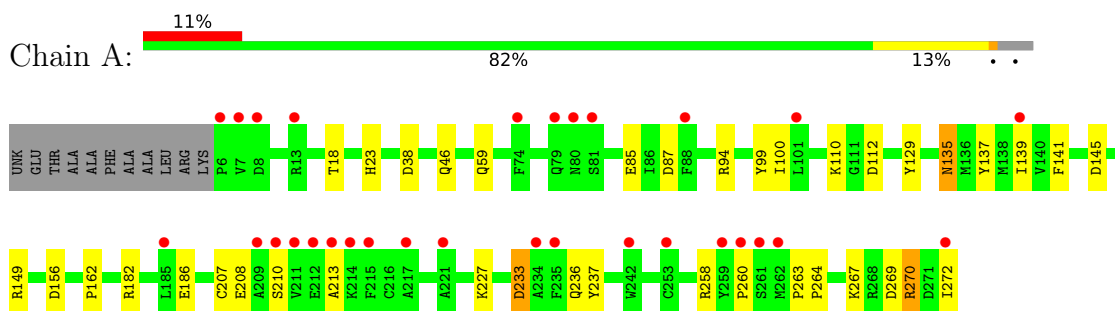
Chain A:

• Molecule 1: XYLOGLUCAN ENDOTRANSGLYCOSYLASE

Chain B:

• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac etamido-2-deoxy-beta-D-glucopyranose

Chain C:
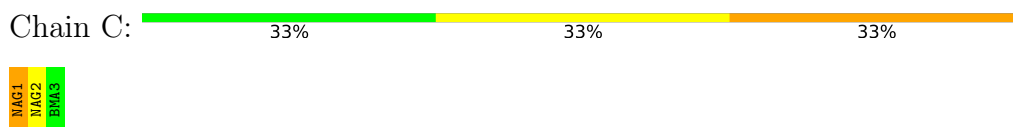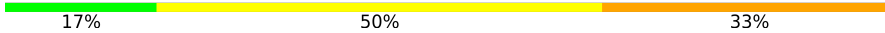
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac etamido-2-deoxy-beta-D-glucopyranose
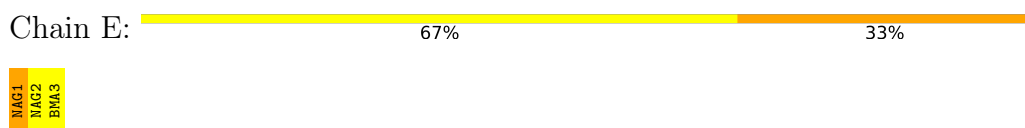
Chain E:

• Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1 -2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain D: 17%   50%   33%
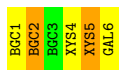
• Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[beta-D-galactopyranose-(1 -2)-alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain F: 83%   17%

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	188.16Å 188.16Å 45.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.99 – 1.80 29.27 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (28.99-1.80) 96.7 (29.27-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.201 , 0.222 0.208 , 0.227	Depositor DCC
R_{free} test set	4216 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	24.3	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4873	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: XYS, BMA, GAL, BGC, NAG

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	0.64	0/2293	0.88	6/3104 (0.2%)
1	B	0.65	0/2285	0.85	7/3095 (0.2%)
All	All	0.65	0/4578	0.87	13/6199 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	156	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	233	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	271	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	112	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	222	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B	189	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	112	ASP	CB-CG-OD2	5.43	123.18	118.30
1	B	225	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	269	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	145	ASP	CB-CG-OD2	5.17	122.96	118.30
1	B	255	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	144	ASP	CB-CG-OD2	5.00	122.80	118.30

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	2220	0	2083	19	0
1	B	2206	0	2070	21	0
2	C	39	0	34	1	0
2	E	39	0	34	2	0
3	D	62	0	52	1	0
3	F	62	0	51	2	0
4	A	111	0	0	1	0
4	B	134	0	0	3	0
All	All	4873	0	4324	43	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 5.

All (43) 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:80:ASN:OD1	1:B:82:GLU:N	1.88	1.06
1:A:260:PRO:O	4:A:2103:HOH:O	1.98	0.81
1:B:80:ASN:OD1	1:B:81:SER:N	2.17	0.77
1:B:233:ASP:H	1:B:236:GLN:HE21	1.32	0.76
3:F:2:BGC:C6	3:F:5:XYS:C1	2.65	0.75
1:A:139:ILE:HD11	1:A:162:PRO:CG	2.17	0.74
1:B:12:GLY:O	1:B:48:LYS:NZ	2.21	0.73
1:B:207:CYS:HG	1:B:216:CYS:HG	0.74	0.73
1:A:139:ILE:HD11	1:A:162:PRO:HG2	1.73	0.70
1:B:174[B]:TRP:CD1	4:B:2076:HOH:O	2.45	0.70
1:B:80:ASN:O	1:B:83:HIS:HB3	1.95	0.66
1:A:23:HIS:HE1	1:A:38:ASP:OD2	1.84	0.60
1:B:97:GLN:NE2	2:E:1:NAG:C6	2.65	0.60
1:B:104:ASN:HD21	1:B:113:ARG:H	1.50	0.59
1:A:18:THR:HG21	1:A:46:GLN:NE2	2.18	0.58
1:A:139:ILE:HD11	1:A:162:PRO:HG3	1.86	0.57
1:A:135:ASN:HD22	1:A:135:ASN:C	2.09	0.56
3:D:2:BGC:C6	3:D:5:XYS:C1	2.82	0.56
1:B:207:CYS:CB	1:B:216:CYS:HG	2.18	0.55
1:B:153:ASN:HD22	1:B:153:ASN:C	2.10	0.54
1:B:233:ASP:H	1:B:236:GLN:NE2	2.05	0.54
1:B:104:ASN:HD22	1:B:105:VAL:H	1.55	0.53
1:A:210:SER:O	1:A:213:ALA:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASN:OD1	1:B:80:ASN:C	2.47	0.52
1:B:100:ILE:HD12	2:E:1:NAG:H82	1.92	0.51
1:A:100:ILE:HD12	2:C:1:NAG:H82	1.94	0.49
1:A:59:GLN:HG3	1:A:129:TYR:CE1	2.47	0.48
1:B:35:LEU:HG	1:B:43:THR:HG23	1.94	0.48
1:A:18:THR:HG21	1:A:46:GLN:HE21	1.77	0.48
1:A:237:TYR:CE1	1:A:270:ARG:HG3	2.49	0.47
3:F:2:BGC:O6	3:F:5:XYS:C2	2.56	0.47
1:A:85:GLU:OE2	1:A:87:ASP:OD1	2.33	0.46
1:A:182:ARG:HD3	1:A:186:GLU:HG2	2.00	0.44
1:B:79:GLN:NE2	4:B:2033:HOH:O	2.09	0.44
1:B:227:LYS:O	1:B:227:LYS:HD3	2.17	0.44
1:A:141:PHE:CD1	1:A:149:ARG:HG2	2.54	0.43
1:A:233:ASP:H	1:A:236:GLN:HE21	1.65	0.43
1:B:85:GLU:OE2	1:B:87:ASP:OD1	2.36	0.42
1:A:263:PRO:HA	1:A:264:PRO:HD3	1.87	0.42
1:A:135:ASN:ND2	1:A:137:TYR:H	2.17	0.42
1:B:234:ALA:O	1:B:238:ARG:HG3	2.20	0.41
1:B:155:LYS:HB3	4:B:2069:HOH:O	2.21	0.40
1:A:182:ARG:HD3	1:A:186:GLU:CG	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/278 (95%)	256 (97%)	9 (3%)	0	100	100
1	B	263/278 (95%)	253 (96%)	10 (4%)	0	100	100
All	All	528/556 (95%)	509 (96%)	19 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/241 (98%)	225 (96%)	10 (4%)	29	14
1	B	233/241 (97%)	221 (95%)	12 (5%)	23	10
All	All	468/482 (97%)	446 (95%)	22 (5%)	26	12

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	TYR
1	A	110	LYS
1	A	135	ASN
1	A	207	CYS
1	A	208	GLU
1	A	227	LYS
1	A	258	ARG
1	A	267	LYS
1	A	270	ARG
1	A	272	ILE
1	B	59	GLN
1	B	80	ASN
1	B	81	SER
1	B	82	GLU
1	B	99	TYR
1	B	104	ASN
1	B	153	ASN
1	B	214	LYS
1	B	216	CYS
1	B	267	LYS
1	B	270	ARG
1	B	272	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	23	HIS
1	A	36	HIS
1	A	46	GLN
1	A	79	GLN
1	A	135	ASN
1	A	175	ASN
1	A	203	HIS
1	A	219	GLN
1	A	236	GLN
1	B	14	ASN
1	B	23	HIS
1	B	36	HIS
1	B	97	GLN
1	B	104	ASN
1	B	153	ASN
1	B	219	GLN
1	B	230	GLN
1	B	236	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

18 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	NAG	C	1	2,1	14,14,15	0.61	0	17,19,21	1.39	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAG	C	2	2	14,14,15	0.74	1 (7%)	17,19,21	1.01	1 (5%)
2	BMA	C	3	2	11,11,12	0.71	0	15,15,17	0.76	0
3	BGC	D	1	3	11,11,12	0.71	0	15,15,17	1.06	2 (13%)
3	BGC	D	2	3	11,11,12	0.66	0	15,15,17	1.02	1 (6%)
3	BGC	D	3	3	11,11,12	0.77	0	15,15,17	0.99	0
3	XYS	D	4	3	9,9,10	1.21	1 (11%)	10,12,14	0.96	1 (10%)
3	XYS	D	5	3	9,9,10	1.28	1 (11%)	10,12,14	1.29	1 (10%)
3	GAL	D	6	3	11,11,12	0.75	0	15,15,17	1.19	1 (6%)
2	NAG	E	1	2,1	14,14,15	0.63	0	17,19,21	1.27	2 (11%)
2	NAG	E	2	2	14,14,15	0.70	0	17,19,21	0.92	1 (5%)
2	BMA	E	3	2	11,11,12	0.68	0	15,15,17	0.99	1 (6%)
3	BGC	F	1	3	11,11,12	0.78	0	15,15,17	1.13	1 (6%)
3	BGC	F	2	3	11,11,12	0.69	0	15,15,17	0.70	0
3	BGC	F	3	3	11,11,12	0.94	1 (9%)	15,15,17	0.98	2 (13%)
3	XYS	F	4	3	9,9,10	1.14	1 (11%)	10,12,14	0.98	1 (10%)
3	XYS	F	5	3	9,9,10	1.06	1 (11%)	10,12,14	1.72	1 (10%)
3	GAL	F	6	3	11,11,12	0.65	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	NAG	C	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	BGC	D	1	3	-	0/2/19/22	0/1/1/1
3	BGC	D	2	3	-	0/2/19/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1
3	XYS	D	4	3	-	-	0/1/1/1
3	XYS	D	5	3	-	-	0/1/1/1
3	GAL	D	6	3	-	0/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	BGC	F	1	3	-	0/2/19/22	0/1/1/1
3	BGC	F	2	3	-	0/2/19/22	0/1/1/1
3	BGC	F	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XYS	F	4	3	-	-	0/1/1/1
3	XYS	F	5	3	-	-	0/1/1/1
3	GAL	F	6	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5	XYS	O5-C1	-3.52	1.36	1.42
3	D	4	XYS	O5-C1	-3.19	1.36	1.42
3	F	4	XYS	O5-C1	-3.13	1.36	1.42
3	F	5	XYS	O5-C1	-2.87	1.37	1.42
3	F	3	BGC	O5-C1	-2.40	1.39	1.43
2	C	2	NAG	O5-C1	-2.03	1.40	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	NAG	O5-C1-C2	-4.47	104.23	111.29
3	F	5	XYS	C5-O5-C1	3.80	117.37	111.52
3	D	5	XYS	C5-O5-C1	3.54	116.96	111.52
3	D	6	GAL	C1-C2-C3	3.02	113.37	109.67
2	C	2	NAG	O5-C1-C2	-2.85	106.80	111.29
3	F	1	BGC	O5-C1-C2	-2.80	106.45	110.77
2	E	1	NAG	C1-C2-N2	2.69	115.09	110.49
3	F	4	XYS	C5-O5-C1	2.52	115.39	111.52
2	E	1	NAG	O5-C1-C2	-2.44	107.44	111.29
3	F	3	BGC	C1-O5-C5	2.43	115.49	112.19
2	E	3	BMA	C1-C2-C3	2.31	112.50	109.67
3	D	4	XYS	C5-O5-C1	2.31	115.07	111.52
3	F	6	GAL	O5-C5-C6	2.30	110.81	107.20
3	D	1	BGC	C1-C2-C3	2.24	112.42	109.67
2	E	2	NAG	O5-C1-C2	-2.20	107.81	111.29
3	D	1	BGC	O5-C5-C6	2.14	110.56	107.20
3	D	2	BGC	C1-C2-C3	2.08	112.22	109.67
2	C	1	NAG	O6-C6-C5	-2.06	104.21	111.29
3	F	3	BGC	O6-C6-C5	-2.04	104.31	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2	BGC	1	0
3	F	2	BGC	2	0
2	C	1	NAG	1	0
2	E	1	NAG	2	0
3	D	5	XYS	1	0
3	F	5	XYS	2	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 C

Bond lengths | Bond angles | Torsions | Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings
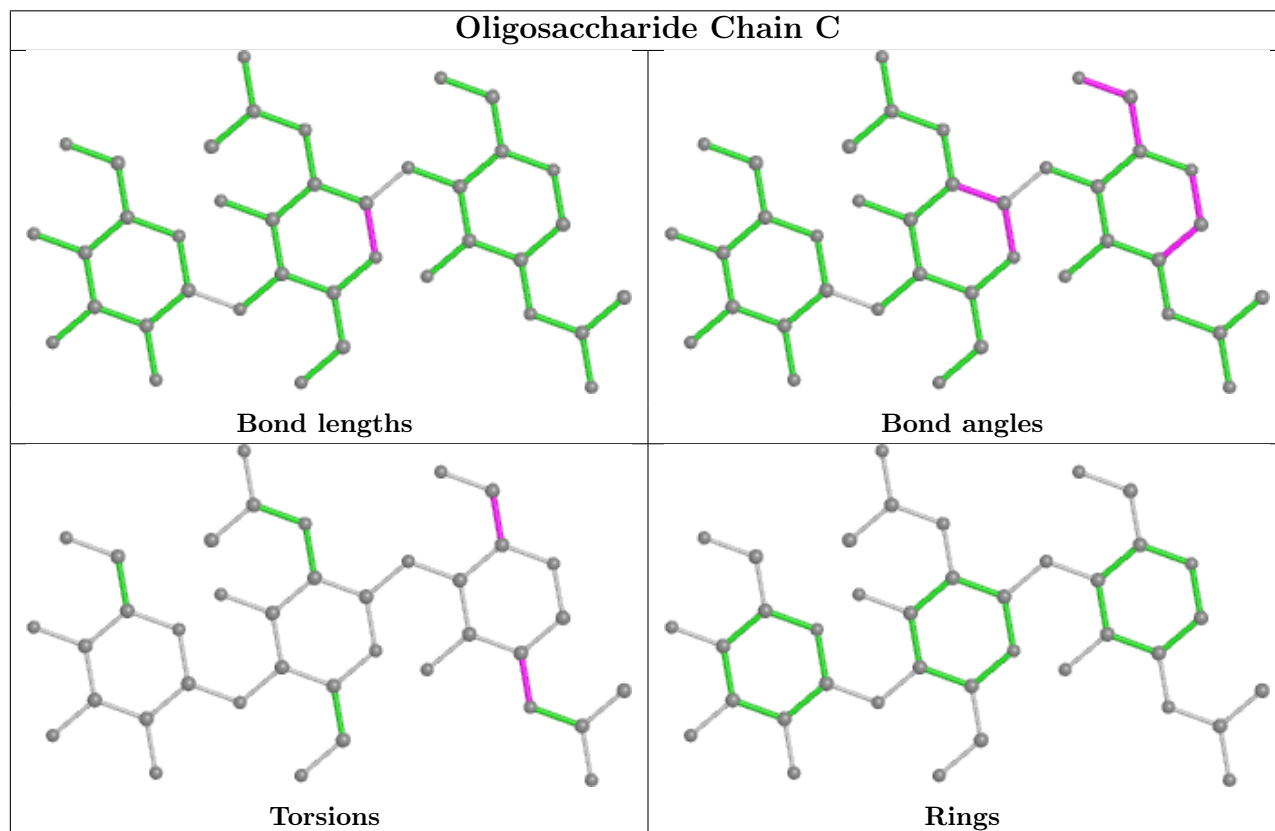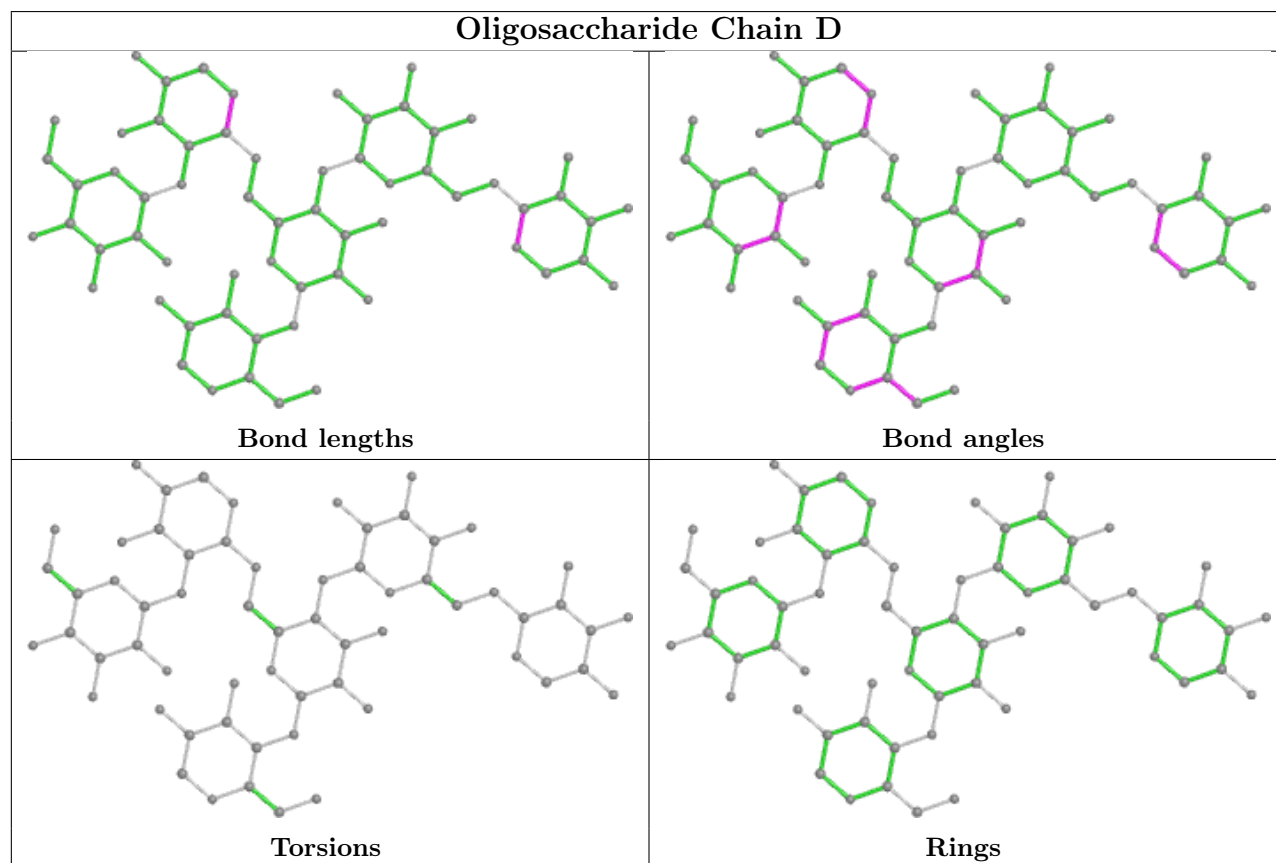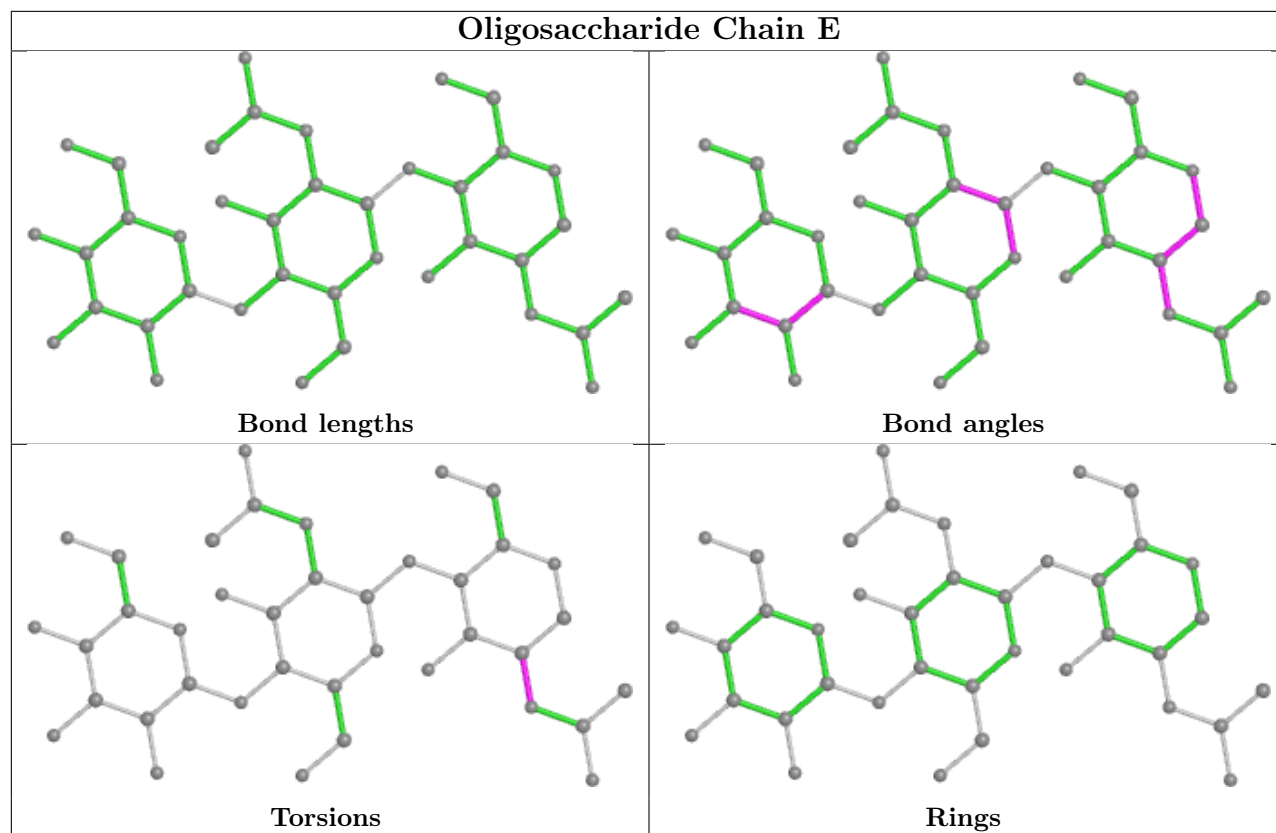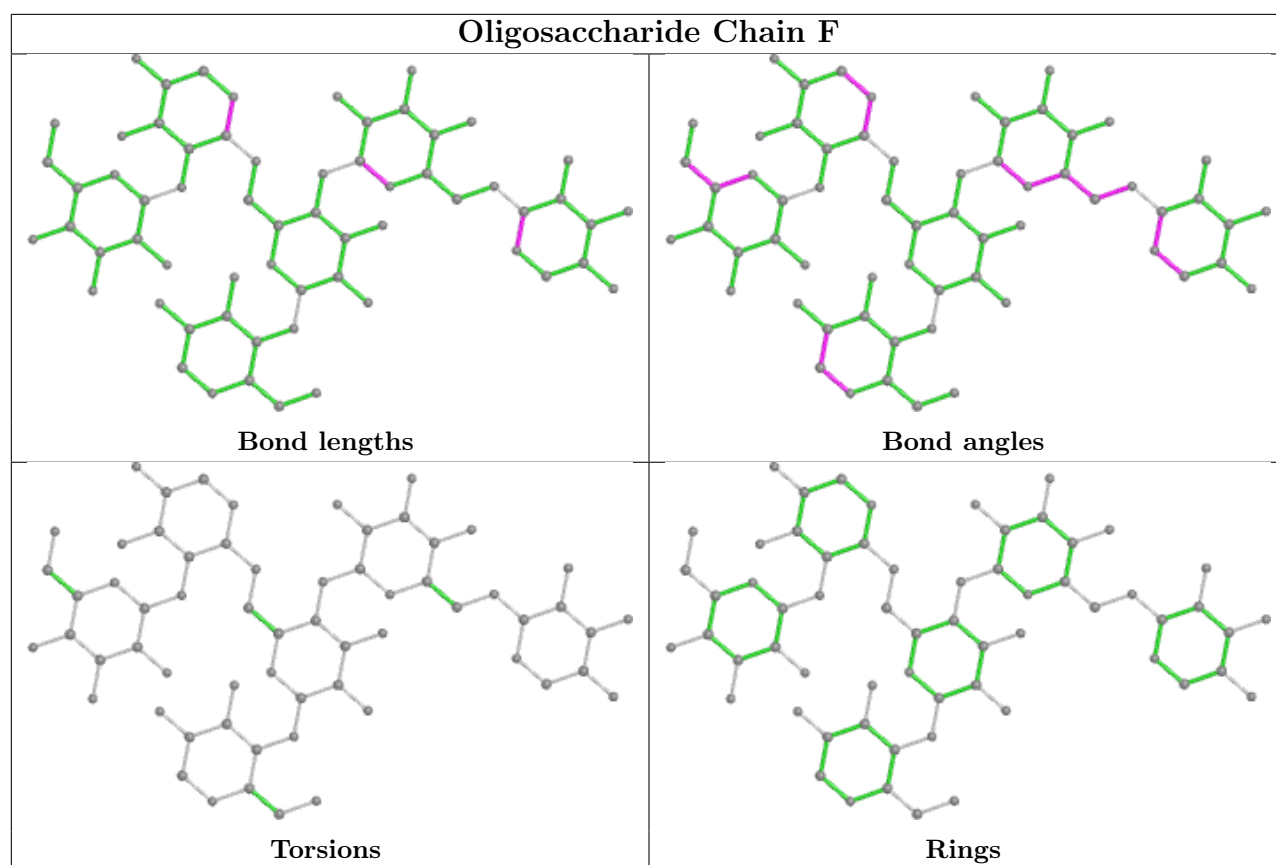
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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(Å²)	Q<0.9
1	A	267/278 (96%)	0.61	30 (11%)	5	4	17, 29, 51, 70	4 (1%)
1	B	264/278 (94%)	0.30	14 (5%)	26	21	16, 28, 42, 49	2 (0%)
All	All	531/556 (95%)	0.46	44 (8%)	11	8	16, 29, 48, 70	6 (1%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	VAL	8.9
1	A	272	ILE	8.3
1	A	213	ALA	7.8
1	A	215	PHE	7.5
1	B	272	ILE	7.0
1	A	212	GLU	6.9
1	A	80	ASN	6.1
1	A	81	SER	5.8
1	B	80	ASN	5.8
1	B	81	SER	5.7
1	A	210	SER	5.4
1	A	261	SER	4.7
1	B	174[A]	TRP	4.3
1	A	217	ALA	4.3
1	A	79	GLN	4.1
1	B	9	VAL	3.8
1	A	235	PHE	3.7
1	A	214	LYS	3.7
1	A	242	TRP	3.4
1	A	7	VAL	3.4
1	A	139	ILE	3.3
1	B	28	ASN	3.2
1	A	262	MET	3.0
1	B	13	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	221	ALA	2.8
1	A	74	PHE	2.8
1	A	259	TYR	2.8
1	A	234	ALA	2.8
1	A	253	CYS	2.7
1	A	88	PHE	2.6
1	A	260	PRO	2.6
1	B	79	GLN	2.5
1	B	139	ILE	2.5
1	A	6	PRO	2.4
1	A	185	LEU	2.3
1	A	13	ARG	2.3
1	A	209	ALA	2.3
1	B	86	ILE	2.2
1	A	8	ASP	2.2
1	B	88	PHE	2.2
1	B	73	ALA	2.2
1	A	101	LEU	2.1
1	B	185	LEU	2.1
1	B	29	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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.
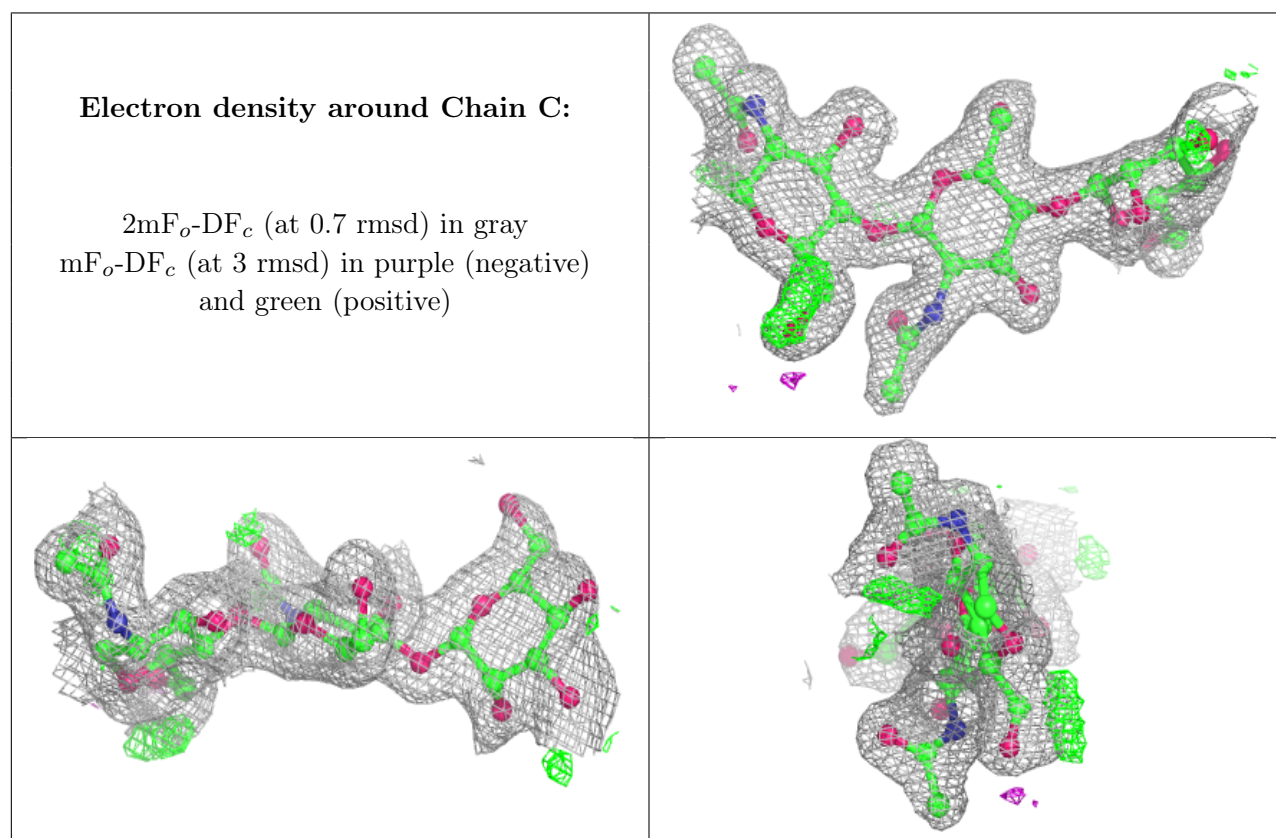
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	D	1	11/12	0.74	0.35	48,50,52,54	0
2	BMA	E	3	11/12	0.81	0.23	48,52,54,57	0
3	XYS	D	5	9/10	0.85	0.19	44,47,49,50	0
3	GAL	D	6	11/12	0.86	0.39	54,55,56,56	0
2	BMA	C	3	11/12	0.87	0.24	51,54,57,59	0
3	BGC	F	1	11/12	0.89	0.23	34,38,43,45	0
3	XYS	D	4	9/10	0.90	0.18	47,48,48,49	0
3	BGC	D	3	11/12	0.90	0.11	29,35,39,42	0

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| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	NAG	C	1	14/15	0.92	0.09	23,26,32,32	0
2	NAG	C	2	14/15	0.92	0.16	35,38,41,45	0
3	XYS	F	4	9/10	0.92	0.15	38,40,43,45	0
3	GAL	F	6	11/12	0.92	0.24	39,42,43,45	0
2	NAG	E	2	14/15	0.93	0.13	30,34,38,41	0
3	XYS	F	5	9/10	0.94	0.10	25,32,35,37	0
3	BGC	D	2	11/12	0.94	0.16	38,41,43,44	0
2	NAG	E	1	14/15	0.96	0.08	22,26,31,32	0
3	BGC	F	2	11/12	0.96	0.13	26,29,32,34	0
3	BGC	F	3	11/12	0.96	0.07	22,27,29,31	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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)
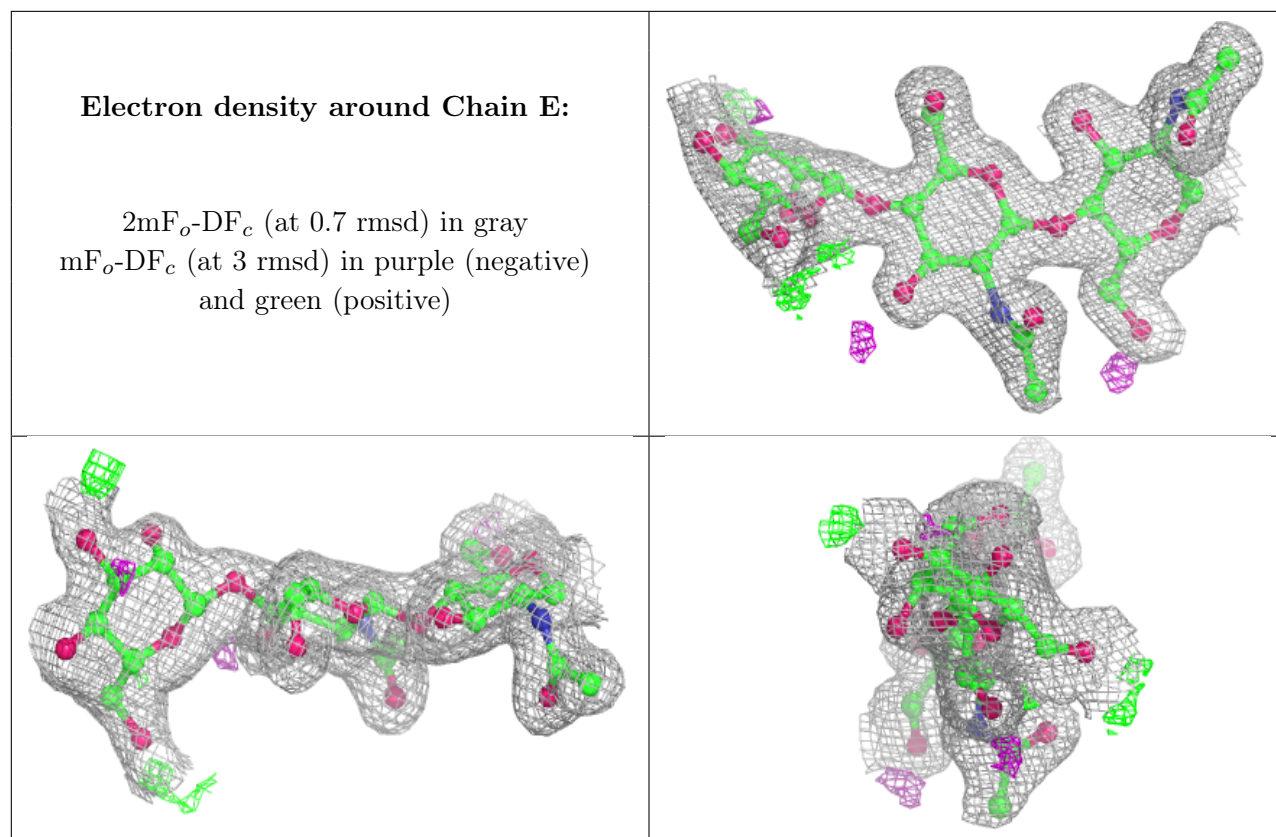
Electron density around Chain D:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)
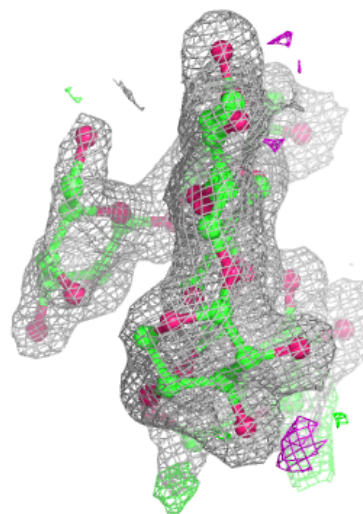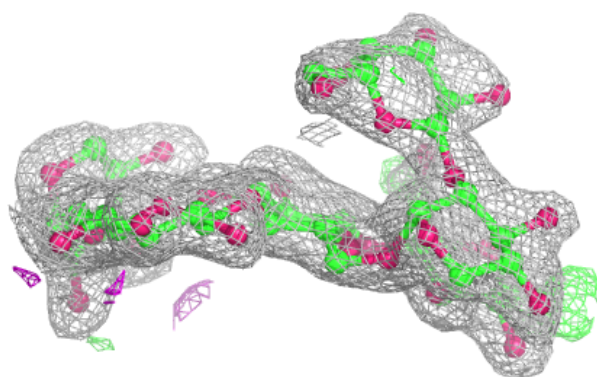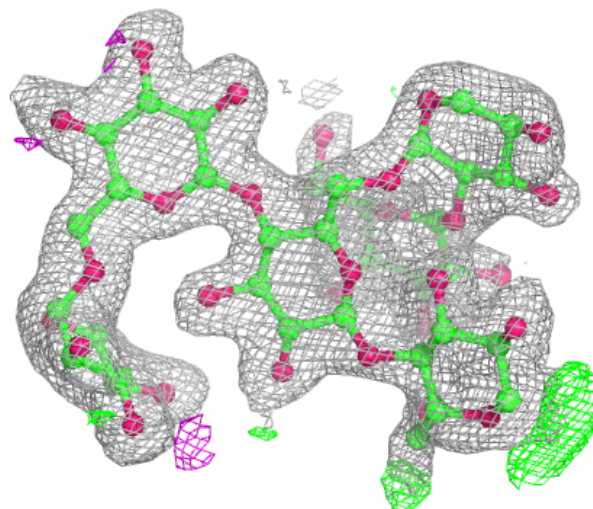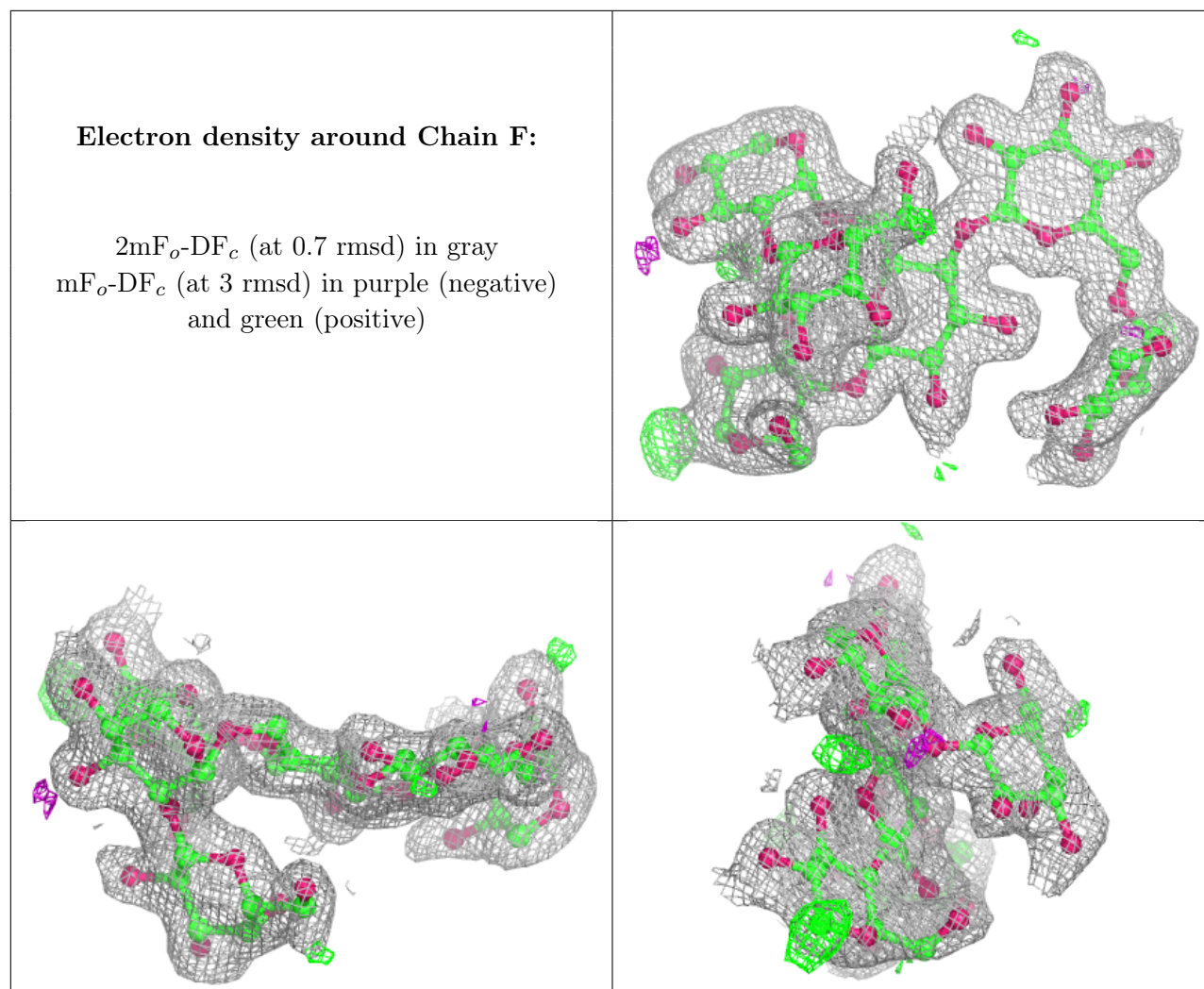
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.