



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 03:42 am GMT

PDB ID : 6G1I
Title : GH124 cellulase from Ruminiclostridium thermocellum in complex with Mn and fructosylated cellopentaose
Authors : Urresti, S.; Davies, G.J.; Walton, P.H.
Deposited on : 2018-03-21
Resolution : 0.99 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 : 2.36
buster-report : 1.1.7 (2018)
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

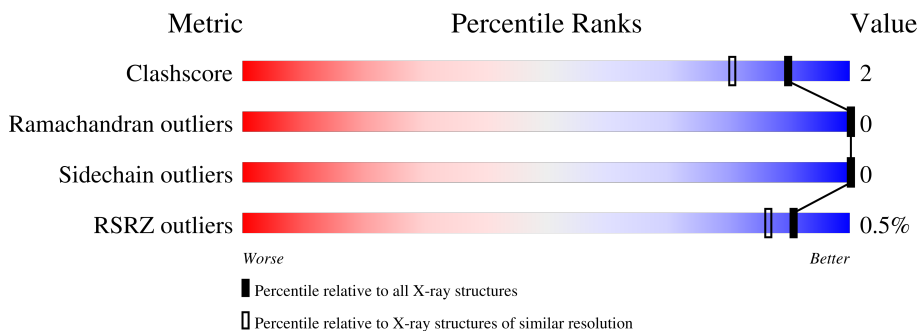
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.99 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))
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	1043 (1.06-0.94)
Sidechain outliers	138945	1045 (1.06-0.94)
RSRZ outliers	127900	1023 (1.06-0.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	
1	B	223	
2	C	4	
2	E	4	
3	D	4	
3	F	4	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 4246 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 Glycosyl Hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	210	Total	C	N	O	S	0	15	0
			1785	1140	305	333	7			
1	B	210	Total	C	N	O	S	0	18	0
			1804	1150	311	335	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	GLY	-	expression tag	UNP A3DCJ4
A	129	PRO	-	expression tag	UNP A3DCJ4
B	128	GLY	-	expression tag	UNP A3DCJ4
B	129	PRO	-	expression tag	UNP A3DCJ4

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	E	4	Total	C	O	0	0	0
			45	24	21			

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

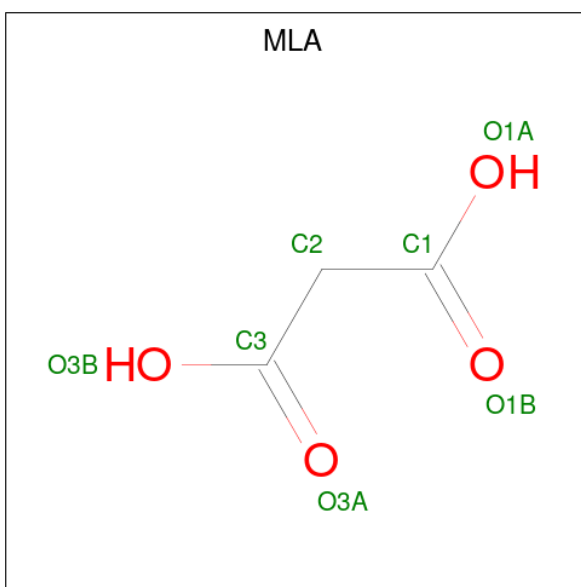


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	4	Total	C	O	0	0	0
			45	24	21			
3	F	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula: C₃H₄O₄).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	244	Total	O	0	0
			244	244		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	217	Total 217	O 217	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: Glycosyl Hydrolase

Chain A:  90% 6%



- Molecule 1: Glycosyl Hydrolase

Chain B:  88% 6% 6%



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-fructofuranose

Chain C:  50% 50%

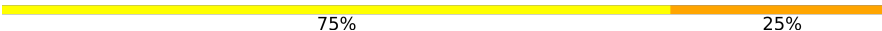


- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-fructofuranose

Chain E:  25% 75%



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

Chain D:  75% 25%



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

Chain F:  75% 25%

BGC1
BGC2
BGC3
BGC4

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.14Å 74.17Å 77.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.59 – 0.99 52.35 – 0.99	Depositor EDS
% Data completeness (in resolution range)	95.1 (53.59-0.99) 95.2 (52.35-0.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 0.99Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.131 , 0.147 0.132 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	9.7	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for k,h,-l	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4246	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: OHI, MN, FRU, BGC, MLA

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	0.80	0/1872	0.92	4/2532 (0.2%)
1	B	0.81	0/1899	0.98	11/2570 (0.4%)
All	All	0.80	0/3771	0.95	15/5102 (0.3%)

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	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309[A]	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	B	309[B]	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	A	323	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	309[A]	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	309[B]	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	275[A]	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	275[B]	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	288	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	A	323	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	268	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	B	193	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	B	178	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	197	PHE	CB-CG-CD1	5.11	124.37	120.80
1	B	178	ASP	CB-CG-OD2	-5.10	113.71	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	TYR	CB-CG-CD2	-5.03	117.98	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	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	1785	0	1696	5	0
1	B	1804	0	1709	6	0
2	C	45	0	39	0	0
2	E	45	0	39	0	0
3	D	45	0	39	2	0
3	F	45	0	39	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	7	0	2	1	0
5	B	7	0	2	1	0
6	A	244	0	0	4	0
6	B	217	0	0	3	0
All	All	4246	0	3565	13	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 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:B:241:HIS:HD2	6:B:588:HOH:O	1.83	0.61
1:B:241:HIS:HE1	6:B:682:HOH:O	1.90	0.55
6:A:563:HOH:O	3:F:1:BGC:H3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159[A]:SER:OG	3:D:1:BGC:H5	2.10	0.50
1:A:187[B]:LYS:CE	6:A:507:HOH:O	2.63	0.47
5:B:410:MLA:O3A	5:B:410:MLA:O1B	2.27	0.46
1:B:151[A]:HIS:CE1	3:D:3:BGC:O2	2.69	0.46
1:B:323[A]:ARG:HD2	6:B:538:HOH:O	2.17	0.43
1:A:306:TRP:CD2	5:A:410:MLA:HC21	2.54	0.43
1:A:325:ASN:HB2	6:A:676:HOH:O	2.18	0.42
1:B:279:GLU:HB3	1:B:280[B]:LYS:HE3	2.01	0.42
1:A:187[B]:LYS:NZ	6:A:507:HOH:O	2.48	0.41
1:A:177:TRP:CD2	1:A:189:LYS:HG2	2.56	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	222/223 (100%)	215 (97%)	7 (3%)	0	100	100
1	B	226/223 (101%)	221 (98%)	5 (2%)	0	100	100
All	All	448/446 (100%)	436 (97%)	12 (3%)	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	187/181 (103%)	187 (100%)	0	100	100
1	B	190/181 (105%)	190 (100%)	0	100	100
All	All	377/362 (104%)	377 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	B	232	ASN
1	B	241	HIS
1	B	248	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	OHI	B	264	1,4	8,11,12	1.47	1 (12%)	5,14,16	1.49	2 (40%)
1	OHI	A	264	1,4	8,11,12	1.58	3 (37%)	5,14,16	1.20	1 (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
1	OHI	B	264	1,4	-	0/3/15/17	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OHI	A	264	1,4	-	0/3/15/17	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	OHI	CE1-ND1	-2.33	1.32	1.39
1	B	264	OHI	CE1-NE2	-2.30	1.32	1.39
1	A	264	OHI	CD2-NE2	2.27	1.39	1.33
1	A	264	OHI	O12-CE1	2.09	1.27	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	OHI	O12-CE1-ND1	-2.31	120.11	126.01
1	A	264	OHI	O12-CE1-ND1	-2.25	120.28	126.01
1	B	264	OHI	CG-CD2-NE2	-2.24	107.14	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

16 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	FRU	C	1	2	11,12,12	0.90	1 (9%)	10,18,18	0.49	0
2	BGC	C	2	2	11,11,12	0.48	0	15,15,17	0.79	0
2	BGC	C	3	2	11,11,12	0.74	0	15,15,17	1.00	0
2	BGC	C	4	2	11,11,12	0.61	0	15,15,17	1.13	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BGC	D	1	3	12,12,12	0.63	0	17,17,17	1.25	1 (5%)
3	BGC	D	2	3	11,11,12	0.76	0	15,15,17	0.99	1 (6%)
3	BGC	D	3	3	11,11,12	0.39	0	15,15,17	0.86	0
3	BGC	D	4	3	11,11,12	0.79	1 (9%)	15,15,17	0.54	0
2	FRU	E	1	2	11,12,12	0.73	0	10,18,18	0.65	0
2	BGC	E	2	2	11,11,12	0.55	0	15,15,17	0.86	1 (6%)
2	BGC	E	3	2	11,11,12	0.63	0	15,15,17	1.00	1 (6%)
2	BGC	E	4	2	11,11,12	1.19	1 (9%)	15,15,17	1.78	4 (26%)
3	BGC	F	1	3	12,12,12	1.18	1 (8%)	17,17,17	1.49	4 (23%)
3	BGC	F	2	3	11,11,12	0.59	0	15,15,17	0.92	0
3	BGC	F	3	3	11,11,12	0.71	0	15,15,17	0.91	0
3	BGC	F	4	3	11,11,12	0.67	0	15,15,17	0.56	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
2	FRU	C	1	2	-	0/5/24/24	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	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
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	D	4	3	-	0/2/19/22	0/1/1/1
2	FRU	E	1	2	-	0/5/24/24	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	E	3	2	-	0/2/19/22	0/1/1/1
2	BGC	E	4	2	-	0/2/19/22	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	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
3	BGC	F	4	3	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	BGC	O2-C2	3.03	1.50	1.43
2	E	4	BGC	O5-C1	-2.87	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	FRU	O2-C2	2.33	1.44	1.40
3	D	4	BGC	O5-C1	-2.06	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4	BGC	O3-C3-C2	4.08	117.82	109.99
2	E	4	BGC	C1-O5-C5	3.14	116.44	112.19
3	F	1	BGC	O3-C3-C4	2.79	116.80	110.35
2	E	4	BGC	O5-C1-C2	-2.66	106.66	110.77
3	D	1	BGC	C3-C4-C5	2.50	114.69	110.24
2	E	4	BGC	O5-C5-C6	2.35	110.89	107.20
3	F	1	BGC	O5-C1-C2	2.34	114.45	110.28
2	C	4	BGC	O4-C4-C5	-2.33	103.51	109.30
3	F	1	BGC	C3-C4-C5	2.19	114.15	110.24
2	E	3	BGC	O5-C1-C2	-2.17	107.41	110.77
2	E	2	BGC	O3-C3-C2	-2.12	105.93	109.99
3	D	2	BGC	O4-C4-C5	-2.01	104.30	109.30
3	F	1	BGC	C1-O5-C5	-2.00	109.88	113.66

There are no chirality outliers.

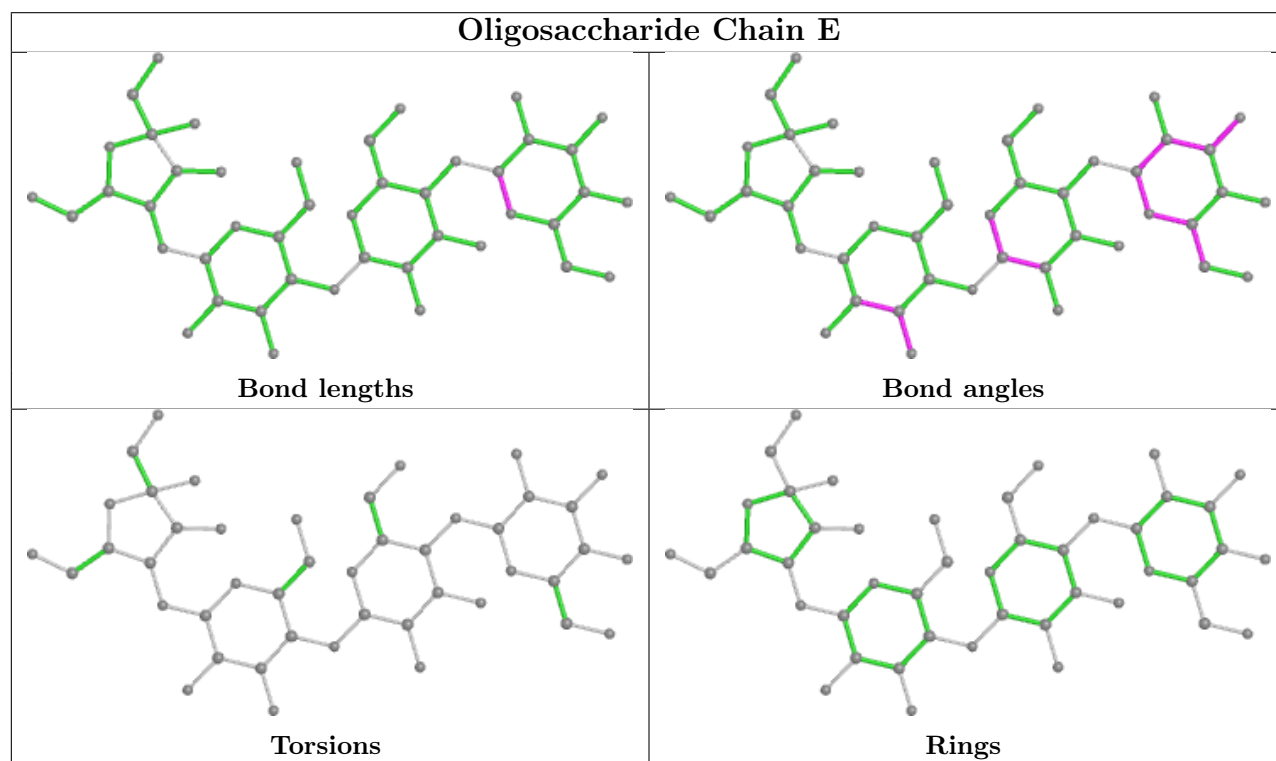
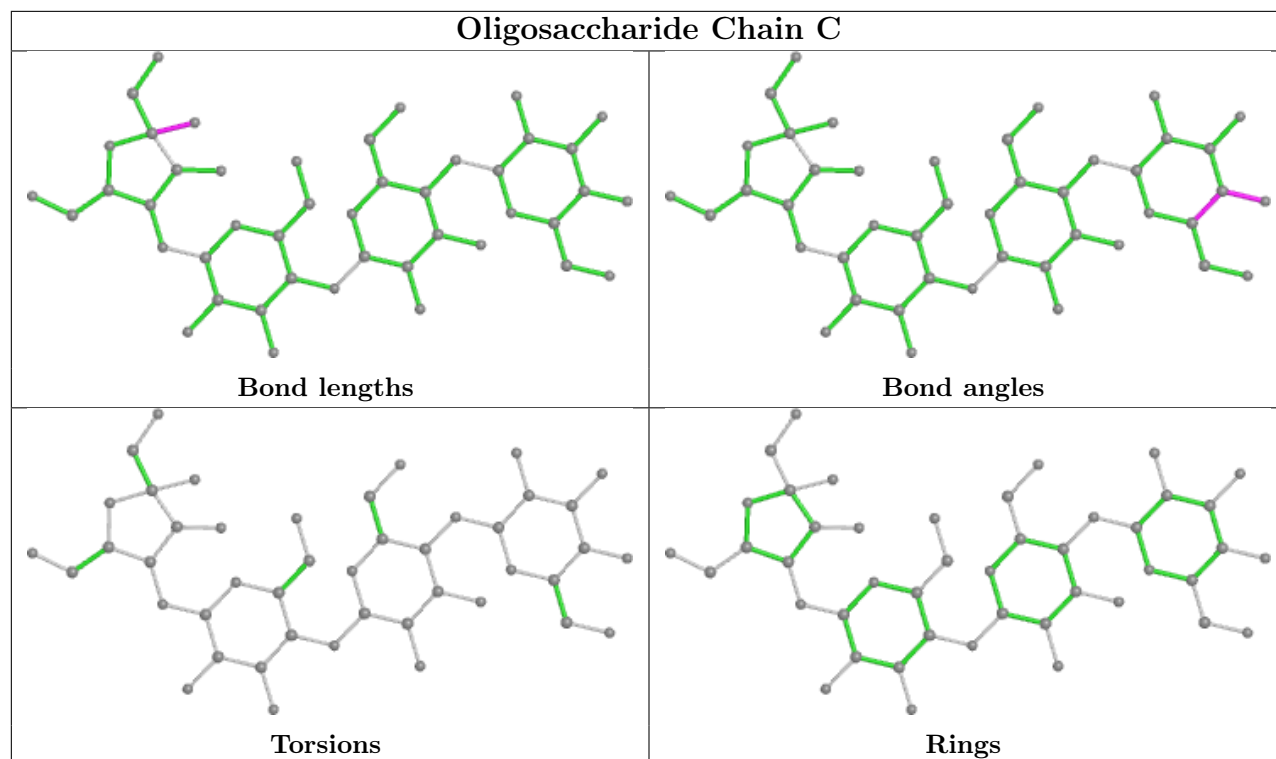
There are no torsion outliers.

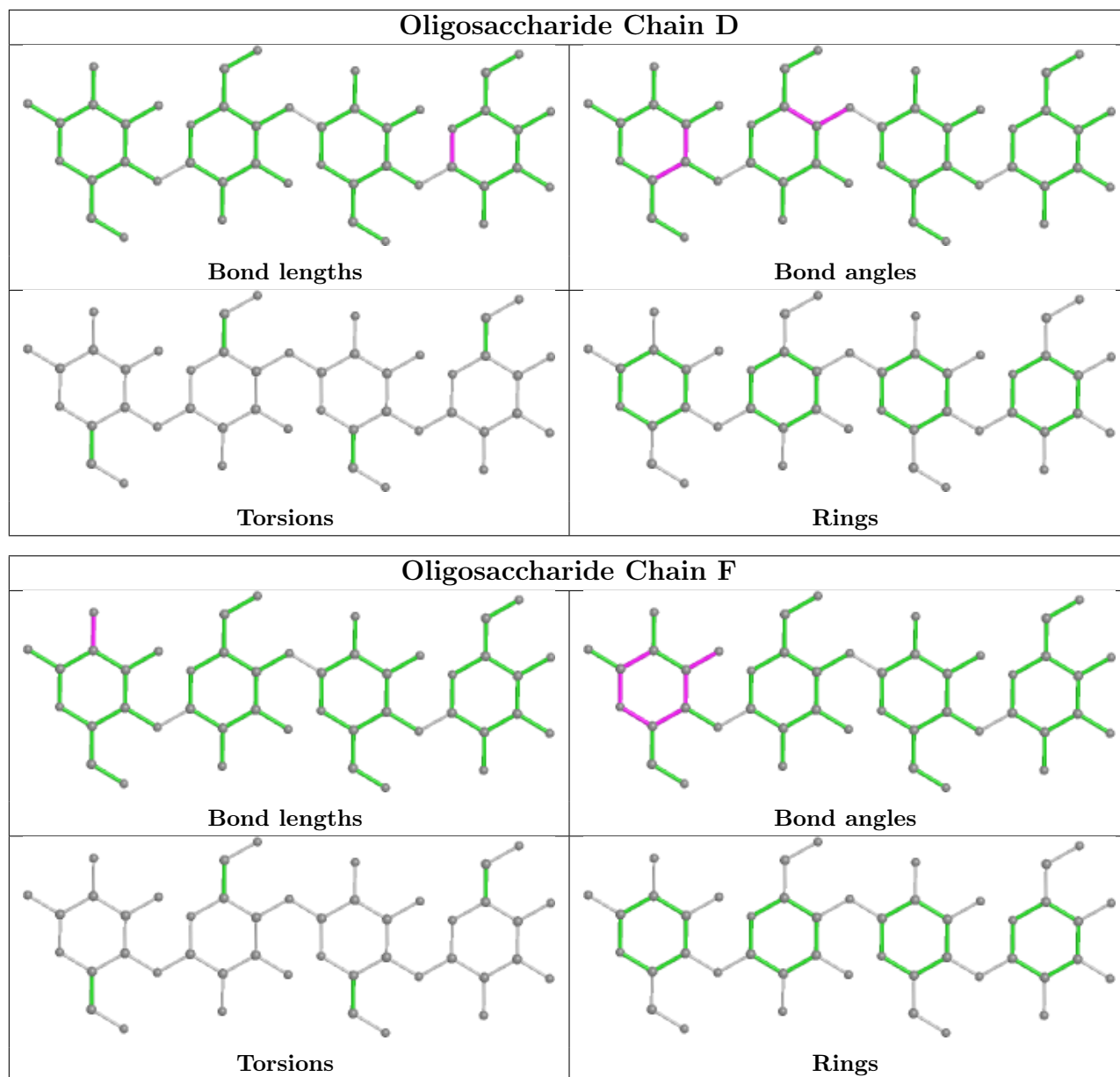
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	BGC	1	0
3	D	1	BGC	1	0
3	D	3	BGC	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, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MLA	A	410	-	6,6,6	1.07	0	7,7,7	1.50	2 (28%)
5	MLA	B	410	-	6,6,6	1.66	1 (16%)	7,7,7	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLA	A	410	-	-	0/4/4/4	-
5	MLA	B	410	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	410	MLA	O3A-C3	2.28	1.29	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	410	MLA	O1B-C1-C2	-2.22	115.60	122.08
5	A	410	MLA	O3B-C3-C2	2.03	121.01	114.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	410	MLA	1	0
5	B	410	MLA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/223 (93%)	-0.08	0 100 100	7, 10, 17, 24	3 (1%)
1	B	209/223 (93%)	-0.10	2 (0%) 82 76	7, 11, 17, 30	4 (1%)
All	All	418/446 (93%)	-0.09	2 (0%) 91 86	7, 11, 17, 30	7 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323[A]	ARG	2.6
1	B	151[A]	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OHI	A	264	11/12	0.99	0.07	6,7,8,10	1
1	OHI	B	264	11/12	0.99	0.08	6,7,8,11	1

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

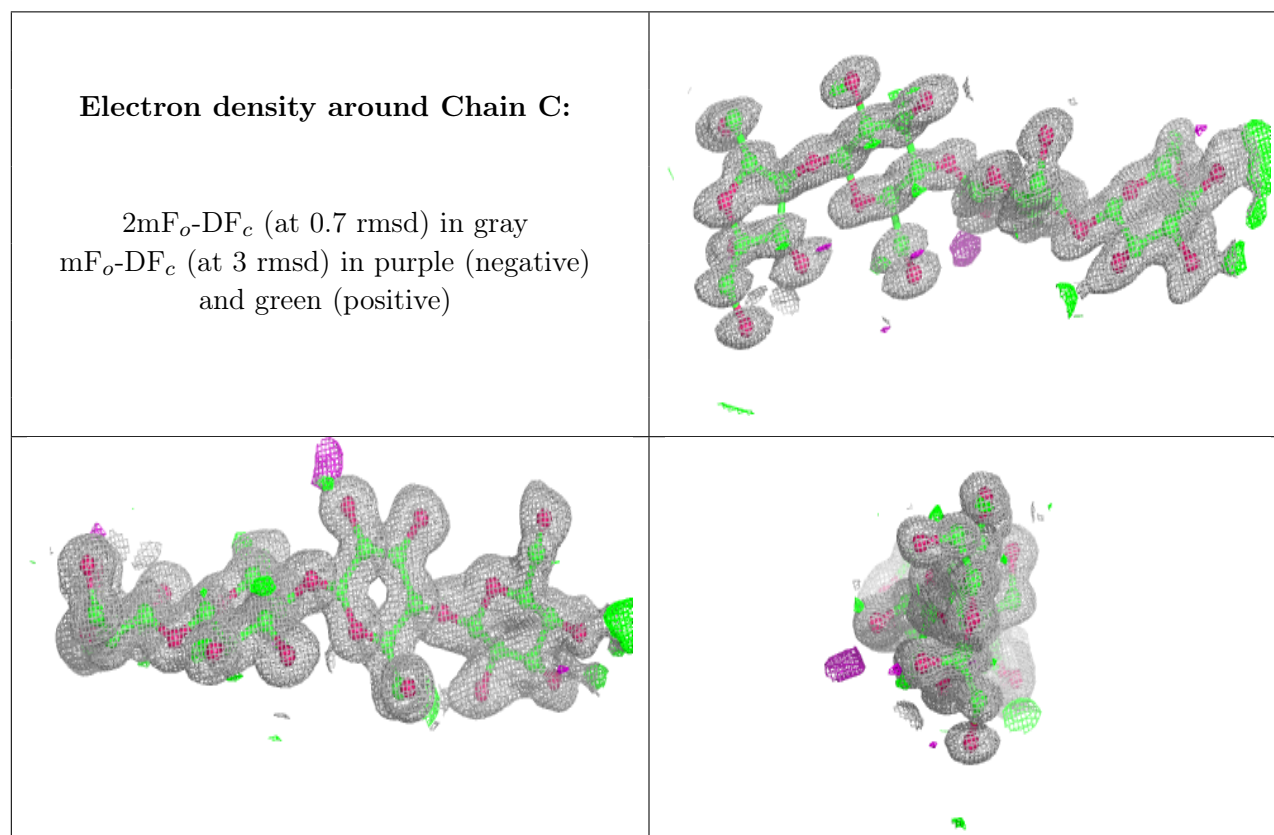
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGC	E	4	11/12	0.90	0.13	16,19,25,28	0

Continued on next page...

Continued from previous page...

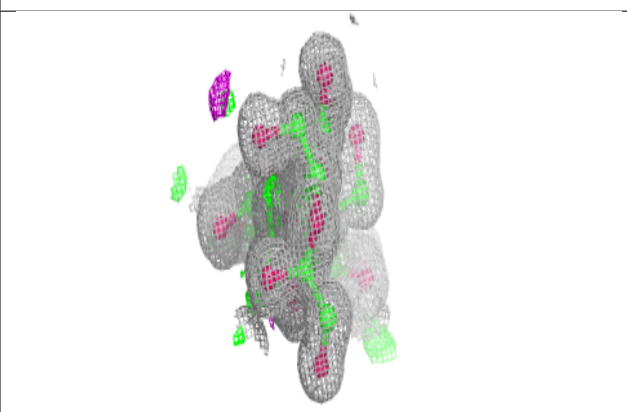
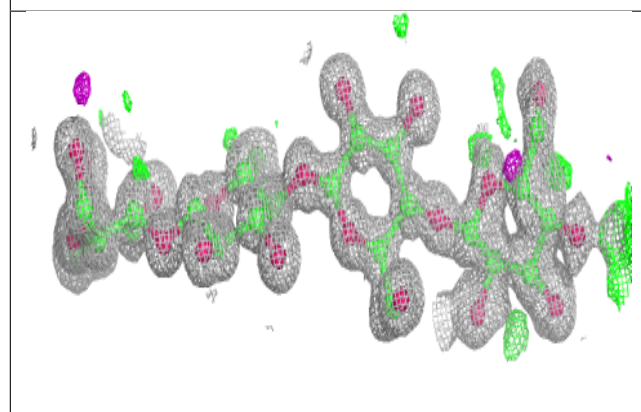
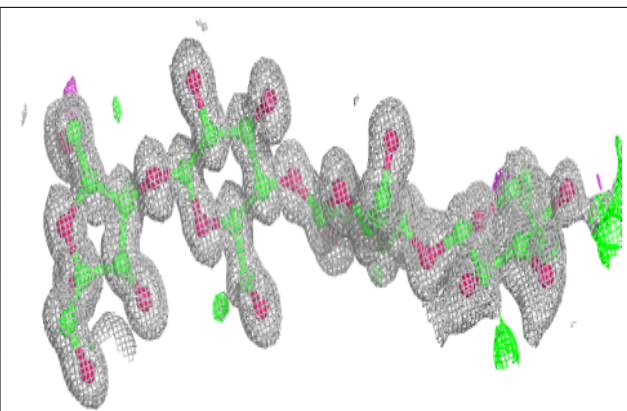
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	BGC	F	1	12/12	0.92	0.10	14,22,77,77	0
2	BGC	C	4	11/12	0.95	0.09	14,19,29,32	0
3	BGC	D	1	12/12	0.97	0.10	13,17,23,28	0
3	BGC	D	4	11/12	0.98	0.06	8,8,9,11	0
3	BGC	D	2	11/12	0.98	0.05	8,10,12,15	0
3	BGC	F	2	11/12	0.98	0.06	10,12,14,15	0
3	BGC	F	3	11/12	0.98	0.06	9,10,11,11	0
2	BGC	C	3	11/12	0.99	0.05	9,10,12,12	0
2	FRU	C	1	12/12	0.99	0.06	7,9,10,13	0
3	BGC	D	3	11/12	0.99	0.06	9,9,10,10	0
2	FRU	E	1	12/12	0.99	0.06	7,9,10,12	0
2	BGC	E	2	11/12	0.99	0.05	7,7,8,9	0
2	BGC	E	3	11/12	0.99	0.06	8,9,10,11	0
2	BGC	C	2	11/12	0.99	0.06	7,8,9,10	0
3	BGC	F	4	11/12	0.99	0.05	8,9,11,11	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.

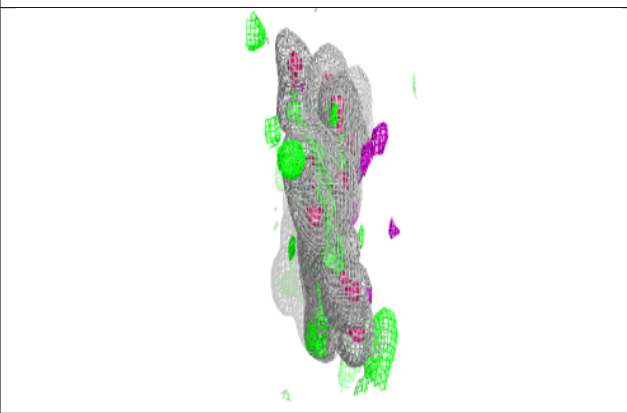
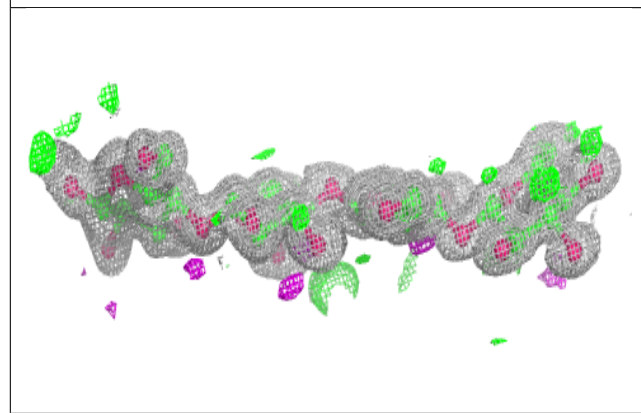
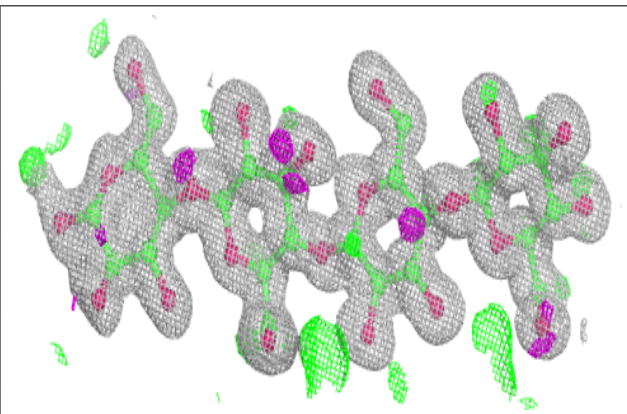


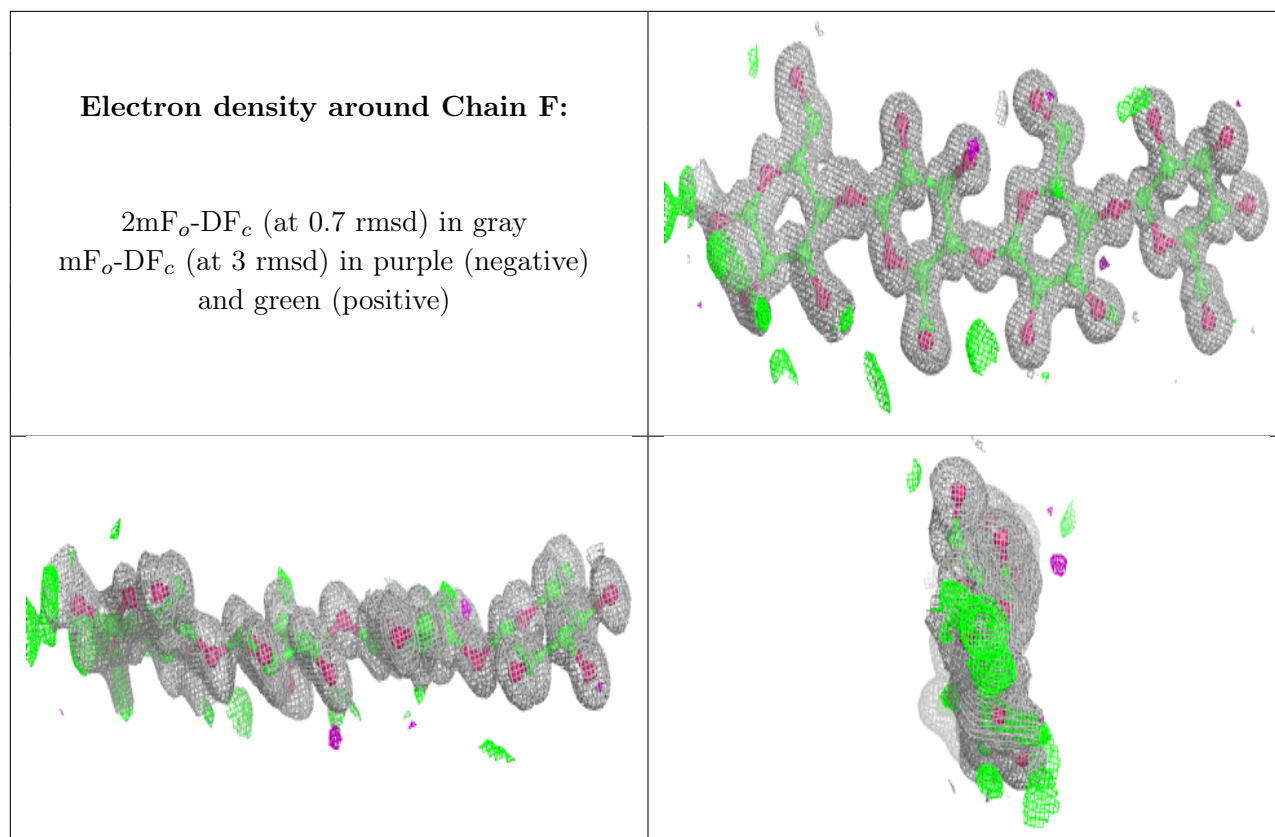
Electron density around Chain E:

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

**Electron density around Chain D:**

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





6.4 Ligands [i](#)

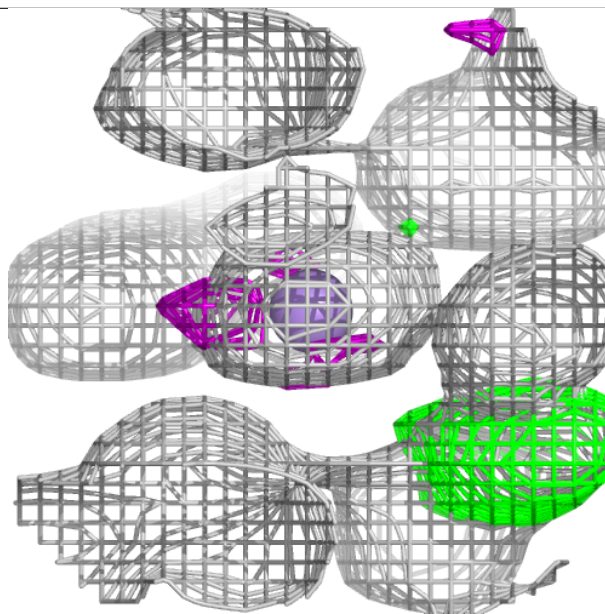
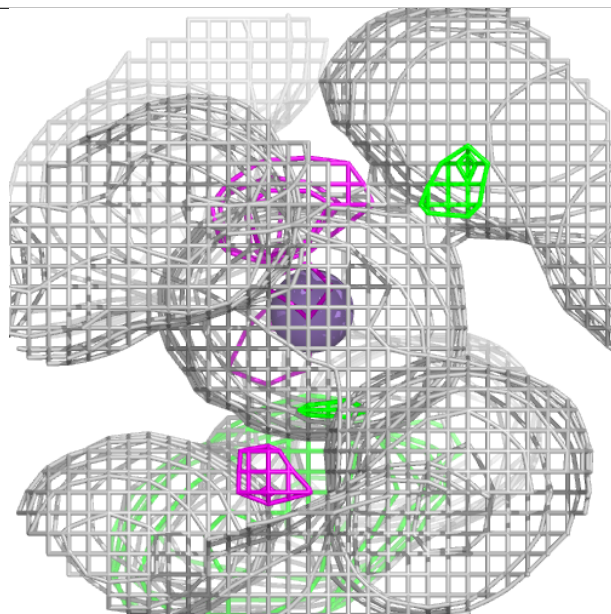
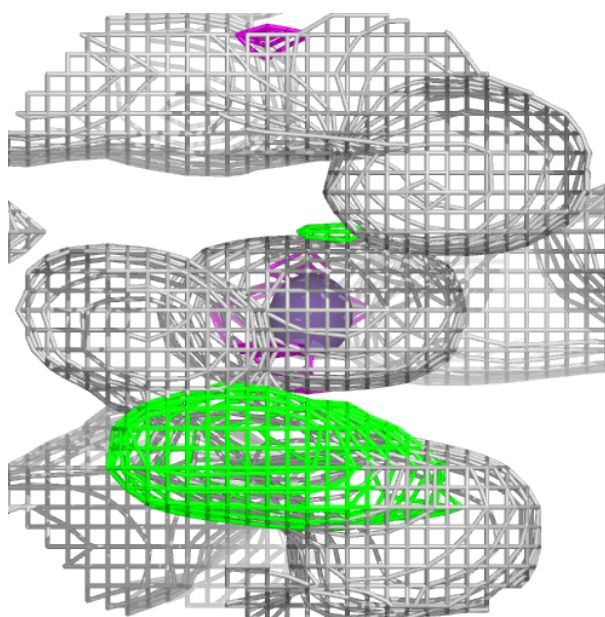
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

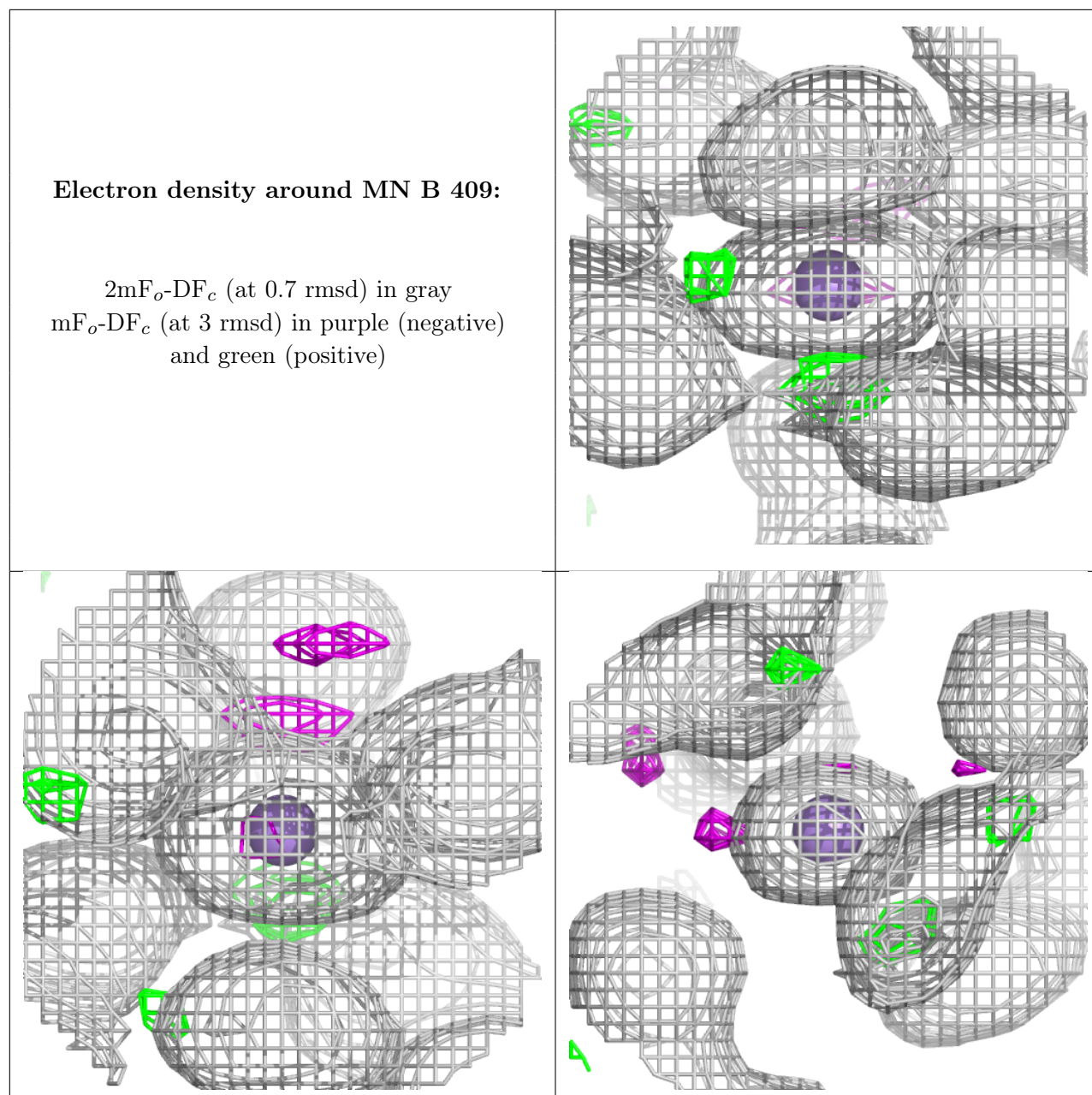
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MLA	A	410	7/7	0.92	0.18	18,25,37,45	7
5	MLA	B	410	7/7	0.93	0.15	11,11,13,14	7
4	MN	A	409	1/1	1.00	0.03	9,9,9,9	1
4	MN	B	409	1/1	1.00	0.04	8,8,8,8	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MN A 409:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.