



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 08:49 PM BST

PDB ID : 6DTQ
Title : Maltose bound T. maritima MalE3
Authors : Cuneo, M.J.; Shukla, S.
Deposited on : 2018-06-18
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2.13.1
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)	:	2.13.1

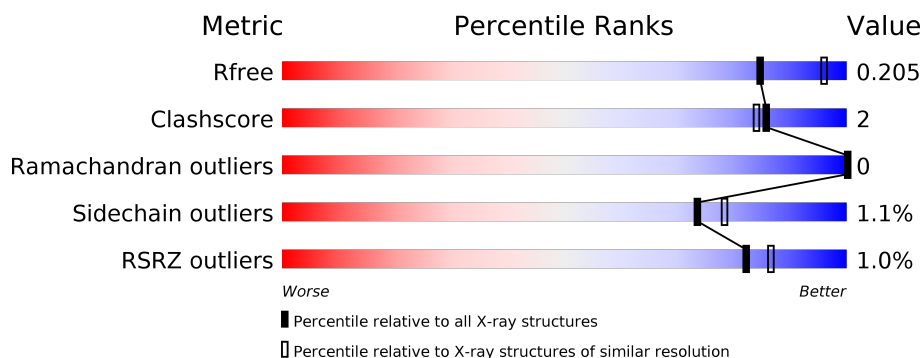
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	400	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>
1	B	400	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>
1	C	400	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>
1	D	400	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div></div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	F	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 50%50%
2	H	2	 50%50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13136 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 maltose-binding protein MalE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	4	0
			3143	2031	513	586	13			
1	B	391	Total	C	N	O	S	0	1	0
			3114	2016	506	580	12			
1	C	391	Total	C	N	O	S	0	3	0
			3129	2025	508	582	14			
1	D	391	Total	C	N	O	S	0	4	0
			3140	2029	512	586	13			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP G4FGN8
A	412	HIS	-	expression tag	UNP G4FGN8
A	413	HIS	-	expression tag	UNP G4FGN8
A	414	HIS	-	expression tag	UNP G4FGN8
A	415	HIS	-	expression tag	UNP G4FGN8
A	416	HIS	-	expression tag	UNP G4FGN8
A	417	HIS	-	expression tag	UNP G4FGN8
B	18	MET	-	initiating methionine	UNP G4FGN8
B	412	HIS	-	expression tag	UNP G4FGN8
B	413	HIS	-	expression tag	UNP G4FGN8
B	414	HIS	-	expression tag	UNP G4FGN8
B	415	HIS	-	expression tag	UNP G4FGN8
B	416	HIS	-	expression tag	UNP G4FGN8
B	417	HIS	-	expression tag	UNP G4FGN8
C	18	MET	-	initiating methionine	UNP G4FGN8
C	412	HIS	-	expression tag	UNP G4FGN8
C	413	HIS	-	expression tag	UNP G4FGN8
C	414	HIS	-	expression tag	UNP G4FGN8
C	415	HIS	-	expression tag	UNP G4FGN8
C	416	HIS	-	expression tag	UNP G4FGN8
C	417	HIS	-	expression tag	UNP G4FGN8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	18	MET	-	initiating methionine	UNP G4FGN8
D	412	HIS	-	expression tag	UNP G4FGN8
D	413	HIS	-	expression tag	UNP G4FGN8
D	414	HIS	-	expression tag	UNP G4FGN8
D	415	HIS	-	expression tag	UNP G4FGN8
D	416	HIS	-	expression tag	UNP G4FGN8
D	417	HIS	-	expression tag	UNP G4FGN8

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	135	Total	O	0	0
			135	135		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	132	Total 132	O 132	0	0
4	C	139	Total 139	O 139	0	0
4	D	108	Total 108	O 108	0	0

Chain E:  50% 50%

 GLC1
GLC2

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

Chain F:  50% 50%

 GLC1
GLC2

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

Chain G:  50% 50%

 GLC1
GLC2

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

Chain H:  50% 50%

 GLC1
GLC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.37Å 124.03Å 174.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.09 – 2.15 39.09 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.2 (39.09-2.15) 95.2 (39.09-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.174 , 0.205 0.174 , 0.205	Depositor DCC
R_{free} test set	4628 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13136	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 18.56% 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: MG, 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	0.25	0/3222	0.43	0/4374
1	B	0.25	0/3193	0.43	0/4336
1	C	0.25	0/3208	0.42	0/4356
1	D	0.25	0/3219	0.44	0/4371
All	All	0.25	0/12842	0.43	0/17437

There are no bond length outliers.

There are no bond angle outliers.

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	3143	0	3111	15	0
1	B	3114	0	3088	11	0
1	C	3129	0	3103	14	0
1	D	3140	0	3108	16	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	135	0	0	3	0
4	B	132	0	0	3	0
4	C	139	0	0	1	0
4	D	108	0	0	2	0
All	All	13136	0	12494	56	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.

The worst 5 of 56 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:268:ASP:OD1	1:A:273:LYS:NZ	2.32	0.62
1:B:369:ARG:NH1	4:B:603:HOH:O	2.33	0.61
1:B:124:ARG:NH1	4:B:604:HOH:O	2.33	0.60
1:A:21:LYS:HE3	1:A:53:GLU:HB2	1.87	0.57
1:B:288:ARG:NH2	4:B:601:HOH:O	2.26	0.56

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	393/400 (98%)	387 (98%)	6 (2%)	0	100	100
1	B	390/400 (98%)	385 (99%)	5 (1%)	0	100	100
1	C	392/400 (98%)	386 (98%)	6 (2%)	0	100	100
1	D	393/400 (98%)	386 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1568/1600 (98%)	1544 (98%)	24 (2%)	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	333/337 (99%)	331 (99%)	2 (1%)	86	90
1	B	330/337 (98%)	324 (98%)	6 (2%)	59	63
1	C	332/337 (98%)	329 (99%)	3 (1%)	78	83
1	D	333/337 (99%)	329 (99%)	4 (1%)	71	76
All	All	1328/1348 (98%)	1313 (99%)	15 (1%)	73	78

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	256	ARG
1	B	374	THR
1	D	204	SER
1	B	204	SER
1	D	133	ASP

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

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 ⓘ

8 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	E	1	2	12,12,12	0.50	0	17,17,17	0.69	0
2	GLC	E	2	2	11,11,12	0.53	0	15,15,17	1.10	1 (6%)
2	GLC	F	1	2	12,12,12	0.50	0	17,17,17	0.68	0
2	GLC	F	2	2	11,11,12	0.53	0	15,15,17	1.10	1 (6%)
2	GLC	G	1	2	12,12,12	0.49	0	17,17,17	0.71	0
2	GLC	G	2	2	11,11,12	0.52	0	15,15,17	1.14	1 (6%)
2	GLC	H	1	2	12,12,12	0.49	0	17,17,17	0.68	0
2	GLC	H	2	2	11,11,12	0.53	0	15,15,17	1.06	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	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLC	E	2	2	-	0/2/19/22	0/1/1/1
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	GLC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	GLC	C1-O5-C5	3.42	116.83	112.19
2	E	2	GLC	C1-O5-C5	3.25	116.59	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GLC	C1-O5-C5	3.16	116.47	112.19
2	H	2	GLC	C1-O5-C5	3.09	116.37	112.19

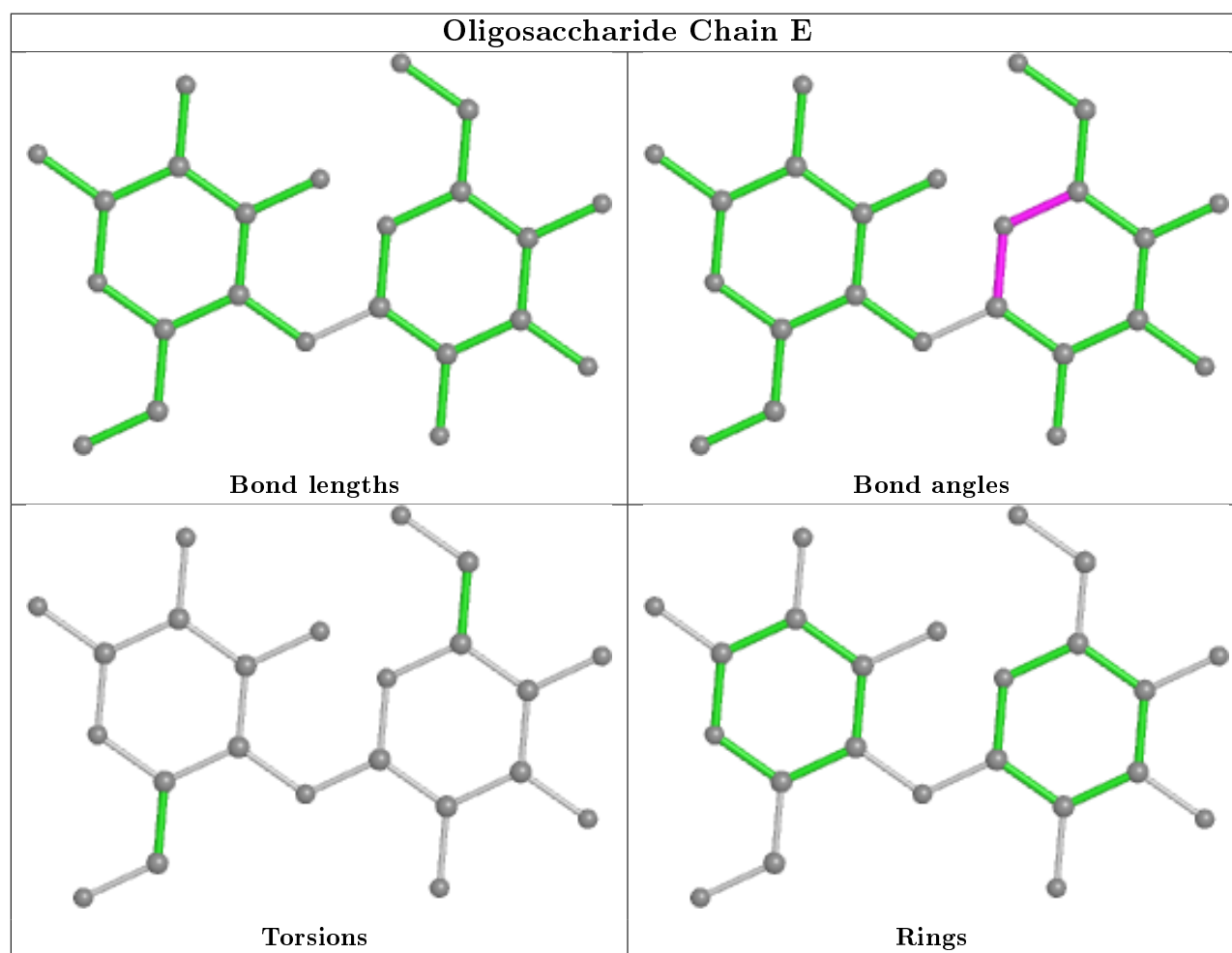
There are no chirality outliers.

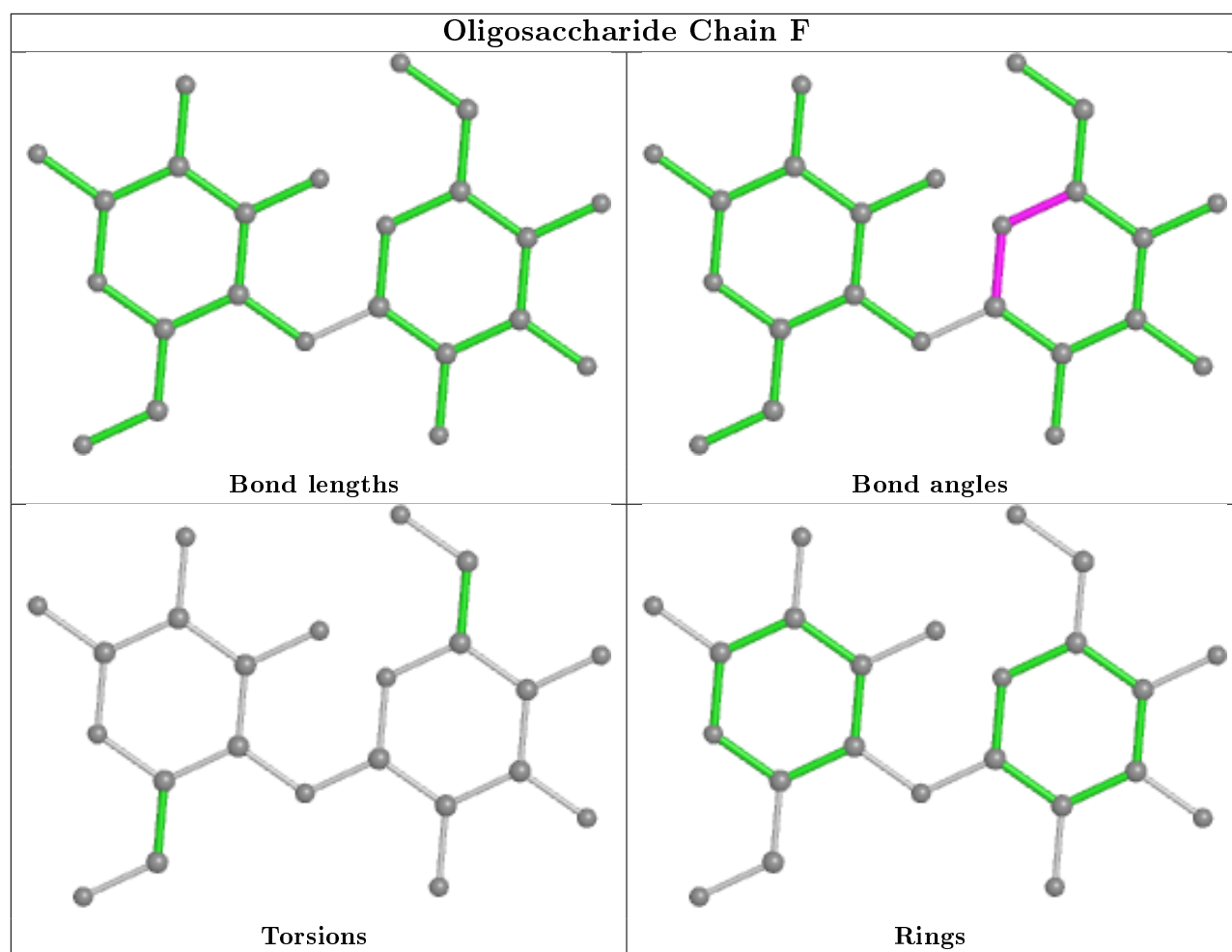
There are no torsion outliers.

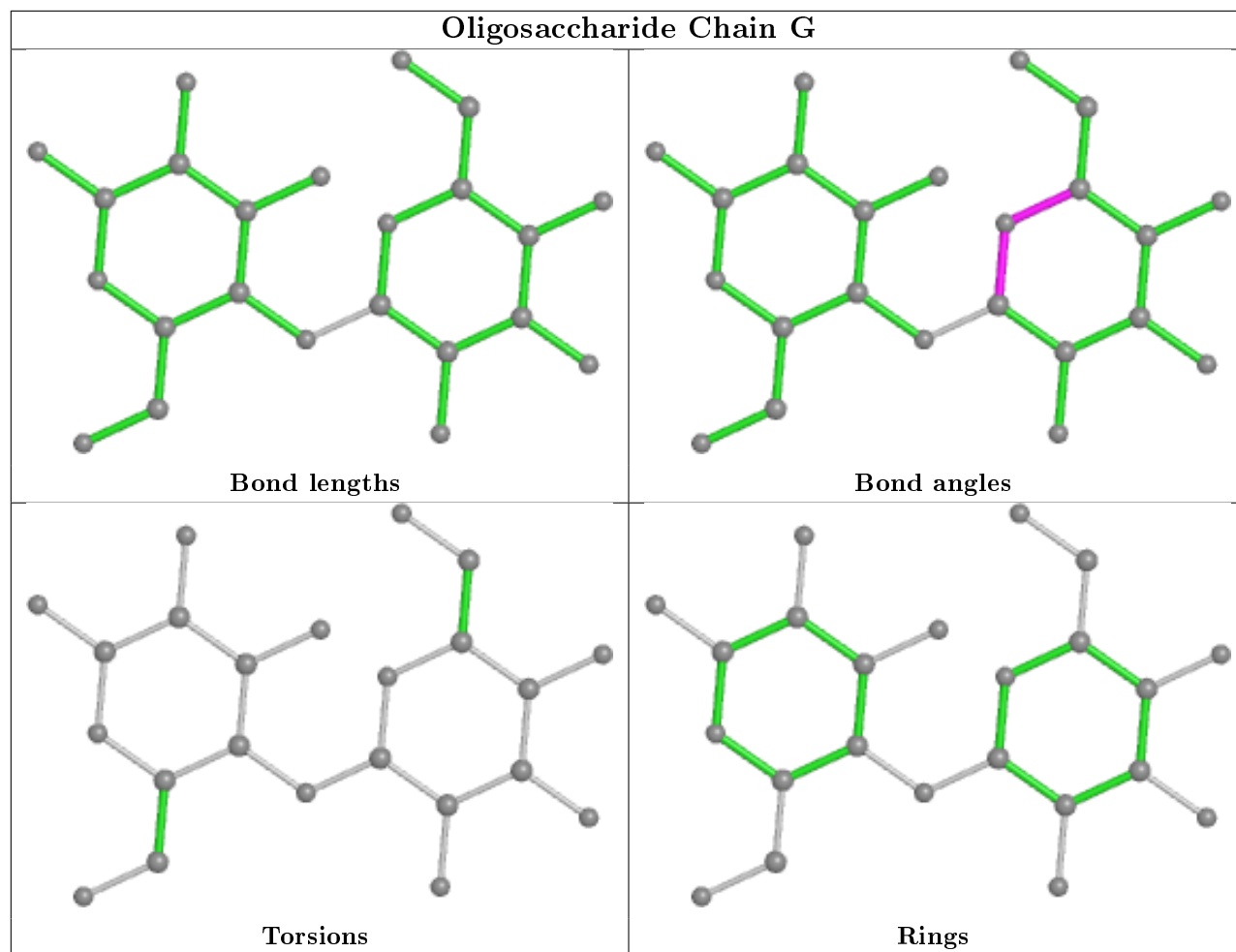
There are no ring outliers.

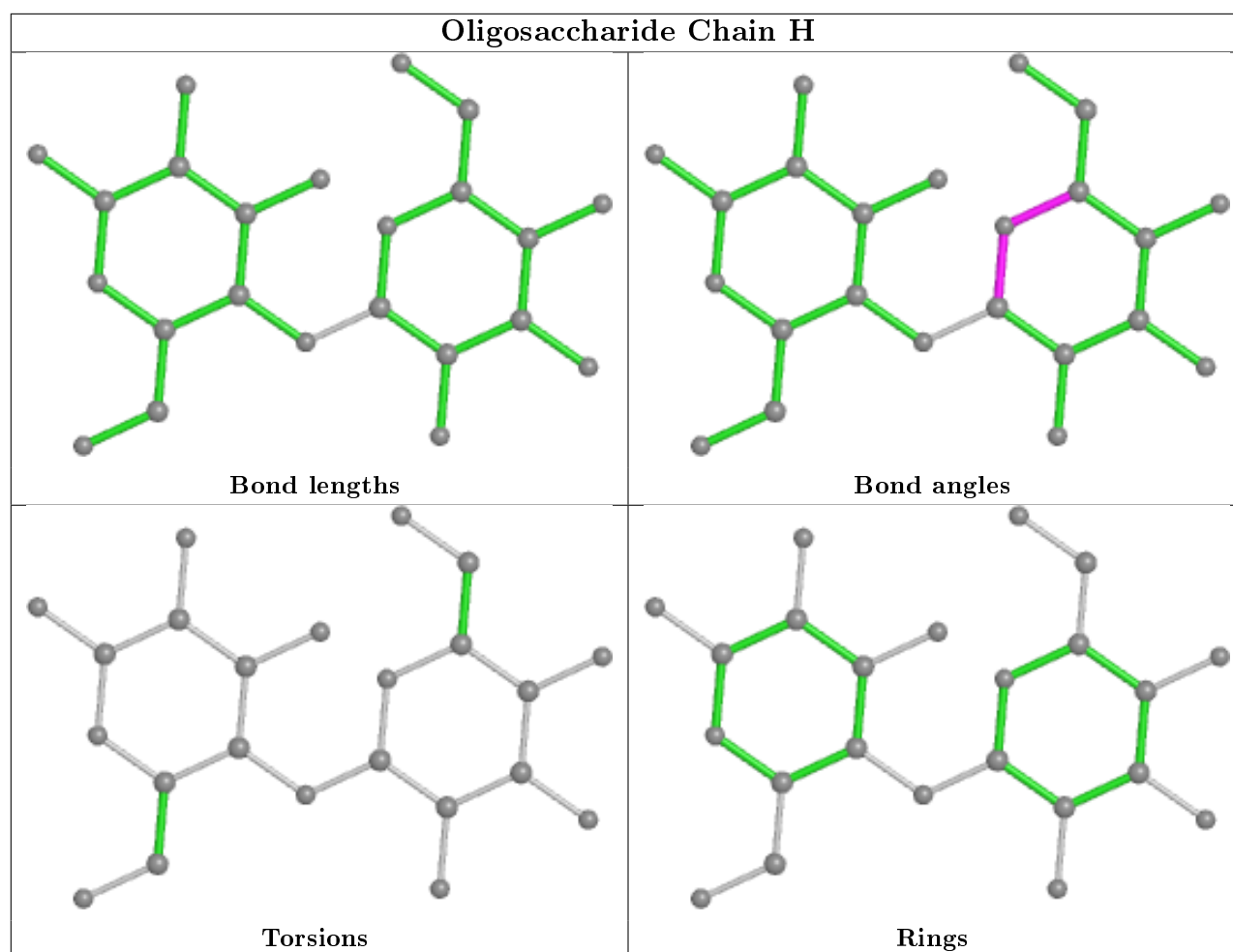
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	391/400 (97%)	-0.28	6 (1%) 73 79	18, 30, 48, 82	0
1	B	391/400 (97%)	-0.41	3 (0%) 86 89	16, 30, 48, 75	0
1	C	391/400 (97%)	-0.45	3 (0%) 86 89	16, 28, 46, 67	0
1	D	391/400 (97%)	-0.27	4 (1%) 82 86	19, 33, 51, 80	0
All	All	1564/1600 (97%)	-0.35	16 (1%) 82 86	16, 30, 49, 82	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	GLU	2.9
1	A	19	ALA	2.7
1	B	203	GLU	2.6
1	D	164	LYS	2.5
1	B	204	SER	2.4

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

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

6.3 Carbohydrates [i](#)

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

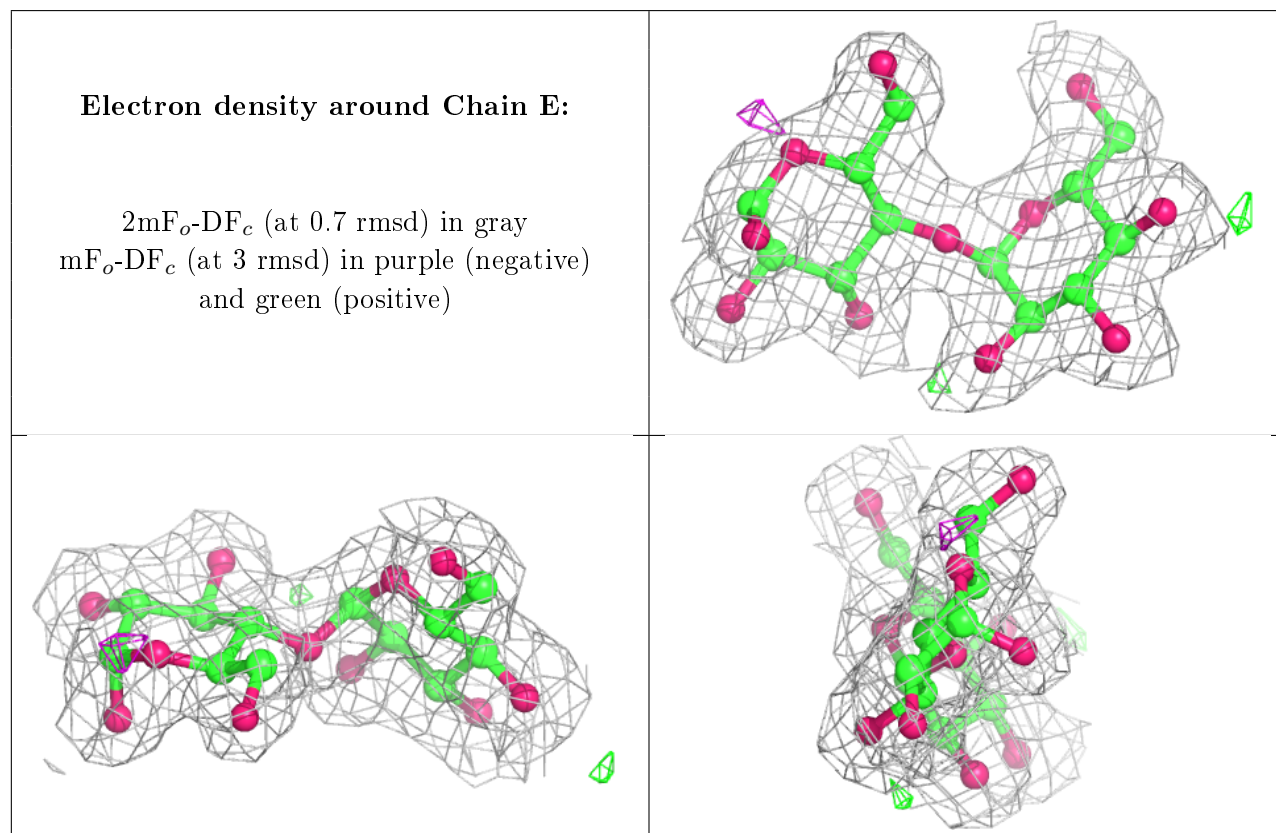
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	F	1	12/12	0.97	0.10	16,18,19,28	0
2	GLC	H	1	12/12	0.97	0.10	19,21,24,30	0

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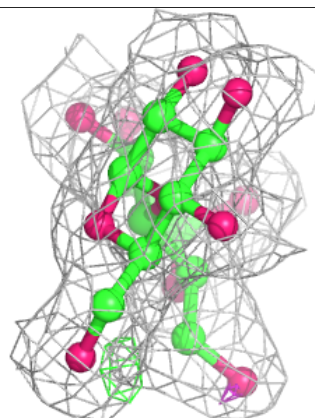
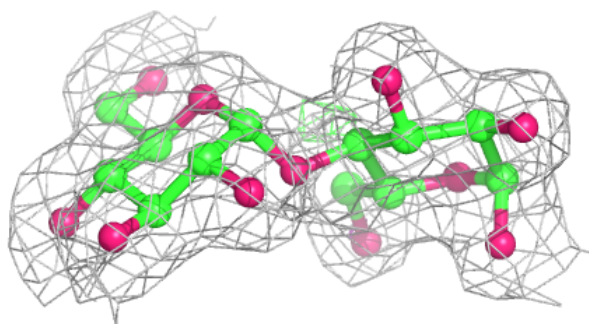
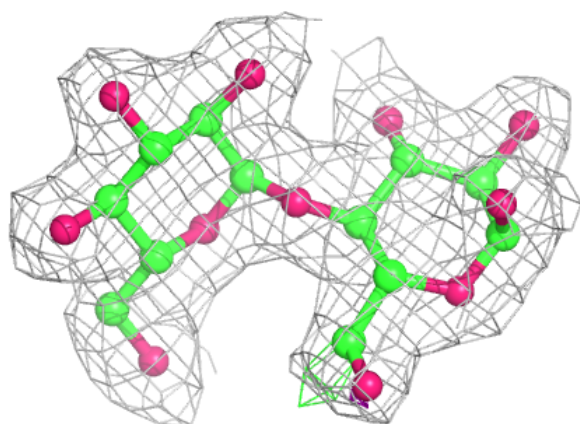
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	H	2	11/12	0.97	0.13	18,19,19,23	0
2	GLC	E	1	12/12	0.97	0.10	18,22,24,32	0
2	GLC	G	1	12/12	0.97	0.08	15,18,22,28	0
2	GLC	F	2	11/12	0.98	0.10	14,17,19,21	0
2	GLC	E	2	11/12	0.98	0.13	17,18,20,20	0
2	GLC	G	2	11/12	0.98	0.10	17,18,19,20	0

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

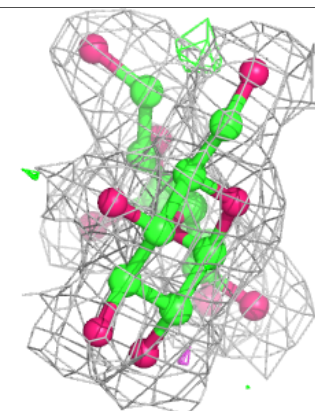
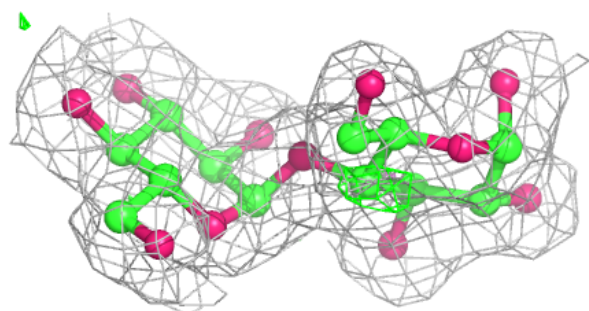
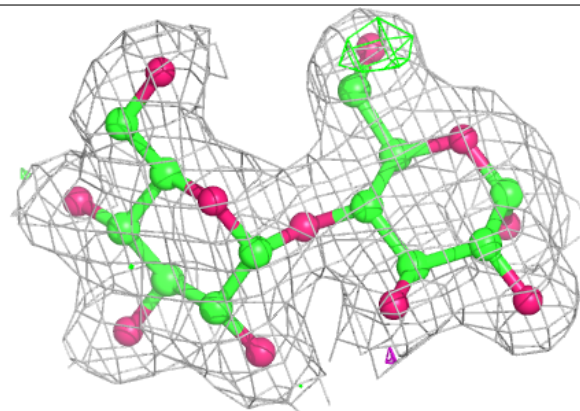


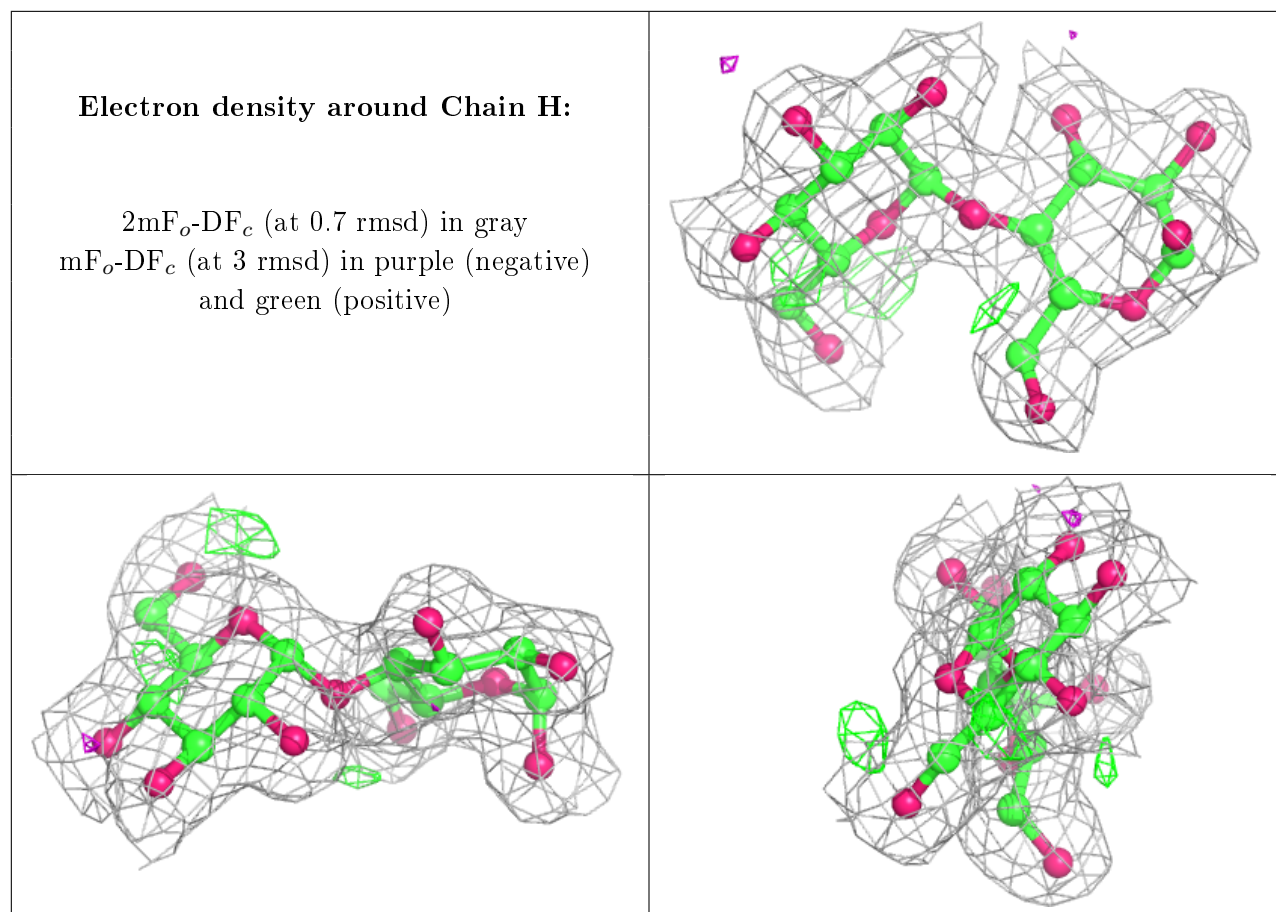
Electron density around Chain F:

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

**Electron density around Chain G:**

$2mF_o-DF_c$ (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(\AA^2)	Q<0.9
3	MG	C	502	1/1	0.95	0.12	24,24,24,24	0
3	MG	A	502	1/1	0.97	0.07	22,22,22,22	0
3	MG	D	502	1/1	0.98	0.13	20,20,20,20	0
3	MG	B	502	1/1	0.98	0.14	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.