



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2023 – 02:59 AM EDT

PDB ID : 6XT1
Title : The structure of the M60 catalytic domain from Clostridium perfringens ZmpC
in complex the sialyl T antigen
Authors : Pluvinage, B.; Boraston, A.B.
Deposited on : 2020-07-16
Resolution : 2.49 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 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

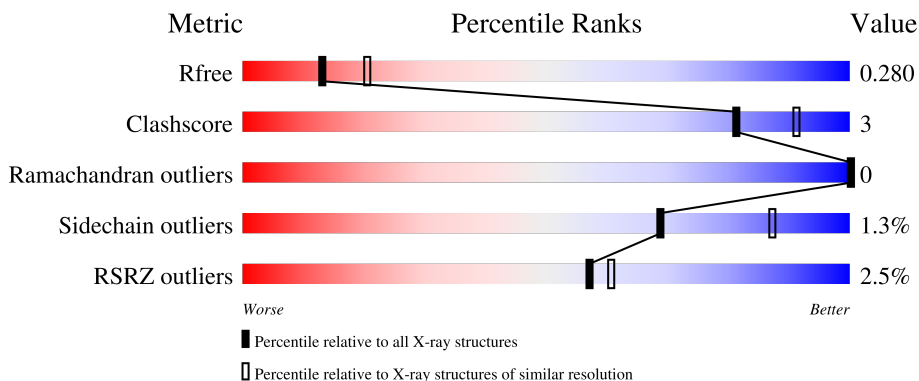
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	531	 2% 89% 7%
1	B	531	 2% 90% 6%
1	C	531	 3% 88% 8%
1	D	531	 4% 86% 9%
2	F	3	 33% 67%

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Mol	Chain	Length	Quality of chain
2	M	3	 33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	F	2	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 16813 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 ZmpC Glycopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	510	4053	2552	673	816	12	0	1	0
1	B	509	4038	2542	670	814	12	0	0	0
1	C	509	4013	2530	667	804	12	0	0	0
1	D	510	4022	2536	673	801	12	0	1	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	MET	-	initiating methionine	UNP F8UNJ8
A	470	GLY	-	expression tag	UNP F8UNJ8
A	471	SER	-	expression tag	UNP F8UNJ8
A	472	SER	-	expression tag	UNP F8UNJ8
A	473	HIS	-	expression tag	UNP F8UNJ8
A	474	HIS	-	expression tag	UNP F8UNJ8
A	475	HIS	-	expression tag	UNP F8UNJ8
A	476	HIS	-	expression tag	UNP F8UNJ8
A	477	HIS	-	expression tag	UNP F8UNJ8
A	478	HIS	-	expression tag	UNP F8UNJ8
A	479	SER	-	expression tag	UNP F8UNJ8
A	480	SER	-	expression tag	UNP F8UNJ8
A	481	GLY	-	expression tag	UNP F8UNJ8
A	482	LEU	-	expression tag	UNP F8UNJ8
A	483	VAL	-	expression tag	UNP F8UNJ8
A	484	PRO	-	expression tag	UNP F8UNJ8
A	485	ARG	-	expression tag	UNP F8UNJ8
A	486	GLY	-	expression tag	UNP F8UNJ8
A	487	SER	-	expression tag	UNP F8UNJ8
A	488	HIS	-	expression tag	UNP F8UNJ8
A	489	MET	-	expression tag	UNP F8UNJ8

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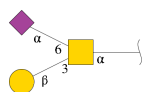
Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ALA	-	expression tag	UNP F8UNJ8
A	491	SER	-	expression tag	UNP F8UNJ8
B	469	MET	-	initiating methionine	UNP F8UNJ8
B	470	GLY	-	expression tag	UNP F8UNJ8
B	471	SER	-	expression tag	UNP F8UNJ8
B	472	SER	-	expression tag	UNP F8UNJ8
B	473	HIS	-	expression tag	UNP F8UNJ8
B	474	HIS	-	expression tag	UNP F8UNJ8
B	475	HIS	-	expression tag	UNP F8UNJ8
B	476	HIS	-	expression tag	UNP F8UNJ8
B	477	HIS	-	expression tag	UNP F8UNJ8
B	478	HIS	-	expression tag	UNP F8UNJ8
B	479	SER	-	expression tag	UNP F8UNJ8
B	480	SER	-	expression tag	UNP F8UNJ8
B	481	GLY	-	expression tag	UNP F8UNJ8
B	482	LEU	-	expression tag	UNP F8UNJ8
B	483	VAL	-	expression tag	UNP F8UNJ8
B	484	PRO	-	expression tag	UNP F8UNJ8
B	485	ARG	-	expression tag	UNP F8UNJ8
B	486	GLY	-	expression tag	UNP F8UNJ8
B	487	SER	-	expression tag	UNP F8UNJ8
B	488	HIS	-	expression tag	UNP F8UNJ8
B	489	MET	-	expression tag	UNP F8UNJ8
B	490	ALA	-	expression tag	UNP F8UNJ8
B	491	SER	-	expression tag	UNP F8UNJ8
C	469	MET	-	initiating methionine	UNP F8UNJ8
C	470	GLY	-	expression tag	UNP F8UNJ8
C	471	SER	-	expression tag	UNP F8UNJ8
C	472	SER	-	expression tag	UNP F8UNJ8
C	473	HIS	-	expression tag	UNP F8UNJ8
C	474	HIS	-	expression tag	UNP F8UNJ8
C	475	HIS	-	expression tag	UNP F8UNJ8
C	476	HIS	-	expression tag	UNP F8UNJ8
C	477	HIS	-	expression tag	UNP F8UNJ8
C	478	HIS	-	expression tag	UNP F8UNJ8
C	479	SER	-	expression tag	UNP F8UNJ8
C	480	SER	-	expression tag	UNP F8UNJ8
C	481	GLY	-	expression tag	UNP F8UNJ8
C	482	LEU	-	expression tag	UNP F8UNJ8
C	483	VAL	-	expression tag	UNP F8UNJ8
C	484	PRO	-	expression tag	UNP F8UNJ8
C	485	ARG	-	expression tag	UNP F8UNJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	486	GLY	-	expression tag	UNP F8UNJ8
C	487	SER	-	expression tag	UNP F8UNJ8
C	488	HIS	-	expression tag	UNP F8UNJ8
C	489	MET	-	expression tag	UNP F8UNJ8
C	490	ALA	-	expression tag	UNP F8UNJ8
C	491	SER	-	expression tag	UNP F8UNJ8
D	469	MET	-	initiating methionine	UNP F8UNJ8
D	470	GLY	-	expression tag	UNP F8UNJ8
D	471	SER	-	expression tag	UNP F8UNJ8
D	472	SER	-	expression tag	UNP F8UNJ8
D	473	HIS	-	expression tag	UNP F8UNJ8
D	474	HIS	-	expression tag	UNP F8UNJ8
D	475	HIS	-	expression tag	UNP F8UNJ8
D	476	HIS	-	expression tag	UNP F8UNJ8
D	477	HIS	-	expression tag	UNP F8UNJ8
D	478	HIS	-	expression tag	UNP F8UNJ8
D	479	SER	-	expression tag	UNP F8UNJ8
D	480	SER	-	expression tag	UNP F8UNJ8
D	481	GLY	-	expression tag	UNP F8UNJ8
D	482	LEU	-	expression tag	UNP F8UNJ8
D	483	VAL	-	expression tag	UNP F8UNJ8
D	484	PRO	-	expression tag	UNP F8UNJ8
D	485	ARG	-	expression tag	UNP F8UNJ8
D	486	GLY	-	expression tag	UNP F8UNJ8
D	487	SER	-	expression tag	UNP F8UNJ8
D	488	HIS	-	expression tag	UNP F8UNJ8
D	489	MET	-	expression tag	UNP F8UNJ8
D	490	ALA	-	expression tag	UNP F8UNJ8
D	491	SER	-	expression tag	UNP F8UNJ8

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose.

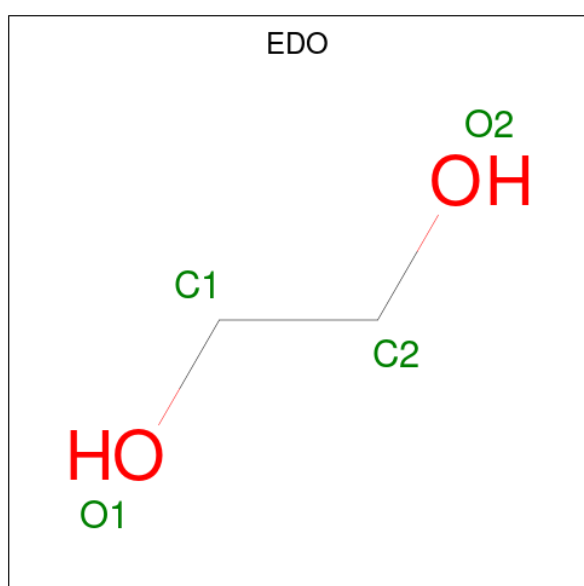


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	0	0	0
			45	25	2	18			
2	M	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



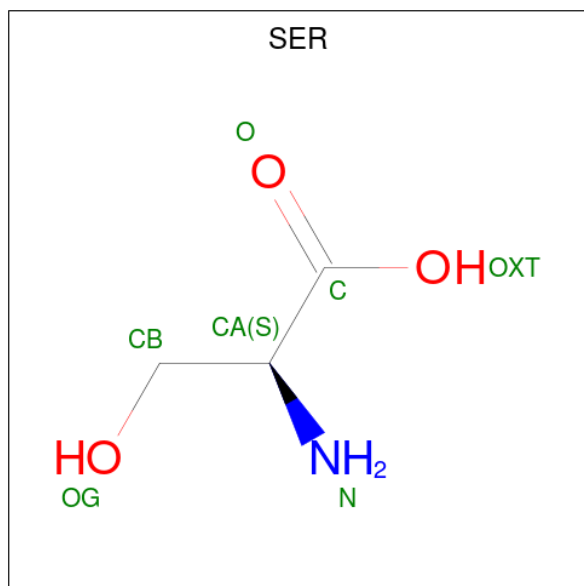
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is SERINE (three-letter code: SER) (formula: C₃H₇NO₃).



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

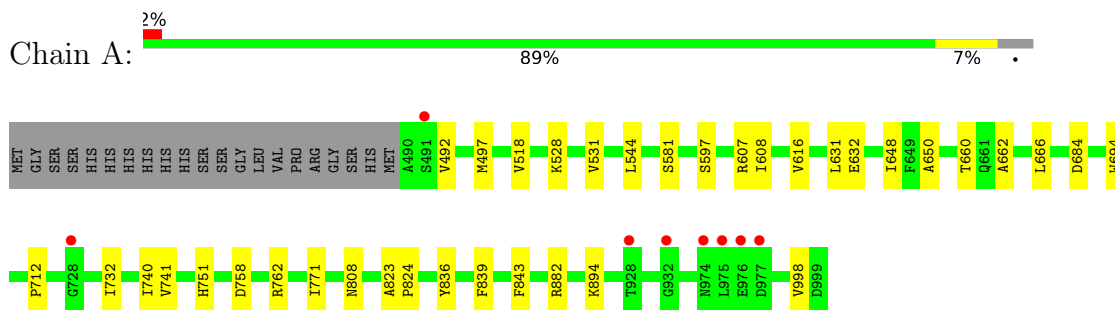
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	130	Total 130	O 130	0	0
6	B	125	Total 125	O 125	0	0
6	C	126	Total 126	O 126	0	0
6	D	134	Total 134	O 134	0	0

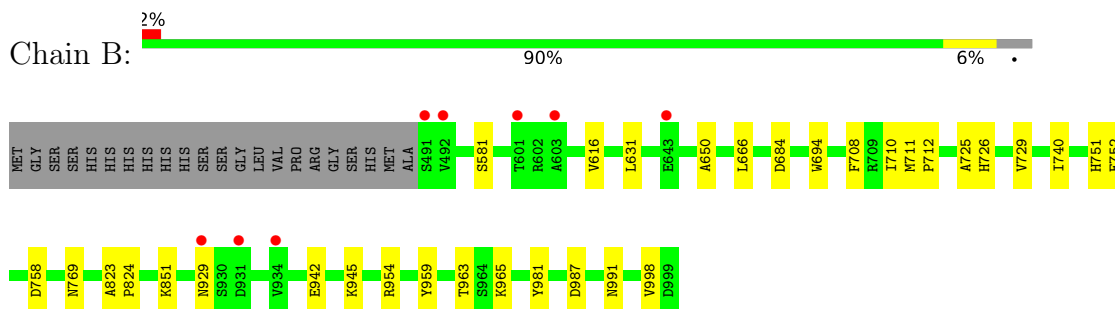
3 Residue-property plots [i](#)

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.

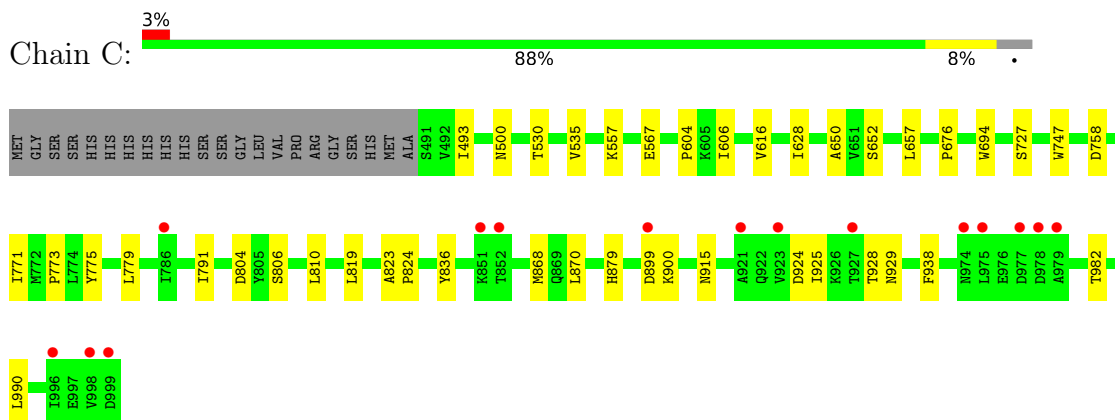
- Molecule 1: ZmpC Glycopeptidase




- Molecule 1: ZmpC Glycopeptidase

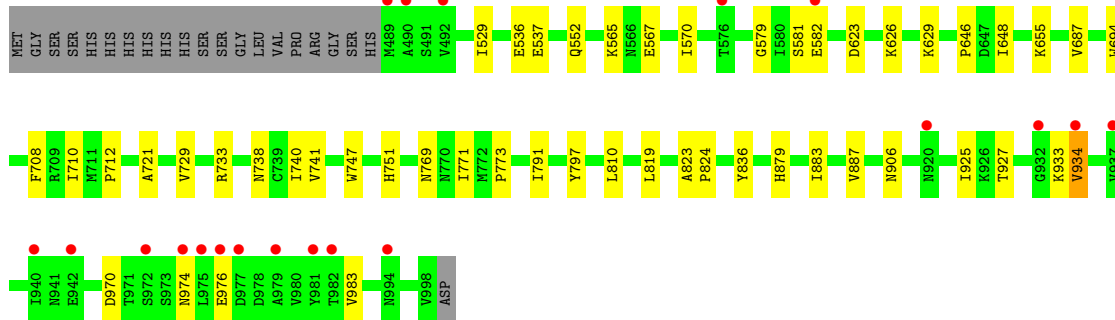


- Molecule 1: ZmpC Glycopeptidase

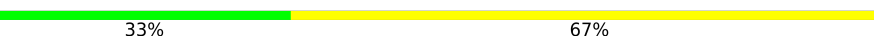


- Molecule 1: ZmpC Glycopeptidase

Chain D:  4% 86% 9%

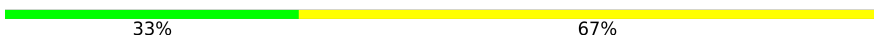


- Molecule 2: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain F:  33% 67%



- Molecule 2: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain M:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.61Å 100.93Å 119.02Å 90.00° 95.91° 90.00°	Depositor
Resolution (Å)	39.07 – 2.49 39.04 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.07-2.49) 96.8 (39.04-2.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.37 (at 2.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.234 , 0.280 0.235 , 0.280	Depositor DCC
R_{free} test set	4404 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtrriage
Anisotropy	0.062	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16813	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: EDO, ZN, GAL, SIA, A2G

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	0/4139	0.42	0/5618
1	B	0.25	0/4124	0.42	0/5599
1	C	0.25	0/4099	0.42	0/5568
1	D	0.25	0/4108	0.43	0/5577
All	All	0.25	0/16470	0.42	0/22362

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	4053	0	3838	17	0
1	B	4038	0	3819	15	0
1	C	4013	0	3786	22	0
1	D	4022	0	3784	27	0
2	F	45	0	37	0	0
2	M	45	0	37	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	8	0	12	1	0
4	B	16	0	24	0	0
4	C	24	0	36	1	0
4	D	16	0	24	1	0
5	A	7	0	3	1	0
5	B	7	0	3	0	0
6	A	130	0	0	0	0
6	B	125	0	0	0	0
6	C	126	0	0	0	0
6	D	134	0	0	0	0
All	All	16813	0	15403	81	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 3.

The worst 5 of 81 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:D:925:ILE:HD11	1:D:983:VAL:HG21	1.70	0.71
1:D:721:ALA:O	1:D:733:ARG:NH1	2.30	0.64
1:A:616:VAL:HG12	1:A:650:ALA:HB3	1.82	0.61
1:B:616:VAL:HG12	1:B:650:ALA:HB3	1.81	0.61
1:B:711:MET:HB2	1:B:729:VAL:HG22	1.82	0.59

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	509/531 (96%)	496 (97%)	13 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	507/531 (96%)	497 (98%)	10 (2%)	0	100	100
1	C	507/531 (96%)	494 (97%)	13 (3%)	0	100	100
1	D	509/531 (96%)	491 (96%)	18 (4%)	0	100	100
All	All	2032/2124 (96%)	1978 (97%)	54 (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	437/464 (94%)	428 (98%)	9 (2%)	53	78
1	B	436/464 (94%)	431 (99%)	5 (1%)	73	89
1	C	429/464 (92%)	423 (99%)	6 (1%)	67	86
1	D	424/464 (91%)	421 (99%)	3 (1%)	84	94
All	All	1726/1856 (93%)	1703 (99%)	23 (1%)	69	87

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	694	TRP
1	C	915	ASN
1	C	758	ASP
1	C	924	ASP
1	A	758	ASP

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	841	GLN
1	B	889	GLN
1	D	738	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](#)

6 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	A2G	F	1	5,2	14,14,15	0.42	0	17,19,21	0.67	0
2	GAL	F	2	2	11,11,12	0.39	0	15,15,17	0.71	1 (6%)
2	SIA	F	3	2	20,20,21	0.79	1 (5%)	24,28,31	0.94	1 (4%)
2	A2G	M	1	5,2	14,14,15	0.41	0	17,19,21	0.73	0
2	GAL	M	2	2	11,11,12	0.39	0	15,15,17	0.82	1 (6%)
2	SIA	M	3	2	20,20,21	0.81	1 (5%)	24,28,31	1.17	3 (12%)

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	A2G	F	1	5,2	-	1/6/23/26	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	SIA	F	3	2	-	0/18/34/38	0/1/1/1
2	A2G	M	1	5,2	-	1/6/23/26	0/1/1/1
2	GAL	M	2	2	-	2/2/19/22	0/1/1/1
2	SIA	M	3	2	-	0/18/34/38	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	SIA	O1B-C1	-2.78	1.21	1.30
2	M	3	SIA	O1B-C1	-2.77	1.21	1.30

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	SIA	C6-O6-C2	2.75	117.23	111.34
2	M	3	SIA	O6-C2-C1	2.67	112.94	107.70
2	M	3	SIA	O1B-C1-C2	2.41	119.90	113.03
2	F	3	SIA	O1B-C1-C2	2.28	119.55	113.03
2	M	2	GAL	C1-O5-C5	2.19	115.16	112.19

There are no chirality outliers.

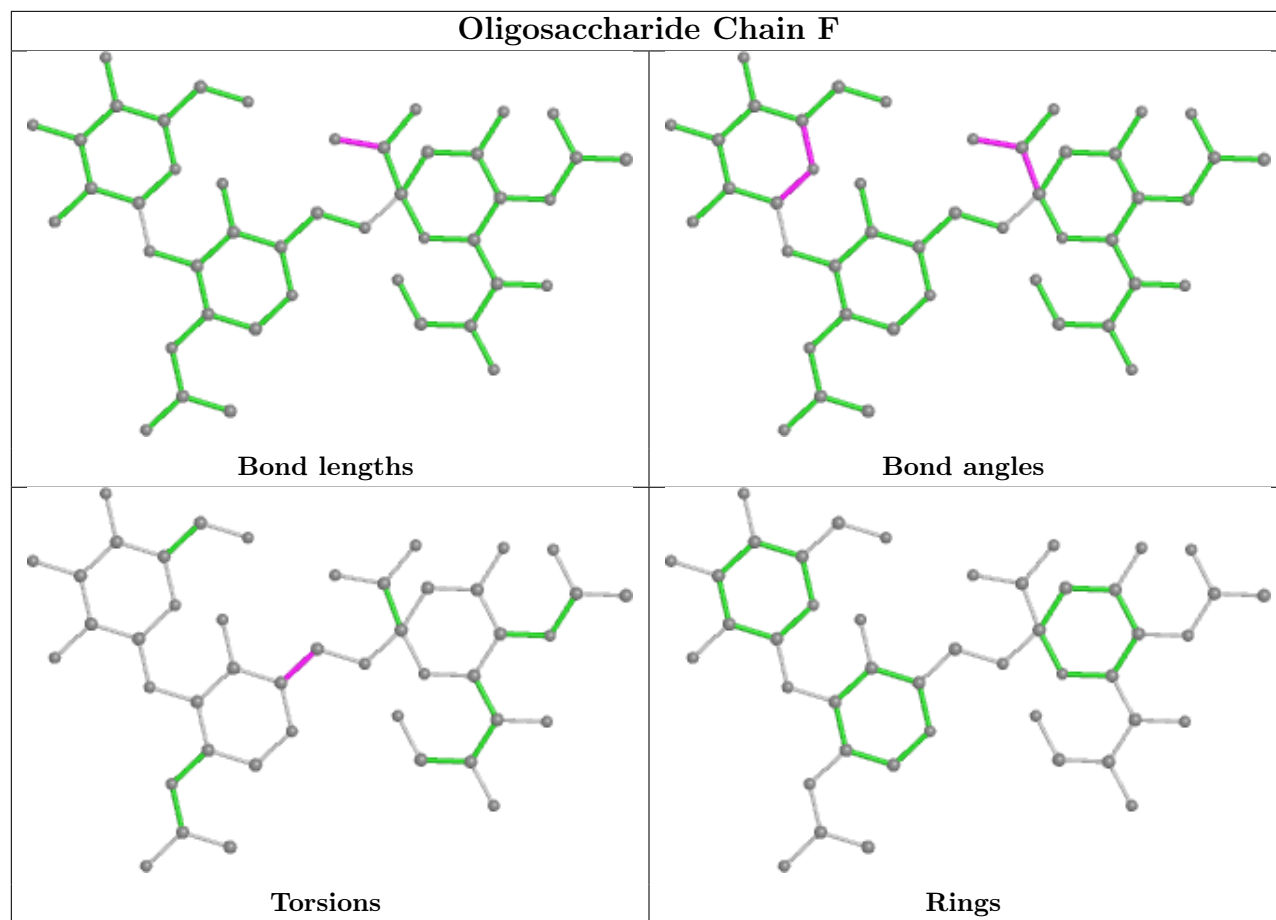
All (4) torsion outliers are listed below:

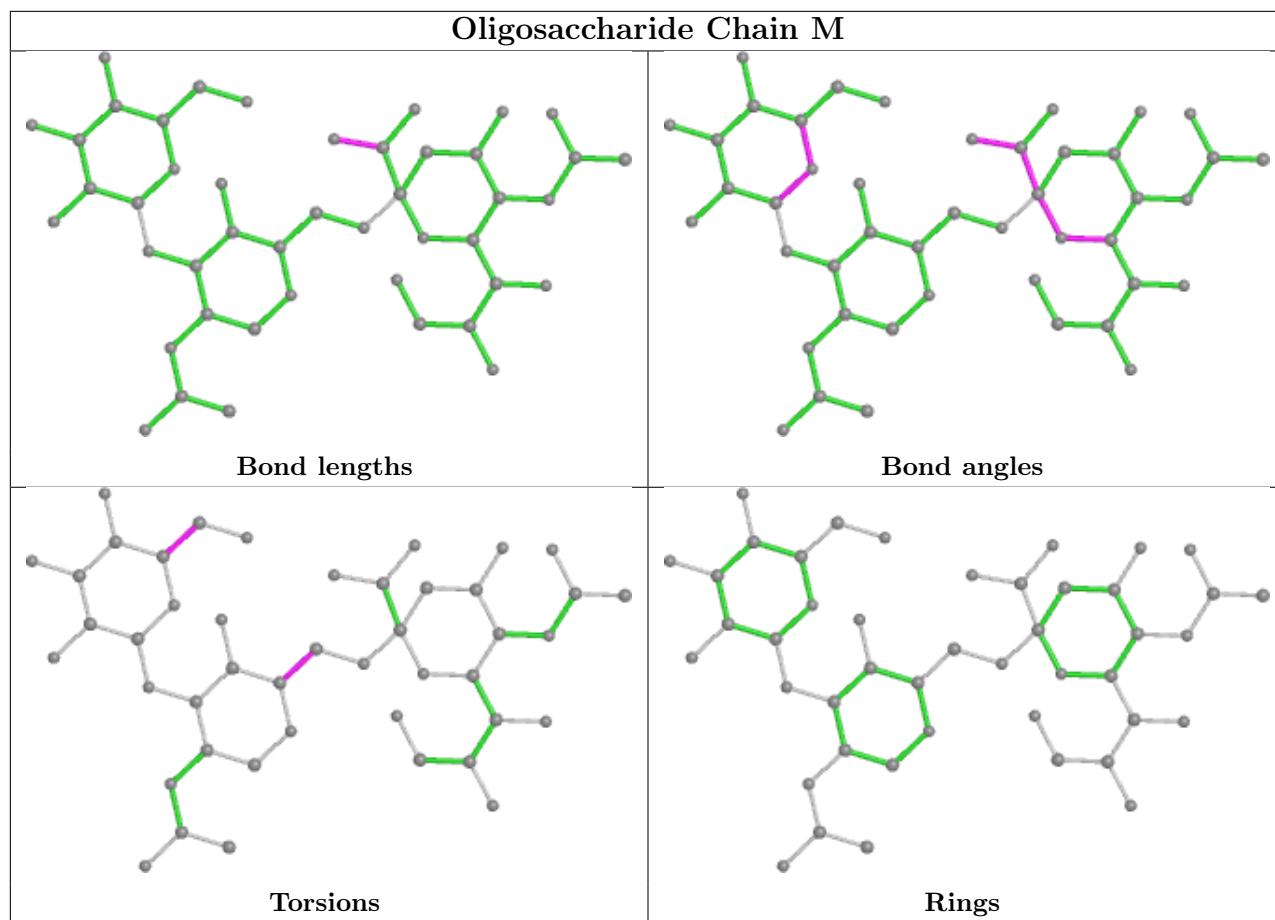
Mol	Chain	Res	Type	Atoms
2	F	1	A2G	O5-C5-C6-O6
2	M	1	A2G	O5-C5-C6-O6
2	M	2	GAL	C4-C5-C6-O6
2	M	2	GAL	O5-C5-C6-O6

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 22 ligands modelled in this entry, 4 are monoatomic - leaving 18 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	$\# Z > 2$
4	EDO	C	1006	-	3,3,3	0.05	0	2,2,2	0.22	0
4	EDO	C	1002	-	3,3,3	0.04	0	2,2,2	0.12	0
4	EDO	B	1005	-	3,3,3	0.05	0	2,2,2	0.18	0
4	EDO	A	1003	-	3,3,3	0.04	0	2,2,2	0.18	0
4	EDO	D	1002	-	3,3,3	0.06	0	2,2,2	0.15	0
4	EDO	D	1004	-	3,3,3	0.05	0	2,2,2	0.14	0
4	EDO	C	1003	-	3,3,3	0.05	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	1003	-	3,3,3	0.06	0	2,2,2	0.19	0
4	EDO	C	1004	-	3,3,3	0.05	0	2,2,2	0.19	0
4	EDO	D	1005	-	3,3,3	0.05	0	2,2,2	0.22	0
5	SER	A	1004	3,2	5,6,6	1.01	1 (20%)	5,7,7	1.65	2 (40%)
5	SER	B	1006	3,2	5,6,6	0.98	1 (20%)	5,7,7	1.67	2 (40%)
4	EDO	C	1007	-	3,3,3	0.06	0	2,2,2	0.19	0
4	EDO	B	1004	-	3,3,3	0.05	0	2,2,2	0.21	0
4	EDO	B	1002	-	3,3,3	0.05	0	2,2,2	0.18	0
4	EDO	C	1005	-	3,3,3	0.05	0	2,2,2	0.21	0
4	EDO	D	1003	-	3,3,3	0.06	0	2,2,2	0.20	0
4	EDO	A	1002	-	3,3,3	0.06	0	2,2,2	0.17	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
4	EDO	C	1006	-	-	1/1/1/1	-
4	EDO	C	1002	-	-	0/1/1/1	-
4	EDO	B	1005	-	-	0/1/1/1	-
4	EDO	A	1003	-	-	1/1/1/1	-
4	EDO	D	1002	-	-	0/1/1/1	-
4	EDO	D	1004	-	-	1/1/1/1	-
4	EDO	C	1003	-	-	0/1/1/1	-
4	EDO	B	1003	-	-	0/1/1/1	-
4	EDO	C	1004	-	-	0/1/1/1	-
4	EDO	D	1005	-	-	0/1/1/1	-
5	SER	A	1004	3,2	-	2/6/6/6	-
5	SER	B	1006	3,2	-	0/6/6/6	-
4	EDO	C	1007	-	-	0/1/1/1	-
4	EDO	B	1004	-	-	1/1/1/1	-
4	EDO	B	1002	-	-	0/1/1/1	-
4	EDO	C	1005	-	-	1/1/1/1	-
4	EDO	D	1003	-	-	0/1/1/1	-
4	EDO	A	1002	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1004	SER	OXT-C	-2.14	1.23	1.30
5	B	1006	SER	OXT-C	-2.09	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1004	SER	OXT-C-O	-2.73	117.90	124.09
5	B	1006	SER	OXT-C-O	-2.69	117.98	124.09
5	B	1006	SER	OXT-C-CA	2.41	121.61	113.38
5	A	1004	SER	OXT-C-CA	2.26	121.07	113.38

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1004	SER	O-C-CA-N
4	A	1003	EDO	O1-C1-C2-O2
4	C	1006	EDO	O1-C1-C2-O2
4	C	1005	EDO	O1-C1-C2-O2
5	A	1004	SER	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1006	EDO	1	0
4	D	1002	EDO	1	0
5	A	1004	SER	1	0
4	A	1002	EDO	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	510/531 (96%)	0.03	8 (1%) 72 74	29, 39, 54, 77	0
1	B	509/531 (95%)	0.10	8 (1%) 72 74	30, 40, 60, 75	0
1	C	509/531 (95%)	0.10	15 (2%) 51 55	28, 40, 63, 89	0
1	D	510/531 (96%)	0.14	20 (3%) 39 42	30, 41, 70, 90	0
All	All	2038/2124 (95%)	0.09	51 (2%) 57 61	28, 40, 63, 90	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	975	LEU	5.1
1	C	979	ALA	4.2
1	A	491	SER	3.4
1	D	975	LEU	3.3
1	D	490	ALA	3.1

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.

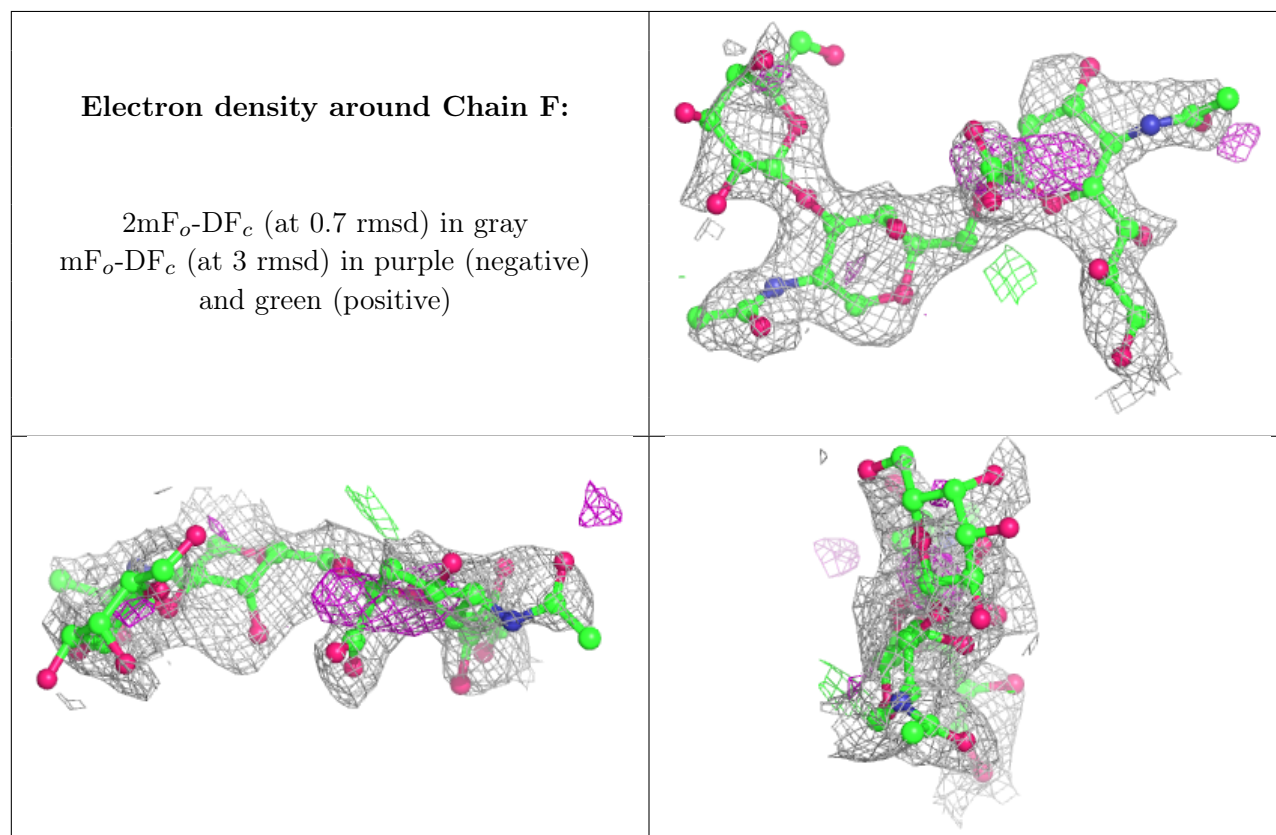
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GAL	M	2	11/12	0.55	0.36	74,78,80,80	0
2	GAL	F	2	11/12	0.66	0.44	92,97,99,100	0

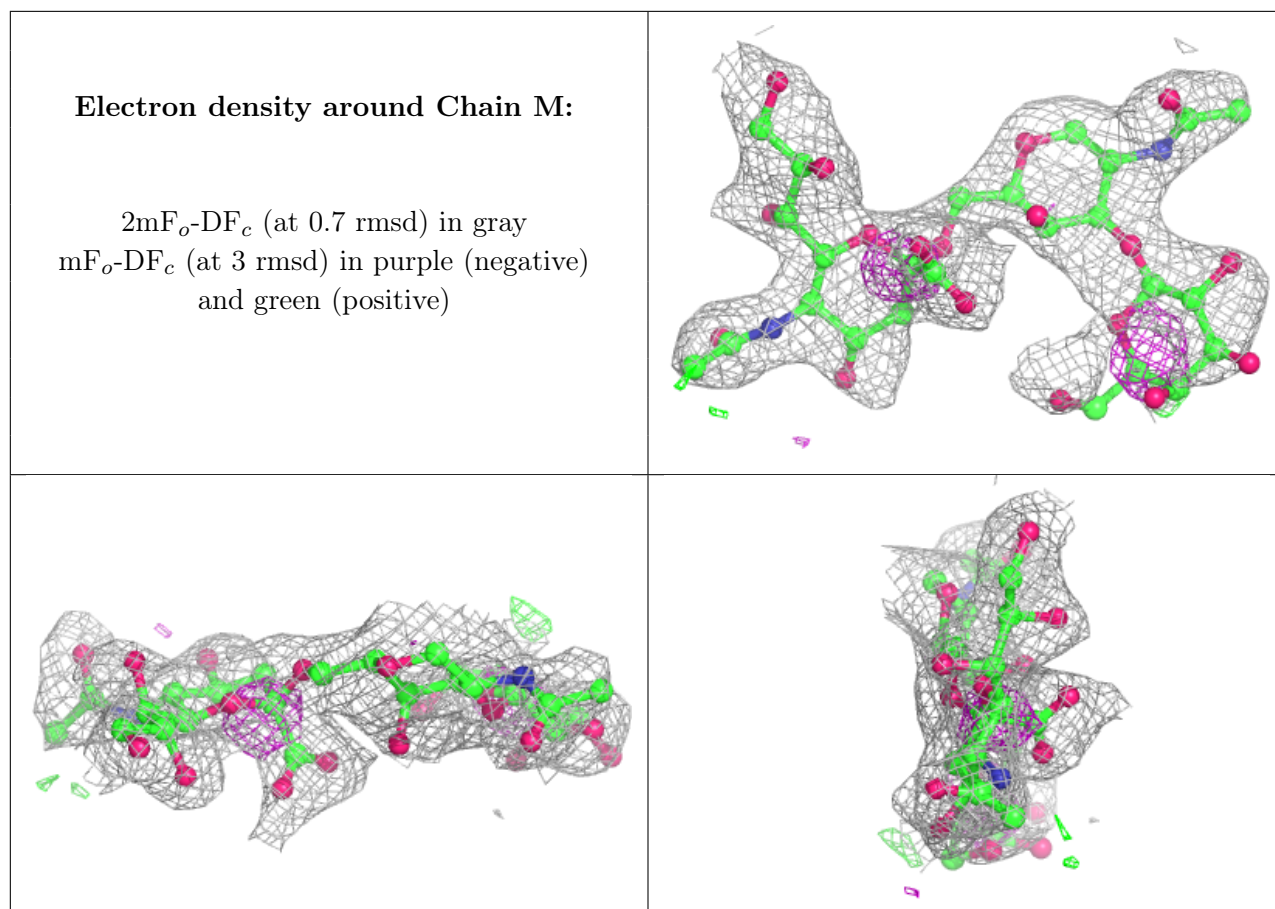
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SIA	F	3	20/21	0.75	0.35	65,71,73,73	0
2	A2G	F	1	14/15	0.77	0.20	66,69,70,77	0
2	SIA	M	3	20/21	0.81	0.20	51,57,59,59	0
2	A2G	M	1	14/15	0.89	0.17	54,56,58,63	0

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.





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
4	EDO	C	1006	4/4	0.64	0.30	50,50,50,51	0
4	EDO	B	1004	4/4	0.77	0.33	53,53,53,53	0
4	EDO	C	1007	4/4	0.78	0.33	49,49,49,49	0
5	SER	A	1004	7/7	0.79	0.25	60,60,63,65	0
4	EDO	C	1003	4/4	0.80	0.22	53,53,53,53	0
4	EDO	B	1002	4/4	0.80	0.22	51,52,52,52	0
4	EDO	C	1004	4/4	0.84	0.30	47,48,48,49	0
4	EDO	D	1005	4/4	0.85	0.23	47,48,48,48	0
4	EDO	A	1003	4/4	0.86	0.17	43,43,43,43	0
4	EDO	C	1005	4/4	0.90	0.31	41,41,41,41	0
4	EDO	D	1002	4/4	0.90	0.16	41,41,41,41	0
4	EDO	D	1003	4/4	0.91	0.21	47,47,47,47	0
4	EDO	B	1003	4/4	0.91	0.25	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	1002	4/4	0.91	0.30	44,44,44,45	0
4	EDO	B	1005	4/4	0.92	0.21	46,46,46,46	0
4	EDO	D	1004	4/4	0.93	0.22	44,45,45,45	0
3	ZN	D	1001	1/1	0.95	0.10	49,49,49,49	0
4	EDO	C	1002	4/4	0.95	0.14	32,33,33,33	0
3	ZN	A	1001	1/1	0.96	0.08	52,52,52,52	0
5	SER	B	1006	7/7	0.96	0.12	51,51,52,54	0
3	ZN	B	1001	1/1	0.97	0.06	52,52,52,52	0
3	ZN	C	1001	1/1	0.99	0.08	46,46,46,46	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.