



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:26 PM UTC

PDB ID : 6XT1 / pdb_00006xt1
Title : The structure of the M60 catalytic domain from Clostridium perfringens ZmpC
in complex the sialyl T antigen
Authors : Pluvinae, B.; Boraston, A.B.
Deposited on : 2020-07-16
Resolution : 2.49 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

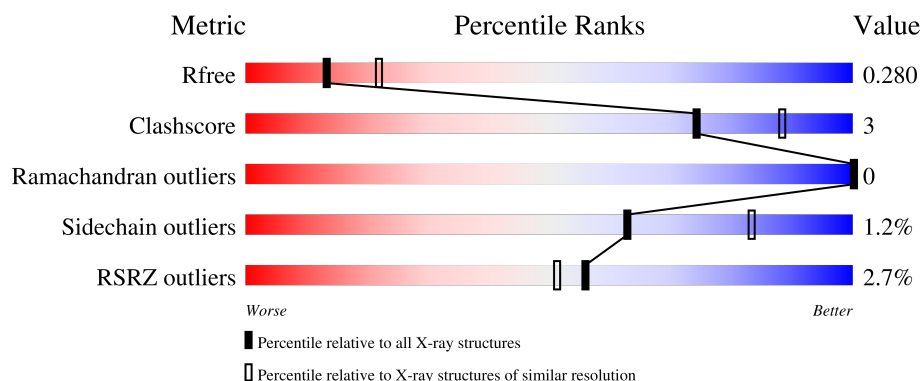
1 Overall quality at a glance

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.



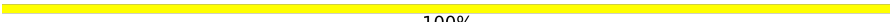
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	0% 87% 9% .
1	B	531	2% 89% 7% .
1	C	531	3% 88% 8% .
1	D	531	4% 85% 11% .
2	F	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	M	3	 100%

2 Entry composition

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

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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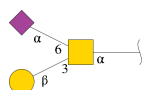
Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ALA	-	expression tag	UNP F8UNJ8
A	491	SER	-	expression tag	UNP F8UNJ8
B	469	MET	-	initiating methionine	UNP F8UNJ8
B	470	GLY	-	expression tag	UNP F8UNJ8
B	471	SER	-	expression tag	UNP F8UNJ8
B	472	SER	-	expression tag	UNP F8UNJ8
B	473	HIS	-	expression 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.

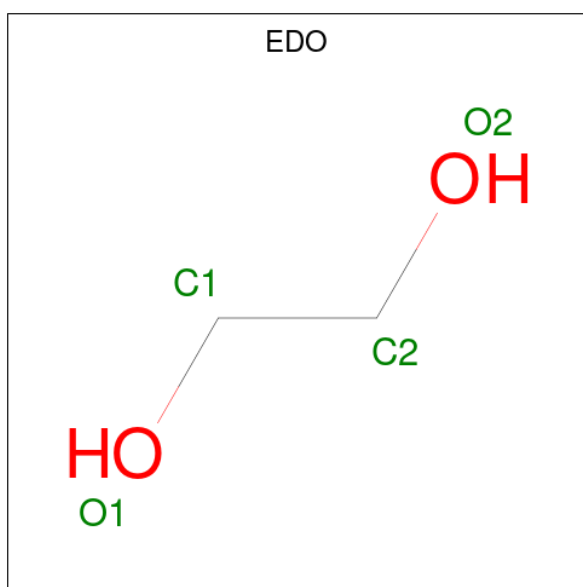


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	0	0	0
			45	25	2	18			
2	M	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 3 is ZINC ION (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



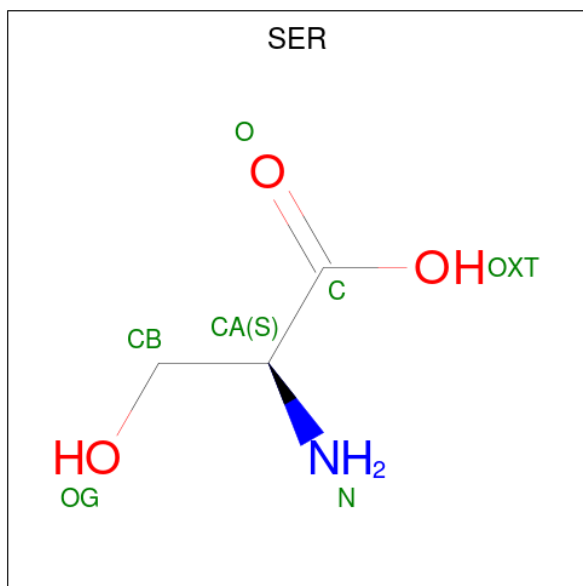
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



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

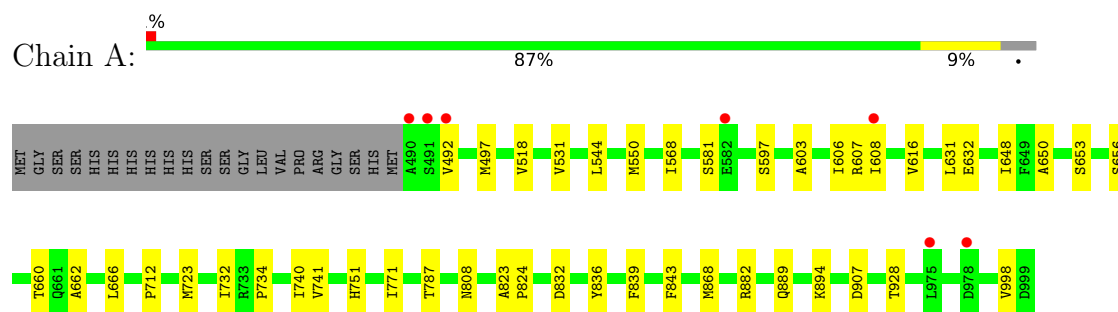
- Molecule 6 is water.

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

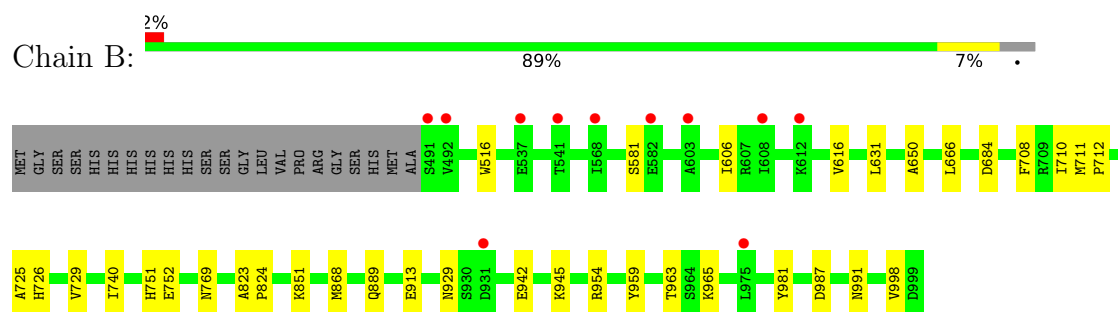
3 Residue-property plots [i](#)

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.

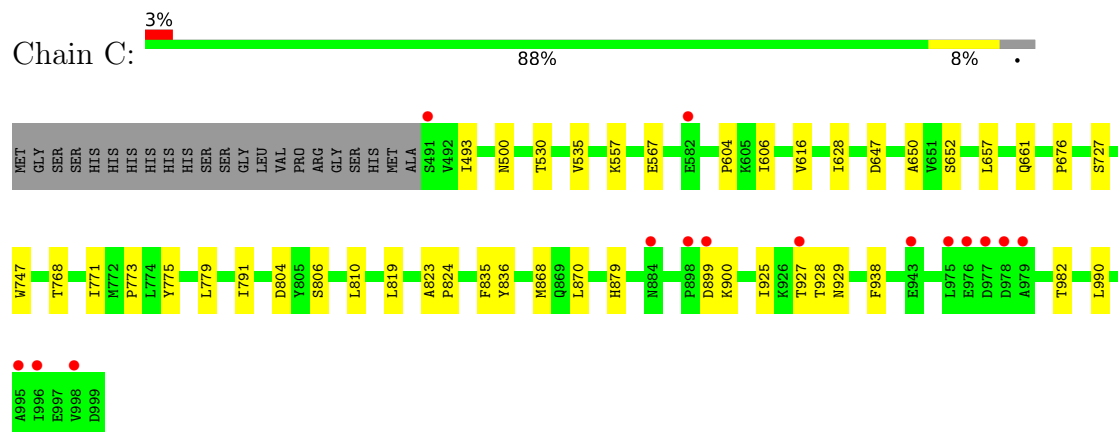
• Molecule 1: ZmpC Glycopeptidase



• Molecule 1: ZmpC Glycopeptidase

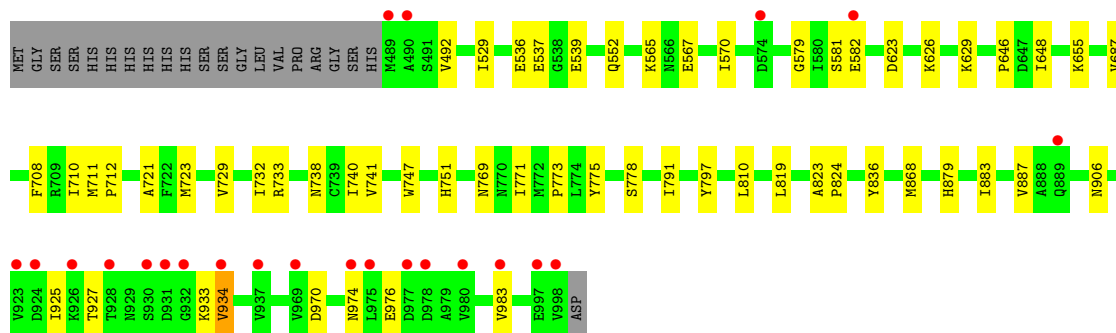


• Molecule 1: ZmpC Glycopeptidase

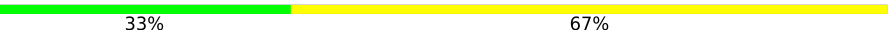


• Molecule 1: ZmpC Glycopeptidase

Chain D:  4% 85% 11% .

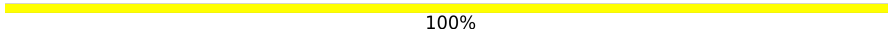


- Molecule 2: beta-D-galactopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)]2-acetamido-2-deoxy-alpha-D-galactopyranose

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:  100%



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 39.07 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.07-2.49) 96.7 (39.07-2.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.37 (at 2.48Å)	Xtriage
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 (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 22.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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: SIA, GAL, A2G, ZN, EDO

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	0.40	0/4139	0.65	0/5618
1	B	0.40	0/4124	0.64	0/5599
1	C	0.40	0/4099	0.64	0/5568
1	D	0.40	0/4108	0.65	0/5577
All	All	0.40	0/16470	0.65	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	24	0
1	B	4038	0	3819	17	0
1	C	4013	0	3786	25	0
1	D	4022	0	3784	33	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	99	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.

All (99) 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:723:MET:HE2	1:A:732:ILE:HG12	1.70	0.73
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
1:A:492:VAL:HG22	1:A:607:ARG:HB2	1.85	0.59
1:A:732:ILE:HD12	1:A:740:ILE:HG12	1.84	0.59
1:A:712:PRO:HB2	1:A:740:ILE:HG23	1.87	0.56
1:C:925:ILE:HD12	1:C:938:PHE:HD1	1.70	0.56
1:A:497:MET:HG2	1:A:597:SER:HB2	1.88	0.56
1:A:832:ASP:HB3	1:A:868:MET:HE1	1.87	0.56
1:C:835:PHE:HA	1:C:868:MET:HE3	1.88	0.55
1:A:653:SER:HG	1:A:656:SER:HG	1.55	0.55
1:B:981:TYR:HB2	1:B:998:VAL:HG12	1.89	0.55
1:B:712:PRO:HB2	1:B:740:ILE:HG23	1.90	0.54
1:D:712:PRO:HB2	1:D:740:ILE:HG23	1.89	0.54
1:A:550:MET:HE1	1:A:734:PRO:HG3	1.90	0.53
1:D:751:HIS:CE1	1:D:769:ASN:HD21	2.26	0.53
1:D:565:LYS:NZ	1:D:567:GLU:OE2	2.35	0.53
1:D:529:ILE:HG13	1:D:570:ILE:HD11	1.90	0.52
1:C:500:ASN:HD21	4:C:1006:EDO:H21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:LEU:HB3	1:B:666:LEU:HD13	1.93	0.51
1:D:646:PRO:HB2	1:D:648:ILE:HG12	1.93	0.51
1:D:536:GLU:HG3	1:D:537:GLU:N	2.26	0.50
1:D:626:LYS:HG3	1:D:629:LYS:HE2	1.93	0.50
1:D:771:ILE:HG21	1:D:836:TYR:OH	2.12	0.49
1:C:925:ILE:HD12	1:C:938:PHE:CD1	2.48	0.49
1:D:729:VAL:HG21	4:D:1002:EDO:H22	1.95	0.48
1:C:616:VAL:HG12	1:C:650:ALA:HB3	1.95	0.48
1:C:791:ILE:HD12	1:C:819:LEU:HB2	1.96	0.48
1:C:804:ASP:OD1	1:C:806:SER:OG	2.29	0.48
1:C:868:MET:HB3	1:C:870:LEU:HD12	1.95	0.48
1:A:631:LEU:HB3	1:A:666:LEU:HD13	1.95	0.47
1:A:823:ALA:N	1:A:824:PRO:HD2	2.29	0.47
1:D:883:ILE:HD12	1:D:887:VAL:HG12	1.95	0.47
1:C:493:ILE:HD12	1:C:606:ILE:HD11	1.96	0.47
1:B:823:ALA:N	1:B:824:PRO:HD2	2.30	0.46
1:C:535:VAL:HG12	1:C:604:PRO:HB3	1.97	0.46
1:D:708:PHE:HE2	1:D:710:ILE:HG12	1.80	0.46
1:D:791:ILE:HD13	1:D:819:LEU:HB2	1.97	0.46
1:A:660:THR:HG21	1:A:741:VAL:HG23	1.98	0.46
1:D:582:GLU:OE1	1:D:582:GLU:N	2.39	0.46
1:B:851:LYS:HE2	1:B:851:LYS:HB3	1.70	0.46
1:C:628:ILE:HD11	1:C:676:PRO:HD3	1.96	0.46
1:C:652:SER:HB2	1:C:657:LEU:HD13	1.98	0.46
1:A:648:ILE:O	1:A:662:ALA:HB2	2.16	0.45
1:C:747:TRP:CE3	1:C:773:PRO:HB2	2.51	0.45
1:D:536:GLU:HB3	1:D:539:GLU:CD	2.42	0.45
1:C:791:ILE:CD1	1:C:819:LEU:HB2	2.47	0.44
1:D:933:LYS:HB3	1:D:970:ASP:O	2.17	0.44
1:A:808:ASN:O	1:A:882:ARG:NH2	2.50	0.44
1:A:894:LYS:NZ	4:A:1002:EDO:O1	2.42	0.44
1:D:723:MET:HE2	1:D:732:ILE:HG12	2.00	0.44
1:B:751:HIS:CE1	1:B:769:ASN:HD21	2.36	0.44
1:D:823:ALA:N	1:D:824:PRO:HD2	2.33	0.44
1:B:516:TRP:CE2	1:B:711:MET:HE1	2.53	0.43
1:D:623:ASP:HB3	1:D:626:LYS:HB3	2.01	0.43
1:A:497:MET:HE2	1:A:603:ALA:HB2	2.00	0.43
1:B:868:MET:HA	1:B:868:MET:HE2	2.01	0.43
1:B:726:HIS:O	1:B:729:VAL:HB	2.19	0.43
1:B:987:ASP:OD2	1:B:991:ASN:HB2	2.18	0.43
1:C:530:THR:OG1	1:C:567:GLU:OE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:647:ASP:CG	1:C:661:GLN:HB2	2.44	0.43
1:A:497:MET:HE3	1:A:497:MET:HB2	1.83	0.43
1:B:963:THR:OG1	1:B:965:LYS:HD2	2.18	0.42
1:A:839:PHE:CZ	1:A:843:PHE:HE2	2.37	0.42
1:C:771:ILE:HG21	1:C:836:TYR:OH	2.20	0.42
1:C:823:ALA:N	1:C:824:PRO:HD2	2.34	0.42
1:D:582:GLU:H	1:D:582:GLU:CD	2.25	0.42
1:B:954:ARG:HG2	1:B:959:TYR:HA	2.02	0.42
1:C:928:THR:OG1	1:C:929:ASN:N	2.52	0.42
1:B:725:ALA:HB2	1:B:752:GLU:HB3	2.01	0.42
1:D:868:MET:HE2	1:D:868:MET:HA	2.02	0.42
1:D:775:TYR:O	1:D:778:SER:OG	2.35	0.42
1:A:751:HIS:CD2	5:A:1004:SER:HB2	2.54	0.41
1:D:927:THR:HG23	1:D:934:VAL:HG23	2.01	0.41
1:B:708:PHE:HE2	1:B:710:ILE:HG12	1.85	0.41
1:C:557:LYS:HA	1:C:557:LYS:HD2	1.79	0.41
1:C:900:LYS:HD2	1:C:990:LEU:HB2	2.02	0.41
1:D:974:ASN:O	1:D:976:GLU:N	2.51	0.41
1:D:655:LYS:HB3	1:D:687:VAL:HG11	2.03	0.41
1:D:747:TRP:CE3	1:D:773:PRO:HB2	2.55	0.41
1:D:797:TYR:OH	1:D:906:ASN:ND2	2.52	0.41
1:A:771:ILE:HG21	1:A:836:TYR:OH	2.21	0.41
1:C:868:MET:HA	1:C:868:MET:HE2	2.02	0.41
1:B:942:GLU:HA	1:B:945:LYS:HD2	2.01	0.41
1:C:810:LEU:HA	1:C:879:HIS:O	2.20	0.41
1:C:899:ASP:OD1	1:C:900:LYS:HG2	2.20	0.41
1:D:738:ASN:HA	1:D:741:VAL:HG12	2.01	0.41
1:D:810:LEU:HA	1:D:879:HIS:O	2.21	0.41
1:A:531:VAL:HG21	1:A:544:LEU:HD22	2.02	0.40
1:A:787:THR:OG1	1:A:907:ASP:OD2	2.36	0.40
1:D:711:MET:HE3	1:D:729:VAL:HG22	2.03	0.40
1:A:632:GLU:HG3	1:A:666:LEU:HD11	2.03	0.40
1:D:738:ASN:HD22	1:D:738:ASN:H	1.69	0.40
1:A:732:ILE:HD12	1:A:740:ILE:CG1	2.51	0.40
1:C:775:TYR:CZ	1:C:779:LEU:HD11	2.56	0.40
1:D:552:GLN:HB3	1:D:579:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
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

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%)	429 (98%)	8 (2%)	51	77
1	B	436/464 (94%)	430 (99%)	6 (1%)	59	81
1	C	429/464 (92%)	425 (99%)	4 (1%)	70	87
1	D	424/464 (91%)	421 (99%)	3 (1%)	76	89
All	All	1726/1856 (93%)	1705 (99%)	21 (1%)	63	83

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	518	VAL
1	A	568	ILE

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Mol	Chain	Res	Type
1	A	581	SER
1	A	606	ILE
1	A	608	ILE
1	A	889	GLN
1	A	928	THR
1	A	998	VAL
1	B	581	SER
1	B	606	ILE
1	B	684	ASP
1	B	889	GLN
1	B	913	GLU
1	B	929	ASN
1	C	727	SER
1	C	768	THR
1	C	927	THR
1	C	982	THR
1	D	492	VAL
1	D	581	SER
1	D	934	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	780	ASN
1	A	842	GLN
1	A	991	ASN
1	B	506	ASN
1	B	514	GLN
1	B	780	ASN
1	B	841	GLN
1	B	889	GLN
1	C	500	ASN
1	C	866	ASN
1	C	915	ASN
1	D	707	ASN
1	D	738	ASN
1	D	991	ASN

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 ⓘ

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	2,5	14,14,15	0.44	0	17,19,21	0.70	0
2	GAL	F	2	2	11,11,12	0.39	0	15,15,17	0.65	1 (6%)
2	SIA	F	3	2	20,20,21	0.78	1 (5%)	21,28,31	0.90	1 (4%)
2	A2G	M	1	2,5	14,14,15	0.43	0	17,19,21	0.77	1 (5%)
2	GAL	M	2	2	11,11,12	0.38	0	15,15,17	0.74	1 (6%)
2	SIA	M	3	2	20,20,21	0.79	1 (5%)	21,28,31	1.09	2 (9%)

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	2,5	-	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	2,5	-	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	-2.88	1.21	1.30
2	M	3	SIA	O1B-C1	-2.87	1.21	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	3	SIA	O6-C2-C1	2.77	112.94	107.72
2	M	3	SIA	O1B-C1-C2	2.76	119.90	112.71
2	F	3	SIA	O1B-C1-C2	2.63	119.55	112.71
2	M	2	GAL	C1-O5-C5	2.22	115.16	112.19
2	M	1	A2G	C1-C2-N2	2.19	113.89	110.43
2	F	2	GAL	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

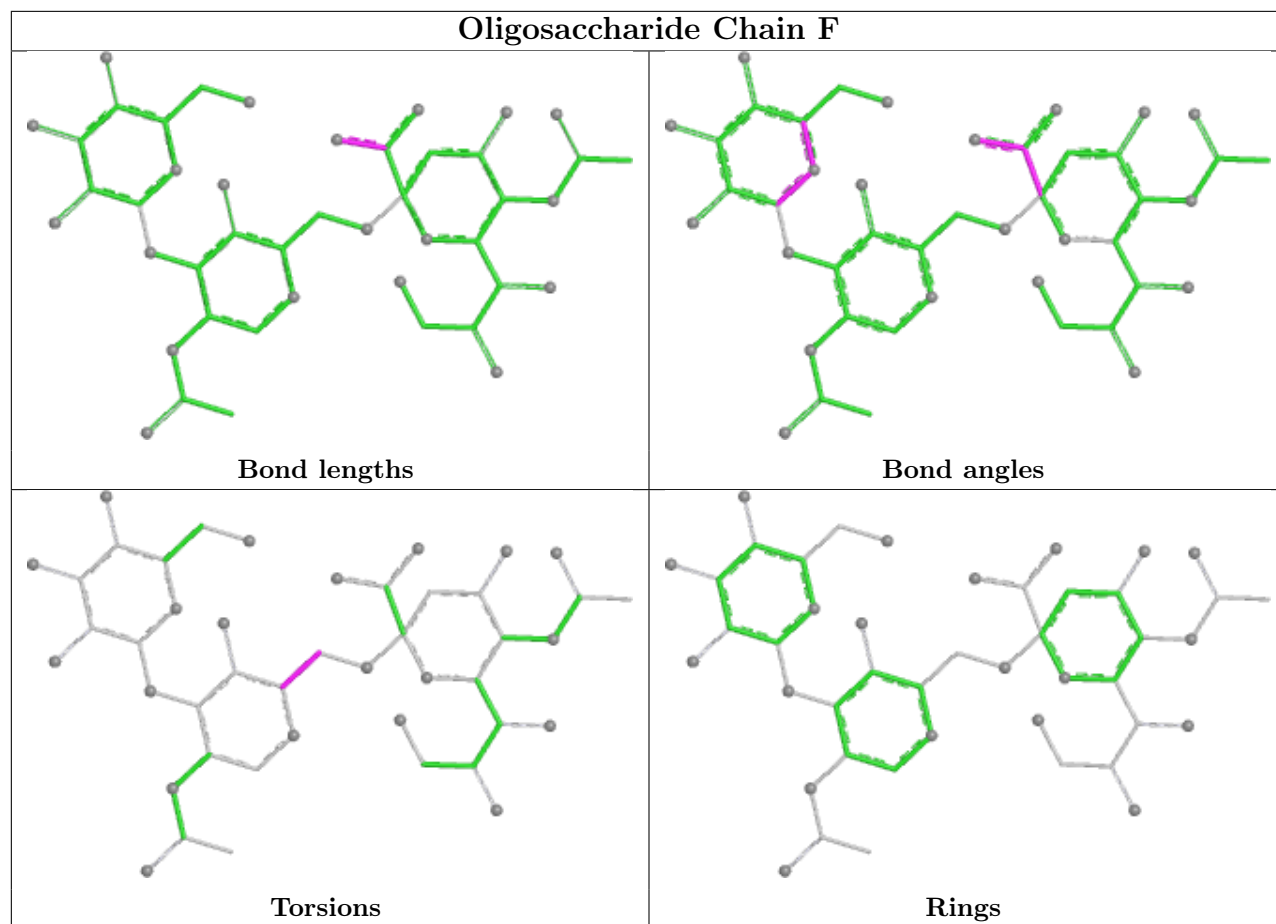
All (4) torsion outliers are listed below:

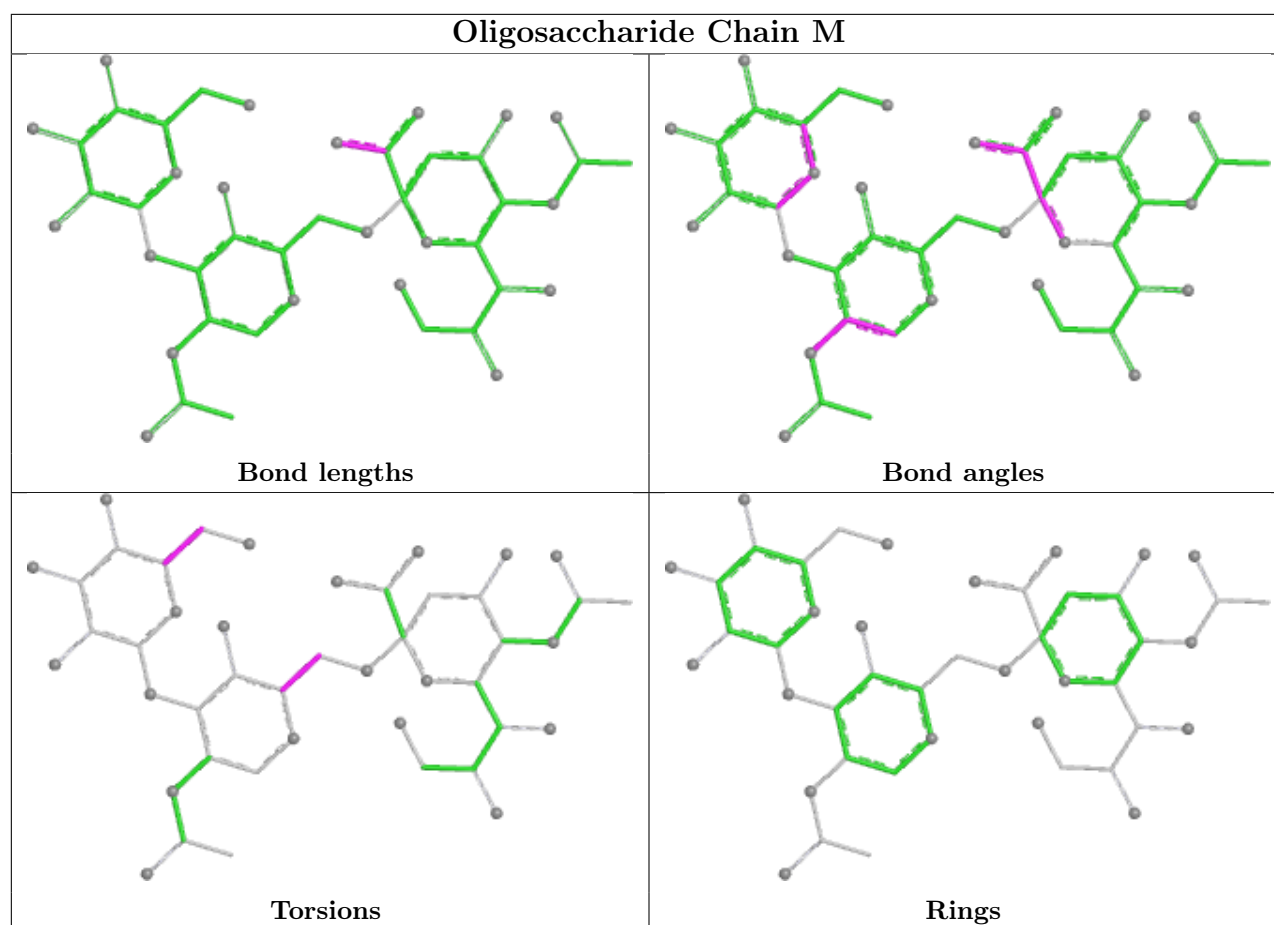
Mol	Chain	Res	Type	Atoms
2	F	1	A2G	O5-C5-C6-O6
2	M	1	A2G	O5-C5-C6-O6
2	M	2	GAL	C4-C5-C6-O6
2	M	2	GAL	O5-C5-C6-O6

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	D	1002	-	3,3,3	0.06	0	2,2,2	0.08	0
4	EDO	C	1003	-	3,3,3	0.05	0	2,2,2	0.10	0
4	EDO	B	1003	-	3,3,3	0.06	0	2,2,2	0.11	0
4	EDO	B	1004	-	3,3,3	0.06	0	2,2,2	0.13	0
4	EDO	C	1004	-	3,3,3	0.05	0	2,2,2	0.12	0
5	SER	B	1006	2,3	4,6,6	1.12	1 (25%)	2,7,7	1.93	1 (50%)
4	EDO	C	1002	-	3,3,3	0.05	0	2,2,2	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	1002	-	3,3,3	0.05	0	2,2,2	0.10	0
4	EDO	C	1007	-	3,3,3	0.07	0	2,2,2	0.12	0
4	EDO	D	1005	-	3,3,3	0.06	0	2,2,2	0.14	0
4	EDO	A	1002	-	3,3,3	0.06	0	2,2,2	0.09	0
4	EDO	C	1005	-	3,3,3	0.05	0	2,2,2	0.14	0
4	EDO	D	1003	-	3,3,3	0.06	0	2,2,2	0.12	0
5	SER	A	1004	2,3	4,6,6	1.15	1 (25%)	2,7,7	1.93	1 (50%)
4	EDO	C	1006	-	3,3,3	0.05	0	2,2,2	0.15	0
4	EDO	B	1005	-	3,3,3	0.05	0	2,2,2	0.10	0
4	EDO	A	1003	-	3,3,3	0.05	0	2,2,2	0.10	0
4	EDO	D	1004	-	3,3,3	0.06	0	2,2,2	0.07	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	D	1002	-	-	0/1/1/1	-
4	EDO	C	1003	-	-	0/1/1/1	-
4	EDO	B	1003	-	-	0/1/1/1	-
4	EDO	B	1004	-	-	1/1/1/1	-
4	EDO	C	1004	-	-	0/1/1/1	-
5	SER	B	1006	2,3	-	0/6/6/6	-
4	EDO	C	1002	-	-	0/1/1/1	-
4	EDO	B	1002	-	-	0/1/1/1	-
4	EDO	C	1007	-	-	0/1/1/1	-
4	EDO	D	1005	-	-	0/1/1/1	-
4	EDO	A	1002	-	-	1/1/1/1	-
4	EDO	C	1005	-	-	1/1/1/1	-
4	EDO	D	1003	-	-	0/1/1/1	-
5	SER	A	1004	2,3	-	2/6/6/6	-
4	EDO	C	1006	-	-	1/1/1/1	-
4	EDO	B	1005	-	-	0/1/1/1	-
4	EDO	A	1003	-	-	1/1/1/1	-
4	EDO	D	1004	-	-	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	-2.22	1.23	1.30
5	B	1006	SER	OXT-C	-2.18	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1004	SER	OXT-C-O	-2.72	117.90	124.08
5	B	1006	SER	OXT-C-O	-2.69	117.98	124.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1004	SER	O-C-CA-N
4	C	1006	EDO	O1-C1-C2-O2
4	A	1003	EDO	O1-C1-C2-O2
5	A	1004	SER	OXT-C-CA-N
4	B	1004	EDO	O1-C1-C2-O2
4	C	1005	EDO	O1-C1-C2-O2
4	A	1002	EDO	O1-C1-C2-O2
4	D	1004	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1002	EDO	1	0
4	A	1002	EDO	1	0
5	A	1004	SER	1	0
4	C	1006	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 ⓘ

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(Å ²)	Q<0.9
1	A	510/531 (96%)	0.23	7 (1%) 73 70	19, 39, 54, 77	1 (0%)
1	B	509/531 (95%)	0.26	11 (2%) 62 58	30, 40, 60, 75	0
1	C	509/531 (95%)	0.34	15 (2%) 53 49	28, 40, 63, 89	0
1	D	510/531 (96%)	0.38	23 (4%) 38 33	20, 41, 70, 90	1 (0%)
All	All	2038/2124 (95%)	0.30	56 (2%) 56 51	19, 40, 63, 90	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	491	SER	4.5
1	D	931	ASP	4.2
1	D	974	ASN	4.2
1	D	998	VAL	3.7
1	A	492	VAL	3.7
1	D	924	ASP	3.6
1	D	490	ALA	3.5
1	C	977	ASP	3.4
1	D	928	THR	3.3
1	D	975	LEU	3.2
1	C	582	GLU	3.2
1	B	582	GLU	3.1
1	D	930	SER	3.1
1	D	969	VAL	3.1
1	A	490	ALA	3.0
1	B	491	SER	3.0
1	D	980	VAL	3.0
1	D	937	VAL	2.9
1	A	975	LEU	2.9
1	C	491	SER	2.8
1	D	489	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	977	ASP	2.8
1	C	976	GLU	2.7
1	D	932	GLY	2.7
1	D	978	ASP	2.7
1	C	978	ASP	2.6
1	D	923	VAL	2.5
1	C	996	ILE	2.5
1	D	926	LYS	2.4
1	C	884	ASN	2.4
1	A	582	GLU	2.4
1	B	975	LEU	2.4
1	C	927	THR	2.4
1	D	582	GLU	2.4
1	D	997	GLU	2.4
1	B	612	LYS	2.3
1	B	537	GLU	2.3
1	B	492	VAL	2.3
1	C	998	VAL	2.3
1	B	541	THR	2.3
1	A	608	ILE	2.3
1	C	975	LEU	2.3
1	C	979	ALA	2.2
1	B	931	ASP	2.2
1	C	899	ASP	2.2
1	C	943	GLU	2.2
1	C	898	PRO	2.2
1	D	934	VAL	2.2
1	D	983	VAL	2.1
1	B	608	ILE	2.1
1	D	889	GLN	2.1
1	B	603	ALA	2.1
1	A	978	ASP	2.1
1	C	995	ALA	2.0
1	B	568	ILE	2.0
1	D	574	ASP	2.0

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

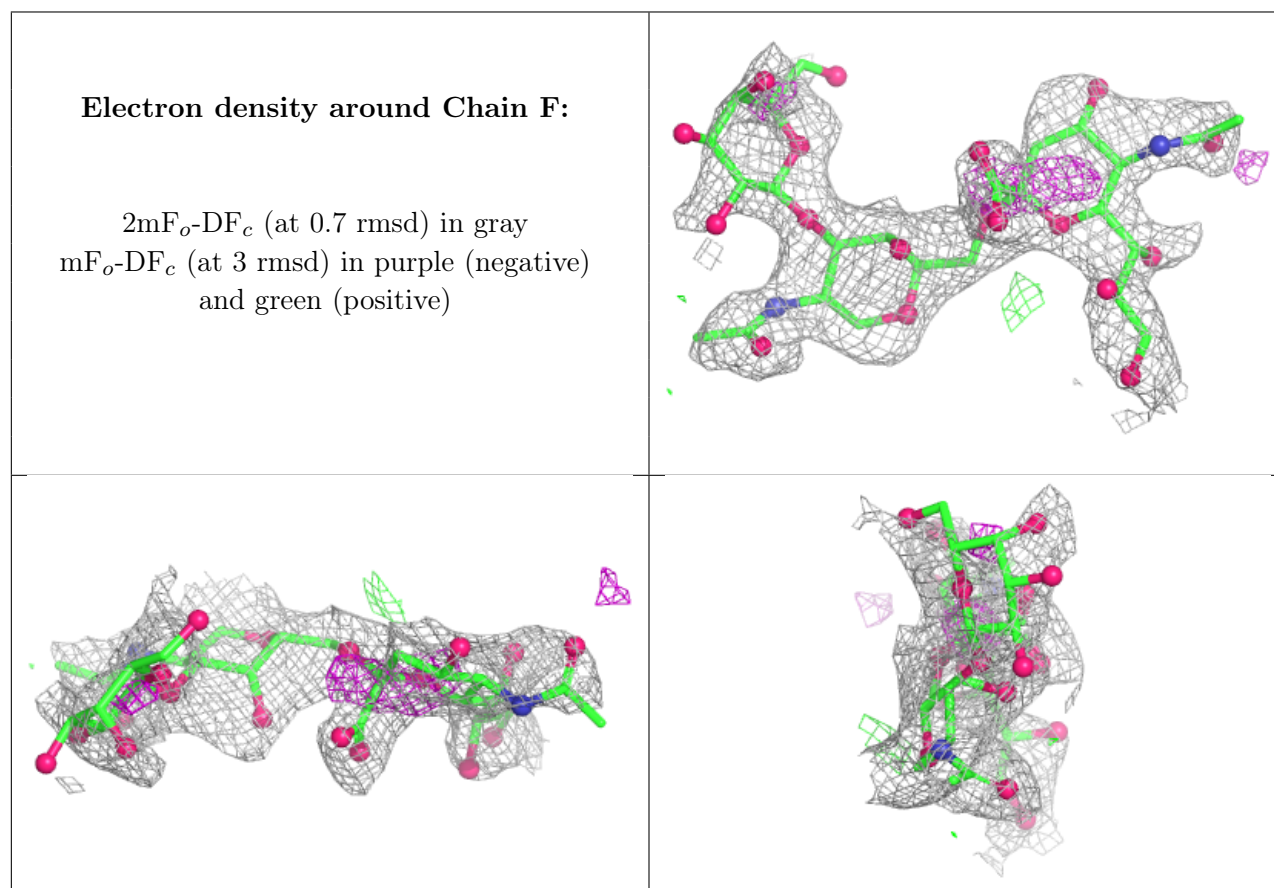
There are no non-standard protein/DNA/RNA residues in this entry.

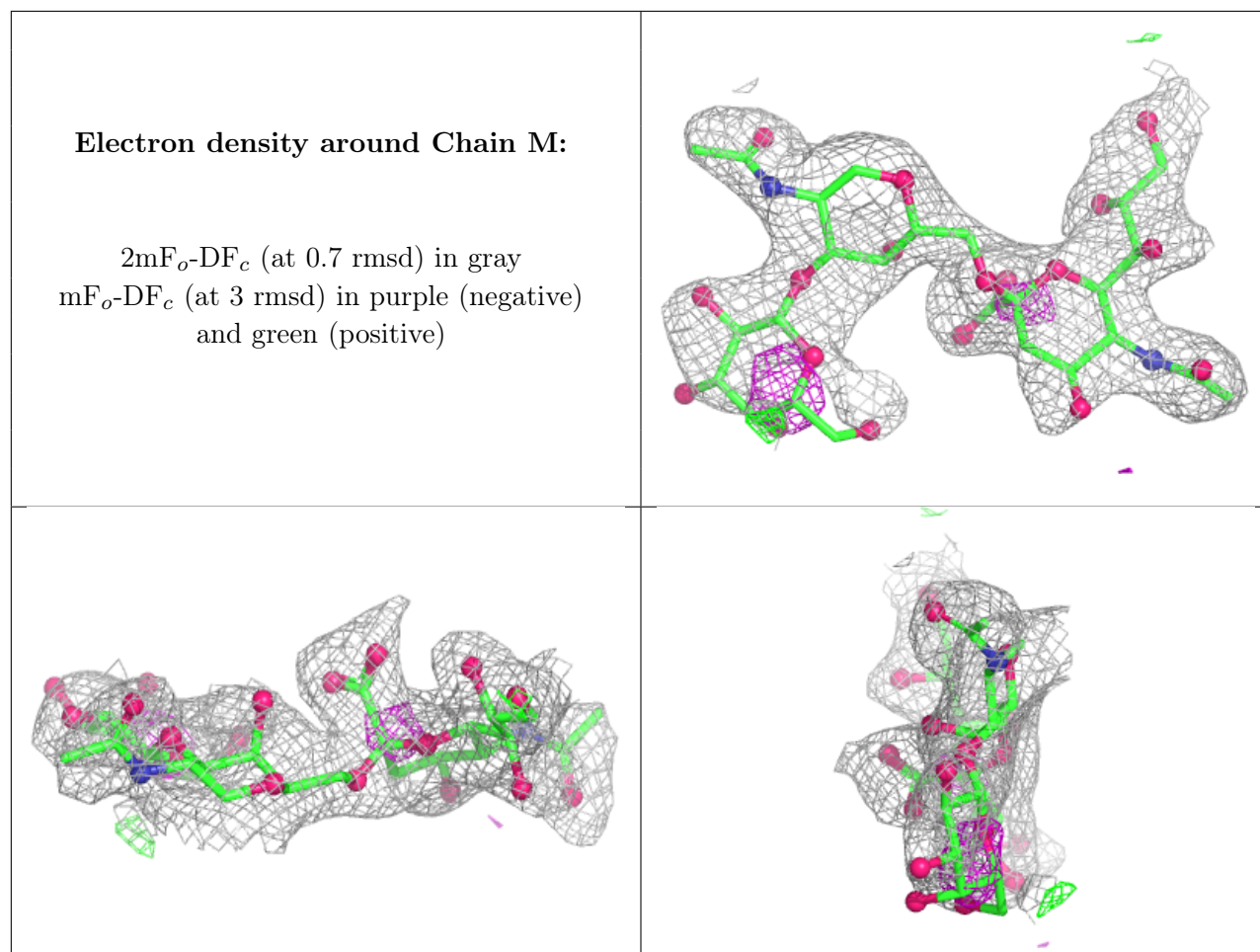
6.3 Carbohydrates [i](#)

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	F	2	11/12	0.52	0.21	92,97,99,100	0
2	SIA	F	3	20/21	0.81	0.13	65,71,73,73	0
2	A2G	F	1	14/15	0.89	0.11	66,69,70,77	0
2	A2G	M	1	14/15	-	-	54,56,58,63	0
2	GAL	M	2	11/12	-	-	74,78,80,80	0
2	SIA	M	3	20/21	-	-	51,57,59,59	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($\text{\AA}^2$)	Q<0.9
4	EDO	B	1002	4/4	0.76	0.14	51,52,52,52	0
4	EDO	C	1006	4/4	0.78	0.19	50,50,50,51	0
4	EDO	C	1004	4/4	0.79	0.24	47,48,48,49	0
4	EDO	A	1002	4/4	0.80	0.13	44,44,44,45	0
5	SER	A	1004	7/7	0.81	0.16	60,60,63,65	0
4	EDO	C	1003	4/4	0.82	0.13	53,53,53,53	0
4	EDO	D	1005	4/4	0.82	0.15	47,48,48,48	0
4	EDO	A	1003	4/4	0.82	0.13	43,43,43,43	0
4	EDO	C	1007	4/4	0.86	0.15	49,49,49,49	0
4	EDO	D	1003	4/4	0.86	0.14	47,47,47,47	0
4	EDO	C	1005	4/4	0.87	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	1004	4/4	0.87	0.13	53,53,53,53	0
4	EDO	D	1004	4/4	0.88	0.14	44,45,45,45	0
5	SER	B	1006	7/7	0.91	0.10	51,51,52,54	0
4	EDO	D	1002	4/4	0.92	0.10	41,41,41,41	0
4	EDO	B	1003	4/4	0.92	0.11	51,51,51,51	0
4	EDO	B	1005	4/4	0.93	0.12	46,46,46,46	0
4	EDO	C	1002	4/4	0.95	0.09	32,33,33,33	0
3	ZN	A	1001	1/1	0.97	0.04	52,52,52,52	0
3	ZN	B	1001	1/1	0.98	0.04	52,52,52,52	0
3	ZN	C	1001	1/1	0.99	0.04	46,46,46,46	0
3	ZN	D	1001	1/1	0.99	0.05	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.