



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:26 AM BST

PDB ID : 4DUW  
Title : E. coli (lacZ) beta-galactosidase (G974A) in complex with allolactose  
Authors : Wheatley, R.W.; Lo, S.; Janzcewicz, L.J.; Dugdale, M.L.; Huber, R.E.  
Deposited on : 2012-02-22  
Resolution : 2.20 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](mailto: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.

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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

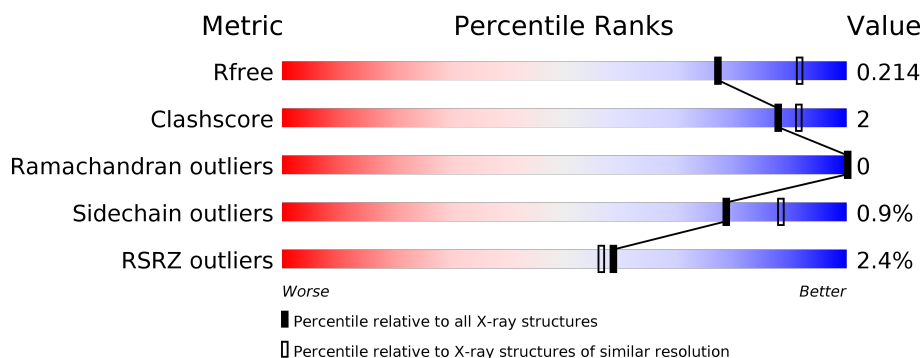
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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.



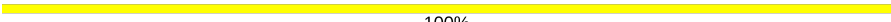
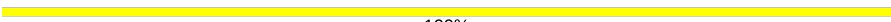
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	1052	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>5%</div> <div></div> </div> </div>
1	B	1052	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div></div> </div> </div>
1	C	1052	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> </div>
1	D	1052	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div></div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%

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
5	DMS	D	8002	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36668 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1015	Total	C	N	O	S	0	0	0
			8158	5160	1445	1515	38			
1	B	1015	Total	C	N	O	S	0	0	0
			8158	5160	1445	1515	38			
1	C	1015	Total	C	N	O	S	0	0	0
			8158	5160	1445	1515	38			
1	D	1015	Total	C	N	O	S	0	0	0
			8158	5160	1445	1515	38			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	initiating methionine	UNP P00722
A	-27	GLY	-	expression tag	UNP P00722
A	-26	GLY	-	expression tag	UNP P00722
A	-25	SER	-	expression tag	UNP P00722
A	-24	HIS	-	expression tag	UNP P00722
A	-23	HIS	-	expression tag	UNP P00722
A	-22	HIS	-	expression tag	UNP P00722
A	-21	HIS	-	expression tag	UNP P00722
A	-20	HIS	-	expression tag	UNP P00722
A	-19	HIS	-	expression tag	UNP P00722
A	-18	GLY	-	expression tag	UNP P00722
A	-17	MET	-	expression tag	UNP P00722
A	-16	ALA	-	expression tag	UNP P00722
A	-15	SER	-	expression tag	UNP P00722
A	-14	MET	-	expression tag	UNP P00722
A	-13	THR	-	expression tag	UNP P00722
A	-12	GLY	-	expression tag	UNP P00722
A	-11	GLY	-	expression tag	UNP P00722
A	-10	GLN	-	expression tag	UNP P00722
A	-9	GLN	-	expression tag	UNP P00722
A	-8	MET	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P00722
A	-6	ARG	-	expression tag	UNP P00722
A	-5	ASP	-	expression tag	UNP P00722
A	-4	LEU	-	expression tag	UNP P00722
A	-3	TYR	-	expression tag	UNP P00722
A	-2	ASP	-	expression tag	UNP P00722
A	-1	ASP	-	expression tag	UNP P00722
A	0	ASP	-	expression tag	UNP P00722
A	1	ASP	-	expression tag	UNP P00722
A	2	LYS	-	expression tag	UNP P00722
A	3	ASP	-	expression tag	UNP P00722
A	4	PRO	-	expression tag	UNP P00722
A	5	MET	-	expression tag	UNP P00722
A	6	ILE	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	794	ALA	GLY	engineered mutation	UNP P00722
B	-28	MET	-	initiating methionine	UNP P00722
B	-27	GLY	-	expression tag	UNP P00722
B	-26	GLY	-	expression tag	UNP P00722
B	-25	SER	-	expression tag	UNP P00722
B	-24	HIS	-	expression tag	UNP P00722
B	-23	HIS	-	expression tag	UNP P00722
B	-22	HIS	-	expression tag	UNP P00722
B	-21	HIS	-	expression tag	UNP P00722
B	-20	HIS	-	expression tag	UNP P00722
B	-19	HIS	-	expression tag	UNP P00722
B	-18	GLY	-	expression tag	UNP P00722
B	-17	MET	-	expression tag	UNP P00722
B	-16	ALA	-	expression tag	UNP P00722
B	-15	SER	-	expression tag	UNP P00722
B	-14	MET	-	expression tag	UNP P00722
B	-13	THR	-	expression tag	UNP P00722
B	-12	GLY	-	expression tag	UNP P00722
B	-11	GLY	-	expression tag	UNP P00722
B	-10	GLN	-	expression tag	UNP P00722
B	-9	GLN	-	expression tag	UNP P00722
B	-8	MET	-	expression tag	UNP P00722
B	-7	GLY	-	expression tag	UNP P00722
B	-6	ARG	-	expression tag	UNP P00722
B	-5	ASP	-	expression tag	UNP P00722
B	-4	LEU	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	TYR	-	expression tag	UNP P00722
B	-2	ASP	-	expression tag	UNP P00722
B	-1	ASP	-	expression tag	UNP P00722
B	0	ASP	-	expression tag	UNP P00722
B	1	ASP	-	expression tag	UNP P00722
B	2	LYS	-	expression tag	UNP P00722
B	3	ASP	-	expression tag	UNP P00722
B	4	PRO	-	expression tag	UNP P00722
B	5	MET	-	expression tag	UNP P00722
B	6	ILE	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	794	ALA	GLY	engineered mutation	UNP P00722
C	-28	MET	-	initiating methionine	UNP P00722
C	-27	GLY	-	expression tag	UNP P00722
C	-26	GLY	-	expression tag	UNP P00722
C	-25	SER	-	expression tag	UNP P00722
C	-24	HIS	-	expression tag	UNP P00722
C	-23	HIS	-	expression tag	UNP P00722
C	-22	HIS	-	expression tag	UNP P00722
C	-21	HIS	-	expression tag	UNP P00722
C	-20	HIS	-	expression tag	UNP P00722
C	-19	HIS	-	expression tag	UNP P00722
C	-18	GLY	-	expression tag	UNP P00722
C	-17	MET	-	expression tag	UNP P00722
C	-16	ALA	-	expression tag	UNP P00722
C	-15	SER	-	expression tag	UNP P00722
C	-14	MET	-	expression tag	UNP P00722
C	-13	THR	-	expression tag	UNP P00722
C	-12	GLY	-	expression tag	UNP P00722
C	-11	GLY	-	expression tag	UNP P00722
C	-10	GLN	-	expression tag	UNP P00722
C	-9	GLN	-	expression tag	UNP P00722
C	-8	MET	-	expression tag	UNP P00722
C	-7	GLY	-	expression tag	UNP P00722
C	-6	ARG	-	expression tag	UNP P00722
C	-5	ASP	-	expression tag	UNP P00722
C	-4	LEU	-	expression tag	UNP P00722
C	-3	TYR	-	expression tag	UNP P00722
C	-2	ASP	-	expression tag	UNP P00722
C	-1	ASP	-	expression tag	UNP P00722
C	0	ASP	-	expression tag	UNP P00722

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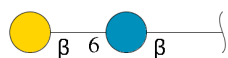
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ASP	-	expression tag	UNP P00722
C	2	LYS	-	expression tag	UNP P00722
C	3	ASP	-	expression tag	UNP P00722
C	4	PRO	-	expression tag	UNP P00722
C	5	MET	-	expression tag	UNP P00722
C	6	ILE	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	794	ALA	GLY	engineered mutation	UNP P00722
D	-28	MET	-	initiating methionine	UNP P00722
D	-27	GLY	-	expression tag	UNP P00722
D	-26	GLY	-	expression tag	UNP P00722
D	-25	SER	-	expression tag	UNP P00722
D	-24	HIS	-	expression tag	UNP P00722
D	-23	HIS	-	expression tag	UNP P00722
D	-22	HIS	-	expression tag	UNP P00722
D	-21	HIS	-	expression tag	UNP P00722
D	-20	HIS	-	expression tag	UNP P00722
D	-19	HIS	-	expression tag	UNP P00722
D	-18	GLY	-	expression tag	UNP P00722
D	-17	MET	-	expression tag	UNP P00722
D	-16	ALA	-	expression tag	UNP P00722
D	-15	SER	-	expression tag	UNP P00722
D	-14	MET	-	expression tag	UNP P00722
D	-13	THR	-	expression tag	UNP P00722
D	-12	GLY	-	expression tag	UNP P00722
D	-11	GLY	-	expression tag	UNP P00722
D	-10	GLN	-	expression tag	UNP P00722
D	-9	GLN	-	expression tag	UNP P00722
D	-8	MET	-	expression tag	UNP P00722
D	-7	GLY	-	expression tag	UNP P00722
D	-6	ARG	-	expression tag	UNP P00722
D	-5	ASP	-	expression tag	UNP P00722
D	-4	LEU	-	expression tag	UNP P00722
D	-3	TYR	-	expression tag	UNP P00722
D	-2	ASP	-	expression tag	UNP P00722
D	-1	ASP	-	expression tag	UNP P00722
D	0	ASP	-	expression tag	UNP P00722
D	1	ASP	-	expression tag	UNP P00722
D	2	LYS	-	expression tag	UNP P00722
D	3	ASP	-	expression tag	UNP P00722
D	4	PRO	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
D	5	MET	-	expression tag	UNP P00722
D	6	ILE	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	794	ALA	GLY	engineered mutation	UNP P00722

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-6)-beta-D-glucopyranose.



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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Mg 3 3	0	0
3	A	3	Total Mg 3 3	0	0
3	D	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total Na 4 4	0	0
4	A	4	Total Na 4 4	0	0

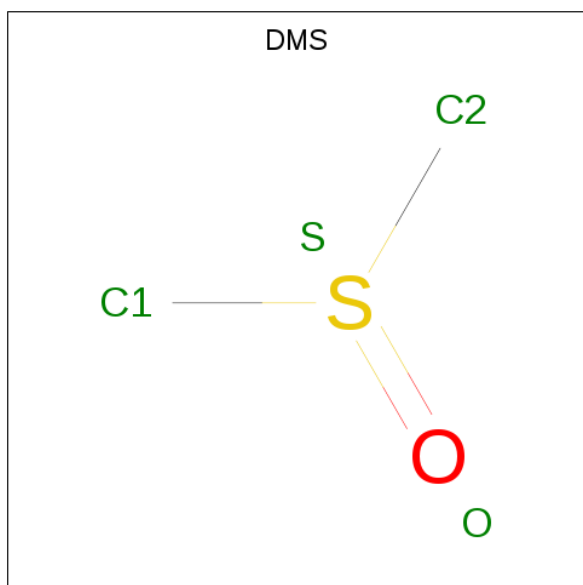
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	4	Total 4	Na 4	0	0
4	C	4	Total 4	Na 4	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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

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

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

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

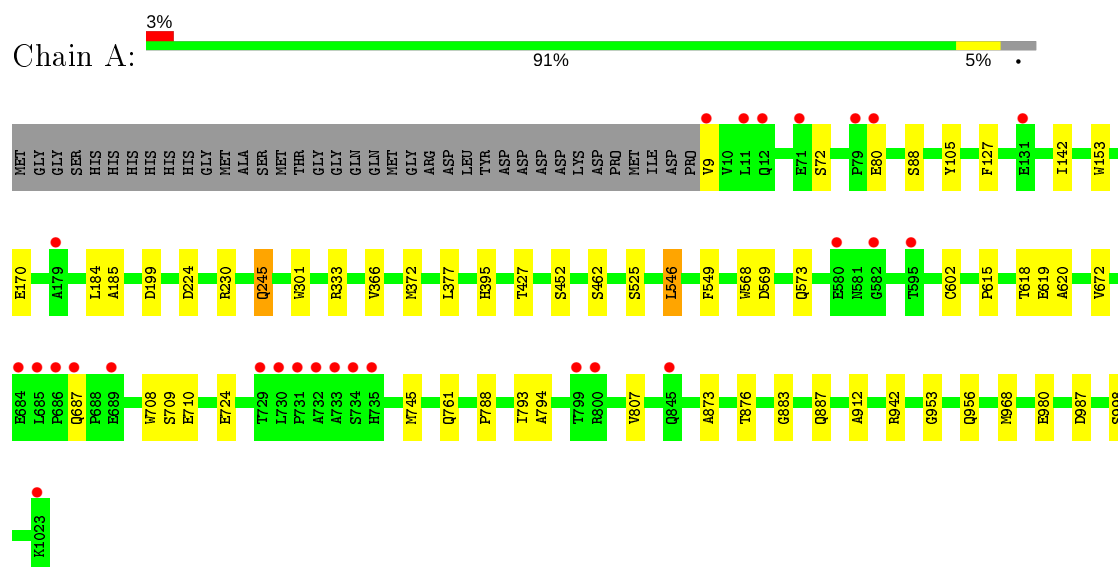
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	824	Total 824	O 824	0	0
6	B	997	Total 997	O 997	0	0
6	C	976	Total 976	O 976	0	0
6	D	813	Total 813	O 813	0	0

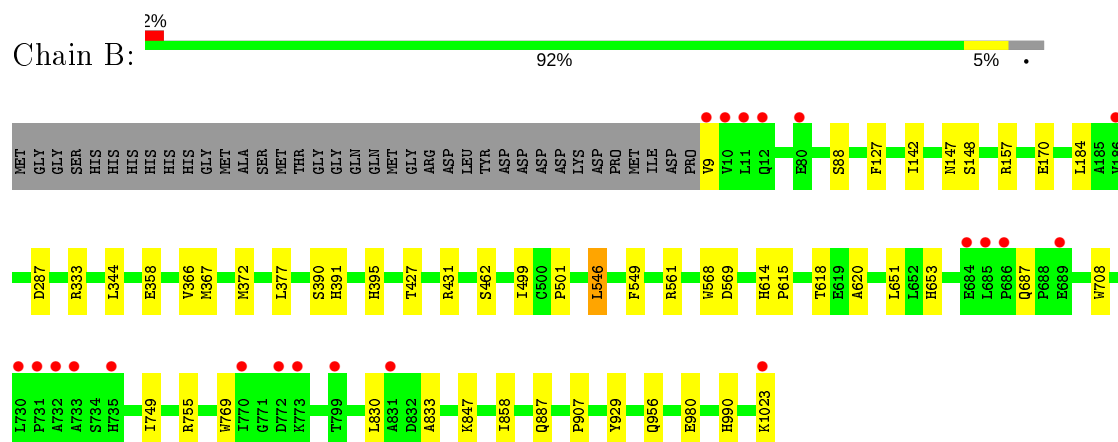
### 3 Residue-property plots [i](#)

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.

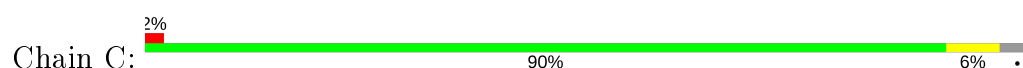
#### • Molecule 1: Beta-galactosidase

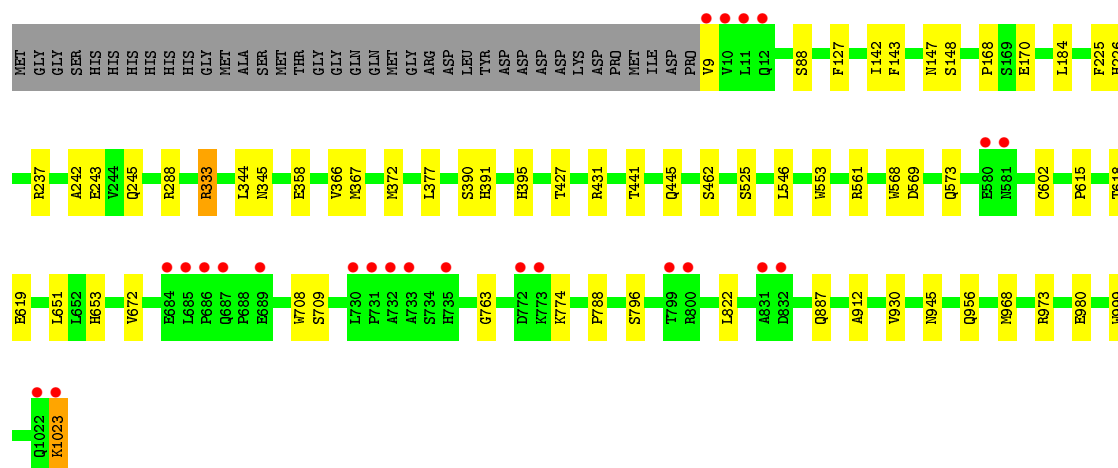


#### • Molecule 1: Beta-galactosidase

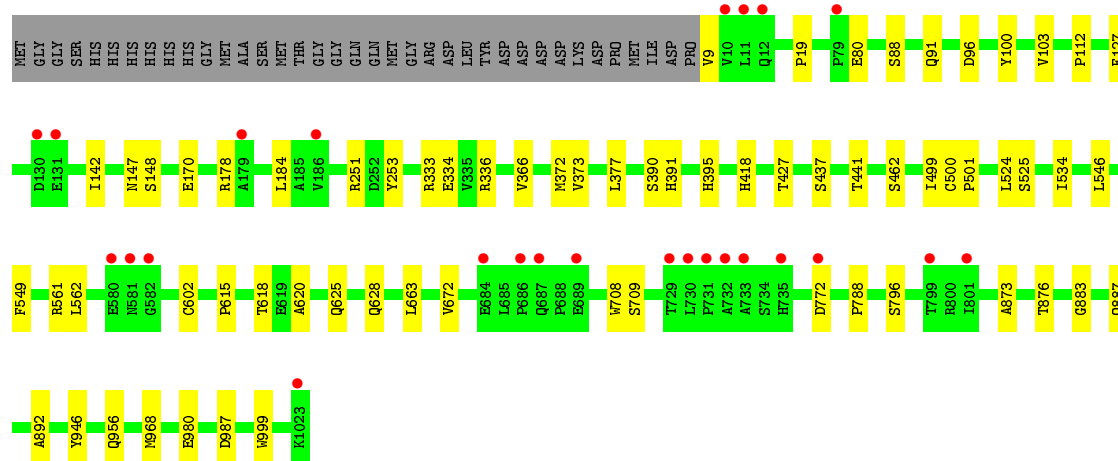
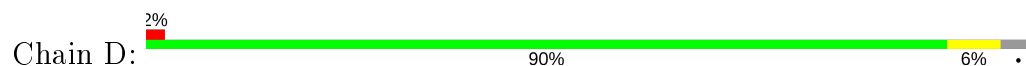


#### • Molecule 1: Beta-galactosidase

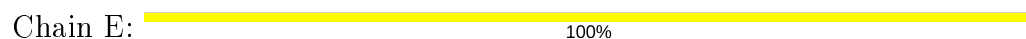




- Molecule 1: Beta-galactosidase



- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-glucopyranose



- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-glucopyranose



B0C1  
GAL2

- Molecule 2: beta-D-galactopyranose-(1-6)-beta-D-glucopyranose

Chain H:

100%

B0C1  
GAL2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.83Å 162.63Å 203.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.81 – 2.20 24.82 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.81-2.20) 92.6 (24.82-2.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.19Å)	Xtrriage
Refinement program	REFMAC 5.5.0109, CNS	Depositor
R, $R_{free}$	0.160 , 0.213 0.163 , 0.214	Depositor DCC
$R_{free}$ test set	3378 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtrriage
Anisotropy	0.003	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	36668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5641e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, MG, BGC, DMS, GAL

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	0.38	0/8400	0.54	0/11460
1	B	0.40	0/8400	0.54	0/11460
1	C	0.40	0/8400	0.54	1/11460 (0.0%)
1	D	0.38	0/8400	0.53	0/11460
All	All	0.39	0/33600	0.54	1/45840 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	553	TRP	CA-CB-CG	-5.09	104.03	113.70

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	8158	0	7755	32	0
1	B	8158	0	7755	31	0
1	C	8158	0	7755	33	0
1	D	8158	0	7755	35	0
2	E	23	0	20	0	0
2	F	23	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	23	0	20	0	0
2	H	23	0	20	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	72	0	108	1	0
5	B	96	0	144	0	0
5	C	80	0	120	1	0
5	D	60	0	90	4	0
6	A	824	0	0	1	0
6	B	997	0	0	6	0
6	C	976	0	0	1	0
6	D	813	0	0	1	0
All	All	36668	0	31562	129	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 (129) 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:142:ILE:HG12	1:B:170:GLU:HG2	1.69	0.74
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.72	0.72
1:A:224:ASP:HB3	1:A:245:GLN:HG3	1.73	0.71
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.73	0.69
5:D:8002:DMS:H22	6:D:4227:HOH:O	1.94	0.66
1:B:887:GLN:NE2	1:B:980:GLU:O	2.30	0.65
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.80	0.64
1:D:887:GLN:NE2	1:D:980:GLU:O	2.30	0.64
1:C:887:GLN:NE2	1:C:980:GLU:O	2.32	0.63
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.36	0.61
1:A:887:GLN:NE2	1:A:980:GLU:O	2.33	0.60
1:D:628:GLN:OE1	5:D:8002:DMS:H21	2.04	0.57
1:B:749:ILE:HD13	1:B:858:ILE:HD12	1.86	0.56
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.41	0.55
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:THR:HG21	1:A:462:SER:HB3	1.90	0.54
1:D:19:PRO:HD3	1:D:112:PRO:HB3	1.90	0.54
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.73	0.54
1:B:651:LEU:HD11	1:B:653:HIS:CE1	2.44	0.53
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.91	0.53
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.90	0.53
1:C:763:GLY:HA3	1:C:822:LEU:HD13	1.91	0.53
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.91	0.53
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.44	0.52
1:A:724:GLU:O	1:B:847:LYS:NZ	2.42	0.52
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.45	0.52
1:B:755:ARG:HB2	1:B:769:TRP:HB2	1.91	0.52
1:C:945:ASN:HB3	1:C:1023:LYS:HE2	1.91	0.52
1:B:615:PRO:O	1:B:618:THR:HG22	2.10	0.52
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.45	0.52
1:D:427:THR:HG21	1:D:462:SER:HB3	1.91	0.51
1:D:500:CYS:HA	1:D:534:ILE:O	2.11	0.51
1:D:373:VAL:O	1:D:377:LEU:HG	2.10	0.51
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.94	0.50
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.94	0.50
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.94	0.50
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.47	0.49
1:C:788:PRO:HD2	1:C:968:MET:HG3	1.94	0.49
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.95	0.48
1:C:88:SER:HA	1:C:366:VAL:HG21	1.94	0.48
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.42	0.48
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.42	0.48
1:B:9:VAL:HG22	1:C:9:VAL:HG22	1.95	0.48
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.95	0.48
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.49	0.48
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.77	0.48
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.49	0.48
1:C:573:GLN:HB2	1:C:602:CYS:O	2.13	0.47
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.96	0.47
1:C:441:THR:O	1:C:445:GLN:HG3	2.15	0.47
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.96	0.47
1:A:873:ALA:O	1:A:876:THR:HG22	2.15	0.47
1:B:367:MET:HE2	1:B:372:MET:HG3	1.96	0.47
1:B:830:LEU:HD12	1:B:833:ALA:HB3	1.95	0.47
1:C:615:PRO:O	1:C:618:THR:HG22	2.15	0.47
1:A:794:ALA:HA	1:A:998:SER:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HD3	6:B:4651:HOH:O	2.15	0.46
1:B:88:SER:HA	1:B:366:VAL:HG21	1.98	0.46
1:C:561:ARG:HD3	1:D:525:SER:O	2.15	0.46
1:D:390:SER:HA	1:D:391:HIS:HA	1.77	0.46
1:A:573:GLN:HB2	1:A:602:CYS:O	2.16	0.46
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.50	0.46
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.98	0.46
1:A:88:SER:HA	1:A:366:VAL:HG21	1.98	0.46
1:C:796:SER:HB3	1:C:999:TRP:HB3	1.98	0.46
6:B:4674:HOH:O	5:C:8013:DMS:H11	2.15	0.45
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.50	0.45
1:D:873:ALA:O	1:D:876:THR:HG22	2.16	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.69	0.45
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.46	0.45
1:A:546:LEU:HA	6:A:4125:HOH:O	2.17	0.45
1:A:745:MET:HA	1:A:761:GLN:HE21	1.82	0.45
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.81	0.45
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.98	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.66	0.44
1:C:427:THR:HG21	1:C:462:SER:HB3	2.00	0.44
1:D:625:GLN:HB2	5:D:8002:DMS:H23	1.98	0.44
1:D:615:PRO:O	1:D:618:THR:HG22	2.17	0.44
1:D:88:SER:HA	1:D:366:VAL:HG21	1.99	0.44
1:A:9:VAL:HG12	1:D:9:VAL:HG12	2.00	0.44
1:C:525:SER:O	1:D:561:ARG:HD3	2.18	0.44
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.80	0.44
1:B:431:ARG:HB2	6:B:4879:HOH:O	2.17	0.44
1:B:427:THR:HG21	1:B:462:SER:HB3	2.00	0.43
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.01	0.43
1:D:437:SER:O	1:D:441:THR:HG23	2.18	0.43
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.53	0.43
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.99	0.43
1:D:796:SER:HB3	1:D:999:TRP:HB3	2.01	0.43
1:B:390:SER:HA	1:B:391:HIS:HA	1.84	0.43
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.54	0.43
2:F:1:BGC:H6C1	2:F:2:GAL:H62	1.99	0.43
1:B:287:ASP:OD1	1:B:287:ASP:N	2.50	0.42
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.55	0.42
1:A:224:ASP:HB3	1:A:245:GLN:CG	2.48	0.42
1:C:431:ARG:NH2	6:C:4487:HOH:O	2.52	0.42
6:B:4098:HOH:O	2:F:1:BGC:H6C2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:GLU:HB3	1:B:367:MET:HG2	2.01	0.42
1:D:628:GLN:OE1	5:D:8002:DMS:C2	2.67	0.42
1:A:153:TRP:HB2	1:A:185:ALA:HB3	2.01	0.42
1:A:372:MET:HE1	1:A:395:HIS:HB3	2.01	0.42
1:A:615:PRO:O	1:A:618:THR:HG22	2.20	0.42
1:B:546:LEU:HA	6:B:4149:HOH:O	2.20	0.42
1:B:147:ASN:HA	1:B:148:SER:HA	1.67	0.42
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.55	0.42
1:D:883:GLY:HA3	1:D:987:ASP:HA	2.02	0.42
1:A:372:MET:CE	1:A:395:HIS:HB3	2.49	0.41
1:A:793:ILE:HA	1:A:807:VAL:HG11	2.03	0.41
1:C:143:PHE:O	1:C:168:PRO:HA	2.20	0.41
1:A:942:ARG:HA	1:A:953:GLY:O	2.21	0.41
1:B:1023:LYS:HA	6:B:4592:HOH:O	2.18	0.41
1:D:524:LEU:HD11	1:D:562:LEU:HG	2.02	0.41
1:C:226:HIS:O	1:C:242:ALA:HA	2.21	0.41
1:D:251:ARG:HD3	1:D:253:TYR:OH	2.21	0.41
1:A:525:SER:O	1:B:561:ARG:HD3	2.21	0.41
1:B:614:HIS:HD1	1:B:929:TYR:HE2	1.69	0.41
1:C:225:PHE:HA	1:C:243:GLU:O	2.21	0.41
1:C:390:SER:HA	1:C:391:HIS:HA	1.82	0.41
1:D:103:VAL:HG22	1:D:418:HIS:CE1	2.56	0.41
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.20	0.41
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.56	0.40
1:B:907:PRO:HG2	1:B:990:HIS:O	2.22	0.40
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.56	0.40
1:C:333:ARG:HA	1:C:345:ASN:OD1	2.21	0.40
1:A:710:GLU:HG3	5:A:8015:DMS:H11	2.04	0.40
1:A:883:GLY:HA3	1:A:987:ASP:HA	2.02	0.40
1:C:358:GLU:HB3	1:C:367:MET:HG2	2.04	0.40
1:A:301:TRP:CH2	1:A:452:SER:HA	2.56	0.40
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.57	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	1013/1052 (96%)	983 (97%)	30 (3%)	0	100	100
1	B	1013/1052 (96%)	981 (97%)	32 (3%)	0	100	100
1	C	1013/1052 (96%)	987 (97%)	26 (3%)	0	100	100
1	D	1013/1052 (96%)	981 (97%)	32 (3%)	0	100	100
All	All	4052/4208 (96%)	3932 (97%)	120 (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	868/898 (97%)	859 (99%)	9 (1%)	76	86
1	B	868/898 (97%)	863 (99%)	5 (1%)	86	93
1	C	868/898 (97%)	860 (99%)	8 (1%)	78	88
1	D	868/898 (97%)	860 (99%)	8 (1%)	78	88
All	All	3472/3592 (97%)	3442 (99%)	30 (1%)	78	88

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	A	80	GLU
1	A	230	ARG
1	A	245	GLN
1	A	333	ARG
1	A	546	LEU
1	A	672	VAL
1	A	687	GLN

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Mol	Chain	Res	Type
1	A	956	GLN
1	B	333	ARG
1	B	344	LEU
1	B	546	LEU
1	B	687	GLN
1	B	956	GLN
1	C	237	ARG
1	C	333	ARG
1	C	344	LEU
1	C	546	LEU
1	C	672	VAL
1	C	774	LYS
1	C	956	GLN
1	C	1023	LYS
1	D	80	GLU
1	D	178	ARG
1	D	333	ARG
1	D	546	LEU
1	D	663	LEU
1	D	672	VAL
1	D	772	ASP
1	D	956	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	761	GLN
1	B	1022	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

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	BGC	E	1	2	12,12,12	0.58	0	17,17,17	1.50	2 (11%)
2	GAL	E	2	2,4	11,11,12	0.54	0	15,15,17	2.68	3 (20%)
2	BGC	F	1	2	12,12,12	0.60	0	17,17,17	1.01	2 (11%)
2	GAL	F	2	2,4	11,11,12	0.49	0	15,15,17	2.70	3 (20%)
2	BGC	G	1	2	12,12,12	0.53	0	17,17,17	0.96	1 (5%)
2	GAL	G	2	2,4	11,11,12	0.39	0	15,15,17	2.75	3 (20%)
2	BGC	H	1	2	12,12,12	0.61	0	17,17,17	1.34	3 (17%)
2	GAL	H	2	2,4	11,11,12	0.50	0	15,15,17	2.64	3 (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
2	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	GAL	E	2	2,4	-	2/2/19/22	0/1/1/1
2	BGC	F	1	2	-	2/2/22/22	0/1/1/1
2	GAL	F	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	G	1	2	-	2/2/22/22	0/1/1/1
2	GAL	G	2	2,4	-	1/2/19/22	0/1/1/1
2	BGC	H	1	2	-	1/2/22/22	0/1/1/1
2	GAL	H	2	2,4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	GAL	C1-O5-C5	9.40	124.92	112.19
2	G	2	GAL	C1-O5-C5	9.31	124.81	112.19
2	H	2	GAL	C1-O5-C5	8.84	124.16	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GAL	C1-O5-C5	8.83	124.15	112.19
2	E	2	GAL	O5-C1-C2	4.15	117.17	110.77
2	E	1	BGC	C3-C4-C5	3.99	117.36	110.24
2	G	2	GAL	O5-C1-C2	3.80	116.64	110.77
2	H	2	GAL	O5-C1-C2	3.66	116.42	110.77
2	H	1	BGC	C3-C4-C5	3.20	115.95	110.24
2	H	1	BGC	C4-C3-C2	3.15	116.32	110.82
2	E	1	BGC	C4-C3-C2	3.15	116.31	110.82
2	F	2	GAL	O5-C1-C2	3.08	115.53	110.77
2	H	2	GAL	C1-C2-C3	2.63	112.90	109.67
2	E	2	GAL	C1-C2-C3	2.57	112.83	109.67
2	G	2	GAL	C1-C2-C3	2.50	112.73	109.67
2	G	1	BGC	C3-C4-C5	2.48	114.67	110.24
2	F	2	GAL	C1-C2-C3	2.38	112.59	109.67
2	F	1	BGC	C3-C4-C5	2.31	114.35	110.24
2	F	1	BGC	C4-C3-C2	2.16	114.60	110.82
2	H	1	BGC	C1-C2-C3	2.08	114.63	110.31

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	BGC	O5-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
2	G	1	BGC	O5-C5-C6-O6
2	F	1	BGC	C4-C5-C6-O6
2	F	2	GAL	O5-C5-C6-O6
2	H	1	BGC	O5-C5-C6-O6
2	H	2	GAL	C4-C5-C6-O6
2	G	2	GAL	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	E	2	GAL	C4-C5-C6-O6
2	G	1	BGC	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

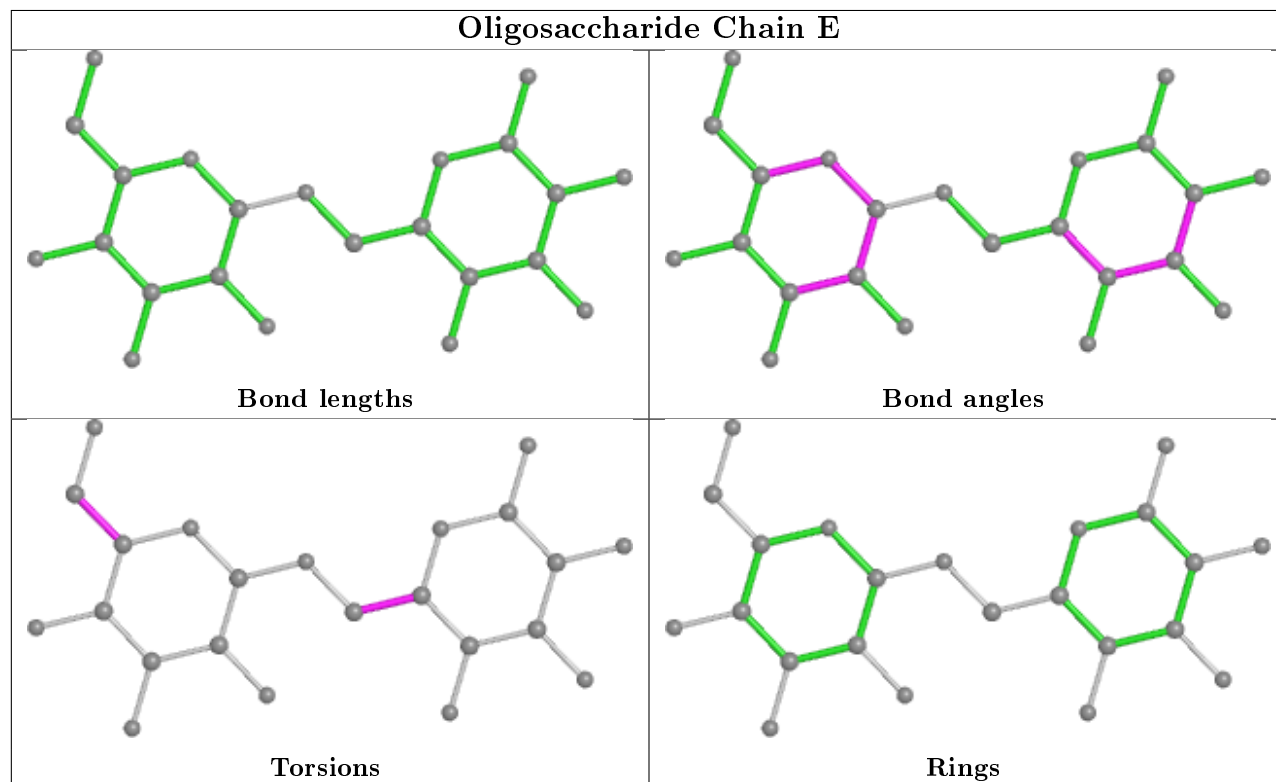
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	BGC	2	0

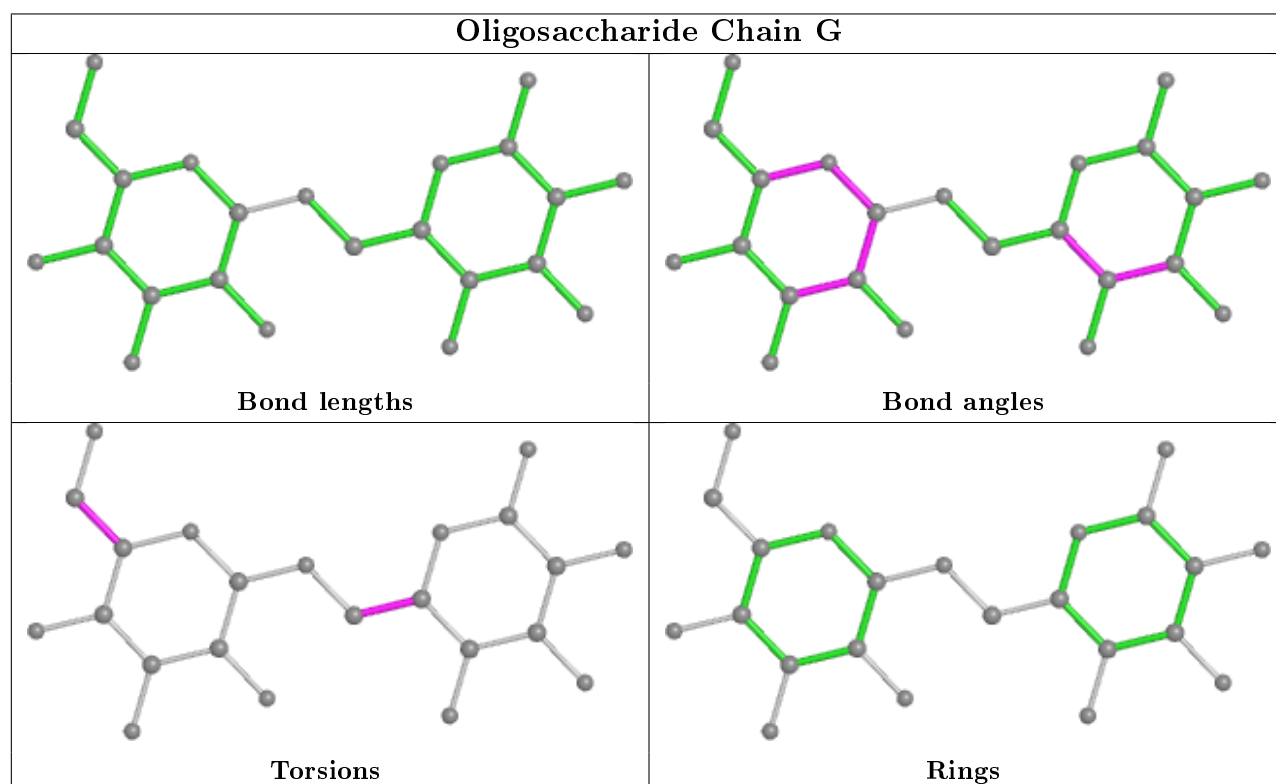
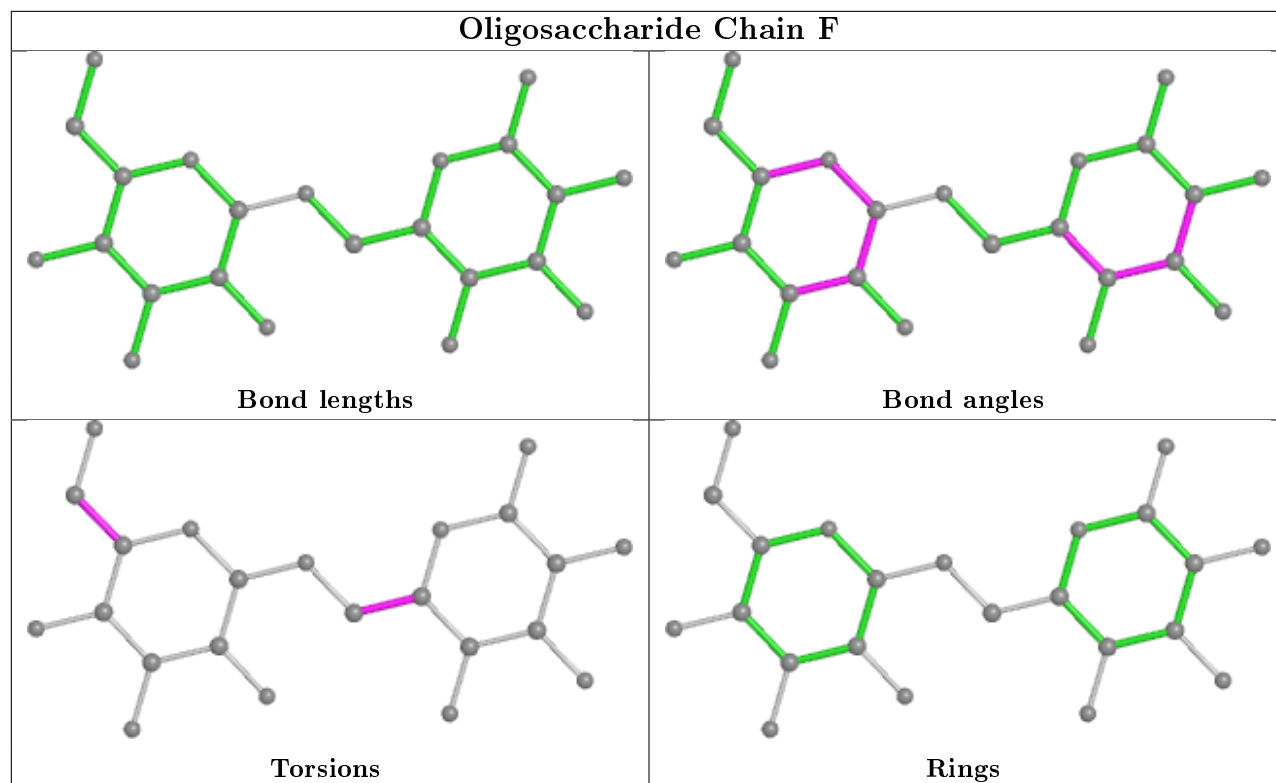
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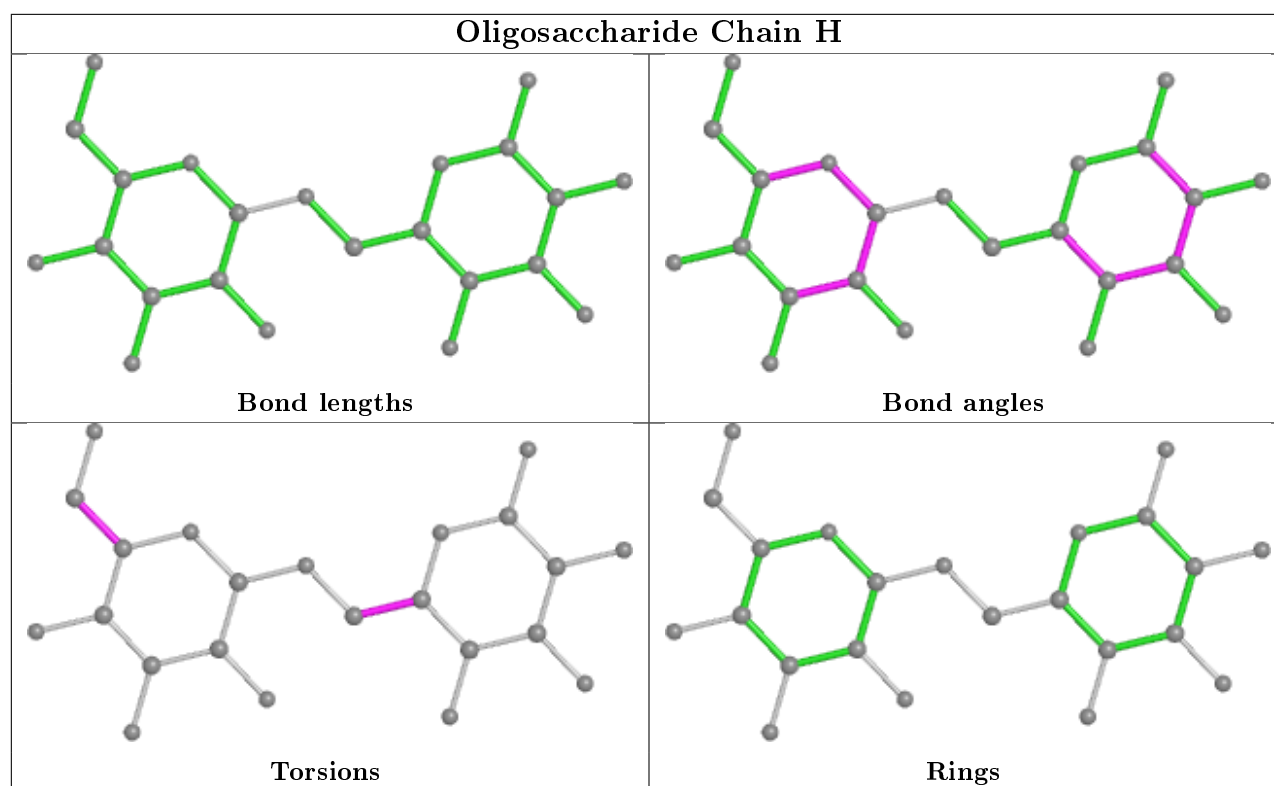
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	GAL	1	0

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 103 ligands modelled in this entry, 26 are monoatomic - leaving 77 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	DMS	A	8014	-	3,3,3	2.65	1 (33%)	3,3,3	0.44	0
5	DMS	C	8020	-	3,3,3	2.43	1 (33%)	3,3,3	0.68	0
5	DMS	C	8008	-	3,3,3	2.57	1 (33%)	3,3,3	0.40	0
5	DMS	A	8018	-	3,3,3	2.67	1 (33%)	3,3,3	0.59	0
5	DMS	C	8002	-	3,3,3	2.60	1 (33%)	3,3,3	0.40	0
5	DMS	D	8010	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
5	DMS	D	8009	-	3,3,3	2.62	1 (33%)	3,3,3	0.51	0
5	DMS	B	8009	-	3,3,3	2.57	1 (33%)	3,3,3	0.31	0
5	DMS	C	8001	-	3,3,3	2.56	1 (33%)	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	D	8005	-	3,3,3	2.63	1 (33%)	3,3,3	0.28	0
5	DMS	B	8019	-	3,3,3	2.57	1 (33%)	3,3,3	0.43	0
5	DMS	D	8012	-	3,3,3	2.65	1 (33%)	3,3,3	0.46	0
5	DMS	D	8015	-	3,3,3	2.64	1 (33%)	3,3,3	0.67	0
5	DMS	B	8023	-	3,3,3	2.67	1 (33%)	3,3,3	0.52	0
5	DMS	B	8005	-	3,3,3	2.62	1 (33%)	3,3,3	0.27	0
5	DMS	D	8011	-	3,3,3	2.64	1 (33%)	3,3,3	0.50	0
5	DMS	A	8003	-	3,3,3	2.63	1 (33%)	3,3,3	0.57	0
5	DMS	B	8003	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
5	DMS	C	8003	-	3,3,3	2.62	1 (33%)	3,3,3	0.36	0
5	DMS	C	8017	-	3,3,3	2.45	1 (33%)	3,3,3	0.36	0
5	DMS	B	8021	-	3,3,3	2.61	1 (33%)	3,3,3	0.46	0
5	DMS	C	8014	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
5	DMS	D	8014	-	3,3,3	2.63	1 (33%)	3,3,3	0.53	0
5	DMS	B	8013	-	3,3,3	2.64	1 (33%)	3,3,3	0.49	0
5	DMS	B	8022	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
5	DMS	C	8006	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
5	DMS	D	8013	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
5	DMS	A	8011	-	3,3,3	2.66	1 (33%)	3,3,3	0.48	0
5	DMS	A	8001	-	3,3,3	2.60	1 (33%)	3,3,3	0.67	0
5	DMS	A	8015	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
5	DMS	C	8005	-	3,3,3	2.63	1 (33%)	3,3,3	0.43	0
5	DMS	A	8005	-	3,3,3	2.65	1 (33%)	3,3,3	0.44	0
5	DMS	B	8001	-	3,3,3	2.54	1 (33%)	3,3,3	0.47	0
5	DMS	B	8011	-	3,3,3	2.63	1 (33%)	3,3,3	0.61	0
5	DMS	A	8004	-	3,3,3	2.67	1 (33%)	3,3,3	0.51	0
5	DMS	B	8006	-	3,3,3	2.65	1 (33%)	3,3,3	0.65	0
5	DMS	B	8008	-	3,3,3	2.67	1 (33%)	3,3,3	0.39	0
5	DMS	A	8007	-	3,3,3	2.69	1 (33%)	3,3,3	0.51	0
5	DMS	D	8008	-	3,3,3	2.64	1 (33%)	3,3,3	0.52	0
5	DMS	C	8011	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
5	DMS	C	8018	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
5	DMS	D	8003	-	3,3,3	2.66	1 (33%)	3,3,3	0.50	0
5	DMS	C	8012	-	3,3,3	2.64	1 (33%)	3,3,3	0.47	0
5	DMS	B	8002	-	3,3,3	2.57	1 (33%)	3,3,3	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	B	8007	-	3,3,3	2.74	1 (33%)	3,3,3	0.63	0
5	DMS	D	8006	-	3,3,3	2.63	1 (33%)	3,3,3	0.44	0
5	DMS	A	8013	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
5	DMS	A	8009	-	3,3,3	2.61	1 (33%)	3,3,3	0.47	0
5	DMS	B	8016	-	3,3,3	2.60	1 (33%)	3,3,3	0.59	0
5	DMS	D	8002	-	3,3,3	2.64	1 (33%)	3,3,3	0.57	0
5	DMS	C	8013	-	3,3,3	2.63	1 (33%)	3,3,3	0.47	0
5	DMS	A	8010	-	3,3,3	2.67	1 (33%)	3,3,3	0.53	0
5	DMS	B	8010	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
5	DMS	C	8010	-	3,3,3	2.64	1 (33%)	3,3,3	0.63	0
5	DMS	C	8004	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
5	DMS	B	8014	-	3,3,3	2.64	1 (33%)	3,3,3	0.44	0
5	DMS	C	8007	-	3,3,3	2.66	1 (33%)	3,3,3	0.57	0
5	DMS	D	8007	-	3,3,3	2.67	1 (33%)	3,3,3	0.49	0
5	DMS	D	8004	-	3,3,3	2.65	1 (33%)	3,3,3	0.56	0
5	DMS	B	8020	-	3,3,3	2.68	1 (33%)	3,3,3	0.61	0
5	DMS	B	8017	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
5	DMS	C	8015	-	3,3,3	2.71	1 (33%)	3,3,3	0.49	0
5	DMS	A	8002	-	3,3,3	2.58	1 (33%)	3,3,3	0.51	0
5	DMS	C	8019	-	3,3,3	2.67	1 (33%)	3,3,3	0.65	0
5	DMS	A	8012	-	3,3,3	2.63	1 (33%)	3,3,3	0.44	0
5	DMS	A	8006	-	3,3,3	2.66	1 (33%)	3,3,3	0.53	0
5	DMS	C	8016	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
5	DMS	D	8001	-	3,3,3	2.59	1 (33%)	3,3,3	0.59	0
5	DMS	A	8016	-	3,3,3	2.66	1 (33%)	3,3,3	0.55	0
5	DMS	B	8012	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
5	DMS	C	8009	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
5	DMS	B	8018	-	3,3,3	2.58	1 (33%)	3,3,3	0.42	0
5	DMS	B	8024	-	3,3,3	2.45	1 (33%)	3,3,3	0.63	0
5	DMS	A	8017	-	3,3,3	2.65	1 (33%)	3,3,3	0.56	0
5	DMS	B	8015	-	3,3,3	2.63	1 (33%)	3,3,3	0.41	0
5	DMS	B	8004	-	3,3,3	2.61	1 (33%)	3,3,3	0.47	0
5	DMS	A	8008	-	3,3,3	2.62	1 (33%)	3,3,3	0.54	0

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8007	DMS	O-S	4.58	1.81	1.50
5	C	8006	DMS	O-S	4.55	1.81	1.50
5	C	8015	DMS	O-S	4.54	1.80	1.50
5	A	8007	DMS	O-S	4.50	1.80	1.50
5	D	8013	DMS	O-S	4.50	1.80	1.50
5	C	8014	DMS	O-S	4.49	1.80	1.50
5	A	8010	DMS	O-S	4.49	1.80	1.50
5	A	8004	DMS	O-S	4.49	1.80	1.50
5	B	8003	DMS	O-S	4.49	1.80	1.50
5	B	8017	DMS	O-S	4.49	1.80	1.50
5	D	8002	DMS	O-S	4.49	1.80	1.50
5	B	8020	DMS	O-S	4.49	1.80	1.50
5	A	8013	DMS	O-S	4.48	1.80	1.50
5	D	8007	DMS	O-S	4.48	1.80	1.50
5	B	8012	DMS	O-S	4.48	1.80	1.50
5	D	8003	DMS	O-S	4.48	1.80	1.50
5	A	8018	DMS	O-S	4.48	1.80	1.50
5	B	8008	DMS	O-S	4.47	1.80	1.50
5	A	8011	DMS	O-S	4.47	1.80	1.50
5	B	8023	DMS	O-S	4.47	1.80	1.50
5	D	8012	DMS	O-S	4.46	1.80	1.50
5	C	8019	DMS	O-S	4.46	1.80	1.50
5	A	8006	DMS	O-S	4.46	1.80	1.50
5	C	8007	DMS	O-S	4.46	1.80	1.50
5	A	8016	DMS	O-S	4.46	1.80	1.50
5	C	8016	DMS	O-S	4.45	1.80	1.50
5	C	8004	DMS	O-S	4.45	1.80	1.50
5	A	8005	DMS	O-S	4.45	1.80	1.50
5	B	8010	DMS	O-S	4.45	1.80	1.50
5	D	8004	DMS	O-S	4.45	1.80	1.50
5	A	8014	DMS	O-S	4.45	1.80	1.50
5	B	8013	DMS	O-S	4.44	1.80	1.50
5	D	8010	DMS	O-S	4.44	1.80	1.50
5	C	8018	DMS	O-S	4.44	1.80	1.50
5	C	8011	DMS	O-S	4.44	1.80	1.50
5	B	8006	DMS	O-S	4.43	1.80	1.50
5	A	8017	DMS	O-S	4.43	1.80	1.50
5	B	8015	DMS	O-S	4.43	1.80	1.50
5	C	8009	DMS	O-S	4.43	1.80	1.50
5	D	8011	DMS	O-S	4.43	1.80	1.50
5	D	8015	DMS	O-S	4.43	1.80	1.50
5	C	8012	DMS	O-S	4.43	1.80	1.50
5	D	8014	DMS	O-S	4.42	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8014	DMS	O-S	4.42	1.80	1.50
5	D	8005	DMS	O-S	4.42	1.80	1.50
5	C	8003	DMS	O-S	4.42	1.80	1.50
5	D	8006	DMS	O-S	4.42	1.80	1.50
5	D	8008	DMS	O-S	4.42	1.80	1.50
5	C	8005	DMS	O-S	4.41	1.80	1.50
5	A	8015	DMS	O-S	4.41	1.80	1.50
5	A	8003	DMS	O-S	4.41	1.80	1.50
5	C	8010	DMS	O-S	4.41	1.80	1.50
5	C	8013	DMS	O-S	4.41	1.80	1.50
5	A	8012	DMS	O-S	4.41	1.80	1.50
5	B	8022	DMS	O-S	4.40	1.80	1.50
5	B	8005	DMS	O-S	4.40	1.80	1.50
5	D	8009	DMS	O-S	4.40	1.79	1.50
5	B	8011	DMS	O-S	4.39	1.79	1.50
5	B	8021	DMS	O-S	4.39	1.79	1.50
5	B	8004	DMS	O-S	4.39	1.79	1.50
5	A	8008	DMS	O-S	4.38	1.79	1.50
5	A	8009	DMS	O-S	4.38	1.79	1.50
5	C	8002	DMS	O-S	4.37	1.79	1.50
5	B	8016	DMS	O-S	4.37	1.79	1.50
5	A	8001	DMS	O-S	4.36	1.79	1.50
5	A	8002	DMS	O-S	4.34	1.79	1.50
5	D	8001	DMS	O-S	4.34	1.79	1.50
5	B	8009	DMS	O-S	4.33	1.79	1.50
5	B	8002	DMS	O-S	4.32	1.79	1.50
5	C	8008	DMS	O-S	4.31	1.79	1.50
5	B	8018	DMS	O-S	4.31	1.79	1.50
5	B	8019	DMS	O-S	4.30	1.79	1.50
5	C	8001	DMS	O-S	4.28	1.79	1.50
5	B	8001	DMS	O-S	4.26	1.79	1.50
5	C	8017	DMS	O-S	4.13	1.78	1.50
5	B	8024	DMS	O-S	4.12	1.78	1.50
5	C	8020	DMS	O-S	4.09	1.77	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8015	DMS	1	0
5	D	8002	DMS	4	0
5	C	8013	DMS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1015/1052 (96%)	-0.44	27 (2%) 54 52	21, 35, 61, 98	0
1	B	1015/1052 (96%)	-0.51	21 (2%) 63 61	20, 30, 58, 97	0
1	C	1015/1052 (96%)	-0.54	24 (2%) 59 56	19, 30, 55, 96	0
1	D	1015/1052 (96%)	-0.39	25 (2%) 57 55	23, 36, 60, 106	0
All	All	4060/4208 (96%)	-0.47	97 (2%) 59 56	19, 33, 59, 106	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	6.1
1	D	735	HIS	6.0
1	B	689	GLU	5.9
1	D	689	GLU	5.6
1	A	733	ALA	5.5
1	A	689	GLU	5.4
1	B	731	PRO	5.3
1	A	799	THR	5.1
1	A	732	ALA	4.8
1	A	9	VAL	4.8
1	B	799	THR	4.7
1	B	733	ALA	4.7
1	B	12	GLN	4.7
1	B	1023	LYS	4.5
1	A	730	LEU	4.5
1	C	731	PRO	4.5
1	D	731	PRO	4.4
1	C	689	GLU	4.4
1	D	732	ALA	4.3
1	A	1023	LYS	4.2
1	C	686	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	731	PRO	4.1
1	D	730	LEU	4.1
1	C	1023	LYS	3.9
1	B	732	ALA	3.9
1	B	684	GLU	3.8
1	A	12	GLN	3.8
1	D	10	VAL	3.6
1	D	687	GLN	3.5
1	C	732	ALA	3.4
1	D	79	PRO	3.4
1	D	799	THR	3.4
1	C	580	GLU	3.4
1	A	684	GLU	3.3
1	A	686	PRO	3.2
1	A	580	GLU	3.2
1	D	733	ALA	3.1
1	D	729	THR	3.1
1	D	801	ILE	3.1
1	B	770	ILE	3.1
1	C	11	LEU	3.1
1	D	11	LEU	3.1
1	C	1022	GLN	3.1
1	C	733	ALA	3.1
1	D	684	GLU	3.1
1	D	772	ASP	3.0
1	D	580	GLU	3.0
1	D	12	GLN	3.0
1	D	179	ALA	3.0
1	B	735	HIS	2.9
1	C	9	VAL	2.9
1	B	80	GLU	2.9
1	C	12	GLN	2.8
1	B	686	PRO	2.8
1	A	687	GLN	2.8
1	A	595	THR	2.8
1	C	772	ASP	2.8
1	C	735	HIS	2.8
1	A	179	ALA	2.8
1	C	684	GLU	2.8
1	B	10	VAL	2.7
1	D	582	GLY	2.7
1	D	186	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	687	GLN	2.7
1	C	831	ALA	2.6
1	A	131	GLU	2.6
1	A	685	LEU	2.6
1	D	581	ASN	2.6
1	C	10	VAL	2.6
1	A	734	SER	2.6
1	D	131	GLU	2.6
1	D	1023	LYS	2.5
1	C	800	ARG	2.5
1	A	71	GLU	2.5
1	D	130	ASP	2.5
1	A	800	ARG	2.4
1	C	685	LEU	2.4
1	C	799	THR	2.4
1	B	730	LEU	2.4
1	D	686	PRO	2.4
1	C	730	LEU	2.4
1	A	11	LEU	2.3
1	C	581	ASN	2.3
1	B	685	LEU	2.3
1	B	831	ALA	2.3
1	B	186	VAL	2.3
1	B	772	ASP	2.2
1	B	9	VAL	2.2
1	A	80	GLU	2.2
1	A	729	THR	2.2
1	A	79	PRO	2.2
1	B	11	LEU	2.2
1	C	832	ASP	2.2
1	A	582	GLY	2.2
1	C	773	LYS	2.1
1	B	773	LYS	2.1
1	A	845	GLN	2.0

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

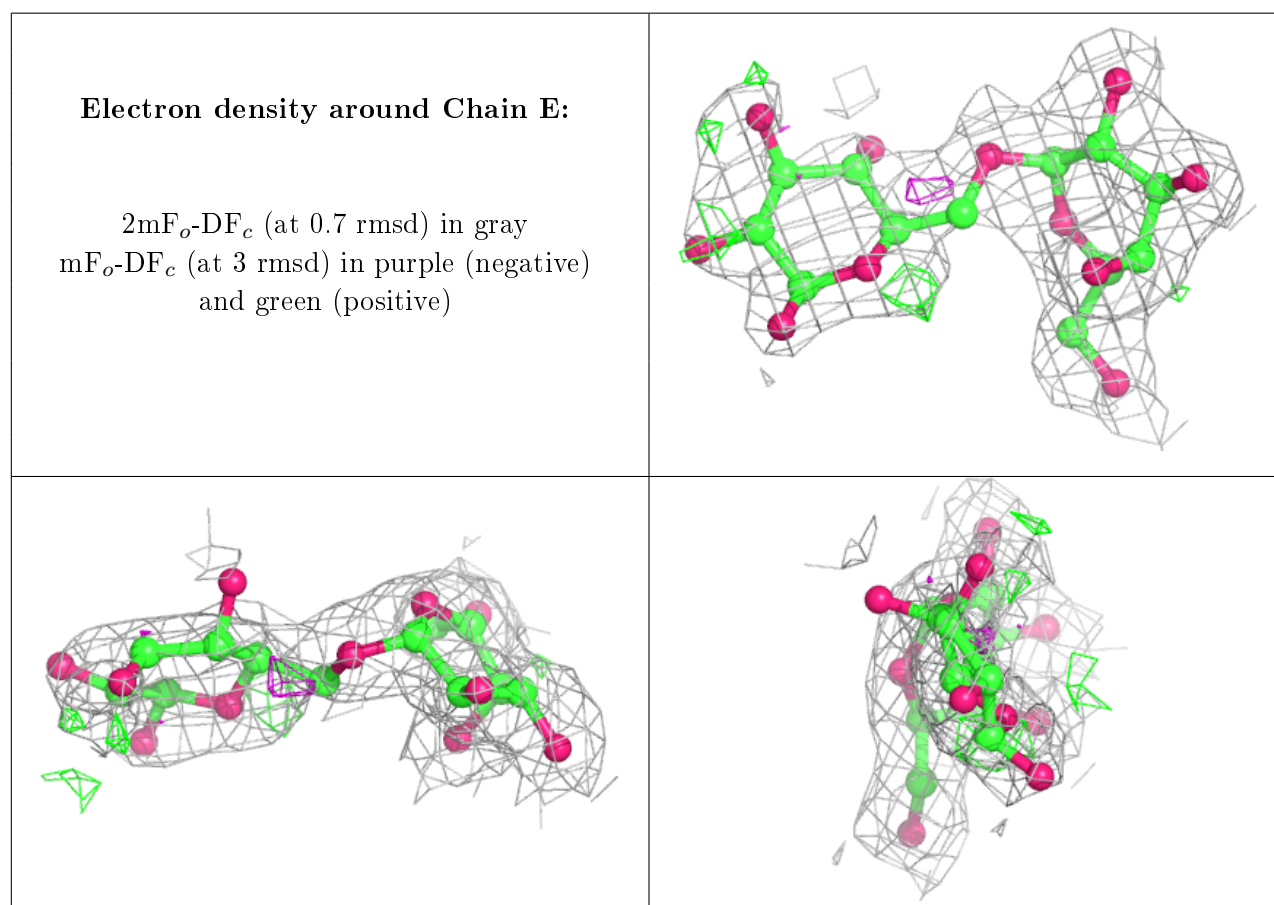
There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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.

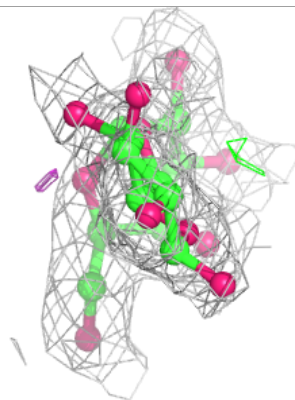
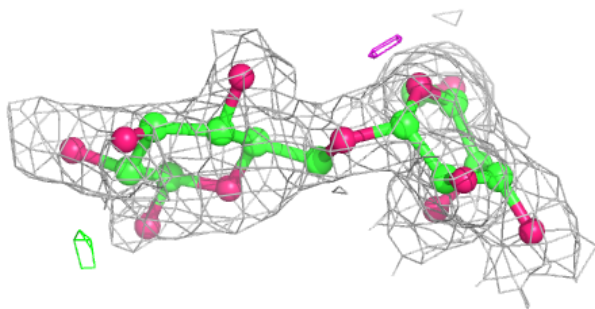
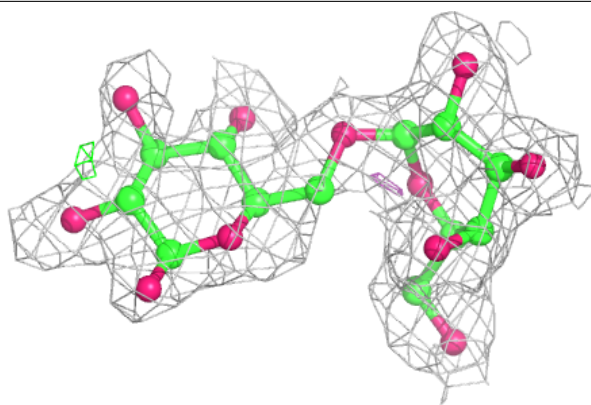
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BGC	H	1	12/12	0.79	0.19	45,66,69,70	0
2	BGC	E	1	12/12	0.81	0.19	45,71,75,78	0
2	BGC	G	1	12/12	0.82	0.19	41,63,67,68	0
2	BGC	F	1	12/12	0.87	0.16	40,57,64,69	0
2	GAL	E	2	11/12	0.94	0.13	30,39,43,44	0
2	GAL	H	2	11/12	0.95	0.11	30,34,41,42	0
2	GAL	F	2	11/12	0.96	0.11	25,32,37,38	0
2	GAL	G	2	11/12	0.97	0.11	25,29,34,35	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.

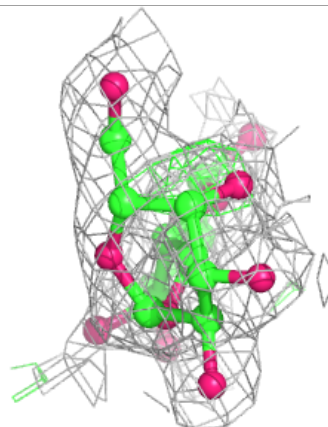
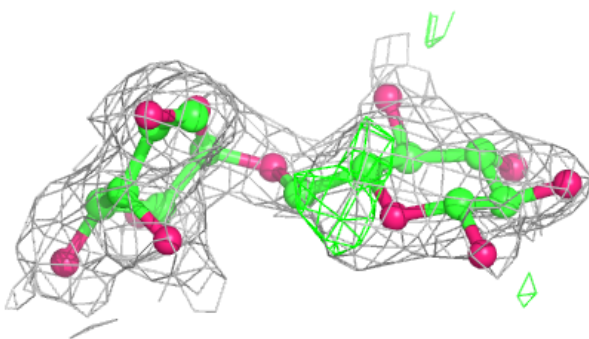
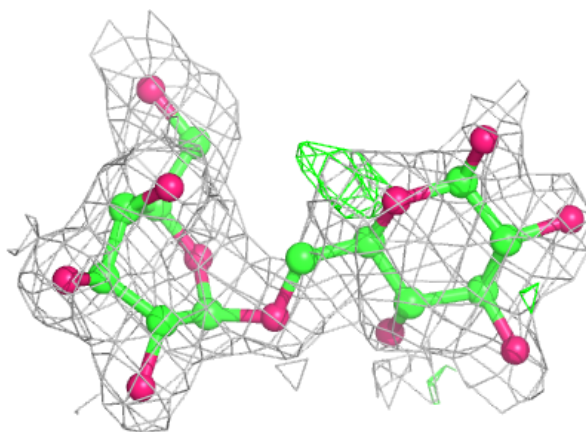


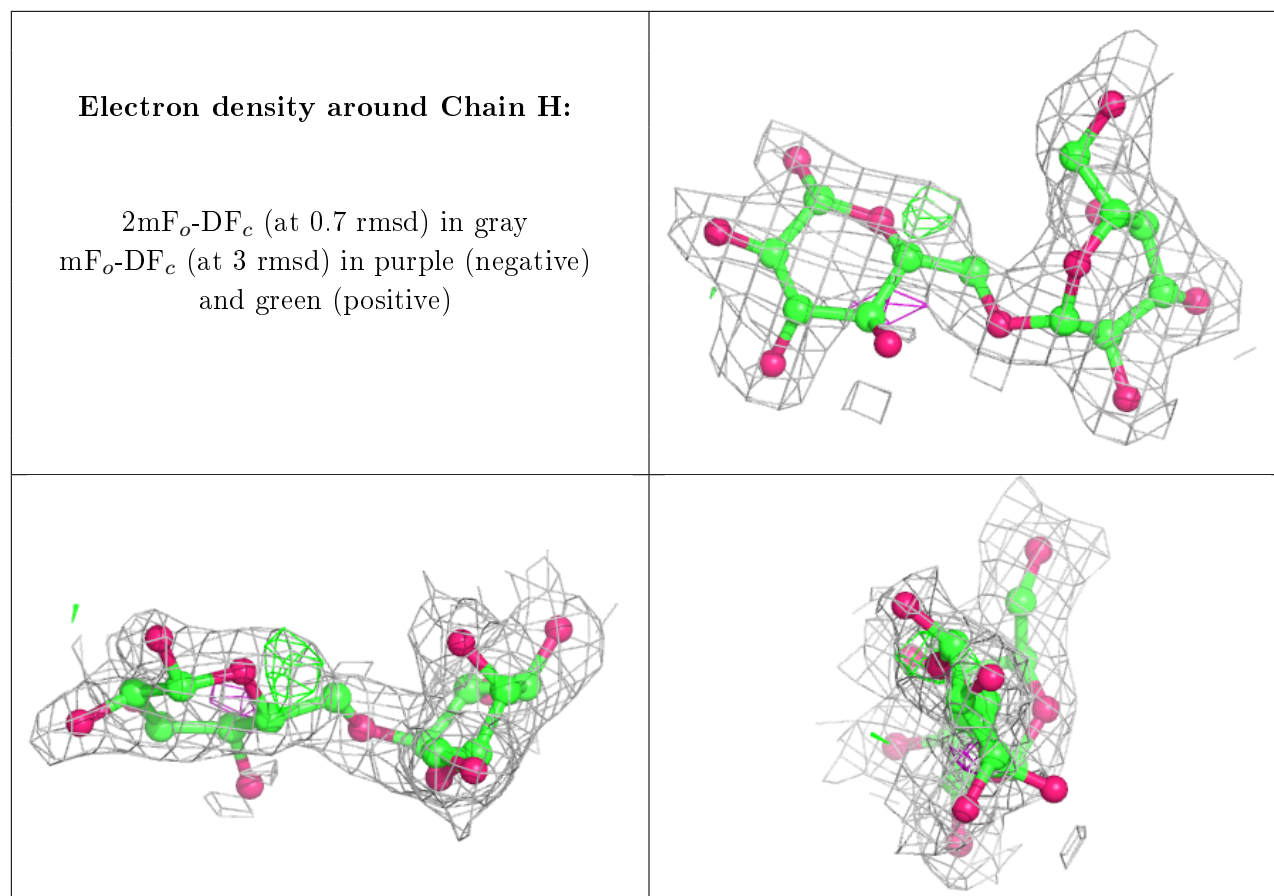
**Electron density around Chain F:**

$2mF_o - DF_c$  (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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	DMS	D	8013	4/4	0.73	0.28	72,74,78,79	0
5	DMS	A	8018	4/4	0.74	0.20	83,83,85,87	0
4	NA	B	3104	1/1	0.75	0.13	55,55,55,55	0
5	DMS	B	8008	4/4	0.82	0.25	74,74,76,76	0
4	NA	D	3104	1/1	0.82	0.14	58,58,58,58	0
5	DMS	A	8017	4/4	0.83	0.28	64,70,73,74	0
5	DMS	A	8013	4/4	0.84	0.20	75,78,79,84	0
4	NA	C	3104	1/1	0.84	0.12	47,47,47,47	0
4	NA	A	3103	1/1	0.85	0.11	49,49,49,49	0
5	DMS	B	8006	4/4	0.85	0.20	57,63,65,67	0
5	DMS	A	8011	4/4	0.85	0.19	78,79,79,81	0
5	DMS	D	8012	4/4	0.87	0.18	59,60,63,65	0
4	NA	B	3103	1/1	0.87	0.20	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	D	8007	4/4	0.88	0.17	69,70,70,71	0
5	DMS	A	8007	4/4	0.88	0.17	72,73,75,77	0
5	DMS	B	8015	4/4	0.88	0.18	81,81,82,83	0
5	DMS	A	8010	4/4	0.88	0.16	65,69,70,71	0
5	DMS	C	8014	4/4	0.88	0.20	81,82,82,83	0
3	MG	A	3006	1/1	0.88	0.07	67,67,67,67	0
5	DMS	B	8018	4/4	0.88	0.19	69,71,72,74	0
5	DMS	B	8023	4/4	0.89	0.13	72,73,74,75	0
5	DMS	D	8006	4/4	0.89	0.19	74,77,79,80	0
5	DMS	B	8019	4/4	0.89	0.20	68,71,71,71	0
5	DMS	D	8004	4/4	0.90	0.17	56,58,59,61	0
5	DMS	C	8004	4/4	0.90	0.20	57,61,62,63	0
5	DMS	B	8013	4/4	0.90	0.19	73,73,74,77	0
5	DMS	B	8011	4/4	0.90	0.27	58,61,64,65	0
4	NA	A	3104	1/1	0.91	0.14	50,50,50,50	0
5	DMS	C	8016	4/4	0.91	0.17	64,64,65,67	0
5	DMS	A	8014	4/4	0.91	0.19	70,72,74,74	0
5	DMS	C	8007	4/4	0.92	0.16	65,69,70,73	0
4	NA	D	3103	1/1	0.92	0.07	45,45,45,45	0
5	DMS	B	8007	4/4	0.92	0.14	47,49,55,57	0
5	DMS	C	8011	4/4	0.92	0.17	52,58,58,61	0
4	NA	A	3101	1/1	0.92	0.09	34,34,34,34	0
5	DMS	B	8016	4/4	0.93	0.15	62,64,65,70	0
5	DMS	A	8004	4/4	0.93	0.13	56,57,63,64	0
5	DMS	B	8004	4/4	0.93	0.16	43,44,49,52	0
5	DMS	D	8010	4/4	0.94	0.35	82,82,85,85	0
5	DMS	D	8015	4/4	0.94	0.24	69,71,71,71	0
5	DMS	A	8012	4/4	0.94	0.22	73,75,77,78	0
5	DMS	A	8009	4/4	0.94	0.16	56,61,63,64	0
5	DMS	A	8016	4/4	0.94	0.19	61,63,63,70	0
5	DMS	C	8006	4/4	0.94	0.13	53,56,56,57	0
3	MG	B	3006	1/1	0.94	0.20	56,56,56,56	0
5	DMS	D	8011	4/4	0.94	0.23	64,67,69,72	0
5	DMS	B	8020	4/4	0.94	0.18	71,72,72,72	0
5	DMS	B	8017	4/4	0.94	0.14	72,73,74,75	0
5	DMS	C	8010	4/4	0.94	0.16	53,55,57,60	0
5	DMS	D	8014	4/4	0.95	0.19	72,73,73,75	0
5	DMS	B	8012	4/4	0.95	0.24	73,74,74,76	0
4	NA	C	3103	1/1	0.95	0.13	43,43,43,43	0
5	DMS	A	8003	4/4	0.95	0.16	40,49,52,53	0
5	DMS	C	8013	4/4	0.95	0.15	67,69,69,72	0
5	DMS	C	8012	4/4	0.95	0.20	70,70,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	B	8014	4/4	0.95	0.22	68,69,71,71	0
5	DMS	C	8015	4/4	0.95	0.11	57,57,58,62	0
5	DMS	A	8006	4/4	0.95	0.16	68,69,70,72	0
5	DMS	A	8015	4/4	0.96	0.25	71,72,72,72	0
5	DMS	C	8017	4/4	0.96	0.14	65,66,66,69	0
5	DMS	C	8018	4/4	0.96	0.14	68,71,71,71	0
4	NA	B	3102	1/1	0.96	0.07	31,31,31,31	0
4	NA	C	3102	1/1	0.96	0.06	31,31,31,31	0
3	MG	A	3002	1/1	0.96	0.06	39,39,39,39	0
3	MG	B	3002	1/1	0.96	0.07	29,29,29,29	0
5	DMS	B	8021	4/4	0.96	0.13	41,42,43,46	0
3	MG	D	3001	1/1	0.96	0.06	32,32,32,32	0
5	DMS	C	8020	4/4	0.96	0.13	51,55,55,57	0
5	DMS	B	8024	4/4	0.97	0.10	60,60,61,62	0
5	DMS	B	8002	4/4	0.97	0.10	38,40,42,42	0
3	MG	D	3002	1/1	0.97	0.19	35,35,35,35	0
5	DMS	B	8010	4/4	0.97	0.18	51,52,53,55	0
5	DMS	D	8009	4/4	0.97	0.15	52,54,57,58	0
5	DMS	A	8008	4/4	0.97	0.14	56,59,60,60	0
4	NA	D	3102	1/1	0.97	0.06	33,33,33,33	0
5	DMS	C	8019	4/4	0.97	0.11	53,53,57,61	0
5	DMS	C	8002	4/4	0.97	0.10	31,34,40,42	0
5	DMS	D	8005	4/4	0.97	0.12	45,45,48,48	0
5	DMS	D	8002	4/4	0.97	0.13	33,33,36,44	0
4	NA	D	3101	1/1	0.97	0.08	32,32,32,32	0
5	DMS	B	8022	4/4	0.98	0.09	51,53,54,55	0
5	DMS	B	8009	4/4	0.98	0.14	49,53,55,55	0
5	DMS	B	8003	4/4	0.98	0.13	44,49,49,49	0
5	DMS	B	8005	4/4	0.98	0.16	44,48,51,53	0
5	DMS	D	8003	4/4	0.98	0.12	54,55,56,56	0
5	DMS	A	8001	4/4	0.98	0.11	33,35,38,39	0
5	DMS	C	8005	4/4	0.98	0.12	39,44,45,46	0
4	NA	C	3101	1/1	0.98	0.15	27,27,27,27	0
5	DMS	D	8008	4/4	0.98	0.10	56,59,60,61	0
5	DMS	D	8001	4/4	0.98	0.13	39,40,41,42	0
5	DMS	A	8002	4/4	0.98	0.08	43,44,45,47	0
3	MG	C	3002	1/1	0.98	0.04	25,25,25,25	0
5	DMS	A	8005	4/4	0.98	0.16	46,47,50,51	0
5	DMS	C	8001	4/4	0.98	0.12	33,36,37,40	0
5	DMS	C	8009	4/4	0.98	0.14	54,57,58,60	0
5	DMS	C	8008	4/4	0.98	0.10	39,39,41,42	0
4	NA	B	3101	1/1	0.98	0.07	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	C	8003	4/4	0.99	0.16	44,47,47,47	0
4	NA	A	3102	1/1	0.99	0.07	30,30,30,30	0
5	DMS	B	8001	4/4	0.99	0.15	37,38,39,41	0
3	MG	C	3001	1/1	0.99	0.04	22,22,22,22	0
3	MG	A	3001	1/1	0.99	0.04	30,30,30,30	0
3	MG	B	3001	1/1	0.99	0.09	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.