



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:28 AM UTC

PDB ID : 8ART / pdb_00008art
Title : ABC transporter binding protein MalE from *Streptomyces scabiei* in complex with maltose
Authors : Jadot, C.; Kerff, F.; Rigali, S.
Deposited on : 2022-08-17
Resolution : 3.17 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

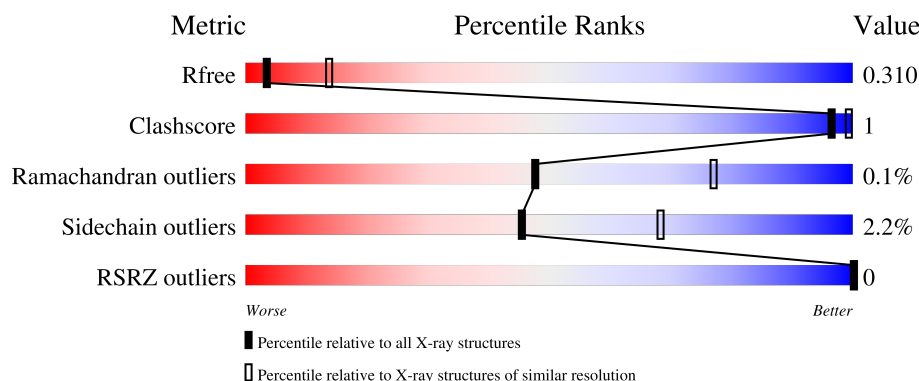
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

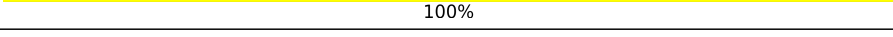
The reported resolution of this entry is 3.17 Å.

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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	429	 88% . 9%
1	B	429	 87% . 8%
2	C	2	 50% 50%
2	D	2	 100%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11866 atoms, of which 5873 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 Putative secreted maltose-binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	H	N	O	S	0	0	0
			5878	1899	2909	488	581	1			
1	B	393	Total	C	H	N	O	S	0	0	0
			5902	1905	2924	490	582	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	424	HIS	-	expression tag	UNP C9ZHD5
A	425	HIS	-	expression tag	UNP C9ZHD5
A	426	HIS	-	expression tag	UNP C9ZHD5
A	427	HIS	-	expression tag	UNP C9ZHD5
A	428	HIS	-	expression tag	UNP C9ZHD5
A	429	HIS	-	expression tag	UNP C9ZHD5
B	424	HIS	-	expression tag	UNP C9ZHD5
B	425	HIS	-	expression tag	UNP C9ZHD5
B	426	HIS	-	expression tag	UNP C9ZHD5
B	427	HIS	-	expression tag	UNP C9ZHD5
B	428	HIS	-	expression tag	UNP C9ZHD5
B	429	HIS	-	expression tag	UNP C9ZHD5

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	O	0	0	0
			43	12	20	11			
2	D	2	Total	C	H	O	0	0	0
			43	12	20	11			

i

- Molecule 1: Putative secreted maltose-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.31Å 68.31Å 260.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.89 – 3.17 48.89 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.89-3.17) 99.4 (48.89-3.17)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.260 , 0.284 0.285 , 0.310	Depositor DCC
R_{free} test set	631 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	126.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.078 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11866	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	0/3042	0.98	4/4137 (0.1%)
1	B	0.67	0/3052	0.97	1/4151 (0.0%)
All	All	0.67	0/6094	0.98	5/8288 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	TYR	CA-C-N	6.75	133.84	121.70
1	A	421	TYR	C-N-CA	6.75	133.84	121.70
1	A	282	LYS	N-CA-C	-6.54	104.23	111.36
1	B	282	LYS	N-CA-C	-6.53	104.24	111.36
1	A	420	ASP	CA-CB-CG	5.55	118.15	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2969	2909	2910	5	0
1	B	2978	2924	2924	7	0
2	C	23	20	21	0	0
2	D	23	20	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5993	5873	5876	12	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 1.

All (12) 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:36:LEU:HD13	1:B:93:ILE:HD11	1.83	0.60
1:B:93:ILE:HD13	1:B:326:PHE:CD1	2.39	0.57
1:A:346:LEU:HD13	1:A:370:LEU:HD11	1.89	0.53
1:A:421:TYR:HB2	1:A:422:SER:HA	1.92	0.51
1:B:150:ALA:HB2	1:B:369:VAL:HG21	1.94	0.49
1:A:150:ALA:HB2	1:A:369:VAL:HG21	1.94	0.49
1:B:346:LEU:HD13	1:B:370:LEU:HD11	1.95	0.48
1:B:346:LEU:HD11	1:B:366:TYR:HB3	1.99	0.44
1:A:217:ILE:CG1	1:A:421:TYR:CD2	3.01	0.43
1:B:226:LYS:NZ	1:B:296:THR:HG21	2.35	0.41
1:A:421:TYR:CB	1:A:422:SER:HA	2.50	0.41
1:B:252:HIS:N	1:B:252:HIS:ND1	2.68	0.41

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	388/429 (90%)	375 (97%)	13 (3%)	0	100	100
1	B	391/429 (91%)	377 (96%)	13 (3%)	1 (0%)	36	66
All	All	779/858 (91%)	752 (96%)	26 (3%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	422	SER

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	301/325 (93%)	295 (98%)	6 (2%)	48	69
1	B	302/325 (93%)	295 (98%)	7 (2%)	44	68
All	All	603/650 (93%)	590 (98%)	13 (2%)	45	68

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	165	GLU
1	A	252	HIS
1	A	412	THR
1	A	418	VAL
1	A	420	ASP
1	B	165	GLU
1	B	208	ASP
1	B	226	LYS
1	B	252	HIS
1	B	308	ASN
1	B	412	THR
1	B	418	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	71	ASN
1	A	76	GLN
1	A	132	GLN
1	A	194	GLN
1	A	220	ASN

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Mol	Chain	Res	Type
1	A	259	ASN
1	B	71	ASN
1	B	76	GLN
1	B	126	GLN
1	B	132	GLN
1	B	194	GLN
1	B	220	ASN
1	B	259	ASN
1	B	367	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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	C	1	2	12,12,12	0.25	0	17,17,17	0.61	0
2	GLC	C	2	2	11,11,12	0.26	0	15,15,17	0.72	1 (6%)
2	GLC	D	1	2	12,12,12	0.21	0	17,17,17	0.95	1 (5%)
2	GLC	D	2	2	11,11,12	0.23	0	15,15,17	0.70	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	C	1	2	-	1/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	1/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	2	GLC	C1-O5-C5	2.36	115.34	112.19
2	D	1	GLC	C1-O5-C5	2.24	117.98	113.65
2	D	2	GLC	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

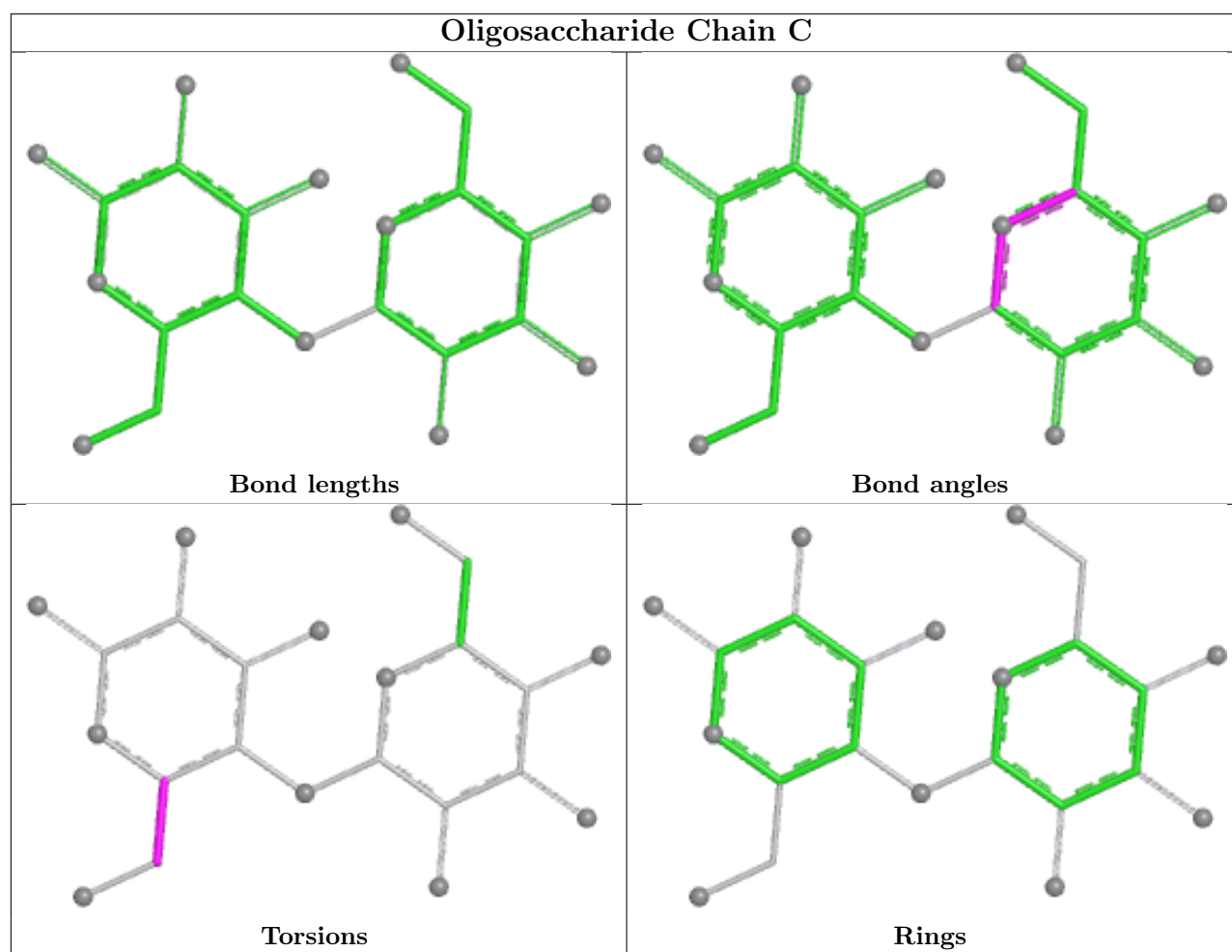
All (2) torsion outliers are listed below:

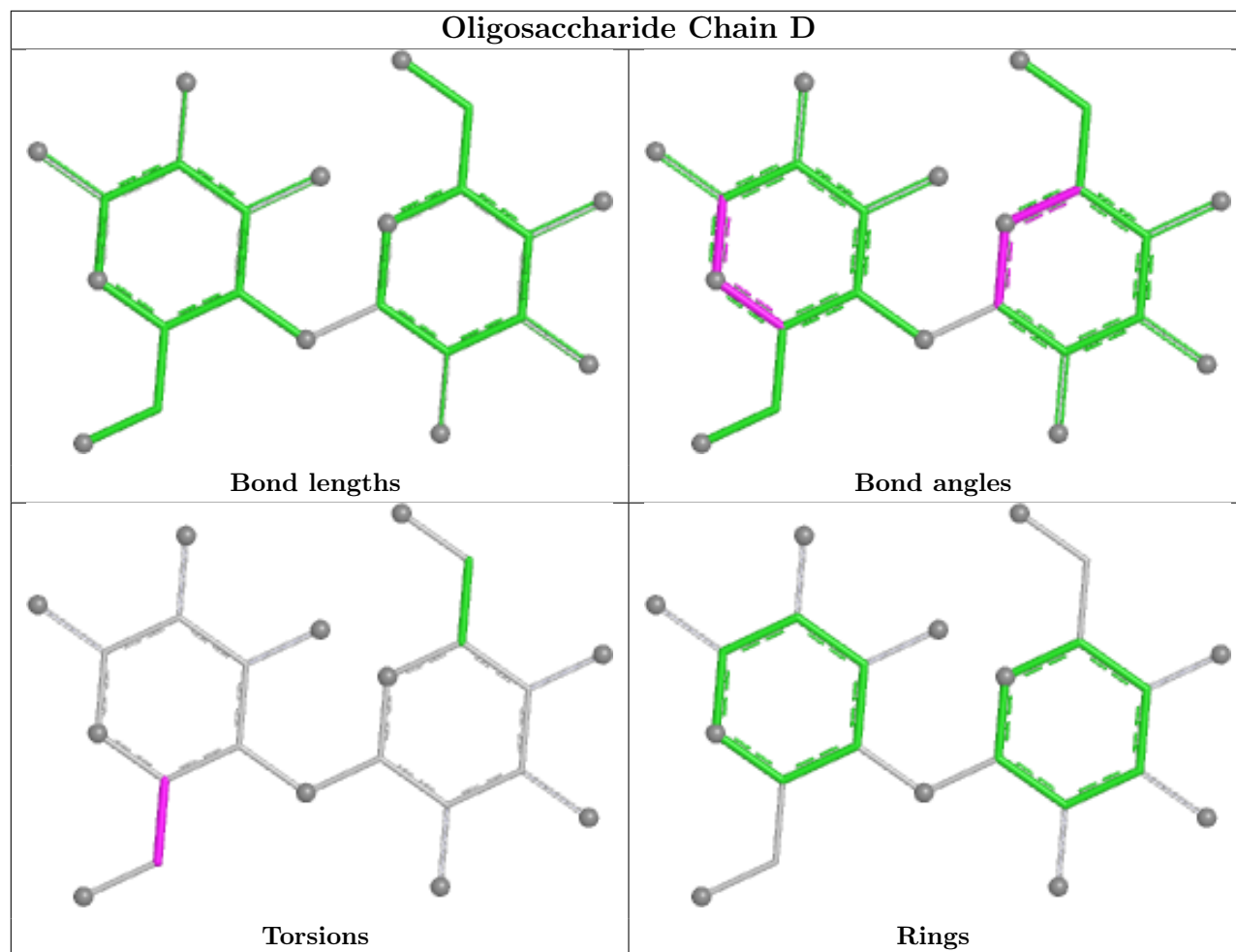
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	O5-C5-C6-O6
2	C	1	GLC	O5-C5-C6-O6

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](#)

There are no ligands in this entry.

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	392/429 (91%)	-0.76	0 100 100	46, 122, 137, 146	0
1	B	393/429 (91%)	-0.66	0 100 100	87, 128, 142, 147	0
All	All	785/858 (91%)	-0.71	0 100 100	46, 126, 140, 147	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

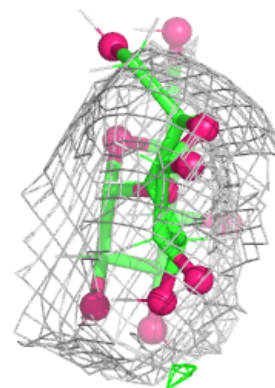
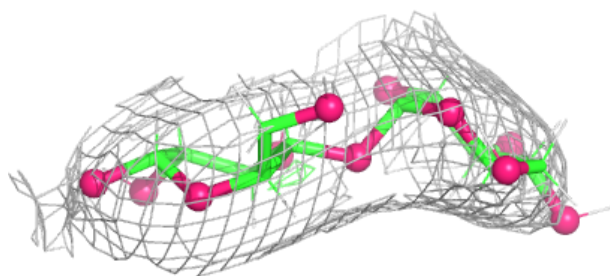
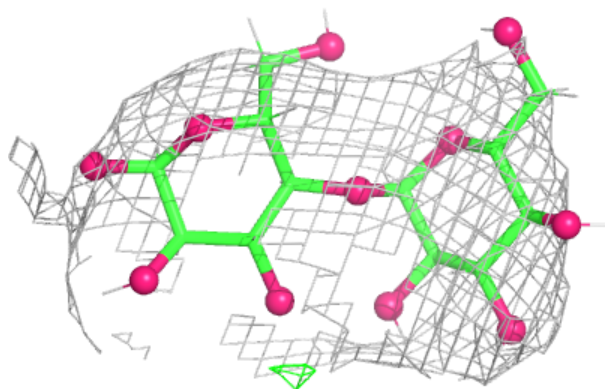
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	C	1	12/12	0.76	0.07	106,111,114,115	0
2	GLC	C	2	11/12	0.83	0.08	96,99,103,104	0
2	GLC	D	1	12/12	0.88	0.06	86,88,95,100	0
2	GLC	D	2	11/12	0.92	0.05	80,84,86,87	0

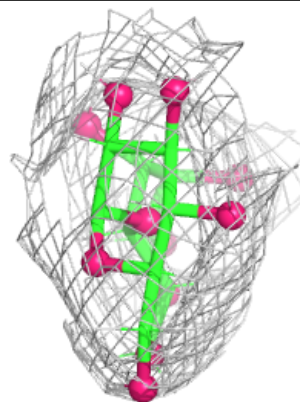
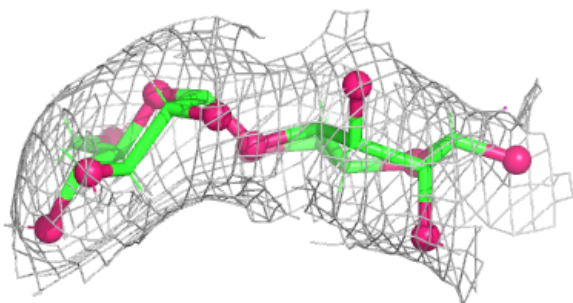
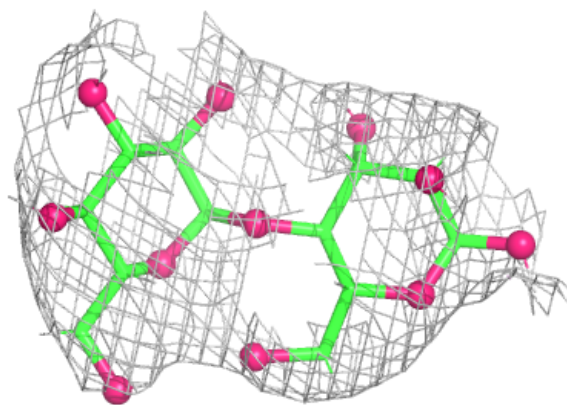
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.