



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:19 AM UTC

PDB ID : 5B0R / pdb_00005b0r
Title : Beta-1,2-Mannobiose phosphorylase from *Listeria innocua* - beta-1,2-mannobiose complex
Authors : Tsuda, T.; Arakawa, T.; Fushinobu, S.
Deposited on : 2015-11-02
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

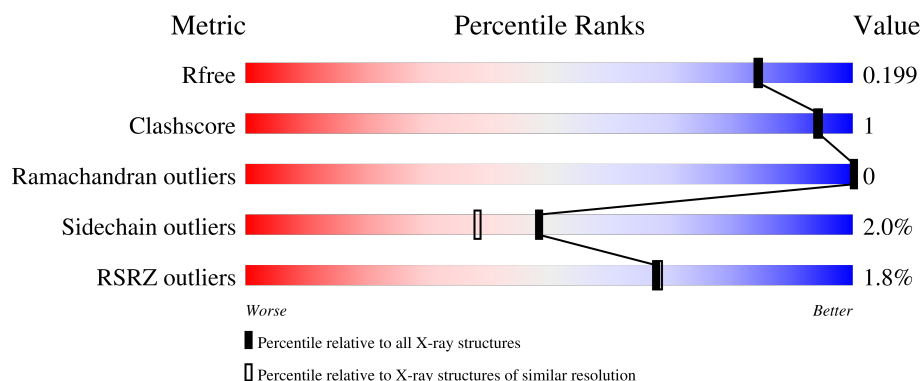
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	363	2% 81% 15% ..
1	B	363	2% 83% 13% ..
2	C	3	100%
2	D	3	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6311 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.

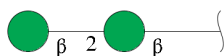
- Molecule 1 is a protein called Lin0857 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	1	0
			2816	1803	461	543	9			
1	B	353	Total	C	N	O	S	0	1	0
			2816	1803	461	543	9			

There are 16 discrepancies between the modelled and reference sequences:

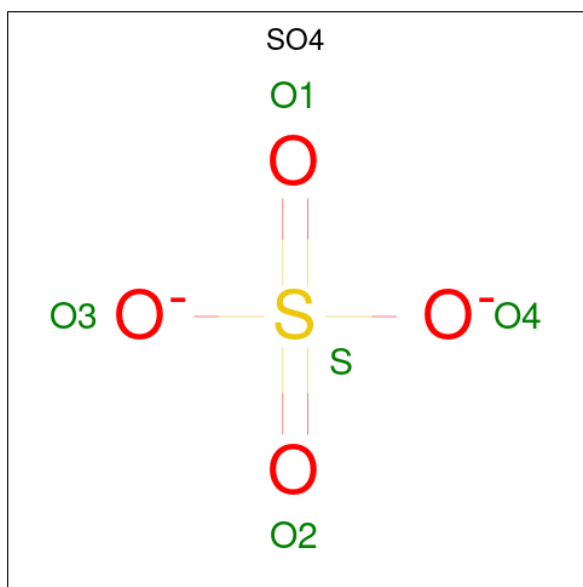
Chain	Residue	Modelled	Actual	Comment	Reference
A	356	LEU	-	expression tag	UNP Q92DF6
A	357	GLU	-	expression tag	UNP Q92DF6
A	358	HIS	-	expression tag	UNP Q92DF6
A	359	HIS	-	expression tag	UNP Q92DF6
A	360	HIS	-	expression tag	UNP Q92DF6
A	361	HIS	-	expression tag	UNP Q92DF6
A	362	HIS	-	expression tag	UNP Q92DF6
A	363	HIS	-	expression tag	UNP Q92DF6
B	356	LEU	-	expression tag	UNP Q92DF6
B	357	GLU	-	expression tag	UNP Q92DF6
B	358	HIS	-	expression tag	UNP Q92DF6
B	359	HIS	-	expression tag	UNP Q92DF6
B	360	HIS	-	expression tag	UNP Q92DF6
B	361	HIS	-	expression tag	UNP Q92DF6
B	362	HIS	-	expression tag	UNP Q92DF6
B	363	HIS	-	expression tag	UNP Q92DF6

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-2)-beta-D-mannopyranose.



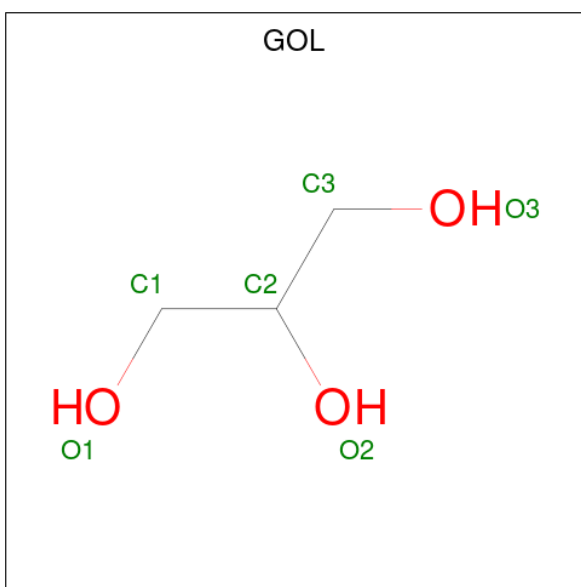
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	2	Total	C	O	0	1	0
			35	18	17			
2	D	2	Total	C	O	0	1	0
			35	18	17			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



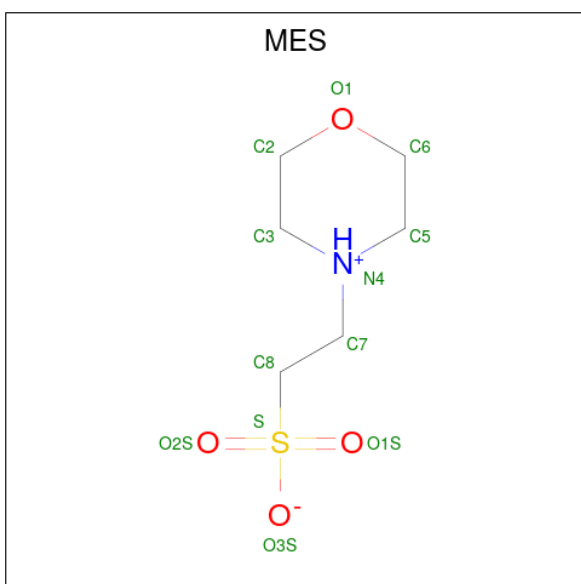
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

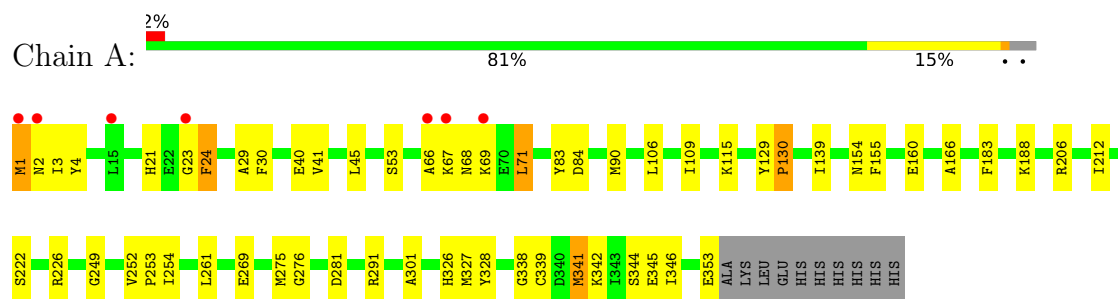
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	281	Total	O	0	0
			281	281		
6	B	240	Total	O	0	0
			240	240		

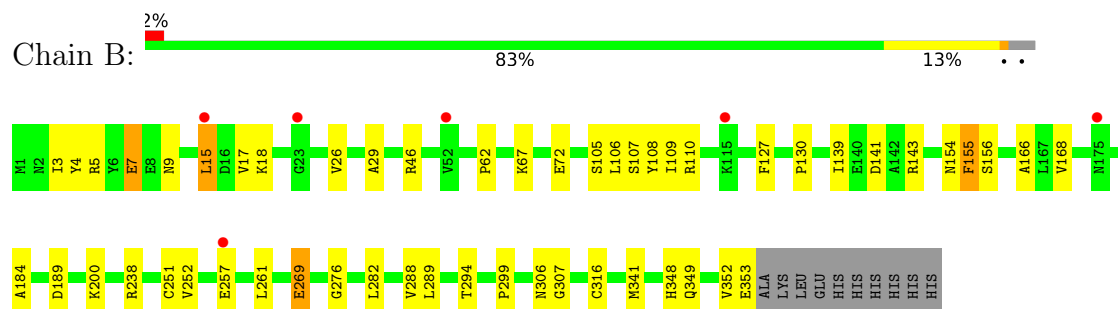
3 Residue-property plots [i](#)

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.

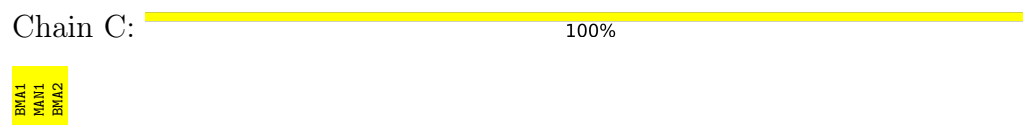
- Molecule 1: Lin0857 protein



- Molecule 1: Lin0857 protein



- Molecule 2: beta-D-mannopyranose-(1-2)-beta-D-mannopyranose



- Molecule 2: beta-D-mannopyranose-(1-2)-beta-D-mannopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.77 Å 145.77 Å 105.77 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.93 – 1.80 32.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.93-1.80) 99.8 (32.93-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.09 (at 1.81 Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.165 , 0.193 (Not available) , 0.199	Depositor DCC
R_{free} test set	5996 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6311	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: BMA, GOL, SO4, MAN, MES

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	1.80	37/2887 (1.3%)	1.45	14/3915 (0.4%)
1	B	1.80	41/2887 (1.4%)	1.41	9/3915 (0.2%)
All	All	1.80	78/5774 (1.4%)	1.43	23/7830 (0.3%)

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	MET	SD-CE	-10.45	1.53	1.79
1	A	67	LYS	N-CA	8.67	1.57	1.46
1	A	291	ARG	CA-C	-8.66	1.41	1.52
1	A	2	ASN	CG-OD1	7.98	1.38	1.23
1	A	66	ALA	CA-C	7.58	1.63	1.52
1	A	2	ASN	CA-C	7.46	1.61	1.52
1	A	326	HIS	CA-C	7.20	1.61	1.52
1	B	15	LEU	N-CA	7.16	1.55	1.46
1	A	2	ASN	N-CA	-7.13	1.37	1.46
1	A	41	VAL	CA-CB	-7.12	1.45	1.54
1	A	40	GLU	CA-C	7.07	1.61	1.52
1	B	257	GLU	CA-C	-7.02	1.42	1.52
1	B	282	LEU	CA-C	-6.98	1.43	1.52
1	A	23	GLY	C-O	6.93	1.33	1.23
1	A	327	MET	N-CA	6.82	1.54	1.46
1	B	26	VAL	CA-C	-6.68	1.45	1.52
1	A	328	TYR	CA-C	6.66	1.60	1.52
1	B	4	TYR	CA-C	6.66	1.61	1.52
1	B	200	LYS	N-CA	6.64	1.54	1.45
1	B	107	SER	CA-C	-6.61	1.45	1.52
1	B	156	SER	N-CA	6.59	1.54	1.46
1	A	41	VAL	N-CA	6.50	1.54	1.46
1	A	261	LEU	CA-C	6.46	1.60	1.52
1	B	288	VAL	CA-CB	-6.38	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	GLY	CA-C	6.27	1.57	1.52
1	A	29	ALA	N-CA	-6.25	1.39	1.46
1	B	72	GLU	CA-C	-6.22	1.46	1.53
1	B	7	GLU	CA-C	6.18	1.61	1.52
1	B	109	ILE	CA-CB	-6.18	1.47	1.54
1	A	249	GLY	CA-C	-6.14	1.46	1.52
1	B	141	ASP	CA-C	-6.13	1.46	1.53
1	B	155	PHE	N-CA	-6.09	1.38	1.46
1	B	46	ARG	N-CA	6.07	1.53	1.46
1	A	276	GLY	CA-C	-5.95	1.46	1.52
1	B	349	GLN	N-CA	-5.94	1.39	1.46
1	B	261	LEU	N-CA	-5.93	1.38	1.46
1	B	289	LEU	N-CA	5.91	1.53	1.46
1	A	3	ILE	C-O	-5.90	1.17	1.24
1	A	345	GLU	N-CA	-5.87	1.39	1.46
1	B	184	ALA	CA-C	-5.84	1.46	1.53
1	B	261	LEU	CA-C	5.78	1.59	1.52
1	A	84	ASP	N-CA	-5.75	1.39	1.46
1	B	62	PRO	N-CA	-5.69	1.40	1.47
1	B	156	SER	CA-CB	-5.69	1.44	1.53
1	A	212	ILE	N-CA	5.58	1.52	1.46
1	A	222	SER	CA-C	5.57	1.58	1.52
1	B	143	ARG	C-O	-5.57	1.17	1.23
1	B	110	ARG	N-CA	5.55	1.53	1.46
1	B	294	THR	CA-CB	5.43	1.61	1.54
1	B	316	CYS	C-O	-5.43	1.16	1.24
1	B	5	ARG	N-CA	5.41	1.53	1.46
1	B	294	THR	C-O	-5.38	1.19	1.24
1	A	344	SER	CA-CB	5.35	1.61	1.53
1	A	222	SER	CA-CB	-5.30	1.46	1.54
1	A	83	TYR	C-O	5.29	1.30	1.23
1	B	168	VAL	N-CA	5.28	1.52	1.46
1	B	252	VAL	CA-C	5.28	1.58	1.52
1	B	348	HIS	CA-C	-5.28	1.46	1.52
1	A	188	LYS	CA-C	5.25	1.59	1.53
1	A	301	ALA	CA-C	-5.22	1.46	1.53
1	A	183	PHE	CA-C	5.21	1.58	1.52
1	A	252	VAL	CA-C	5.21	1.58	1.52
1	B	307	GLY	CA-C	5.19	1.58	1.52
1	A	90	MET	SD-CE	-5.18	1.66	1.79
1	B	29	ALA	N-CA	-5.17	1.40	1.46
1	A	254	ILE	N-CA	5.16	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	30	PHE	CA-C	-5.13	1.46	1.52
1	B	127	PHE	N-CA	-5.12	1.39	1.46
1	B	238	ARG	CA-CB	-5.11	1.47	1.53
1	B	105	SER	CA-C	-5.11	1.46	1.52
1	B	108	TYR	CA-C	5.10	1.58	1.52
1	B	189	ASP	N-CA	5.10	1.54	1.46
1	B	67	LYS	N-CA	5.08	1.52	1.46
1	A	24	PHE	N-CA	5.06	1.52	1.45
1	A	281	ASP	N-CA	5.04	1.52	1.46
1	B	306	ASN	N-CA	5.02	1.52	1.46
1	B	299	PRO	N-CA	5.02	1.52	1.47
1	A	160	GLU	CD-OE2	5.01	1.34	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	MET	CG-SD-CE	-8.26	82.72	100.90
1	B	353	GLU	CA-C-O	-7.91	107.36	120.80
1	A	67	LYS	N-CA-C	7.79	119.86	111.36
1	A	353	GLU	CA-C-O	-7.71	107.69	120.80
1	B	352	VAL	N-CA-C	7.34	117.47	110.42
1	A	3	ILE	N-CA-CB	-6.94	102.71	111.46
1	A	275	MET	CA-C-N	6.73	128.16	122.17
1	A	275	MET	C-N-CA	6.73	128.16	122.17
1	A	226	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	B	282	LEU	N-CA-C	6.11	117.94	111.28
1	B	110	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	A	2	ASN	CA-C-O	5.66	126.47	120.36
1	B	251	CYS	N-CA-C	5.55	118.04	110.55
1	A	342	LYS	N-CA-C	5.48	117.89	109.07
1	A	222	SER	O-C-N	5.46	125.67	121.85
1	A	206	ARG	O-C-N	5.35	127.47	121.32
1	A	2	ASN	CB-CG-ND2	-5.35	108.38	116.40
1	B	276	GLY	O-C-N	-5.32	118.97	123.59
1	A	1	MET	CB-CA-C	-5.25	100.12	110.10
1	B	9	ASN	CA-C-O	5.23	125.09	120.02
1	A	276	GLY	O-C-N	-5.19	119.95	123.95
1	B	269	GLU	CB-CG-CD	5.13	121.33	112.60
1	B	17	VAL	CB-CA-C	-5.05	103.60	110.42

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	2816	0	2731	11	0
1	B	2816	0	2731	4	0
2	C	35	0	32	0	0
2	D	35	0	32	0	0
3	A	15	0	0	0	0
3	B	25	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	0	0
5	A	12	0	13	0	0
5	B	12	0	13	0	0
6	A	281	0	0	2	0
6	B	240	0	0	0	0
All	All	6311	0	5584	15	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 (15) 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:269:GLU:HG3	6:A:629:HOH:O	1.97	0.63
1:B:3:ILE:HD12	1:B:341:MET:HE2	1.86	0.57
1:A:21:HIS:CD2	1:A:71:LEU:HD22	2.51	0.46
1:B:269:GLU:H	1:B:269:GLU:CD	2.25	0.45
1:B:139:ILE:HG23	1:B:155:PHE:CD1	2.54	0.42
1:A:154:ASN:HA	1:A:166:ALA:O	2.20	0.42
1:A:4:TYR:O	1:A:339:CYS:HA	2.20	0.42
1:A:341:MET:HE3	1:A:346:ILE:HD11	2.01	0.42
1:A:68:ASN:O	1:A:69:LYS:C	2.63	0.41
1:B:154:ASN:HA	1:B:166:ALA:O	2.20	0.41
1:A:24:PHE:CZ	1:A:71:LEU:HD23	2.55	0.41
1:A:139:ILE:HG23	1:A:155:PHE:CD1	2.56	0.41
1:A:129:TYR:O	1:A:130:PRO:C	2.63	0.41
1:A:45:LEU:O	1:A:109:ILE:HA	2.20	0.40
1:A:269:GLU:CG	6:A:629:HOH:O	2.64	0.40

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	352/363 (97%)	338 (96%)	14 (4%)	0	100	100
1	B	352/363 (97%)	339 (96%)	13 (4%)	0	100	100
All	All	704/726 (97%)	677 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/311 (97%)	296 (98%)	7 (2%)	44	33
1	B	303/311 (97%)	298 (98%)	5 (2%)	53	45
All	All	606/622 (97%)	594 (98%)	12 (2%)	48	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	53	SER
1	A	71	LEU
1	A	106	LEU
1	A	115	LYS

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Mol	Chain	Res	Type
1	A	130	PRO
1	A	253	PRO
1	B	7	GLU
1	B	15	LEU
1	B	18	LYS
1	B	106	LEU
1	B	130	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	214	ASN
1	A	320	GLN
1	A	348	HIS
1	B	214	ASN
1	B	306	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	BMA	C	1[A]	2	12,12,12	1.01	1 (8%)	17,17,17	2.18	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	C	1[B]	2	12,12,12	1.15	2 (16%)	17,17,17	1.37	2 (11%)
2	BMA	C	2	2	11,11,12	1.36	2 (18%)	15,15,17	1.88	3 (20%)
2	BMA	D	1[A]	2	12,12,12	0.73	0	17,17,17	2.78	6 (35%)
2	MAN	D	1[B]	2	12,12,12	1.00	1 (8%)	17,17,17	1.43	2 (11%)
2	BMA	D	2	2	11,11,12	1.56	3 (27%)	15,15,17	1.69	6 (40%)

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	BMA	C	1[A]	2	-	0/2/22/22	0/1/1/1
2	MAN	C	1[B]	2	-	0/2/22/22	0/1/1/1
2	BMA	C	2	2	-	0/2/19/22	1/1/1/1
2	BMA	D	1[A]	2	-	0/2/22/22	0/1/1/1
2	MAN	D	1[B]	2	-	0/2/22/22	0/1/1/1
2	BMA	D	2	2	-	0/2/19/22	1/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	BMA	O5-C1	-2.78	1.39	1.43
2	C	1[A]	BMA	O4-C4	2.71	1.49	1.43
2	C	1[B]	MAN	O4-C4	2.71	1.49	1.43
2	C	2	BMA	O5-C5	2.64	1.48	1.43
2	D	1[B]	MAN	O1-C1	2.54	1.47	1.39
2	C	1[B]	MAN	O1-C1	2.38	1.47	1.39
2	D	2	BMA	O4-C4	2.25	1.48	1.43
2	C	2	BMA	C2-C3	2.18	1.55	1.52
2	D	2	BMA	O2-C2	-2.11	1.38	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1[A]	BMA	O1-C1-O5	-6.06	92.40	110.41
2	C	2	BMA	C1-O5-C5	5.17	119.11	112.19
2	D	1[A]	BMA	C1-O5-C5	-4.81	104.35	113.65
2	D	1[A]	BMA	C1-C2-C3	-4.74	100.69	110.36
2	D	1[A]	BMA	O5-C1-C2	3.90	117.16	110.30
2	C	1[A]	BMA	C1-O5-C5	-3.79	106.32	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1[A]	BMA	O1-C1-O5	-3.69	99.46	110.41
2	D	1[A]	BMA	O2-C2-C1	3.59	117.52	109.25
2	D	2	BMA	C1-O5-C5	3.33	116.65	112.19
2	C	1[A]	BMA	O5-C1-C2	3.24	116.00	110.30
2	C	1[A]	BMA	C3-C4-C5	3.00	115.68	110.23
2	D	1[A]	BMA	C3-C4-C5	3.00	115.67	110.23
2	C	2	BMA	C2-C3-C4	2.96	116.06	110.86
2	C	1[A]	BMA	O2-C2-C1	2.85	115.83	109.25
2	D	1[B]	MAN	O1-C1-O5	2.81	118.75	110.41
2	C	1[A]	BMA	C1-C2-C3	-2.72	104.80	110.36
2	C	1[B]	MAN	C3-C4-C5	2.70	115.13	110.23
2	D	1[B]	MAN	C3-C4-C5	2.65	115.04	110.23
2	C	1[B]	MAN	O2-C2-C3	-2.58	104.30	110.38
2	D	2	BMA	O3-C3-C2	2.41	114.98	110.05
2	D	2	BMA	O2-C2-C3	2.35	115.02	110.15
2	C	1[A]	BMA	O2-C2-C3	-2.28	105.01	110.38
2	D	2	BMA	O3-C3-C4	2.26	115.70	110.38
2	C	2	BMA	O2-C2-C3	2.25	114.81	110.15
2	D	2	BMA	O2-C2-C1	2.24	114.35	109.22
2	D	2	BMA	C3-C4-C5	2.12	114.08	110.23

There are no chirality outliers.

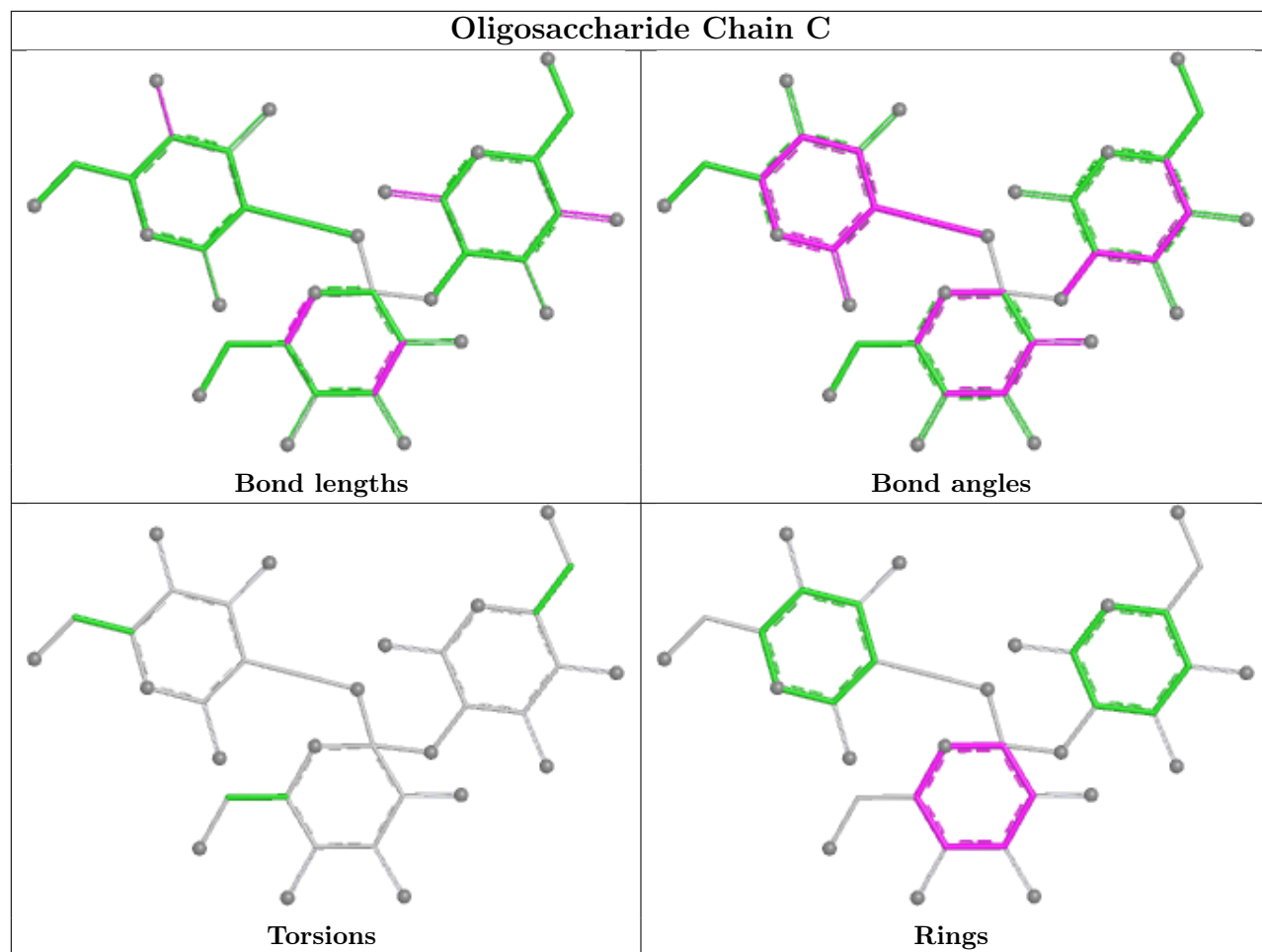
There are no torsion outliers.

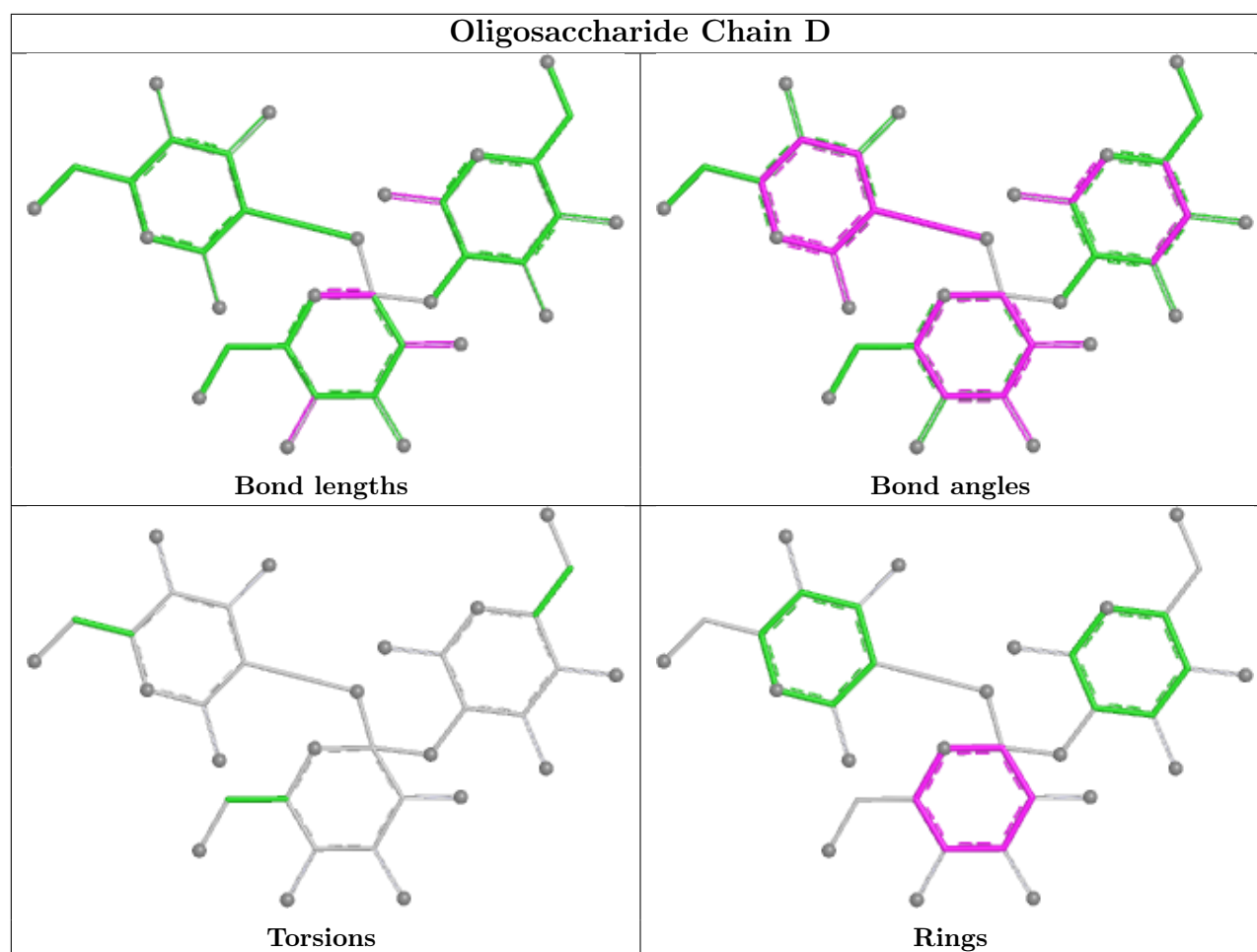
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	BMA	C1-C2-C3-C4-C5-O5
2	C	2	BMA	C1-C2-C3-C4-C5-O5

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](#)

14 ligands 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	$\# Z > 2$
3	SO4	A	504	-	4,4,4	0.56	0	6,6,6	0.57	0
3	SO4	B	508	-	4,4,4	1.55	1 (25%)	6,6,6	1.19	1 (16%)
4	GOL	B	509	-	5,5,5	0.63	0	5,5,5	1.24	0
5	MES	B	511	-	12,12,12	1.77	2 (16%)	15,16,16	1.78	4 (26%)
3	SO4	A	506	-	4,4,4	1.07	0	6,6,6	1.44	1 (16%)
3	SO4	B	507	-	4,4,4	0.60	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	505	-	4,4,4	0.66	0	6,6,6	0.95	0
4	GOL	B	510	-	5,5,5	0.55	0	5,5,5	1.27	1 (20%)
3	SO4	A	505	-	4,4,4	1.11	0	6,6,6	0.69	0
3	SO4	B	504	-	4,4,4	0.54	0	6,6,6	0.83	0
4	GOL	A	508	-	5,5,5	0.59	0	5,5,5	0.83	0
4	GOL	A	507	-	5,5,5	1.10	0	5,5,5	1.29	0
5	MES	A	509	-	12,12,12	1.66	3 (25%)	15,16,16	2.65	5 (33%)
3	SO4	B	506	-	4,4,4	0.96	0	6,6,6	1.34	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	GOL	B	509	-	-	0/4/4/4	-
5	MES	B	511	-	-	0/6/14/14	0/1/1/1
4	GOL	B	510	-	-	4/4/4/4	-
4	GOL	A	508	-	-	2/4/4/4	-
4	GOL	A	507	-	-	4/4/4/4	-
5	MES	A	509	-	-	0/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	511	MES	C8-S	-4.61	1.71	1.77
5	A	509	MES	C8-S	-4.29	1.71	1.77
3	B	508	SO4	O1-S	2.44	1.59	1.44
5	A	509	MES	C3-N4	2.16	1.52	1.46
5	A	509	MES	O2S-S	2.14	1.51	1.45
5	B	511	MES	O1S-S	2.09	1.51	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	509	MES	O2S-S-C8	7.39	117.90	106.73
5	B	511	MES	O2S-S-C8	3.66	112.27	106.73
5	A	509	MES	C2-C3-N4	-3.54	104.75	110.12
5	A	509	MES	O3S-S-O1S	3.42	119.97	111.40
5	B	511	MES	O3S-S-O1S	3.38	119.86	111.40
5	A	509	MES	O3S-S-O2S	-3.25	103.28	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	511	MES	O2S-S-O1S	-3.14	103.62	113.82
3	B	508	SO4	O3-S-O2	2.46	122.44	109.56
3	A	506	SO4	O3-S-O2	2.44	122.29	109.56
4	B	510	GOL	O1-C1-C2	-2.30	100.02	110.38
5	A	509	MES	O2S-S-O1S	-2.23	106.57	113.82
5	B	511	MES	O3S-S-C8	-2.05	102.00	106.00

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	507	GOL	O1-C1-C2-C3
4	A	507	GOL	C1-C2-C3-O3
4	A	507	GOL	O1-C1-C2-O2
4	A	507	GOL	O2-C2-C3-O3
4	B	510	GOL	O1-C1-C2-O2
4	A	508	GOL	O1-C1-C2-C3
4	B	510	GOL	O1-C1-C2-C3
4	B	510	GOL	C1-C2-C3-O3
4	A	508	GOL	O1-C1-C2-O2
4	B	510	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	353/363 (97%)	-0.11	7 (1%) 65 65	18, 26, 42, 59	1 (0%)
1	B	353/363 (97%)	0.06	6 (1%) 69 69	19, 28, 46, 75	1 (0%)
All	All	706/726 (97%)	-0.02	13 (1%) 67 68	18, 27, 43, 75	2 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ASN	3.7
1	B	23	GLY	3.2
1	B	15	LEU	3.0
1	A	67	LYS	2.8
1	A	23	GLY	2.7
1	A	15	LEU	2.7
1	B	175	ASN	2.4
1	A	69	LYS	2.3
1	B	115	LYS	2.2
1	B	52	VAL	2.1
1	B	257	GLU	2.1
1	A	66	ALA	2.0
1	A	1	MET	2.0

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

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

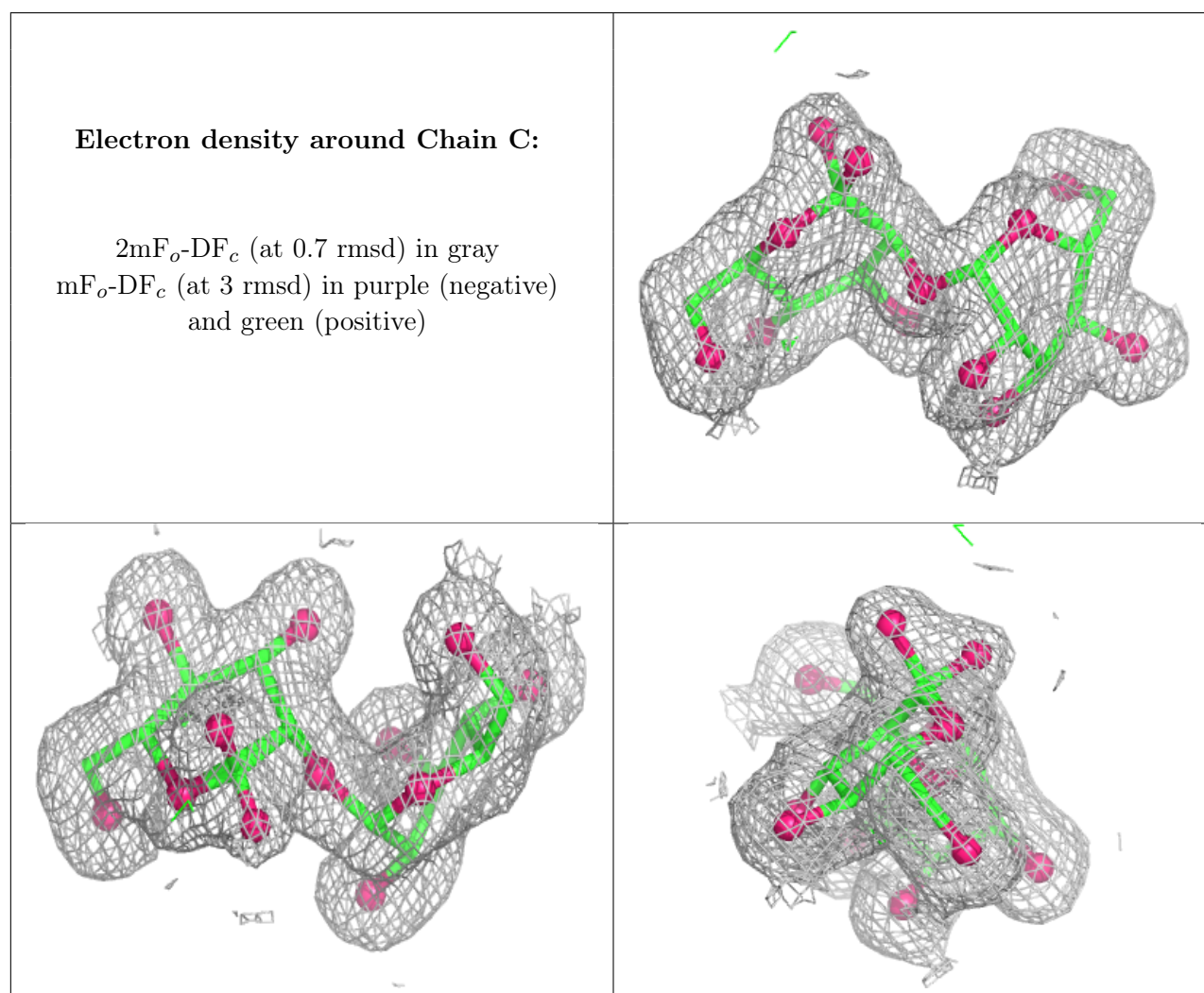
6.3 Carbohydrates [i](#)

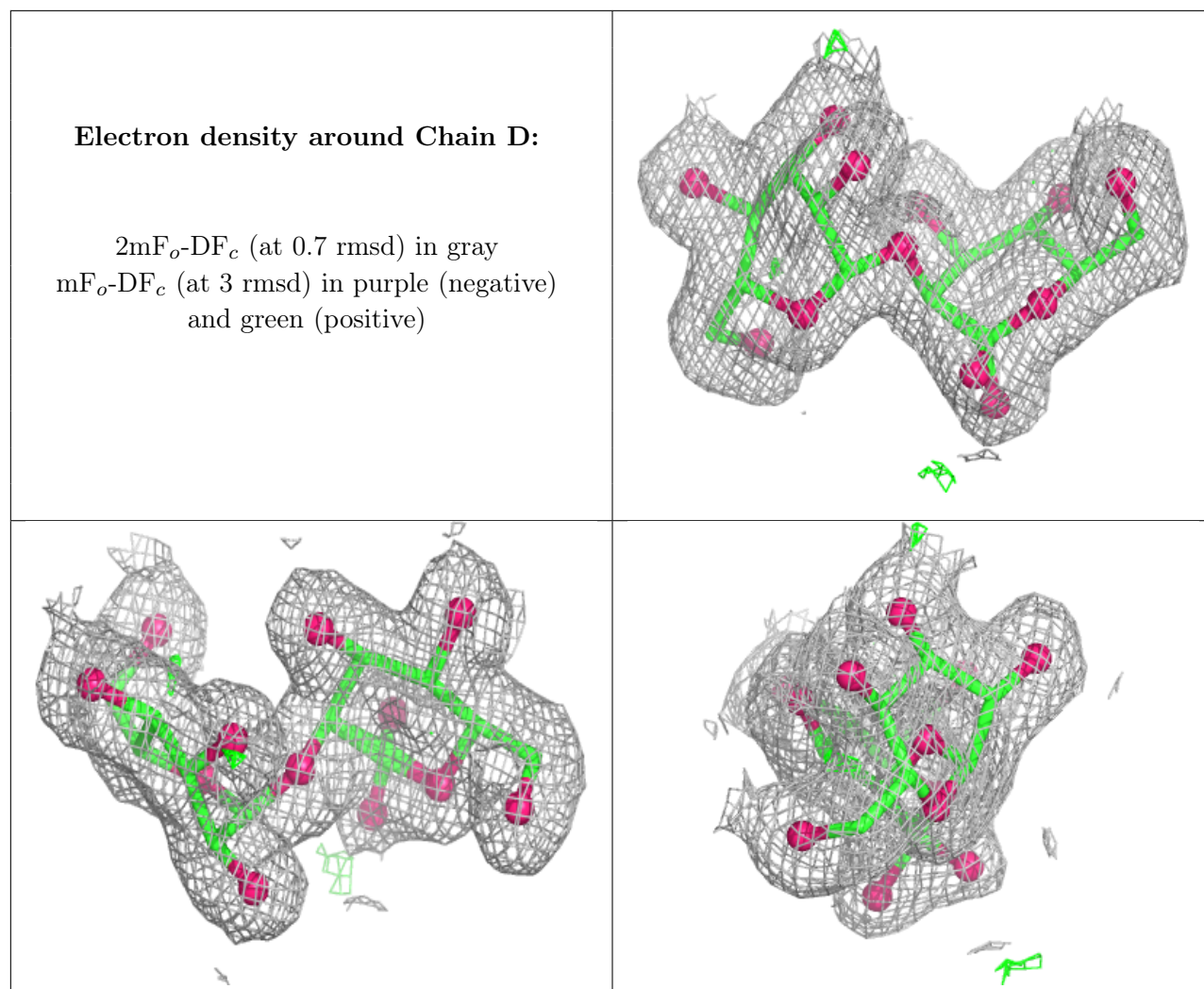
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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($\text{\AA}^2$)	Q<0.9
2	BMA	D	1[A]	12/12	0.97	0.06	19,21,23,24	12
2	MAN	C	1[B]	12/12	-	-	15,18,19,21	12
2	BMA	C	1[A]	12/12	0.98	0.04	17,19,19,22	12
2	BMA	D	2	11/12	0.98	0.05	19,21,22,23	0
2	MAN	D	1[B]	12/12	-	-	17,20,21,23	12
2	BMA	C	2	11/12	0.99	0.04	17,18,19,20	0

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





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
3	SO4	B	506	5/5	0.81	0.13	52,59,66,79	0
3	SO4	B	507	5/5	0.83	0.10	77,80,88,90	0
4	GOL	A	508	6/6	0.84	0.19	47,60,66,72	0
3	SO4	A	506	5/5	0.86	0.11	44,57,60,62	0
4	GOL	B	510	6/6	0.87	0.15	40,55,58,62	0
3	SO4	B	508	5/5	0.88	0.12	40,47,52,60	0
4	GOL	A	507	6/6	0.93	0.11	29,42,43,43	0
5	MES	B	511	12/12	0.93	0.13	47,48,51,56	0
5	MES	A	509	12/12	0.94	0.13	40,51,58,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	505	5/5	0.96	0.07	41,45,51,52	0
3	SO4	A	505	5/5	0.96	0.07	34,40,45,47	0
4	GOL	B	509	6/6	0.96	0.09	29,47,49,49	0
3	SO4	A	504	5/5	1.00	0.03	18,18,18,19	0
3	SO4	B	504	5/5	1.00	0.04	20,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.