



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:15 AM UTC

PDB ID : 4TVC / pdb_00004tvc
Title : N-terminally truncated dextranucrase DSR-E from *Leuconostoc mesenteroides* NRRL B-1299 in complex with gluco-oligosaccharides
Authors : Brison, Y.; Remaud-Simeon, M.; Mourey, L.; Tranier, S.
Deposited on : 2014-06-26
Resolution : 1.85 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

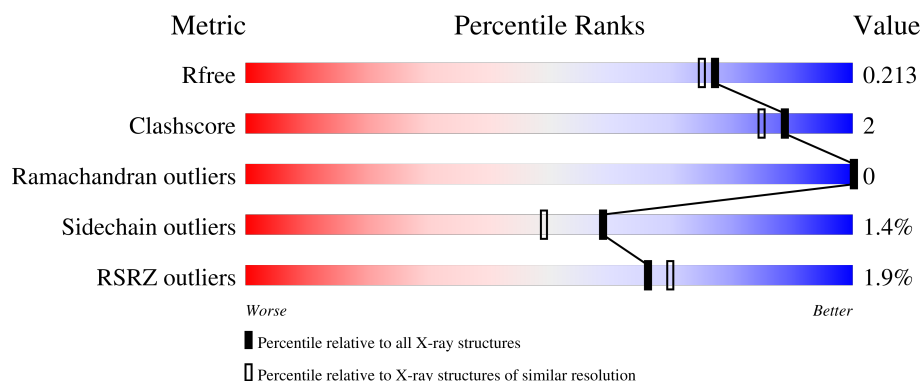
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	1108	2% 87% 6% 6%
2	B	3	67% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9183 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 Dextransucrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1036	Total	C	I	N	O	S	0	9	0
			8189	5125	3	1397	1644	20			

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1758	ALA	-	expression tag	UNP Q8G9Q2
A	2836	LYS	-	expression tag	UNP Q8G9Q2
A	2837	GLY	-	expression tag	UNP Q8G9Q2
A	2838	GLU	-	expression tag	UNP Q8G9Q2
A	2839	LEU	-	expression tag	UNP Q8G9Q2
A	2840	LYS	-	expression tag	UNP Q8G9Q2
A	2841	LEU	-	expression tag	UNP Q8G9Q2
A	2842	GLU	-	expression tag	UNP Q8G9Q2
A	2843	GLY	-	expression tag	UNP Q8G9Q2
A	2844	LYS	-	expression tag	UNP Q8G9Q2
A	2845	PRO	-	expression tag	UNP Q8G9Q2
A	2846	ILE	-	expression tag	UNP Q8G9Q2
A	2847	PRO	-	expression tag	UNP Q8G9Q2
A	2848	ASN	-	expression tag	UNP Q8G9Q2
A	2849	PRO	-	expression tag	UNP Q8G9Q2
A	2850	LEU	-	expression tag	UNP Q8G9Q2
A	2851	LEU	-	expression tag	UNP Q8G9Q2
A	2852	GLY	-	expression tag	UNP Q8G9Q2
A	2853	LEU	-	expression tag	UNP Q8G9Q2
A	2854	ASP	-	expression tag	UNP Q8G9Q2
A	2855	SER	-	expression tag	UNP Q8G9Q2
A	2856	THR	-	expression tag	UNP Q8G9Q2
A	2857	ARG	-	expression tag	UNP Q8G9Q2
A	2858	THR	-	expression tag	UNP Q8G9Q2
A	2859	GLY	-	expression tag	UNP Q8G9Q2
A	2860	HIS	-	expression tag	UNP Q8G9Q2
A	2861	HIS	-	expression tag	UNP Q8G9Q2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2862	HIS	-	expression tag	UNP Q8G9Q2
A	2863	HIS	-	expression tag	UNP Q8G9Q2
A	2864	HIS	-	expression tag	UNP Q8G9Q2
A	2865	HIS	-	expression tag	UNP Q8G9Q2

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	1
			12	6	6		

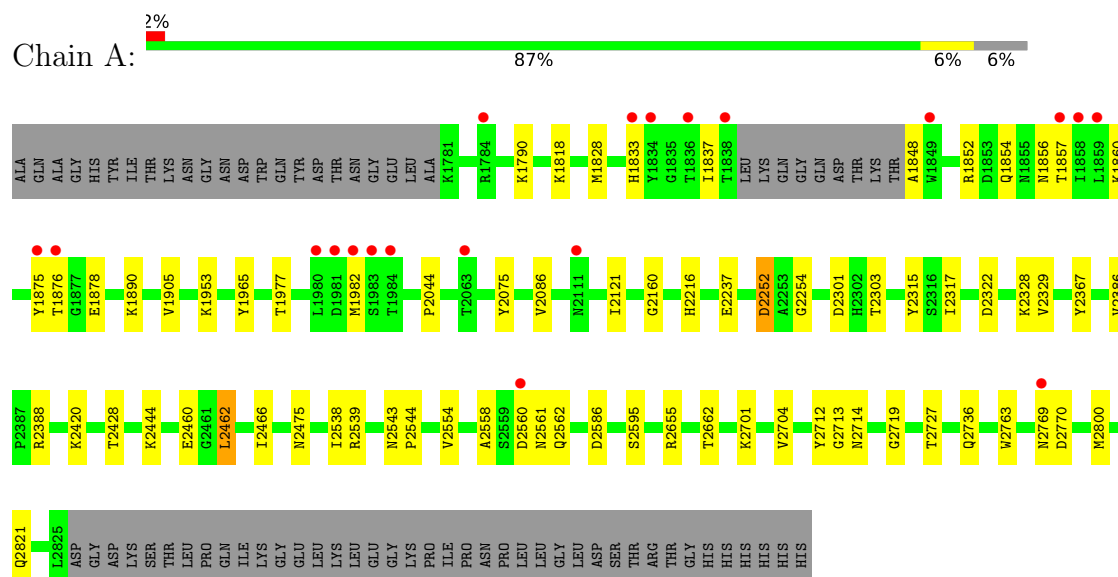
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	922	Total 922	O 922	0	0

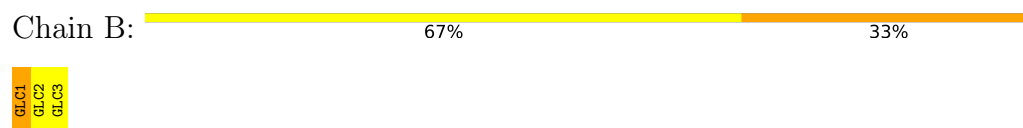
3 Residue-property plots

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: Dextranucrase



• Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranos e



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.31Å 100.14Å 186.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.20 – 1.85 27.20 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.20-1.85) 99.7 (27.20-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.161 , 0.205 0.170 , 0.213	Depositor DCC
R_{free} test set	5458 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9183	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: GOL, GLC, TYI, CA, NA, IYR

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	1.23	12/8368 (0.1%)	1.07	7/11372 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2714	ASN	CA-CB	6.46	1.63	1.53
1	A	1977	THR	CA-C	-6.37	1.44	1.52
1	A	2586	ASP	CG-OD2	6.13	1.36	1.25
1	A	2662	THR	CA-C	5.98	1.58	1.52
1	A	2595	SER	CA-C	5.49	1.59	1.52
1	A	2322	ASP	C-O	5.43	1.30	1.23
1	A	2428	THR	N-CA	-5.39	1.39	1.45
1	A	2655	ARG	CZ-NH1	-5.38	1.25	1.32
1	A	2086	VAL	CA-CB	5.18	1.60	1.54
1	A	2562	GLN	C-O	-5.17	1.17	1.23
1	A	2558	ALA	CA-CB	-5.04	1.44	1.53
1	A	2736	GLN	C-O	5.03	1.30	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2538	ILE	CB-CA-C	-6.20	102.41	110.84
1	A	2713	GLY	CA-C-N	6.13	130.10	121.02
1	A	2713	GLY	C-N-CA	6.13	130.10	121.02
1	A	2821	GLN	N-CA-C	5.52	117.74	108.96
1	A	2329	VAL	N-CA-C	-5.41	105.10	110.62
1	A	2466	ILE	CA-C-N	-5.41	117.45	121.61
1	A	2466	ILE	C-N-CA	-5.41	117.45	121.61

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	8189	0	7701	27	0
2	B	34	0	30	3	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	12	0	12	1	0
6	A	24	0	32	0	0
7	A	922	0	0	3	0
All	All	9183	0	7775	30	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 (30) 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:2328:LYS:HD3	1:A:2367:TYR:O	1.87	0.75
2:B:1:GLC:H61	2:B:2:GLC:H5	1.71	0.72
1:A:1953:LYS:NZ	5:A:3005:GLC:O2	2.25	0.69
1:A:1982:MET:HE3	7:A:3679:HOH:O	1.97	0.64
1:A:2044:PRO:HG3	1:A:2121:ILE:HD11	1.85	0.59
1:A:2561:ASN:OD1	1:A:2561:ASN:N	2.30	0.56
1:A:1848:ALA:HB1	1:A:1878:GLU:HG3	1.88	0.55
1:A:1818:LYS:HD3	1:A:1890:LYS:HG3	1.89	0.54
2:B:1:GLC:C6	2:B:2:GLC:H5	2.37	0.53
1:A:1852:ARG:HA	1:A:1857:THR:O	2.09	0.52
1:A:2160:GLY:HA3	1:A:2216:HIS:CD2	2.47	0.50
1:A:2317:ILE:HG22	1:A:2388:ARG:HB3	1.94	0.49
1:A:2444:LYS:HB2	1:A:2460:GLU:OE1	2.12	0.49
1:A:2301:ASP:OD1	1:A:2303:THR:HG23	2.13	0.48
1:A:2254:GLY:HA3	1:A:2763:TRP:O	2.14	0.47
2:B:1:GLC:C6	2:B:2:GLC:C5	2.94	0.46
1:A:2044:PRO:CG	1:A:2121:ILE:HD11	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2543:ASN:HB2	1:A:2544:PRO:CD	2.47	0.45
1:A:2462:LEU:HB3	1:A:2554:VAL:HG12	1.98	0.44
1:A:1965:TYR:CG	1:A:2719:GLY:HA2	2.53	0.43
1:A:2315:TYR:HA	1:A:2386:VAL:O	2.18	0.43
1:A:2539:ARG:O	1:A:2539:ARG:HD3	2.18	0.43
1:A:2475:ASN:OD1	1:A:2475:ASN:C	2.62	0.43
1:A:2420:LYS:NZ	7:A:3153:HOH:O	2.53	0.42
1:A:2237:GLU:HG2	7:A:3103:HOH:O	2.19	0.42
1:A:1828:MET:HE2	1:A:1828:MET:HB3	1.93	0.41
1:A:1875:TYR:O	1:A:1876:THR:C	2.63	0.41
1:A:2769:ASN:OD1	1:A:2770:ASP:N	2.54	0.41
1:A:2701:LYS:HA	1:A:2727:THR:O	2.21	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	1039/1108 (94%)	1004 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	868/923 (94%)	855 (98%)	13 (2%)	57 47

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

Mol	Chain	Res	Type
1	A	1790	LYS
1	A	1833	HIS
1	A	1837	ILE
1	A	1854	GLN
1	A	1856	ASN
1	A	1860	LYS
1	A	1905	VAL
1	A	2252[A]	ASP
1	A	2252[B]	ASP
1	A	2462	LEU
1	A	2560	ASP
1	A	2704	VAL
1	A	2800	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1805	GLN
1	A	1927	GLN
1	A	1942	GLN
1	A	1955	GLN
1	A	1971	ASN
1	A	2074	GLN
1	A	2109	GLN
1	A	2112	ASN
1	A	2169	ASN
1	A	2278	ASN
1	A	2360	GLN
1	A	2368	ASN
1	A	2508	ASN
1	A	2528	GLN
1	A	2609	ASN
1	A	2632	GLN
1	A	2801	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	IYR	A	2712	1	12,13,14	1.25	2 (16%)	12,17,19	2.78	3 (25%)
1	TYI	A	2075	1	13,14,15	2.03	2 (15%)	14,19,21	1.85	3 (21%)

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
1	IYR	A	2712	1	-	0/5/6/8	0/1/1/1
1	TYI	A	2075	1	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2075	TYI	CZ-CE2	5.10	1.51	1.40
1	A	2075	TYI	CZ-CE1	4.18	1.49	1.40
1	A	2712	IYR	CF-CE	2.94	1.45	1.39
1	A	2712	IYR	CG-CF	-2.08	1.36	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2712	IYR	CF-CE-IE	-7.41	112.61	119.76
1	A	2712	IYR	CD-CE-IE	4.77	127.41	118.46
1	A	2075	TYI	CZ-CE2-I2	4.49	125.88	119.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2075	TYI	CD2-CE2-CZ	-3.28	115.15	121.33
1	A	2712	IYR	CB-CC-CH	-2.59	116.09	120.90
1	A	2075	TYI	CD2-CG-CD1	2.41	122.28	119.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

3 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	B	1	2	12,12,12	0.38	0	17,17,17	1.31	1 (5%)
2	GLC	B	2	2	11,11,12	0.70	0	15,15,17	0.85	0
2	GLC	B	3	2	11,11,12	0.44	0	15,15,17	1.76	4 (26%)

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	B	1	2	-	2/2/22/22	0/1/1/1
2	GLC	B	2	2	-	2/2/19/22	0/1/1/1
2	GLC	B	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	GLC	C1-C2-C3	-3.52	104.52	109.64
2	B	3	GLC	O5-C5-C6	3.51	114.50	107.66
2	B	1	GLC	C4-C3-C2	-2.64	106.20	110.83
2	B	3	GLC	C2-C3-C4	-2.24	106.93	110.86
2	B	3	GLC	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

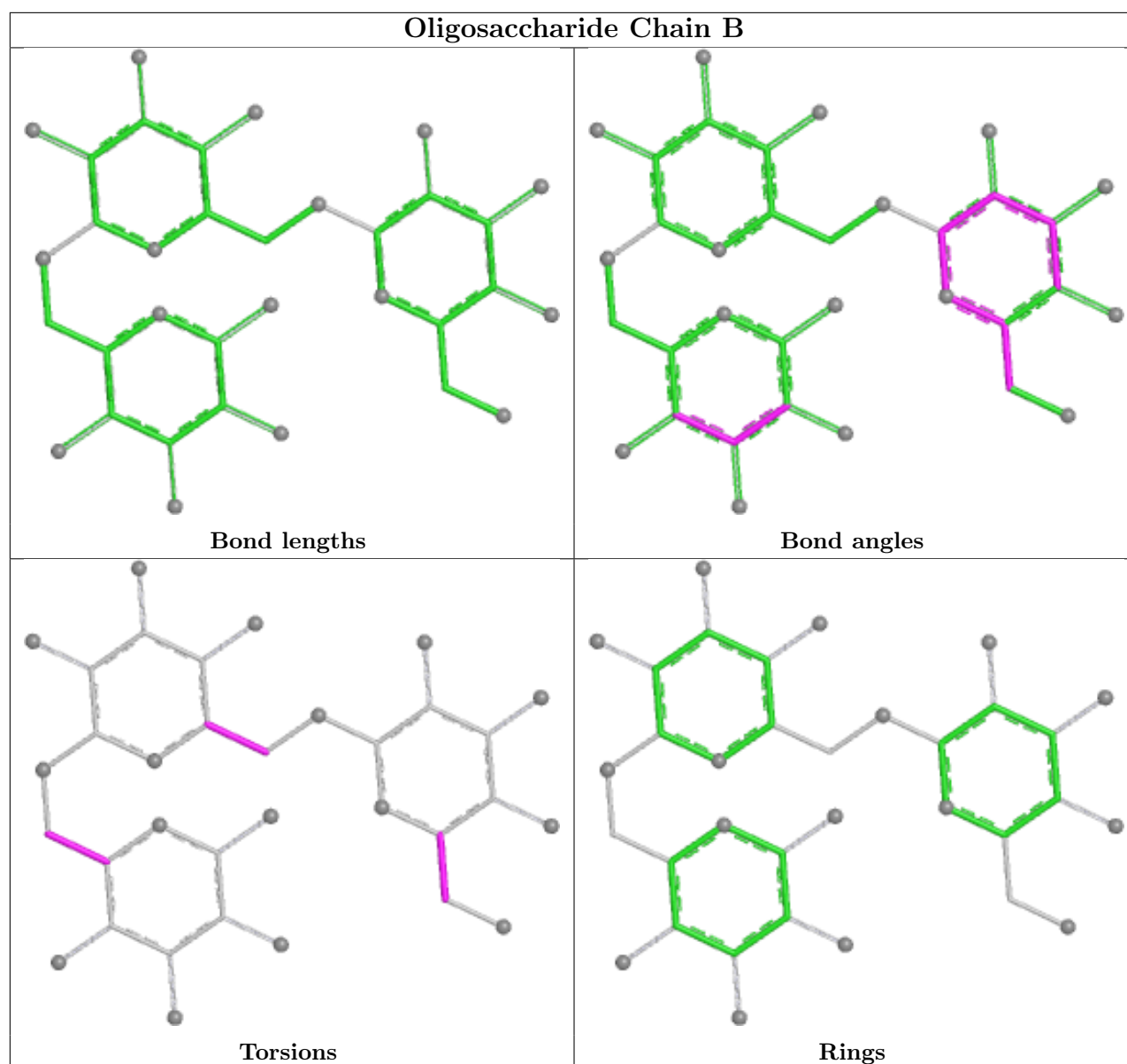
Mol	Chain	Res	Type	Atoms
2	B	1	GLC	O5-C5-C6-O6
2	B	1	GLC	C4-C5-C6-O6
2	B	3	GLC	C4-C5-C6-O6
2	B	2	GLC	C4-C5-C6-O6
2	B	2	GLC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	GLC	3	0
2	B	1	GLC	3	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
6	GOL	A	3006	-	5,5,5	0.38	0	5,5,5	0.84	0
6	GOL	A	3008[B]	-	5,5,5	0.40	0	5,5,5	0.40	0
6	GOL	A	3008[A]	-	5,5,5	0.61	0	5,5,5	0.68	0
5	GLC	A	3005	-	12,12,12	0.82	0	17,17,17	1.29	2 (11%)
6	GOL	A	3007	-	5,5,5	0.26	0	5,5,5	0.43	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
6	GOL	A	3006	-	-	4/4/4/4	-
6	GOL	A	3008[B]	-	-	2/4/4/4	-
6	GOL	A	3008[A]	-	-	2/4/4/4	-
5	GLC	A	3005	-	-	2/2/22/22	0/1/1/1
6	GOL	A	3007	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3005	GLC	C1-C2-C3	2.48	115.42	110.36
5	A	3005	GLC	O2-C2-C3	-2.30	104.94	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	3006	GOL	C1-C2-C3-O3
6	A	3008[A]	GOL	O1-C1-C2-C3
6	A	3008[B]	GOL	O1-C1-C2-C3
5	A	3005	GLC	C4-C5-C6-O6
5	A	3005	GLC	O5-C5-C6-O6
6	A	3006	GOL	O1-C1-C2-C3
6	A	3006	GOL	O2-C2-C3-O3
6	A	3008[A]	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	3008[B]	GOL	O1-C1-C2-O2
6	A	3006	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3005	GLC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1034/1108 (93%)	-0.26	20 (1%) 66 70	12, 25, 54, 87	9 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1838	THR	3.4
1	A	1849	TRP	3.2
1	A	2063	THR	3.1
1	A	1984	THR	3.0
1	A	1875	TYR	3.0
1	A	1876	THR	2.9
1	A	1858	ILE	2.9
1	A	1983	SER	2.6
1	A	1982	MET	2.6
1	A	1834	TYR	2.4
1	A	1980	LEU	2.4
1	A	1836	THR	2.4
1	A	1833	HIS	2.3
1	A	2560	ASP	2.3
1	A	2111	ASN	2.3
1	A	1859	LEU	2.3
1	A	1981[A]	ASP	2.2
1	A	1784	ARG	2.2
1	A	2769	ASN	2.1
1	A	1857	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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.

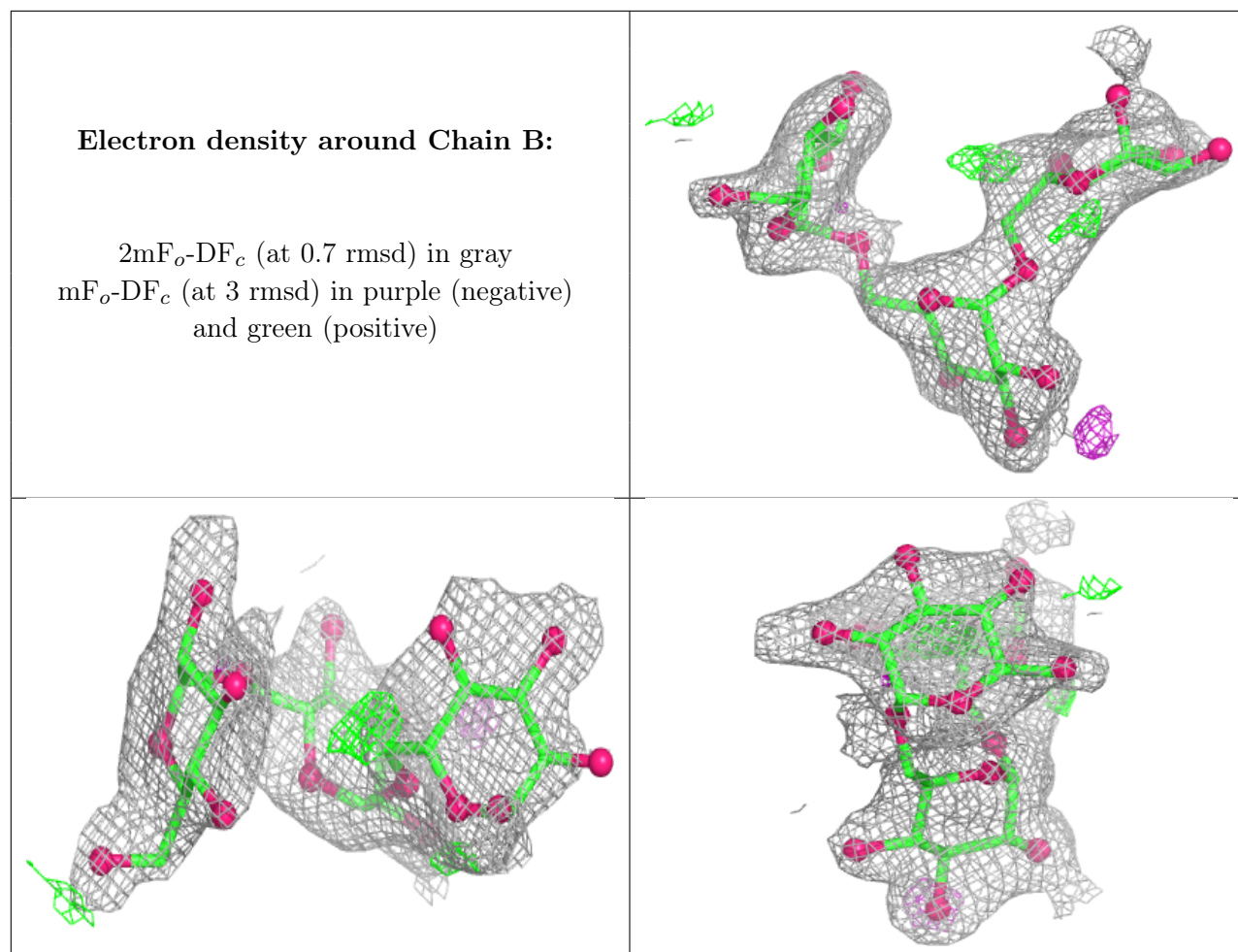
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TYI	A	2075	14/15	0.88	0.13	29,52,77,113	2
1	IYR	A	2712	13/14	0.88	0.11	21,29,49,80	1

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, 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	GLC	B	1	12/12	0.68	0.14	64,78,85,85	0
2	GLC	B	3	11/12	0.77	0.10	68,71,72,73	0
2	GLC	B	2	11/12	0.88	0.09	50,59,71,74	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(Å ²)	Q<0.9
5	GLC	A	3005	12/12	0.85	0.12	32,59,65,66	0
6	GOL	A	3006	6/6	0.88	0.10	38,43,46,47	0
6	GOL	A	3007	6/6	0.89	0.10	50,53,54,55	0
6	GOL	A	3008[A]	6/6	0.91	0.12	18,27,28,34	6
6	GOL	A	3008[B]	6/6	0.91	0.12	38,45,48,50	6
4	NA	A	3001	1/1	0.98	0.10	33,33,33,33	0
3	CA	A	3000	1/1	1.00	0.02	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.