



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:06 PM BST

PDB ID : 4TVD  
Title : N-terminally truncated dextransucrase DSR-E from *Leuconostoc mesenteroides* NRRL B-1299 in complex with D-glucose  
Authors : Brison, Y.; Remaud-Simeon, M.; Mourey, L.; Tranier, S.  
Deposited on : 2014-06-26  
Resolution : 2.30 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

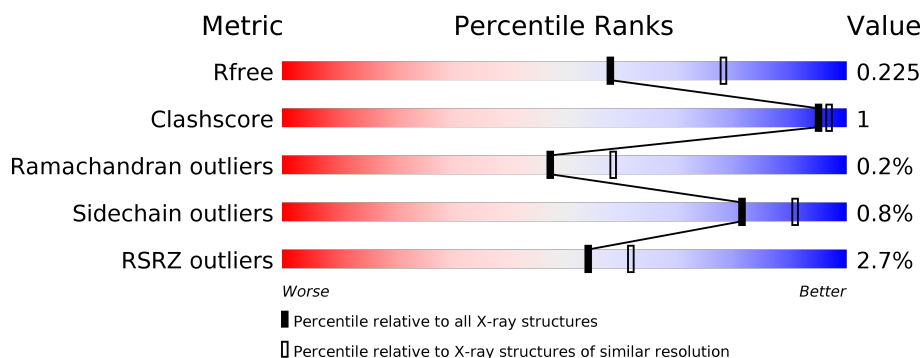
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	1108	<div> <div>3%</div> <div>89%</div> <div>5%</div> <div>7%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8631 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 Dextranucrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1032	Total	C	I	N	O	S	0	2	0
			8108	5071	5	1386	1628	18			

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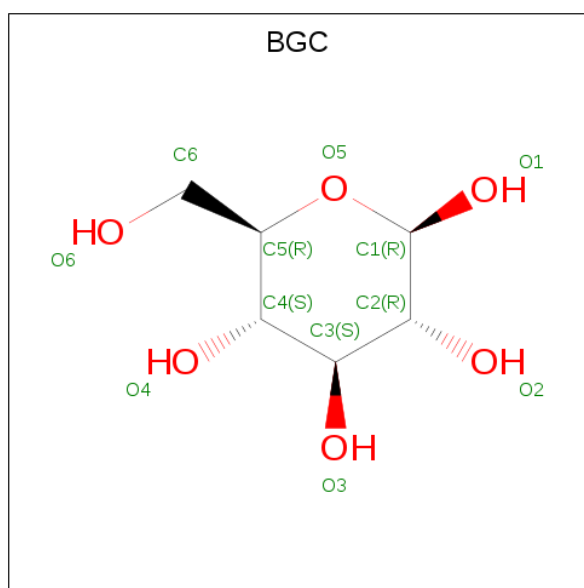
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Chain	Residue	Modelled	Actual	Comment	Reference
A	2862	HIS	-	expression tag	UNP Q8G9Q2
A	2863	HIS	-	expression tag	UNP Q8G9Q2
A	2864	HIS	-	expression tag	UNP Q8G9Q2
A	2865	HIS	-	expression tag	UNP Q8G9Q2

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



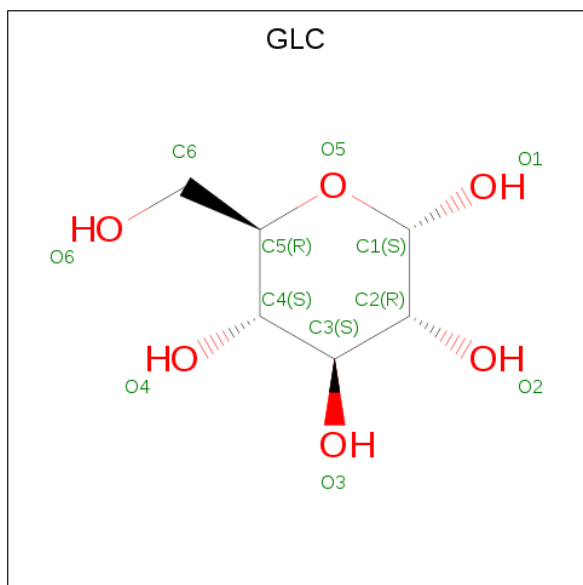
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	A	1	Total C O 12 6 6	0	0
3	A	1	Total C O 12 6 6	0	0
3	A	1	Total C O 12 6 6	0	0
3	A	1	Total C O 12 6 6	0	0
3	A	1	Total C O 12 6 6	0	0

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

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	395	Total	O	0	0
			395	395		

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.

Chain A:

89% 5% 7% 3%

ALA GLN ALA GLY HIS TYR ILE THR LYS ASN GLY ASN ASP TRP GLN TYR ASP THR ASN GLY GLU LEU ALA LYS G1782 Q1785 D1786 S1787 N1788 G1789 Y1793 I1809 G1810 D1819 T1830 H1833 Y1834 G1835 T1836 ILE THR LEU LYS GLN GLY GLN ASP THR LYS THR W1849 F1850

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.77Å 98.98Å 181.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.70 – 2.30 47.75 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.70-2.30) 99.6 (47.75-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.169 , 0.223 0.175 , 0.225	Depositor DCC
$R_{free}$ test set	2772 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: BGC, TYI, CA, GLC, IYR, PEG

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	0.69	0/8234	0.77	5/11187 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	2388	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	2200	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	2301	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	2208	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	2083	ASP	CB-CG-OD1	5.13	122.92	118.30

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	8108	0	7582	19	0
2	A	1	0	0	0	0
3	A	108	0	108	2	0
4	A	12	0	12	0	0
5	A	7	0	10	0	0
6	A	395	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8631	0	7712	19	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 (19) 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:1985:ASN:O	1:A:1989:THR:HG23	1.78	0.83
1:A:2160:GLY:HA3	1:A:2216:HIS:CD2	2.32	0.64
1:A:1852:ARG:HA	1:A:1857:THR:O	2.07	0.55
1:A:1793:TYR:CD2	1:A:1809:ILE:HD11	2.42	0.55
1:A:2462:LEU:HB3	1:A:2554:VAL:HG12	1.88	0.53
1:A:2251:LEU:HD12	1:A:2294:ASP:HB3	1.92	0.52
1:A:2237:GLU:HG3	1:A:2568:ALA:HB1	1.94	0.50
1:A:2213:ASP:OD2	1:A:2252:ASP:OD2	2.31	0.49
1:A:1858:ILE:HG13	1:A:1858:ILE:O	2.12	0.48
1:A:2315:TYR:HA	1:A:2386:VAL:O	2.15	0.47
1:A:2324:GLY:O	1:A:2328:LYS:HE2	2.17	0.44
1:A:2248:GLU:OE1	3:A:2906:BGC:O1	2.35	0.44
1:A:1965:TYR:O	1:A:1972:GLY:HA2	2.18	0.43
1:A:2052:TYR:CE1	1:A:2056:MET:HE2	2.54	0.43
1:A:2002:ASP:C	1:A:2002:ASP:OD1	2.58	0.42
1:A:2204:PHE:CG	1:A:2688:ALA:HB2	2.54	0.42
1:A:2815:LYS:HB3	1:A:2822:TYR:CD1	2.53	0.42
1:A:2098:THR:OG1	3:A:2908:BGC:C6	2.69	0.41
1:A:2257:THR:O	1:A:2258:ILE:C	2.59	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	1024/1108 (92%)	991 (97%)	31 (3%)	2 (0%)	47 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1819	ASP
1	A	1810	GLY

### 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	850/921 (92%)	843 (99%)	7 (1%)	81 91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1854	GLN
1	A	2026	THR
1	A	2167	LEU
1	A	2462	LEU
1	A	2539	ARG
1	A	2560	ASP
1	A	2770	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1854	GLN
1	A	2067	GLN
1	A	2302	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	2764	1	12,13,14	1.62	1 (8%)	14,17,19	1.79	4 (28%)
1	TYI	A	2075	1	13,14,15	1.24	2 (15%)	16,19,21	1.55	4 (25%)
1	IYR	A	2767	1	12,13,14	1.56	1 (8%)	14,17,19	1.84	4 (28%)
1	IYR	A	2712	1	12,13,14	1.12	2 (16%)	14,17,19	3.22	4 (28%)

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	2764	1	-	0/5/6/8	0/1/1/1
1	TYI	A	2075	1	-	0/5/6/8	0/1/1/1
1	IYR	A	2767	1	-	0/5/6/8	0/1/1/1
1	IYR	A	2712	1	-	0/5/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2764	IYR	CF-CE	5.16	1.50	1.39
1	A	2767	IYR	CF-CE	5.15	1.50	1.39
1	A	2075	TYI	CZ-CE1	2.77	1.46	1.40
1	A	2075	TYI	CZ-CE2	2.71	1.46	1.40
1	A	2712	IYR	CE-IE	-2.54	2.04	2.10
1	A	2712	IYR	CF-CE	2.45	1.44	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2712	IYR	CF-CE-IE	-9.70	110.19	119.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2712	IYR	CD-CE-IE	4.49	126.90	118.61
1	A	2764	IYR	CF-CE-IE	4.39	124.16	119.81
1	A	2767	IYR	CF-CE-IE	3.58	123.36	119.81
1	A	2075	TYI	CD2-CE2-I2	3.53	125.11	118.61
1	A	2767	IYR	OF-CF-CE	3.41	123.33	119.19
1	A	2764	IYR	CD-CE-CF	-3.06	117.11	120.59
1	A	2767	IYR	CC-CB-CA	-2.92	108.20	114.10
1	A	2075	TYI	CD2-CG-CD1	2.55	122.48	118.98
1	A	2075	TYI	CZ-CE2-I2	-2.34	115.81	119.42
1	A	2767	IYR	CH-CC-CD	2.21	121.63	118.54
1	A	2764	IYR	CC-CB-CA	2.17	118.50	114.10
1	A	2712	IYR	CC-CB-CA	-2.14	109.76	114.10
1	A	2764	IYR	CB-CC-CD	-2.10	116.83	120.44
1	A	2075	TYI	CB-CG-CD1	-2.08	116.86	120.44
1	A	2712	IYR	CH-CC-CD	2.07	121.44	118.54

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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z  > 2$
3	BGC	A	2905	-	12,12,12	0.82	0	17,17,17	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BGC	A	2911	-	12,12,12	0.80	0	17,17,17	1.70	4 (23%)
3	BGC	A	2902	-	12,12,12	0.65	0	17,17,17	1.33	3 (17%)
5	PEG	A	2912	-	6,6,6	0.78	0	5,5,5	0.74	0
3	BGC	A	2906	-	12,12,12	0.85	0	17,17,17	1.76	6 (35%)
4	GLC	A	2903	-	12,12,12	1.45	2 (16%)	17,17,17	1.69	2 (11%)
3	BGC	A	2908	-	12,12,12	0.74	0	17,17,17	1.42	3 (17%)
3	BGC	A	2910	-	12,12,12	1.00	1 (8%)	17,17,17	1.86	5 (29%)
3	BGC	A	2909	-	12,12,12	0.77	0	17,17,17	0.87	0
3	BGC	A	2907	-	12,12,12	0.96	0	17,17,17	2.09	4 (23%)
3	BGC	A	2904	-	12,12,12	0.53	0	17,17,17	1.16	2 (11%)

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
3	BGC	A	2905	-	-	0/2/22/22	0/1/1/1
3	BGC	A	2911	-	-	1/2/22/22	0/1/1/1
3	BGC	A	2902	-	-	2/2/22/22	0/1/1/1
5	PEG	A	2912	-	-	2/4/4/4	-
3	BGC	A	2906	-	-	2/2/22/22	0/1/1/1
4	GLC	A	2903	-	-	2/2/22/22	0/1/1/1
3	BGC	A	2908	-	-	0/2/22/22	0/1/1/1
3	BGC	A	2910	-	-	0/2/22/22	0/1/1/1
3	BGC	A	2909	-	-	0/2/22/22	0/1/1/1
3	BGC	A	2907	-	-	2/2/22/22	0/1/1/1
3	BGC	A	2904	-	-	2/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2903	GLC	O5-C5	-2.62	1.38	1.44
3	A	2910	BGC	O5-C5	-2.36	1.38	1.44
4	A	2903	GLC	C4-C5	-2.05	1.48	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2907	BGC	C1-C2-C3	-5.27	99.37	110.31
3	A	2911	BGC	C3-C4-C5	4.38	118.05	110.24
4	A	2903	GLC	C6-C5-C4	-4.33	102.87	113.00
3	A	2907	BGC	O5-C1-C2	-3.81	103.49	110.28
3	A	2910	BGC	O5-C5-C4	3.69	116.40	109.69
3	A	2910	BGC	O5-C1-C2	3.47	116.48	110.28
4	A	2903	GLC	O5-C1-C2	3.38	116.32	110.28
3	A	2908	BGC	O5-C1-C2	-2.97	104.98	110.28
3	A	2907	BGC	O2-C2-C3	2.93	117.13	110.35
3	A	2911	BGC	C1-C2-C3	-2.92	104.25	110.31
3	A	2906	BGC	O1-C1-O5	-2.90	101.66	110.38
3	A	2906	BGC	C1-O5-C5	2.82	118.99	113.66
3	A	2910	BGC	O3-C3-C4	2.82	116.87	110.35
3	A	2907	BGC	C3-C4-C5	2.71	115.08	110.24
3	A	2904	BGC	C4-C3-C2	-2.68	106.14	110.82
3	A	2902	BGC	C3-C4-C5	2.68	115.02	110.24
3	A	2906	BGC	C1-C2-C3	-2.65	104.82	110.31
3	A	2908	BGC	O4-C4-C5	2.60	115.76	109.30
3	A	2910	BGC	C3-C4-C5	2.53	114.76	110.24
3	A	2902	BGC	O5-C5-C4	2.52	114.28	109.69
3	A	2908	BGC	O4-C4-C3	-2.51	104.54	110.35
3	A	2911	BGC	O5-C1-C2	-2.47	105.87	110.28
3	A	2906	BGC	O5-C5-C4	2.35	113.97	109.69
3	A	2906	BGC	O3-C3-C2	2.29	115.64	110.35
3	A	2906	BGC	C3-C4-C5	2.21	114.17	110.24
3	A	2911	BGC	O4-C4-C3	-2.11	105.46	110.35
3	A	2902	BGC	O5-C1-C2	2.10	114.03	110.28
3	A	2905	BGC	O5-C5-C6	2.08	111.60	106.44
3	A	2905	BGC	O3-C3-C4	2.06	115.11	110.35
3	A	2910	BGC	C6-C5-C4	-2.04	108.23	113.00
3	A	2904	BGC	O2-C2-C1	2.03	113.88	109.16

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2904	BGC	O5-C5-C6-O6
3	A	2904	BGC	C4-C5-C6-O6
3	A	2902	BGC	C4-C5-C6-O6
3	A	2907	BGC	O5-C5-C6-O6
5	A	2912	PEG	O2-C3-C4-O4
3	A	2902	BGC	O5-C5-C6-O6
3	A	2906	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	2911	BGC	O5-C5-C6-O6
3	A	2906	BGC	O5-C5-C6-O6
3	A	2907	BGC	C4-C5-C6-O6
5	A	2912	PEG	O1-C1-C2-O2
4	A	2903	GLC	O5-C5-C6-O6
4	A	2903	GLC	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2906	BGC	1	0
3	A	2908	BGC	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	1028/1108 (92%)	-0.22	28 (2%) 54 62	23, 36, 71, 109	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1789	GLY	4.4
1	A	1830	THR	4.1
1	A	1874	PRO	3.8
1	A	2343	ASN	3.8
1	A	1983	SER	3.8
1	A	1875	TYR	3.7
1	A	1849	TRP	3.5
1	A	1876	THR	3.4
1	A	1854	GLN	3.2
1	A	1834	TYR	3.1
1	A	2341	TRP	3.1
1	A	1858	ILE	2.9
1	A	1984	THR	2.9
1	A	1788	ASN	2.9
1	A	2342	THR	2.8
1	A	2771	GLY	2.7
1	A	1857	THR	2.5
1	A	1785	GLN	2.5
1	A	1835	GLY	2.4
1	A	1833	HIS	2.4
1	A	2018	LYS	2.3
1	A	1867	GLY	2.3
1	A	2337	THR	2.2
1	A	1856	ASN	2.2
1	A	2826	ASP	2.1
1	A	2110	ASN	2.1
1	A	1786	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2067	GLN	2.0

## 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, 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
1	IYR	A	2764	13/14	0.93	0.16	33,60,82,82	1
1	IYR	A	2767	13/14	0.93	0.12	49,54,65,95	1
1	IYR	A	2712	13/14	0.95	0.11	26,35,48,64	1
1	TYI	A	2075	14/15	0.97	0.09	40,61,77,85	2

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 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, 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	PEG	A	2912	7/7	0.82	0.15	48,52,54,58	0
3	BGC	A	2904	12/12	0.87	0.16	68,81,84,85	0
3	BGC	A	2911	12/12	0.88	0.19	52,57,60,62	0
3	BGC	A	2910	12/12	0.89	0.21	43,57,62,68	0
4	GLC	A	2903	12/12	0.91	0.19	41,49,55,58	0
3	BGC	A	2907	12/12	0.93	0.13	37,47,55,59	0
3	BGC	A	2906	12/12	0.93	0.14	34,39,49,58	0
3	BGC	A	2908	12/12	0.94	0.15	45,54,61,66	0
3	BGC	A	2909	12/12	0.95	0.12	54,59,61,62	0
3	BGC	A	2902	12/12	0.95	0.10	35,41,46,55	0
3	BGC	A	2905	12/12	0.95	0.14	44,52,54,56	0
2	CA	A	2901	1/1	0.99	0.12	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.