wwPDB X-ray Structure Validation Summary Report (i)

Sep 4, 2023 – 07:03 PM EDT

PDB ID	:	3TTO
Title	:	Crystal structure of Leuconostoc mesenteroides NRRL B-1299 N-terminally truncated dextransucrase DSR-E in triclinic form
Authors	:	Brison, Y.; Pijning, T.; Fabre, E.; Mourey, L.; Morel, S.; Potocki-Veronese, G.; Monsan, P.; Tranier, S.; Remaud-Simeon, M.; Dijkstra, B.W.
Deposited on	:	2011-09-15
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

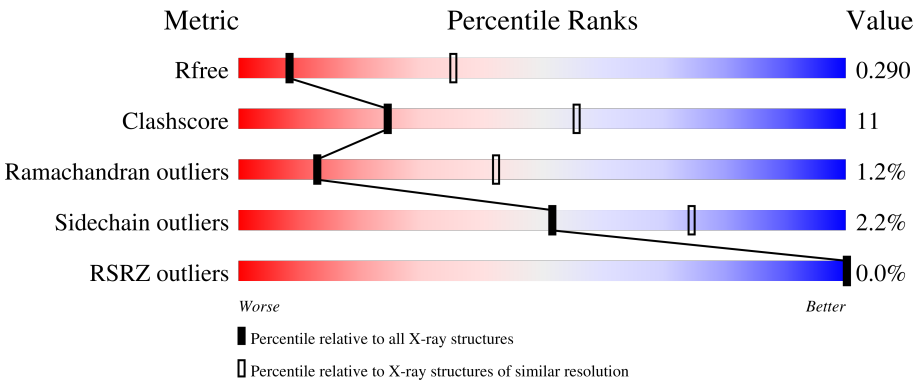
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	74% 20% • 5%
1	B	1108	75% 19% • 5%
1	C	1108	73% 21% • 5%
1	D	1108	70% 23% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32341 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
			Total	C	N	O	S			
1	A	1055	8122	5088	1377	1638	19	0	1	0
1	B	1053	8105	5088	1364	1635	18	0	1	0
1	C	1052	8071	5062	1358	1633	18	0	1	0
1	D	1043	7952	4988	1339	1607	18	0	1	0

There are 124 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
B	1758	ALA	-	expression tag	UNP Q8G9Q2
B	2836	LYS	-	expression tag	UNP Q8G9Q2
B	2837	GLY	-	expression tag	UNP Q8G9Q2
B	2838	GLU	-	expression tag	UNP Q8G9Q2
B	2839	LEU	-	expression tag	UNP Q8G9Q2
B	2840	LYS	-	expression tag	UNP Q8G9Q2
B	2841	LEU	-	expression tag	UNP Q8G9Q2
B	2842	GLU	-	expression tag	UNP Q8G9Q2
B	2843	GLY	-	expression tag	UNP Q8G9Q2
B	2844	LYS	-	expression tag	UNP Q8G9Q2
B	2845	PRO	-	expression tag	UNP Q8G9Q2
B	2846	ILE	-	expression tag	UNP Q8G9Q2
B	2847	PRO	-	expression tag	UNP Q8G9Q2
B	2848	ASN	-	expression tag	UNP Q8G9Q2
B	2849	PRO	-	expression tag	UNP Q8G9Q2
B	2850	LEU	-	expression tag	UNP Q8G9Q2
B	2851	LEU	-	expression tag	UNP Q8G9Q2
B	2852	GLY	-	expression tag	UNP Q8G9Q2
B	2853	LEU	-	expression tag	UNP Q8G9Q2
B	2854	ASP	-	expression tag	UNP Q8G9Q2
B	2855	SER	-	expression tag	UNP Q8G9Q2
B	2856	THR	-	expression tag	UNP Q8G9Q2
B	2857	ARG	-	expression tag	UNP Q8G9Q2
B	2858	THR	-	expression tag	UNP Q8G9Q2
B	2859	GLY	-	expression tag	UNP Q8G9Q2
B	2860	HIS	-	expression tag	UNP Q8G9Q2
B	2861	HIS	-	expression tag	UNP Q8G9Q2
B	2862	HIS	-	expression tag	UNP Q8G9Q2
B	2863	HIS	-	expression tag	UNP Q8G9Q2
B	2864	HIS	-	expression tag	UNP Q8G9Q2
B	2865	HIS	-	expression tag	UNP Q8G9Q2
C	1758	ALA	-	expression tag	UNP Q8G9Q2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2836	LYS	-	expression tag	UNP Q8G9Q2
C	2837	GLY	-	expression tag	UNP Q8G9Q2
C	2838	GLU	-	expression tag	UNP Q8G9Q2
C	2839	LEU	-	expression tag	UNP Q8G9Q2
C	2840	LYS	-	expression tag	UNP Q8G9Q2
C	2841	LEU	-	expression tag	UNP Q8G9Q2
C	2842	GLU	-	expression tag	UNP Q8G9Q2
C	2843	GLY	-	expression tag	UNP Q8G9Q2
C	2844	LYS	-	expression tag	UNP Q8G9Q2
C	2845	PRO	-	expression tag	UNP Q8G9Q2
C	2846	ILE	-	expression tag	UNP Q8G9Q2
C	2847	PRO	-	expression tag	UNP Q8G9Q2
C	2848	ASN	-	expression tag	UNP Q8G9Q2
C	2849	PRO	-	expression tag	UNP Q8G9Q2
C	2850	LEU	-	expression tag	UNP Q8G9Q2
C	2851	LEU	-	expression tag	UNP Q8G9Q2
C	2852	GLY	-	expression tag	UNP Q8G9Q2
C	2853	LEU	-	expression tag	UNP Q8G9Q2
C	2854	ASP	-	expression tag	UNP Q8G9Q2
C	2855	SER	-	expression tag	UNP Q8G9Q2
C	2856	THR	-	expression tag	UNP Q8G9Q2
C	2857	ARG	-	expression tag	UNP Q8G9Q2
C	2858	THR	-	expression tag	UNP Q8G9Q2
C	2859	GLY	-	expression tag	UNP Q8G9Q2
C	2860	HIS	-	expression tag	UNP Q8G9Q2
C	2861	HIS	-	expression tag	UNP Q8G9Q2
C	2862	HIS	-	expression tag	UNP Q8G9Q2
C	2863	HIS	-	expression tag	UNP Q8G9Q2
C	2864	HIS	-	expression tag	UNP Q8G9Q2
C	2865	HIS	-	expression tag	UNP Q8G9Q2
D	1758	ALA	-	expression tag	UNP Q8G9Q2
D	2836	LYS	-	expression tag	UNP Q8G9Q2
D	2837	GLY	-	expression tag	UNP Q8G9Q2
D	2838	GLU	-	expression tag	UNP Q8G9Q2
D	2839	LEU	-	expression tag	UNP Q8G9Q2
D	2840	LYS	-	expression tag	UNP Q8G9Q2
D	2841	LEU	-	expression tag	UNP Q8G9Q2
D	2842	GLU	-	expression tag	UNP Q8G9Q2
D	2843	GLY	-	expression tag	UNP Q8G9Q2
D	2844	LYS	-	expression tag	UNP Q8G9Q2
D	2845	PRO	-	expression tag	UNP Q8G9Q2
D	2846	ILE	-	expression tag	UNP Q8G9Q2

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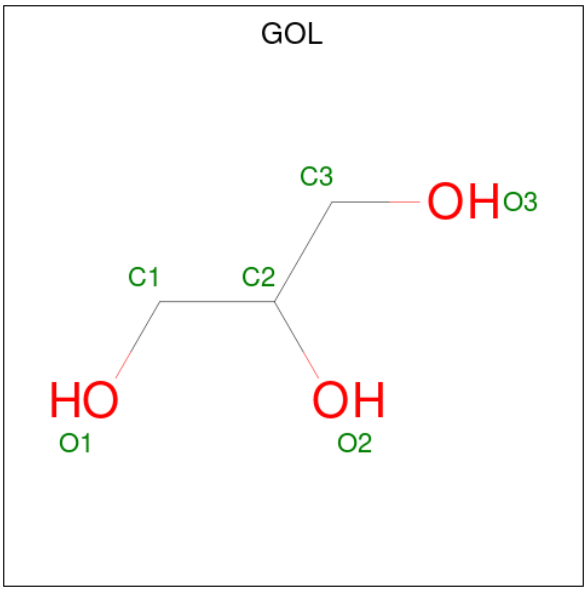
Chain	Residue	Modelled	Actual	Comment	Reference
D	2847	PRO	-	expression tag	UNP Q8G9Q2
D	2848	ASN	-	expression tag	UNP Q8G9Q2
D	2849	PRO	-	expression tag	UNP Q8G9Q2
D	2850	LEU	-	expression tag	UNP Q8G9Q2
D	2851	LEU	-	expression tag	UNP Q8G9Q2
D	2852	GLY	-	expression tag	UNP Q8G9Q2
D	2853	LEU	-	expression tag	UNP Q8G9Q2
D	2854	ASP	-	expression tag	UNP Q8G9Q2
D	2855	SER	-	expression tag	UNP Q8G9Q2
D	2856	THR	-	expression tag	UNP Q8G9Q2
D	2857	ARG	-	expression tag	UNP Q8G9Q2
D	2858	THR	-	expression tag	UNP Q8G9Q2
D	2859	GLY	-	expression tag	UNP Q8G9Q2
D	2860	HIS	-	expression tag	UNP Q8G9Q2
D	2861	HIS	-	expression tag	UNP Q8G9Q2
D	2862	HIS	-	expression tag	UNP Q8G9Q2
D	2863	HIS	-	expression tag	UNP Q8G9Q2
D	2864	HIS	-	expression tag	UNP Q8G9Q2
D	2865	HIS	-	expression tag	UNP Q8G9Q2

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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	9	9	9	0	0
4	B	10	10	10	0	0
4	C	6	6	6	0	0

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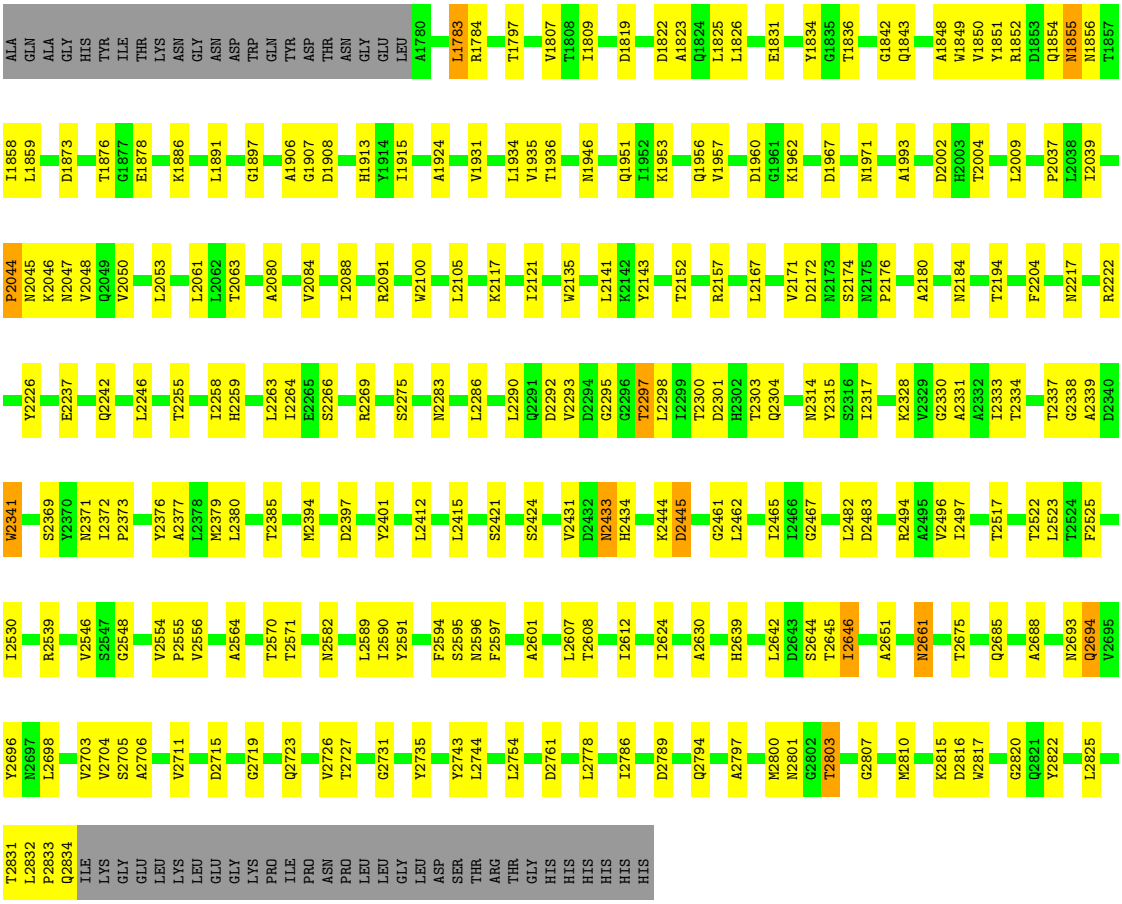
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	8	8	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

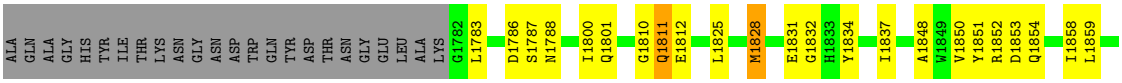
- Molecule 1: Dextransucrase

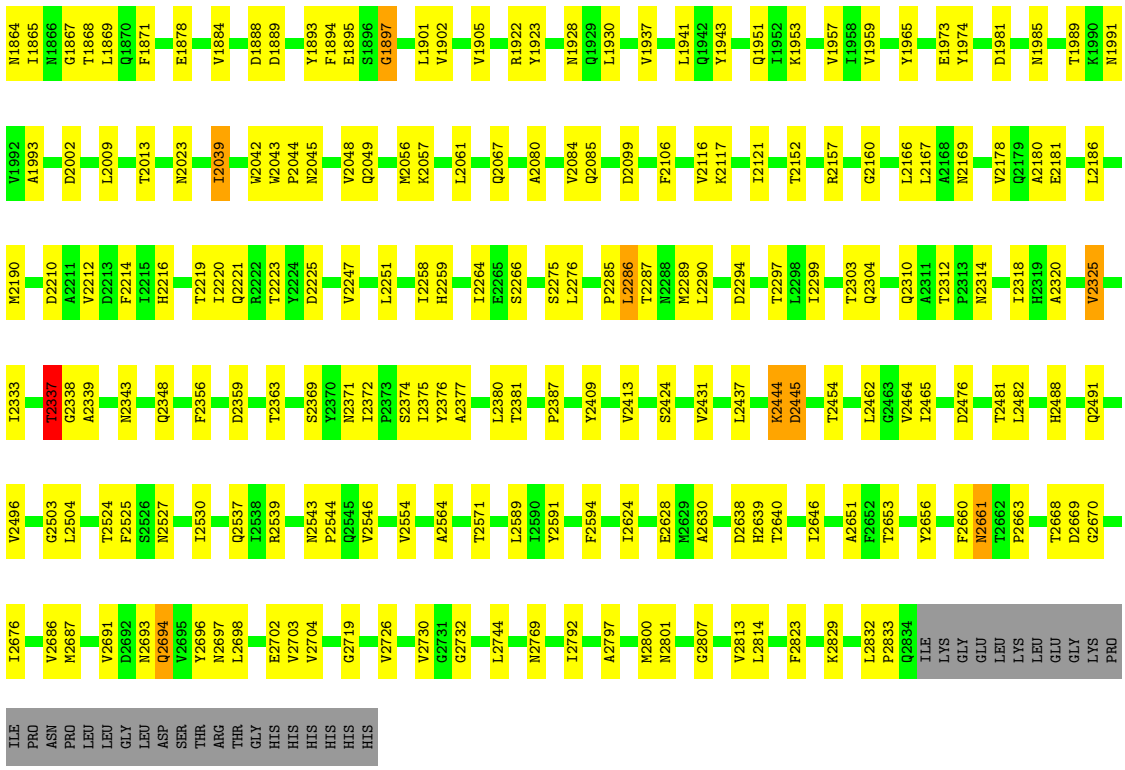
Chain A:



- Molecule 1: Dextransucrase

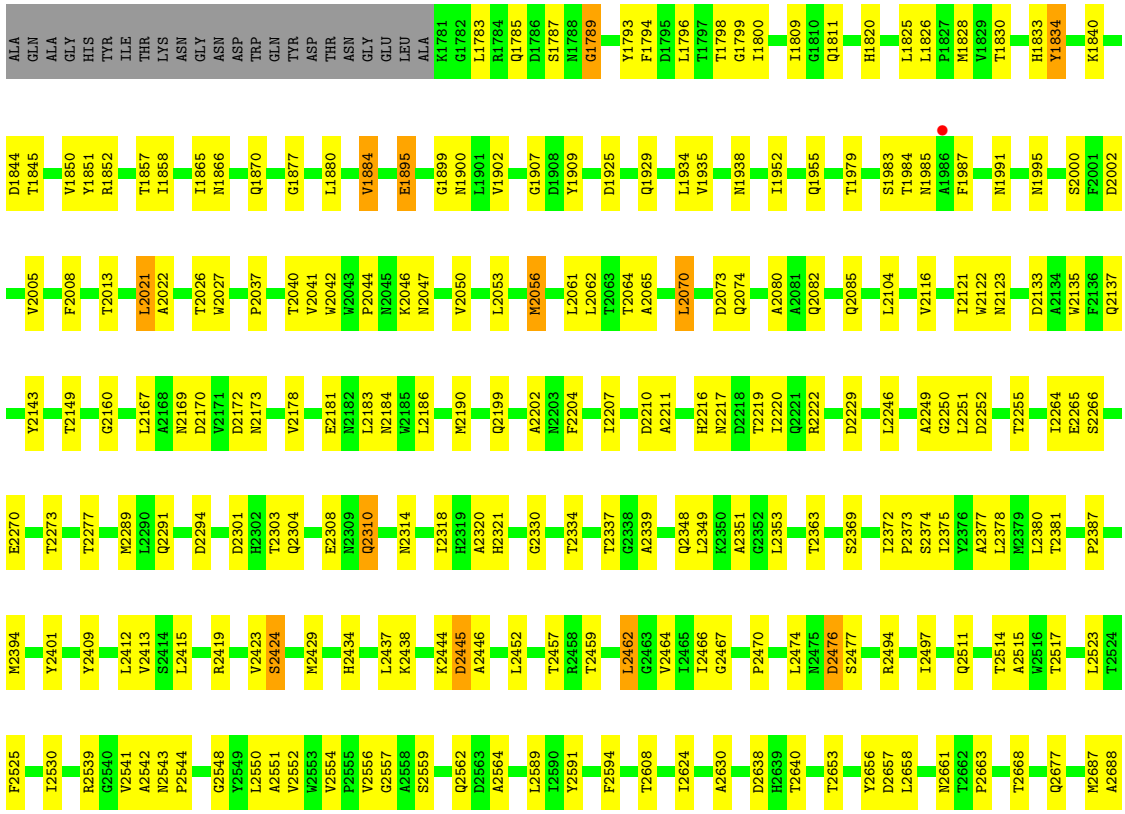
Chain B:

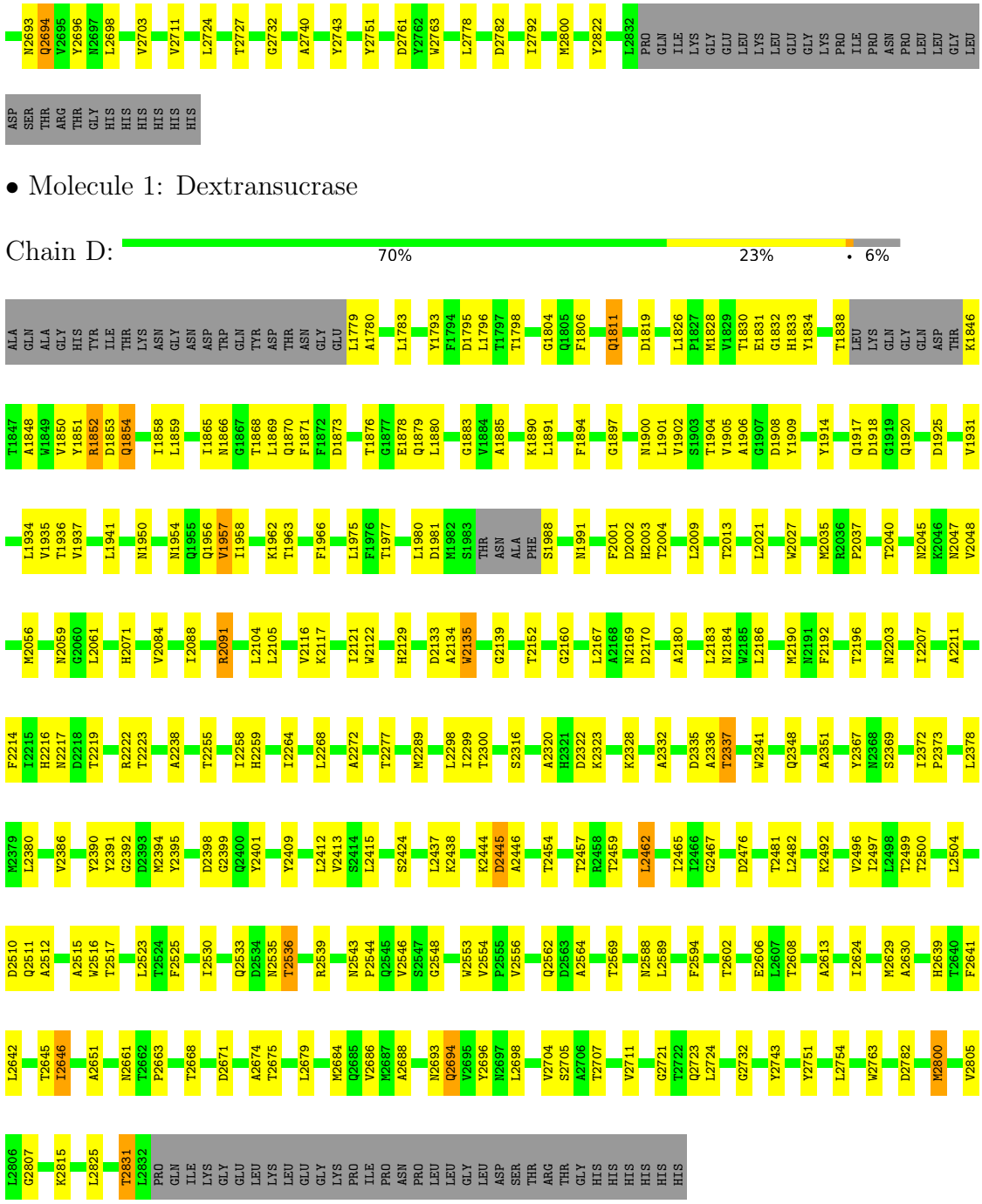




- Molecule 1: Dextransucrase

Chain C:





• Molecule 1: Dextransucrase

Chain D: 70% 23% • 6%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.84Å 140.04Å 155.46Å 85.36° 90.92° 76.85°	Depositor
Resolution (Å)	51.62 – 3.30 51.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (51.62-3.30) 97.5 (51.62-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.291 0.227 , 0.290	Depositor DCC
R_{free} test set	4029 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , -12.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.055 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	32341	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, GOL

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	0.54	1/8308 (0.0%)	0.61	0/11325
1	B	0.54	2/8291 (0.0%)	0.60	0/11302
1	C	0.54	2/8255 (0.0%)	0.59	0/11260
1	D	0.54	4/8131 (0.0%)	0.59	0/11091
All	All	0.54	9/32985 (0.0%)	0.60	0/44978

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1973	GLU	CD-OE2	7.00	1.33	1.25
1	A	2341	TRP	CD2-CE2	5.53	1.48	1.41
1	D	2553	TRP	CD2-CE2	5.34	1.47	1.41
1	D	2516	TRP	CD2-CE2	5.29	1.47	1.41
1	C	2042	TRP	CD2-CE2	5.19	1.47	1.41

There are no bond angle outliers.

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	8122	0	7431	170	0
1	B	8105	0	7419	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	8071	0	7358	167	0
1	D	7952	0	7198	191	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	0	0
3	B	12	0	16	1	0
3	C	18	0	24	1	0
3	D	18	0	24	0	0
4	A	9	0	0	0	0
4	B	10	0	0	0	0
4	C	6	0	0	0	0
4	D	8	0	0	0	0
All	All	32341	0	29478	676	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 11.

The worst 5 of 676 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:1850:VAL:HG11	1:B:1858:ILE:HG23	1.25	1.16
1:D:2059:ASN:HD22	1:D:2104:LEU:HD11	1.17	1.07
1:B:1812:GLU:CG	1:B:1825:LEU:HD11	1.86	1.06
1:A:1850:VAL:CG1	1:A:1858:ILE:HG23	1.93	0.98
1:D:2533:GLN:O	1:D:2536:THR:HG23	1.64	0.96

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	1054/1108 (95%)	965 (92%)	73 (7%)	16 (2%)	10	38
1	B	1052/1108 (95%)	963 (92%)	75 (7%)	14 (1%)	12	40
1	C	1051/1108 (95%)	961 (91%)	79 (8%)	11 (1%)	15	46
1	D	1038/1108 (94%)	953 (92%)	77 (7%)	8 (1%)	19	51
All	All	4195/4432 (95%)	3842 (92%)	304 (7%)	49 (1%)	13	42

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1819	ASP
1	A	1852	ARG
1	A	1855	ASN
1	A	2337	THR
1	B	1787	SER

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	823/925 (89%)	800 (97%)	23 (3%)	43	70
1	B	819/925 (88%)	801 (98%)	18 (2%)	52	74
1	C	814/925 (88%)	797 (98%)	17 (2%)	53	75
1	D	790/925 (85%)	775 (98%)	15 (2%)	57	77
All	All	3246/3700 (88%)	3173 (98%)	73 (2%)	52	74

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2800	MET
1	D	2800	MET
1	D	1957	VAL
1	D	2476	ASP
1	B	1828	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1985	ASN
1	C	2260	ASN
1	D	2259	HIS
1	C	2074	GLN
1	C	2184	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	GOL	D	2868	-	5,5,5	0.24	0	5,5,5	0.64	0
3	GOL	D	2869	-	5,5,5	0.23	0	5,5,5	0.48	0
3	GOL	C	2869	-	5,5,5	0.42	0	5,5,5	0.28	0
3	GOL	A	2867	-	5,5,5	0.18	0	5,5,5	0.46	0
3	GOL	B	2868	-	5,5,5	0.45	0	5,5,5	0.46	0
3	GOL	D	2867	-	5,5,5	0.32	0	5,5,5	0.17	0
3	GOL	C	2868	-	5,5,5	0.45	0	5,5,5	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	C	2867	-	5,5,5	0.24	0	5,5,5	0.46	0
3	GOL	B	2867	-	5,5,5	0.12	0	5,5,5	0.54	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
3	GOL	D	2868	-	-	0/4/4/4	-
3	GOL	D	2869	-	-	2/4/4/4	-
3	GOL	C	2869	-	-	2/4/4/4	-
3	GOL	A	2867	-	-	0/4/4/4	-
3	GOL	B	2868	-	-	0/4/4/4	-
3	GOL	D	2867	-	-	3/4/4/4	-
3	GOL	C	2868	-	-	4/4/4/4	-
3	GOL	C	2867	-	-	2/4/4/4	-
3	GOL	B	2867	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2868	GOL	O1-C1-C2-C3
3	D	2867	GOL	C1-C2-C3-O3
3	C	2868	GOL	O2-C2-C3-O3
3	C	2867	GOL	C1-C2-C3-O3
3	C	2868	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2868	GOL	1	0
3	C	2868	GOL	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	1055/1108 (95%)	-0.24	0	100	100	18, 30, 48, 82	0
1	B	1053/1108 (95%)	-0.31	0	100	100	15, 27, 45, 64	0
1	C	1052/1108 (94%)	-0.22	1 (0%)	95	97	16, 33, 56, 79	0
1	D	1043/1108 (94%)	-0.23	0	100	100	21, 34, 55, 80	0
All	All	4203/4432 (94%)	-0.25	1 (0%)	100	100	15, 31, 52, 82	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1986	ALA	2.5

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)

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, 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
3	GOL	B	2868	6/6	0.90	0.30	27,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	2868	6/6	0.92	0.38	29,31,33,34	0
2	CA	B	2866	1/1	0.95	0.12	44,44,44,44	0
3	GOL	B	2867	6/6	0.96	0.23	13,13,13,13	0
3	GOL	C	2869	6/6	0.96	0.14	20,21,21,21	0
3	GOL	D	2867	6/6	0.96	0.15	20,21,21,21	0
3	GOL	D	2868	6/6	0.96	0.27	20,21,22,24	0
2	CA	A	2866	1/1	0.97	0.14	51,51,51,51	0
3	GOL	C	2867	6/6	0.97	0.19	25,26,26,26	0
3	GOL	A	2867	6/6	0.98	0.17	15,15,15,16	0
2	CA	C	2866	1/1	0.98	0.12	30,30,30,30	0
3	GOL	D	2869	6/6	0.98	0.23	25,25,26,26	0
2	CA	D	2866	1/1	0.99	0.11	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.