



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 11:25 pm BST

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](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.

---

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	:	2.11
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)	:	2.11

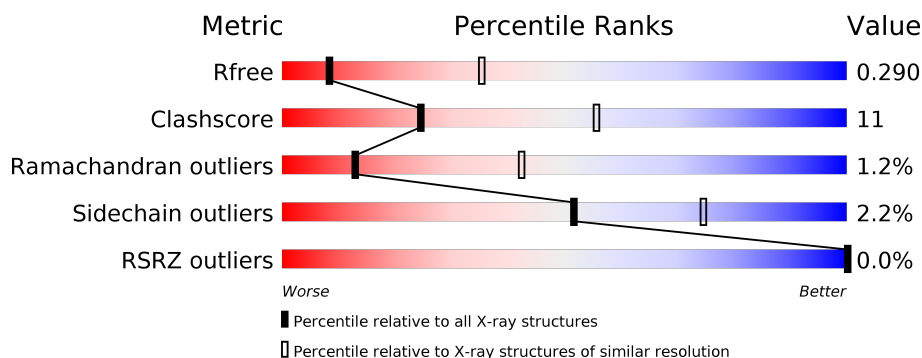
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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 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 style="width: 74%;"></div> <div style="width: 20%;"></div> <div style="width: 5%;"></div> </div> <div>74% 20% • 5%</div>
1	B	1108	<div> <div style="width: 75%;"></div> <div style="width: 19%;"></div> <div style="width: 5%;"></div> </div> <div>75% 19% • 5%</div>
1	C	1108	<div> <div style="width: 73%;"></div> <div style="width: 21%;"></div> <div style="width: 5%;"></div> </div> <div>73% 21% • 5%</div>
1	D	1108	<div> <div style="width: 70%;"></div> <div style="width: 23%;"></div> <div style="width: 6%;"></div> </div> <div>70% 23% • 6%</div>

## 2 Entry composition

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
1	A	1055	Total	C	N	O	S	0	1	0
			8122	5088	1377	1638	19			
1	B	1053	Total	C	N	O	S	0	1	0
			8105	5088	1364	1635	18			
1	C	1052	Total	C	N	O	S	0	1	0
			8071	5062	1358	1633	18			
1	D	1043	Total	C	N	O	S	0	1	0
			7952	4988	1339	1607	18			

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is water.

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

*Continued on next page...*

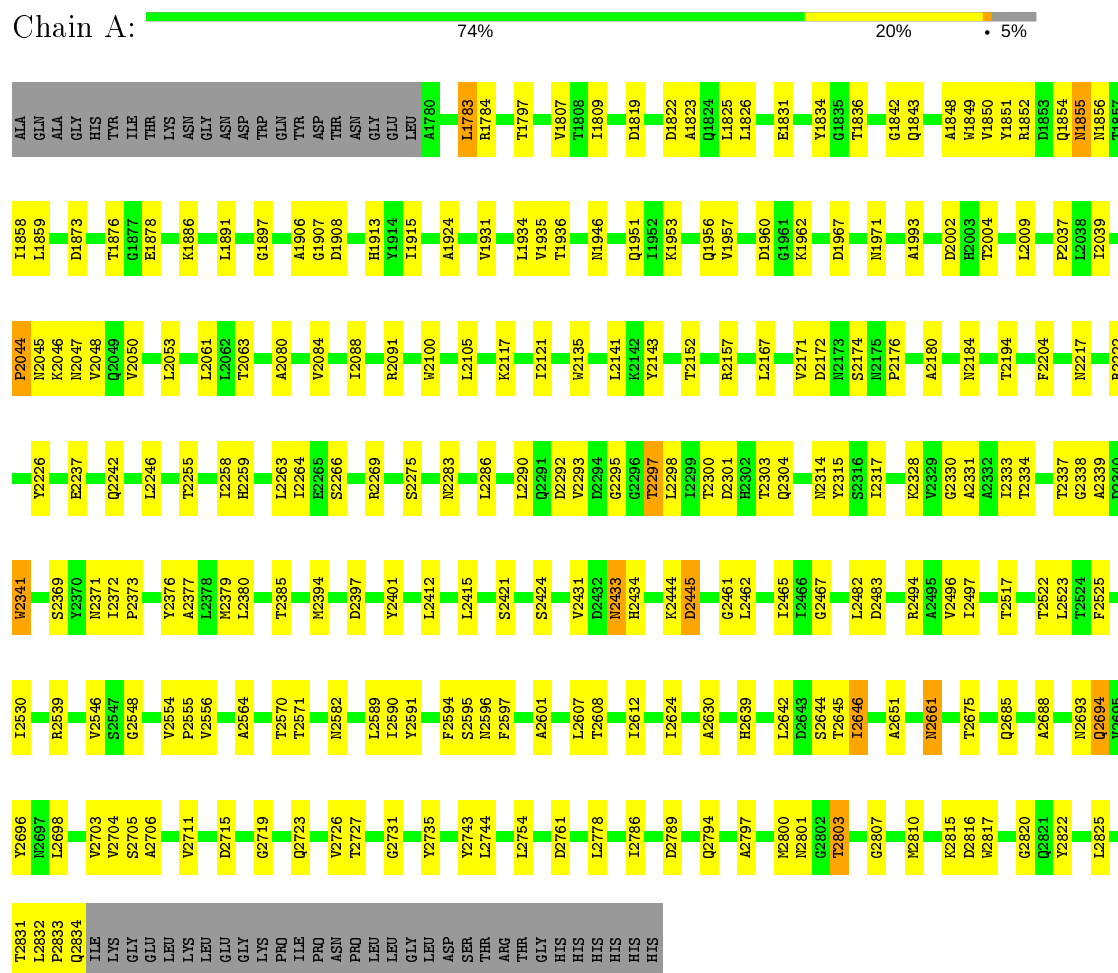
*Continued from previous page...*

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



I1864	V1992	I2333	V2496	I2676	I1864
I1865	A1993	T2337	Q2503	V2686	I1845
I1866	D2002	A2339	L2504	M2687	V1850
I1867	L2009	N2343	T2524	V2691	I1851
I1868	T2013	N2343	P2525	D2692	R1852
I1869	N2023	Q2348	S2526	N2693	T1857
I1870	E1878	Q2348	N2527	Q2694	I1858
I1871	L2039	F2356	I2530	V2696	T1865
I1878	D2042	D2359	Q2537	T2697	I1866
I1884	W2043	T2363	I2538	L2698	Q1870
D1888	P2044	S2369	R2539	E2702	G1877
D1889	N2045	N2370	N2543	V2703	T2040
Y1893	V2048	I2371	P2544	V2704	V2042
F1894	Q2049	I2372	Q2545	G2719	W2043
I1895	M2056	P2373	V2546	V2726	P2044
S1896	K2057	S2374	V2554	V2730	P2046
G1897	L2061	I2376	A2564	G2731	K2046
L1901	Q2067	A2377	T2571	G2732	N2047
V1902	A2080	L2380	L2589	L2744	V2050
V1905	V2084	T2381	I2590	N2769	L2053
R1922	Q2085	S2275	Y2591	I2792	M2056
Y1923	D2099	L2276	F2594	A2797	L2061
N1928	D2106	P2285	I2624	M2800	L2062
I1929	V2116	T2286	E2628	F1794	T2063
I1930	K2117	N2288	N2629	N2801	A2065
V1937	I2121	L2290	A2630	G2807	L2070
L1941	Q1951	D2294	D2638	V2813	D2073
I1942	I1952	T2297	H2639	L2814	Q2074
Y1943	K1953	L2386	T2640	F2823	A2080
Q1951	T2152	I2299	I2646	H1809	A2081
V1957	R2157	T2303	A2651	Q1810	Q2082
I1958	G2160	Q2304	T2652	Q1811	Q2085
V1959	L2166	V2463	T2653	H1820	L2104
Y1965	L2167	I2465	Y2656	L1825	V2116
Y1973	A2168	D2476	F2660	L1826	Q2250
Y1974	N2169	T2481	N2661	F1827	L2251
D1981	V2178	L2482	T2662	M1828	L2252
Q2179	A2180	L2348	L2663	V1829	D2255
I1985	E2181	H2488	T2668	T1830	T2255
T1989	L2186	Q2491	G2670	H1833	I2264
K1990				Y1834	E2265
N1991				K1840	S2266

• Molecule 1: Dextransucrase

Chain C:  73% 21% 5%

ALA	D1844	V2005	Y2143	E2270	N2394	F2525
GLN	T1845	F2008	T2149	T2273	Y2401	I2530
ALA	V1850	T2013	G2160	T2277	Y2409	R2539
GLY	I1851	L2021	L2167	M2289	L2412	G2540
HIS	R1852	A2022	A2168	L2290	V2413	V2541
LEU	T1857	T2026	N2169	Q2291	S2414	A2542
ILE	I1858	W2027	D2170	D2294	L2415	N2543
THR	T1865	P2037	V2171	D2301	R2419	P2544
ASP	I1866	G1870	N2172	E2302	Y2423	Q2548
ASP	Q1870	G1877	N2173	Q2303	V2423	Y2549
TRP	T2040	T2042	V2178	Q2304	S2424	L2550
GLN	V2042	W2043	E2181	E2308	N2429	A2551
ASP	P2044	P2046	L2183	N2309	H2434	V2553
ASN	N2045	K2046	N2184	Q2310	L2437	V2554
GLY	N2047	N2047	N2185	N2314	K2438	P2555
LEU	ALA	V2050	L2186	N2318	K2444	V2556
ALA	K1781	L2053	N2190	I2319	D2445	G2557
G1782	L1783	L1902	Q2199	A2320	A2446	A2558
I1785	Q1784	V1902	G2330	E2321	L2452	S2559
D1786	G1907	G1907	N2203	G2334	T2457	Q2562
S1787	I1908	L2061	F2204	T2337	R2458	I2589
N1788	Y1909	L2062	T2207	A2338	T2459	L2590
G1789	D1925	T2063	D2210	G2339	L2463	Y2591
Y1793	I1929	A2065	A2211	L2464	V2464	F2594
D1795	L1934	L2070	H2216	Q2348	I2465	T2608
L1796	V1935	D2073	N2217	L2349	L2466	I2624
T1797	N1938	Q2074	D2218	F2350	G2467	A2630
G1799	N1952	A2080	I2220	A2351	P2470	D2638
I1800	Q1955	A2081	Q2221	G2352	T2475	H2639
H1810	Q1955	Q2082	R2222	L2353	N2476	T2640
Q1811	T1979	Q2085	D2229	T2363	D2476	T2653
H1820	S1983	L2104	L2246	S2369	S2477	Y2656
L1825	T1984	V2116	Q2250	I2372	R2494	D2657
L1826	N1985	I2121	L2251	P2373	L2497	L2658
F1827	A1986	W2122	D2252	S2374	Q2511	N2661
M1828	F1987	N2123	T2255	I2375	T2514	T2662
V1829	N1991	N2123	T2255	Y2376	A2515	P2663
T1830	N1991	D2133	I2264	I2378	N2516	T2668
H1833	N1995	A2134	E2265	L2378	T2517	Q2677
Y1834	S2000	F2136	S2266	L2380	L2523	M2687
K1840	D2002	Q2137		T2381	T2524	A2688



Chain D:  70% 23% • 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	42.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , -12.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	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 <sup>2</sup> )	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.*

<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: GOL, CA

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

*Continued on next page...*

*Continued from previous page...*

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 ⓘ

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	B	2310	GLN
1	B	2800	MET
1	D	2539	ARG
1	B	2539	ARG
1	C	1834	TYR

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

Mol	Chain	Res	Type
1	B	2742	GLN
1	C	2082	GLN
1	D	2260	ASN
1	B	2766	ASN
1	C	1805	GLN

### 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 carbohydrates 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	C	2868	-	5,5,5	0.45	0	5,5,5	0.42	0
3	GOL	A	2867	-	5,5,5	0.18	0	5,5,5	0.46	0
3	GOL	C	2867	-	5,5,5	0.24	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	D	2868	-	5,5,5	0.24	0	5,5,5	0.64	0
3	GOL	C	2869	-	5,5,5	0.42	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	B	2867	-	5,5,5	0.12	0	5,5,5	0.54	0
3	GOL	D	2869	-	5,5,5	0.23	0	5,5,5	0.48	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	C	2868	-	-	4/4/4/4	-
3	GOL	A	2867	-	-	0/4/4/4	-
3	GOL	C	2867	-	-	2/4/4/4	-
3	GOL	B	2868	-	-	0/4/4/4	-
3	GOL	D	2867	-	-	3/4/4/4	-
3	GOL	D	2868	-	-	0/4/4/4	-
3	GOL	C	2869	-	-	2/4/4/4	-
3	GOL	B	2867	-	-	0/4/4/4	-
3	GOL	D	2869	-	-	2/4/4/4	-

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	2868	GOL	C1-C2-C3-O3
3	C	2867	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	C	2868	GOL	1	0
3	B	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, 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	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 carbohydrates 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
3	GOL	B	2868	6/6	0.90	0.30	27,29,29,29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	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	D	2868	6/6	0.96	0.27	20,21,22,24	0
3	GOL	C	2869	6/6	0.96	0.14	20,21,21,21	0
3	GOL	B	2867	6/6	0.96	0.23	13,13,13,13	0
3	GOL	D	2867	6/6	0.96	0.15	20,21,21,21	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.