



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:24 PM GMT

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 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

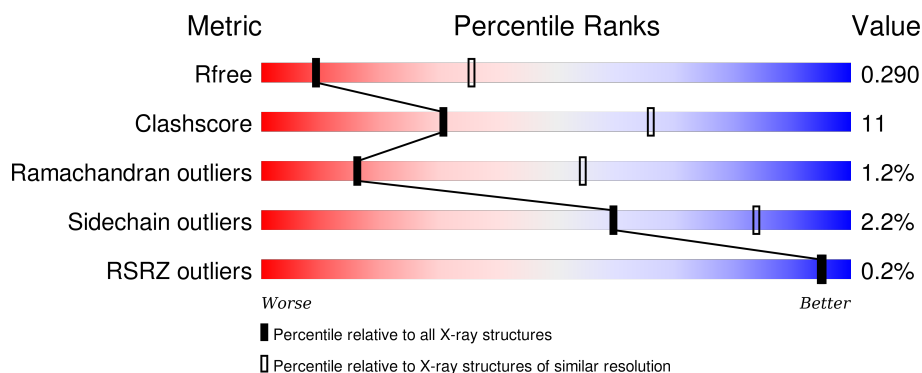
1 Overall quality at a glance

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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 74% 20% • 5%
1	B	1108	 75% 19% • 5%
1	C	1108	 73% 21% • 5%
1	D	1108	 70% 23% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	2868	-	-	-	X
3	GOL	C	2868	-	-	-	X

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

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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
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: C₃H₈O₃).



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		

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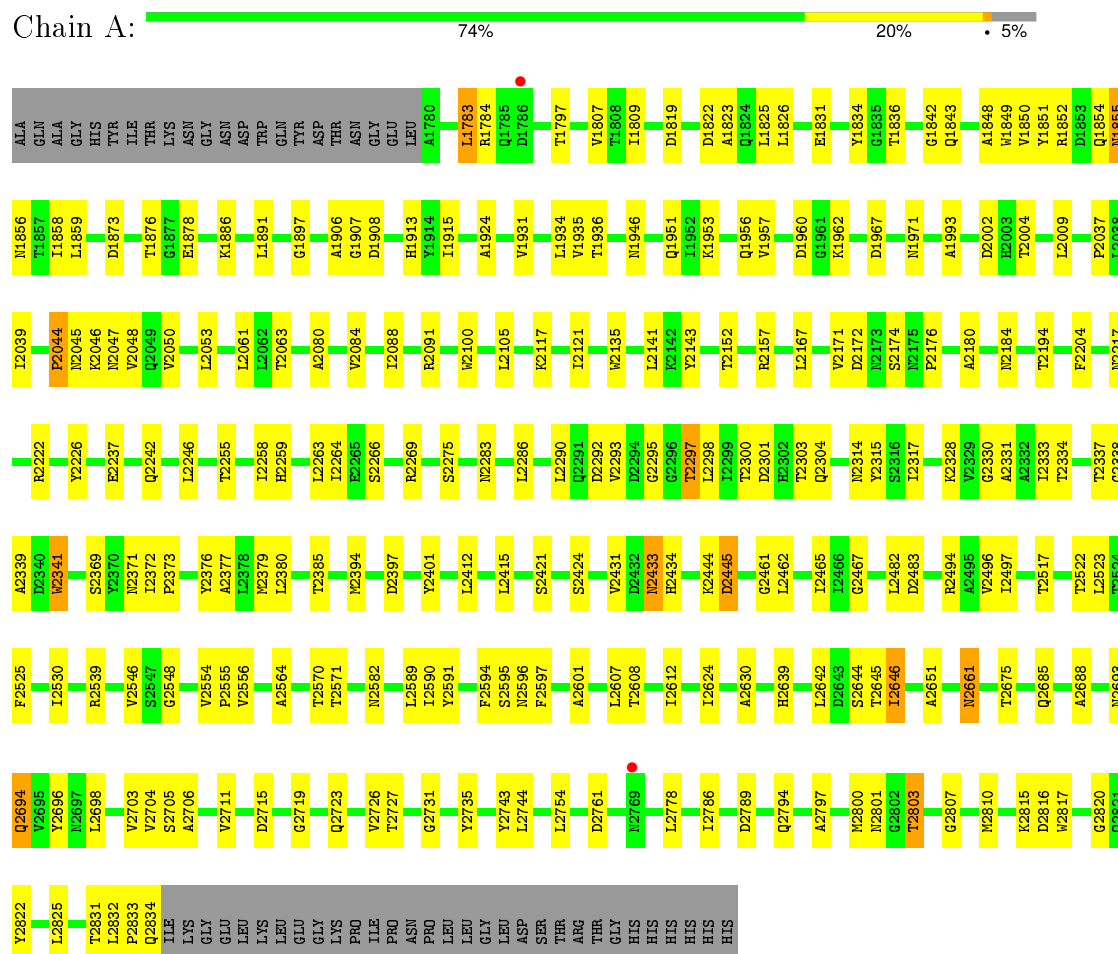
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	8	Total	O	0	0
			8	8		

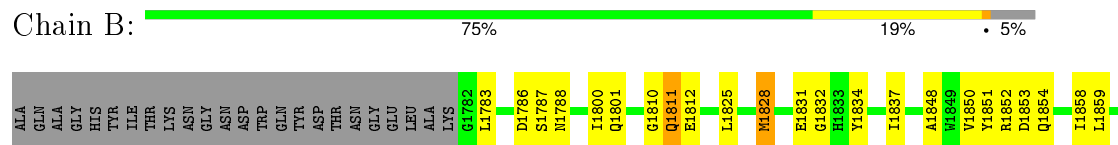
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



• Molecule 1: Dextransucrase



ILE	I2676	V2496	I2333	M2190	V1992	M1864
PRO	V2686	G2503	T2337	D2210	A1993	I1866
ASN	M2687	L2504	G2338	A2211	D2002	G1867
PRO			A2339	V2212		T1868
LEU				D2213		L1869
LEU	V2691	T2524	M2343	F2214	L2009	Q1870
GLY	D2692	F2525		L2215	T2013	F1871
LEU	M2693	S2526		H2216		
ASP	Q2694	N2527	Q2348		M2023	E1878
SER	V2695					
THR	V2696	L2530	F2356	T2219	I2039	V1884
ARG	N2697	Q2537		L2220		
THR	L2698	L2538	D2359	Q2221		
GLY		R2539		T2222	W2042	D1888
HIS	E2702	R2539	T2363	T2223	W2043	D1889
HIS	V2703			V2224	P2044	
HIS	V2704	M2543	S2369	D2225	M2045	Y1893
HIS		P2544	E2370			F1894
HIS	G2719	Q2545	M2371	V2247	Q2048	E1895
HIS		V2546	L2372		Q2049	S1896
HIS	V2726		S2373	L2251		G1897
		V2554	S2374		M2056	
	V2730	L2559	T2375	I2258	K2057	L1901
	G2731	A2564	V2376	H2259		V1902
	G2732		A2377		L2061	
	L2744	T2571		I2264		V1905
		L2589	L2380	E2265	Q2067	R1922
	N2769	T2590	T2381	S2266		Y1923
		Y2591				
	I2792	F2594	P2387	S2275	V2084	M1928
	A2797		Y2409	L2276	Q2085	Q1929
		L2624	V2413	T2285		L1930
	M2800	E2628		L2286	D2099	V1937
	N2801	F2629	S2424	T2287	F2106	
	G2807	A2630	V2431	M2289	V2116	L1941
				L2290	K2117	Q1942
	V2813	D2638	L2437	D2294		Y1943
	L2814	H2639			I2121	Q1951
		T2640			T2152	I1952
	F2823		K2444	T2297		K1953
			D2445	L2299		
		L2646			R2157	V1957
	K2829	A2651	T2454	T2303		I1958
	L2832	F2652	L2462	Q2304	G2160	V1959
	P2833	T2653	G2465			
	Q2834		V2464	Q2310	L2166	Y1965
ILE			I2465	A2311	L2167	E1973
LYS		Y2656		T2312	A2168	
GLY		F2660	D2476	P2313	M2169	Y1974
GLU		N2661		M2314		
LEU		T2662	T2481		V2178	D1981
LEU		P2663	L2482	I2318	Q2179	
LEU			H2319	A2180	E2179	N1985
GLU		T2668	H2483	A2320	E2181	
GLY		D2669				T1989
LEU		G2670	Q2491	V2325	L2186	F1990
PRO						N1991

- Molecule 1: Dextranucrase

Chain C:  73% 21% • 5%

L2523	P2387	S2266	F2136	F2001	G1842	ALA
T2524	M2394	E2270	Q2137	D2002	Q1843	GLN
F2525	M2394	E2270	Y2143	V2005	T1845	GLY
L2530	Y2401	T2273	T2149	F2008	V1850	TYR
R2539	Y2409	T2277	G2160	T2013	V1851	ILE
Q2540	L2412	M2289	L2167	L2021	R1852	THR
V2541	V2413	L2290	A2168	A2022	T1857	LYS
A2542	S2414	Q2291	R2169	T2026	T1858	ASN
L2543	L2415	D2294	D2170	W2027	T1865	GLY
P2544	R2419	D2301	V2171	W2027	M1866	ASN
Q2548	V2423	R2302	D2172	P2037	Q1870	TRP
R2549	S2424	T2303	M2173	T2040	Q1877	GLN
V2550	M2429	Q2304	V2178	W2041	G1887	TYR
A2551	H2434	E2308	E2181	W2042	L1880	ASP
V2552	H2434	M2309	R2182	W2043	L1880	ASN
V2553	L2437	Q2310	L2183	P2044	L1880	GLY
P2556	K2438	M2314	M2185	W2045	V1884	GLU
G2557	K2438	M2314	L2186	M2047	H1895	LEU
A2558	K2444	T2318	M2190	V2050	G1899	ALA
S2559	T2445	H2319	M2199	L2061	L1783	K1781
Q2562	A2446	A2320	Q2199	L2062	L1783	K1782
L2563	L2452	H2321	Q2199	L2063	L1901	L1784
A2564	L2452	G2330	A2202	A2064	V1902	Q1785
L2589	T2457	T2334	M2203	A2064	G1907	D1786
Y2591	T2458	T2334	F2204	A2064	D1908	S1787
F2594	T2459	T2337	I2207	A2064	V1909	H1788
T2608	L2462	G2338	I2207	T2063	D1925	G1789
L2624	G2463	G2339	D2210	L2064	D1925	Y1793
A2630	V2464	A2339	A2211	L2064	F1794	F1794
L2624	L2465	Q2348	H2216	L2070	D1795	D1795
A2630	L2466	L2349	M2217	L2070	T1797	L1796
L2638	G2467	K2350	D2218	D2073	L1934	T1798
R2639	P2470	A2351	T2219	Q2074	G1799	G1799
T2640	L2474	L2352	T2220	A2080	V1935	I1800
T2653	L2475	T2363	Q2221	A2081	M1938	I1809
Y2656	D2476	T2369	R2222	Q2082	L1952	Q1810
D2657	S2477	T2372	D2229	Q2085	Q1955	Q1811
L2658	R2494	T2373	L2246	L2104	T1979	H1820
L2661	L2497	S2374	A2249	V2116	S1983	L1825
T2662	Q2511	T2375	G2250	T2121	T1984	P1827
P2663	T2514	T2376	L2251	T2121	M1828	M1828
T2668	A2515	L2377	D2252	T2122	A1986	V1829
Q2677	A2516	T2378	T2255	T2122	F1987	T1830
	T2517	L2380	T2264	M1991	M1991	H1833
		T2381	F2265	D2133	Y1834	Y1834
			F2265	A2134		K1840
				T2135		G1843

4 Data and refinement statistics

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) 90.0 (51.62-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.29%)	DCC
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.055 for h,h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 80174 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, 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

All (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
1	B	2042	TRP	CD2-CE2	5.16	1.47	1.41
1	D	2135	TRP	CD2-CE2	5.12	1.47	1.41
1	D	2763	TRP	CD2-CE2	5.05	1.47	1.41
1	C	2763	TRP	CD2-CE2	5.04	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

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
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.

All (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
1:A:2601:ALA:HB3	1:A:2607:LEU:HD23	1.48	0.92
1:B:2445:ASP:CG	1:B:2454:THR:HG23	1.93	0.89
1:B:2571:THR:HG23	1:C:2476:ASP:HB2	1.54	0.89
1:A:2601:ALA:CB	1:A:2607:LEU:HD23	2.05	0.87
1:A:2693:ASN:HD22	1:A:2694:GLN:HE21	1.17	0.87
1:D:2059:ASN:ND2	1:D:2104:LEU:HD11	1.88	0.87
1:A:2831:THR:CG2	1:A:2833:PRO:HD2	2.05	0.86
1:C:1985:ASN:HD21	1:C:2082:GLN:HE22	1.20	0.85
1:D:2445:ASP:OD1	1:D:2454:THR:HG23	1.78	0.84
1:B:2266:SER:HB3	1:B:2314:ASN:HD22	1.42	0.84
1:A:1850:VAL:HG11	1:A:1858:ILE:HG23	1.61	0.82
1:D:2515:ALA:HB2	1:D:2530:ILE:HG21	1.60	0.81
1:C:2056:MET:HE1	1:C:2104:LEU:HD21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2046:LYS:O	1:C:2050:VAL:HG23	1.80	0.81
1:A:2831:THR:HG23	1:A:2833:PRO:HD2	1.59	0.80
1:B:1865:ILE:O	1:B:1868:THR:HG22	1.83	0.79
1:A:2444:LYS:O	1:A:2445:ASP:HB2	1.81	0.79
1:B:2043:TRP:CE3	1:B:2049:GLN:NE2	2.52	0.78
1:A:2693:ASN:HD22	1:A:2694:GLN:NE2	1.81	0.78
1:C:1985:ASN:HD21	1:C:2082:GLN:NE2	1.83	0.77
1:D:2056:MET:CE	1:D:2105:LEU:HD21	2.14	0.77
1:C:1850:VAL:HG11	1:C:1858:ILE:HG23	1.66	0.76
1:B:2290:LEU:HD21	1:B:2431:VAL:HG23	1.69	0.75
1:D:2424[A]:SER:HB2	1:D:2564:ALA:HB1	1.69	0.75
1:C:2021:LEU:HD22	1:C:2027:TRP:CE2	2.23	0.73
1:B:2445:ASP:OD2	1:B:2454:THR:HG23	1.87	0.73
1:D:2629:MET:CE	1:D:2675:THR:HG21	2.19	0.73
1:C:1985:ASN:ND2	1:C:2082:GLN:HE22	1.86	0.73
1:D:2444:LYS:O	1:D:2445:ASP:HB2	1.86	0.73
1:A:1854:GLN:O	1:A:1855:ASN:HB3	1.89	0.72
1:A:2601:ALA:HB3	1:A:2607:LEU:CD2	2.19	0.71
1:C:2589:LEU:HD23	1:C:2624:ILE:HD13	1.71	0.71
1:B:2369:SER:HB2	1:B:2372:ILE:HD11	1.73	0.71
1:D:2629:MET:HE3	1:D:2675:THR:HG21	1.73	0.71
1:A:2496:VAL:O	1:A:2497:ILE:HD13	1.90	0.70
1:B:2444:LYS:O	1:B:2445:ASP:HB2	1.89	0.70
1:A:2167:LEU:HD13	1:A:2696:TYR:OH	1.92	0.69
1:B:1850:VAL:HG11	1:B:1858:ILE:CG2	2.16	0.69
1:D:2186:LEU:CD2	1:D:2223:THR:HG23	2.22	0.69
1:A:1850:VAL:HG11	1:A:1858:ILE:CG2	2.23	0.69
1:C:1907:GLY:H	1:C:1935:VAL:HG12	1.58	0.69
1:D:2009:LEU:N	1:D:2009:LEU:HD22	2.08	0.68
1:A:1876:THR:HG23	1:A:1878:GLU:H	1.59	0.68
1:C:2401:TYR:CG	1:C:2608:THR:HG23	2.29	0.68
1:D:2184:ASN:HD21	1:D:2743:TYR:H	1.42	0.68
1:D:2341:TRP:O	1:D:2642:LEU:HD13	1.94	0.68
1:B:2571:THR:HG21	1:C:2477:SER:N	2.08	0.68
1:D:2009:LEU:HD12	1:D:2013:THR:HG21	1.76	0.68
1:A:2152:THR:HB	1:A:2704:VAL:HG22	1.77	0.67
1:A:2266:SER:HB3	1:A:2314:ASN:HD22	1.58	0.67
1:C:2202:ALA:HB2	1:C:2677:GLN:HE21	1.60	0.67
1:C:1880:LEU:HD21	1:C:1884:VAL:O	1.92	0.67
1:A:2303:THR:HG22	1:A:2304:GLN:HG3	1.76	0.67
1:D:1804:GLY:O	1:D:1890:LYS:NZ	2.20	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2500:THR:HG22	1:D:2535:ASN:CG	2.16	0.66
1:B:2337:THR:HG23	1:B:2339:ALA:H	1.61	0.66
1:A:2152:THR:CB	1:A:2704:VAL:HG22	2.25	0.66
1:A:1850:VAL:CG1	1:A:1858:ILE:CG2	2.73	0.65
1:A:2831:THR:HG22	1:A:2833:PRO:HD2	1.77	0.65
1:A:1967:ASP:OD1	1:A:1971:ASN:N	2.29	0.65
1:B:2589:LEU:HD23	1:B:2624:ILE:HD13	1.78	0.65
1:C:2591:TYR:HB2	1:C:2624:ILE:HD12	1.78	0.65
1:D:2693:ASN:HD22	1:D:2694:GLN:HE21	1.45	0.65
1:C:2167:LEU:HD13	1:C:2696:TYR:OH	1.97	0.65
1:B:2693:ASN:HD22	1:B:2694:GLN:HE21	1.44	0.65
1:B:2445:ASP:OD2	1:B:2454:THR:CG2	2.44	0.65
1:B:2660:PHE:O	1:B:2661:ASN:HB2	1.97	0.65
1:D:2002:ASP:O	1:D:2013:THR:HG23	1.96	0.64
1:C:2199:GLN:NE2	1:C:2677:GLN:HE22	1.95	0.64
1:A:2009:LEU:HD11	1:A:2825:LEU:CD2	2.27	0.64
1:C:2169:ASN:HD22	1:C:2698:LEU:HD12	1.61	0.64
1:A:2831:THR:CG2	1:A:2833:PRO:CD	2.74	0.64
1:C:2444:LYS:O	1:C:2445:ASP:CB	2.44	0.64
1:C:2266:SER:HB3	1:C:2314:ASN:HD22	1.62	0.64
1:B:2221:GLN:NE2	1:B:2225:ASP:OD2	2.31	0.64
1:A:1854:GLN:O	1:A:1855:ASN:CB	2.45	0.63
1:A:2204:PHE:CG	1:A:2688:ALA:HB2	2.33	0.63
1:A:2693:ASN:ND2	1:A:2694:GLN:HE21	1.94	0.63
1:D:2594:PHE:CG	1:D:2630:ALA:HB2	2.34	0.63
1:C:2217:ASN:HB3	1:C:2255:THR:HG21	1.80	0.63
1:A:2184:ASN:HD21	1:A:2743:TYR:H	1.47	0.63
1:D:2613:ALA:HB2	1:D:2675:THR:HA	1.80	0.63
1:D:2693:ASN:HD22	1:D:2694:GLN:NE2	1.96	0.62
1:D:2679:LEU:HD22	1:D:2684:MET:HE3	1.81	0.62
1:A:2143:TYR:CE1	1:A:2727:THR:HG21	2.33	0.62
1:A:2831:THR:CG2	1:A:2833:PRO:HG2	2.30	0.62
1:B:2703:VAL:HG22	1:B:2726:VAL:HG22	1.80	0.62
1:A:2831:THR:HG22	1:A:2833:PRO:CD	2.29	0.62
1:B:2571:THR:HG21	1:C:2477:SER:H	1.64	0.62
1:D:2515:ALA:CB	1:D:2530:ILE:HG21	2.29	0.62
1:A:2494:ARG:HB3	1:A:2556:VAL:HG22	1.81	0.62
1:C:1895:GLU:O	1:C:1899:GLY:HA2	1.99	0.62
1:B:1993:ALA:HB2	1:B:2833:PRO:HG2	1.82	0.61
1:C:2056:MET:HE1	1:C:2104:LEU:CD2	2.30	0.61
1:D:1906:ALA:HB3	1:D:1935:VAL:HG12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2594:PHE:CG	1:C:2630:ALA:HB2	2.34	0.61
1:A:1850:VAL:HG13	1:A:1858:ILE:HG23	1.80	0.61
1:D:1832:GLY:HA3	1:D:1851:TYR:OH	1.99	0.61
1:C:2056:MET:CE	1:C:2104:LEU:HD21	2.31	0.61
1:B:1848:ALA:HB1	1:B:1878:GLU:HG3	1.82	0.61
1:D:2671:ASP:O	1:D:2674:ALA:HB3	2.00	0.61
1:B:2333:ILE:O	1:B:2337:THR:HG22	2.01	0.61
1:B:2376:TYR:O	1:B:2380:LEU:HD12	2.01	0.61
1:B:2669:ASP:OD1	1:B:2670:GLY:N	2.34	0.61
1:C:2046:LYS:NZ	1:C:2070:LEU:O	2.33	0.61
1:D:1865:ILE:O	1:D:1868:THR:HG22	2.00	0.61
1:C:2401:TYR:CD1	1:C:2608:THR:HG23	2.36	0.60
1:B:2181:GLU:OE2	1:B:2656:TYR:OH	2.18	0.60
1:C:2494:ARG:HB3	1:C:2556:VAL:HG22	1.84	0.60
1:B:2653:THR:HG23	1:B:2698:LEU:HD23	1.81	0.60
1:D:1988:SER:HA	1:D:1991:ASN:HD22	1.67	0.60
1:B:2488:HIS:ND1	1:B:2491:GLN:NE2	2.45	0.60
1:D:2525:PHE:CD1	1:D:2530:ILE:HD11	2.36	0.60
1:B:2465:ILE:HD11	1:B:2482:LEU:HG	1.84	0.60
1:B:1922:ARG:HD3	1:B:1930:LEU:HD11	1.84	0.60
1:C:2291:GLN:HG2	1:C:2301:ASP:OD1	2.02	0.60
1:B:2160:GLY:HA3	1:B:2216:HIS:CE1	2.37	0.59
1:C:2022:ALA:HB3	1:C:2026:THR:O	2.01	0.59
1:B:2056:MET:SD	1:B:2061:LEU:HD12	2.42	0.59
1:D:2679:LEU:HD22	1:D:2684:MET:CE	2.33	0.59
1:A:2143:TYR:HE1	1:A:2727:THR:HG21	1.67	0.59
1:B:1991:ASN:HD21	1:B:2085:GLN:HE22	1.50	0.59
1:A:2591:TYR:HB2	1:A:2624:ILE:HD12	1.84	0.59
1:B:2186:LEU:HD22	1:B:2223:THR:HG23	1.84	0.59
1:C:2693:ASN:HD22	1:C:2694:GLN:HE21	1.49	0.58
1:C:2070:LEU:HD12	1:C:2070:LEU:H	1.67	0.58
1:D:2061:LEU:HD21	1:D:2091:ARG:HE	1.68	0.58
1:C:2135:TRP:CD2	1:C:2711:VAL:HG11	2.38	0.58
1:A:2317:ILE:HA	1:A:2379:MET:HE1	1.86	0.58
1:A:1822:ASP:O	1:A:1823:ALA:HB3	2.04	0.58
1:C:2334:THR:HG22	1:C:2339:ALA:O	2.04	0.58
1:D:2289:MET:HE3	1:D:2378:LEU:HD13	1.86	0.58
1:C:1783:LEU:C	1:C:1783:LEU:HD23	2.23	0.58
1:A:2157:ARG:HG2	1:A:2801:ASN:HD22	1.69	0.58
1:A:2009:LEU:HD11	1:A:2825:LEU:HD21	1.85	0.58
1:C:2349:LEU:HD11	1:C:2353:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1783:LEU:HD23	1:A:1784:ARG:N	2.18	0.58
1:D:2693:ASN:ND2	1:D:2694:GLN:HE21	2.01	0.57
1:A:2594:PHE:CG	1:A:2630:ALA:HB2	2.39	0.57
1:A:2172:ASP:OD1	1:A:2174:SER:OG	2.21	0.57
1:C:2056:MET:HE2	1:C:2061:LEU:HD12	1.86	0.57
1:B:2591:TYR:HB2	1:B:2624:ILE:HD12	1.87	0.57
1:A:2334:THR:O	1:A:2338:GLY:N	2.36	0.57
1:B:2503:GLY:O	1:B:2504:LEU:HD23	2.05	0.56
1:B:2465:ILE:CG1	1:B:2482:LEU:HD21	2.36	0.56
1:D:2348:GLN:O	1:D:2351:ALA:HB3	2.05	0.56
1:B:1828:MET:HE1	1:B:1867:GLY:H	1.70	0.56
1:C:2143:TYR:CE1	1:C:2727:THR:HG21	2.41	0.56
1:B:2318:ILE:CD1	1:B:2375:ILE:HD13	2.35	0.56
1:D:1828:MET:HE2	1:D:1866:ASN:HA	1.86	0.56
1:A:2369:SER:HB2	1:A:2372:ILE:HD11	1.87	0.56
1:A:2831:THR:CG2	1:A:2833:PRO:CG	2.84	0.56
1:C:1985:ASN:HD21	1:C:1987:PHE:HB3	1.71	0.55
1:A:2180:ALA:O	1:A:2744:LEU:HD21	2.06	0.55
1:D:1900:ASN:N	1:D:1900:ASN:HD22	2.03	0.55
1:B:2039:ILE:HD11	1:B:2106:PHE:CZ	2.40	0.55
1:D:2462:LEU:HB3	1:D:2554:VAL:HG12	1.88	0.55
1:A:1951:GLN:HE21	1:A:1953:LYS:HE2	1.71	0.55
1:D:1880:LEU:HD11	1:D:1883:GLY:HA3	1.88	0.55
1:D:2238:ALA:HB2	1:D:2569:THR:O	2.06	0.55
1:B:2152:THR:HB	1:B:2704:VAL:HG22	1.89	0.55
1:B:2303:THR:HG22	1:B:2304:GLN:HG3	1.87	0.55
1:D:2167:LEU:HD13	1:D:2696:TYR:OH	2.07	0.55
1:B:2275:SER:HB2	1:B:2286:LEU:HD23	1.88	0.55
1:B:2318:ILE:HB	1:B:2375:ILE:HG21	1.89	0.55
1:D:1838:THR:HG23	1:D:1846:LYS:O	2.07	0.55
1:D:2401:TYR:CD1	1:D:2608:THR:HG23	2.42	0.55
1:C:2363:THR:HG23	1:C:2543:ASN:HA	1.89	0.55
1:C:1850:VAL:HG11	1:C:1858:ILE:CG2	2.35	0.55
1:C:1880:LEU:CD2	1:C:1884:VAL:O	2.54	0.55
1:B:2333:ILE:O	1:B:2337:THR:CG2	2.54	0.55
1:A:2376:TYR:O	1:A:2380:LEU:HD12	2.07	0.54
1:D:2533:GLN:O	1:D:2536:THR:CG2	2.48	0.54
1:D:2500:THR:HG22	1:D:2535:ASN:ND2	2.22	0.54
1:B:2663:PRO:HB3	1:B:2668:THR:HG23	1.90	0.54
1:A:2264:ILE:HD12	1:A:2264:ILE:O	2.07	0.54
1:B:2444:LYS:O	1:B:2445:ASP:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2264:ILE:HD12	1:A:2264:ILE:C	2.28	0.54
1:B:2045:ASN:OD1	1:B:2048:VAL:HG23	2.08	0.54
1:A:1906:ALA:HB3	1:A:1934:LEU:O	2.08	0.54
1:C:1798:THR:OG1	1:C:1799:GLY:N	2.40	0.54
1:C:2303:THR:HG22	1:C:2304:GLN:HG3	1.89	0.54
1:B:1864:ASN:HA	1:B:1869:LEU:HD23	1.90	0.54
1:A:2424[B]:SER:OG	1:A:2444:LYS:N	2.40	0.54
1:C:2464:VAL:HG22	1:C:2552:VAL:HG22	1.89	0.54
1:D:2135:TRP:CG	1:D:2711:VAL:HG11	2.42	0.53
1:A:2554:VAL:HB	1:A:2555:PRO:HD2	1.89	0.53
1:C:2246:LEU:HD23	1:C:2687:MET:HE1	1.89	0.53
1:C:2220:ILE:HG21	1:C:2255:THR:OG1	2.09	0.53
1:A:1891:LEU:HD13	1:A:1908:ASP:HB2	1.90	0.53
1:A:1783:LEU:HD12	1:A:1809:ILE:HG21	1.88	0.53
1:D:1901:LEU:HD23	1:D:1902:VAL:N	2.23	0.53
1:D:1850:VAL:CG1	1:D:1858:ILE:HG23	2.38	0.53
1:D:2021:LEU:HD13	1:D:2027:TRP:CD1	2.43	0.53
1:D:2084:VAL:HG12	1:D:2088:ILE:CD1	2.38	0.53
1:C:1995:ASN:OD1	1:C:2000:SER:OG	2.27	0.53
1:B:1828:MET:HE3	1:B:1828:MET:HA	1.91	0.53
1:B:1828:MET:HE1	1:B:1867:GLY:N	2.24	0.53
1:A:2462:LEU:HB3	1:A:2554:VAL:HG12	1.91	0.53
1:C:2424[A]:SER:HB2	1:C:2564:ALA:HB1	1.89	0.53
1:A:2330:GLY:HA2	1:A:2333:ILE:HD12	1.90	0.53
1:A:2290:LEU:HD21	1:A:2431:VAL:HG23	1.91	0.53
1:B:2409:TYR:O	1:B:2413:VAL:HG23	2.09	0.53
1:B:2152:THR:CB	1:B:2704:VAL:HG22	2.39	0.53
1:C:2446:ALA:HB2	1:C:2457:THR:HG21	1.90	0.53
1:C:2374:SER:OG	1:C:2550:LEU:HD22	2.09	0.53
1:C:2133:ASP:O	1:C:2711:VAL:HG13	2.09	0.52
1:D:1956:GLN:O	1:D:1957:VAL:HG13	2.09	0.52
1:A:2377:ALA:HA	1:A:2415:LEU:HD13	1.90	0.52
1:C:2008:PHE:CD2	1:C:2703:VAL:HG11	2.44	0.52
1:B:1800:ILE:HG22	1:B:1801:GLN:O	2.09	0.52
1:C:2229:ASP:HB3	1:C:2751:TYR:CD1	2.45	0.52
1:C:1850:VAL:HG12	1:C:1851:TYR:N	2.23	0.52
1:C:2330:GLY:O	1:C:2334:THR:HG23	2.09	0.52
1:A:2334:THR:HG22	1:A:2339:ALA:O	2.10	0.52
1:C:2184:ASN:HD21	1:C:2743:TYR:H	1.56	0.52
1:C:2318:ILE:HB	1:C:2375:ILE:HG21	1.91	0.52
1:C:1834:TYR:CE1	1:C:1865:ILE:HD13	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2021:LEU:CD2	1:C:2027:TRP:CE2	2.93	0.52
1:B:1985:ASN:O	1:B:1989:THR:HG23	2.10	0.52
1:A:1956:GLN:O	1:A:1957:VAL:HG13	2.09	0.52
1:C:2380:LEU:HD12	1:C:2415:LEU:HB3	1.91	0.52
1:D:2465:ILE:HG13	1:D:2482:LEU:HD11	1.91	0.52
1:A:2483:ASP:OD1	1:A:2522:THR:HG23	2.08	0.52
1:C:2409:TYR:CZ	1:C:2413:VAL:HG21	2.45	0.52
1:A:2275:SER:HB2	1:A:2286:LEU:HD23	1.92	0.52
1:C:2310:GLN:HA	1:C:2310:GLN:HE21	1.75	0.52
1:C:2047:ASN:HD21	1:C:2070:LEU:HD23	1.75	0.51
1:D:2589:LEU:HD23	1:D:2624:ILE:HD13	1.91	0.51
1:D:2629:MET:HE1	1:D:2675:THR:HG21	1.89	0.51
1:D:2438:LYS:NZ	1:D:2481:THR:O	2.37	0.51
1:C:2264:ILE:HD12	1:C:2265:GLU:O	2.09	0.51
1:B:2212:VAL:HG23	1:B:2220:ILE:HD13	1.90	0.51
1:A:2263:LEU:HD22	1:A:2314:ASN:O	2.11	0.51
1:B:2589:LEU:CD2	1:B:2624:ILE:HD13	2.41	0.51
1:D:1934:LEU:HD11	1:D:1941:LEU:HD11	1.92	0.51
1:D:2298:LEU:HD12	1:D:2299:ILE:N	2.26	0.51
1:C:2047:ASN:ND2	1:C:2070:LEU:HD23	2.25	0.51
1:B:2299:ILE:HG23	1:B:2312:THR:HB	1.93	0.51
1:D:1811:GLN:HE21	1:D:1811:GLN:H	1.59	0.51
1:C:2160:GLY:HA3	1:C:2216:HIS:CE1	2.46	0.51
1:A:2704:VAL:HG12	1:A:2705:SER:N	2.25	0.51
1:D:1934:LEU:CD1	1:D:1941:LEU:HD11	2.40	0.51
1:A:2661:ASN:ND2	1:A:2735:TYR:OH	2.44	0.51
1:A:2815:LYS:HE2	1:A:2817:TRP:CH2	2.46	0.51
1:D:2328:LYS:NZ	1:D:2369:SER:OG	2.43	0.51
1:C:1909:TYR:O	1:C:1938:ASN:N	2.31	0.51
1:C:2724:LEU:HD12	1:C:2822:TYR:CD1	2.45	0.51
1:D:2045:ASN:OD1	1:D:2048:VAL:HG23	2.11	0.51
1:C:2434:HIS:CG	1:C:2474:LEU:HD21	2.46	0.51
1:C:2462:LEU:HB3	1:C:2554:VAL:HG12	1.93	0.51
1:C:1825:LEU:HD12	1:C:1826:LEU:N	2.26	0.51
1:C:2181:GLU:OE2	1:C:2656:TYR:OH	2.21	0.51
1:B:2247:VAL:CG2	1:B:2264:ILE:HG22	2.41	0.51
1:C:2594:PHE:CD1	1:C:2630:ALA:HB2	2.47	0.50
1:A:1783:LEU:C	1:A:1783:LEU:CD2	2.80	0.50
1:D:1908:ASP:HA	1:D:1936:THR:HB	1.92	0.50
1:B:2318:ILE:HD13	1:B:2375:ILE:HD13	1.94	0.50
1:D:1811:GLN:N	1:D:1811:GLN:HE21	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2332:ALA:HA	1:D:2367:TYR:CE1	2.45	0.50
1:A:1907:GLY:N	1:A:1935:VAL:HG12	2.26	0.50
1:A:1851:TYR:CD2	1:A:1859:LEU:HD12	2.46	0.50
1:A:2444:LYS:O	1:A:2445:ASP:CB	2.54	0.50
1:A:2091:ARG:HB3	1:A:2100:TRP:CZ2	2.46	0.50
1:A:2258:ILE:HG23	1:A:2259:HIS:CD2	2.47	0.50
1:C:2116:VAL:HG13	1:C:2122:TRP:CE3	2.47	0.50
1:B:2258:ILE:HG23	1:B:2259:HIS:CD2	2.46	0.50
1:D:1828:MET:CE	1:D:1866:ASN:HA	2.42	0.50
1:A:1913:HIS:CE1	1:A:1924:ALA:HB3	2.47	0.50
1:A:2002:ASP:O	1:A:2004:THR:HG23	2.12	0.50
1:D:1869:LEU:HD12	1:D:2071:HIS:NE2	2.27	0.50
1:A:2237:GLU:OE1	1:A:2582:ASN:ND2	2.44	0.50
1:C:2638:ASP:OD1	1:C:2640:THR:HG22	2.12	0.50
1:B:2424[A]:SER:HB2	1:B:2564:ALA:HB1	1.94	0.49
1:D:1977:THR:H	1:D:2047:ASN:ND2	2.10	0.49
1:A:2246:LEU:HD13	1:A:2315:TYR:CE1	2.46	0.49
1:D:2002:ASP:O	1:D:2004:THR:HG23	2.12	0.49
1:D:2298:LEU:HD12	1:D:2299:ILE:H	1.78	0.49
1:A:2723:GLN:NE2	1:A:2822:TYR:OH	2.45	0.49
1:D:1958:ILE:HA	1:D:1962:LYS:O	2.11	0.49
1:A:2046:LYS:O	1:A:2050:VAL:HG23	2.12	0.49
1:D:2001:PHE:CZ	1:D:2831:THR:HG21	2.47	0.49
1:B:2462:LEU:HD12	1:B:2462:LEU:C	2.33	0.49
1:B:2704:VAL:HG21	1:B:2797:ALA:HB1	1.94	0.49
1:B:1851:TYR:CD1	1:B:1865:ILE:HD13	2.47	0.49
1:D:1851:TYR:O	1:D:1852:ARG:O	2.29	0.49
1:C:2137:GLN:NE2	1:C:2640:THR:OG1	2.46	0.49
1:D:1870:GLN:HE22	1:D:1879:GLN:HE21	1.61	0.49
1:C:1785:GLN:NE2	1:C:1789:GLY:O	2.46	0.49
1:A:2226:TYR:HA	1:A:2754:LEU:HD21	1.95	0.49
1:A:2009:LEU:HD11	1:A:2825:LEU:HD22	1.95	0.49
1:D:2394:MET:HG2	1:D:2412:LEU:HD12	1.94	0.49
1:C:2037:PRO:HB2	1:C:2040:THR:HG23	1.95	0.49
1:C:1865:ILE:HD12	1:C:1870:GLN:OE1	2.13	0.49
1:C:2250:GLY:C	1:C:2264:ILE:HD13	2.33	0.49
1:C:2429:MET:SD	1:C:2437:LEU:HD21	2.53	0.49
1:D:2320:ALA:HB3	1:D:2323:LYS:H	1.78	0.49
1:A:1873:ASP:OD1	1:A:1876:THR:HG22	2.12	0.48
1:A:2009:LEU:CD1	1:A:2825:LEU:CD2	2.91	0.48
1:B:2527:ASN:O	1:B:2537:GLN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2467:GLY:O	1:A:2548:GLY:HA3	2.13	0.48
1:D:2264:ILE:HD12	1:D:2264:ILE:C	2.33	0.48
1:C:2653:THR:HG23	1:C:2698:LEU:HD23	1.95	0.48
1:B:1923:TYR:O	1:B:1930:LEU:HD23	2.12	0.48
1:D:1931:VAL:HG11	1:D:1935:VAL:HG11	1.95	0.48
1:D:2116:VAL:HG13	1:D:2122:TRP:CE3	2.48	0.48
1:D:1917:GLN:HG2	1:D:1918:ASP:OD1	2.13	0.48
1:D:2258:ILE:HG23	1:D:2259:HIS:CD2	2.48	0.48
1:D:2594:PHE:CD1	1:D:2630:ALA:HB2	2.48	0.48
1:D:1851:TYR:HD2	1:D:1859:LEU:HD12	1.78	0.48
1:B:1923:TYR:CZ	1:B:1937:VAL:HG13	2.48	0.48
1:D:1806:PHE:HE1	1:D:1826:LEU:HD11	1.79	0.48
1:A:2421:SER:O	1:A:2564:ALA:HB2	2.13	0.48
1:D:1832:GLY:HA3	1:D:1851:TYR:CZ	2.48	0.48
1:D:2084:VAL:HG12	1:D:2088:ILE:HD11	1.96	0.48
1:A:1931:VAL:HG11	1:A:1935:VAL:HG21	1.94	0.48
1:B:1786:ASP:O	1:B:1788:ASN:N	2.47	0.48
1:A:2045:ASN:HD21	1:A:2121:ILE:HD13	1.79	0.48
1:A:1907:GLY:H	1:A:1935:VAL:HG12	1.78	0.48
1:B:2251:LEU:HD12	1:B:2294:ASP:HB3	1.96	0.48
1:B:2525:PHE:CD1	1:B:2530:ILE:HD11	2.49	0.48
1:A:2293:VAL:HG22	1:A:2298:LEU:HD13	1.96	0.48
1:C:2369:SER:HB2	1:C:2372:ILE:HD11	1.95	0.48
1:B:2424[B]:SER:OG	1:B:2444:LYS:N	2.47	0.47
1:A:1993:ALA:HB2	1:A:2833:PRO:HG3	1.96	0.47
1:B:2167:LEU:HD13	1:B:2696:TYR:OH	2.14	0.47
1:B:1943:TYR:CD1	1:B:1957:VAL:HG11	2.49	0.47
1:C:2044:PRO:HG3	1:C:2121:ILE:HD11	1.96	0.47
1:D:1853:ASP:O	1:D:1854:GLN:CB	2.61	0.47
1:D:2160:GLY:HA3	1:D:2216:HIS:CE1	2.49	0.47
1:D:2639:HIS:ND1	1:D:2645:THR:HG23	2.29	0.47
1:D:2437:LEU:HD23	1:D:2437:LEU:C	2.34	0.47
1:D:2602:THR:OG1	1:D:2606:GLU:OE1	2.24	0.47
1:C:2251:LEU:HD12	1:C:2294:ASP:HB3	1.95	0.47
1:A:2496:VAL:HG12	1:A:2497:ILE:HG12	1.97	0.47
1:D:2332:ALA:HB2	1:D:2367:TYR:CD1	2.49	0.47
1:A:2394:MET:HG2	1:A:2412:LEU:HD12	1.96	0.47
1:B:1951:GLN:HE21	1:B:1953:LYS:HE2	1.79	0.47
1:B:2445:ASP:CG	1:B:2454:THR:CG2	2.74	0.47
1:C:2170:ASP:OD1	1:C:2693:ASN:OD1	2.33	0.47
1:D:2504:LEU:HD21	1:D:2546:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2702:GLU:HG3	1:B:2730:VAL:HG23	1.95	0.47
1:B:1810:GLY:O	1:B:1811:GLN:HG2	2.15	0.47
1:C:1840:LYS:HA	1:C:1845:THR:HA	1.96	0.47
1:C:2363:THR:HG23	1:C:2543:ASN:CA	2.44	0.47
1:A:2045:ASN:HD21	1:A:2121:ILE:HG21	1.80	0.47
1:A:2292:ASP:O	1:A:2298:LEU:HD12	2.14	0.47
1:D:1830:THR:O	1:D:1831:GLU:CB	2.62	0.47
1:D:2517:THR:HG22	1:D:2523:LEU:HG	1.96	0.47
1:D:2272:ALA:O	1:D:2277:THR:HG23	2.15	0.47
1:B:2210:ASP:OD1	1:B:2691:VAL:HG13	2.14	0.47
1:C:1828:MET:HE3	1:C:1866:ASN:HA	1.96	0.47
1:C:2002:ASP:O	1:C:2013:THR:HG23	2.15	0.47
1:C:2761:ASP:HB3	1:C:2778:LEU:HD11	1.96	0.47
1:A:2009:LEU:HD12	1:A:2009:LEU:N	2.29	0.47
1:C:2525:PHE:CD1	1:C:2530:ILE:HD11	2.49	0.47
1:D:1779:LEU:O	1:D:1780:ALA:HB3	2.14	0.47
1:A:2269:ARG:HD3	1:A:2317:ILE:HG13	1.96	0.47
1:D:2216:HIS:O	1:D:2219:THR:HG22	2.15	0.47
1:D:2386:VAL:HG13	1:D:2588:ASN:O	2.15	0.47
1:B:2726:VAL:HG23	1:B:2813:VAL:HG22	1.95	0.47
1:B:1783:LEU:CD2	1:B:1783:LEU:O	2.63	0.47
1:C:2216:HIS:O	1:C:2219:THR:HG22	2.15	0.46
1:B:1783:LEU:O	1:B:1783:LEU:HD23	2.16	0.46
1:B:1965:TYR:CG	1:B:2719:GLY:HA2	2.50	0.46
1:A:2517:THR:HG23	1:A:2523:LEU:CD2	2.43	0.46
1:B:2638:ASP:OD1	1:B:2640:THR:HG22	2.14	0.46
1:D:2335:ASP:O	1:D:2336:ALA:HB3	2.15	0.46
1:B:2169:ASN:HD22	1:B:2698:LEU:HD12	1.80	0.46
1:C:2053:LEU:HD22	1:C:2080:ALA:HB1	1.97	0.46
1:D:2751:TYR:HB2	1:D:2754:LEU:HD12	1.97	0.46
1:C:2663:PRO:HB3	1:C:2668:THR:HG23	1.97	0.46
1:D:2391:TYR:CE1	1:D:2395:TYR:HB2	2.51	0.46
1:A:2143:TYR:CE1	1:A:2803:THR:HG22	2.50	0.46
1:C:2348:GLN:O	1:C:2351:ALA:HB3	2.15	0.46
1:D:1871:PHE:HB2	1:D:1894:PHE:CZ	2.50	0.46
1:B:2320:ALA:O	1:B:2325:VAL:HG21	2.16	0.46
1:A:2141:LEU:HB3	1:A:2706:ALA:HB1	1.95	0.46
1:C:2541:VAL:HG12	1:C:2542:ALA:N	2.30	0.46
1:C:2394:MET:HG2	1:C:2412:LEU:HD12	1.96	0.46
1:A:1783:LEU:HD23	1:A:1783:LEU:C	2.36	0.46
1:A:2039:ILE:HD11	1:A:2105:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1836:THR:HG22	1:A:1849:TRP:CD2	2.50	0.46
1:A:2646:ILE:HD12	1:A:2646:ILE:C	2.36	0.46
1:D:1806:PHE:CE1	1:D:1826:LEU:HD11	2.51	0.46
1:B:2166:LEU:HD13	1:B:2214:PHE:CE2	2.50	0.46
1:C:2190:MET:HA	1:C:2190:MET:HE2	1.97	0.46
1:D:2398:ASP:OD1	1:D:2399:GLY:N	2.48	0.46
1:A:2731:GLY:O	1:A:2794:GLN:HB2	2.16	0.46
1:B:2080:ALA:O	1:B:2084:VAL:HG23	2.16	0.46
1:D:2424[B]:SER:OG	1:D:2564:ALA:HB1	2.16	0.46
1:D:1851:TYR:CD2	1:D:1859:LEU:HD12	2.51	0.46
1:B:2371:ASN:ND2	1:B:2546:VAL:HG23	2.31	0.46
1:D:2651:ALA:HA	1:D:2696:TYR:CD1	2.51	0.46
1:B:2543:ASN:HB2	1:B:2544:PRO:CD	2.46	0.46
1:D:2525:PHE:CE1	1:D:2530:ILE:HD11	2.51	0.45
1:A:2703:VAL:HG22	1:A:2726:VAL:HG22	1.98	0.45
1:A:2328:LYS:O	1:A:2331:ALA:HB3	2.15	0.45
1:C:2123:ASN:OD1	1:C:2123:ASN:C	2.55	0.45
1:C:1850:VAL:HG22	1:C:1877:GLY:O	2.16	0.45
1:D:1850:VAL:HG12	1:D:1851:TYR:N	2.31	0.45
1:D:2222:ARG:NH1	1:D:2754:LEU:O	2.48	0.45
1:D:2170:ASP:O	1:D:2800:MET:HG3	2.15	0.45
1:D:2322:ASP:N	1:D:2322:ASP:OD1	2.49	0.45
1:D:2059:ASN:HD22	1:D:2104:LEU:CD1	2.07	0.45
1:C:1850:VAL:HG12	1:C:1851:TYR:H	1.80	0.45
1:A:2246:LEU:C	1:A:2246:LEU:HD12	2.37	0.45
1:A:2644:SER:HB3	1:A:2651:ALA:HB1	1.98	0.45
1:C:1979:THR:HG23	1:C:2074:GLN:NE2	2.31	0.45
1:D:1980:LEU:HG	1:D:1981:ASP:H	1.81	0.45
1:D:2207:ILE:HA	1:D:2688:ALA:O	2.16	0.45
1:B:2409:TYR:CZ	1:B:2413:VAL:HG21	2.52	0.45
1:C:2470:PRO:HB2	1:C:2542:ALA:HB2	1.97	0.45
1:A:2401:TYR:CD2	1:A:2608:THR:HG23	2.50	0.45
1:D:2409:TYR:O	1:D:2413:VAL:HG23	2.17	0.45
1:B:2044:PRO:HG3	1:B:2121:ILE:HD11	1.99	0.45
1:A:2433:ASN:HD22	1:A:2434:HIS:N	2.13	0.45
1:D:2009:LEU:CD2	1:D:2009:LEU:N	2.77	0.45
1:C:2467:GLY:O	1:C:2548:GLY:HA3	2.17	0.45
1:A:1809:ILE:HD12	1:A:1809:ILE:N	2.32	0.45
1:B:2039:ILE:H	1:B:2039:ILE:HD13	1.81	0.45
1:C:2459:THR:HG21	1:C:2557:GLY:O	2.17	0.45
1:C:1991:ASN:ND2	1:C:2085:GLN:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2726:VAL:HG23	1:B:2813:VAL:CG2	2.46	0.45
1:A:2719:GLY:O	1:A:2810:MET:HE1	2.16	0.45
1:A:1825:LEU:HD12	1:A:1826:LEU:N	2.32	0.45
1:D:2446:ALA:HB2	1:D:2457:THR:HG21	1.99	0.45
1:D:1920:GLN:HG3	1:D:1950:ASN:ND2	2.30	0.45
1:D:2289:MET:CE	1:D:2378:LEU:HD13	2.46	0.45
1:D:2135:TRP:CD2	1:D:2711:VAL:HG11	2.52	0.45
1:D:1963:THR:HG22	1:D:1975:LEU:HD12	1.99	0.45
1:C:2378:LEU:HG	1:C:2466:ILE:CD1	2.47	0.45
1:C:2589:LEU:CD2	1:C:2624:ILE:HD13	2.45	0.44
1:C:1793:TYR:CE2	1:C:1794:PHE:O	2.70	0.44
1:C:1985:ASN:ND2	1:C:1987:PHE:HB3	2.31	0.44
1:A:2222:ARG:NH1	1:A:2754:LEU:O	2.50	0.44
1:D:2499:THR:HA	1:D:2504:LEU:HD23	2.00	0.44
1:D:1848:ALA:HB1	1:D:1878:GLU:HG3	1.98	0.44
1:C:1809:ILE:N	1:C:1809:ILE:HD12	2.33	0.44
1:D:2217:ASN:HB3	1:D:2255:THR:HG21	1.98	0.44
1:B:1832:GLY:HA3	1:B:1851:TYR:CE2	2.53	0.44
1:B:2343:ASN:ND2	1:B:2639:HIS:ND1	2.65	0.44
1:D:1793:TYR:OH	1:D:1796:LEU:CD1	2.65	0.44
1:A:2217:ASN:HB3	1:A:2255:THR:HG21	1.98	0.44
1:B:2465:ILE:HG12	1:B:2482:LEU:HD21	1.99	0.44
1:B:2106:PHE:CD1	1:B:2116:VAL:HG21	2.52	0.44
1:C:2062:LEU:O	1:C:2064:THR:HG22	2.18	0.44
1:B:2180:ALA:O	1:B:2744:LEU:HD21	2.18	0.44
1:C:2377:ALA:O	1:C:2381:THR:HG23	2.17	0.44
1:C:1850:VAL:CG1	1:C:1858:ILE:HG23	2.42	0.44
1:D:2037:PRO:HB2	1:D:2040:THR:HG23	1.99	0.44
1:B:1893:TYR:CE1	1:B:1941:LEU:HD22	2.51	0.44
1:C:2135:TRP:CG	1:C:2711:VAL:HG11	2.52	0.44
1:B:2009:LEU:HB3	1:B:2814:LEU:HD12	2.00	0.44
1:D:1891:LEU:O	1:D:1904:THR:HG23	2.18	0.44
1:C:2289:MET:HE2	1:C:2289:MET:HB3	1.92	0.44
1:D:2056:MET:HE1	1:D:2105:LEU:HD21	1.95	0.44
1:D:2003:HIS:HB2	1:D:2013:THR:HA	2.00	0.44
1:D:1935:VAL:O	1:D:1941:LEU:HD12	2.18	0.44
1:D:1850:VAL:HG11	1:D:1858:ILE:HD13	1.99	0.44
1:A:2045:ASN:OD1	1:A:2048:VAL:HG23	2.18	0.44
1:B:2363:THR:HG23	1:B:2543:ASN:CA	2.48	0.44
1:A:2831:THR:HG22	1:A:2833:PRO:HG2	1.99	0.43
1:A:2494:ARG:HB3	1:A:2556:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2424[B]:SER:HB3	1:C:2564:ALA:HB1	2.00	0.43
1:A:2401:TYR:CG	1:A:2608:THR:HG23	2.53	0.43
1:D:2510:ASP:O	1:D:2512:ALA:N	2.51	0.43
1:D:2152:THR:HB	1:D:2704:VAL:HG22	1.98	0.43
1:D:2705:SER:HA	1:D:2724:LEU:HD23	1.99	0.43
1:C:1900:ASN:O	1:C:1902:VAL:HG13	2.18	0.43
1:D:2401:TYR:CG	1:D:2608:THR:HG23	2.53	0.43
1:C:2515:ALA:HB2	1:C:2530:ILE:HG21	2.00	0.43
1:C:2657:ASP:C	1:C:2658:LEU:HD12	2.38	0.43
1:C:2401:TYR:CD2	1:C:2608:THR:HG23	2.54	0.43
1:C:1796:LEU:HD12	1:C:2073:ASP:OD2	2.19	0.43
1:B:2646:ILE:HD12	1:B:2646:ILE:C	2.38	0.43
1:A:2496:VAL:C	1:A:2497:ILE:HD13	2.39	0.43
1:A:2590:ILE:HG22	1:A:2591:TYR:N	2.34	0.43
1:C:1825:LEU:HD12	1:C:1826:LEU:H	1.83	0.43
1:C:2270:GLU:O	1:C:2273:THR:HB	2.18	0.43
1:A:2789:ASP:N	1:A:2789:ASP:OD1	2.49	0.43
1:B:2057:LYS:NZ	1:B:2067:GLN:OE1	2.51	0.43
1:A:1851:TYR:HD2	1:A:1859:LEU:HD12	1.82	0.43
1:D:2167:LEU:HD11	1:D:2641:PHE:CE2	2.54	0.43
1:D:1834:TYR:OH	1:D:1870:GLN:OE1	2.37	0.43
1:D:2134:ALA:HB1	1:D:2139:GLY:N	2.34	0.43
1:C:2249:ALA:HB1	1:C:2252:ASP:OD1	2.18	0.43
1:B:2374:SER:O	1:B:2377:ALA:HB3	2.18	0.43
1:D:1925:ASP:OD1	1:D:1925:ASP:N	2.51	0.43
1:B:2266:SER:CB	1:B:2314:ASN:HD22	2.20	0.43
1:A:2317:ILE:HA	1:A:2379:MET:CE	2.47	0.43
1:C:2320:ALA:O	1:C:2321:HIS:C	2.54	0.43
1:B:1888:ASP:O	1:B:1889:ASP:CB	2.67	0.43
1:B:2676:ILE:HG23	1:B:2686:VAL:HG21	2.01	0.43
1:D:2496:VAL:O	1:D:2497:ILE:HD13	2.18	0.43
1:C:1840:LYS:HA	1:C:1844:ASP:O	2.18	0.43
1:A:2371:ASN:ND2	1:A:2546:VAL:HG23	2.34	0.43
1:A:2397:ASP:HB3	1:A:2597:PHE:O	2.19	0.43
1:B:1901:LEU:HD23	1:B:1902:VAL:N	2.33	0.43
1:D:2492:LYS:HG2	1:D:2556:VAL:HG21	2.01	0.43
1:D:2190:MET:O	1:D:2203:ASN:HB3	2.19	0.43
1:B:2289:MET:HE2	1:B:2289:MET:HB3	1.92	0.43
1:A:2157:ARG:HA	1:A:2801:ASN:ND2	2.33	0.43
1:D:2169:ASN:ND2	1:D:2698:LEU:HD12	2.34	0.43
1:C:2183:LEU:HD11	1:C:2222:ARG:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2117:LYS:NZ	1:A:2807:GLY:O	2.51	0.43
1:D:2467:GLY:O	1:D:2548:GLY:HA3	2.19	0.43
1:A:2009:LEU:CD1	1:A:2009:LEU:N	2.82	0.43
1:B:2276:LEU:HD12	1:B:2375:ILE:HG12	2.01	0.43
1:D:2133:ASP:O	1:D:2711:VAL:HG13	2.19	0.43
1:A:2242:GLN:O	1:A:2685:GLN:NE2	2.51	0.43
1:D:2707:THR:HG23	1:D:2721:GLY:O	2.19	0.43
1:A:2053:LEU:HD11	1:A:2080:ALA:HB3	2.00	0.43
1:B:2660:PHE:CD1	1:B:2669:ASP:OD2	2.72	0.43
1:D:2002:ASP:OD2	1:D:2035:MET:CE	2.66	0.42
1:A:1886:LYS:HA	1:A:1891:LEU:HD23	2.01	0.42
1:D:2021:LEU:HD13	1:D:2027:TRP:CE2	2.54	0.42
1:C:2308:GLU:O	1:C:2310:GLN:HG2	2.19	0.42
1:B:1901:LEU:C	1:B:1901:LEU:HD23	2.39	0.42
1:B:2594:PHE:CG	1:B:2630:ALA:HB2	2.54	0.42
1:C:2172:ASP:O	1:C:2178:VAL:HG11	2.19	0.42
1:C:1934:LEU:O	1:C:1935:VAL:HG13	2.19	0.42
1:D:1900:ASN:N	1:D:1900:ASN:ND2	2.66	0.42
1:B:2663:PRO:HB3	1:B:2668:THR:CG2	2.50	0.42
1:D:2268:LEU:HD13	1:D:2316:SER:HB3	2.01	0.42
1:D:1869:LEU:HD12	1:D:2071:HIS:CD2	2.54	0.42
1:A:2045:ASN:ND2	1:A:2121:ILE:HD13	2.33	0.42
1:D:1954:ASN:N	1:D:1966:PHE:O	2.52	0.42
1:D:2646:ILE:CD1	1:D:2646:ILE:C	2.88	0.42
1:C:2204:PHE:CG	1:C:2688:ALA:HB2	2.54	0.42
1:A:1850:VAL:HG12	1:A:1851:TYR:N	2.35	0.42
1:C:1830:THR:HA	1:C:1866:ASN:HD21	1.84	0.42
1:A:2698:LEU:HD22	1:A:2731:GLY:HA3	2.01	0.42
1:D:1850:VAL:HG11	1:D:1858:ILE:HG12	2.01	0.42
1:C:2121:ILE:HG23	3:C:2868:GOL:H12	2.00	0.42
1:B:2638:ASP:CG	1:B:2640:THR:HG22	2.39	0.42
1:C:2419:ARG:HA	1:C:2423:VAL:CG2	2.50	0.42
1:D:2380:LEU:CD1	1:D:2415:LEU:HB3	2.50	0.42
1:D:1783:LEU:HD23	1:D:1783:LEU:C	2.40	0.42
1:B:1837:ILE:C	1:B:1837:ILE:HD12	2.40	0.42
1:A:2525:PHE:CD1	1:A:2530:ILE:HD11	2.54	0.42
1:A:2176:PRO:HA	1:A:2786:ILE:HG22	2.01	0.42
1:B:1850:VAL:HG12	1:B:1851:TYR:N	2.35	0.42
1:D:1905:VAL:CG1	1:D:1935:VAL:HA	2.50	0.42
1:D:2437:LEU:HD23	1:D:2438:LYS:N	2.34	0.42
1:C:2173:ASN:HB3	1:C:2219:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1943:TYR:CE1	1:B:1957:VAL:HG11	2.55	0.42
1:A:1825:LEU:HD12	1:A:1826:LEU:H	1.84	0.42
1:A:2465:ILE:HG13	1:A:2482:LEU:HD11	2.01	0.42
1:D:2459:THR:O	1:D:2562:GLN:NE2	2.49	0.42
1:B:2437:LEU:C	1:B:2437:LEU:HD23	2.40	0.42
1:B:1853:ASP:O	1:B:1854:GLN:C	2.58	0.42
1:B:2660:PHE:O	1:B:2661:ASN:CB	2.67	0.42
1:C:1865:ILE:O	1:C:1865:ILE:HG22	2.19	0.42
1:A:2815:LYS:HE2	1:A:2817:TRP:CZ2	2.55	0.42
1:D:2045:ASN:ND2	1:D:2121:ILE:HD13	2.34	0.42
1:C:1952:ILE:HG23	1:C:1955:GLN:OE1	2.20	0.42
1:D:2723:GLN:HE22	1:D:2815:LYS:NZ	2.18	0.42
1:D:2192:PHE:O	1:D:2196:THR:HG23	2.19	0.42
1:C:1833:HIS:O	1:C:1834:TYR:CB	2.68	0.42
1:B:1783:LEU:C	1:B:1783:LEU:HD23	2.39	0.42
1:C:2273:THR:HA	1:C:2277:THR:OG1	2.19	0.42
1:B:2117:LYS:NZ	1:B:2807:GLY:O	2.53	0.42
1:D:2372:ILE:N	1:D:2373:PRO:CD	2.82	0.42
1:C:2387:PRO:HG2	1:C:2589:LEU:HD12	2.02	0.42
1:A:2372:ILE:N	1:A:2373:PRO:CD	2.82	0.42
1:A:2298:LEU:HD21	1:A:2301:ASP:HB2	2.01	0.42
1:B:2651:ALA:HA	1:B:2696:TYR:CD1	2.55	0.42
1:C:2183:LEU:HD11	1:C:2222:ARG:HD3	2.02	0.42
1:C:2419:ARG:HA	1:C:2423:VAL:HG23	2.01	0.42
1:D:1873:ASP:HB3	1:D:1876:THR:CG2	2.50	0.42
1:B:2387:PRO:HG2	1:B:2589:LEU:CD1	2.50	0.41
1:C:2169:ASN:ND2	1:C:2698:LEU:HD12	2.32	0.41
1:C:2149:THR:HG21	1:C:2724:LEU:HD22	2.02	0.41
1:A:2341:TRP:CE3	1:A:2642:LEU:HD22	2.55	0.41
1:C:1925:ASP:OD1	1:C:1929:GLN:N	2.42	0.41
1:D:1914:TYR:CZ	1:D:1937:VAL:HG11	2.55	0.41
1:D:2679:LEU:HD12	1:D:2686:VAL:HG22	2.02	0.41
1:C:2040:THR:OG1	1:C:2041:VAL:HG13	2.20	0.41
1:B:2638:ASP:OD2	1:B:2640:THR:CG2	2.67	0.41
1:D:1873:ASP:CG	1:D:1876:THR:HG22	2.40	0.41
1:B:1871:PHE:HB2	1:B:1894:PHE:CZ	2.56	0.41
1:C:1811:GLN:NE2	1:C:2065:ALA:HB3	2.35	0.41
1:B:2356:PHE:O	1:B:2359:ASP:HB3	2.20	0.41
1:B:2002:ASP:O	1:B:2013:THR:HG23	2.20	0.41
1:A:2084:VAL:HG12	1:A:2088:ILE:CD1	2.50	0.41
1:B:1868:THR:HA	3:B:2868:GOL:H32	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2517:THR:HG22	1:D:2523:LEU:CD2	2.50	0.41
1:B:2481:THR:HG22	1:B:2524:THR:HA	2.01	0.41
1:B:1959:VAL:HG12	1:B:1959:VAL:O	2.20	0.41
1:C:1987:PHE:HB3	1:C:2082:GLN:NE2	2.36	0.41
1:C:2494:ARG:HB3	1:C:2514:THR:HG22	2.01	0.41
1:A:2589:LEU:CD2	1:A:2624:ILE:HD13	2.50	0.41
1:C:2409:TYR:O	1:C:2413:VAL:HG23	2.19	0.41
1:D:1833:HIS:O	1:D:1834:TYR:HB2	2.20	0.41
1:D:1871:PHE:CZ	1:D:1885:ALA:HB1	2.55	0.41
1:B:1893:TYR:CZ	1:B:1941:LEU:HD22	2.55	0.41
1:C:2517:THR:HG22	1:C:2523:LEU:HG	2.01	0.41
1:B:1895:GLU:OE2	1:B:1897:GLY:N	2.52	0.41
1:D:2663:PRO:HB3	1:D:2668:THR:HG23	2.01	0.41
1:A:2831:THR:HG23	1:A:2833:PRO:CD	2.39	0.41
1:A:2831:THR:HG22	1:A:2833:PRO:CG	2.51	0.41
1:D:2186:LEU:HD22	1:D:2223:THR:HG23	2.01	0.41
1:A:1873:ASP:HB3	1:A:1876:THR:HG22	2.02	0.41
1:A:2517:THR:HG23	1:A:2523:LEU:HD21	2.03	0.41
1:A:2639:HIS:CE1	1:A:2645:THR:HG23	2.56	0.41
1:A:2595:SER:OG	1:A:2596:ASN:N	2.53	0.41
1:D:2129:HIS:CE1	1:D:2805:VAL:HG21	2.56	0.41
1:A:1848:ALA:HB1	1:A:1878:GLU:HG3	2.01	0.41
1:B:2339:ALA:HB2	1:B:2348:GLN:NE2	2.36	0.41
1:A:1807:VAL:HG12	1:A:1809:ILE:HD12	2.02	0.41
1:A:2045:ASN:ND2	1:A:2121:ILE:HG21	2.35	0.41
1:A:2394:MET:CG	1:A:2412:LEU:HD12	2.50	0.41
1:A:2761:ASP:HB3	1:A:2778:LEU:HD11	2.03	0.41
1:A:2061:LEU:HA	1:A:2061:LEU:HD23	1.96	0.41
1:B:1848:ALA:HB1	1:B:1878:GLU:CG	2.50	0.41
1:D:2390:TYR:CE2	1:D:2392:GLY:HA3	2.55	0.41
1:A:2171:VAL:HG23	1:A:2693:ASN:O	2.20	0.41
1:A:1993:ALA:HB2	1:A:2833:PRO:CG	2.50	0.41
1:D:2045:ASN:HD21	1:D:2121:ILE:HD13	1.86	0.41
1:D:2001:PHE:CE1	1:D:2825:LEU:HD21	2.56	0.41
1:C:2429:MET:HA	1:C:2438:LYS:O	2.21	0.41
1:D:2152:THR:CB	1:D:2704:VAL:HG22	2.51	0.41
1:C:2497:ILE:O	1:C:2551:ALA:HA	2.21	0.41
1:B:2823:PHE:CE2	1:B:2832:LEU:CG	3.04	0.41
1:C:2186:LEU:HD11	1:C:2207:ILE:HG21	2.02	0.41
1:A:2816:ASP:O	1:A:2820:GLY:N	2.53	0.41
1:A:2832:LEU:O	1:A:2834:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2381:THR:HG21	1:B:2464:VAL:HG21	2.03	0.41
1:D:1795:ASP:CG	1:D:1798:THR:HG22	2.41	0.41
1:C:2740:ALA:HB1	1:C:2792:ILE:O	2.21	0.41
1:D:2180:ALA:O	1:D:2183:LEU:N	2.54	0.41
1:B:2190:MET:HA	1:B:2190:MET:HE2	2.02	0.41
1:A:2704:VAL:HG21	1:A:2797:ALA:HB1	2.03	0.41
1:D:2651:ALA:HA	1:D:2696:TYR:CE1	2.56	0.41
1:D:2021:LEU:HD13	1:D:2027:TRP:CG	2.55	0.41
1:D:2646:ILE:HD12	1:D:2646:ILE:C	2.41	0.41
1:C:2210:ASP:O	1:C:2211:ALA:HB3	2.21	0.41
1:B:2178:VAL:HG22	1:B:2792:ILE:HD11	2.03	0.41
1:D:2211:ALA:HB1	1:D:2214:PHE:HB2	2.03	0.41
1:B:1851:TYR:HD2	1:B:1859:LEU:HD12	1.86	0.40
1:A:2266:SER:CB	1:A:2314:ASN:HD22	2.31	0.40
1:A:2044:PRO:CG	1:A:2121:ILE:HD11	2.51	0.40
1:B:2628:GLU:HA	1:B:2687:MET:HB3	2.03	0.40
1:A:2612:ILE:HG22	1:A:2675:THR:HG23	2.03	0.40
1:C:2559:SER:HB3	1:C:2562:GLN:HB2	2.03	0.40
1:C:1800:ILE:H	1:C:1800:ILE:HD12	1.86	0.40
1:D:2424[B]:SER:CB	1:D:2564:ALA:HB1	2.51	0.40
1:C:2591:TYR:HB2	1:C:2624:ILE:CD1	2.46	0.40
1:A:2217:ASN:ND2	1:A:2255:THR:HG23	2.36	0.40
1:B:1902:VAL:HG11	1:B:1974:TYR:CE2	2.56	0.40
1:B:2285:PRO:C	1:B:2287:THR:H	2.24	0.40
1:A:1822:ASP:O	1:A:1823:ALA:CB	2.69	0.40
1:C:2005:VAL:HG12	1:C:2703:VAL:HG23	2.03	0.40
1:A:2293:VAL:HG13	1:A:2297:THR:O	2.22	0.40
1:C:2372:ILE:HB	1:C:2373:PRO:HD3	2.03	0.40
1:D:2409:TYR:CZ	1:D:2413:VAL:HG21	2.55	0.40
1:C:1811:GLN:HE21	1:C:2065:ALA:HB3	1.85	0.40
1:A:2135:TRP:CD2	1:A:2711:VAL:HG11	2.56	0.40
1:B:2337:THR:CG2	1:B:2338:GLY:N	2.85	0.40
1:D:1909:TYR:HE2	1:D:1931:VAL:HG11	1.86	0.40
1:C:2543:ASN:HB2	1:C:2544:PRO:CD	2.50	0.40
1:B:2496:VAL:CG2	1:B:2554:VAL:HG13	2.52	0.40
1:D:2117:LYS:NZ	1:D:2807:GLY:O	2.55	0.40
1:D:2543:ASN:HB2	1:D:2544:PRO:CD	2.51	0.40
1:D:2445:ASP:OD1	1:D:2454:THR:CG2	2.59	0.40
1:D:1906:ALA:HB3	1:D:1935:VAL:CG1	2.49	0.40
1:B:1869:LEU:HA	1:B:1869:LEU:HD23	1.92	0.40
1:A:2646:ILE:CD1	1:A:2646:ILE:C	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2543:ASN:HB2	1:B:2544:PRO:HD2	2.04	0.40
1:B:2157:ARG:HA	1:B:2801:ASN:ND2	2.37	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	1054/1108 (95%)	965 (92%)	73 (7%)	16 (2%)	13	49
1	B	1052/1108 (95%)	963 (92%)	75 (7%)	14 (1%)	15	52
1	C	1051/1108 (95%)	961 (91%)	79 (8%)	11 (1%)	19	58
1	D	1038/1108 (94%)	953 (92%)	77 (7%)	8 (1%)	24	62
All	All	4195/4432 (95%)	3842 (92%)	304 (7%)	49 (1%)	16	54

All (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
1	B	1928	ASN
1	C	1983	SER
1	D	1819	ASP
1	D	1852	ARG
1	A	1842	GLY
1	A	2445	ASP
1	B	1852	ARG
1	B	2829	LYS

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Mol	Chain	Res	Type
1	C	1857	THR
1	C	1984	THR
1	C	2445	ASP
1	C	2511	GLN
1	D	2337	THR
1	D	2511	GLN
1	A	1797	THR
1	A	1856	ASN
1	A	1897	GLY
1	A	2661	ASN
1	B	1831	GLU
1	B	1981	ASP
1	B	2445	ASP
1	B	2661	ASN
1	C	1852	ARG
1	D	1854	GLN
1	A	1843	GLN
1	A	2571	THR
1	B	2286	LEU
1	C	2337	THR
1	C	2661	ASN
1	D	2661	ASN
1	A	1831	GLU
1	B	2337	THR
1	B	2697	ASN
1	C	1787	SER
1	C	1789	GLY
1	D	1897	GLY
1	A	2295	GLY
1	A	2461	GLY
1	D	2732	GLY
1	A	2044	PRO
1	B	2325	VAL
1	B	1897	GLY
1	B	2732	GLY
1	C	2732	GLY

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%)	51	80
1	B	819/925 (88%)	801 (98%)	18 (2%)	60	84
1	C	814/925 (88%)	797 (98%)	17 (2%)	61	84
1	D	790/925 (85%)	775 (98%)	15 (2%)	65	85
All	All	3246/3700 (88%)	3173 (98%)	73 (2%)	60	84

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1783	LEU
1	A	1834	TYR
1	A	1915	ILE
1	A	1936	THR
1	A	1946	ASN
1	A	1960	ASP
1	A	1962	LYS
1	A	2037	PRO
1	A	2047	ASN
1	A	2063	THR
1	A	2194	THR
1	A	2283	ASN
1	A	2297	THR
1	A	2300	THR
1	A	2385	THR
1	A	2433	ASN
1	A	2539	ARG
1	A	2570	THR
1	A	2646	ILE
1	A	2694	GLN
1	A	2715	ASP
1	A	2800	MET
1	A	2803	THR
1	B	1811	GLN
1	B	1828	MET
1	B	1834	TYR
1	B	1884	VAL
1	B	1905	VAL
1	B	2023	ASN
1	B	2039	ILE

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Mol	Chain	Res	Type
1	B	2099	ASP
1	B	2219	THR
1	B	2297	THR
1	B	2310	GLN
1	B	2337	THR
1	B	2444	LYS
1	B	2476	ASP
1	B	2539	ARG
1	B	2694	GLN
1	B	2769	ASN
1	B	2800	MET
1	C	1820	HIS
1	C	1834	TYR
1	C	1884	VAL
1	C	1895	GLU
1	C	2021	LEU
1	C	2056	MET
1	C	2070	LEU
1	C	2310	GLN
1	C	2424[A]	SER
1	C	2424[B]	SER
1	C	2452	LEU
1	C	2462	LEU
1	C	2476	ASP
1	C	2539	ARG
1	C	2694	GLN
1	C	2782	ASP
1	C	2800	MET
1	D	1811	GLN
1	D	1957	VAL
1	D	2091	ARG
1	D	2300	THR
1	D	2337	THR
1	D	2445	ASP
1	D	2462	LEU
1	D	2476	ASP
1	D	2536	THR
1	D	2539	ARG
1	D	2646	ILE
1	D	2694	GLN
1	D	2782	ASP
1	D	2800	MET

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Mol	Chain	Res	Type
1	D	2831	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1785	GLN
1	A	1788	ASN
1	A	1913	HIS
1	A	1951	GLN
1	A	1978	ASN
1	A	1991	ASN
1	A	2047	ASN
1	A	2078	ASN
1	A	2079	GLN
1	A	2184	ASN
1	A	2199	GLN
1	A	2217	ASN
1	A	2259	HIS
1	A	2283	ASN
1	A	2314	ASN
1	A	2343	ASN
1	A	2371	ASN
1	A	2433	ASN
1	A	2434	HIS
1	A	2491	GLN
1	A	2533	GLN
1	A	2573	ASN
1	A	2580	HIS
1	A	2661	ASN
1	A	2694	GLN
1	A	2723	GLN
1	A	2742	GLN
1	A	2801	ASN
1	B	1801	GLN
1	B	1805	GLN
1	B	1920	GLN
1	B	1951	GLN
1	B	2047	ASN
1	B	2085	GLN
1	B	2112	ASN
1	B	2169	ASN
1	B	2217	ASN

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Mol	Chain	Res	Type
1	B	2221	GLN
1	B	2259	HIS
1	B	2283	ASN
1	B	2314	ASN
1	B	2343	ASN
1	B	2371	ASN
1	B	2491	GLN
1	B	2528	GLN
1	B	2573	ASN
1	B	2680	HIS
1	B	2693	ASN
1	B	2723	GLN
1	B	2742	GLN
1	B	2766	ASN
1	B	2769	ASN
1	B	2773	ASN
1	B	2801	ASN
1	C	1801	GLN
1	C	1805	GLN
1	C	1811	GLN
1	C	1985	ASN
1	C	1991	ASN
1	C	2074	GLN
1	C	2078	ASN
1	C	2082	GLN
1	C	2085	GLN
1	C	2112	ASN
1	C	2137	GLN
1	C	2184	ASN
1	C	2191	ASN
1	C	2199	GLN
1	C	2217	ASN
1	C	2232	GLN
1	C	2259	HIS
1	C	2260	ASN
1	C	2283	ASN
1	C	2310	GLN
1	C	2371	ASN
1	C	2396	GLN
1	C	2434	HIS
1	C	2491	GLN
1	C	2528	GLN

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Mol	Chain	Res	Type
1	C	2573	ASN
1	C	2620	ASN
1	C	2677	GLN
1	C	2694	GLN
1	C	2723	GLN
1	C	2766	ASN
1	C	2801	ASN
1	D	1811	GLN
1	D	1870	GLN
1	D	1900	ASN
1	D	1991	ASN
1	D	2047	ASN
1	D	2049	GLN
1	D	2059	ASN
1	D	2067	GLN
1	D	2085	GLN
1	D	2112	ASN
1	D	2184	ASN
1	D	2217	ASN
1	D	2232	GLN
1	D	2259	HIS
1	D	2260	ASN
1	D	2283	ASN
1	D	2491	GLN
1	D	2528	GLN
1	D	2680	HIS
1	D	2694	GLN
1	D	2723	GLN
1	D	2766	ASN
1	D	2801	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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	A	2867	-	5,5,5	0.19	0	5,5,5	0.45	0
3	GOL	B	2867	-	5,5,5	0.16	0	5,5,5	0.49	0
3	GOL	B	2868	-	5,5,5	0.40	0	5,5,5	0.45	0
3	GOL	C	2867	-	5,5,5	0.20	0	5,5,5	0.43	0
3	GOL	C	2868	-	5,5,5	0.40	0	5,5,5	0.43	0
3	GOL	C	2869	-	5,5,5	0.37	0	5,5,5	0.33	0
3	GOL	D	2867	-	5,5,5	0.27	0	5,5,5	0.15	0
3	GOL	D	2868	-	5,5,5	0.28	0	5,5,5	0.58	0
3	GOL	D	2869	-	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
3	GOL	A	2867	-	-	0/4/4/4	0/0/0/0
3	GOL	B	2867	-	-	0/4/4/4	0/0/0/0
3	GOL	B	2868	-	-	0/4/4/4	0/0/0/0
3	GOL	C	2867	-	-	0/4/4/4	0/0/0/0
3	GOL	C	2868	-	-	0/4/4/4	0/0/0/0
3	GOL	C	2869	-	-	0/4/4/4	0/0/0/0
3	GOL	D	2867	-	-	0/4/4/4	0/0/0/0
3	GOL	D	2868	-	-	0/4/4/4	0/0/0/0
3	GOL	D	2869	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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%)	-0.16	2 (0%) 95 95	18, 30, 48, 82	0
1	B	1053/1108 (95%)	-0.25	0 100 100	15, 27, 45, 64	0
1	C	1052/1108 (94%)	-0.12	4 (0%) 93 92	16, 33, 56, 79	0
1	D	1043/1108 (94%)	-0.15	3 (0%) 94 94	21, 34, 55, 80	0
All	All	4203/4432 (94%)	-0.17	9 (0%) 95 95	15, 31, 52, 82	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2830	SER	2.6
1	A	1786	ASP	2.5
1	C	1842	GLY	2.4
1	C	2831	THR	2.4
1	D	1914	TYR	2.4
1	C	1986	ALA	2.3
1	A	2769	ASN	2.2
1	D	2344	PHE	2.1
1	D	2831	THR	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	B	2868	6/6	0.89	0.36	4.52	27,29,29,29	0
3	GOL	C	2868	6/6	0.92	0.36	2.38	29,31,33,34	0
3	GOL	D	2869	6/6	0.97	0.23	-0.29	25,25,26,26	0
2	CA	A	2866	1/1	0.98	0.16	-1.33	51,51,51,51	0
2	CA	C	2866	1/1	0.98	0.12	-1.96	30,30,30,30	0
2	CA	D	2866	1/1	0.98	0.12	-2.21	29,29,29,29	0
2	CA	B	2866	1/1	0.94	0.14	-2.70	44,44,44,44	0
3	GOL	C	2869	6/6	0.96	0.14	-	20,21,21,21	0
3	GOL	B	2867	6/6	0.96	0.21	-	13,13,13,13	0
3	GOL	A	2867	6/6	0.98	0.17	-	15,15,15,16	0
3	GOL	C	2867	6/6	0.96	0.17	-	25,26,26,26	0
3	GOL	D	2867	6/6	0.95	0.17	-	20,21,21,21	0
3	GOL	D	2868	6/6	0.94	0.27	-	20,21,22,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.