Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

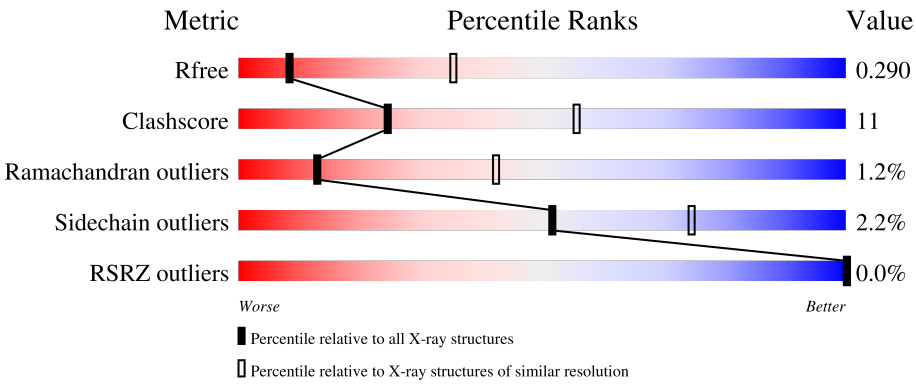
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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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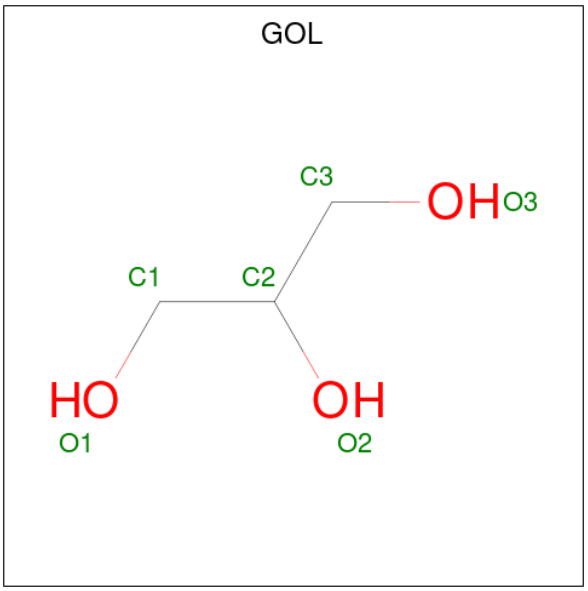
Chain	Residue	Modelled	Actual	Comment	Reference
D	2847	PRO	-	expression tag	UNP Q8G9Q2
D	2848	ASN	-	expression tag	UNP Q8G9Q2
D	2849	PRO	-	expression tag	UNP Q8G9Q2
D	2850	LEU	-	expression tag	UNP Q8G9Q2
D	2851	LEU	-	expression tag	UNP Q8G9Q2
D	2852	GLY	-	expression tag	UNP Q8G9Q2
D	2853	LEU	-	expression 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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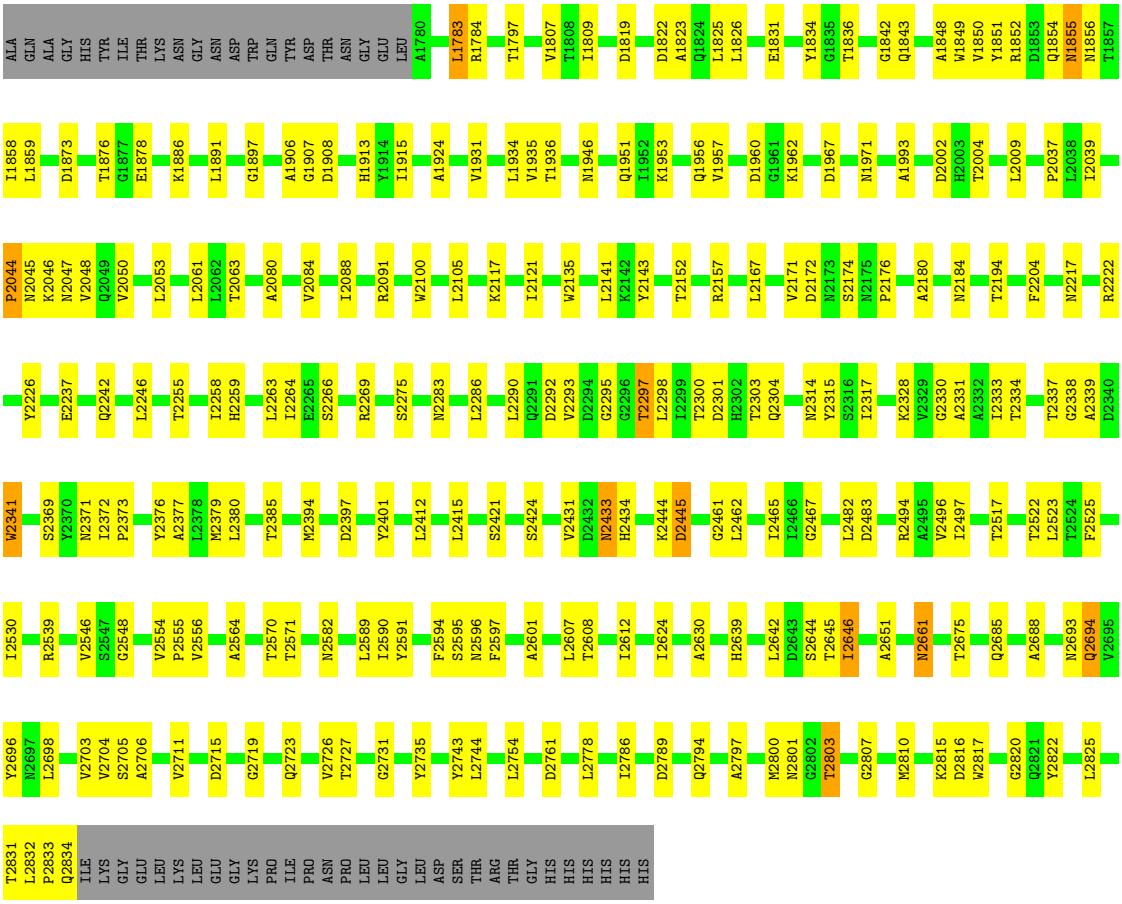
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	8	8	8	0	0

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.

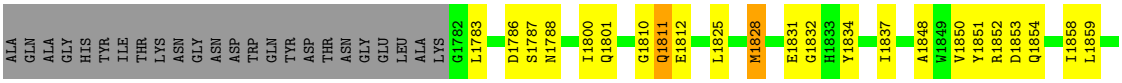
- Molecule 1: Dextransucrase

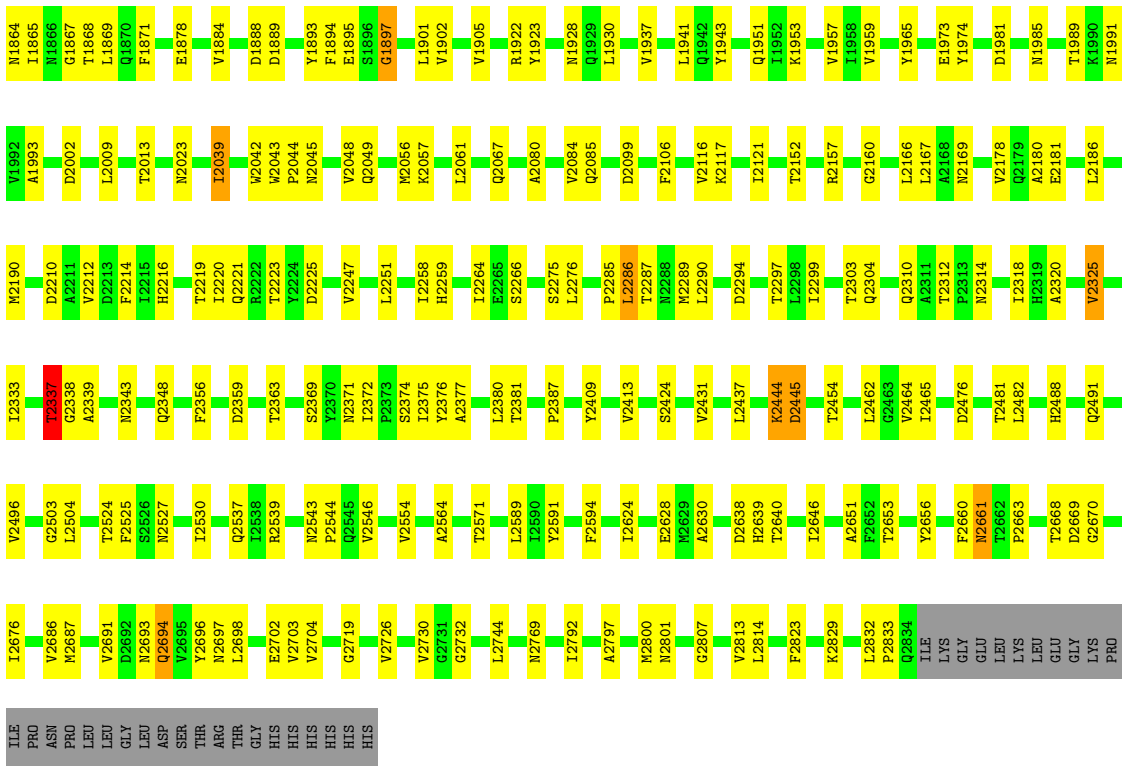
Chain A:



- Molecule 1: Dextransucrase

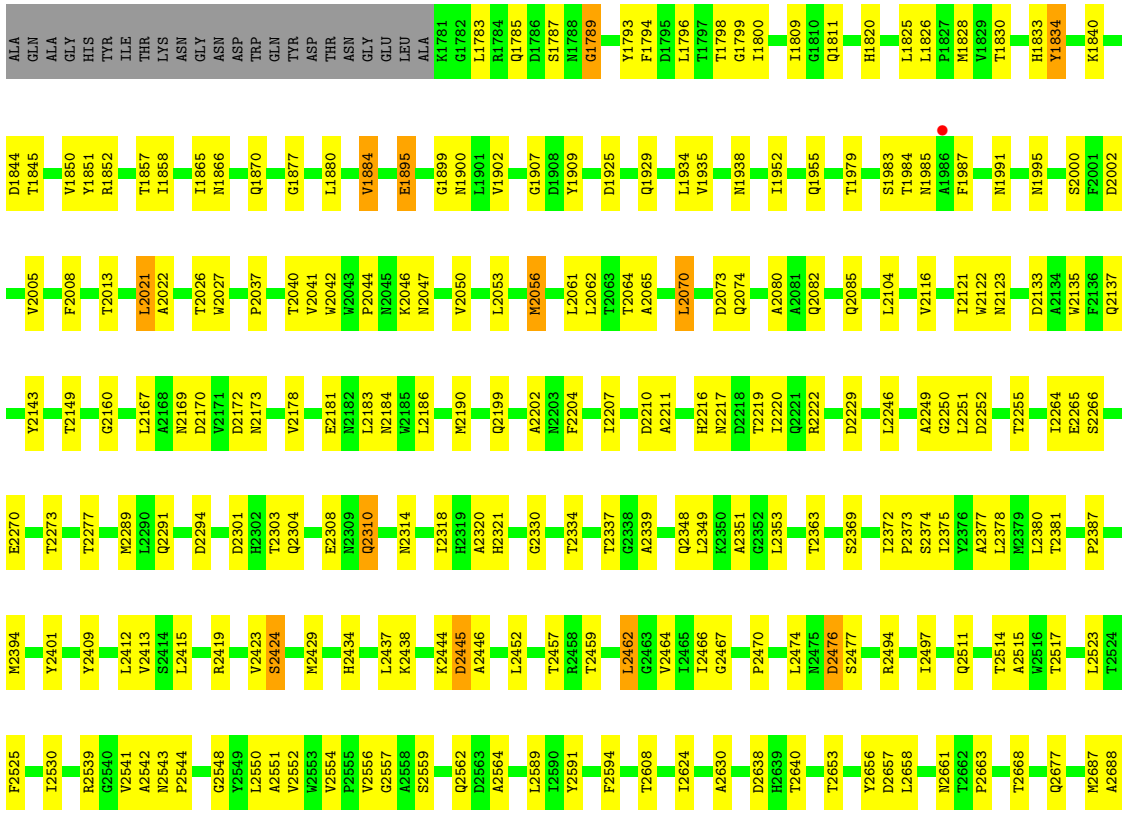
Chain B:

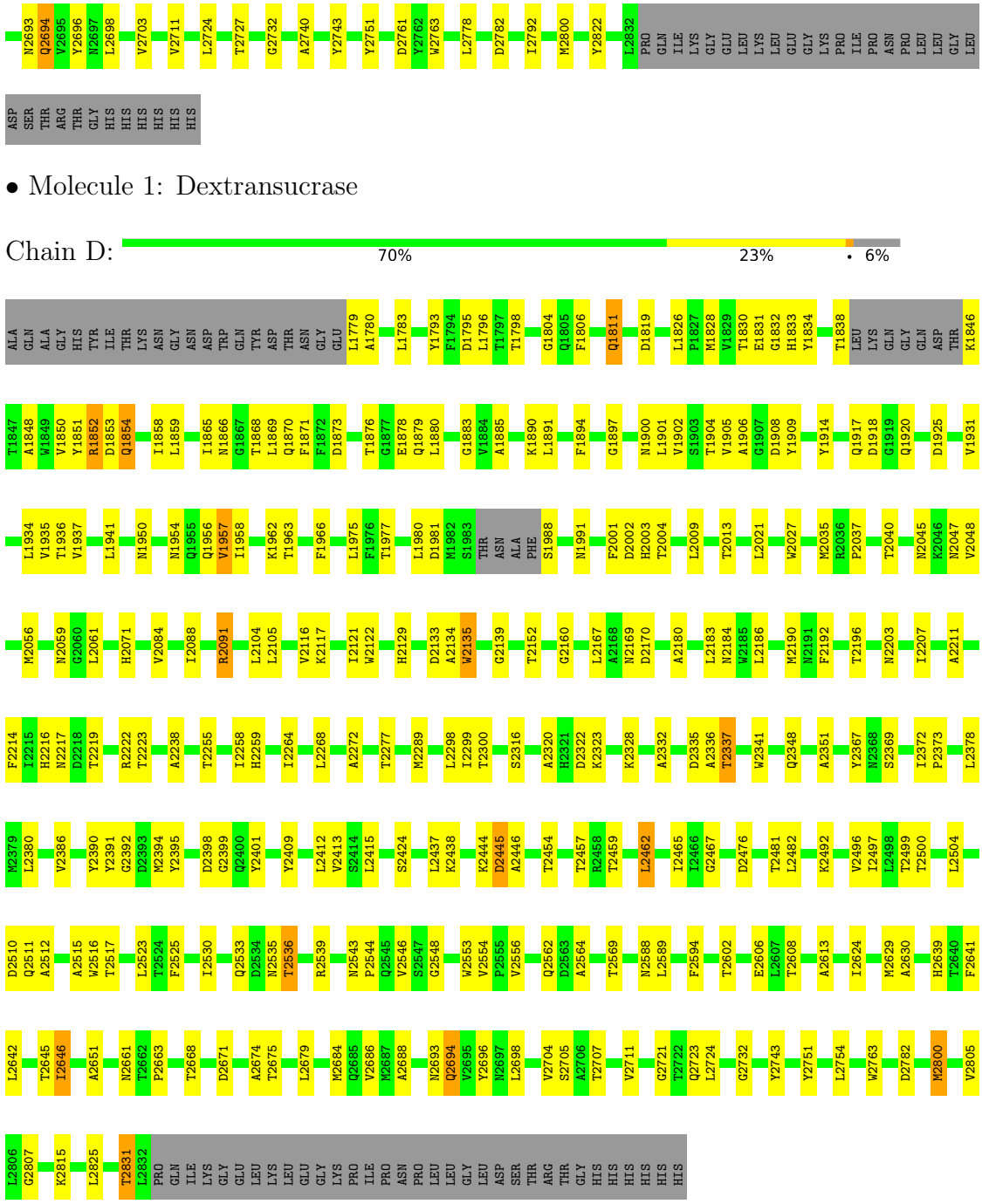




• Molecule 1: Dextransucrase

Chain C: 73% 21% • 5%




N2693 Q2694 V2695 Y2696 N2697 L2698 V2703 V2711 L2724 T2727 G2732 A2740 Y2743 Y2751 D2761 Y2762 W2763 L2778 D2782 I2792 M2800 Y2822 L2832 PRO GLN ILE LYS GLY GLU LEU LYS LEU GLU GLY LYS PRO ILE PRO ASN PRO LEU LEU GLY LEU
ASP SER THR ARG THR GLY HIS HIS HIS HIS HIS HIS
• Molecule 1: Dextransucrase
Chain D:
70%
23%
• 6%
ALA GLN ALA GLY HIS TYR ILE THR LYS ASN GLY ASN ASP TRP GLN TYR ASP THR ASN GLY GLU L1779 A1780 L1783 Y1793 F1794 D1795 L1796 T1797 T1798 G1804 Q1805 F1806 Q1811 D1819 L1826 P1827 M1828 V1829 T1830 E1831 G1832 H1833 Y1834 T1838 LEU LYS GLN GLY GLN ASP THR K1846
T1847 A1848 W1849 V1850 Y1851 R1852 D1853 Q1854 I1858 L1859 I1865 N1866 G1867 T1868 L1869 Q1870 F1871 F1872 D1873 T1876 G1877 E1878 Q1879 L1880 G1883 Y1884 A1885 K1890 L1891 F1894 G1897 N1900 L1901 V1902 S1903 T1904 V1905 A1906 G1907 D1908 Y1909 Y1914 Q1917 D1918 G1919 Q1920 D1925 V1931
L1934 V1935 T1936 V1937 L1941 N1950 N1954 Q1955 Q1956 V1957 I1958 K1962 T1963 F1966 L1975 F1976 T1977 L1980 D1981 M1982 S1983 THR ASN ALA PHE S1988 N1991 F2001 D2002 H2003 T2004 L2009 T2013 L2021 W2027 M2035 R2036 P2037 T2040 N2045 K2046 N2047 V2048
M2056 N2059 G2060 L2061 H2071 V2084 I2088 R2091 L2104 L2105 V2116 K2117 I2121 W2122 H2129 D2133 A2134 W2135 G2139 T2152 G2160 L2167 A2168 N2169 D2170 A2180 L2183 N2184 W2185 L2186 M2190 N2191 F2192 T2196 N2203 I2207 A2211
F2214 I2215 H2216 N2217 D2218 T2219 R2222 T2223 A2238 T2255 I2258 H2259 I2264 L2268 A2272 T2277 M2289 L2298 I2299 T2300 S2316 A2320 H2321 D2322 K2323 K2328 A2332 D2335 A2336 T2337 W2341 Q2348 A2351 Y2367 N2368 S2369 I2372 P2373 L2378
M2379 L2380 V2386 Y2390 Y2391 G2392 D2393 M2394 Y2395 D2398 G2399 Q2400 Y2401 Y2409 L2412 V2413 S2414 L2415 S2424 L2437 K2438 K2444 D2445 A2446 T2454 T2457 R2458 T2459 L2462 I2465 I2466 G2467 D2476 T2481 L2482 K2492 V2496 I2497 L2498 T2499 T2500 L2504
D2510 Q2511 A2512 A2515 W2516 T2517 L2523 T2524 F2525 I2530 Q2533 D2534 N2535 T2536 R2539 N2543 P2544 Q2545 V2546 S2547 G2548 W2553 V2554 P2555 V2556 Q2562 D2563 A2564 T2569 N2588 L2589 F2594 T2602 E2606 L2607 T2608 A2613 I2624 M2629 A2630 H2639 T2640 F2641
L2642 T2645 I2646 A2651 N2661 T2662 P2663 T2668 D2671 A2674 T2675 L2679 M2684 Q2685 V2686 M2687 A2688 N2693 Q2694 V2695 Y2696 N2697 L2698 V2704 S2705 A2706 T2707 V2711 G2721 T2722 Q2723 L2724 G2732 Y2743 Y2751 L2754 W2763 D2782 M2800 V2805
L2806 G2807 K2815 L2825 T2831 L2832 PRO GLN ILE LYS GLY GLU LEU LYS LEU GLU GLY LYS PRO ILE PRO ASN PRO LEU LEU GLY LEU ASP SER THR ARG THR GLY HIS HIS HIS HIS HIS HIS

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

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 (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
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:HD22	1:D:2009:LEU:N	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: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:C:2199:GLN:NE2	1:C:2677:GLN:HE22	1.95	0.64
1:D:2002:ASP:O	1:D:2013:THR:HG23	1.96	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:A:2184:ASN:HD21	1:A:2743:TYR:H	1.47	0.63
1:C:2217:ASN:HB3	1:C:2255:THR:HG21	1.80	0.63
1:D:2613:ALA:HB2	1:D:2675:THR:HA	1.80	0.63
1:D:2679:LEU:HD22	1:D:2684:MET:HE3	1.81	0.62
1:D:2693:ASN:HD22	1:D:2694:GLN:NE2	1.96	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:A:2494:ARG:HB3	1:A:2556:VAL:HG22	1.81	0.62
1:D:2515:ALA:CB	1:D:2530:ILE:HG21	2.29	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:C:2594:PHE:CG	1:C:2630:ALA:HB2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1906:ALA:HB3	1:D:1935:VAL:HG12	1.81	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:B:1848:ALA:HB1	1:B:1878:GLU:HG3	1.82	0.61
1:C:2056:MET:CE	1:C:2104:LEU:HD21	2.31	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:B:2181:GLU:OE2	1:B:2656:TYR:OH	2.18	0.60
1:C:2401:TYR:CD1	1:C:2608:THR:HG23	2.36	0.60
1:B:2653:THR:HG23	1:B:2698:LEU:HD23	1.81	0.60
1:C:2494:ARG:HB3	1:C:2556:VAL:HG22	1.84	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:B:2465:ILE:HD11	1:B:2482:LEU:HG	1.84	0.60
1:D:2525:PHE:CD1	1:D:2530:ILE:HD11	2.36	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: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:D:2679:LEU:HD22	1:D:2684:MET:CE	2.33	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:A:2157:ARG:HG2	1:A:2801:ASN:HD22	1.69	0.58
1:C:1783:LEU:HD23	1:C:1783:LEU:C	2.23	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:A:2009:LEU:HD11	1:A:2825:LEU:HD21	1.85	0.58
1:A:1783:LEU:HD23	1:A:1784:ARG:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2349:LEU:HD11	1:C:2353:LEU:HD11	1.86	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:B:2591:TYR:HB2	1:B:2624:ILE:HD12	1.87	0.57
1:C:2056:MET:HE2	1:C:2061:LEU:HD12	1.86	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:B:2275:SER:HB2	1:B:2286:LEU:HD23	1.88	0.55
1:D:2167:LEU:HD13	1:D:2696:TYR:OH	2.07	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:B:2333:ILE:O	1:B:2337:THR:CG2	2.54	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: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:A:1906:ALA:HB3	1:A:1934:LEU:O	2.08	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:1864:ASN:HA	1:B:1869:LEU:HD23	1.90	0.54
1:B:2045:ASN:OD1	1:B:2048:VAL:HG23	2.08	0.54
1:B:2444:LYS:O	1:B:2445:ASP:CB	2.56	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: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: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:D:2135:TRP:CG	1:D:2711:VAL:HG11	2.42	0.53
1:A:1891:LEU:HD13	1:A:1908:ASP:HB2	1.90	0.53
1:C:2220:ILE:HG21	1:C:2255:THR:OG1	2.09	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:C:1995:ASN:OD1	1:C:2000:SER:OG	2.27	0.53
1:D:2084:VAL:HG12	1:D:2088:ILE:CD1	2.38	0.53
1:B:1828:MET:HE3	1:B:1828:MET:HA	1.91	0.53
1:A:2330:GLY:HA2	1:A:2333:ILE:HD12	1.90	0.53
1:A:2462:LEU:HB3	1:A:2554:VAL:HG12	1.91	0.53
1:B:1828:MET:HE1	1:B:1867:GLY:N	2.24	0.53
1:C:2424[A]:SER:HB2	1:C:2564:ALA:HB1	1.89	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:2374:SER:OG	1:C:2550:LEU:HD22	2.09	0.53
1:C:2446:ALA:HB2	1:C:2457:THR:HG21	1.90	0.53
1:A:2377:ALA:HA	1:A:2415:LEU:HD13	1.90	0.52
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:B:1800:ILE:HG22	1:B:1801:GLN:O	2.09	0.52
1:C:2008:PHE:CD2	1:C:2703:VAL:HG11	2.44	0.52
1:C:2229:ASP:HB3	1:C:2751:TYR:CD1	2.45	0.52
1:A:2334:THR:HG22	1:A:2339:ALA:O	2.10	0.52
1:C:1850:VAL:HG12	1:C:1851:TYR:N	2.23	0.52
1:C:2184:ASN:HD21	1:C:2743:TYR:H	1.56	0.52
1:C:2330:GLY:O	1:C:2334:THR:HG23	2.09	0.52
1:C:1834:TYR:CE1	1:C:1865:ILE:HD13	2.44	0.52
1:C:2318:ILE:HB	1:C:2375:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1956:GLN:O	1:A:1957:VAL:HG13	2.09	0.52
1:A:2483:ASP:OD1	1:A:2522:THR:HG23	2.08	0.52
1:B:1985:ASN:O	1:B:1989:THR:HG23	2.10	0.52
1:C:2021:LEU:CD2	1:C:2027:TRP:CE2	2.93	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:2275:SER:HB2	1:A:2286:LEU:HD23	1.92	0.52
1:C:2409:TYR:CZ	1:C:2413:VAL:HG21	2.45	0.52
1:C:2310:GLN:HE21	1:C:2310:GLN:HA	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:2438:LYS:NZ	1:D:2481:THR:O	2.37	0.51
1:D:2629:MET:HE1	1:D:2675:THR:HG21	1.89	0.51
1:B:2212:VAL:HG23	1:B:2220:ILE:HD13	1.90	0.51
1:C:2264:ILE:HD12	1:C:2265:GLU:O	2.09	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:B:2299:ILE:HG23	1:B:2312:THR:HB	1.93	0.51
1:C:2047:ASN:ND2	1:C:2070:LEU:HD23	2.25	0.51
1:C:2160:GLY:HA3	1:C:2216:HIS:CE1	2.46	0.51
1:D:1811:GLN:H	1:D:1811:GLN:HE21	1.59	0.51
1:A:2661:ASN:ND2	1:A:2735:TYR:OH	2.44	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:2815:LYS:HE2	1:A:2817:TRP:CH2	2.46	0.51
1:C:1909:TYR:O	1:C:1938:ASN:N	2.31	0.51
1:D:2328:LYS:NZ	1:D:2369:SER:OG	2.43	0.51
1:C:1825:LEU:HD12	1:C:1826:LEU:N	2.26	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: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:B:2247:VAL:CG2	1:B:2264:ILE:HG22	2.41	0.51
1:C:2181:GLU:OE2	1:C:2656:TYR:OH	2.21	0.51
1:A:1783:LEU:C	1:A:1783:LEU:CD2	2.80	0.50
1:C:2594:PHE:CD1	1:C:2630:ALA:HB2	2.47	0.50
1:D:1908:ASP:HA	1:D:1936:THR:HB	1.92	0.50
1:A:1907:GLY:N	1:A:1935:VAL:HG12	2.26	0.50
1:B:2318:ILE:HD13	1:B:2375:ILE:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1811:GLN:HE21	1:D:1811:GLN:N	2.09	0.50
1:D:2332:ALA:HA	1:D:2367:TYR:CE1	2.45	0.50
1:A:1851:TYR:CD2	1:A:1859:LEU:HD12	2.46	0.50
1:A:2091:ARG:HB3	1:A:2100:TRP:CZ2	2.46	0.50
1:A:2444:LYS:O	1:A:2445:ASP:CB	2.54	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:A:1913:HIS:CE1	1:A:1924:ALA:HB3	2.47	0.50
1:D:1828:MET:CE	1:D:1866:ASN:HA	2.42	0.50
1:A:2002:ASP:O	1:A:2004:THR:HG23	2.12	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:D:1869:LEU:HD12	1:D:2071:HIS:NE2	2.27	0.50
1:B:2424[A]:SER:HB2	1:B:2564:ALA:HB1	1.94	0.49
1:A:2246:LEU:HD13	1:A:2315:TYR:CE1	2.46	0.49
1:D:1977:THR:H	1:D:2047:ASN:ND2	2.10	0.49
1:A:2046:LYS:O	1:A:2050:VAL:HG23	2.12	0.49
1:A:2723:GLN:NE2	1:A:2822:TYR:OH	2.45	0.49
1:B:2462:LEU:HD12	1:B:2462:LEU:C	2.33	0.49
1:D:1958:ILE:HA	1:D:1962:LYS:O	2.11	0.49
1:D:2001:PHE:CZ	1:D:2831:THR:HG21	2.47	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: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:C:1785:GLN:NE2	1:C:1789:GLY:O	2.46	0.49
1:C:2137:GLN:NE2	1:C:2640:THR:OG1	2.46	0.49
1:D:1851:TYR:O	1:D:1852:ARG:O	2.29	0.49
1:D:1870:GLN:HE22	1:D:1879:GLN:HE21	1.61	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:C:2037:PRO:HB2	1:C:2040:THR:HG23	1.95	0.49
1:D:2394:MET:HG2	1:D:2412:LEU:HD12	1.94	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:A:2467:GLY:O	1:A:2548:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2527:ASN:O	1:B:2537:GLN:HB2	2.13	0.48
1:D:2264:ILE:C	1:D:2264:ILE:HD12	2.33	0.48
1:B:1923:TYR:O	1:B:1930:LEU:HD23	2.12	0.48
1:C:2653:THR:HG23	1:C:2698:LEU:HD23	1.95	0.48
1:D:1917:GLN:HG2	1:D:1918:ASP:OD1	2.13	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:2258:ILE:HG23	1:D:2259:HIS:CD2	2.48	0.48
1:B:1923:TYR:CZ	1:B:1937:VAL:HG13	2.48	0.48
1:D:1851:TYR:HD2	1:D:1859:LEU:HD12	1.78	0.48
1:D:2594:PHE:CD1	1:D:2630:ALA:HB2	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:A:1931:VAL:HG11	1:A:1935:VAL:HG21	1.94	0.48
1:A:2045:ASN:HD21	1:A:2121:ILE:HD13	1.79	0.48
1:B:1786:ASP:O	1:B:1788:ASN:N	2.47	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:1907:GLY:H	1:A:1935:VAL:HG12	1.78	0.48
1:A:2293:VAL:HG22	1:A:2298:LEU:HD13	1.96	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:C:2369:SER:HB2	1:C:2372:ILE:HD11	1.95	0.48
1:A:1993:ALA:HB2	1:A:2833:PRO:HG3	1.96	0.47
1:B:1943:TYR:CD1	1:B:1957:VAL:HG11	2.49	0.47
1:B:2167:LEU:HD13	1:B:2696:TYR:OH	2.14	0.47
1:B:2424[B]:SER:OG	1:B:2444:LYS:N	2.47	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:C:2251:LEU:HD12	1:C:2294:ASP:HB3	1.95	0.47
1:D:2437:LEU:C	1:D:2437:LEU:HD23	2.34	0.47
1:D:2602:THR:OG1	1:D:2606:GLU:OE1	2.24	0.47
1:A:2394:MET:HG2	1:A:2412:LEU:HD12	1.96	0.47
1:A:2496:VAL:HG12	1:A:2497:ILE:HG12	1.97	0.47
1:B:1951:GLN:HE21	1:B:1953:LYS:HE2	1.79	0.47
1:D:2332:ALA:HB2	1:D:2367:TYR:CD1	2.49	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:B:1810:GLY:O	1:B:1811:GLN:HG2	2.15	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:C:1840:LYS:HA	1:C:1845:THR:HA	1.96	0.47
1:D:2504:LEU:HD21	1:D:2546:VAL:HG11	1.97	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: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:2363:THR:HG23	1:C:2543:ASN:CA	2.44	0.47
1:C:2761:ASP:HB3	1:C:2778:LEU:HD11	1.96	0.47
1:D:1830:THR:O	1:D:1831:GLU:CB	2.62	0.47
1:D:2272:ALA:O	1:D:2277:THR:HG23	2.15	0.47
1:D:2517:THR:HG22	1:D:2523:LEU:HG	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:1783:LEU:O	1:B:1783:LEU:CD2	2.63	0.47
1:B:2726:VAL:HG23	1:B:2813:VAL:HG22	1.95	0.47
1:C:2216:HIS:O	1:C:2219:THR:HG22	2.15	0.46
1:A:2517:THR:HG23	1:A:2523:LEU:CD2	2.43	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: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: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:D:2751:TYR:HB2	1:D:2754:LEU:HD12	1.97	0.46
1:A:2141:LEU:HB3	1:A:2706:ALA:HB1	1.95	0.46
1:A:2143:TYR:CE1	1:A:2803:THR:HG22	2.50	0.46
1:B:2320:ALA:O	1:B:2325:VAL:HG21	2.16	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:C:2394:MET:HG2	1:C:2412:LEU:HD12	1.96	0.46
1:C:2541:VAL:HG12	1:C:2542:ALA:N	2.30	0.46
1:A:1783:LEU:HD23	1:A:1783:LEU:C	2.36	0.46
1:A:1836:THR:HG22	1:A:1849:TRP:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2039:ILE:HD11	1:A:2105:LEU:HD13	1.98	0.46
1:A:2646:ILE:C	1:A:2646:ILE:HD12	2.36	0.46
1:B:2166:LEU:HD13	1:B:2214:PHE:CE2	2.50	0.46
1:C:2190:MET:HE2	1:C:2190:MET:HA	1.97	0.46
1:D:1806:PHE:CE1	1:D:1826:LEU:HD11	2.51	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:B:2371:ASN:ND2	1:B:2546:VAL:HG23	2.31	0.46
1:D:1851:TYR:CD2	1:D:1859:LEU:HD12	2.51	0.46
1:D:2424[B]:SER:OG	1:D:2564:ALA:HB1	2.16	0.46
1:B:2543:ASN:HB2	1:B:2544:PRO:CD	2.46	0.46
1:D:2651:ALA:HA	1:D:2696:TYR:CD1	2.51	0.46
1:A:2328:LYS:O	1:A:2331:ALA:HB3	2.15	0.45
1:A:2703:VAL:HG22	1:A:2726:VAL:HG22	1.98	0.45
1:C:2123:ASN:OD1	1:C:2123:ASN:C	2.55	0.45
1:D:2525:PHE:CE1	1:D:2530:ILE:HD11	2.51	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:2170:ASP:O	1:D:2800:MET:HG3	2.15	0.45
1:D:2222:ARG:NH1	1:D:2754:LEU:O	2.48	0.45
1:D:2322:ASP:OD1	1:D:2322:ASP:N	2.49	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:1850:VAL:HG12	1:C:1851:TYR:H	1.80	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:2059:ASN:HD22	1:D:2104:LEU:CD1	2.07	0.45
1:D:2207:ILE:HA	1:D:2688:ALA:O	2.16	0.45
1:A:2401:TYR:CD2	1:A:2608:THR:HG23	2.50	0.45
1:A:2433:ASN:HD22	1:A:2434:HIS:N	2.13	0.45
1:B:2044:PRO:HG3	1:B:2121:ILE:HD11	1.99	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:D:2409:TYR:O	1:D:2413:VAL:HG23	2.17	0.45
1:D:2009:LEU:N	1:D:2009:LEU:CD2	2.77	0.45
1:C:2467:GLY:O	1:C:2548:GLY:HA3	2.17	0.45
1:A:1809:ILE:N	1:A:1809:ILE:HD12	2.32	0.45
1:B:2039:ILE:HD13	1:B:2039:ILE:H	1.81	0.45
1:C:1991:ASN:ND2	1:C:2085:GLN:OE1	2.50	0.45
1:C:2459:THR:HG21	1:C:2557:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1825:LEU:HD12	1:A:1826:LEU:N	2.32	0.45
1:A:2719:GLY:O	1:A:2810:MET:HE1	2.16	0.45
1:B:2726:VAL:HG23	1:B:2813:VAL:CG2	2.46	0.45
1:D:1920:GLN:HG3	1:D:1950:ASN:ND2	2.30	0.45
1:D:2446:ALA:HB2	1:D:2457:THR:HG21	1.99	0.45
1:C:2378:LEU:HG	1:C:2466:ILE:CD1	2.47	0.45
1:D:1963:THR:HG22	1:D:1975:LEU:HD12	1.99	0.45
1:D:2135:TRP:CD2	1:D:2711:VAL:HG11	2.52	0.45
1:D:2289:MET:CE	1:D:2378:LEU:HD13	2.46	0.45
1:C:1793:TYR:CE2	1:C:1794:PHE:O	2.70	0.44
1:C:2589:LEU:CD2	1:C:2624:ILE:HD13	2.45	0.44
1:A:2222:ARG:NH1	1:A:2754:LEU:O	2.50	0.44
1:C:1809:ILE:N	1:C:1809:ILE:HD12	2.33	0.44
1:C:1985:ASN:ND2	1:C:1987:PHE:HB3	2.31	0.44
1:D:1848:ALA:HB1	1:D:1878:GLU:HG3	1.98	0.44
1:D:2217:ASN:HB3	1:D:2255:THR:HG21	1.98	0.44
1:D:2499:THR:HA	1:D:2504:LEU:HD23	2.00	0.44
1:A:2217:ASN:HB3	1:A: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:B:2106:PHE:CD1	1:B:2116:VAL:HG21	2.52	0.44
1:B:2180:ALA:O	1:B:2744:LEU:HD21	2.18	0.44
1:B:2465:ILE:HG12	1:B:2482:LEU:HD21	1.99	0.44
1:C:2062:LEU:O	1:C:2064:THR:HG22	2.18	0.44
1:C:2377:ALA:O	1:C:2381:THR:HG23	2.17	0.44
1:B:1893:TYR:CE1	1:B:1941:LEU:HD22	2.51	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:2009:LEU:HB3	1:B:2814:LEU:HD12	2.00	0.44
1:C:2135:TRP:CG	1:C:2711:VAL:HG11	2.52	0.44
1:C:2289:MET:HB3	1:C:2289:MET:HE2	1.92	0.44
1:D:1891:LEU:O	1:D:1904:THR:HG23	2.18	0.44
1:A:2045:ASN:OD1	1:A:2048:VAL:HG23	2.18	0.44
1:D:1850:VAL:HG11	1:D:1858:ILE:HD13	1.99	0.44
1:D:1935:VAL:O	1:D:1941:LEU:HD12	2.18	0.44
1:D:2003:HIS:HB2	1:D:2013:THR:HA	2.00	0.44
1:D:2056:MET:HE1	1:D:2105:LEU:HD21	1.95	0.44
1:B:2363:THR:HG23	1:B:2543:ASN:CA	2.48	0.44
1:A:2401:TYR:CG	1:A:2608:THR:HG23	2.53	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:A:2831:THR:HG22	1:A:2833:PRO:HG2	1.99	0.43
1:C:1900:ASN:O	1:C:1902:VAL:HG13	2.18	0.43
1:C:2424[B]:SER:HB3	1:C:2564:ALA:HB1	2.00	0.43
1:D:2152:THR:HB	1:D:2704:VAL:HG22	1.98	0.43
1:D:2510:ASP:O	1:D:2512:ALA:N	2.51	0.43
1:D:2705:SER:HA	1:D:2724:LEU:HD23	1.99	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:D:2401:TYR:CG	1:D:2608:THR:HG23	2.53	0.43
1:B:2646:ILE:HD12	1:B:2646:ILE:C	2.38	0.43
1:C:1796:LEU:HD12	1:C:2073:ASP:OD2	2.19	0.43
1:C:2401:TYR:CD2	1:C:2608:THR:HG23	2.54	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:A:2789:ASP:OD1	1:A:2789:ASP:N	2.49	0.43
1:B:2057:LYS:NZ	1:B:2067:GLN:OE1	2.51	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:1851:TYR:HD2	1:A:1859:LEU:HD12	1.82	0.43
1:B:2374:SER:O	1:B:2377:ALA:HB3	2.18	0.43
1:C:2249:ALA:HB1	1:C:2252:ASP:OD1	2.18	0.43
1:D:1834:TYR:OH	1:D:1870:GLN:OE1	2.37	0.43
1:D:1925:ASP:OD1	1:D:1925:ASP:N	2.51	0.43
1:D:2134:ALA:HB1	1:D:2139:GLY:N	2.34	0.43
1:D:2167:LEU:HD11	1:D:2641:PHE:CE2	2.54	0.43
1:A:2317:ILE:HA	1:A:2379:MET:CE	2.47	0.43
1:B:1888:ASP:O	1:B:1889:ASP:CB	2.67	0.43
1:B:2266:SER:CB	1:B:2314:ASN:HD22	2.20	0.43
1:B:2676:ILE:HG23	1:B:2686:VAL:HG21	2.01	0.43
1:C:2320:ALA:O	1:C:2321:HIS:C	2.54	0.43
1:D:2496:VAL:O	1:D:2497:ILE:HD13	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:B:2289:MET:HB3	1:B:2289:MET:HE2	1.92	0.43
1:C:1840:LYS:HA	1:C:1844:ASP:O	2.18	0.43
1:D:2190:MET:O	1:D:2203:ASN:HB3	2.19	0.43
1:D:2492:LYS:HG2	1:D:2556:VAL:HG21	2.01	0.43
1:A:2117:LYS:NZ	1:A:2807:GLY:O	2.51	0.43
1:A:2157:ARG:HA	1:A:2801:ASN:ND2	2.33	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:D:2169:ASN:ND2	1:D:2698:LEU:HD12	2.34	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:A:2053:LEU:HD11	1:A:2080:ALA:HB3	2.00	0.43
1:A:2242:GLN:O	1:A:2685:GLN:NE2	2.51	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:D:2707:THR:HG23	1:D:2721:GLY:O	2.19	0.43
1:B:2660:PHE:CD1	1:B:2669:ASP:OD2	2.72	0.43
1:A:1886:LYS:HA	1:A:1891:LEU:HD23	2.01	0.42
1:B:1901:LEU:HD23	1:B:1901:LEU:C	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:2308:GLU:O	1:C:2310:GLN:HG2	2.19	0.42
1:D:2002:ASP:OD2	1:D:2035:MET:CE	2.66	0.42
1:D:2021:LEU:HD13	1:D:2027:TRP:CE2	2.54	0.42
1:B:2663:PRO:HB3	1:B:2668:THR:CG2	2.50	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:D:2268:LEU:HD13	1:D:2316:SER:HB3	2.01	0.42
1:A:2045:ASN:ND2	1:A:2121:ILE:HD13	2.33	0.42
1:C:2204:PHE:CG	1:C:2688:ALA:HB2	2.54	0.42
1:D:1869:LEU:HD12	1:D:2071:HIS:CD2	2.54	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:A:1850:VAL:HG12	1:A:1851:TYR:N	2.35	0.42
1:A:2698:LEU:HD22	1:A:2731:GLY:HA3	2.01	0.42
1:C:1830:THR:HA	1:C:1866:ASN:HD21	1.84	0.42
1:A:2176:PRO:HA	1:A:2786:ILE:HG22	2.01	0.42
1:A:2525:PHE:CD1	1:A:2530:ILE:HD11	2.54	0.42
1:B:1837:ILE:C	1:B:1837:ILE:HD12	2.40	0.42
1:B:2638:ASP:CG	1:B:2640:THR:HG22	2.39	0.42
1:C:2121:ILE:HG23	3:C:2868:GOL:H12	2.00	0.42
1:C:2419:ARG:HA	1:C:2423:VAL:CG2	2.50	0.42
1:D:1783:LEU:C	1:D:1783:LEU:HD23	2.40	0.42
1:D:1850:VAL:HG11	1:D:1858:ILE:HG12	2.01	0.42
1:D:2380:LEU:CD1	1:D:2415:LEU:HB3	2.50	0.42
1:B:1850:VAL:HG12	1:B:1851:TYR:N	2.35	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:B:1853:ASP:O	1:B:1854:GLN:C	2.58	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:B:2437:LEU:C	1:B:2437:LEU:HD23	2.40	0.42
1:C:2173:ASN:HB3	1:C:2219:THR:HG21	2.01	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:D:2459:THR:O	1:D:2562:GLN:NE2	2.49	0.42
1:A:2815:LYS:HE2	1:A:2817:TRP:CZ2	2.55	0.42
1:B:2660:PHE:O	1:B:2661:ASN:CB	2.67	0.42
1:C:1865:ILE:HG22	1:C:1865:ILE:O	2.19	0.42
1:C:1952:ILE:HG23	1:C:1955:GLN:OE1	2.20	0.42
1:D:2045:ASN:ND2	1:D:2121:ILE:HD13	2.34	0.42
1:D:2192:PHE:O	1:D:2196:THR:HG23	2.19	0.42
1:D:2723:GLN:HE22	1:D:2815:LYS:NZ	2.18	0.42
1:B:1783:LEU:HD23	1:B:1783:LEU:C	2.39	0.42
1:B:2117:LYS:NZ	1:B:2807:GLY:O	2.53	0.42
1:C:1833:HIS:O	1:C:1834:TYR:CB	2.68	0.42
1:C:2273:THR:HA	1:C:2277:THR:OG1	2.19	0.42
1:D:2372:ILE:N	1:D:2373:PRO:CD	2.82	0.42
1:A:2298:LEU:HD21	1:A:2301:ASP:HB2	2.01	0.42
1:A:2372:ILE:N	1:A:2373:PRO:CD	2.82	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:2387:PRO:HG2	1:C:2589:LEU:HD12	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:A:2341:TRP:CE3	1:A:2642:LEU:HD22	2.55	0.41
1:B:2387:PRO:HG2	1:B:2589:LEU:CD1	2.50	0.41
1:C:1925:ASP:OD1	1:C:1929:GLN:N	2.42	0.41
1:C:2149:THR:HG21	1:C:2724:LEU:HD22	2.02	0.41
1:C:2169:ASN:ND2	1:C:2698:LEU:HD12	2.32	0.41
1:D:1914:TYR:CZ	1:D:1937:VAL:HG11	2.55	0.41
1:A:2084:VAL:HG12	1:A:2088:ILE:CD1	2.50	0.41
1:B:1871:PHE:HB2	1:B:1894:PHE:CZ	2.56	0.41
1:B:2002:ASP:O	1:B:2013:THR:HG23	2.20	0.41
1:B:2356:PHE:O	1:B:2359:ASP:HB3	2.20	0.41
1:B:2638:ASP:OD2	1:B:2640:THR:CG2	2.67	0.41
1:C:1811:GLN:NE2	1:C:2065:ALA:HB3	2.35	0.41
1:C:2040:THR:OG1	1:C:2041:VAL:HG13	2.20	0.41
1:D:1873:ASP:CG	1:D:1876:THR:HG22	2.40	0.41
1:D:2679:LEU:HD12	1:D:2686:VAL:HG22	2.02	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:B:1959:VAL:O	1:B:1959:VAL:HG12	2.20	0.41
1:B:2481:THR:HG22	1:B:2524:THR:HA	2.01	0.41
1:D:2517:THR:HG22	1:D:2523:LEU:CD2	2.50	0.41
1:A:2589:LEU:CD2	1:A:2624:ILE:HD13	2.50	0.41
1:B:1893:TYR:CZ	1:B:1941:LEU:HD22	2.55	0.41
1:B:1895:GLU:OE2	1:B:1897:GLY:N	2.52	0.41
1:C:1987:PHE:HB3	1:C:2082:GLN:NE2	2.36	0.41
1:C:2409:TYR:O	1:C:2413:VAL:HG23	2.19	0.41
1:C:2494:ARG:HB3	1:C:2514:THR:HG22	2.01	0.41
1:C:2517:THR:HG22	1:C:2523:LEU:HG	2.01	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: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: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:2595:SER:OG	1:A:2596:ASN:N	2.53	0.41
1:A:2639:HIS:CE1	1:A:2645:THR:HG23	2.56	0.41
1:A:2831:THR:HG22	1:A:2833:PRO:CG	2.51	0.41
1:D:2129:HIS:CE1	1:D:2805:VAL:HG21	2.56	0.41
1:D:2186:LEU:HD22	1:D:2223:THR:HG23	2.01	0.41
1:A:1807:VAL:HG12	1:A:1809:ILE:HD12	2.02	0.41
1:A:1848:ALA:HB1	1:A:1878:GLU:HG3	2.01	0.41
1:A:2045:ASN:ND2	1:A:2121:ILE:HG21	2.35	0.41
1:A:2061:LEU:HD23	1:A:2061:LEU:HA	1.96	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:B:2339:ALA:HB2	1:B:2348:GLN:NE2	2.36	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:1993:ALA:HB2	1:A:2833:PRO:CG	2.50	0.41
1:A:2171:VAL:HG23	1:A:2693:ASN:O	2.20	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
1:B:2190:MET:HA	1:B:2190:MET:HE2	2.02	0.41
1:B:2381:THR:HG21	1:B:2464:VAL:HG21	2.03	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:C:2429:MET:HA	1:C:2438:LYS:O	2.21	0.41
1:C:2497:ILE:O	1:C:2551:ALA:HA	2.21	0.41
1:C:2740:ALA:HB1	1:C:2792:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1795:ASP:CG	1:D:1798:THR:HG22	2.41	0.41
1:D:2001:PHE:CE1	1:D:2825:LEU:HD21	2.56	0.41
1:D:2045:ASN:HD21	1:D:2121:ILE:HD13	1.86	0.41
1:D:2152:THR:CB	1:D:2704:VAL:HG22	2.51	0.41
1:D:2180:ALA:O	1:D:2183:LEU:N	2.54	0.41
1:A:2704:VAL:HG21	1:A:2797:ALA:HB1	2.03	0.41
1:B:2178:VAL:HG22	1:B:2792:ILE:HD11	2.03	0.41
1:C:2210:ASP:O	1:C:2211:ALA:HB3	2.21	0.41
1:D:2021:LEU:HD13	1:D:2027:TRP:CG	2.55	0.41
1:D:2211:ALA:HB1	1:D:2214:PHE:HB2	2.03	0.41
1:D:2646:ILE:C	1:D:2646:ILE:HD12	2.41	0.41
1:D:2651:ALA:HA	1:D:2696:TYR:CE1	2.56	0.41
1:A:2044:PRO:CG	1:A:2121:ILE:HD11	2.51	0.40
1:A:2266:SER:CB	1:A:2314:ASN:HD22	2.31	0.40
1:A:2612:ILE:HG22	1:A:2675:THR:HG23	2.03	0.40
1:B:1851:TYR:HD2	1:B:1859:LEU:HD12	1.86	0.40
1:B:2628:GLU:HA	1:B:2687:MET:HB3	2.03	0.40
1:C:1800:ILE:HD12	1:C:1800:ILE:H	1.86	0.40
1:C:2559:SER:HB3	1:C:2562:GLN:HB2	2.03	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:C:2591:TYR:HB2	1:C:2624:ILE:CD1	2.46	0.40
1:D:2424[B]:SER:CB	1:D:2564:ALA:HB1	2.51	0.40
1:A:1822:ASP:O	1:A:1823:ALA:CB	2.69	0.40
1:A:2135:TRP:CD2	1:A:2711:VAL:HG11	2.56	0.40
1:A:2293:VAL:HG13	1:A:2297:THR:O	2.22	0.40
1:C:1811:GLN:HE21	1:C:2065:ALA:HB3	1.85	0.40
1:C:2005:VAL:HG12	1:C:2703:VAL:HG23	2.03	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:B:2337:THR:CG2	1:B:2338:GLY:N	2.85	0.40
1:B:2496:VAL:CG2	1:B:2554:VAL:HG13	2.52	0.40
1:C:2543:ASN:HB2	1:C:2544:PRO:CD	2.50	0.40
1:D:1909:TYR:HE2	1:D:1931:VAL:HG11	1.86	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:A:2646:ILE:C	1:A:2646:ILE:CD1	2.90	0.40
1:B:1869:LEU:HD23	1:B:1869:LEU:HA	1.92	0.40
1:B:2157:ARG:HA	1:B:2801:ASN:ND2	2.37	0.40
1:B:2543:ASN:HB2	1:B:2544:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1906:ALA:HB3	1:D:1935:VAL:CG1	2.49	0.40
1:D:2445:ASP:OD1	1:D:2454:THR:CG2	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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%)	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

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

Sometimes 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 (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
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.

All (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
3	C	2869	GOL	C1-C2-C3-O3
3	D	2869	GOL	O1-C1-C2-C3
3	C	2869	GOL	O2-C2-C3-O3
3	C	2867	GOL	O2-C2-C3-O3
3	C	2868	GOL	O1-C1-C2-O2
3	D	2867	GOL	O2-C2-C3-O3
3	D	2869	GOL	O1-C1-C2-O2
3	D	2867	GOL	O1-C1-C2-C3

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.