



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:20 pm BST

PDB ID : 3AU5
Title : Structure of the human myosin-X MyTH4-FERM cassette
Authors : Hirano, Y.; Takahashi, A.; Hakoshima, T.
Deposited on : 2011-01-28
Resolution : 2.55 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

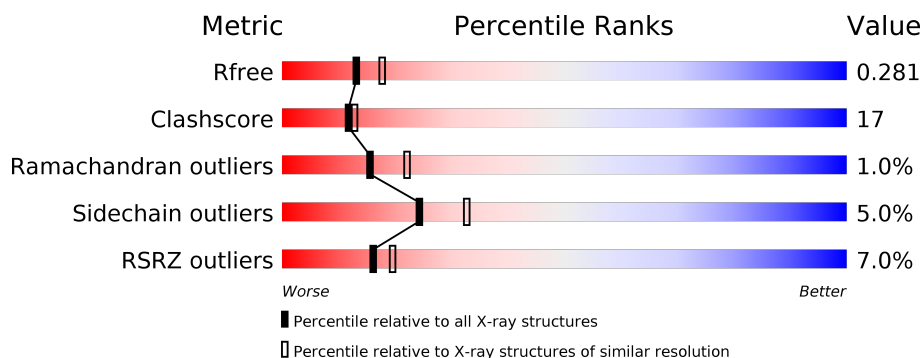
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	555	<div> <div>8%</div> <div> <div></div> <div>54%</div> <div>30%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7782 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 Myosin-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3856	2479	644	713	20			
1	B	484	Total	C	N	O	S	0	0	0
			3832	2465	642	706	19			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1484	GLY	-	EXPRESSION TAG	UNP Q9HD67
A	1485	PRO	-	EXPRESSION TAG	UNP Q9HD67
A	1663	THR	SER	SEE REMARK 999	UNP Q9HD67
A	?	-	THR	DELETION	UNP Q9HD67
A	?	-	PRO	DELETION	UNP Q9HD67
A	?	-	CYS	DELETION	UNP Q9HD67
A	?	-	GLU	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
A	?	-	LEU	DELETION	UNP Q9HD67
A	?	-	GLU	DELETION	UNP Q9HD67
A	?	-	LYS	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
A	?	-	THR	DELETION	UNP Q9HD67
A	?	-	SER	DELETION	UNP Q9HD67
A	?	-	PHE	DELETION	UNP Q9HD67
A	?	-	LEU	DELETION	UNP Q9HD67
A	?	-	GLU	DELETION	UNP Q9HD67
A	?	-	GLY	DELETION	UNP Q9HD67
A	?	-	THR	DELETION	UNP Q9HD67
A	?	-	LEU	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
A	?	-	ARG	DELETION	UNP Q9HD67
B	1484	GLY	-	EXPRESSION TAG	UNP Q9HD67
B	1485	PRO	-	EXPRESSION TAG	UNP Q9HD67

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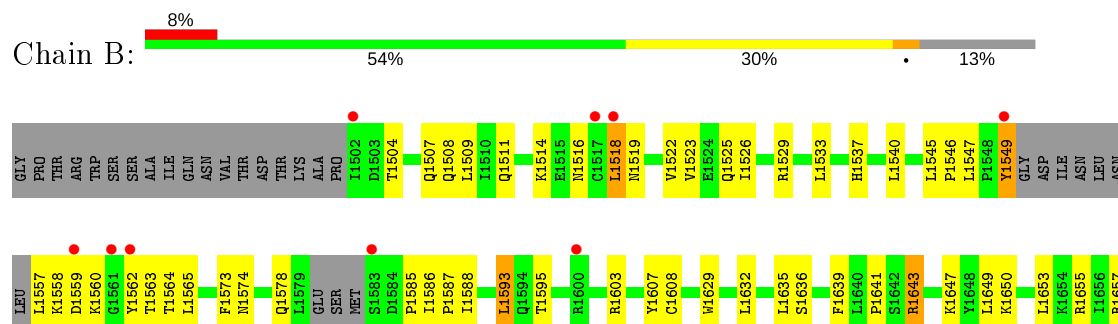
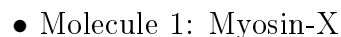
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1663	THR	SER	SEE REMARK 999	UNP Q9HD67
B	?	-	THR	DELETION	UNP Q9HD67
B	?	-	PRO	DELETION	UNP Q9HD67
B	?	-	CYS	DELETION	UNP Q9HD67
B	?	-	GLU	DELETION	UNP Q9HD67
B	?	-	ARG	DELETION	UNP Q9HD67
B	?	-	LEU	DELETION	UNP Q9HD67
B	?	-	GLU	DELETION	UNP Q9HD67
B	?	-	LYS	DELETION	UNP Q9HD67
B	?	-	ARG	DELETION	UNP Q9HD67
B	?	-	ARG	DELETION	UNP Q9HD67
B	?	-	THR	DELETION	UNP Q9HD67
B	?	-	SER	DELETION	UNP Q9HD67
B	?	-	PHE	DELETION	UNP Q9HD67
B	?	-	LEU	DELETION	UNP Q9HD67
B	?	-	GLU	DELETION	UNP Q9HD67
B	?	-	GLY	DELETION	UNP Q9HD67
B	?	-	THR	DELETION	UNP Q9HD67
B	?	-	LEU	DELETION	UNP Q9HD67
B	?	-	ARG	DELETION	UNP Q9HD67
B	?	-	ARG	DELETION	UNP Q9HD67

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	62	Total O 62 62	0	0
2	B	32	Total O 32 32	0	0

- Molecule 1: Myosin-X



E1658	Q1659	F1660	E1666	L1670	F1671	Y1672	Y1673	L1676	P1686	E1690	H1696	Q1697	Q1698	E1699	M1700	H1707	I1716	T1721	E1724	V1725	V1726	I1730	R1731	G1732	L1733	A1734	M1735	E1736	D1737	N1740	A1743	L1744	F1745	E1746	Y1747	N1748	G1749	H1750	V1751	D1752	K1753	A1754	I1755	E1756	S1757	R1758																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
T1759	V1760	V1761	L1765	A1766	K1767	F1768	L1771	A1772	A1773	THR	SER	GLU	VAL	GLY	ASP	L1780	P1781	M1782	K1783	F1784	K1787	L1788	Y1789	C1790	K1799	D1800	S1801	F1808	A1811	H1812	E1813	A1814	V1815	I1816	H1819	H1820	P1821	A1822	P1823	E1824	Q1828	V1829	L1835	D1841	Y1842	T1843	L1844	P1850																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
L1851	E1852	E1853	V1854	Y1855	S1856	L1857	Q1858	K1861	A1862	R1863	ILE	SER	GLN	SER	THR	LYS	THR	PHE	SER	PHE	ARG	THR	GLY	SER	VAL	VAL	GLN	ARG	L1891	L1892	L1893	L1894	L1895	L1896	L1897	L1898	L1899	L1900	L1901	L1902	L1903	L1904	L1905	L1906	L1907	L1908	L1909	L1910	L1911	L1912	L1913	L1914	L1915	L1916	L1917	L1918	L1919	L1920	L1921	L1922	L1923	L1924	L1925	L1926	L1927	L1928	L1929	L1930	L1931	L1932	L1933	L1934	L1935	L1936	L1937	L1938	L1939	L1940	L1941	L1942	L1943	L1944	L1945	L1946	L1947	L1948	L1949	L1950	L1951	L1952	L1953	L1954	L1955	L1956	L1957	L1958	L1959	L1960	L1961	L1962	L1963	L1964	L1965	L1966	L1967	L1968	L1969	L1970	L1971	L1972	L1973	L1974	L1975	L1976	L1977	L1978	L1979	L1980	L1981	L1982	L1983	L1984	L1985	L1986	L1987	L1988	L1989	L1990	L1991	L1992	L1993	L1994	L1995	L1996	L1997	L1998	L1999	L2000	L2001	L2002	L2003	L2004	L2005	L2006	L2007	L2008	L2009	L2010	L2011	L2012	L2013	L2014	L2015	L2016	L2017	L2018	L2019	L2020	L2021	L2022	L2023	L2024	L2025	L2026	L2027	L2028	L2029	L2030	L2031	L2032	L2033	L2034	L2035	L2036	L2037	L2038	L2039	L2040	L2041	L2042	L2043	L2044	L2045	L2046	L2047	L2048	L2049	L2050	L2051	L2052	L2053	L2054	L2055	L2056	L2057	L2058	L2059	L2060	L2061	L2062	L2063	L2064	L2065	L2066	L2067	L2068	L2069	L2070	L2071	L2072	L2073	L2074	L2075	L2076	L2077	L2078	L2079	L2080	L2081	L2082	L2083	L2084	L2085	L2086	L2087	L2088	L2089	L2090	L2091	L2092	L2093	L2094	L2095	L2096	L2097	L2098	L2099	L2100	L2101	L2102	L2103	L2104	L2105	L2106	L2107	L2108	L2109	L2110	L2111	L2112	L2113	L2114	L2115	L2116	L2117	L2118	L2119	L2120	L2121	L2122	L2123	L2124	L2125	L2126	L2127	L2128	L2129	L2130	L2131	L2132	L2133	L2134	L2135	L2136	L2137	L2138	L2139	L2140	L2141	L2142	L2143	L2144	L2145	L2146	L2147	L2148	L2149	L2150	L2151	L2152	L2153	L2154	L2155	L2156	L2157	L2158	L2159	L2160	L2161	L2162	L2163	L2164	L2165	L2166	L2167	L2168	L2169	L2170	L2171	L2172	L2173	L2174	L2175	L2176	L2177	L2178	L2179	L2180	L2181	L2182	L2183	L2184	L2185	L2186	L2187	L2188	L2189	L2190	L2191	L2192	L2193	L2194	L2195	L2196	L2197	L2198	L2199	L2200	L2201	L2202	L2203	L2204	L2205	L2206	L2207	L2208	L2209	L2210	L2211	L2212	L2213	L2214	L2215	L2216	L2217	L2218	L2219	L2220	L2221	L2222	L2223	L2224	L2225	L2226	L2227	L2228	L2229	L2230	L2231	L2232	L2233	L2234	L2235	L2236	L2237	L2238	L2239	L2240	L2241	L2242	L2243	L2244	L2245	L2246	L2247	L2248	L2249	L2250	L2251	L2252	L2253	L2254	L2255	L2256	L2257	L2258	L2259	L2260	L2261	L2262	L2263	L2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	L2282	L2283	L2284	L2285	L2286	L2287	L2288	L2289	L2290	L2291	L2292	L2293	L2294	L2295	L2296	L2297	L2298	L2299	L2300	L2301	L2302	L2303	L2304	L2305	L2306	L2307	L2308	L2309	L2310	L2311	L2312	L2313	L2314	L2315	L2316	L2317	L2318	L2319	L2320	L2321	L2322	L2323	L2324	L2325	L2326	L2327	L2328	L2329	L2330	L2331	L2332	L2333	L2334	L2335	L2336	L2337	L2338	L2339	L2340	L2341	L2342	L2343	L2344	L2345	L2346	L2347	L2348	L2349	L2350	L2351	L2352	L2353	L2354	L2355	L2356	L2357	L2358	L2359	L2360	L2361	L2362	L2363	L2364	L2365	L2366	L2367	L2368	L2369	L2370	L2371	L2372	L2373	L2374	L2375	L2376	L2377	L2378	L2379	L2380	L2381	L2382	L2383	L2384	L2385	L2386	L2387	L2388	L2389	L2390	L2391	L2392	L2393	L2394	L2395	L2396	L2397	L2398	L2399	L2400	L2401	L2402	L2403	L2404	L2405	L2406	L2407	L2408	L2409	L2410	L2411	L2412	L2413	L2414	L2415	L2416	L2417	L2418	L2419	L2420	L2421	L2422	L2423	L2424	L2425	L2426	L2427	L2428	L2429	L2430	L2431	L2432	L2433	L2434	L2435	L2436	L2437	L2438	L2439	L2440	L2441	L2442	L2443	L2444	L2445	L2446	L2447	L2448	L2449	L2450	L2451	L2452	L2453	L2454	L2455	L2456	L2457	L2458	L2459	L2460	L2461	L2462	L2463	L2464	L2465	L2466	L2467	L2468	L2469	L2470	L2471	L2472	L2473	L2474	L2475	L2476	L2477	L2478	L2479	L2480	L2481	L2482	L2483	L2484	L2485	L2486	L2487	L2488	L2489	L2490	L2491	L2492	L2493	L2494	L2495	L2496	L2497	L2498	L2499	L2500	L2501	L2502	L2503	L2504	L2505	L2506	L2507	L2508	L2509	L2510	L2511	L2512	L2513	L2514	L2515	L2516	L2517	L2518	L2519	L2520	L2521	L2522	L2523	L2524	L2525	L2526	L2527	L2528	L2529	L2530	L2531	L2532	L2533	L2534	L2535	L2536	L2537	L2538	L2539	L2540	L2541	L2542	L2543	L2544	L2545	L2546	L2547	L2548	L2549	L2550	L2551	L2552	L2553	L2554	L2555	L2556	L2557	L2558	L2559	L2560	L2561	L2562	L2563	L2564	L2565	L2566	L2567	L2568	L2569	L2570	L2571	L2572	L2573	L2574	L2575	L2576	L2577	L2578	L2579	L2580	L2581	L2582	L2583	L2584	L2585	L2586	L2587	L2588	L2589	L2590	L2591	L2592	L2593	L2594	L2595	L2596	L2597	L2598	L2599	L2600	L2601	L2602	L2603	L2604	L2605	L2606	L2607	L2608	L2609	L2610	L2611	L2612	L2613	L2614	L2615	L2616	L2617	L2618	L2619	L2620	L2621	L2622	L2623	L2624	L2625	L2626	L2627	L2628	L2629	L2630	L2631	L2632	L2633	L2634	L2635	L2636	L2637	L2638	L2639	L2640	L2641	L2642	L2643	L2644	L2645	L2646	L2647	L2648	L2649	L2650	L2651	L2652	L2653	L2654	L2655	L2656	L2657	L2658	L2659	L2660	L2661	L2662	L2663	L2664	L2665	L2666	L2667	L2668	L2669	L2670	L2671	L2672	L2673	L2674	L2675	L2676	L2677	L2678	L2679	L2680	L2681	L2682	L2683	L2684	L2685	L2686	L2687	L2688	L2689	L2690	L2691	L2692	L2693	L2694	L2695	L2696	L2697	L2698	L2699	L2700	L2701	L2702	L2703	L2704	L2705	L2706	L2707	L2708	L2709	L2710	L2711	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753	L2754	L2755	L2756	L2757	L2758	L2759	L2760	L2761	L2762	L2763	L2764	L2765	L2766	L2767	L2768	L2769	L2770	L2771	L2772	L2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780	L2781	L2782	L2783	L2784	L2785	L2786	L2787	L2788	L2789	L2790	L2791	L2792	L2793	L2794	L2795	L2796	L2797	L2798	L2799	L2800	L2801	L2802	L2803	L2804	L2805	L2806	L2807	L2808	L2809	L2810	L2811	L2812	L2813	L2814	L2815	L2816	L2817	L2818	L2819	L2820	L2821	L2822	L2823	L2824	L2825	L2826	L2827	L2828	L2829	L2830	L2831	L2832	L2833	L2834	L2835	L2836	L2837	L2838	L2839	L2840	L2841	L2842	L2843	L2844	L2845	L2846	L2847	L2848	L2849	L2850	L2851	L2852	L2853	L2854	L2855	L2856	L2857	L2858	L2859	L2860	L2861	L2862	L2863	L2864	L2865	L2866	L2867	L2868	L2869	L2870	L2871	L2872	L2873	L2874	L2875	L2876	L2877	L2878	L2879	L2880	L2881	L2882	L2883	L2884	L2885	L2886	L2887	L2888	L2889	L2890	L2891	L2892	L2893	L2894	L2895	L2896	L2897	L2898	L2899	L2900	L2901	L2902	L2903	L2904	L2905	L2906	L2907	L2908	L2909	L2910	L2911	L2912	L2913	L2914	L2915	L2916	L2917	L2918	L2919	L2920	L2921	L2922	L2923	L2924	L2925	L2926	L2927	L2928	L2929	L2930	L2931	L2932	L2933	L2934	L2935	L2936	L2937	L2938	L2939	L2940	L2941	L2942	L2943	L2944	L2945	L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	L2990	L2991	L2992	L2993	L2994	L2995	L2996	L2997	L2998	L2999	L3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	L3012	L3013	L3014	L3015	L3016	L3017	L3018	L3019	L3020	L3021	L3022	L3023	L3024	L3025	L3026	L3027	L3028	L3029	L3030	L3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053	L3054	L3055	L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113	L3114	L3115	L3116	L3117	L3118	L3119	L3120	L3121	L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.56Å 49.31Å 158.41Å 90.00° 93.58° 90.00°	Depositor
Resolution (Å)	32.68 – 2.55 32.68 – 2.55	Depositor EDS
% Data completeness (in resolution range)	91.9 (32.68-2.55) 92.0 (32.68-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.54Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.236 , 0.281 0.236 , 0.281	Depositor DCC
R_{free} test set	2021 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7782	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0648e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/3945	0.62	0/5355
1	B	0.39	0/3921	0.55	0/5314
All	All	0.45	0/7866	0.59	0/10669

There are no bond length outliers.

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	3856	0	3751	101	0
1	B	3832	0	3740	167	0
2	A	62	0	0	2	0
2	B	32	0	0	2	0
All	All	7782	0	7491	264	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 17.

All (264) 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:1643:ARG:H	1:B:1643:ARG:HD2	1.21	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1962:CYS:HB2	1:A:1971:LEU:HD22	1.47	0.97
1:B:2027:VAL:HG12	1:B:2031:LYS:HE3	1.52	0.91
1:B:2006:LEU:HD13	1:B:2008:ASN:H	1.37	0.89
1:B:1504:THR:HG22	1:B:1507:GLN:HB2	1.55	0.88
1:B:1518:LEU:HD22	1:B:1518:LEU:H	1.36	0.88
1:A:1540:LEU:H	1:A:1574:ASN:HD21	1.18	0.86
1:B:2000:LEU:HD12	1:B:2013:VAL:HG12	1.60	0.83
1:B:1747:TYR:HD1	1:B:1752:ASP:HB3	1.42	0.83
1:B:1960:VAL:HG23	1:B:1971:LEU:HB3	1.62	0.82
1:B:1516:ASN:HB3	1:B:1522:VAL:HG11	1.62	0.81
1:B:2009:THR:HG23	1:B:2020:LEU:HD11	1.63	0.80
1:A:1707:HIS:HE1	1:A:1787:LYS:HE3	1.47	0.80
1:A:1835:LEU:HD13	1:A:1854:VAL:HG11	1.64	0.79
1:B:1549:TYR:HB3	1:B:1565:LEU:HD22	1.66	0.77
1:A:1567:ASP:OD2	1:A:1571:LYS:HE3	1.85	0.77
1:A:1860:LEU:HD13	1:A:1913:ILE:HD12	1.68	0.75
1:A:1636:SER:HB2	1:A:1676:LEU:HD13	1.67	0.75
1:B:1636:SER:HB2	1:B:1676:LEU:HD13	1.68	0.75
1:B:1984:LYS:HG3	1:B:1987:GLU:CD	2.07	0.75
1:A:1739:ARG:HH21	1:A:1796:ASN:HB2	1.51	0.74
1:B:2006:LEU:HB3	1:B:2009:THR:HB	1.70	0.73
1:A:1843:THR:OG1	1:A:1846:ALA:HB2	1.89	0.73
1:A:1647:LYS:NZ	1:A:1647:LYS:HB3	2.04	0.72
1:B:2006:LEU:CD1	1:B:2008:ASN:H	2.02	0.72
1:B:1747:TYR:CD1	1:B:1752:ASP:HB3	2.25	0.71
1:B:1643:ARG:CD	1:B:1643:ARG:H	2.02	0.71
1:A:1504:THR:HG21	1:A:1544:LEU:O	1.90	0.71
1:B:1721:THR:HB	1:B:1757:SER:O	1.90	0.71
1:B:1984:LYS:H	1:B:1984:LYS:CD	2.04	0.71
1:A:1504:THR:HG22	1:A:1507:GLN:HG3	1.72	0.71
1:A:1739:ARG:HH21	1:A:1796:ASN:CB	2.06	0.69
1:B:1607:TYR:CD2	1:B:1641:PRO:HB3	2.28	0.68
1:B:2020:LEU:HD13	1:B:2021:PHE:N	2.07	0.68
1:B:1509:LEU:HB3	1:B:1533:LEU:HD11	1.75	0.68
1:B:1782:TRP:O	1:B:1783:LYS:HG3	1.94	0.68
1:B:1522:VAL:HG13	1:B:1523:VAL:N	2.09	0.68
1:A:1835:LEU:CD1	1:A:1854:VAL:HG11	2.24	0.67
1:B:1657:ARG:HG2	1:B:1666:GLU:HG2	1.76	0.67
1:B:1746:GLU:HG2	1:B:1782:TRP:CE3	2.29	0.67
1:A:1593:LEU:HD12	1:A:1635:LEU:HD12	1.76	0.66
1:B:1744:LEU:HB3	1:B:1755:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1636:SER:HB3	1:A:1672:THR:HG23	1.78	0.65
1:A:1647:LYS:HD2	1:B:2000:LEU:HD21	1.78	0.65
1:B:1522:VAL:HG13	1:B:1523:VAL:H	1.60	0.65
1:B:1979:ALA:HB2	1:B:1995:GLN:HA	1.78	0.65
1:A:1519:ASN:HB3	1:A:1522:VAL:CG1	2.27	0.65
1:B:1507:GLN:HE22	1:B:1546:PRO:HG2	1.62	0.64
1:A:1962:CYS:HB2	1:A:1971:LEU:CD2	2.27	0.64
1:B:1962:CYS:SG	1:B:1967:PHE:HB2	2.38	0.63
1:B:1657:ARG:NH1	1:B:1670:LEU:HD13	2.14	0.63
1:B:1984:LYS:HD2	1:B:1991:LEU:HD13	1.80	0.63
1:B:1649:LEU:O	1:B:1653:LEU:HG	1.98	0.63
1:A:1519:ASN:HB3	1:A:1522:VAL:HG12	1.80	0.63
1:B:1696:HIS:O	1:B:1698:GLN:HG3	1.99	0.62
1:B:1850:PRO:O	1:B:1853:GLU:HB2	1.99	0.61
1:B:2009:THR:HG23	1:B:2020:LEU:CD1	2.30	0.61
1:B:2005:PRO:HD2	1:B:2009:THR:HG22	1.83	0.61
1:A:1502:ILE:HG13	1:A:1503:ASP:H	1.64	0.60
1:A:1647:LYS:HD2	1:B:2000:LEU:CD2	2.31	0.60
1:A:1977:ALA:HA	1:A:2036:TYR:CD1	2.37	0.60
1:B:1546:PRO:O	1:B:1547:LEU:HD23	2.02	0.60
1:A:1603:ARG:HG2	1:A:1639:PHE:CE2	2.37	0.60
1:A:1575:SER:O	1:A:1578:GLN:HG2	2.02	0.59
1:A:2010:TYR:HB2	1:A:2026:VAL:HG12	1.84	0.59
1:B:1660:PHE:O	1:B:1666:GLU:HB2	2.02	0.59
1:A:1707:HIS:CE1	1:A:1787:LYS:HE3	2.33	0.59
1:B:1863:ARG:O	1:B:1863:ARG:HD2	2.03	0.59
1:A:1553:ASN:HB3	1:A:1556:LEU:HB2	1.85	0.58
1:A:1645:ILE:HD12	1:A:1645:ILE:N	2.18	0.58
1:B:1593:LEU:HD12	1:B:1635:LEU:HD12	1.85	0.58
1:B:1707:HIS:ND1	1:B:1813:GLU:HG3	2.18	0.58
1:B:2006:LEU:HD13	1:B:2007:ALA:N	2.19	0.58
1:B:1767:LYS:HG2	1:B:1771:LEU:HD12	1.84	0.58
1:A:1980:VAL:O	1:A:1980:VAL:HG23	2.02	0.58
1:A:1727:GLU:O	1:A:1731:ARG:HG2	2.04	0.57
1:B:1984:LYS:HD3	1:B:1984:LYS:H	1.68	0.57
1:A:1549:TYR:HD1	1:A:1552:ILE:HG21	1.70	0.57
1:A:1962:CYS:HB3	1:A:1968:PRO:O	2.05	0.57
1:B:1504:THR:HG21	1:B:1545:LEU:HA	1.87	0.56
1:B:1522:VAL:O	1:B:1526:ILE:HG13	2.05	0.56
1:B:1511:GLN:HE22	1:B:1514:LYS:HD3	1.69	0.56
1:B:1920:ALA:O	1:B:1924:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1518:LEU:CD2	1:B:1518:LEU:H	2.13	0.56
1:A:2023:THR:HG23	1:A:2026:VAL:HG13	1.88	0.55
1:A:2029:VAL:HG12	1:A:2033:MET:HE3	1.87	0.55
1:A:1811:ALA:O	1:A:1815:VAL:HG23	2.05	0.55
1:B:1816:ILE:HA	1:B:1856:SER:HB2	1.89	0.55
1:B:1562:TYR:CE1	1:B:1595:THR:HG23	2.42	0.55
1:B:1959:ASP:HB3	1:B:1985:ARG:HH22	1.72	0.55
1:A:1582:MET:HE1	1:A:1588:ILE:HD12	1.87	0.55
1:A:1647:LYS:HB3	1:A:1647:LYS:HZ2	1.71	0.55
1:B:1516:ASN:HB3	1:B:1522:VAL:CG1	2.35	0.55
1:A:1553:ASN:CB	1:A:1556:LEU:HD12	2.37	0.55
1:A:1824:GLU:O	1:A:1828:GLN:HG3	2.06	0.55
1:B:1643:ARG:HD2	1:B:1643:ARG:N	2.05	0.55
1:B:2037:ILE:O	1:B:2041:VAL:HG23	2.06	0.55
1:B:1782:TRP:C	1:B:1783:LYS:HG3	2.27	0.54
1:A:2017:ARG:HG2	1:A:2019:LEU:HD21	1.88	0.54
1:B:2025:GLU:HB2	1:B:2028:ASP:OD2	2.07	0.54
1:B:1650:LYS:HE2	1:B:1673:TYR:HE1	1.72	0.54
1:B:2004:ALA:HA	1:B:2009:THR:O	2.08	0.54
1:B:1852:GLU:HA	1:B:1855:TYR:O	2.08	0.54
1:B:1984:LYS:HG3	1:B:1987:GLU:OE2	2.07	0.54
1:A:1607:TYR:CD2	1:A:1641:PRO:HB3	2.44	0.53
1:B:1690:GLU:HG3	1:B:1700:MET:SD	2.48	0.53
1:B:1984:LYS:CD	1:B:1991:LEU:HD13	2.38	0.53
1:B:1979:ALA:CB	1:B:1995:GLN:HA	2.39	0.53
1:B:2006:LEU:HD13	1:B:2008:ASN:N	2.17	0.53
1:A:1824:GLU:OE2	1:A:1855:TYR:OH	2.27	0.53
1:A:1518:LEU:HD11	1:B:1997:GLU:HG2	1.91	0.53
1:B:1726:VAL:HG21	1:B:1743:ALA:HA	1.91	0.53
1:B:2023:THR:O	1:B:2026:VAL:HG13	2.09	0.53
1:B:2006:LEU:HB3	1:B:2009:THR:CB	2.37	0.53
1:B:1765:LEU:HD13	1:B:1784:PHE:CE2	2.44	0.52
1:B:1925:ILE:O	1:B:1929:ARG:HG3	2.09	0.52
1:B:1959:ASP:CG	1:B:1985:ARG:HH12	2.13	0.52
1:A:1682:ARG:HD3	2:A:49:HOH:O	2.08	0.52
1:B:1746:GLU:HG3	1:B:1768:PHE:CE1	2.45	0.52
1:B:1740:ASN:HB3	1:B:1790:CYS:O	2.09	0.52
1:B:1842:TYR:CD1	1:B:1842:TYR:C	2.84	0.52
1:B:1821:PRO:HA	2:B:92:HOH:O	2.09	0.51
1:A:1645:ILE:H	1:A:1645:ILE:HD12	1.76	0.51
1:B:1700:MET:HE1	1:B:1765:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1572:ILE:HD13	1:A:1606:LEU:HD21	1.92	0.50
1:A:1518:LEU:CD1	1:B:1997:GLU:HG2	2.41	0.50
1:B:1700:MET:CE	1:B:1765:LEU:HD23	2.42	0.50
1:A:1649:LEU:HD23	1:A:1676:LEU:HD21	1.93	0.50
1:A:1617:VAL:HG11	1:A:1625:ASN:ND2	2.26	0.50
1:A:1593:LEU:CD1	1:A:1635:LEU:HD12	2.40	0.50
1:A:2029:VAL:CG1	1:A:2033:MET:HE3	2.42	0.50
1:B:1545:LEU:HD11	1:B:1608:CYS:SG	2.52	0.50
1:B:1746:GLU:HG3	1:B:1768:PHE:HE1	1.76	0.50
1:A:2036:TYR:O	1:A:2040:ILE:HG13	2.11	0.49
1:B:2020:LEU:HD13	1:B:2021:PHE:H	1.74	0.49
1:A:1557:LEU:C	1:A:1557:LEU:HD23	2.33	0.49
1:B:1812:HIS:HA	1:B:1943:TYR:OH	2.12	0.49
1:B:1799:LYS:O	1:B:1800:ASP:CG	2.50	0.49
1:A:1736:GLU:HG2	1:A:1737:ASP:N	2.28	0.49
1:A:2017:ARG:NH1	1:A:2019:LEU:HD21	2.27	0.49
1:B:1504:THR:HG22	1:B:1507:GLN:CB	2.33	0.49
1:B:1841:ASP:OD1	1:B:1932:GLN:HA	2.12	0.49
1:A:2028:ASP:HA	1:A:2031:LYS:HZ2	1.76	0.49
1:A:1860:LEU:HD11	1:A:1916:GLU:CB	2.43	0.48
1:B:1507:GLN:HE22	1:B:1546:PRO:CG	2.25	0.48
1:B:1861:LYS:HG2	1:B:1861:LYS:O	2.12	0.48
1:B:1984:LYS:N	1:B:1984:LYS:CD	2.72	0.48
1:B:1995:GLN:O	1:B:1999:ILE:HG13	2.12	0.48
1:A:1553:ASN:HB3	1:A:1556:LEU:HD12	1.96	0.48
1:A:1649:LEU:CD2	1:A:1676:LEU:HD21	2.44	0.48
1:B:1518:LEU:HD22	1:B:1518:LEU:N	2.17	0.48
1:B:1504:THR:HG23	1:B:1507:GLN:H	1.79	0.48
1:A:1962:CYS:CB	1:A:1971:LEU:HD22	2.32	0.48
1:B:1716:ILE:HD13	1:B:1761:VAL:CG1	2.43	0.48
1:B:1934:MET:HA	1:B:1938:GLN:NE2	2.28	0.47
1:B:1657:ARG:HH11	1:B:1670:LEU:HD13	1.79	0.47
1:B:1824:GLU:HG3	1:B:1828:GLN:NE2	2.29	0.47
1:B:1800:ASP:C	1:B:1800:ASP:OD2	2.53	0.47
1:A:1960:VAL:HG12	1:A:2023:THR:HB	1.97	0.47
1:A:1801:SER:HB2	2:A:52:HOH:O	2.14	0.47
1:B:1765:LEU:HD13	1:B:1784:PHE:HE2	1.79	0.47
1:B:1707:HIS:CG	1:B:1813:GLU:HG3	2.50	0.47
1:B:1970:GLU:O	1:B:1984:LYS:O	2.32	0.47
1:A:1860:LEU:HD11	1:A:1916:GLU:HB2	1.97	0.47
1:B:1574:ASN:O	1:B:1578:GLN:HG2	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2017:ARG:HG2	1:A:2019:LEU:CD2	2.44	0.46
1:B:1522:VAL:CG1	1:B:1523:VAL:N	2.77	0.46
1:B:1950:TRP:HE1	1:B:1988:GLY:HA2	1.79	0.46
1:A:1821:PRO:CG	1:A:1988:GLY:HA2	2.45	0.46
1:B:1603:ARG:HG2	1:B:1639:PHE:CE2	2.50	0.46
1:B:1756:GLU:OE2	1:B:2031:LYS:HE2	2.15	0.46
1:B:2002:PHE:HA	1:B:2011:LYS:O	2.15	0.46
1:A:1509:LEU:HB3	1:A:1533:LEU:HD11	1.98	0.46
1:A:1647:LYS:HZ3	1:A:1647:LYS:HB3	1.80	0.46
1:B:1974:GLY:O	1:B:1980:VAL:HA	2.14	0.46
1:B:1808:PHE:HE1	1:B:1943:TYR:CG	2.33	0.46
1:A:1806:PHE:O	1:A:1810:GLN:HB2	2.16	0.46
1:B:1523:VAL:HA	1:B:1526:ILE:HD12	1.98	0.45
1:B:1799:LYS:O	1:B:1800:ASP:OD2	2.34	0.45
1:A:1569:ALA:HB2	1:A:1602:LEU:HD21	1.99	0.45
1:B:1767:LYS:HG2	1:B:1771:LEU:CD1	2.46	0.45
1:A:1839:GLN:OE1	1:A:1849:PRO:HD3	2.16	0.45
1:A:2015:ASP:OD1	1:A:2017:ARG:HB2	2.17	0.45
1:A:1519:ASN:CB	1:A:1522:VAL:HG12	2.44	0.45
1:A:1751:VAL:HG11	1:A:1782:TRP:HH2	1.82	0.45
1:B:1578:GLN:NE2	2:B:67:HOH:O	2.50	0.45
1:A:1545:LEU:HD11	1:A:1608:CYS:SG	2.57	0.45
1:B:2038:SER:O	1:B:2042:LYS:HD3	2.17	0.45
1:A:1586:ILE:HB	1:A:1587:PRO:HD3	1.98	0.45
1:B:1746:GLU:HG2	1:B:1782:TRP:CZ3	2.52	0.45
1:A:1828:GLN:NE2	1:A:1923:SER:OG	2.47	0.45
1:A:1980:VAL:O	1:A:1980:VAL:CG2	2.65	0.45
1:A:1687:SER:HB3	1:A:1766:ALA:HA	1.99	0.44
1:B:1525:GLN:O	1:B:1529:ARG:HB2	2.17	0.44
1:A:1502:ILE:HG13	1:A:1503:ASP:N	2.32	0.44
1:B:2006:LEU:HD22	1:B:2007:ALA:H	1.83	0.44
1:B:2027:VAL:O	1:B:2031:LYS:HG3	2.18	0.44
1:A:2025:GLU:O	1:A:2029:VAL:HG23	2.17	0.44
1:B:1522:VAL:HG13	1:B:1523:VAL:HG23	1.99	0.44
1:B:1911:MET:O	1:B:1915:GLU:CB	2.66	0.44
1:A:1648:TYR:O	1:A:1651:PHE:HB3	2.17	0.44
1:B:1636:SER:HB3	1:B:1672:THR:HG23	1.98	0.44
1:B:1519:ASN:HB3	1:B:1522:VAL:CG1	2.48	0.43
1:B:1819:HIS:HD2	1:B:1957:LEU:HB2	1.83	0.43
1:B:1558:LYS:C	1:B:1560:LYS:H	2.21	0.43
1:B:1745:PHE:CE2	1:B:1787:LYS:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1972:TRP:HB2	1:B:1983:TYR:HB2	2.00	0.43
1:B:1655:ARG:HH11	1:B:1655:ARG:HG2	1.83	0.43
1:B:1740:ASN:HB3	1:B:1788:LEU:HD11	2.01	0.43
1:B:1983:TYR:CE2	1:B:1990:PRO:HB3	2.54	0.43
1:A:2006:LEU:HB3	1:A:2009:THR:OG1	2.19	0.43
1:A:2010:TYR:CE2	1:A:2033:MET:HE3	2.54	0.43
1:A:1575:SER:C	1:A:1577:GLN:H	2.22	0.43
1:B:1753:LYS:HE3	1:B:1753:LYS:HB2	1.81	0.43
1:B:1823:PRO:O	1:B:1824:GLU:C	2.57	0.43
1:B:1522:VAL:CG1	1:B:1523:VAL:H	2.27	0.43
1:B:1721:THR:HA	1:B:1759:THR:O	2.19	0.43
1:B:2006:LEU:HD13	1:B:2006:LEU:C	2.39	0.43
1:B:1686:PRO:HA	1:B:1690:GLU:OE1	2.19	0.42
1:B:1984:LYS:HG2	1:B:1987:GLU:HB2	2.00	0.42
1:B:2009:THR:CG2	1:B:2020:LEU:HD11	2.42	0.42
1:A:1569:ALA:HB2	1:A:1602:LEU:CD2	2.49	0.42
1:B:1842:TYR:HB2	1:B:1928:TRP:CD2	2.54	0.42
1:B:1557:LEU:HG	1:B:1558:LYS:N	2.34	0.42
1:A:1573:PHE:O	1:A:1577:GLN:HB2	2.19	0.42
1:B:1730:ILE:C	1:B:1732:GLY:H	2.23	0.42
1:B:1911:MET:O	1:B:1915:GLU:HB3	2.19	0.42
1:A:1707:HIS:CD2	1:A:1813:GLU:HG3	2.55	0.42
1:B:1636:SER:CB	1:B:1672:THR:HG23	2.49	0.42
1:A:1960:VAL:HG21	1:A:1973:LEU:HD13	2.01	0.42
1:B:1643:ARG:O	1:B:1647:LYS:HG3	2.19	0.42
1:A:1991:LEU:O	1:A:1992:GLU:HB2	2.20	0.41
1:A:2015:ASP:C	1:A:2017:ARG:H	2.24	0.41
1:A:1956:THR:HB	1:A:2032:LEU:HD21	2.02	0.41
1:B:1586:ILE:HB	1:B:1587:PRO:HD3	2.02	0.41
1:B:1562:TYR:OH	1:B:1595:THR:HA	2.19	0.41
1:B:1629:TRP:CZ3	1:B:1632:LEU:HD23	2.54	0.41
1:B:1657:ARG:CG	1:B:1666:GLU:HG2	2.47	0.41
1:A:1794:THR:O	1:A:1948:LYS:NZ	2.33	0.41
1:B:1649:LEU:HD23	1:B:1676:LEU:HD21	2.02	0.41
1:B:1563:THR:OG1	1:B:1564:THR:N	2.53	0.41
1:B:1971:LEU:HA	1:B:1984:LYS:O	2.20	0.41
1:A:1516:ASN:HB3	1:A:1522:VAL:HG11	2.03	0.41
1:B:1835:LEU:HD12	1:B:1835:LEU:HA	1.94	0.41
1:A:1960:VAL:HG12	1:A:2023:THR:CB	2.51	0.41
1:B:1540:LEU:HB2	1:B:1573:PHE:CD2	2.56	0.41
1:B:1950:TRP:NE1	1:B:1988:GLY:HA2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1585:PRO:O	1:B:1588:ILE:N	2.53	0.41
1:B:1562:TYR:HE1	1:B:1595:THR:HG23	1.83	0.41
1:B:1984:LYS:CE	1:B:1991:LEU:HD13	2.50	0.41
1:A:1600:ARG:HB2	1:A:1601:PRO:HD3	2.03	0.41
1:B:1800:ASP:OD2	1:B:1801:SER:N	2.53	0.41
1:A:1915:GLU:HA	1:A:1915:GLU:OE2	2.19	0.41
1:B:1991:LEU:HA	1:B:1991:LEU:HD12	1.91	0.41
1:A:1503:ASP:HA	1:A:1507:GLN:OE1	2.21	0.41
1:B:1657:ARG:NE	1:B:1666:GLU:OE2	2.54	0.41
1:A:1527:TYR:O	1:A:1534:ARG:NE	2.49	0.40
1:B:1733:LEU:HD13	1:B:1735:MET:HE2	2.03	0.40
1:B:1811:ALA:O	1:B:1815:VAL:HG23	2.21	0.40
1:A:1513:ILE:HG23	1:A:1523:VAL:HG22	2.03	0.40
1:A:1516:ASN:HB3	1:A:1522:VAL:CG1	2.51	0.40
1:B:1829:VAL:HG22	1:B:1927:LYS:HD3	2.03	0.40
1:B:1522:VAL:HG22	1:B:1526:ILE:HD11	2.03	0.40
1:B:1748:ASN:ND2	1:B:1780:LEU:HD13	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	485/555 (87%)	450 (93%)	29 (6%)	6 (1%)	13	17
1	B	474/555 (85%)	424 (90%)	46 (10%)	4 (1%)	19	27
All	All	959/1110 (86%)	874 (91%)	75 (8%)	10 (1%)	15	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1985	ARG

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Mol	Chain	Res	Type
1	A	1985	ARG
1	B	1844	LEU
1	A	2015	ASP
1	A	2016	GLU
1	B	1686	PRO
1	B	1965	GLY
1	A	1965	GLY
1	A	1992	GLU
1	A	1968	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/492 (83%)	387 (95%)	20 (5%)	25	34
1	B	406/492 (82%)	385 (95%)	21 (5%)	23	30
All	All	813/984 (83%)	772 (95%)	41 (5%)	24	33

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1503	ASP
1	A	1518	LEU
1	A	1520	SER
1	A	1529	ARG
1	A	1544	LEU
1	A	1582	MET
1	A	1593	LEU
1	A	1610	LEU
1	A	1635	LEU
1	A	1647	LYS
1	A	1676	LEU
1	A	1747	TYR
1	A	1765	LEU
1	A	1788	LEU

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Mol	Chain	Res	Type
1	A	1835	LEU
1	A	1842	TYR
1	A	1860	LEU
1	A	1957	LEU
1	A	1972	TRP
1	A	1995	GLN
1	B	1508	GLN
1	B	1518	LEU
1	B	1537	HIS
1	B	1549	TYR
1	B	1559	ASP
1	B	1593	LEU
1	B	1643	ARG
1	B	1676	LEU
1	B	1724	GLU
1	B	1737	ASP
1	B	1788	LEU
1	B	1835	LEU
1	B	1842	TYR
1	B	1858	GLN
1	B	1972	TRP
1	B	1980	VAL
1	B	1984	LYS
1	B	1991	LEU
1	B	2020	LEU
1	B	2026	VAL
1	B	2042	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1508	GLN
1	A	1538	HIS
1	A	1574	ASN
1	A	1707	HIS
1	A	1817	HIS
1	A	1828	GLN
1	A	1938	GLN
1	B	1507	GLN
1	B	1508	GLN
1	B	1511	GLN
1	B	1574	ASN

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Mol	Chain	Res	Type
1	B	1597	HIS
1	B	1659	GLN
1	B	1748	ASN
1	B	1796	ASN
1	B	1817	HIS
1	B	1819	HIS
1	B	1826	ASN
1	B	1858	GLN
1	B	1969	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	493/555 (88%)	0.12	23 (4%)	31 38	12, 36, 77, 109	2 (0%)
1	B	484/555 (87%)	0.50	45 (9%)	8 10	30, 55, 86, 106	3 (0%)
All	All	977/1110 (88%)	0.31	68 (6%)	16 19	12, 47, 83, 109	5 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2045	TYR	8.2
1	A	1501	PRO	6.8
1	B	1912	TRP	5.7
1	A	2047	THR	5.7
1	A	2007	ALA	5.6
1	B	1913	ILE	5.6
1	B	2048	THR	5.6
1	A	1780	LEU	5.5
1	B	1549	TYR	5.4
1	B	2046	SER	5.3
1	B	1562	TYR	5.0
1	A	2045	TYR	4.8
1	A	2046	SER	4.7
1	A	2005	PRO	4.4
1	A	2048	THR	4.3
1	B	1518	LEU	3.9
1	B	2047	THR	3.9
1	B	1844	LEU	3.9
1	B	2041	VAL	3.8
1	B	1968	PRO	3.7
1	B	1758	ARG	3.7
1	B	1862	ALA	3.6
1	B	2005	PRO	3.5
1	B	1914	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1750	HIS	3.4
1	B	2042	LYS	3.2
1	B	1857	LEU	3.2
1	B	2043	LYS	3.1
1	B	1780	LEU	3.1
1	B	1583	SER	3.1
1	A	2006	LEU	3.0
1	A	1775	SER	3.0
1	A	2004	ALA	3.0
1	B	1737	ASP	3.0
1	B	2022	GLU	3.0
1	B	1600	ARG	2.9
1	B	2004	ALA	2.9
1	B	1559	ASP	2.8
1	B	1502	ILE	2.8
1	A	1994	PHE	2.7
1	B	1969	GLN	2.7
1	A	1980	VAL	2.7
1	B	1965	GLY	2.7
1	A	1549	TYR	2.6
1	A	1582	MET	2.6
1	A	1991	LEU	2.5
1	A	1750	HIS	2.3
1	A	2008	ASN	2.2
1	A	1772	ALA	2.2
1	B	2019	LEU	2.2
1	B	1659	GLN	2.2
1	B	1961	GLU	2.2
1	B	1971	LEU	2.2
1	B	1800	ASP	2.2
1	B	1955	SER	2.2
1	A	1781	PRO	2.2
1	B	1988	GLY	2.2
1	B	2007	ALA	2.2
1	A	2043	LYS	2.1
1	A	2018	GLU	2.1
1	B	1561	GLY	2.1
1	B	1957	LEU	2.1
1	B	2006	LEU	2.1
1	A	1749	GLY	2.1
1	B	2010	TYR	2.1
1	B	1858	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1517	CYS	2.0
1	B	1962	CYS	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.