



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:59 PM UTC

PDB ID : 5NUG / pdb_00005nug
EMDB ID : EMD-3698
Title : Motor domains from human cytoplasmic dynein-1 in the phi-particle conformation
Authors : Zhang, K.; Foster, H.E.; Carter, A.P.
Deposited on : 2017-04-30
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

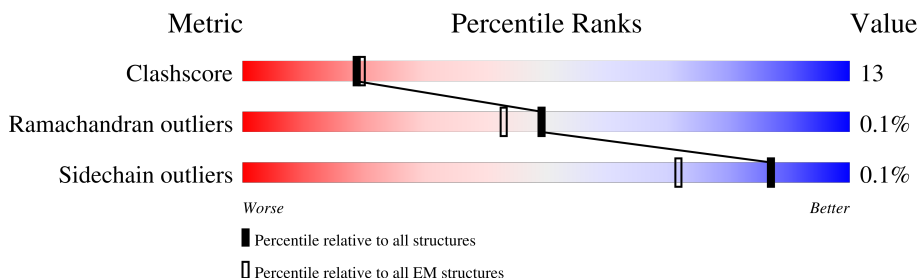
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	63% 51% 11% 37%
1	B	4646	63% 51% 11% 37%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	4801	-	-	X	-
2	ADP	B	4801	-	-	X	-

2 Entry composition [i](#)

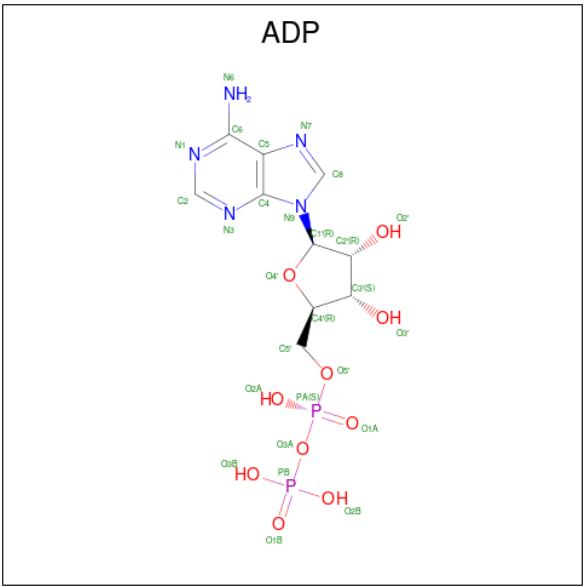
There are 4 unique types of molecules in this entry. The entry contains 46232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		
1	B	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		

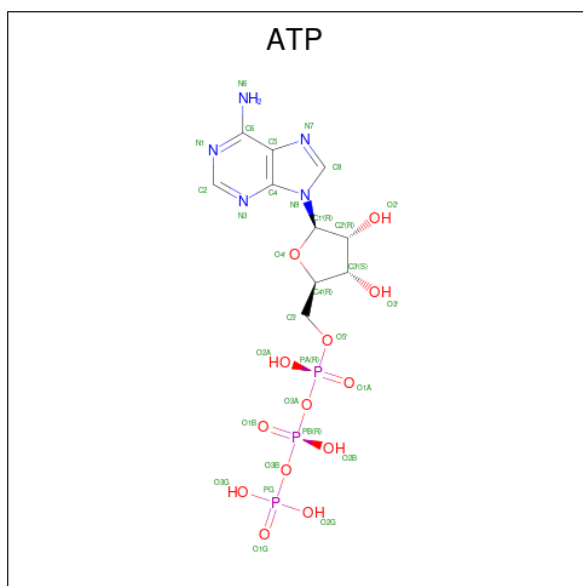
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	



L2521	M2461	I2341	T2281	M2221	L2161	G2101	M2041	A1981	H1921	M1861	P1801
T2522	L2462	M2342	H2282	M2222	S2162	N2102	T2042	L1982	Q1922	A1862	P1802
T2523	H2463	F2343	V2283	V2223	D2163	V2103	K2043	R1983	L1923	N1863	L1803
V2524	Q2464	E2344	L2284	G2224	V2164	K2104	P2044	E1984	G1924	K1864	R1804
L2525	A2465	V2345	R2285	P2225	P2165	E2106	D2045	H1985	R1925	K1865	R1805
L2526	C2466	Q2346	K2286	P2226	P2166	E2106	R2046	S1986	F1926	F1866	R1806
P2527	R2467	D2347	L2287	G2227	G2167	R2107	Q2047	N1987	V1927	N1867	K1807
T2528	N2468	L2348	L2288	S2228	V2168	T2108	L2048	PRO	L1928	Y1868	L1808
A2529	V2469	K2349	D2289	G2229	Q2169	Q2109	I2049	ASN	L1929	Y1869	E1809
P2530	A2470	R2350	S2290	K2230	Q2170	Q2110	A2050	TVR	F1930	F1870	H1810
M2531	Q2471	A2351	V2291	S2231	H2171	I2111	Q2051	LYS	M1931	E1871	L1811
L2532	Y2472	T2352	R2292	M2232	R2172	K2112	V2052	THR	C1932	Y1872	I1812
P2533	N2473	L2353	G2293	A2233	G2173	R2113	M2053	SER	D1933	G1874	T1813
L2534	A2474	A2354	E2294	W2234	E2174	E2114	L2054	ALA	E1934	G1874	E1814
T2535	N2475	T2355	L2295	A2235	M2175	LYS	Y2055	P1996	T1935	V1875	L1815
D2536	H2476	V2356	Q2296	V2236	T2176	GLU	S2056	I1997	F1936	Q1876	V1816
V2537	D2477	S2357	K2297	L2237	A2177	ARG	Q2057	T1998	D1937	D1877	H1817
E2538	P2478	R2358	R2298	L2238	L2178	GLY	G2058	C1999	F1938	K1878	Q1818
V2539	F2479	C2359	Q2299	K2239	R2179	GLU	F2059	E2000	Q1939	L1879	R1819
S2540	P2480	G2360	V2300	A2240	E2180	ALA	R2060	L2001	A1940	V1880	D1820
L2541	M2481	M2361	I2301	L2241	E2181	VAL	T2061	L2002	M1941	Q1881	V1821
S2542	Q2482	V2362	F2302	E2242	L2182	ASP	A2062	N2003	G1942	T1882	T1822
G2543	L2483	K2363	F2303	A2243	K2183	GLU	E2063	K2004	R1943	P1883	R1823
E2544	E2484	F2364	D2304	L2244	K2184	GLY	V2064	Q2005	I1944	L1884	S1824
M2545	Q2485	S2365	G2305	E2245	V2185	TLE	L2065	V2006	F1945	T1885	L1825
L2546	F2477	S2366	D2306	G2246	C2186	E2129	A2066	K2007	V1946	T1886	I1826
P2547	T2428	D2367	V2307	V2247	Q2187	N2130	N2067	V2008	G1947	D1886	K1827
W2548	T2429	V2368	D2308	E2248	E2188	L2131	K2068	S2009	L1948	R1887	S1828
Q2549	N2489	L2369	P2309	G2249	M2189	L2132	I2069	P2010	C1949	C1888	K1829
A2550	I2490	S2370	E2310	V2250	L2190	E2133	V2070	D2011	Q1950	L1890	I1830
K2551	Q2491	T2371	W2311	A2251	L2191	Q2134	P2071	M2012	V1951	T1891	D1831
V2552	R2492	D2372	E2312	H2252	T2192	E2135	F2072	A2013	G1952	M1892	N1832
P2553	Y2493	M2373	E2313	L2253	Y2193	L2136	T2073	T2014	A1953	T1893	A1833
Q2554	L2494	L2374	N2314	I2254	Q2194	L2137	K2074	F2015	W1954	Q1894	K1834
L2555	V2495	F2375	L2315	D2255	D2195	L2138	L2075	T2016	G1955	A1895	S1835
E2556	Y2496	M2376	N2316	P2256	Q2196	Q2139	C2076	T2017	C1956	L1896	F1836
A2557	A2497	N2377	S2317	K2257	E2197	S2140	D2077	N2019	F1957	E1897	E1837
I2558	I2498	F2378	L2318	A2258	E2198	V2141	E2078	P2020	D1958	A1898	W1838
T2559	L2499	L2379	L2319	I2259	V2199	C2142	Q2079	G2021	E1959	R1899	L1839
H2560	V2500	A2380	D2320	S2260	G2200	E2143	L2080	Y2022	F1960	L1900	S1840
S2501	Q2442	R2381	D2321	K2261	G2201	T2144	S2081	A2023	N1961	G1901	Q1841
L2502	L2443	L2382	N2322	D2262	W2202	W2145	S2082	Q2024	R1962	G1902	M1842
S2503	H2444	R2383	K2323	H2263	W2203	V2146	Q2083	R2025	L1963	S1903	R1843
Q2504	T2446	S2384	L2324	L2264	V2204	P2147	S2084	S2026	E1964	P1904	F1844
D2505	M2447	I2385	L2325	Y2265	E2205	K2148	H2085	N2027	E1965	F1905	F1845
S2506	D2448	T2386	T2326	G2266	K2206	L2149	Y2086	M2028	R1966	G1906	Y1846
R2507	L2449	L2387	L2327	T2267	V2207	V2150	D2087	P2029	M1967	P1907	D1847
L2508	T2450	D2388	L2328	L2268	Q2208	A2151	F2088	D2030	L1968	A1908	P1848
M2509	R2451	E2389	P2329	D2269	Q2209	E2152	G2089	N2031	S1969	G1909	K1849
M2510	L2452	GLY	M2330	G2266	L2210	D2153	L2090	M2032	A1970	T1910	Q1850
T2511	R2453	ASP	Q2330	T2267	Y2211	T2154	R2091	K2033	V1971	G1911	T1851
A2512	C2454	GLU	E2331	T2272	Q2212	P2155	A2092	K2034	S1972	G1912	D1852
L2513	L2455	ALA	R2332	E2274	I2213	L2156	L2093	L2035	Q1973	T1913	V1853
E2514	G2456	GLN	S2334	E2274	T2214	L2157	K2094	F2036	Q1974	E1914	L1854
Q2515	S2457	ARG	L2335	W2275	Q2215	F2158	S2095	R2037	V1975	S1915	Q1855
E2516	L2458	ARG	P2336	T2276	I2216	S2159	V2096	T2037	Q1976	V1916	Q1856
L2517	F2459	LYS	P2337	D2277	N2217	L2160	L2097	L2039	C1977	K1917	L1857
I2518	S2460	GLY	N2338	G2278	H2218		V2098	A2040	I1978	A1918	S1858
R2519			V2339	L2279	G2219		S2099		Q1979	L1919	T1859
L2520			R2340	F2280	L2220		A2100		E1980	G1920	Q1860

LYS	K3241	N3181	I3121	N3061	D3001	A2941	Y2881	S2761	V2701	L2581
GLN	K3242	H3182	V3122	L3062	S3002	G2942	T2882	L2762	K2702	Y2641
HIS	M3243	Y3183	P3123	H3063	G3003	K2943	P2883	R2763	L2703	R2642
LEU	V3244	A3184	D3124	V3064	F3004	T2944	V2884	T2764	E2704	T2643
GLU	K3245	N3185	Y3125	V3065	L3005	T2945	L2885	Y2765	R2705	T2644
VAL	K3246	L3186	M3126	F3066	E3006	L2946	Q2886	A2766	L2706	P2645
ARG	D3247	F3187	K3127	T3067	R3007	S2947	E2887	E2767	Q2707	G2647
SER	K3248	H3188	V3128	M3068	N3008	R2948	E2888	P2768	P2708	H2588
MET	E3249	K3189	V3129	N3069	M3009	F2949	E2889	V2649	V2709	K2589
ASN	K3250	E3190	Y3130	P3070	T3010	V2950	R2890	L2650	G2710	P2590
PRO	E3251	R3191	D3131	S3071	L3011	A2951	D2891	A2771	A2711	L2591
ALA	K3252	S3192	K3132	S3072	L3012	W2952	Y2892	A2772	C2712	V2592
ALA	K3253	E3193	L3133	E3073	A3013	M2953	Y2893	M2773	N2713	L2593
VAL	L3254	L3194	P3134	G3074	N3014	N2954	K2894	V2774	P2714	C2594
LYS	VAL	E3195	Q3135	G3075	G3015	G2955	A2895	E2775	P2715	G2595
VAL	MET	E3196	P3136	K3076	E3016	L2956	R2896	F2776	T2716	P2596
MET	SER	E3197	P3137	D3077	V3017	S2957	L2897	Y2777	D2717	P2597
GLN	GLU	Q3198	S3138	R3078	P3018	V2958	K2898	T2778	P2718	G2598
ILE	SER	Q3199	H3139	A3079	G3019	Y2959	V2899	M2779	G2719	S2599
GLN	CYS	M3199	H3140	A3080	L3020	Q2960	F2900	S2780	R2720	G2600
LEU	GLU	H3200	R3141	T3081	F3021	I2961	Y2901	E2841	K2721	L2601
LEU	LEU	L3201	A3142	S3082	E3022	K2962	E2902	E2782	P2722	T2602
LEU	LEU	N3202	I3143	F3083	G3023	V2963	E2903	R2783	L2723	C2603
GLY	GLY	V3203	I3144	P3084	D3024	H2964	E2904	F2784	S2724	T2604
GLY	SER	G3204	V3145	A3084	E3025	R2965	L2905	T2785	H2725	L2605
GLN	GLN	L3205	K3146	F3086	Y3026	K2966	D2906	Q2786	R2726	P2606
THR	GLU	R3206	S3146	L3087	A3027	Y2967	V2907	D2787	F2727	S2607
ASP	VAL	K3207	C3147	N3087	T3028	T2968	P2908	L2788	L2728	A2608
ILE	ASP	I3208	V3148	R3088	L3029	G2969	L2909	Q2789	R2729	L2609
ALA	ASP	E3209	F3149	C3089	M3030	E2970	V2910	P2790	K2730	R2610
GLN	LYS	K3210	V3150	V3090	L3031	D2971	L2911	H2791	V2731	A2611
ARG	MET	T3211	H3151	L3091	T3032	F2972	F2912	T2792	V2732	L2612
SER	SER	V3212	K3152	N3092	Q3032	D2973	M2913	L2793	P2733	P2613
ILE	VAL	D3213	T3153	W3093	C3033	E2974	E2914	Y2794	V2734	D2614
GLU	GLU	Q3214	L3154	F3094	K3034	D2975	V2915	S2795	Y2735	M2615
ARG	ASP	V3215	H3155	G3095	E3035	D2976	L2916	P2796	V2736	E2616
GLU	LEU	V3216	Q3156	D3096	G3036	L2977	D2917	R2797	Q2677	V2617
ASN	ASP	E3217	A3157	W3097	A3037	T2978	H2918	E2798	R2678	L2618
PHE	PHE	E3218	S3158	S3098	Q3038	R2979	V2919	M2799	P2739	G2619
ILE	ILE	L3219	A3159	T3099	K3039	V2979	N2920	T2800	Q2740	L2620
THR	PRO	R3219	R3160	E3100	E3040	L2980	L2921	R2801	P2741	N2621
ILE	VAL	R3220	L3161	A3101	G3041	R2981	T2922	K2802	A2742	S2681
VAL	VAL	D3221	A3162	L3102	L3042	R2982	L2923	V2803	S2743	S2682
ASN	ILE	L3222	I3163	Y3103	M3043	S2983	D2924	R2804	L2744	R2684
GLU	GLU	R3223	R3164	Q3104	L3044	G2984	R2925	G2805	T2745	A2625
ALA	GLN	T3224	G3165	V3105	D3045	C2985	F2926	T2806	Q2746	Q2685
ASN	ASN	K3225	G3166	G3106	S3046	K2986	R2927	F2807	V2687	M2686
VAL	VAL	S3226	K3167	K3107	H3047	N2987	Q2928	E2808	Y2687	T2687
VAL	VAL	Q3227	T3168	E3108	E3048	K2988	P2929	A2809	G2749	P2628
LYS	SER	E3228	M3169	F3109	E3049	E2989	Q2930	L2810	T2750	E2629
ILE	ILE	L3229	A3170	T3110	L3050	I2990	Q2931	R2811	F2751	L2630
LYS	LYS	V3231	I3171	S3111	Y3051	A2991	H2932	P2812	N2752	L2631
ILE	ILE	K3232	T3172	K3112	K3052	F2992	H2933	L2813	R2753	L2632
LYS	LYS	N3233	P3173	D3113	W3053	I2993	L2934	E2814	A2754	L2633
ASN	ASN	A3234	R3174	M3114	F3054	N2994	T2935	T2815	M2755	T2634
ASN	ASN	A3235	H3175	L3115	T3055	D2995	L2936	L2816	L2756	P2635
ASN	ASN	A3236	Y3176	E3116	S3056	E2996	T2937	P2817	T2757	D2636
ASN	ASN	N3237	D3177	K3117	Q3057	S2997	Q2938	L2818	R2758	H2637
ASN	ASN	D3238	L3178	P3118	V3058	N2998	T2939	V2819	L2759	L2638
ASN	ASN	K3239	F3179	N3119	I3059	V2999	G2940	E2820	P2760	C2639
ASN	ASN	L3240	I3180	Y3120	R3060	L3000				E2640





M221	M222	V2223	G2224	F2225	S2226	G2227	S2228	G2229	S2230	S2231	M2232	A2233	A2234	R2235	V2236	L2237	L2238	K2239	A2240	L2241	E2242	K2243	L2244	E2245	G2246	V2247	E2248	G2249	V2250	A2251	H2252	L2253	L2254	D2255	P2256	K2257	A2258	L2259	S2260	K2261	H2262	H2263	L2264	L2265	G2266	T2267	L2268	L2269	P2270	N2271	L2272	R2273	E2274	K2275	T2276	D2277	G2278	L2279	F2280
L2161	S2162	D2163	V2164	F2165	T2166	G2167	V2168	Q2169	Q2170	H2171	R2172	G2173	E2174	M2175	T2176	A2177	L2178	R2179	E2180	E2181	L2182	K2183	K2184	V2185	L2186	Q2187	E2188	M2189	V2190	L2191	T2192	Y2193	G2194	L2195	G2196	E2197	E2198	V2199	G2200	G2201	M2202	G2203	V2204	E2205	K2206	V2207	L2208	Q2209	L2210	V2211	Q2212	L2213	T2214	Q2215	I2216	N2217	H2218	G2219	L2220
G2101	N2102	V2103	K2104	R2105	E2106	R2107	T2108	Q2109	K2110	I2111	K2112	R2113	E2114	LYS	GLU	GLY	ARG	GLY	GLU	ALA	VAL	ASP	GLY	GLU	ILE	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	E2135	L2136	L2137	I2138	Q2139	S2140	V2141	C2142	E2143	T2144	N2145	V2146	P2147	K2148	L2149	V2150	A2151	E2152	D2153	L2154	P2155	L2156	L2157	F2158	S2159	L2160	
M2041	T2042	K2043	P2044	D2045	Q2047	L2048	T2049	A2050	Q2051	V2052	L2053	M2054	Y2055	S2056	Q2057	Q2058	F2059	R2060	T2061	A2062	E2063	V2064	L2065	L2066	N2067	K2068	I2069	D2011	M2012	A2013	T2014	F2015	K2074	L2075	C2076	E2077	D2078	Q2079	L2080	S2081	S2082	Q2083	S2084	H2085	Y2086	D2087	F2088	G2089	L2090	R2091	A2092	L2093	K2094	F2095	S2095	V2096	L2097	S2098	A2100
A1981	L1982	R1983	E1984	H1985	S1986	N1987	PRO	ASN	TYP	ASP	LYS	THR	SER	ALA	P1996	I1997	T1998	C1999	E2000	L2001	L2002	N2003	K2004	Q2005	V2006	K2007	V2008	S2009	P2010	D2011	M2012	A2013	T2014	F2015	T2016	T2017	M2018	N2019	G2020	Y2021	Y2022	A2023	G2024	R2025	S2026	N2027	L2028	P2029	D2030	N2031	L2032	K2033	K2034	F2035	R2037	S2038	L2039	A2040	
M2041	T2042	K2043	P2044	D2045	Q2047	L2048	T2049	A2050	Q2051	V2052	L2053	M2054	Y2055	S2056	Q2057	Q2058	F2059	R2060	T2061	A2062	E2063	V2064	L2065	L2066	N2067	K2068	I2069	D2011	M2012	A2013	T2014	F2015	K2074	L2075	C2076	E2077	D2078	Q2079	L2080	S2081	S2082	Q2083	S2084	H2085	Y2086	D2087	F2088	G2089	L2090	R2091	A2092	L2093	K2094	F2095	S2095	V2096	L2097	S2098	A2100
G2101	N2102	V2103	K2104	R2105	E2106	R2107	T2108	Q2109	K2110	I2111	K2112	R2113	E2114	LYS	GLU	GLY	ARG	GLY	GLU	ALA	VAL	ASP	GLY	GLU	ILE	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	E2135	L2136	L2137	I2138	Q2139	S2140	V2141	C2142	E2143	T2144	N2145	V2146	P2147	K2148	L2149	V2150	A2151	E2152	D2153	L2154	P2155	L2156	L2157	F2158	S2159	L2160	
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G2101	N2102	V2103	K2104	R2105	E2106	R2107	T2108	Q2109	K2110	I2111	K2112	R2113	E2114	LYS	GLU	GLY	ARG	GLY	GLU	ALA	VAL	ASP	GLY	GLU	ILE	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	E2135	L2136	L2137	I2138	Q2139	S2140	V2141	C2142	E2143	T2144	N2145	V2146	P2147	K2148	L2149	V2150	A2151	E2152	D2153	L2154	P2155	L2156	L2157	F2158	S2159	L2160	
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L1561	P1562	V1563	E1564	T1565	Q1566	P1567	F1568	Q1569	S1570	I1571	S1572	L1573	E1574	F1575	F1576	A1577	L1578	M1579	K1580	K1581	V1582	S1583	K1584	D1585	P1586	L1587	V1588	M1589	D1590	V1591	L1592	N1593	I1594	Q1595	G1596	V1597	Q1598	R1599	S1600	L1601	R1602	R1603	L1604	A1605	L1606	L1607	L1608	G1609	K1610	I1611	Q1612	K1613	A1614	L1615	G1616	E1617	L1618	L1619	E1620
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A1981	L1982	R1983	E1984	H1985	S1986	N1987	PRO	ASN	TYP	ASP	LYS	THR	SER	ALA	P1996	I1997	T1998	C1999	E2000	L2001	L2002	N2003	K2004	Q2005	V2006	K2007	V2008	S2009	P2010	D2011	M2012	A2013	T2014	F2015	T2016	T2017	M2018	N2019	G2020	Y2021	Y2022	A2023	G2024	R2025	S2026	N2027	L2028	P2029	D2030	N2031	L2032	K2033	K2034	F2035	R2037	S2038	L2039	A2040	
M2041	T2042	K2043	P2044	D2045	Q2047	L2048	T2049	A2050	Q2051	V2052	L2053	M2054	Y2055	S2056	Q2057	Q2058	F2059	R2060	T2061	A2062	E2063	V2064	L2065	L2066	N2067	K2068	I2069	D2011	M2012	A2013	T2014	F2015	K2074	L2075	C2076	E2077	D2078	Q2079	L2080	S2081	S2082	Q2083	S2084	H2085	Y2086	D2087	F2088	G2089	L2090	R2091	A2092	L2093	K2094	F2095	S2095	V2096	L2097	S2098	A2100
G2101	N2102	V2103	K2104	R2105	E2106	R2107	T2108	Q2109	K2110	I2111	K2112	R2113	E2114	LYS	GLU	GLY	ARG	GLY	GLU	ALA	VAL	ASP	GLY	GLU	ILE	A2128	E2129	N2130	L2131	P2132	E2133	Q2134	E2135	L2136	L2137	I2138	Q2139	S2140	V2141	C2142	E2143	T2144	N2145	V2146	P2147	K2148	L2149	V2150	A2151	E2152	D2153	L2154	P2155	L2156	L2157	F2158	S2159	L2160	
L2161	S2162	D2163	V2164	F2165	T2166	G2167	V2168	Q2169	Q2170	H2171	R2172	G2173	E2174	M2175	T2176	A2177	L2178	R2179	E2180	E2181	L2182	K2183	K2184	V2185	L2186	Q2187	E2188	M2189	V2190	L2191	T2192	Y2193	G2194	L2195	G2196	E2197	E2198	V2199	G2200	G2201	M2202	G2203	V2204	E2205	K2206	V2207													

D3001	T2281	L2581	Y2641	V2701	S2761	L2821	Y2881	A2941	D3001
S3002	H2282	Y2582	R2642	K2702	L2762	I2822	I2882	G2942	S3002
G3003	V2283	T2583	R2643	L2703	R2763	E2823	P2883	K2943	G3003
F3004	L2284	W2584	T2644	E2704	T2764	I2824	V2884	T2944	F3004
L3005	R2285	L2585	P2645	R2705	Y2765	W2825	D2885	L2945	L3005
E3006	K2286	A2586	N2646	I2706	A2766	A2826	Q2886	L2946	E3006
R3007	I2287	E2587	G2647	Q2707	E2767	H2827	E2887	S2947	R3007
N3008	I2288	K2588	V2648	F2708	L2768	E2828	E2888	R2948	N3008
K3009	I2289	K2589	V2649	V2709	P2769	A2829	E2889	F2949	K3009
T3010	S2290	P2590	L2650	G2710	L2770	L2830	R2890	V2950	T3010
L3011	M2291	L2591	A2651	A2711	A2771	R2831	D2891	A2951	L3011
L3012	R2292	V2592	P2652	G2712	M2772	L2832	V2892	W2952	L3012
A3013	G2293	L2593	P2653	N2713	A2773	F2833	Y2893	M2953	A3013
N3014	E2294	C2594	Q2654	P2714	V2774	Q2834	K2894	N2954	N3014
G3015	L2295	Q2595	L2655	P2715	E2775	D2835	A2895	G2955	G3015
E3016	Q2296	P2596	G2656	T2716	F2776	R2836	R2896	L2956	E3016
V3017	R2297	P2597	K2657	D2717	Y2777	L2837	L2897	S2957	V3017
P3018	K2298	G2598	W2658	P2718	T2778	V2838	K2898	V2958	P3018
G3019	Q2299	S2599	L2659	G2719	M2779	E2839	V2899	Y2959	G3019
L3020	W2300	Q2600	V2660	R2720	S2780	D2840	F2900	Q2960	L3020
F3021	I2301	L2601	L2661	K2721	Q2781	E2841	Y2901	I2961	F3021
E3022	V2302	T2602	F2662	P2722	E2782	E2842	K2902	K2962	E3022
G3023	F2303	K2603	C2663	L2723	R2783	R2843	E2903	V2963	G3023
D3024	D2304	T2604	D2664	S2724	F2784	R2844	E2904	H2964	D3024
S3025	G2305	L2605	E2665	H2725	T2785	W2845	L2905	R2965	S3025
Y3026	D2306	F2606	I2666	R2726	Q2786	T2846	V2906	K2966	Y3026
A3027	V2307	S2607	N2667	F2727	D2787	D2847	V2907	Y2967	A3027
T3028	D2308	A2608	L2668	L2728	T2788	E2848	P2908	T2968	T3028
L3029	P2309	L2609	P2669	R2729	Q2789	N2849	V2909	G2969	L3029
K3030	E2310	R2610	D2670	H2730	T2790	I2850	V2910	E2970	K3030
T3031	W2311	A2611	M2671	V2731	H2791	D2851	L2911	D2971	T3031
Q3032	V2312	V2612	D2672	P2732	Y2792	T2852	F2912	F2972	Q3032
C3033	E2313	P2613	K2673	V2733	I2793	V2853	M2913	D2973	C3033
E3035	L2315	Q2614	Y2674	V2734	Y2794	A2854	E2914	E2974	E3035
G3036	N2316	L2615	G2675	Y2735	S2795	L2855	V2915	D2975	G3036
A3037	S2317	E2616	T2676	V2736	P2796	K2856	L2916	L2976	A3037
Q3038	W2318	V2617	Q2677	D2737	E2797	H2857	H2917	T2977	Q3038
K3039	L2319	I2498	R2678	V2738	R2798	P2858	D2918	R2978	K3039
E3040	D2320	L2499	G2619	P2739	M2799	P2859	V2919	V2979	E3040
G3041	D2321	W2500	I2680	Q2740	T2800	N2860	L2920	L2980	G3041
L3042	R2381	S2501	S2681	P2621	R2801	I2861	R2921	R2981	L3042
K3043	W2382	L2502	K2561	F2622	W2802	D2862	I2922	R2982	K3043
D3044	R2383	S2503	A2563	S2623	V2803	R2863	D2923	S2983	D3044
S3045	L2324	G2504	A2564	S2624	R2804	E2864	R2924	G2984	S3045
K3046	L2325	D2505	P2565	A2625	Q2805	K2865	L2925	C2985	K3046
H3047	T2326	S2506	D2566	T2626	T2806	A2866	F2926	K2986	H3047
E3048	L2327	R2507	V2567	T2627	F2807	M2867	R2927	N2987	E3048
E3049	P2328	L2508	V2568	P2628	E2808	S2868	Q2928	E2988	E3049
Y3051	R2329	K2509	W2569	E2629	A2809	R2869	P2929	R2989	Y3051
K3052	GLU	M2510	P2570	T2630	L2810	E2870	Q2930	I2990	K3052
W3053	E2331	R2511	T2571	L2631	G2691	F2751	G2931	A2991	W3053
F3054	R2332	A2512	L2572	P2632	F2692	N2752	H2932	F2992	F3054
T3055	L2333	E2513	D2573	K2633	Y2693	L2873	L2933	I2993	T3055
S3056	S2334	L2514	T2574	T2634	R2694	S2874	L2934	M2994	S3056
Q3057	L2335	G2515	V2575	P2635	T2695	N2875	L2935	D2995	Q3057
Y3058	P2336	E2516	R2576	D2636	S2696	W2876	I2936	E2996	Y3058
N2337	R2337	Y2517	H2577	L2637	D2697	L2877	G2937	S2997	N2337
W2338	N2338	L2518	E2578	Y2638	Q2698	S2878	V2938	N2998	W2338
V2339	V2339	R2519	A2579	C2639	T2699	K2879	S2939	V2999	V2339
		R2520	L2580	E2640	W2700	D2880	G2940	L3000	



T4561	K4441	H4381	L4321	D4261	W4201	A4141	D4081	M4021	L3961	Y3901	T4562	K4442	T4382	H4382	L4322	Q4262	S4202	A4142	G4142	D4082	E4022	D3902	Y3841	K4443	T4383	L4323	Q4263	H4383	L4323	R4263	K4203	A4083	D3962	D3962	E3942	K4444	A4384	P4324	L4264	L4264	I4144	I4084	S3964	A3903	F3904	E3904	K4445	S4385	M4325	N4325	P4324	L4265	F4145	I4145	G4145	A4084	S3965	F3905	E3905	K4446	M4386	N4266	E4206	Y4206	L4265	M4085	L4086	D4026	P3966	S3966	F3906	Q3906	L3846	N3845	K4505	M4506	I4507	G4567	S4567	L4566	K4566	T4567	S4576	V4516	L4455	E4454	N4453	L4451	T4450	R4449	L4448	Y4447	K4447	N4446	M4466	H4466	Q4526	R4525	L4585	A4465	V4464	S4463	R4462	T4522	L4521	T4461	L4460	I4459	G4458	K4457	V4456	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4452	L4451	T4450	V4509	H4508	L4507	M4506	K4566	G4567	S4567	L4566	T4567	S4576	V4516	L4455	E4454	N4453	L4452	I4451	L4511	G4512	N4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T4621	Y4622	D4623	F4624	E4625	T4626	A4627	T4628	R4629	E4630	D4631	P4632	R4633	S4634	F4635	Y4636	E4637	R4638	C4639	Y4640	A4641	Y4642	L4643	C4644	T4645	E4646
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	233227	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	106061	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.309	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP

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	0.57	0/23474	1.03	33/31851 (0.1%)
1	B	0.57	0/23474	1.03	33/31851 (0.1%)
All	All	0.57	0/46948	1.03	66/63702 (0.1%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3821	ILE	N-CA-C	16.76	126.51	110.42
1	A	3821	ILE	N-CA-C	16.76	126.51	110.42
1	A	4250	SER	N-CA-C	13.35	125.91	111.36
1	B	4250	SER	N-CA-C	13.35	125.91	111.36
1	B	3578	ILE	CB-CA-C	-8.26	101.40	111.97
1	A	3578	ILE	CB-CA-C	-8.26	101.40	111.97
1	B	2795	SER	N-CA-C	7.38	114.77	108.13
1	A	2795	SER	N-CA-C	7.32	114.72	108.13
1	B	2824	ILE	N-CA-CB	6.72	119.68	110.54
1	A	2824	ILE	N-CA-CB	6.71	119.66	110.54
1	A	2795	SER	CA-C-N	6.38	127.82	119.84
1	A	2795	SER	C-N-CA	6.38	127.82	119.84
1	B	2795	SER	CA-C-N	6.38	127.82	119.84
1	B	2795	SER	C-N-CA	6.38	127.82	119.84
1	B	2552	VAL	CA-C-N	-6.37	114.22	120.52
1	B	2552	VAL	C-N-CA	-6.37	114.22	120.52
1	A	2552	VAL	CA-C-N	-6.36	114.23	120.52
1	A	2552	VAL	C-N-CA	-6.36	114.23	120.52
1	A	2197	GLU	N-CA-C	-6.26	104.46	111.28
1	B	2197	GLU	N-CA-C	-6.26	104.46	111.28
1	A	2609	LEU	N-CA-C	6.18	118.09	111.36
1	B	2609	LEU	N-CA-C	6.17	118.09	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2019	ASN	CA-C-N	-5.96	113.80	119.76
1	A	2019	ASN	C-N-CA	-5.96	113.80	119.76
1	B	2019	ASN	CA-C-N	-5.94	113.82	119.76
1	B	2019	ASN	C-N-CA	-5.94	113.82	119.76
1	A	2687	VAL	N-CA-C	5.92	116.04	110.30
1	B	2687	VAL	N-CA-C	5.92	116.04	110.30
1	A	2569	VAL	CA-C-N	-5.87	113.72	119.76
1	A	2569	VAL	C-N-CA	-5.87	113.72	119.76
1	B	2569	VAL	CA-C-N	-5.87	113.72	119.76
1	B	2569	VAL	C-N-CA	-5.87	113.72	119.76
1	A	2596	PRO	O-C-N	5.84	123.89	121.15
1	B	2596	PRO	O-C-N	5.84	123.89	121.15
1	A	1626	PHE	CA-C-N	5.81	127.11	119.84
1	A	1626	PHE	C-N-CA	5.81	127.11	119.84
1	B	1626	PHE	CA-C-N	5.78	127.07	119.84
1	B	1626	PHE	C-N-CA	5.78	127.07	119.84
1	A	2154	ILE	O-C-N	5.75	124.15	120.07
1	B	2154	ILE	O-C-N	5.73	124.14	120.07
1	B	3756	VAL	N-CA-C	5.70	115.89	110.53
1	A	3756	VAL	N-CA-C	5.66	115.85	110.53
1	B	3013	ALA	N-CA-C	5.49	116.95	110.97
1	A	3013	ALA	N-CA-C	5.47	116.93	110.97
1	A	2498	ILE	N-CA-CB	5.43	117.93	110.54
1	B	2498	ILE	N-CA-CB	5.43	117.93	110.54
1	A	1519	ASP	N-CA-C	5.32	117.16	111.36
1	B	1519	ASP	N-CA-C	5.30	117.14	111.36
1	A	3162	ALA	N-CA-C	5.26	117.76	111.71
1	B	3162	ALA	N-CA-C	5.26	117.76	111.71
1	A	3147	CYS	CB-CA-C	-5.23	102.66	110.88
1	B	3147	CYS	CB-CA-C	-5.23	102.66	110.88
1	A	3879	ASP	CA-C-N	5.23	127.29	120.28
1	A	3879	ASP	C-N-CA	5.23	127.29	120.28
1	B	3879	ASP	CA-C-N	5.23	127.29	120.28
1	B	3879	ASP	C-N-CA	5.23	127.29	120.28
1	A	2856	LYS	N-CA-C	5.20	116.64	110.97
1	B	2856	LYS	N-CA-C	5.20	116.64	110.97
1	A	2886	GLN	N-CA-C	5.13	116.56	111.07
1	B	2886	GLN	N-CA-C	5.13	116.56	111.07
1	A	3514	ILE	N-CA-C	5.09	115.23	110.30
1	B	3514	ILE	N-CA-C	5.09	115.23	110.30
1	B	3811	ILE	CB-CA-C	-5.08	105.46	111.97
1	A	3811	ILE	CB-CA-C	-5.06	105.49	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1698	ILE	N-CA-C	5.03	116.35	110.62
1	B	1698	ILE	N-CA-C	5.03	116.35	110.62

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23003	0	22805	604	0
1	B	23003	0	22805	597	0
2	A	81	0	36	13	0
2	B	81	0	36	13	0
3	A	31	0	12	4	0
3	B	31	0	12	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	46232	0	45706	1184	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 13.

All (1184) 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:A:3638:VAL:HG12	1:A:3681:THR:CG2	1.29	1.60
1:A:3815:MET:HE2	1:A:3871:VAL:CG2	1.34	1.55
1:B:3815:MET:HE2	1:B:3871:VAL:CG2	1.34	1.54
1:B:3638:VAL:HG12	1:B:3681:THR:CG2	1.29	1.54
1:B:3749:LEU:HD13	1:B:3773:LEU:CD1	1.44	1.46
1:B:2584:TRP:CZ3	1:B:2732:PRO:HG2	1.50	1.45
1:A:3749:LEU:HD13	1:A:3773:LEU:CD1	1.44	1.43
1:A:2584:TRP:CZ3	1:A:2732:PRO:HG2	1.50	1.43
1:A:1931:ASN:ND2	1:A:2317:SER:HB3	1.28	1.42
1:B:1931:ASN:ND2	1:B:2317:SER:HB3	1.28	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3815:MET:CE	1:A:3871:VAL:CG2	2.07	1.33
1:B:3815:MET:CE	1:B:3871:VAL:CG2	2.07	1.32
1:A:3456:SER:CB	1:B:3459:GLN:HG3	1.64	1.27
1:A:2584:TRP:CZ3	1:A:2732:PRO:CG	2.17	1.25
1:A:3459:GLN:HG3	1:B:3456:SER:CB	1.65	1.25
1:A:3638:VAL:CG1	1:A:3681:THR:CG2	2.14	1.25
1:B:2584:TRP:CZ3	1:B:2732:PRO:CG	2.18	1.24
1:B:3638:VAL:CG1	1:B:3681:THR:CG2	2.14	1.24
1:A:3115:LEU:HD13	1:A:3143:ILE:CD1	1.67	1.24
1:B:3115:LEU:HD13	1:B:3143:ILE:CD1	1.67	1.24
1:A:3456:SER:OG	1:B:3459:GLN:HG3	1.34	1.22
1:A:4622:VAL:HG12	1:A:4624:PHE:CE2	1.75	1.21
1:A:3459:GLN:HG3	1:B:3456:SER:OG	1.38	1.19
1:B:4622:VAL:HG12	1:B:4624:PHE:CE2	1.76	1.19
1:A:2609:LEU:HD11	1:A:2615:MET:HB2	1.23	1.17
1:B:3815:MET:CE	1:B:3871:VAL:HG21	1.72	1.16
1:B:2325:LEU:HD23	1:B:2333:LEU:HD12	1.28	1.15
1:A:3821:ILE:HD12	1:A:4342:LYS:CG	1.77	1.14
1:A:3749:LEU:HD13	1:A:3773:LEU:HD11	1.26	1.13
1:A:3815:MET:CE	1:A:3871:VAL:HG21	1.72	1.13
1:A:3815:MET:HE2	1:A:3871:VAL:HG22	1.29	1.12
1:B:3821:ILE:HD12	1:B:4342:LYS:CG	1.78	1.12
1:A:2549:GLN:NE2	1:A:2572:LEU:HD22	1.65	1.12
1:A:3456:SER:OG	1:B:3459:GLN:CG	1.96	1.12
1:A:4607:LEU:HD21	1:A:4635:PHE:HZ	1.08	1.11
1:A:4511:LEU:HD22	1:A:4644:CYS:SG	1.90	1.11
1:B:2549:GLN:NE2	1:B:2572:LEU:HD22	1.65	1.11
1:B:2196:GLY:HA2	1:B:2201:GLY:HA3	1.32	1.11
1:A:3821:ILE:HD12	1:A:4342:LYS:HG3	1.33	1.10
1:B:2457:SER:HB3	1:B:2584:TRP:CH2	1.86	1.10
1:B:2457:SER:CB	1:B:2584:TRP:HH2	1.63	1.10
1:A:2457:SER:HB3	1:A:2584:TRP:CH2	1.86	1.10
1:A:2457:SER:CB	1:A:2584:TRP:HH2	1.63	1.10
1:A:3115:LEU:HD13	1:A:3143:ILE:HD11	1.31	1.10
1:A:4607:LEU:HD21	1:A:4635:PHE:CZ	1.85	1.10
1:B:2609:LEU:HD11	1:B:2615:MET:HB2	1.23	1.10
1:B:3821:ILE:CD1	1:B:4342:LYS:HD2	1.81	1.10
1:A:3459:GLN:CG	1:B:3456:SER:OG	1.99	1.10
1:B:4511:LEU:HD22	1:B:4644:CYS:SG	1.90	1.10
1:B:4607:LEU:HD21	1:B:4635:PHE:CZ	1.85	1.10
1:B:3115:LEU:HD13	1:B:3143:ILE:HD11	1.31	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3749:LEU:HD13	1:A:3773:LEU:HD13	1.33	1.09
1:B:1931:ASN:ND2	1:B:2317:SER:CB	2.14	1.09
1:B:4424:LEU:HD13	1:B:4486:ILE:CD1	1.83	1.09
1:A:3821:ILE:CD1	1:A:4342:LYS:HD2	1.81	1.09
1:A:1931:ASN:ND2	1:A:2317:SER:CB	2.14	1.09
1:A:2196:GLY:HA2	1:A:2201:GLY:HA3	1.32	1.09
1:A:4424:LEU:HD13	1:A:4486:ILE:CD1	1.83	1.08
1:A:4622:VAL:CG1	1:A:4624:PHE:CE2	2.34	1.08
1:B:3749:LEU:HD13	1:B:3773:LEU:HD11	1.26	1.08
1:B:4607:LEU:HD21	1:B:4635:PHE:HZ	1.08	1.08
1:B:4622:VAL:CG1	1:B:4624:PHE:CE2	2.34	1.08
1:A:2325:LEU:HD23	1:A:2333:LEU:HD12	1.28	1.08
1:B:3821:ILE:HD12	1:B:4342:LYS:HG3	1.34	1.08
1:B:3749:LEU:HD13	1:B:3773:LEU:HD13	1.33	1.08
1:B:1766:LEU:HD23	1:B:1833:ALA:HA	1.36	1.07
1:B:3815:MET:HE2	1:B:3871:VAL:HG22	1.29	1.07
1:B:3815:MET:HE2	1:B:3871:VAL:HG21	1.09	1.07
1:B:2580:LEU:O	1:B:2584:TRP:HD1	1.36	1.07
1:A:3815:MET:HE2	1:A:3871:VAL:HG21	1.09	1.06
1:A:1879:LEU:HD12	1:A:1918:ALA:HB2	1.36	1.06
1:B:3638:VAL:CG1	1:B:3681:THR:HG23	1.79	1.06
1:A:3638:VAL:CG1	1:A:3681:THR:HG23	1.79	1.05
1:A:1766:LEU:HD23	1:A:1833:ALA:HA	1.36	1.05
1:A:2580:LEU:O	1:A:2584:TRP:HD1	1.36	1.04
1:B:1879:LEU:HD12	1:B:1918:ALA:HB2	1.36	1.03
1:A:2609:LEU:HD11	1:A:2615:MET:CB	1.87	1.03
1:A:2549:GLN:HE21	1:A:2572:LEU:HD22	1.18	1.03
1:B:4605:VAL:CG1	1:B:4635:PHE:CE2	2.42	1.03
1:B:4424:LEU:HD13	1:B:4486:ILE:HD11	1.38	1.02
1:A:4605:VAL:CG1	1:A:4635:PHE:CE2	2.42	1.02
1:A:3749:LEU:CD1	1:A:3773:LEU:CD1	2.37	1.01
1:A:4424:LEU:HD13	1:A:4486:ILE:HD11	1.38	1.01
1:B:2609:LEU:HD11	1:B:2615:MET:CB	1.88	1.01
1:B:3749:LEU:CD1	1:B:3773:LEU:CD1	2.37	1.01
1:A:3099:THR:HG22	1:A:3152:GLN:NE2	1.75	1.01
1:B:2549:GLN:HE21	1:B:2572:LEU:HD22	1.18	1.01
1:B:3099:THR:HG22	1:B:3152:GLN:NE2	1.75	1.01
1:A:1778:LEU:CD1	1:A:1830:ILE:HD12	1.91	1.00
1:B:4605:VAL:HG11	1:B:4635:PHE:CE2	1.96	1.00
1:B:1778:LEU:CD1	1:B:1830:ILE:HD12	1.91	1.00
1:A:3638:VAL:CG1	1:A:3681:THR:HG21	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4605:VAL:HG11	1:A:4635:PHE:CE2	1.96	0.99
1:A:2549:GLN:HG3	1:A:2572:LEU:HD13	1.44	0.98
1:B:1879:LEU:HD12	1:B:1918:ALA:CB	1.93	0.98
1:A:3638:VAL:HG12	1:A:3681:THR:HG21	1.45	0.98
1:B:2819:GLU:OE2	1:B:2862:ASP:CB	2.12	0.98
1:B:3638:VAL:CG1	1:B:3681:THR:HG21	1.91	0.97
1:B:2457:SER:CB	1:B:2584:TRP:CH2	2.44	0.97
1:B:3638:VAL:HG12	1:B:3681:THR:HG21	1.45	0.97
1:B:2584:TRP:HZ3	1:B:2732:PRO:HG2	1.15	0.97
1:A:3749:LEU:CD1	1:A:3773:LEU:HD11	1.95	0.97
1:B:2358:ARG:NH2	2:B:4801:ADP:O1B	1.97	0.97
1:A:2819:GLU:OE2	1:A:2862:ASP:CB	2.12	0.97
1:A:3817:SER:OG	1:A:4349:LEU:HD12	1.65	0.97
1:B:2549:GLN:HG3	1:B:2572:LEU:HD13	1.44	0.97
1:A:2358:ARG:NH2	2:A:4801:ADP:O1B	1.97	0.96
1:A:4247:MET:HE3	1:A:4252:TYR:CE2	2.00	0.96
1:A:1879:LEU:HD12	1:A:1918:ALA:CB	1.93	0.96
1:A:2302:VAL:HG22	1:A:2342:MET:HB2	1.46	0.96
1:B:4247:MET:HE3	1:B:4252:TYR:CE2	2.00	0.96
1:A:3459:GLN:HG3	1:B:3456:SER:HB3	1.46	0.96
1:B:3817:SER:OG	1:B:4349:LEU:CD1	2.14	0.96
1:B:3822:HIS:O	1:B:3823:PHE:CG	2.19	0.96
1:B:3749:LEU:CD1	1:B:3773:LEU:HD11	1.95	0.95
1:A:3172:THR:HG21	1:A:3694:SER:OG	1.66	0.95
1:A:3822:HIS:O	1:A:3823:PHE:CG	2.19	0.95
1:A:3817:SER:OG	1:A:4349:LEU:CD1	2.14	0.95
1:A:3821:ILE:HD12	1:A:4342:LYS:CD	1.97	0.95
1:A:2457:SER:CB	1:A:2584:TRP:CH2	2.44	0.95
1:B:1931:ASN:HD22	1:B:2317:SER:HB3	1.15	0.95
1:A:2609:LEU:CD1	1:A:2615:MET:HB2	1.97	0.95
1:A:2220:LEU:HD23	1:A:2342:MET:HG2	1.48	0.95
1:A:3456:SER:HB3	1:B:3459:GLN:HG3	1.49	0.95
1:A:3638:VAL:HG12	1:A:3681:THR:HG23	0.97	0.95
1:B:3817:SER:OG	1:B:4349:LEU:HD12	1.65	0.94
1:B:4247:MET:HE3	1:B:4252:TYR:HE2	1.32	0.94
1:B:1981:ALA:HB2	1:B:1999:CYS:SG	2.07	0.94
1:B:3638:VAL:HG12	1:B:3681:THR:HG23	0.97	0.94
1:B:2302:VAL:HG22	1:B:2342:MET:HB2	1.46	0.94
1:B:3822:HIS:O	1:B:3823:PHE:CD2	2.21	0.94
1:A:4622:VAL:HG11	1:A:4624:PHE:CZ	2.03	0.94
1:B:3821:ILE:HD12	1:B:4342:LYS:CD	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2609:LEU:CD1	1:B:2615:MET:HB2	1.97	0.94
1:B:1931:ASN:HD22	1:B:2317:SER:CB	1.76	0.94
1:B:3172:THR:HG21	1:B:3694:SER:OG	1.66	0.94
1:A:1981:ALA:HB2	1:A:1999:CYS:SG	2.07	0.93
1:A:4247:MET:HE3	1:A:4252:TYR:HE2	1.32	0.93
1:A:3822:HIS:O	1:A:3823:PHE:CD2	2.21	0.93
1:B:4622:VAL:HG11	1:B:4624:PHE:CZ	2.03	0.93
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.48	0.93
1:A:3115:LEU:CD1	1:A:3143:ILE:HD11	1.99	0.92
1:A:1778:LEU:HD11	1:A:1830:ILE:HD12	1.52	0.92
1:A:1931:ASN:HD22	1:A:2317:SER:HB3	1.15	0.92
1:A:1931:ASN:HD22	1:A:2317:SER:CB	1.77	0.92
1:A:4622:VAL:CG1	1:A:4624:PHE:CZ	2.53	0.92
1:B:3115:LEU:CD1	1:B:3143:ILE:HD11	1.99	0.91
1:B:4622:VAL:CG1	1:B:4624:PHE:CZ	2.53	0.91
1:B:2220:LEU:HD23	1:B:2342:MET:HG2	1.49	0.91
1:B:2464:GLN:HG2	1:B:2583:THR:HG23	1.51	0.91
1:B:2605:LEU:CD2	1:B:2662:PHE:CE1	2.54	0.91
1:B:3708:LEU:HD23	1:B:3809:SER:HA	1.49	0.91
1:B:1778:LEU:HD11	1:B:1830:ILE:HD12	1.52	0.91
1:A:2584:TRP:HZ3	1:A:2732:PRO:HG2	1.15	0.90
1:A:3123:PRO:HB3	1:A:3540:ASN:ND2	1.85	0.90
1:A:2605:LEU:CD2	1:A:2662:PHE:CE1	2.54	0.90
1:B:3123:PRO:HB3	1:B:3540:ASN:ND2	1.85	0.90
1:B:2580:LEU:O	1:B:2584:TRP:CD1	2.24	0.90
1:A:2584:TRP:HZ3	1:A:2732:PRO:CG	1.70	0.89
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	1.51	0.89
1:A:2580:LEU:O	1:A:2584:TRP:CD1	2.24	0.89
1:B:3115:LEU:CD1	1:B:3143:ILE:CD1	2.50	0.89
1:A:4186:PHE:HZ	1:A:4265:LEU:CD1	1.85	0.89
1:B:4186:PHE:HZ	1:B:4265:LEU:CD1	1.85	0.89
1:A:2457:SER:HB3	1:A:2584:TRP:HH2	1.29	0.89
1:A:1632:VAL:CG1	1:A:1636:ASP:HB2	2.03	0.88
1:A:4186:PHE:HZ	1:A:4265:LEU:HD11	1.39	0.88
1:B:2584:TRP:HZ3	1:B:2732:PRO:CG	1.70	0.88
1:B:1632:VAL:CG1	1:B:1636:ASP:HB2	2.03	0.88
1:B:2752:ASN:ND2	1:B:2770:THR:HG22	1.90	0.87
1:A:4067:THR:HB	1:A:4094:VAL:HG22	1.56	0.87
1:B:4186:PHE:HZ	1:B:4265:LEU:HD11	1.38	0.87
1:A:3115:LEU:HD13	1:A:3143:ILE:HD13	1.55	0.87
1:B:3115:LEU:HD13	1:B:3143:ILE:HD13	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:VAL:HG12	1:A:3681:THR:HG22	1.57	0.86
1:A:3708:LEU:CD2	1:A:3809:SER:HA	2.05	0.86
1:B:4067:THR:HB	1:B:4094:VAL:HG22	1.56	0.85
1:A:4424:LEU:CD1	1:A:4486:ILE:HD13	2.07	0.85
1:B:3821:ILE:HD13	1:B:4342:LYS:HD2	1.59	0.85
1:B:3708:LEU:CD2	1:B:3809:SER:HA	2.05	0.85
1:B:2863:ARG:O	1:B:2863:ARG:HD3	1.76	0.85
1:B:3808:CYS:SG	1:B:3836:TYR:OH	2.35	0.85
1:A:2863:ARG:O	1:A:2863:ARG:HD3	1.76	0.85
1:B:4424:LEU:CD1	1:B:4486:ILE:HD13	2.07	0.85
1:A:2091:ARG:NH1	2:A:4801:ADP:O1A	2.10	0.84
1:A:2752:ASN:ND2	1:A:2770:THR:HG22	1.90	0.84
1:A:3115:LEU:CD1	1:A:3143:ILE:CD1	2.50	0.84
1:A:3821:ILE:HD13	1:A:4342:LYS:HD2	1.59	0.84
1:B:2091:ARG:NH1	2:B:4801:ADP:O1A	2.10	0.84
1:B:3815:MET:CE	1:B:3871:VAL:HG23	2.06	0.84
1:A:3821:ILE:CD1	1:A:4342:LYS:CD	2.55	0.84
1:A:4605:VAL:HG11	1:A:4635:PHE:CZ	2.13	0.83
1:B:2091:ARG:NH1	2:B:4801:ADP:H5'2	1.94	0.83
1:B:4605:VAL:HG11	1:B:4635:PHE:CZ	2.13	0.83
1:A:3815:MET:CE	1:A:3871:VAL:HG23	2.06	0.83
1:A:3808:CYS:SG	1:A:3836:TYR:OH	2.35	0.83
1:A:2446:ILE:HD11	1:A:2735:TYR:CD1	2.14	0.82
1:B:1879:LEU:CD1	1:B:1918:ALA:HB2	2.10	0.82
1:B:2446:ILE:HD11	1:B:2735:TYR:CD1	2.14	0.82
1:A:2851:ASP:OD2	1:A:2863:ARG:NH1	2.12	0.82
1:A:2091:ARG:NH1	2:A:4801:ADP:H5'2	1.94	0.81
1:B:3821:ILE:CD1	1:B:4342:LYS:CD	2.55	0.81
1:A:1879:LEU:CD1	1:A:1918:ALA:HB2	2.10	0.81
1:B:2851:ASP:OD2	1:B:2863:ARG:NH1	2.12	0.81
1:B:3638:VAL:HG12	1:B:3681:THR:HG22	1.57	0.81
1:A:3008:MET:HE2	1:A:3066:PHE:CZ	2.16	0.80
1:A:3882:THR:HG22	1:A:4339:MET:HG3	1.64	0.80
1:B:3822:HIS:ND1	1:B:3824:LEU:HB3	1.97	0.80
1:B:4424:LEU:HD13	1:B:4486:ILE:HD13	1.61	0.80
1:B:2609:LEU:CD2	1:B:2617:VAL:HG23	2.12	0.80
1:B:3151:HIS:HD1	1:B:3516:TYR:HH	1.24	0.80
1:A:1931:ASN:OD1	1:A:1958:ASP:HB2	1.82	0.80
1:B:2551:LYS:O	1:B:2551:LYS:HD3	1.82	0.80
1:B:3008:MET:HE2	1:B:3066:PHE:CZ	2.16	0.80
1:B:3882:THR:HG22	1:B:4339:MET:HG3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3175:HIS:CD2	1:B:3585:ARG:NH2	2.50	0.80
1:A:2571:THR:HG1	1:A:2574:THR:HG1	1.20	0.79
1:B:2609:LEU:CD2	1:B:2617:VAL:CG2	2.60	0.79
1:A:2609:LEU:CD2	1:A:2617:VAL:HG23	2.12	0.79
1:B:1879:LEU:HD11	1:B:1914:GLU:O	1.83	0.79
1:B:3815:MET:HE1	1:B:3871:VAL:CG2	2.11	0.79
1:A:3822:HIS:ND1	1:A:3824:LEU:HB3	1.97	0.79
1:A:2551:LYS:O	1:A:2551:LYS:HD3	1.82	0.79
1:A:3815:MET:HE1	1:A:3871:VAL:CG2	2.11	0.79
1:B:1636:ASP:OD2	1:B:1656:LYS:NZ	2.14	0.79
1:B:2593:LEU:HD23	1:B:2734:VAL:CG2	2.13	0.79
1:A:2609:LEU:CD2	1:A:2617:VAL:CG2	2.60	0.79
1:B:1931:ASN:OD1	1:B:1958:ASP:HB2	1.82	0.78
1:A:3675:PHE:O	1:A:3676:VAL:HG13	1.83	0.78
1:B:3675:PHE:O	1:B:3676:VAL:HG13	1.83	0.78
1:A:1825:LEU:HD12	1:A:1830:ILE:HD11	1.64	0.78
1:A:2605:LEU:CD2	1:A:2662:PHE:CD1	2.66	0.78
1:A:1879:LEU:HD11	1:A:1914:GLU:O	1.83	0.78
1:A:3175:HIS:CD2	1:A:3585:ARG:NH2	2.50	0.78
1:A:2265:TYR:CE2	1:A:2314:ASN:ND2	2.52	0.78
1:A:2609:LEU:HD21	1:A:2617:VAL:HG23	1.66	0.78
1:B:2265:TYR:CE2	1:B:2314:ASN:ND2	2.52	0.78
1:B:2605:LEU:CD2	1:B:2662:PHE:CD1	2.66	0.78
1:A:2593:LEU:HD23	1:A:2734:VAL:CG2	2.13	0.78
1:B:2549:GLN:HE21	1:B:2572:LEU:CD2	1.97	0.78
1:A:3815:MET:HE1	1:A:3871:VAL:HG23	1.65	0.77
1:B:1825:LEU:HD12	1:B:1830:ILE:HD11	1.64	0.77
1:B:2609:LEU:HD21	1:B:2617:VAL:HG23	1.66	0.77
1:A:1636:ASP:OD2	1:A:1656:LYS:NZ	2.14	0.77
1:B:2058:GLY:O	1:B:2104:LYS:HE3	1.85	0.77
1:B:4622:VAL:HG11	1:B:4624:PHE:CE2	2.17	0.77
1:A:2581:LEU:HD21	1:A:2593:LEU:HD21	1.67	0.76
1:B:2581:LEU:HD21	1:B:2593:LEU:HD21	1.67	0.76
1:A:4622:VAL:HG11	1:A:4624:PHE:CE2	2.17	0.76
1:B:4605:VAL:HG13	1:B:4635:PHE:CE2	2.19	0.76
1:A:4605:VAL:HG13	1:A:4635:PHE:CE2	2.19	0.76
1:A:2584:TRP:CE3	1:A:2732:PRO:HG2	2.17	0.76
1:A:4035:VAL:HG22	1:A:4143:ARG:HG3	1.68	0.76
1:B:2609:LEU:CD1	1:B:2615:MET:CB	2.59	0.76
1:B:2549:GLN:CG	1:B:2572:LEU:HD13	2.16	0.76
1:A:2461:MET:HE3	1:A:2584:TRP:CZ2	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3562:TRP:HB3	1:A:3567:LEU:HD23	1.69	0.75
1:B:2461:MET:HE3	1:B:2584:TRP:CZ2	2.21	0.75
1:B:3815:MET:HE1	1:B:3871:VAL:HG23	1.65	0.75
1:A:4424:LEU:CD1	1:A:4486:ILE:CD1	2.61	0.75
1:A:2058:GLY:O	1:A:2104:LYS:HE3	1.85	0.75
1:A:4190:ILE:HD11	1:A:4252:TYR:HE1	1.52	0.75
1:B:2149:LEU:HD11	1:B:2157:LEU:HD22	1.68	0.75
1:B:4035:VAL:HG22	1:B:4143:ARG:HG3	1.68	0.75
1:A:2609:LEU:CD1	1:A:2615:MET:CB	2.59	0.75
1:A:3008:MET:CE	1:A:3066:PHE:CZ	2.69	0.75
1:A:1778:LEU:HD13	1:A:1830:ILE:HD12	1.68	0.75
1:B:4190:ILE:HD11	1:B:4252:TYR:HE1	1.52	0.75
1:A:1933:ASP:OD1	1:A:1962:ARG:NH2	2.20	0.75
1:A:2549:GLN:CG	1:A:2572:LEU:HD13	2.16	0.75
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.68	0.74
1:B:2584:TRP:CZ3	1:B:2732:PRO:HG3	2.20	0.74
1:B:2584:TRP:CE3	1:B:2732:PRO:HG2	2.17	0.74
1:B:1933:ASP:OD1	1:B:1962:ARG:NH2	2.20	0.74
1:B:3008:MET:CE	1:B:3066:PHE:CZ	2.69	0.74
1:B:1778:LEU:HD13	1:B:1830:ILE:HD12	1.68	0.74
1:B:2749:GLY:HA2	1:B:2770:THR:HG21	1.70	0.74
1:B:2605:LEU:HD23	1:B:2662:PHE:CE1	2.21	0.74
1:B:3562:TRP:HB3	1:B:3567:LEU:HD23	1.69	0.74
1:A:2549:GLN:HE21	1:A:2572:LEU:CD2	1.97	0.74
1:A:3456:SER:OG	1:B:3459:GLN:CD	2.30	0.74
1:A:2605:LEU:HD23	1:A:2662:PHE:CE1	2.21	0.74
1:A:3082:SER:OG	1:A:3085:LEU:HD12	1.87	0.74
1:B:4388:LEU:O	1:B:4392:PRO:HD3	1.88	0.74
1:A:3459:GLN:CG	1:B:3456:SER:CB	2.58	0.73
1:A:4388:LEU:O	1:A:4392:PRO:HD3	1.88	0.73
1:B:2457:SER:OG	1:B:2584:TRP:HH2	1.71	0.73
1:B:3082:SER:OG	1:B:3085:LEU:HD12	1.87	0.73
1:B:3154:LEU:HD22	1:B:3516:TYR:CD2	2.23	0.73
1:B:4424:LEU:CD1	1:B:4486:ILE:CD1	2.61	0.73
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.30	0.72
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.70	0.72
1:A:3154:LEU:HD22	1:A:3516:TYR:CD2	2.23	0.72
1:A:3459:GLN:CD	1:B:3456:SER:OG	2.32	0.72
1:A:2078:GLU:OE1	1:A:4522:THR:HG21	1.90	0.72
1:A:2312:VAL:HG11	1:A:2355:THR:HG23	1.70	0.72
1:A:2605:LEU:HD22	1:A:2662:PHE:HE1	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2078:GLU:OE1	1:B:4522:THR:HG21	1.90	0.72
1:A:2457:SER:OG	1:A:2584:TRP:HH2	1.71	0.72
1:B:2312:VAL:HG11	1:B:2355:THR:HG23	1.70	0.72
1:B:3550:THR:OG1	1:B:3574:THR:HG22	1.90	0.72
1:A:3638:VAL:HG13	1:A:3681:THR:HG21	1.71	0.72
1:B:2605:LEU:HD22	1:B:2662:PHE:HE1	1.55	0.71
1:A:3822:HIS:CE1	1:A:3824:LEU:HB3	2.25	0.71
1:B:3099:THR:HG22	1:B:3152:GLN:HE22	1.54	0.71
1:A:3550:THR:OG1	1:A:3574:THR:HG22	1.89	0.71
1:B:3099:THR:CG2	1:B:3152:GLN:NE2	2.52	0.71
1:A:3099:THR:CG2	1:A:3152:GLN:HE22	2.04	0.71
1:B:2863:ARG:HD3	1:B:2863:ARG:C	2.16	0.71
1:A:2863:ARG:HD3	1:A:2863:ARG:C	2.16	0.71
1:B:3638:VAL:HG13	1:B:3681:THR:HG21	1.71	0.70
1:B:4607:LEU:CD2	1:B:4635:PHE:CZ	2.70	0.70
1:B:3822:HIS:CE1	1:B:3824:LEU:HB3	2.25	0.70
1:A:2584:TRP:CZ3	1:A:2732:PRO:HG3	2.20	0.70
1:B:2571:THR:HG1	1:B:2574:THR:HG1	1.22	0.70
1:A:3562:TRP:HB3	1:A:3567:LEU:CD2	2.22	0.70
1:A:2933:LEU:HD23	1:A:3065:VAL:HG13	1.73	0.70
1:A:3099:THR:CG2	1:A:3152:GLN:NE2	2.52	0.70
1:A:1762:VAL:O	1:A:1766:LEU:HD13	1.92	0.69
1:B:3099:THR:CG2	1:B:3152:GLN:HE22	2.04	0.69
1:B:1766:LEU:CD2	1:B:1833:ALA:HA	2.19	0.69
1:B:2912:PHE:HB2	1:B:3104:GLN:OE1	1.93	0.69
1:A:1766:LEU:CD2	1:A:1833:ALA:HA	2.19	0.69
1:B:2457:SER:HB3	1:B:2584:TRP:CZ2	2.28	0.69
1:A:3456:SER:CB	1:B:3459:GLN:CG	2.58	0.69
1:A:4607:LEU:CD2	1:A:4635:PHE:CZ	2.70	0.69
1:B:3562:TRP:HB3	1:B:3567:LEU:CD2	2.22	0.69
1:A:1931:ASN:HD21	1:A:2317:SER:HB3	1.51	0.69
1:A:4190:ILE:HD11	1:A:4252:TYR:CE1	2.28	0.69
1:B:2933:LEU:HD23	1:B:3065:VAL:HG13	1.73	0.69
1:A:3099:THR:HG22	1:A:3152:GLN:HE22	1.54	0.69
1:B:1762:VAL:O	1:B:1766:LEU:HD13	1.92	0.69
1:A:2912:PHE:HB2	1:A:3104:GLN:OE1	1.93	0.69
1:B:3824:LEU:CD2	1:B:4130:ILE:HG12	2.23	0.69
1:B:1632:VAL:CG1	1:B:1636:ASP:CB	2.71	0.68
1:B:2995:ASP:OD1	1:B:3067:THR:HB	1.94	0.68
1:A:2626:THR:O	1:A:2627:THR:HG23	1.93	0.68
1:A:1632:VAL:CG1	1:A:1636:ASP:CB	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2995:ASP:OD1	1:A:3067:THR:HB	1.94	0.68
1:B:2626:THR:O	1:B:2627:THR:HG23	1.93	0.68
1:A:2457:SER:HB3	1:A:2584:TRP:CZ2	2.28	0.68
1:A:2196:GLY:CA	1:A:2201:GLY:HA3	2.19	0.68
1:A:3550:THR:OG1	1:A:3574:THR:CG2	2.42	0.68
1:B:3478:LEU:HD13	1:B:3770:LEU:HD13	1.75	0.68
1:A:3824:LEU:CD2	1:A:4130:ILE:HG12	2.23	0.68
1:B:3522:GLN:OE1	1:B:3704:THR:HG21	1.94	0.68
1:B:2196:GLY:CA	1:B:2201:GLY:HA3	2.19	0.68
1:B:3550:THR:OG1	1:B:3574:THR:CG2	2.42	0.68
1:B:4190:ILE:HD11	1:B:4252:TYR:CE1	2.28	0.68
1:B:2994:MET:HE2	1:B:3008:MET:SD	2.34	0.67
1:A:2580:LEU:HG	1:A:2584:TRP:HE1	1.59	0.67
1:A:2457:SER:HG	1:A:2584:TRP:HH2	1.39	0.67
1:A:2605:LEU:HD22	1:A:2662:PHE:CE1	2.27	0.67
1:A:3522:GLN:OE1	1:A:3704:THR:HG21	1.94	0.67
1:B:2549:GLN:NE2	1:B:2572:LEU:CD2	2.53	0.67
1:B:4042:LEU:HD11	1:B:4128:MET:HE3	1.76	0.67
1:B:3175:HIS:HD2	1:B:3585:ARG:NH2	1.92	0.67
1:A:2994:MET:HE2	1:A:3008:MET:SD	2.34	0.67
1:A:4186:PHE:CZ	1:A:4265:LEU:HD11	2.28	0.67
1:B:2555:ILE:HG21	1:B:2570:PRO:HD2	1.76	0.67
1:B:2580:LEU:HG	1:B:2584:TRP:HE1	1.59	0.67
1:A:2910:VAL:HG11	1:A:3105:VAL:HG23	1.77	0.67
1:A:2555:ILE:HG21	1:A:2570:PRO:HD2	1.76	0.67
1:A:2612:LEU:HD13	1:A:2615:MET:CE	2.25	0.67
1:A:3200:HIS:O	1:A:3204:GLY:N	2.28	0.67
1:B:1931:ASN:HD21	1:B:2317:SER:HB3	1.51	0.67
1:A:3675:PHE:O	1:A:3676:VAL:CG1	2.43	0.66
1:B:2910:VAL:HG11	1:B:3105:VAL:HG23	1.77	0.66
1:B:4099:VAL:HB	1:B:4106:LEU:HD21	1.77	0.66
1:B:3200:HIS:O	1:B:3204:GLY:N	2.28	0.66
1:B:4186:PHE:CZ	1:B:4265:LEU:HD11	2.28	0.66
1:A:3924:ILE:O	1:A:3924:ILE:HG22	1.95	0.66
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.77	0.66
1:A:3478:LEU:HD13	1:A:3770:LEU:HD13	1.76	0.66
1:A:4042:LEU:HD11	1:A:4128:MET:HE3	1.76	0.66
1:B:1632:VAL:HG12	1:B:1636:ASP:HB2	1.77	0.66
1:B:3675:PHE:O	1:B:3676:VAL:CG1	2.43	0.66
1:A:3021:PHE:CD1	1:A:3029:LEU:HD12	2.31	0.65
1:B:2612:LEU:HD13	1:B:2615:MET:CE	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3021:PHE:CD1	1:B:3029:LEU:HD12	2.31	0.65
1:B:3817:SER:HG	1:B:4349:LEU:HD12	1.60	0.65
1:A:2584:TRP:CH2	1:A:2732:PRO:CG	2.79	0.65
1:A:2593:LEU:HD23	1:A:2734:VAL:HG23	1.78	0.65
1:A:2549:GLN:CD	1:A:2572:LEU:HD22	2.22	0.65
1:A:2787:ASP:OD1	1:A:2787:ASP:O	2.15	0.65
1:A:3175:HIS:HD2	1:A:3585:ARG:NH2	1.92	0.65
1:B:3021:PHE:CE1	1:B:3029:LEU:HD12	2.32	0.65
1:B:3113:MET:HE1	1:B:3183:TYR:CD2	2.32	0.65
1:A:2609:LEU:HD22	1:A:2617:VAL:CG2	2.27	0.65
1:B:2091:ARG:NH1	2:B:4801:ADP:C5'	2.60	0.65
1:B:2593:LEU:HD23	1:B:2734:VAL:HG23	1.78	0.65
1:A:2551:LYS:HD3	1:A:2551:LYS:C	2.22	0.64
1:A:3021:PHE:CE1	1:A:3029:LEU:HD12	2.32	0.64
1:B:2549:GLN:CD	1:B:2572:LEU:HD22	2.22	0.64
1:B:3924:ILE:HG22	1:B:3924:ILE:O	1.95	0.64
1:A:1632:VAL:HG12	1:A:1636:ASP:HB2	1.77	0.64
1:B:2568:VAL:HG22	1:B:2603:MET:HE2	1.80	0.64
1:B:2584:TRP:HZ3	1:B:2732:PRO:HG3	1.60	0.64
1:B:4388:LEU:HD21	1:B:4434:VAL:HG13	1.79	0.64
1:B:4565:LEU:HD23	1:B:4642:VAL:HG22	1.79	0.64
1:A:3113:MET:HE1	1:A:3183:TYR:CD2	2.32	0.64
1:B:2584:TRP:CH2	1:B:2732:PRO:CG	2.79	0.64
1:A:1778:LEU:HD11	1:A:1830:ILE:CD1	2.27	0.64
1:B:2602:THR:OG1	2:B:4804:ADP:O1A	2.16	0.64
1:A:2091:ARG:NH1	2:A:4801:ADP:C5'	2.60	0.64
1:B:2551:LYS:HD3	1:B:2551:LYS:C	2.22	0.64
1:B:2609:LEU:HD22	1:B:2617:VAL:CG2	2.27	0.64
1:B:2787:ASP:O	1:B:2787:ASP:OD1	2.15	0.64
1:A:2568:VAL:HG22	1:A:2603:MET:HE2	1.80	0.64
1:A:3580:LEU:HD21	1:A:3589:ILE:HD11	1.80	0.64
1:A:1766:LEU:HD23	1:A:1833:ALA:CA	2.22	0.63
1:A:4560:VAL:O	1:A:4587:LEU:HD12	1.98	0.63
1:A:4388:LEU:HD21	1:A:4434:VAL:HG13	1.79	0.63
1:A:2602:THR:OG1	2:A:4804:ADP:O1A	2.16	0.63
1:A:2667:ASN:ND2	1:A:2713:ASN:O	2.32	0.63
1:B:4560:VAL:O	1:B:4587:LEU:HD12	1.98	0.63
1:B:2667:ASN:ND2	1:B:2713:ASN:O	2.32	0.63
1:B:3580:LEU:HD21	1:B:3589:ILE:HD11	1.81	0.63
1:A:4565:LEU:HD23	1:A:4642:VAL:HG22	1.79	0.63
1:B:3708:LEU:HD23	1:B:3809:SER:CA	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4190:ILE:CD1	1:B:4252:TYR:CE1	2.82	0.62
1:A:3811:ILE:HD12	1:A:3887:LEU:HD22	1.81	0.62
1:B:2295:LEU:C	1:B:2338:ASN:HD21	2.07	0.62
1:B:3824:LEU:HD22	1:B:4130:ILE:HG12	1.79	0.62
1:A:2295:LEU:C	1:A:2338:ASN:HD21	2.07	0.62
1:B:3482:LEU:O	1:B:3486:ARG:N	2.32	0.62
1:A:3824:LEU:HD22	1:A:4130:ILE:HG12	1.80	0.62
1:B:2605:LEU:HD22	1:B:2662:PHE:CE1	2.27	0.62
1:A:4247:MET:CE	1:A:4252:TYR:HE2	2.07	0.62
1:A:1879:LEU:HD12	1:A:1918:ALA:HB3	1.82	0.62
1:A:4508:HIS:CE1	1:A:4587:LEU:HD21	2.35	0.62
1:B:3811:ILE:CD1	1:B:3887:LEU:HD22	2.30	0.62
1:A:2568:VAL:HG22	1:A:2603:MET:CE	2.30	0.61
1:B:2568:VAL:HG22	1:B:2603:MET:CE	2.30	0.61
1:B:3203:VAL:C	1:B:3204:GLY:N	2.58	0.61
1:A:2549:GLN:NE2	1:A:2572:LEU:CD2	2.53	0.61
1:B:2103:VAL:HG13	1:B:2136:ILE:HG23	1.82	0.61
1:B:2593:LEU:CD1	1:B:2605:LEU:HB2	2.30	0.61
1:A:1931:ASN:ND2	1:A:2317:SER:CA	2.63	0.61
1:A:3203:VAL:C	1:A:3204:GLY:N	2.58	0.61
1:B:4247:MET:CE	1:B:4252:TYR:HE2	2.07	0.61
1:A:4190:ILE:CD1	1:A:4252:TYR:CE1	2.82	0.61
1:B:3811:ILE:HD12	1:B:3887:LEU:HD22	1.81	0.61
1:A:2072:PHE:HZ	1:A:2157:LEU:HD11	1.64	0.61
1:B:2100:ALA:HA	1:B:2140:SER:OG	2.01	0.61
1:A:1927:VAL:HG12	1:A:1954:TRP:HB2	1.83	0.61
1:A:2103:VAL:HG13	1:A:2136:ILE:HG23	1.82	0.61
1:A:3482:LEU:O	1:A:3486:ARG:N	2.32	0.61
1:B:3824:LEU:HD22	1:B:4130:ILE:HG23	1.82	0.60
1:B:4508:HIS:CE1	1:B:4587:LEU:HD21	2.35	0.60
1:A:2593:LEU:CD1	1:A:2605:LEU:HB2	2.30	0.60
1:B:1879:LEU:HD12	1:B:1918:ALA:HB3	1.82	0.60
1:B:1879:LEU:HD11	1:B:1914:GLU:C	2.27	0.60
1:A:3459:GLN:CG	1:B:3456:SER:HB3	2.28	0.60
1:B:1931:ASN:ND2	1:B:2317:SER:CA	2.63	0.60
1:A:2571:THR:CG2	1:A:2747:ILE:HG12	2.32	0.60
1:B:1766:LEU:HD23	1:B:1833:ALA:CA	2.22	0.60
1:B:2571:THR:CG2	1:B:2747:ILE:HG12	2.32	0.60
1:A:1879:LEU:HD11	1:A:1914:GLU:C	2.27	0.60
1:A:2936:ILE:HG21	1:A:3093:TRP:CZ3	2.36	0.60
1:A:3708:LEU:HD23	1:A:3809:SER:CA	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3824:LEU:HD22	1:A:4130:ILE:HG23	1.82	0.60
1:B:2072:PHE:HZ	1:B:2157:LEU:HD11	1.64	0.60
1:B:2936:ILE:HG21	1:B:3093:TRP:CZ3	2.36	0.60
1:A:3639:GLU:OE2	1:A:4137:ASN:ND2	2.22	0.60
1:A:4561:THR:CG2	1:A:4587:LEU:HD13	2.32	0.60
1:A:3811:ILE:CD1	1:A:3887:LEU:HD22	2.30	0.60
1:B:4561:THR:CG2	1:B:4587:LEU:HD13	2.32	0.60
1:A:2100:ALA:HA	1:A:2140:SER:OG	2.01	0.60
1:A:2605:LEU:HD21	1:A:2662:PHE:CD1	2.37	0.60
1:B:2830:LEU:HD12	1:B:2871:ILE:HG21	1.84	0.60
1:A:2300:TRP:CZ3	1:A:2342:MET:HE1	2.37	0.59
1:A:2300:TRP:CH2	1:A:2342:MET:HE1	2.37	0.59
1:B:4622:VAL:HG12	1:B:4624:PHE:CZ	2.28	0.59
1:B:1927:VAL:HG12	1:B:1954:TRP:HB2	1.83	0.59
1:B:2300:TRP:CH2	1:B:2342:MET:HE1	2.37	0.59
1:B:4507:ILE:HG13	1:B:4509:VAL:HG23	1.83	0.59
1:A:4507:ILE:HG13	1:A:4509:VAL:HG23	1.83	0.59
1:B:2472:TYR:HB2	1:B:2541:ILE:HD11	1.84	0.59
1:B:3822:HIS:CE1	1:B:3824:LEU:CB	2.86	0.59
1:B:3099:THR:HG22	1:B:3152:GLN:HE21	1.65	0.59
1:A:3099:THR:HG22	1:A:3152:GLN:HE21	1.65	0.59
1:A:3822:HIS:CE1	1:A:3824:LEU:CB	2.86	0.59
1:B:2300:TRP:CZ3	1:B:2342:MET:HE1	2.37	0.59
1:B:4186:PHE:CZ	1:B:4265:LEU:CD1	2.77	0.59
1:B:1778:LEU:HD11	1:B:1830:ILE:CD1	2.27	0.59
1:B:1830:ILE:HG22	1:B:1831:ASP:N	2.18	0.59
1:B:2584:TRP:CZ3	1:B:2732:PRO:CB	2.86	0.59
1:B:3150:VAL:HG22	1:B:3532:TRP:CD1	2.38	0.59
1:A:3817:SER:HG	1:A:4349:LEU:HD12	1.64	0.59
1:B:3822:HIS:HB3	1:B:3825:TYR:CZ	2.38	0.59
1:A:2190:TYR:O	1:A:2377:ASN:CG	2.46	0.58
1:A:3150:VAL:HG22	1:A:3532:TRP:CD1	2.38	0.58
1:B:2549:GLN:HG3	1:B:2572:LEU:CD1	2.29	0.58
1:A:2830:LEU:HD12	1:A:2871:ILE:HG21	1.84	0.58
1:A:3683:ASP:HB2	1:A:4137:ASN:OD1	2.03	0.58
1:A:2294:GLU:OE1	1:A:2299:GLN:NE2	2.37	0.58
1:B:2819:GLU:CD	1:B:2862:ASP:CB	2.77	0.58
1:B:3639:GLU:OE2	1:B:4137:ASN:ND2	2.22	0.58
1:A:2472:TYR:HB2	1:A:2541:ILE:HD11	1.84	0.58
1:A:4027:LEU:HD23	1:A:4058:LEU:HD13	1.86	0.58
1:B:2588:HIS:HA	1:B:2707:GLN:NE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3803:PRO:C	1:B:3804:LEU:N	2.62	0.58
1:A:2588:HIS:HA	1:A:2707:GLN:NE2	2.18	0.58
1:B:3822:HIS:C	1:B:3823:PHE:CD2	2.81	0.58
1:B:2279:LEU:O	1:B:2283:VAL:HG23	2.04	0.58
1:A:3803:PRO:C	1:A:3804:LEU:N	2.62	0.58
1:A:3822:HIS:HB3	1:A:3825:TYR:CZ	2.38	0.58
1:B:2294:GLU:OE1	1:B:2299:GLN:NE2	2.37	0.58
1:B:4027:LEU:HD23	1:B:4058:LEU:HD13	1.86	0.58
1:A:1896:LEU:HD21	1:A:1954:TRP:CZ2	2.39	0.58
1:A:2819:GLU:CD	1:A:2862:ASP:CB	2.76	0.58
1:A:2963:VAL:HG23	1:A:2967:TYR:CD2	2.39	0.58
1:B:2573:ASP:OD1	1:B:2576:ARG:NH2	2.36	0.58
1:B:2605:LEU:HD21	1:B:2662:PHE:CD1	2.37	0.58
1:B:4388:LEU:CD2	1:B:4434:VAL:HG13	2.33	0.58
1:A:1830:ILE:HG22	1:A:1831:ASP:N	2.18	0.58
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.36	0.58
1:A:3822:HIS:C	1:A:3823:PHE:CD2	2.81	0.58
1:B:1935:THR:HG22	1:B:2328:PRO:HG2	1.86	0.58
1:B:2912:PHE:CE2	1:B:3101:ALA:HB1	2.39	0.58
1:A:2912:PHE:CE2	1:A:3101:ALA:HB1	2.39	0.57
1:A:3459:GLN:HG3	1:B:3456:SER:HG	1.64	0.57
1:A:4388:LEU:CD2	1:A:4434:VAL:HG13	2.33	0.57
1:A:4424:LEU:HD11	1:A:4486:ILE:HD13	1.86	0.57
1:B:2963:VAL:HG23	1:B:2967:TYR:CD2	2.39	0.57
1:A:2295:LEU:HA	1:A:2338:ASN:HD22	1.70	0.57
1:A:4605:VAL:HG13	1:A:4635:PHE:CD2	2.39	0.57
1:B:2190:TYR:O	1:B:2377:ASN:CG	2.46	0.57
1:A:2279:LEU:O	1:A:2283:VAL:HG23	2.04	0.57
1:A:4247:MET:HE3	1:A:4252:TYR:CD2	2.38	0.57
1:B:1889:TYR:O	1:B:1893:THR:HG23	2.05	0.57
1:B:3639:GLU:CD	1:B:4137:ASN:HD21	2.11	0.57
1:B:3683:ASP:HB2	1:B:4137:ASN:OD1	2.04	0.57
1:B:4605:VAL:HG13	1:B:4635:PHE:CD2	2.39	0.57
1:A:1571:ILE:HD13	1:A:1607:LEU:HD22	1.87	0.57
1:B:1896:LEU:HD21	1:B:1954:TRP:CZ2	2.39	0.57
1:B:2571:THR:HG21	1:B:2747:ILE:HG12	1.87	0.57
1:B:4086:THR:O	1:B:4090:SER:N	2.37	0.57
1:B:4186:PHE:HE2	1:B:4252:TYR:CD2	2.23	0.57
1:A:4508:HIS:CE1	1:A:4587:LEU:CD2	2.88	0.57
1:B:1571:ILE:HD13	1:B:1607:LEU:HD22	1.87	0.57
1:A:1935:THR:HG22	1:A:2328:PRO:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3082:SER:OG	1:A:3085:LEU:CD1	2.53	0.57
1:B:4247:MET:HE3	1:B:4252:TYR:CD2	2.38	0.57
1:B:4508:HIS:CE1	1:B:4587:LEU:CD2	2.88	0.57
1:A:4186:PHE:HE2	1:A:4252:TYR:CD2	2.23	0.56
1:B:1778:LEU:CD1	1:B:1830:ILE:CD1	2.75	0.56
1:A:3451:TYR:CE1	1:A:3455:ILE:HD11	2.40	0.56
1:A:4067:THR:HG21	1:A:4083:ALA:HB1	1.87	0.56
1:B:2499:LEU:HD12	1:B:2514:LEU:HD23	1.87	0.56
1:A:1892:MET:O	1:A:1896:LEU:HD13	2.05	0.56
1:A:2499:LEU:HD12	1:A:2514:LEU:HD23	1.87	0.56
1:A:2584:TRP:CZ3	1:A:2732:PRO:CB	2.86	0.56
1:A:2626:THR:O	1:A:2627:THR:CG2	2.53	0.56
1:B:2295:LEU:HA	1:B:2338:ASN:HD22	1.70	0.56
1:B:3451:TYR:CE1	1:B:3455:ILE:HD11	2.40	0.56
1:A:3818:LEU:O	1:A:3821:ILE:HG22	2.06	0.56
1:A:4507:ILE:CD1	1:A:4509:VAL:CG2	2.84	0.56
1:A:1778:LEU:CD1	1:A:1830:ILE:CD1	2.75	0.56
1:A:1889:TYR:O	1:A:1893:THR:HG23	2.05	0.56
1:A:2591:LEU:HG	1:A:2709:VAL:HG12	1.88	0.56
1:A:3456:SER:HB3	1:B:3459:GLN:CG	2.30	0.56
1:A:4589:GLN:C	1:A:4590:LEU:HD12	2.31	0.56
1:B:4067:THR:HG21	1:B:4083:ALA:HB1	1.87	0.56
1:B:4560:VAL:HG12	1:B:4563:LEU:HD11	1.88	0.56
1:A:1644:SER:HA	1:A:1650:LEU:HD11	1.88	0.56
1:B:4589:GLN:C	1:B:4590:LEU:HD12	2.31	0.56
1:A:3822:HIS:HB3	1:A:3825:TYR:CE1	2.41	0.56
1:A:4186:PHE:CZ	1:A:4265:LEU:CD1	2.77	0.56
1:B:1644:SER:HA	1:B:1650:LEU:HD11	1.88	0.56
1:B:4507:ILE:CD1	1:B:4509:VAL:CG2	2.84	0.56
1:B:2626:THR:O	1:B:2627:THR:CG2	2.53	0.56
1:A:2571:THR:HG21	1:A:2747:ILE:HG12	1.87	0.55
1:B:2994:MET:CE	1:B:3008:MET:SD	2.94	0.55
1:B:4561:THR:HG22	1:B:4587:LEU:HD13	1.88	0.55
1:A:2091:ARG:CZ	2:A:4801:ADP:H5'2	2.36	0.55
1:B:2609:LEU:HD11	1:B:2615:MET:HB3	1.83	0.55
1:B:2591:LEU:HG	1:B:2709:VAL:HG12	1.88	0.55
1:A:1830:ILE:CG2	1:A:1831:ASP:N	2.69	0.55
1:A:4561:THR:HG22	1:A:4587:LEU:HD13	1.88	0.55
1:B:2464:GLN:HG2	1:B:2583:THR:CG2	2.32	0.55
1:A:2091:ARG:HH11	2:A:4801:ADP:H5'2	1.71	0.55
1:A:2897:LEU:HD23	1:A:2901:TYR:OH	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1892:MET:O	1:B:1896:LEU:HD13	2.05	0.55
1:A:1765:ALA:CB	1:A:1778:LEU:HD23	2.37	0.55
1:B:2897:LEU:HD23	1:B:2901:TYR:OH	2.07	0.55
1:A:2994:MET:CE	1:A:3008:MET:SD	2.94	0.55
1:B:1830:ILE:CG2	1:B:1831:ASP:N	2.69	0.55
1:B:3082:SER:OG	1:B:3085:LEU:CD1	2.53	0.55
1:B:4395:LEU:HD21	1:B:4483:SER:HA	1.88	0.55
1:A:2609:LEU:HD11	1:A:2615:MET:HB3	1.83	0.55
1:A:4560:VAL:HG12	1:A:4563:LEU:HD11	1.88	0.55
1:B:3822:HIS:HB3	1:B:3825:TYR:CE1	2.41	0.55
1:B:4424:LEU:HD11	1:B:4486:ILE:HD13	1.86	0.55
1:A:3236:ALA:HB1	1:A:3451:TYR:HE1	1.72	0.55
1:A:4186:PHE:HZ	1:A:4265:LEU:HD12	1.71	0.54
1:B:2091:ARG:CZ	2:B:4801:ADP:H5'2	2.36	0.54
1:A:2220:LEU:CD2	1:A:2342:MET:HE2	2.37	0.54
1:A:4395:LEU:HD21	1:A:4483:SER:HA	1.88	0.54
1:B:4560:VAL:HG12	1:B:4563:LEU:CD1	2.38	0.54
1:B:1765:ALA:CB	1:B:1778:LEU:HD23	2.37	0.54
1:B:3818:LEU:O	1:B:3821:ILE:HG22	2.06	0.54
1:A:2457:SER:CA	1:A:2584:TRP:CH2	2.91	0.54
1:A:2893:VAL:O	1:A:2897:LEU:HD13	2.07	0.54
1:A:4560:VAL:HG12	1:A:4563:LEU:CD1	2.38	0.54
1:B:3030:MET:HE3	1:B:3050:LEU:HD23	1.90	0.54
1:A:4067:THR:HG21	1:A:4083:ALA:CB	2.37	0.54
1:B:2893:VAL:O	1:B:2897:LEU:HD13	2.07	0.54
1:B:3818:LEU:HA	1:B:4346:MET:HE1	1.90	0.54
1:A:2192:THR:OG1	1:A:2373:MET:HG3	2.07	0.54
1:A:2312:VAL:HG11	1:A:2355:THR:CG2	2.38	0.54
1:A:2464:GLN:OE1	1:A:2586:ALA:HB3	2.08	0.54
1:A:2552:VAL:HG23	1:A:2552:VAL:O	2.08	0.54
1:B:2464:GLN:OE1	1:B:2586:ALA:HB3	2.08	0.54
1:B:3150:VAL:O	1:B:3153:THR:OG1	2.25	0.54
1:B:3745:LEU:HD11	1:B:3773:LEU:HA	1.89	0.54
1:B:3822:HIS:C	1:B:3823:PHE:CG	2.86	0.54
1:A:2295:LEU:HA	1:A:2338:ASN:ND2	2.23	0.54
1:A:4086:THR:O	1:A:4090:SER:N	2.37	0.54
1:B:2767:GLU:N	1:B:2768:PRO:HD2	2.23	0.54
1:A:3030:MET:HE3	1:A:3050:LEU:HD23	1.90	0.54
1:A:3745:LEU:HD11	1:A:3773:LEU:HA	1.89	0.54
1:B:2220:LEU:CD2	1:B:2342:MET:HE2	2.37	0.54
1:B:1765:ALA:HB3	1:B:1778:LEU:HD23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2295:LEU:HA	1:B:2338:ASN:ND2	2.23	0.53
1:B:3222:LEU:HD12	1:B:3465:LEU:HD23	1.90	0.53
1:B:4067:THR:HG21	1:B:4083:ALA:CB	2.37	0.53
1:A:2767:GLU:N	1:A:2768:PRO:HD2	2.23	0.53
1:A:3639:GLU:CD	1:A:4137:ASN:HD21	2.11	0.53
1:A:2540:SER:OG	1:A:2544:GLU:O	2.16	0.53
1:A:3150:VAL:O	1:A:3153:THR:OG1	2.25	0.53
1:A:1765:ALA:HB3	1:A:1778:LEU:HD23	1.89	0.53
1:A:2265:TYR:CD2	1:A:2314:ASN:ND2	2.76	0.53
1:A:2549:GLN:HG3	1:A:2572:LEU:CD1	2.29	0.53
1:A:3818:LEU:HA	1:A:4346:MET:HE1	1.90	0.53
1:B:1879:LEU:CD1	1:B:1914:GLU:O	2.55	0.53
1:B:2552:VAL:HG23	1:B:2552:VAL:O	2.08	0.53
1:B:4622:VAL:HG11	1:B:4624:PHE:HZ	1.69	0.53
1:B:2091:ARG:HH11	2:B:4801:ADP:H5'2	1.71	0.53
1:A:2182:LEU:HD11	1:A:2207:VAL:HG11	1.91	0.53
1:A:3175:HIS:CD2	1:A:3585:ARG:CZ	2.92	0.53
1:B:2192:THR:OG1	1:B:2373:MET:HG3	2.07	0.53
1:B:3205:LEU:O	1:B:3208:ILE:HG22	2.09	0.53
1:A:2464:GLN:HG2	1:A:2583:THR:CG2	2.32	0.53
1:B:2457:SER:CA	1:B:2584:TRP:CH2	2.91	0.53
1:A:2238:LEU:HD13	1:A:2300:TRP:CE3	2.44	0.53
1:A:2584:TRP:HZ3	1:A:2732:PRO:HG3	1.60	0.53
1:A:2612:LEU:HD13	1:A:2615:MET:HE3	1.90	0.53
1:A:3811:ILE:CD1	1:A:3887:LEU:CD2	2.87	0.53
1:B:2046:ARG:HA	1:B:2049:ILE:HG22	1.90	0.53
1:B:2238:LEU:HD13	1:B:2300:TRP:CE3	2.44	0.53
1:B:2591:LEU:C	1:B:2591:LEU:HD12	2.34	0.53
1:B:3236:ALA:HB1	1:B:3451:TYR:HE1	1.72	0.53
1:B:4607:LEU:CD2	1:B:4635:PHE:CE2	2.92	0.53
1:A:1762:VAL:O	1:A:1766:LEU:CD1	2.58	0.52
1:A:3205:LEU:O	1:A:3208:ILE:HG22	2.09	0.52
1:B:3236:ALA:HB1	1:B:3451:TYR:CE1	2.44	0.52
1:B:3749:LEU:HD13	1:B:3773:LEU:HD12	1.74	0.52
1:A:3822:HIS:C	1:A:3823:PHE:CG	2.86	0.52
1:B:2265:TYR:CD2	1:B:2314:ASN:ND2	2.76	0.52
1:B:2302:VAL:HG22	1:B:2342:MET:CB	2.31	0.52
1:A:2591:LEU:C	1:A:2591:LEU:HD12	2.34	0.52
1:B:3008:MET:HE1	1:B:3066:PHE:CZ	2.44	0.52
1:B:3175:HIS:CD2	1:B:3585:ARG:CZ	2.92	0.52
1:B:3882:THR:OG1	1:B:4342:LYS:NZ	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1825:LEU:HD12	1:A:1830:ILE:CD1	2.38	0.52
1:B:2345:VAL:HG11	1:B:2348:LEU:HD21	1.91	0.52
1:B:3010:THR:HG22	1:B:3016:GLU:O	2.10	0.52
1:A:1970:ALA:CB	1:A:4073:SER:HB2	2.40	0.52
1:A:2046:ARG:HA	1:A:2049:ILE:HG22	1.90	0.52
1:A:2584:TRP:CH2	1:A:2732:PRO:HB3	2.45	0.52
1:A:3236:ALA:HB1	1:A:3451:TYR:CE1	2.44	0.52
1:A:3459:GLN:CG	1:B:3456:SER:HG	2.18	0.52
1:B:1969:SER:O	1:B:1972:SER:OG	2.21	0.52
1:B:2312:VAL:HG11	1:B:2355:THR:CG2	2.38	0.52
1:A:4607:LEU:CD2	1:A:4635:PHE:CE2	2.92	0.52
1:B:3824:LEU:HD21	1:B:4130:ILE:HG12	1.92	0.52
1:A:2091:ARG:CZ	2:A:4801:ADP:H4'	2.40	0.52
1:A:2345:VAL:HG11	1:A:2348:LEU:HD21	1.91	0.52
1:A:3008:MET:HE1	1:A:3066:PHE:CZ	2.44	0.52
1:A:3222:LEU:HD12	1:A:3465:LEU:HD23	1.90	0.52
1:B:2182:LEU:HD11	1:B:2207:VAL:HG11	1.91	0.52
1:B:2307:VAL:HG13	1:B:2312:VAL:HG21	1.92	0.52
1:A:2302:VAL:HG22	1:A:2342:MET:CB	2.31	0.52
1:A:3102:LEU:O	1:A:3105:VAL:HG12	2.10	0.52
1:B:2091:ARG:CZ	2:B:4801:ADP:H4'	2.40	0.52
1:A:2230:LYS:NZ	3:A:4802:ATP:O3G	2.43	0.51
1:A:2549:GLN:CG	1:A:2572:LEU:HD22	2.40	0.51
1:A:2648:VAL:HG11	1:A:2694:ARG:NH2	2.26	0.51
1:A:3882:THR:OG1	1:A:4342:LYS:NZ	2.35	0.51
1:B:3068:MET:HE3	1:B:3075:LEU:HD12	1.91	0.51
1:B:3811:ILE:CD1	1:B:3887:LEU:CD2	2.87	0.51
1:B:2078:GLU:OE1	1:B:4522:THR:CG2	2.58	0.51
1:A:1490:TRP:CG	1:A:1538:ILE:HD12	2.45	0.51
1:A:2588:HIS:HA	1:A:2707:GLN:HE22	1.76	0.51
1:A:2849:ASN:O	1:A:2852:THR:HG22	2.11	0.51
1:A:3021:PHE:CG	1:A:3029:LEU:CD1	2.93	0.51
1:B:1970:ALA:CB	1:B:4073:SER:HB2	2.40	0.51
1:A:4186:PHE:HE2	1:A:4252:TYR:CG	2.28	0.51
1:A:4622:VAL:HG11	1:A:4624:PHE:HZ	1.70	0.51
1:B:2584:TRP:CH2	1:B:2732:PRO:HB3	2.45	0.51
1:B:2584:TRP:CH2	1:B:2732:PRO:CB	2.93	0.51
1:B:4042:LEU:CD2	1:B:4139:LEU:HD23	2.41	0.51
1:A:3068:MET:HE3	1:A:3075:LEU:HD12	1.91	0.51
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.75	0.51
1:A:4609:VAL:HG23	1:A:4622:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1750:VAL:HG12	1:A:1811:LEU:HD13	1.93	0.51
1:B:1750:VAL:HG12	1:B:1811:LEU:HD13	1.93	0.51
1:B:2605:LEU:HD21	1:B:2662:PHE:HD1	1.75	0.51
1:B:3021:PHE:CG	1:B:3029:LEU:CD1	2.93	0.51
1:B:4186:PHE:HE2	1:B:4252:TYR:CG	2.28	0.51
1:A:2612:LEU:HD13	1:A:2615:MET:HE2	1.93	0.51
1:B:2149:LEU:HD11	1:B:2157:LEU:CD2	2.40	0.51
1:B:2230:LYS:NZ	3:B:4802:ATP:O3G	2.43	0.51
1:B:2612:LEU:HD13	1:B:2615:MET:HE3	1.90	0.51
1:A:2307:VAL:HG13	1:A:2312:VAL:HG21	1.92	0.51
1:A:2584:TRP:CH2	1:A:2732:PRO:CB	2.93	0.51
1:B:2612:LEU:HD13	1:B:2615:MET:HE2	1.93	0.51
1:B:4609:VAL:HG23	1:B:4622:VAL:HG23	1.93	0.51
1:B:1490:TRP:CG	1:B:1538:ILE:HD12	2.45	0.51
1:B:1762:VAL:O	1:B:1766:LEU:CD1	2.57	0.51
1:B:2540:SER:OG	1:B:2544:GLU:O	2.16	0.51
1:B:2588:HIS:HA	1:B:2707:GLN:HE22	1.76	0.51
1:B:2648:VAL:HG11	1:B:2694:ARG:NH2	2.26	0.51
1:B:3021:PHE:CG	1:B:3029:LEU:HD13	2.46	0.51
1:B:3102:LEU:O	1:B:3105:VAL:HG12	2.10	0.51
1:B:4507:ILE:HD12	1:B:4509:VAL:HG22	1.93	0.51
1:B:4560:VAL:CG1	1:B:4563:LEU:HD11	2.41	0.51
1:B:4622:VAL:CG1	1:B:4624:PHE:HE2	2.15	0.51
1:A:2593:LEU:HD11	1:A:2605:LEU:HB2	1.93	0.50
1:A:4607:LEU:HD21	1:A:4635:PHE:CE2	2.41	0.50
1:B:1752:LEU:CD2	1:B:1756:ILE:HD11	2.41	0.50
1:B:2549:GLN:CG	1:B:2572:LEU:HD22	2.41	0.50
1:A:1752:LEU:CD2	1:A:1756:ILE:HD11	2.41	0.50
1:A:2593:LEU:CD2	1:A:2734:VAL:CG2	2.89	0.50
1:A:4622:VAL:HG12	1:A:4624:PHE:CZ	2.28	0.50
1:B:3888:ALA:HB1	1:B:4012:ASN:HD22	1.75	0.50
1:B:4186:PHE:HZ	1:B:4265:LEU:HD12	1.71	0.50
1:A:3010:THR:HG22	1:A:3016:GLU:O	2.10	0.50
1:A:3021:PHE:CG	1:A:3029:LEU:HD13	2.46	0.50
1:A:3097:TRP:CE3	1:A:3173:PRO:HB3	2.47	0.50
1:A:1879:LEU:CD1	1:A:1914:GLU:O	2.55	0.50
1:B:2849:ASN:O	1:B:2852:THR:HG22	2.11	0.50
1:A:3521:ASP:OD1	1:A:3702:THR:HG21	2.11	0.50
1:A:4560:VAL:CG1	1:A:4563:LEU:HD11	2.41	0.50
1:A:2072:PHE:CZ	1:A:2157:LEU:HD11	2.45	0.50
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3824:LEU:HD21	1:A:4130:ILE:HG12	1.92	0.50
1:A:1537:TRP:CH2	1:A:1578:LEU:HD21	2.47	0.50
1:A:4042:LEU:CD2	1:A:4139:LEU:HD23	2.41	0.50
1:A:2472:TYR:CD2	1:A:2481:MET:HE2	2.47	0.50
1:A:3456:SER:HG	1:B:3459:GLN:HG3	1.65	0.50
1:B:1537:TRP:CH2	1:B:1578:LEU:HD21	2.47	0.50
1:B:2961:ILE:HD11	1:B:2998:ASN:HB3	1.93	0.49
1:A:3821:ILE:HG23	1:A:3822:HIS:N	2.28	0.49
1:B:3097:TRP:CE3	1:B:3173:PRO:HB3	2.47	0.49
1:B:4447:TYR:CE2	1:B:4451:LEU:HD11	2.47	0.49
1:A:2078:GLU:OE1	1:A:4522:THR:CG2	2.58	0.49
1:B:2472:TYR:CD2	1:B:2481:MET:HE2	2.47	0.49
1:B:3478:LEU:CD1	1:B:3770:LEU:HD13	2.43	0.49
1:B:3521:ASP:OD1	1:B:3702:THR:HG21	2.11	0.49
1:A:1792:LEU:HD13	1:A:1812:ILE:HG13	1.95	0.49
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.94	0.49
1:A:4507:ILE:HD12	1:A:4509:VAL:HG22	1.93	0.49
1:A:3208:ILE:HD12	1:A:3482:LEU:HB3	1.95	0.49
1:A:3680:SER:O	1:A:3681:THR:HG23	2.12	0.49
1:A:3708:LEU:HD21	1:A:3809:SER:HA	1.93	0.49
1:B:1792:LEU:HD13	1:B:1812:ILE:HG13	1.95	0.49
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.94	0.49
1:A:3008:MET:HE2	1:A:3066:PHE:HZ	1.72	0.49
1:B:2493:TYR:HA	1:B:2539:VAL:HG11	1.95	0.49
1:B:3008:MET:HE2	1:B:3066:PHE:HZ	1.72	0.49
1:B:3821:ILE:HG23	1:B:3822:HIS:N	2.28	0.49
1:A:2457:SER:HA	1:A:2584:TRP:CH2	2.47	0.49
1:A:2580:LEU:C	1:A:2584:TRP:HD1	2.17	0.49
1:A:4434:VAL:HA	1:A:4437:VAL:HG22	1.95	0.49
1:B:2072:PHE:CZ	1:B:2157:LEU:HD11	2.45	0.49
1:B:2457:SER:HA	1:B:2584:TRP:CH2	2.47	0.49
1:B:2593:LEU:HD11	1:B:2605:LEU:HB2	1.93	0.49
1:A:3509:LEU:HB3	1:A:3529:PHE:CE1	2.48	0.49
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	1.95	0.49
1:B:3208:ILE:HD12	1:B:3482:LEU:HB3	1.95	0.49
1:B:3572:LEU:HD23	1:B:3572:LEU:C	2.38	0.49
1:A:2662:PHE:CZ	1:A:2711:ALA:HB2	2.48	0.48
1:B:1825:LEU:HD12	1:B:1830:ILE:CD1	2.38	0.48
1:A:2585:LEU:HB2	1:A:2612:LEU:HD11	1.95	0.48
1:B:2551:LYS:C	1:B:2551:LYS:CD	2.86	0.48
1:B:3509:LEU:HB3	1:B:3529:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3680:SER:O	1:B:3681:THR:HG23	2.13	0.48
1:B:3683:ASP:CG	1:B:4137:ASN:OD1	2.56	0.48
1:B:4635:PHE:CZ	1:B:4640:VAL:HB	2.48	0.48
1:A:2605:LEU:HD21	1:A:2662:PHE:HD1	1.75	0.48
1:A:3572:LEU:C	1:A:3572:LEU:HD23	2.38	0.48
1:A:4635:PHE:CZ	1:A:4640:VAL:HB	2.48	0.48
1:B:2580:LEU:C	1:B:2584:TRP:HD1	2.17	0.48
1:B:2662:PHE:CZ	1:B:2711:ALA:HB2	2.48	0.48
1:B:4434:VAL:HA	1:B:4437:VAL:HG22	1.95	0.48
1:A:3745:LEU:HD22	1:A:3776:GLU:CB	2.44	0.48
1:B:4248:ALA:HB1	1:B:4266:ASN:OD1	2.14	0.48
1:A:2230:LYS:N	3:A:4802:ATP:O1B	2.46	0.48
1:A:3638:VAL:H	1:A:3681:THR:HG22	1.79	0.48
1:B:4609:VAL:CG2	1:B:4622:VAL:CG2	2.92	0.48
1:A:4447:TYR:CE2	1:A:4451:LEU:HD11	2.47	0.48
1:B:2626:THR:HG22	1:B:2679:VAL:HG21	1.96	0.48
1:A:2602:THR:HG22	1:A:2662:PHE:CZ	2.49	0.48
1:A:4622:VAL:CG1	1:A:4624:PHE:HE2	2.15	0.48
1:B:3745:LEU:HD22	1:B:3776:GLU:CB	2.44	0.48
1:A:2493:TYR:HA	1:A:2539:VAL:HG11	1.95	0.48
1:A:3021:PHE:CD1	1:A:3029:LEU:CD1	2.97	0.48
1:B:2668:LEU:N	1:B:2669:PRO:CD	2.77	0.48
1:B:3811:ILE:HD12	1:B:3887:LEU:CD2	2.44	0.48
1:B:4041:VAL:HG11	1:B:4125:PHE:CE2	2.49	0.48
1:B:4186:PHE:CZ	1:B:4265:LEU:HD12	2.48	0.48
1:A:2069:ILE:HD12	1:A:2137:LEU:HD21	1.96	0.47
1:A:3683:ASP:CG	1:A:4137:ASN:OD1	2.56	0.47
1:A:4041:VAL:HG11	1:A:4125:PHE:CE2	2.49	0.47
1:B:2585:LEU:HB2	1:B:2612:LEU:HD11	1.95	0.47
1:B:2599:SER:N	2:B:4804:ADP:O2A	2.43	0.47
1:B:3021:PHE:CD1	1:B:3029:LEU:CD1	2.97	0.47
1:B:3638:VAL:H	1:B:3681:THR:HG22	1.79	0.47
1:B:4247:MET:CE	1:B:4252:TYR:CE2	2.86	0.47
1:A:4609:VAL:CG2	1:A:4622:VAL:CG2	2.92	0.47
1:B:2602:THR:HG22	1:B:2662:PHE:CZ	2.49	0.47
1:B:3509:LEU:HD21	1:B:3536:LEU:HD12	1.96	0.47
1:A:2149:LEU:HD11	1:A:2157:LEU:CD2	2.40	0.47
1:A:2635:PHE:CZ	1:A:2686:MET:HE1	2.50	0.47
1:B:1778:LEU:HD13	1:B:1830:ILE:CD1	2.40	0.47
1:B:2635:PHE:CZ	1:B:2686:MET:HE1	2.50	0.47
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2551:LYS:C	1:A:2551:LYS:CD	2.86	0.47
1:A:2729:ARG:NH1	3:A:4802:ATP:O1G	2.40	0.47
1:A:4387:TRP:CZ3	1:A:4391:ILE:HD13	2.49	0.47
1:B:2230:LYS:N	3:B:4802:ATP:O1B	2.46	0.47
1:B:2295:LEU:C	1:B:2338:ASN:ND2	2.72	0.47
1:B:2729:ARG:NH1	3:B:4802:ATP:O1G	2.40	0.47
1:B:3824:LEU:HD22	1:B:4130:ILE:CG2	2.45	0.47
1:B:4042:LEU:HD12	1:B:4126:LEU:HB2	1.95	0.47
1:A:2191:LEU:HD22	3:A:4802:ATP:C5	2.50	0.47
1:A:4508:HIS:ND1	1:A:4587:LEU:CD2	2.77	0.47
1:B:1766:LEU:HD12	1:B:1778:LEU:HD21	1.96	0.47
1:B:2231:SER:OG	1:B:2344:GLU:OE2	2.32	0.47
1:B:4508:HIS:ND1	1:B:4587:LEU:CD2	2.77	0.47
1:A:4247:MET:CE	1:A:4252:TYR:CE2	2.86	0.47
1:A:4248:ALA:HB1	1:A:4266:ASN:OD1	2.14	0.47
1:B:2069:ILE:HD12	1:B:2137:LEU:HD21	1.96	0.47
1:A:2154:ILE:N	1:A:2155:PRO:CD	2.78	0.47
1:A:3554:SER:HB2	1:A:3578:ILE:HD12	1.96	0.47
1:A:4042:LEU:HD12	1:A:4126:LEU:HB2	1.95	0.47
1:A:4566:GLN:HE21	1:A:4643:LEU:HD11	1.80	0.47
1:B:2154:ILE:N	1:B:2155:PRO:CD	2.78	0.47
1:B:2191:LEU:HD22	3:B:4802:ATP:C5	2.50	0.47
1:B:3478:LEU:HD22	1:B:3770:LEU:HD13	1.96	0.47
1:B:3716:VAL:HG21	1:B:3804:LEU:HD23	1.95	0.47
1:B:4387:TRP:CZ3	1:B:4391:ILE:HD13	2.49	0.47
1:A:1541:GLN:O	1:A:1545:VAL:HG23	2.15	0.47
1:A:2626:THR:HG22	1:A:2679:VAL:HG21	1.96	0.47
1:A:3478:LEU:HD22	1:A:3770:LEU:HD13	1.96	0.47
1:B:3554:SER:HB2	1:B:3578:ILE:HD12	1.96	0.47
1:A:1766:LEU:HD12	1:A:1778:LEU:HD21	1.96	0.47
1:A:4427:VAL:O	1:A:4431:LEU:HG	2.15	0.47
1:B:3522:GLN:HB2	1:B:3704:THR:HG22	1.97	0.47
1:B:3888:ALA:HA	1:B:4013:LEU:HD21	1.97	0.47
1:A:2668:LEU:N	1:A:2669:PRO:CD	2.77	0.47
1:A:3478:LEU:CD1	1:A:3770:LEU:HD22	2.45	0.47
1:A:3645:LEU:HD23	1:A:3648:VAL:HB	1.97	0.47
1:B:2922:ILE:HD12	1:B:2933:LEU:HD21	1.96	0.47
1:A:3888:ALA:HA	1:A:4013:LEU:HD21	1.97	0.46
1:B:1504:VAL:HG11	1:B:1524:GLU:HB2	1.97	0.46
1:B:2103:VAL:HG13	1:B:2136:ILE:CG2	2.46	0.46
1:A:2308:ASP:OD2	1:A:2310:GLU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2752:ASN:HD22	1:B:2770:THR:HG22	1.76	0.46
1:A:3811:ILE:HD12	1:A:3887:LEU:CD2	2.44	0.46
1:A:4507:ILE:HD12	1:A:4509:VAL:CG2	2.46	0.46
1:B:2863:ARG:C	1:B:2863:ARG:CD	2.87	0.46
1:B:2958:VAL:HG13	1:B:2993:ILE:HG12	1.98	0.46
1:B:4427:VAL:O	1:B:4431:LEU:HG	2.15	0.46
1:A:2058:GLY:O	1:A:2104:LYS:CE	2.61	0.46
1:A:2295:LEU:C	1:A:2338:ASN:ND2	2.72	0.46
1:A:3509:LEU:HD21	1:A:3536:LEU:HD12	1.96	0.46
1:A:4183:LEU:CD1	1:A:4247:MET:HE1	2.46	0.46
1:A:2922:ILE:HD12	1:A:2933:LEU:HD21	1.96	0.46
1:A:3478:LEU:CD1	1:A:3770:LEU:HD13	2.43	0.46
1:A:3824:LEU:HD22	1:A:4130:ILE:CG2	2.45	0.46
1:B:3645:LEU:HD23	1:B:3648:VAL:HB	1.97	0.46
1:A:4387:TRP:CH2	1:A:4391:ILE:HG21	2.51	0.46
1:B:2191:LEU:HD23	1:B:2377:ASN:ND2	2.30	0.46
1:B:4566:GLN:HE21	1:B:4643:LEU:HD11	1.80	0.46
1:A:2103:VAL:HG13	1:A:2136:ILE:CG2	2.46	0.46
1:B:3478:LEU:CD1	1:B:3770:LEU:HD22	2.45	0.46
1:B:3817:SER:OG	1:B:4349:LEU:HD13	2.10	0.46
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.97	0.46
1:B:1541:GLN:O	1:B:1545:VAL:HG23	2.15	0.46
1:B:3203:VAL:O	1:B:3207:LYS:N	2.47	0.46
1:B:1792:LEU:HD22	1:B:1808:LEU:HD22	1.97	0.46
1:B:4607:LEU:HD12	1:B:4624:PHE:CE2	2.51	0.46
1:A:3522:GLN:HB2	1:A:3704:THR:HG22	1.97	0.46
1:A:3683:ASP:CB	1:A:4137:ASN:OD1	2.64	0.46
1:B:3683:ASP:CB	1:B:4137:ASN:OD1	2.64	0.46
1:A:2304:ASP:OD1	1:A:2684:ARG:NH2	2.47	0.45
1:A:2958:VAL:HG13	1:A:2993:ILE:HG12	1.98	0.45
1:A:3745:LEU:HD22	1:A:3776:GLU:HB2	1.98	0.45
1:B:2058:GLY:O	1:B:2104:LYS:CE	2.61	0.45
1:B:2308:ASP:OD2	1:B:2310:GLU:HB3	2.16	0.45
1:B:3745:LEU:HD11	1:B:3773:LEU:HD22	1.98	0.45
1:A:1778:LEU:HD13	1:A:1830:ILE:CD1	2.40	0.45
1:A:2191:LEU:HD23	1:A:2377:ASN:ND2	2.30	0.45
1:A:4186:PHE:CZ	1:A:4265:LEU:HD12	2.48	0.45
1:A:3814:THR:OG1	1:A:3890:ILE:HD11	2.16	0.45
1:A:3817:SER:OG	1:A:4349:LEU:HD13	2.10	0.45
1:B:4387:TRP:CH2	1:B:4391:ILE:HG21	2.51	0.45
1:B:4507:ILE:HD12	1:B:4509:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3675:PHE:C	1:A:3676:VAL:HG13	2.41	0.45
1:B:3717:LEU:HD11	1:B:3797:VAL:HG11	1.99	0.45
1:A:2254:ILE:HG12	1:A:2279:LEU:HD21	1.98	0.45
1:B:1931:ASN:HD22	1:B:2317:SER:CA	2.26	0.45
1:A:1931:ASN:HD22	1:A:2317:SER:N	2.15	0.45
1:A:2213:ILE:CG2	1:A:2220:LEU:HD13	2.47	0.45
1:A:4607:LEU:HD12	1:A:4624:PHE:CE2	2.51	0.45
1:B:2079:GLN:OE1	1:B:4526:GLN:NE2	2.47	0.45
1:A:2709:VAL:HG23	1:A:2709:VAL:O	2.17	0.45
1:A:3745:LEU:HD11	1:A:3773:LEU:HD22	1.98	0.45
1:B:1985:HIS:CD2	1:B:1997:ILE:HD12	2.52	0.45
1:B:2213:ILE:CG2	1:B:2220:LEU:HD13	2.47	0.45
1:B:2254:ILE:HG12	1:B:2279:LEU:HD21	1.98	0.45
1:B:3871:VAL:HG11	1:B:3883:PHE:CE2	2.52	0.45
1:A:1792:LEU:HD22	1:A:1808:LEU:HD22	1.97	0.45
1:A:3871:VAL:HG11	1:A:3883:PHE:CE2	2.52	0.45
1:B:3814:THR:OG1	1:B:3890:ILE:HD11	2.16	0.45
1:B:4178:ARG:HG2	1:B:4278:PHE:CE1	2.52	0.45
1:B:4183:LEU:CD1	1:B:4247:MET:HE1	2.46	0.45
1:A:3680:SER:O	1:A:3681:THR:CG2	2.65	0.45
1:A:3801:TYR:CD1	1:A:3856:LEU:HD22	2.52	0.45
1:B:4240:TRP:CZ3	1:B:4273:PHE:O	2.70	0.45
1:A:2568:VAL:CG2	1:A:2603:MET:HE2	2.47	0.45
1:A:3203:VAL:O	1:A:3207:LYS:N	2.47	0.45
1:A:3822:HIS:NE2	1:A:3876:LEU:CD1	2.79	0.45
1:A:4097:LYS:HA	1:A:4127:THR:HG22	1.98	0.45
1:B:2593:LEU:CD2	1:B:2734:VAL:CG2	2.89	0.45
1:B:3822:HIS:NE2	1:B:3876:LEU:CD1	2.79	0.45
1:B:4088:VAL:HG22	1:B:4122:PHE:CE2	2.52	0.45
1:B:4097:LYS:HA	1:B:4127:THR:HG22	1.98	0.45
1:A:4178:ARG:HG2	1:A:4278:PHE:CE1	2.52	0.44
1:B:2569:VAL:O	1:B:2569:VAL:HG13	2.17	0.44
1:B:3102:LEU:HB3	1:B:3148:VAL:HG22	1.99	0.44
1:A:2458:LEU:HD13	1:A:2498:ILE:HG22	1.99	0.44
1:B:2515:GLY:HA2	1:B:2534:ILE:HD12	1.99	0.44
1:A:2358:ARG:HH22	2:A:4801:ADP:PB	2.40	0.44
1:A:2453:ARG:HD2	1:A:2733:VAL:HG12	2.00	0.44
1:A:2515:GLY:HA2	1:A:2534:ILE:HD12	1.99	0.44
1:A:3567:LEU:HB2	1:A:3599:PHE:CD1	2.52	0.44
1:A:4042:LEU:HD11	1:A:4128:MET:CE	2.47	0.44
1:B:2622:PHE:CE2	1:B:2679:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2320:ASP:CG	1:A:2321:ASP:N	2.76	0.44
1:A:2766:ALA:O	1:A:2770:THR:HG23	2.18	0.44
1:A:4088:VAL:HG22	1:A:4122:PHE:CE2	2.52	0.44
1:A:4508:HIS:ND1	1:A:4587:LEU:HD21	2.33	0.44
1:B:1931:ASN:ND2	1:B:2317:SER:N	2.65	0.44
1:B:3745:LEU:HD22	1:B:3776:GLU:HB2	1.98	0.44
1:A:1931:ASN:HD22	1:A:2317:SER:CA	2.27	0.44
1:A:1985:HIS:CD2	1:A:1997:ILE:HD12	2.52	0.44
1:A:3822:HIS:O	1:A:3822:HIS:CG	2.71	0.44
1:B:2304:ASP:OD1	1:B:2684:ARG:NH2	2.47	0.44
1:B:2358:ARG:NH2	2:B:4801:ADP:PB	2.89	0.44
1:B:3567:LEU:HB2	1:B:3599:PHE:CD1	2.52	0.44
1:B:3675:PHE:C	1:B:3676:VAL:HG13	2.41	0.44
1:A:2358:ARG:NH2	2:A:4801:ADP:PB	2.89	0.44
1:A:2874:SER:OG	1:A:2875:ASN:N	2.51	0.44
1:A:3717:LEU:HD11	1:A:3797:VAL:HG11	1.99	0.44
1:A:4612:ASN:C	1:A:4643:LEU:HD22	2.43	0.44
1:A:2605:LEU:HD23	1:A:2662:PHE:CD1	2.44	0.44
1:A:2622:PHE:CE2	1:A:2679:VAL:HG11	2.52	0.44
1:A:3102:LEU:HB3	1:A:3148:VAL:HG22	1.99	0.44
1:B:1861:MET:HE2	1:B:1890:LEU:HA	2.00	0.44
1:B:1931:ASN:HD22	1:B:2317:SER:N	2.15	0.44
1:B:2358:ARG:HH22	2:B:4801:ADP:PB	2.40	0.44
1:B:2453:ARG:HD2	1:B:2733:VAL:HG12	2.00	0.44
1:B:2874:SER:OG	1:B:2875:ASN:N	2.51	0.44
1:B:3680:SER:O	1:B:3681:THR:CG2	2.65	0.44
1:B:4609:VAL:CG2	1:B:4622:VAL:HG23	2.48	0.44
1:B:4612:ASN:C	1:B:4643:LEU:HD22	2.43	0.44
1:B:1879:LEU:HD21	1:B:1914:GLU:CG	2.47	0.44
1:B:2569:VAL:HG11	1:B:2747:ILE:HG23	1.99	0.44
1:B:4508:HIS:ND1	1:B:4587:LEU:HD21	2.33	0.44
1:A:2079:GLN:OE1	1:A:4526:GLN:NE2	2.47	0.44
1:A:2568:VAL:CG2	1:A:2603:MET:CE	2.95	0.44
1:A:3609:ILE:HG12	1:A:3632:PRO:HG2	1.99	0.44
1:A:4240:TRP:CZ3	1:A:4273:PHE:O	2.70	0.44
1:B:3708:LEU:HD21	1:B:3809:SER:HA	1.93	0.44
1:B:3801:TYR:CD1	1:B:3856:LEU:HD22	2.52	0.44
1:A:2284:LEU:HB3	1:A:2333:LEU:HD13	2.00	0.43
1:A:3822:HIS:CB	1:A:3825:TYR:CZ	3.01	0.43
1:B:1550:ILE:HD13	1:B:1638:LEU:HD22	2.00	0.43
1:B:3609:ILE:HG12	1:B:3632:PRO:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3822:HIS:O	1:B:3822:HIS:CG	2.71	0.43
1:A:1879:LEU:HD21	1:A:1914:GLU:CG	2.47	0.43
1:A:2335:LEU:HD11	1:A:2341:ILE:HD11	2.00	0.43
1:A:2863:ARG:C	1:A:2863:ARG:CD	2.87	0.43
1:A:2871:ILE:HG23	1:A:2871:ILE:O	2.18	0.43
1:B:2335:LEU:HD11	1:B:2341:ILE:HD11	2.00	0.43
1:B:2709:VAL:HG23	1:B:2709:VAL:O	2.17	0.43
1:B:2910:VAL:CG1	1:B:3105:VAL:HG23	2.47	0.43
1:B:3832:PHE:O	1:B:3835:ILE:HB	2.18	0.43
1:A:2519:ARG:HA	1:A:2526:LEU:CD1	2.49	0.43
1:B:2568:VAL:CG2	1:B:2603:MET:CE	2.95	0.43
1:B:3822:HIS:CB	1:B:3825:TYR:CZ	3.01	0.43
1:A:1931:ASN:ND2	1:A:2317:SER:N	2.65	0.43
1:A:3832:PHE:O	1:A:3835:ILE:HB	2.18	0.43
1:B:2320:ASP:CG	1:B:2321:ASP:N	2.76	0.43
1:B:2571:THR:OG1	1:B:2574:THR:OG1	2.06	0.43
1:B:3574:THR:O	1:B:3578:ILE:HG12	2.19	0.43
1:A:2569:VAL:HG11	1:A:2747:ILE:HG23	1.99	0.43
1:A:2635:PHE:CE1	1:A:2706:ILE:HD13	2.54	0.43
1:A:3825:TYR:CE2	1:A:3875:MET:SD	3.12	0.43
1:B:1818:GLN:O	1:B:1822:THR:HG23	2.19	0.43
1:A:1818:GLN:O	1:A:1822:THR:HG23	2.19	0.43
1:A:1923:LEU:HD12	1:A:1954:TRP:CZ2	2.53	0.43
1:A:2302:VAL:HG12	1:A:2303:PHE:N	2.33	0.43
1:A:2910:VAL:CG1	1:A:3105:VAL:HG23	2.47	0.43
1:B:2302:VAL:HG12	1:B:2303:PHE:N	2.33	0.43
1:B:2766:ALA:O	1:B:2770:THR:HG23	2.18	0.43
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	2.00	0.43
1:B:1526:LYS:O	1:B:1529:ARG:HG2	2.19	0.43
1:B:1632:VAL:HG13	1:B:1636:ASP:HB2	1.95	0.43
1:B:2284:LEU:HB3	1:B:2333:LEU:HD13	2.00	0.43
1:B:2568:VAL:CG2	1:B:2603:MET:HE2	2.47	0.43
1:B:3654:ARG:HB2	1:B:3661:LEU:HB2	2.01	0.43
1:A:1861:MET:HE2	1:A:1890:LEU:HA	2.00	0.43
1:A:1970:ALA:HB2	1:A:4073:SER:HB2	2.00	0.43
1:A:4609:VAL:CG2	1:A:4622:VAL:HG23	2.48	0.43
1:B:1970:ALA:HB2	1:B:4073:SER:HB2	2.00	0.43
1:B:4430:ASP:O	1:B:4434:VAL:HG12	2.19	0.43
1:A:2308:ASP:HB2	1:A:2309:PRO:HD2	2.00	0.43
1:A:2569:VAL:O	1:A:2569:VAL:HG13	2.17	0.43
1:A:3574:THR:O	1:A:3578:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4430:ASP:O	1:A:4434:VAL:HG12	2.19	0.43
1:B:1923:LEU:HD12	1:B:1954:TRP:CZ2	2.53	0.43
1:B:2458:LEU:HD13	1:B:2498:ILE:HG22	1.99	0.43
1:B:2519:ARG:HA	1:B:2526:LEU:CD1	2.49	0.43
1:B:2635:PHE:CE1	1:B:2706:ILE:HD13	2.54	0.43
1:B:3769:THR:O	1:B:3773:LEU:HG	2.19	0.43
1:B:3825:TYR:CE2	1:B:3875:MET:SD	3.12	0.43
1:A:1632:VAL:HG11	1:A:1636:ASP:CB	2.48	0.43
1:B:2461:MET:CE	1:B:2584:TRP:CZ2	2.98	0.43
1:A:2213:ILE:HG21	1:A:2220:LEU:HD13	2.01	0.42
1:A:2256:PRO:HB3	1:A:2264:LEU:HD22	2.00	0.42
1:A:4088:VAL:HG13	1:A:4118:PRO:CB	2.49	0.42
1:B:1713:LEU:HD22	1:B:1749:LEU:HD21	2.00	0.42
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	2.01	0.42
1:B:2213:ILE:HG21	1:B:2220:LEU:HD13	2.01	0.42
1:A:2234:TRP:HH2	1:A:2253:ILE:HD11	1.84	0.42
1:B:2319:LEU:HD13	1:B:2359:CYS:SG	2.59	0.42
1:B:2571:THR:HG22	1:B:2747:ILE:HG12	2.00	0.42
1:B:2871:ILE:HG23	1:B:2871:ILE:O	2.18	0.42
1:B:4088:VAL:HG13	1:B:4118:PRO:CB	2.49	0.42
1:A:1526:LYS:O	1:A:1529:ARG:HG2	2.19	0.42
1:A:2496:TYR:CZ	1:A:2500:TRP:CD1	3.08	0.42
1:A:3109:PHE:CD2	1:A:3180:ILE:HG21	2.54	0.42
1:B:2275:TRP:NE1	1:B:2277:ASP:OD1	2.53	0.42
1:B:3550:THR:OG1	1:B:3574:THR:HG21	2.19	0.42
1:A:2588:HIS:HB3	1:A:2658:TRP:CZ3	2.54	0.42
1:B:1961:ASN:ND2	1:B:2025:ARG:CB	2.82	0.42
1:B:2234:TRP:HH2	1:B:2253:ILE:HD11	1.84	0.42
1:B:2526:LEU:HA	1:B:2545:TRP:CZ3	2.54	0.42
1:B:2907:VAL:O	1:B:2907:VAL:HG23	2.20	0.42
1:B:4577:LEU:HD21	1:B:4635:PHE:HD1	1.84	0.42
1:A:1452:VAL:HG13	1:A:1512:TYR:CE1	2.55	0.42
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.53	0.42
1:A:3609:ILE:HG12	1:A:3632:PRO:HB2	2.01	0.42
1:B:2308:ASP:HB2	1:B:2309:PRO:HD2	2.00	0.42
1:B:2571:THR:O	1:B:2572:LEU:C	2.62	0.42
1:B:2626:THR:C	1:B:2627:THR:HG23	2.44	0.42
1:B:4529:ALA:O	1:B:4533:SER:N	2.52	0.42
1:A:1550:ILE:HD13	1:A:1638:LEU:HD22	2.00	0.42
1:A:2381:ARG:HG2	1:A:2385:ILE:HD11	2.02	0.42
1:B:1452:VAL:HG13	1:B:1512:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4609:VAL:CG2	1:B:4622:VAL:HG21	2.50	0.42
1:B:4611:LEU:HB2	1:B:4619:ILE:HD11	2.01	0.42
1:A:2549:GLN:HG2	1:A:2572:LEU:HB2	2.02	0.42
1:A:2824:ILE:HG13	1:A:2825:TRP:N	2.34	0.42
1:A:3769:THR:O	1:A:3773:LEU:HG	2.19	0.42
1:B:1632:VAL:HG11	1:B:1636:ASP:CB	2.48	0.42
1:B:2605:LEU:HD23	1:B:2662:PHE:CD1	2.44	0.42
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	2.02	0.42
1:A:3178:ASP:OD1	1:A:3584:ASN:HB3	2.20	0.42
1:B:2256:PRO:HB3	1:B:2264:LEU:HD22	2.01	0.42
1:B:3178:ASP:OD1	1:B:3584:ASN:HB3	2.20	0.42
1:B:3588:LEU:HD23	1:B:3589:ILE:N	2.35	0.42
1:B:3609:ILE:HG12	1:B:3632:PRO:HB2	2.01	0.42
1:A:2626:THR:C	1:A:2627:THR:HG23	2.44	0.42
1:A:4609:VAL:CG2	1:A:4622:VAL:HG21	2.50	0.42
1:B:2285:ARG:NH1	1:B:2333:LEU:HD21	2.35	0.42
1:B:3508:LEU:HD23	1:B:3536:LEU:HD21	2.02	0.42
1:A:1961:ASN:ND2	1:A:2025:ARG:CB	2.82	0.42
1:A:2091:ARG:NH1	2:A:4801:ADP:PA	2.93	0.42
1:A:2571:THR:HG22	1:A:2747:ILE:HG12	2.00	0.42
1:A:2938:VAL:O	1:A:2941:ALA:HB2	2.20	0.42
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	2.02	0.42
1:A:3654:ARG:HB2	1:A:3661:LEU:HB2	2.01	0.42
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.01	0.42
1:B:2091:ARG:NH1	2:B:4801:ADP:PA	2.93	0.42
1:B:2938:VAL:O	1:B:2941:ALA:HB2	2.20	0.42
1:B:3109:PHE:CD2	1:B:3180:ILE:HG21	2.54	0.42
1:B:3175:HIS:CD2	1:B:3585:ARG:HH22	2.36	0.42
1:B:1628:ARG:NH2	1:B:1871:GLU:OE2	2.53	0.41
1:B:2549:GLN:HG2	1:B:2572:LEU:HB2	2.02	0.41
1:A:1636:ASP:CG	1:A:1656:LYS:NZ	2.77	0.41
1:A:1931:ASN:HD21	1:A:2317:SER:CB	2.21	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.01	0.41
1:A:2623:SER:OG	1:A:2624:SER:N	2.53	0.41
1:A:2907:VAL:HG23	1:A:2907:VAL:O	2.20	0.41
1:B:1761:ASN:HB3	1:B:1781:VAL:HG22	2.02	0.41
1:B:3713:LEU:O	1:B:3717:LEU:HG	2.20	0.41
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.59	0.41
1:B:2381:ARG:HG2	1:B:2385:ILE:HD11	2.02	0.41
1:B:2496:TYR:CZ	1:B:2500:TRP:CD1	3.08	0.41
1:A:1641:ILE:HA	1:A:1698:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1960:PHE:CE1	1:B:1963:LEU:CD2	3.03	0.41
1:B:2588:HIS:HB3	1:B:2658:TRP:CZ3	2.54	0.41
1:B:4387:TRP:CZ3	1:B:4391:ILE:HG21	2.56	0.41
1:A:1632:VAL:HG11	1:A:1636:ASP:HB3	2.02	0.41
1:A:1960:PHE:CE1	1:A:1963:LEU:CD2	3.03	0.41
1:A:2454:CYS:HB3	1:A:2502:LEU:HD23	2.03	0.41
1:A:3550:THR:OG1	1:A:3574:THR:HG21	2.19	0.41
1:A:4387:TRP:CZ3	1:A:4391:ILE:HG21	2.56	0.41
1:A:4577:LEU:HD21	1:A:4635:PHE:HD1	1.84	0.41
1:B:2623:SER:OG	1:B:2624:SER:N	2.53	0.41
1:B:2824:ILE:HG13	1:B:2825:TRP:N	2.34	0.41
1:A:1628:ARG:NH2	1:A:1871:GLU:OE2	2.53	0.41
1:A:2526:LEU:HA	1:A:2545:TRP:CZ3	2.54	0.41
1:A:2538:GLU:N	1:A:2546:SER:O	2.53	0.41
1:A:4529:ALA:O	1:A:4533:SER:N	2.52	0.41
1:B:2091:ARG:HH11	2:B:4801:ADP:PA	2.43	0.41
1:B:2147:PRO:HG3	1:B:2209:GLN:HB3	2.02	0.41
1:B:4176:ARG:HD3	1:B:4223:LEU:HD22	2.03	0.41
1:A:3924:ILE:O	1:A:3924:ILE:CG2	2.67	0.41
1:A:4528:VAL:HG21	1:A:4592:TRP:CD1	2.56	0.41
1:A:2091:ARG:HH11	2:A:4801:ADP:PA	2.43	0.41
1:A:2369:LEU:O	1:A:2451:ARG:NH1	2.43	0.41
1:A:3745:LEU:CD1	1:A:3773:LEU:HD22	2.51	0.41
1:B:3633:LEU:O	1:B:3677:ILE:HA	2.21	0.41
1:B:4528:VAL:HG21	1:B:4592:TRP:CD1	2.56	0.41
1:B:4561:THR:HG23	1:B:4587:LEU:HD13	2.03	0.41
1:A:1761:ASN:HB3	1:A:1781:VAL:HG22	2.02	0.41
1:A:2635:PHE:O	1:A:2639:CYS:N	2.50	0.41
1:A:3151:HIS:CE1	1:A:3516:TYR:HH	2.36	0.41
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.01	0.41
1:A:3588:LEU:HD23	1:A:3589:ILE:N	2.35	0.41
1:A:3591:ASP:CG	1:A:3596:ALA:HB3	2.45	0.41
1:A:3633:LEU:O	1:A:3677:ILE:HA	2.21	0.41
1:B:3638:VAL:N	1:B:3681:THR:HG22	2.36	0.41
1:A:1931:ASN:OD1	1:A:1958:ASP:CB	2.62	0.41
1:A:3871:VAL:HG11	1:A:3883:PHE:CD2	2.56	0.41
1:B:1641:ILE:HA	1:B:1698:ILE:CD1	2.50	0.41
1:A:1632:VAL:HG13	1:A:1636:ASP:HB2	1.95	0.40
1:A:2285:ARG:NH1	1:A:2333:LEU:HD21	2.35	0.40
1:A:2599:SER:N	2:A:4804:ADP:O2A	2.43	0.40
1:A:2752:ASN:HD22	1:A:2770:THR:HG22	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3648:VAL:HA	1:A:3662:ILE:HD11	2.03	0.40
1:B:3871:VAL:HG11	1:B:3883:PHE:CD2	2.56	0.40
1:A:2370:SER:O	1:A:2373:MET:HB3	2.21	0.40
1:A:3154:LEU:HD11	1:A:3520:PHE:CE2	2.56	0.40
1:A:4042:LEU:HD21	1:A:4139:LEU:HD23	2.03	0.40
1:B:1879:LEU:HD13	1:B:1915:SER:HA	2.03	0.40
1:B:2454:CYS:HB3	1:B:2502:LEU:HD23	2.03	0.40
1:B:2538:GLU:N	1:B:2546:SER:O	2.53	0.40
1:A:2091:ARG:NH2	1:A:2320:ASP:OD1	2.53	0.40
1:A:2639:CYS:SG	1:A:2652:PRO:HA	2.62	0.40
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	2.03	0.40
1:A:4176:ARG:HD3	1:A:4223:LEU:HD22	2.03	0.40
1:B:3151:HIS:CE1	1:B:3516:TYR:HH	2.36	0.40
1:B:3154:LEU:HD11	1:B:3520:PHE:CE2	2.56	0.40
1:B:3553:LEU:HD13	1:B:3578:ILE:HG21	2.04	0.40
1:B:3868:PHE:CE1	1:B:3884:ALA:HB2	2.56	0.40
1:B:4009:VAL:HG13	1:B:4013:LEU:HD12	2.03	0.40
1:A:2571:THR:O	1:A:2572:LEU:C	2.62	0.40
1:A:3868:PHE:CE1	1:A:3884:ALA:HB2	2.56	0.40
1:A:4565:LEU:CD2	1:A:4642:VAL:HG22	2.50	0.40
1:B:1632:VAL:HG11	1:B:1636:ASP:HB3	2.02	0.40
1:B:2370:SER:O	1:B:2373:MET:HB3	2.21	0.40
1:B:2635:PHE:O	1:B:2639:CYS:N	2.50	0.40
1:A:2182:LEU:O	1:A:2185:VAL:HG22	2.22	0.40
1:A:4468:THR:HG21	1:A:4611:LEU:HD23	2.04	0.40
1:B:2016:ILE:HD12	1:B:2036:PHE:CD2	2.56	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 PDB entries followed by that with respect to all EM entries.

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	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	48	79
1	B	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	48	79
All	All	5776/9292 (62%)	5428 (94%)	342 (6%)	6 (0%)	49	79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1647	VAL
1	B	1647	VAL
1	A	1964	GLU
1	B	1964	GLU
1	A	1511	PRO
1	B	1511	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 PDB entries followed by that with respect to all EM entries.

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	2472/4125 (60%)	2469 (100%)	3 (0%)	88	89
1	B	2472/4125 (60%)	2469 (100%)	3 (0%)	88	89
All	All	4944/8250 (60%)	4938 (100%)	6 (0%)	87	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2445	HIS
1	A	2702	LYS
1	A	2796	PRO
1	B	2445	HIS
1	B	2702	LYS
1	B	2796	PRO

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	1479	ASN
1	A	1612	GLN
1	A	1670	ASN
1	A	1699	ASN
1	A	1746	GLN
1	A	1748	GLN
1	A	1784	ASN
1	A	1790	ASN
1	A	1856	GLN
1	A	1863	ASN
1	A	1881	GLN
1	A	1894	GLN
1	A	1921	HIS
1	A	1931	ASN
1	A	1961	ASN
1	A	1973	GLN
1	A	1974	GLN
1	A	1979	GLN
1	A	1985	HIS
1	A	2079	GLN
1	A	2134	GLN
1	A	2212	GLN
1	A	2217	ASN
1	A	2377	ASN
1	A	2485	GLN
1	A	2549	GLN
1	A	2667	ASN
1	A	2677	GLN
1	A	2752	ASN
1	A	2913	ASN
1	A	2998	ASN
1	A	3014	ASN
1	A	3047	HIS
1	A	3057	GLN
1	A	3152	GLN
1	A	3175	HIS
1	A	3182	HIS
1	A	3198	GLN
1	A	3459	GLN
1	A	3540	ASN
1	A	3542	GLN
1	A	3646	ASN
1	A	3792	GLN

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Mol	Chain	Res	Type
1	A	3880	HIS
1	A	4012	ASN
1	A	4029	HIS
1	A	4119	HIS
1	A	4131	ASN
1	A	4156	ASN
1	A	4397	HIS
1	A	4436	GLN
1	A	4488	GLN
1	A	4490	GLN
1	A	4526	GLN
1	A	4566	GLN
1	B	1479	ASN
1	B	1612	GLN
1	B	1670	ASN
1	B	1699	ASN
1	B	1746	GLN
1	B	1748	GLN
1	B	1784	ASN
1	B	1790	ASN
1	B	1856	GLN
1	B	1863	ASN
1	B	1881	GLN
1	B	1894	GLN
1	B	1921	HIS
1	B	1931	ASN
1	B	1973	GLN
1	B	1974	GLN
1	B	1979	GLN
1	B	1985	HIS
1	B	2079	GLN
1	B	2134	GLN
1	B	2217	ASN
1	B	2485	GLN
1	B	2549	GLN
1	B	2667	ASN
1	B	2677	GLN
1	B	2752	ASN
1	B	2913	ASN
1	B	2998	ASN
1	B	3014	ASN
1	B	3047	HIS

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Mol	Chain	Res	Type
1	B	3057	GLN
1	B	3152	GLN
1	B	3175	HIS
1	B	3182	HIS
1	B	3198	GLN
1	B	3459	GLN
1	B	3542	GLN
1	B	3646	ASN
1	B	3709	GLN
1	B	3792	GLN
1	B	3843	ASN
1	B	3880	HIS
1	B	4012	ASN
1	B	4029	HIS
1	B	4062	GLN
1	B	4119	HIS
1	B	4131	ASN
1	B	4156	ASN
1	B	4397	HIS
1	B	4436	GLN
1	B	4488	GLN
1	B	4490	GLN
1	B	4526	GLN
1	B	4566	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
2	ADP	A	4804	-	28,29,29	1.41	5 (17%)	43,45,45	1.79	10 (23%)
2	ADP	A	4801	-	28,29,29	1.54	6 (21%)	43,45,45	1.95	8 (18%)
2	ADP	A	4805	-	28,29,29	1.35	4 (14%)	43,45,45	1.96	11 (25%)
2	ADP	B	4805	-	28,29,29	1.35	4 (14%)	43,45,45	1.96	11 (25%)
2	ADP	B	4801	-	28,29,29	1.54	6 (21%)	43,45,45	1.95	8 (18%)
2	ADP	B	4804	-	28,29,29	1.41	5 (17%)	43,45,45	1.79	11 (25%)
3	ATP	A	4802	4	32,33,33	1.52	6 (18%)	48,52,52	1.71	11 (22%)
3	ATP	B	4802	4	32,33,33	1.51	6 (18%)	48,52,52	1.71	11 (22%)

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
2	ADP	A	4804	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4801	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4805	-	-	3/16/32/32	0/3/3/3
2	ADP	B	4805	-	-	3/16/32/32	0/3/3/3
2	ADP	B	4801	-	-	3/16/32/32	0/3/3/3
2	ADP	B	4804	-	-	3/16/32/32	0/3/3/3
3	ATP	A	4802	4	-	2/22/38/38	0/3/3/3
3	ATP	B	4802	4	-	2/22/38/38	0/3/3/3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4801	ADP	C5-C4	4.86	1.47	1.39
2	A	4801	ADP	C5-C4	4.85	1.47	1.39
3	A	4802	ATP	C5-C4	4.70	1.47	1.39
3	B	4802	ATP	C5-C4	4.65	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4804	ADP	C5-C4	4.19	1.46	1.39
2	B	4804	ADP	C5-C4	4.19	1.46	1.39
2	A	4805	ADP	C5-C4	3.99	1.46	1.39
2	B	4805	ADP	C5-C4	3.99	1.46	1.39
2	B	4805	ADP	C5-N7	-3.56	1.32	1.39
2	A	4805	ADP	C5-N7	-3.52	1.32	1.39
2	A	4804	ADP	C4-N9	-3.28	1.30	1.37
2	B	4804	ADP	C4-N9	-3.28	1.30	1.37
3	B	4802	ATP	C4-N9	-3.18	1.31	1.37
3	A	4802	ATP	C4-N9	-3.17	1.31	1.37
2	B	4801	ADP	C5-N7	-3.13	1.33	1.39
2	A	4801	ADP	C5-N7	-3.10	1.33	1.39
3	A	4802	ATP	C5-C6	2.79	1.48	1.41
3	B	4802	ATP	C5-C6	2.79	1.48	1.41
3	A	4802	ATP	C5-N7	-2.74	1.34	1.39
3	B	4802	ATP	C5-N7	-2.71	1.34	1.39
2	A	4804	ADP	C5-N7	-2.70	1.34	1.39
2	B	4804	ADP	C5-N7	-2.70	1.34	1.39
2	B	4801	ADP	C5-C6	2.54	1.48	1.41
2	A	4801	ADP	C5-C6	2.54	1.48	1.41
3	A	4802	ATP	C8-N7	2.47	1.36	1.31
3	B	4802	ATP	C8-N7	2.46	1.36	1.31
2	A	4804	ADP	C5-C6	2.44	1.47	1.41
2	B	4804	ADP	C5-C6	2.44	1.47	1.41
3	B	4802	ATP	PB-O3B	2.33	1.62	1.59
3	A	4802	ATP	PB-O3B	2.32	1.62	1.59
2	A	4801	ADP	C8-N7	2.29	1.36	1.31
2	B	4801	ADP	C8-N7	2.29	1.36	1.31
2	A	4805	ADP	C5-C6	2.24	1.47	1.41
2	B	4805	ADP	C5-C6	2.24	1.47	1.41
2	A	4804	ADP	C8-N7	2.20	1.35	1.31
2	B	4804	ADP	C8-N7	2.20	1.35	1.31
2	A	4805	ADP	C4-N9	-2.16	1.33	1.37
2	B	4805	ADP	C4-N9	-2.16	1.33	1.37
2	B	4801	ADP	C4-N9	-2.10	1.33	1.37
2	A	4801	ADP	C4-N9	-2.10	1.33	1.37
2	A	4801	ADP	C8-N9	-2.06	1.34	1.37
2	B	4801	ADP	C8-N9	-2.05	1.34	1.37

All (81) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4801	ADP	C5-C4-N3	-6.36	117.96	126.72
2	A	4801	ADP	C5-C4-N3	-6.36	117.97	126.72
2	A	4805	ADP	C5-C4-N3	-6.30	118.04	126.72
2	B	4805	ADP	C5-C4-N3	-6.30	118.04	126.72
2	A	4805	ADP	N3-C4-N9	5.04	135.75	127.17
2	B	4805	ADP	N3-C4-N9	5.04	135.75	127.17
2	B	4801	ADP	N3-C4-N9	4.96	135.60	127.17
2	A	4801	ADP	N3-C4-N9	4.95	135.59	127.17
2	B	4804	ADP	C5-C4-N3	-4.80	120.10	126.72
2	A	4804	ADP	C5-C4-N3	-4.79	120.12	126.72
3	A	4802	ATP	C5-C4-N3	-4.50	120.53	126.72
3	B	4802	ATP	C5-C4-N3	-4.49	120.54	126.72
3	A	4802	ATP	N3-C2-N1	-4.14	122.31	128.58
3	B	4802	ATP	N3-C2-N1	-4.14	122.31	128.58
2	A	4805	ADP	C2-N3-C4	4.00	121.60	111.83
2	B	4805	ADP	C2-N3-C4	4.00	121.60	111.83
2	B	4801	ADP	C2-N3-C4	3.92	121.41	111.83
2	A	4801	ADP	C2-N3-C4	3.90	121.35	111.83
2	A	4805	ADP	N3-C2-N1	-3.76	122.88	128.58
2	B	4805	ADP	N3-C2-N1	-3.76	122.88	128.58
3	A	4802	ATP	C2-N3-C4	3.65	120.73	111.83
3	B	4802	ATP	C2-N3-C4	3.63	120.71	111.83
2	B	4804	ADP	N3-C4-N9	3.58	133.26	127.17
2	A	4804	ADP	N3-C4-N9	3.57	133.24	127.17
2	B	4801	ADP	N3-C2-N1	-3.54	123.22	128.58
2	A	4801	ADP	N3-C2-N1	-3.53	123.24	128.58
2	A	4804	ADP	N3-C2-N1	-3.49	123.30	128.58
2	B	4804	ADP	C2-N3-C4	3.49	120.35	111.83
2	A	4804	ADP	C2-N3-C4	3.49	120.34	111.83
2	B	4804	ADP	N3-C2-N1	-3.47	123.33	128.58
2	A	4801	ADP	C4-C5-N7	-3.46	106.62	110.58
3	A	4802	ATP	C4-C5-N7	-3.43	106.66	110.58
2	B	4801	ADP	C4-C5-N7	-3.43	106.66	110.58
3	B	4802	ATP	C4-C5-N7	-3.42	106.67	110.58
3	A	4802	ATP	N3-C4-N9	3.41	132.97	127.17
2	A	4805	ADP	C4-C5-N7	-3.40	106.69	110.58
3	B	4802	ATP	N3-C4-N9	3.40	132.95	127.17
2	B	4805	ADP	C4-C5-N7	-3.38	106.72	110.58
3	A	4802	ATP	C4-N9-C8	3.13	109.03	105.74
3	B	4802	ATP	C4-N9-C8	3.13	109.02	105.74
2	A	4804	ADP	C4-C5-N7	-3.08	107.06	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4804	ADP	C4-C5-N7	-3.08	107.06	110.58
2	A	4805	ADP	C5-N7-C8	2.97	108.12	103.45
2	B	4805	ADP	C5-N7-C8	2.95	108.08	103.45
3	A	4802	ATP	C6-C5-N7	2.91	137.71	132.09
3	B	4802	ATP	C6-C5-N7	2.90	137.68	132.09
2	A	4804	ADP	C4-N9-C8	2.75	108.63	105.74
2	B	4804	ADP	C4-N9-C8	2.75	108.63	105.74
2	A	4801	ADP	C3'-C2'-C1'	2.70	106.57	101.46
2	B	4801	ADP	C3'-C2'-C1'	2.69	106.56	101.46
2	A	4805	ADP	C4-N9-C8	2.45	108.31	105.74
3	A	4802	ATP	C2-N1-C6	2.42	122.70	118.73
3	B	4802	ATP	C2-N1-C6	2.42	122.70	118.73
2	B	4805	ADP	C4-N9-C8	2.41	108.27	105.74
2	A	4801	ADP	C5-N7-C8	2.37	107.18	103.45
2	B	4801	ADP	C5-N7-C8	2.35	107.14	103.45
2	A	4804	ADP	O4'-C1'-N9	-2.31	103.66	108.09
2	A	4805	ADP	N9-C8-N7	-2.30	110.68	113.94
2	B	4804	ADP	O4'-C1'-N9	-2.28	103.71	108.09
2	B	4805	ADP	N9-C8-N7	-2.27	110.72	113.94
2	A	4804	ADP	C6-C5-N7	2.25	136.42	132.09
2	B	4804	ADP	C6-C5-N7	2.25	136.42	132.09
3	A	4802	ATP	C5-N7-C8	2.18	106.88	103.45
3	A	4802	ATP	C4-N9-C1'	-2.16	121.57	126.63
3	B	4802	ATP	C4-N9-C1'	-2.16	121.57	126.63
3	B	4802	ATP	C5-N7-C8	2.16	106.84	103.45
2	B	4804	ADP	C4-N9-C1'	-2.13	121.64	126.63
2	A	4805	ADP	O3B-PB-O2B	2.13	115.80	107.80
2	B	4805	ADP	O3B-PB-O2B	2.13	115.80	107.80
2	A	4804	ADP	C4-N9-C1'	-2.12	121.67	126.63
3	A	4802	ATP	N9-C8-N7	-2.12	110.93	113.94
3	B	4802	ATP	N9-C8-N7	-2.11	110.94	113.94
2	B	4805	ADP	O2A-PA-O1A	2.09	122.18	112.44
2	A	4805	ADP	O2A-PA-O1A	2.09	122.16	112.44
2	A	4801	ADP	C4-N9-C8	2.09	107.93	105.74
2	B	4801	ADP	C4-N9-C8	2.05	107.89	105.74
2	A	4804	ADP	C3'-C2'-C1'	2.01	105.27	101.46
2	B	4804	ADP	C3'-C2'-C1'	2.01	105.27	101.46
2	B	4804	ADP	O5'-C5'-C4'	2.00	115.81	108.99
2	A	4805	ADP	O4'-C1'-C2'	-2.00	102.33	106.62
2	B	4805	ADP	O4'-C1'-C2'	-2.00	102.33	106.62

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4804	ADP	PA-O3A-PB-O2B
2	A	4804	ADP	C5'-O5'-PA-O1A
2	A	4805	ADP	C5'-O5'-PA-O2A
2	A	4805	ADP	C5'-O5'-PA-O3A
2	B	4804	ADP	PA-O3A-PB-O2B
2	B	4804	ADP	C5'-O5'-PA-O1A
2	B	4805	ADP	C5'-O5'-PA-O2A
2	B	4805	ADP	C5'-O5'-PA-O3A
2	A	4801	ADP	O4'-C4'-C5'-O5'
2	B	4801	ADP	O4'-C4'-C5'-O5'
2	A	4801	ADP	C3'-C4'-C5'-O5'
2	B	4801	ADP	C3'-C4'-C5'-O5'
2	A	4801	ADP	C4'-C5'-O5'-PA
2	B	4801	ADP	C4'-C5'-O5'-PA
3	A	4802	ATP	PG-O3B-PB-O2B
3	B	4802	ATP	PG-O3B-PB-O2B
2	A	4804	ADP	C2'-C1'-N9-C8
2	B	4804	ADP	C2'-C1'-N9-C8
2	A	4805	ADP	O4'-C4'-C5'-O5'
2	B	4805	ADP	O4'-C4'-C5'-O5'
3	A	4802	ATP	PG-O3B-PB-O1B
3	B	4802	ATP	PG-O3B-PB-O1B

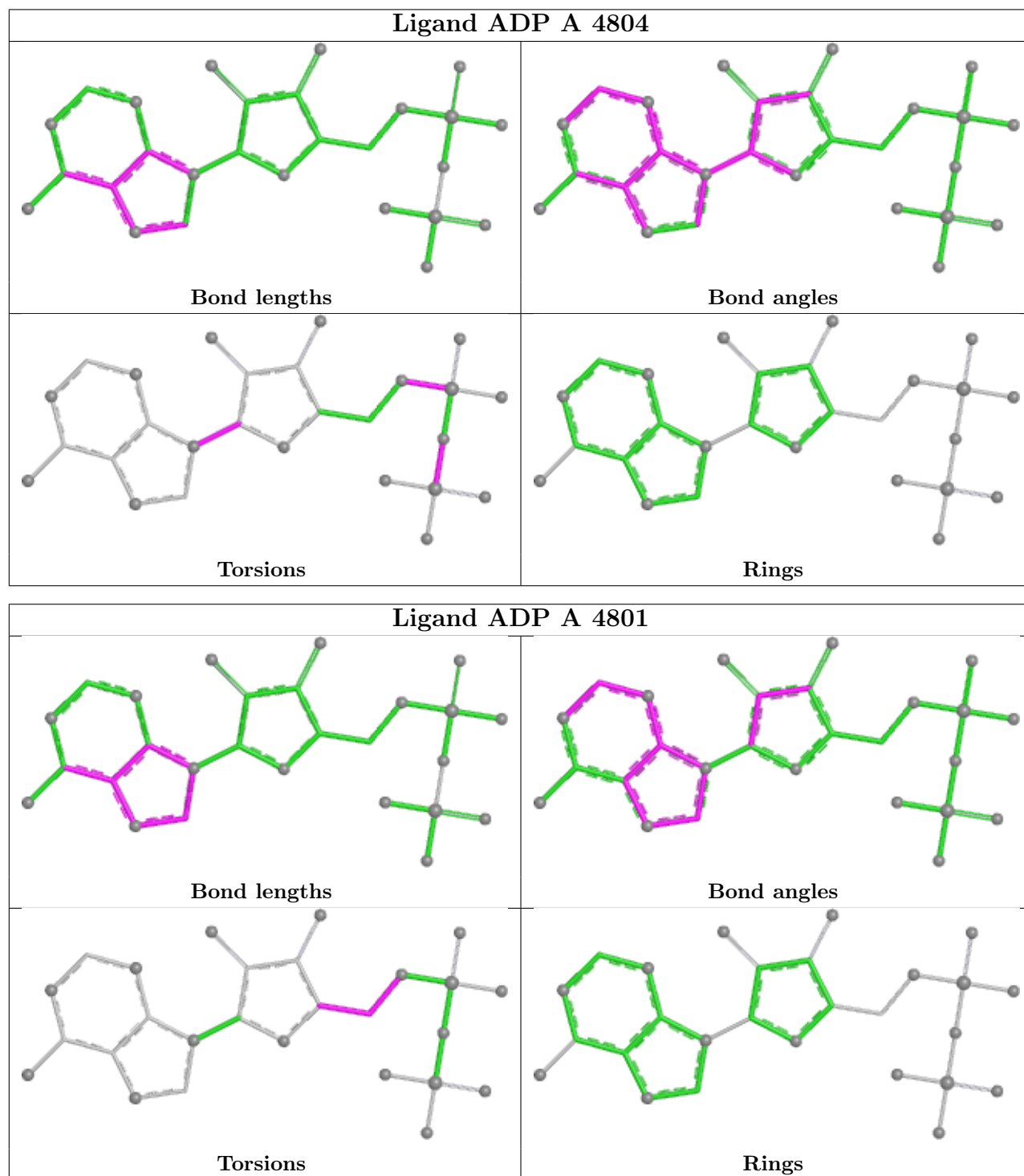
There are no ring outliers.

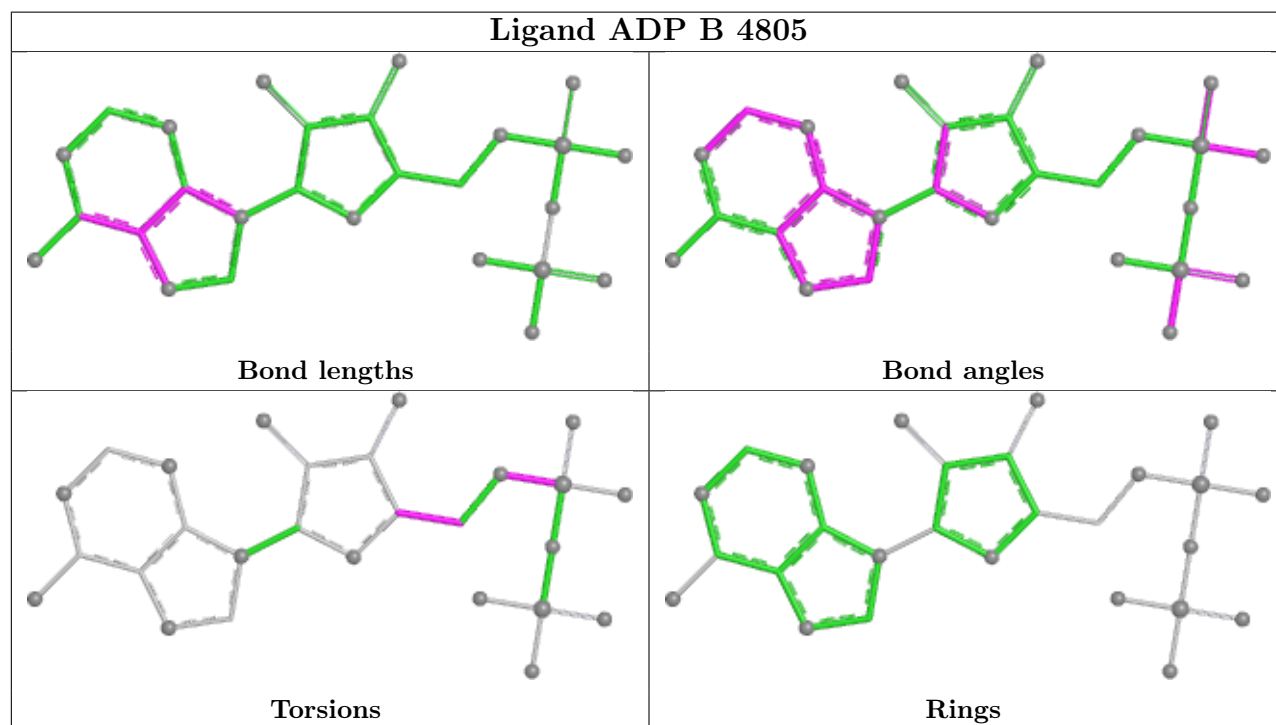
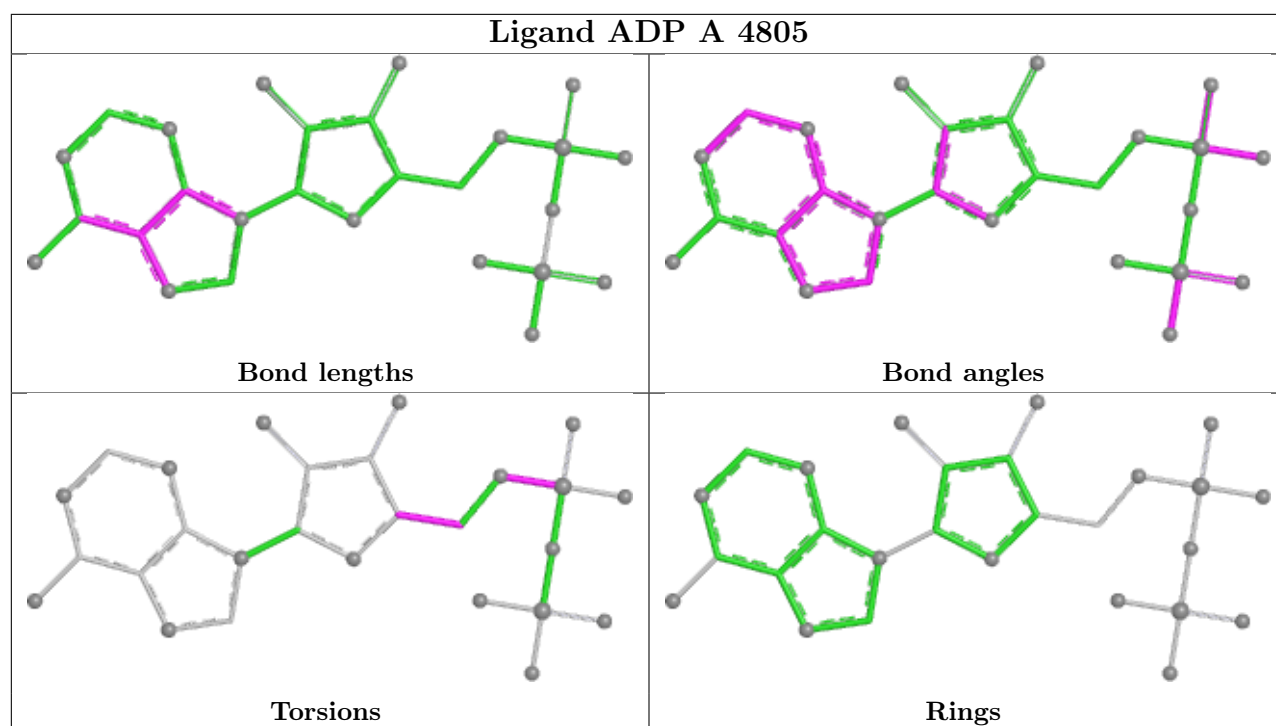
6 monomers are involved in 34 short contacts:

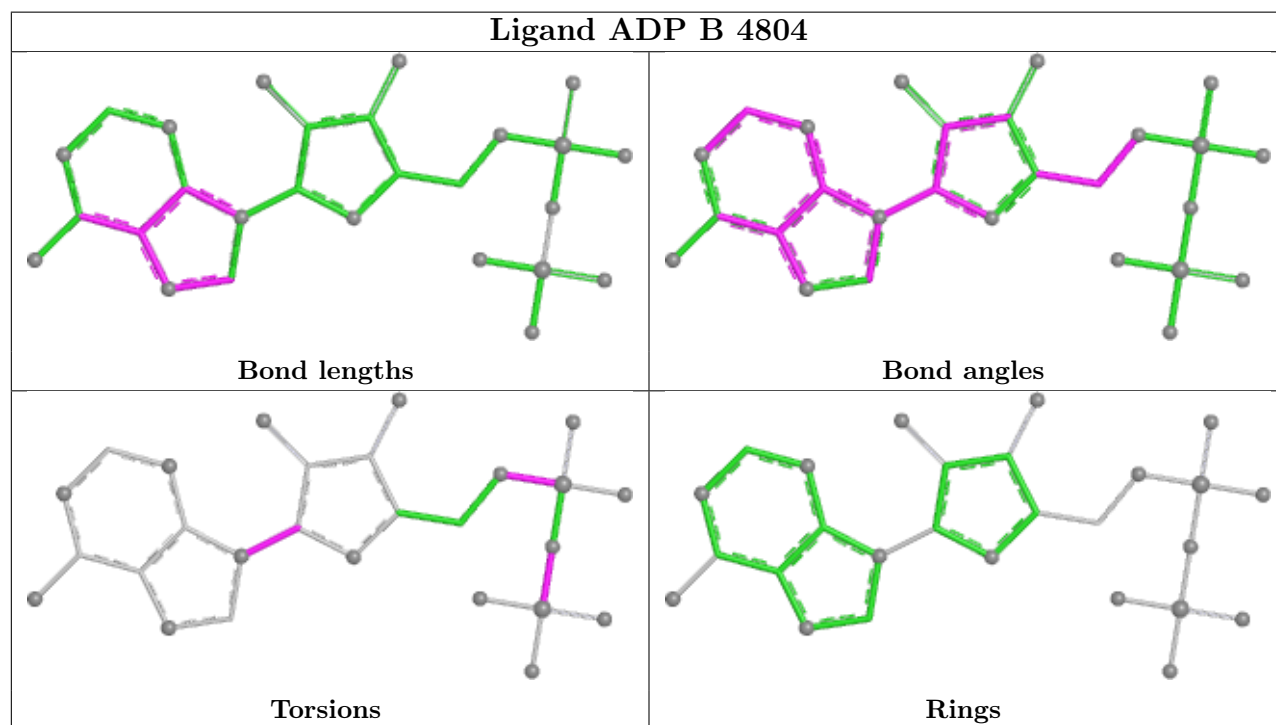
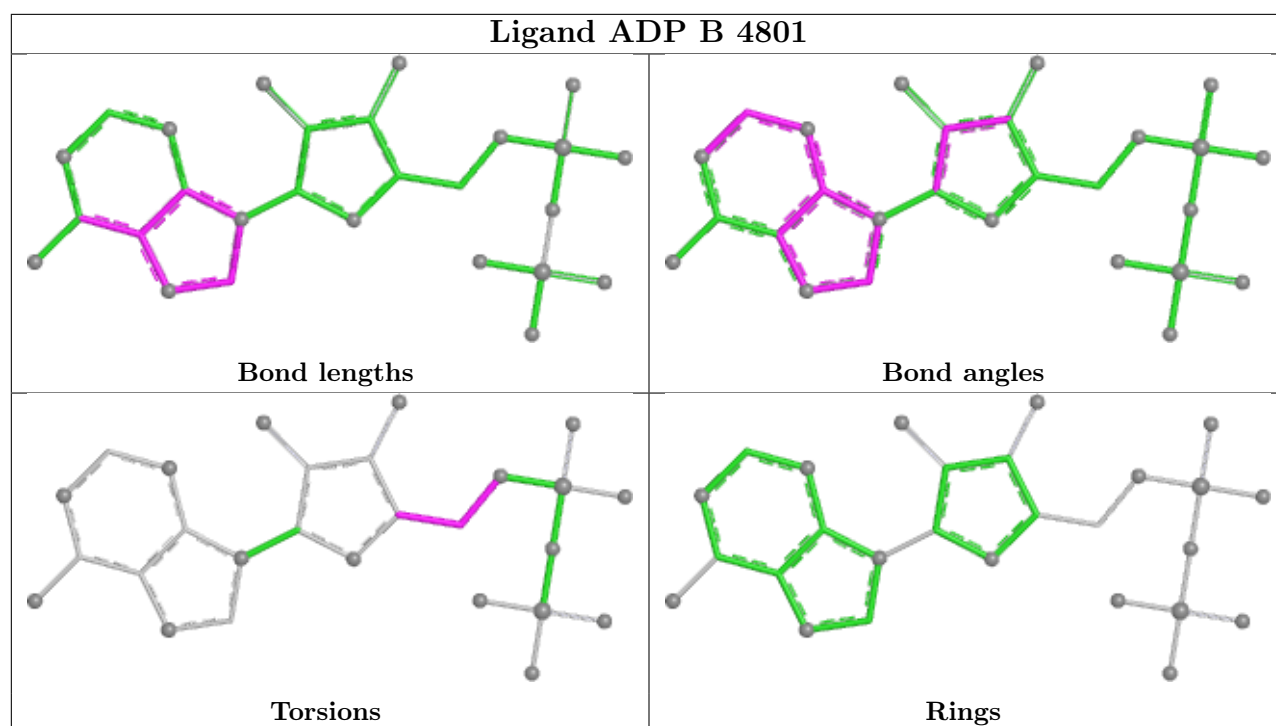
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4804	ADP	2	0
2	A	4801	ADP	11	0
2	B	4801	ADP	11	0
2	B	4804	ADP	2	0
3	A	4802	ATP	4	0
3	B	4802	ATP	4	0

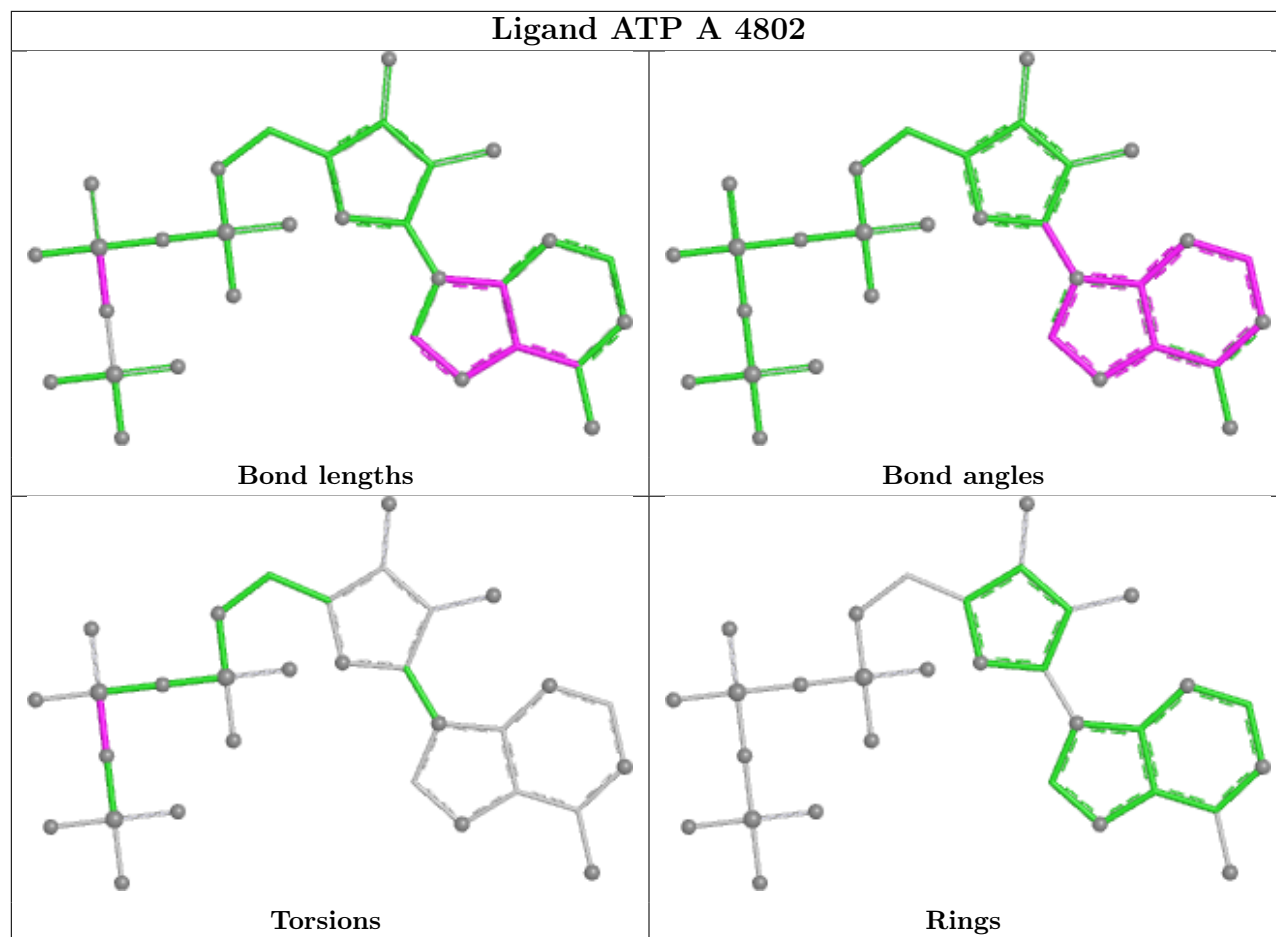
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

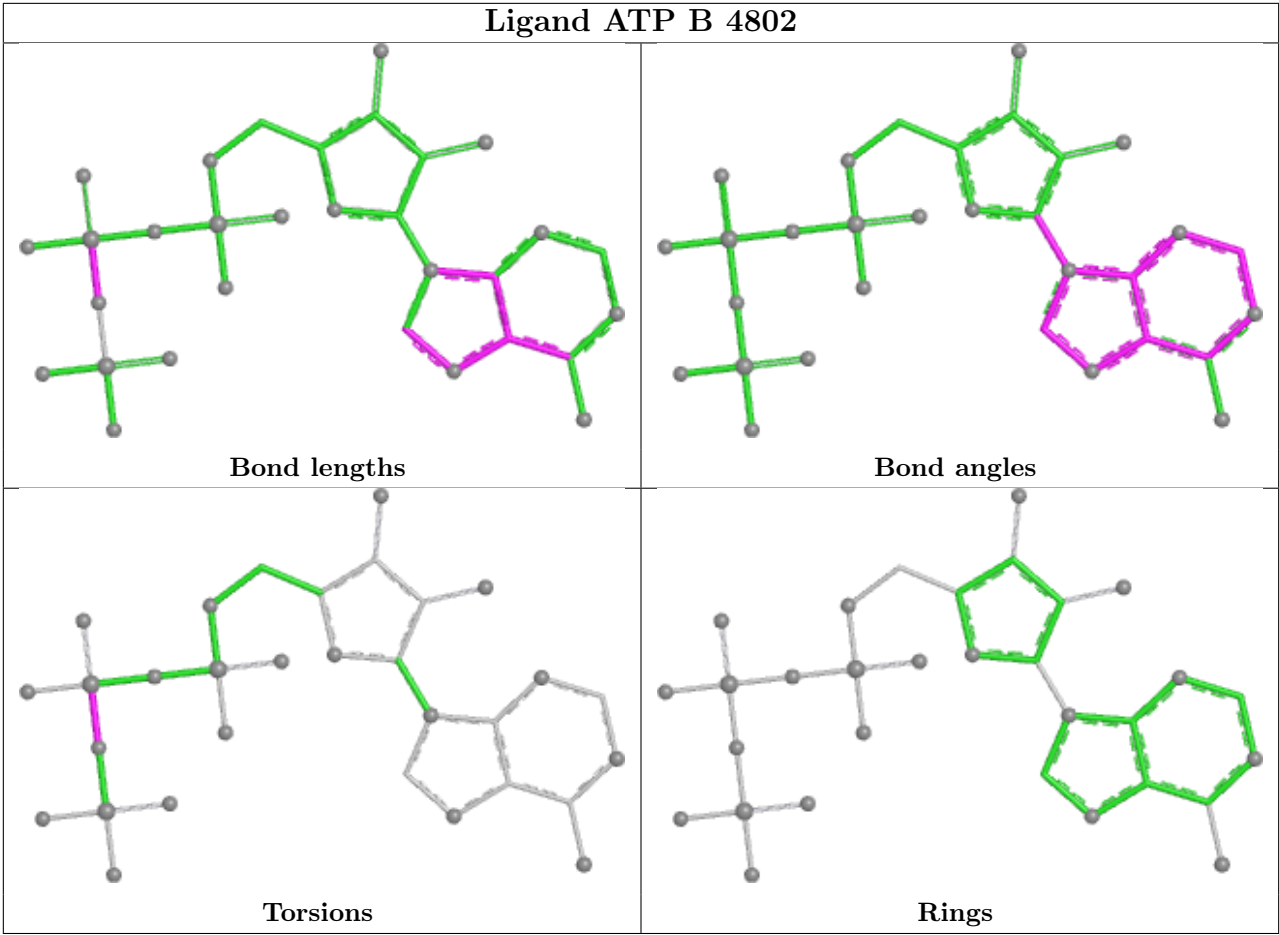
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3803:PRO	C	3804:LEU	N	2.62
1	B	3803:PRO	C	3804:LEU	N	2.62
1	A	3203:VAL	C	3204:GLY	N	2.58
1	B	3203:VAL	C	3204:GLY	N	2.58

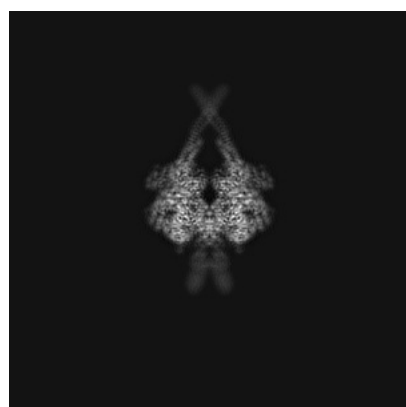
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3698. These allow visual inspection of the internal detail of the map and identification of artifacts.

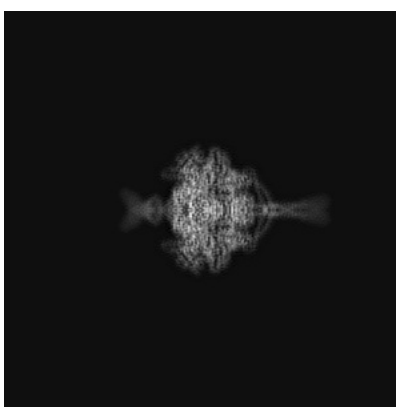
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

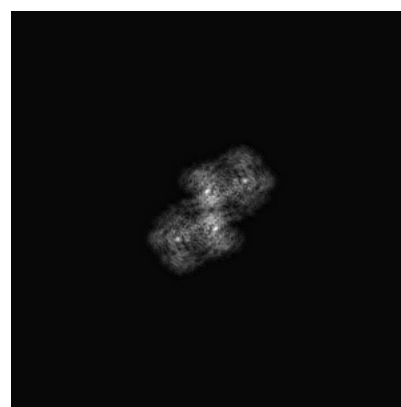
6.1.1 Primary map



X



Y

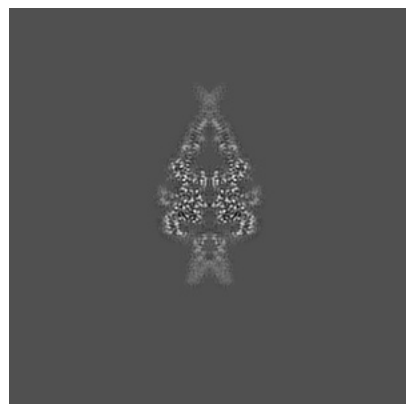


Z

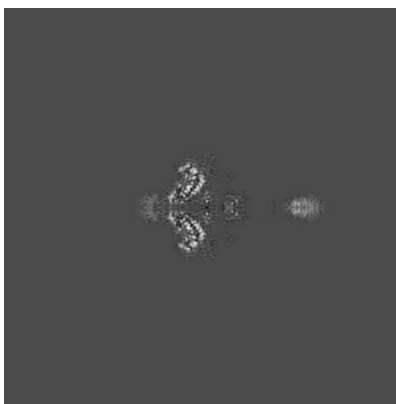
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

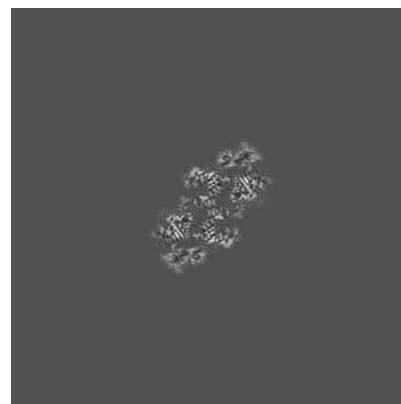
6.2.1 Primary map



X Index: 200



Y Index: 200

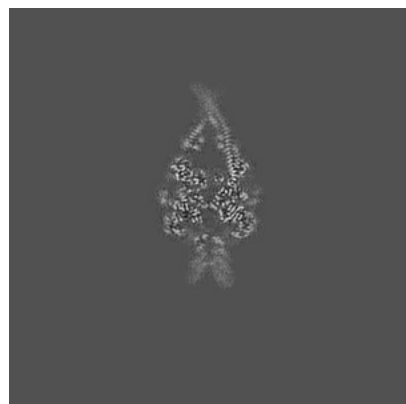


Z Index: 200

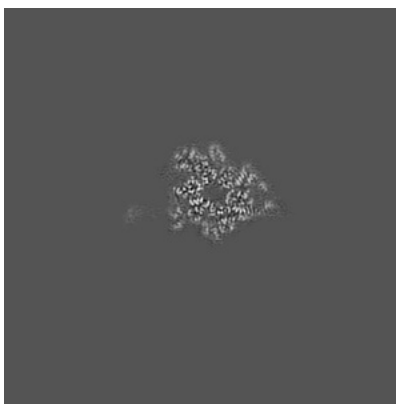
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 198



Y Index: 223

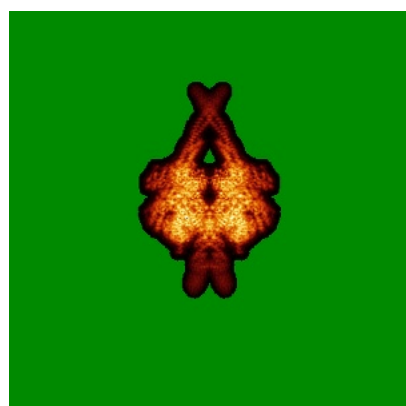


Z Index: 189

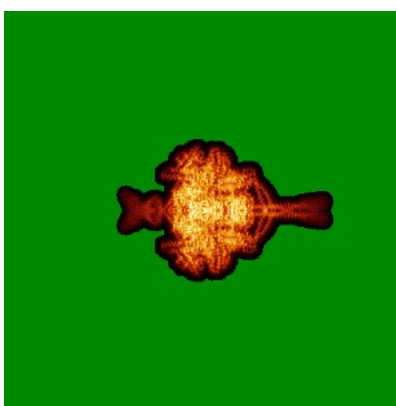
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

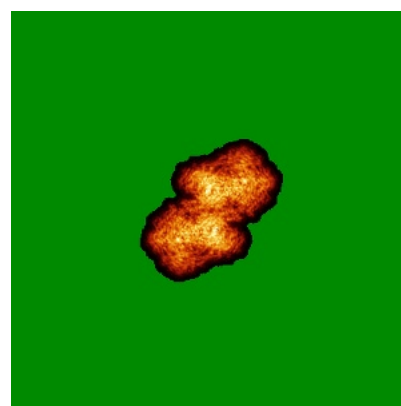
6.4.1 Primary map



X



Y

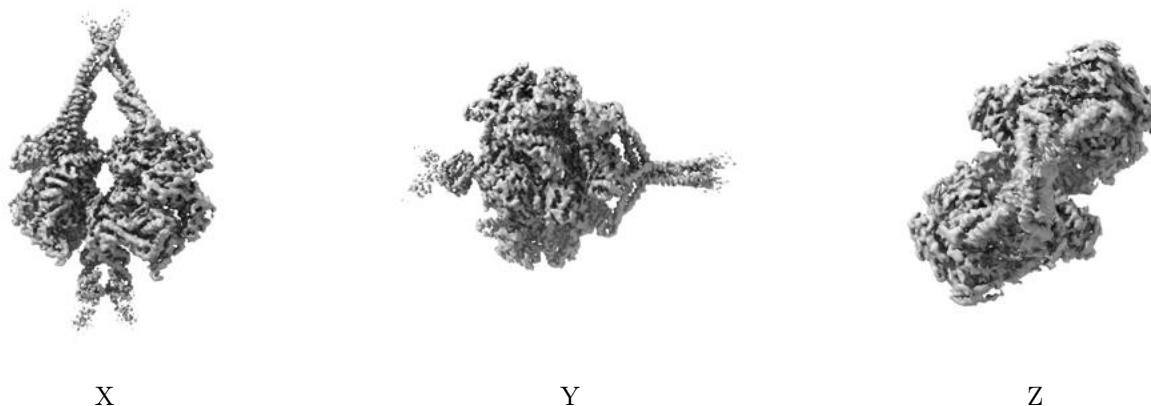


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

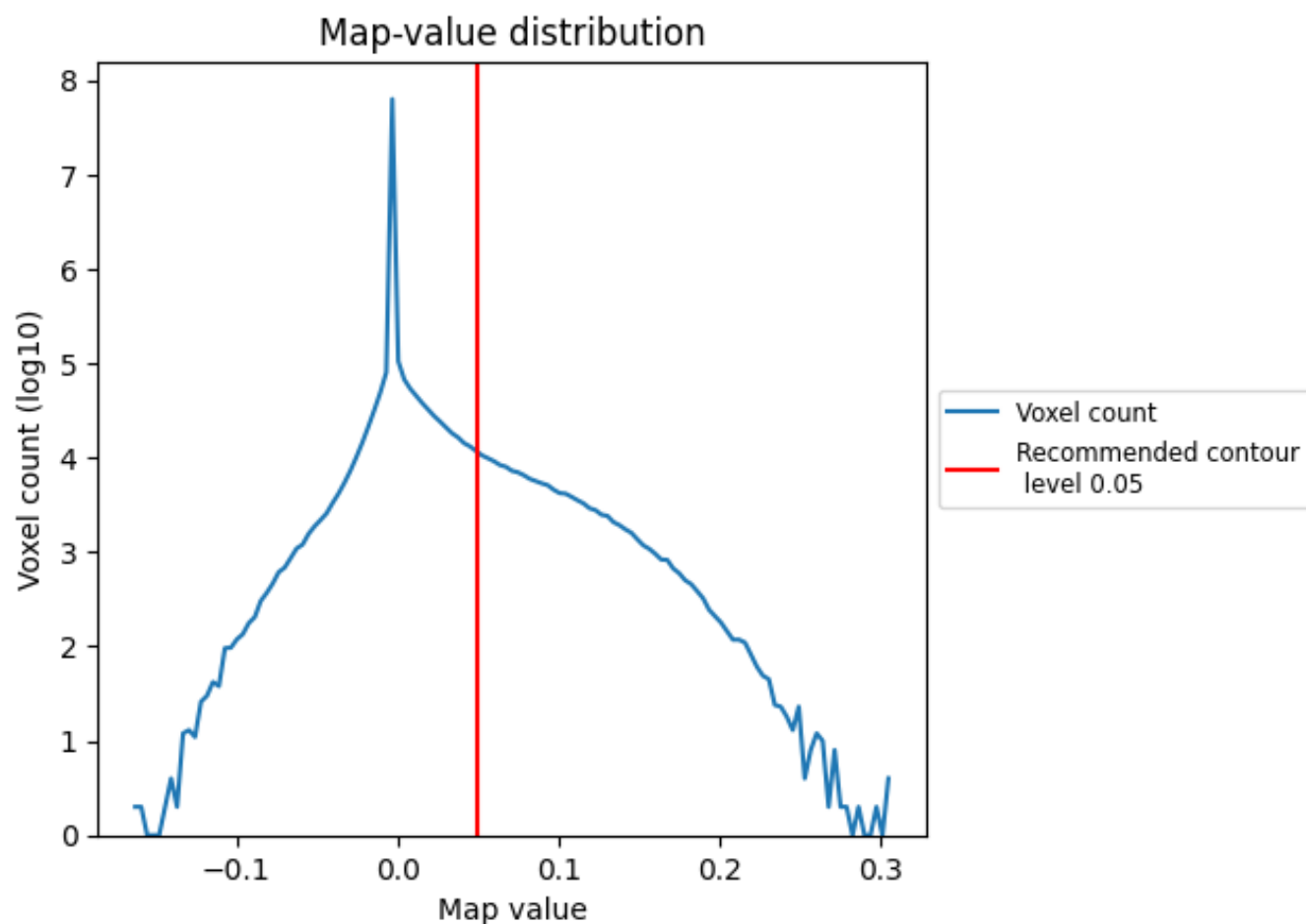
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

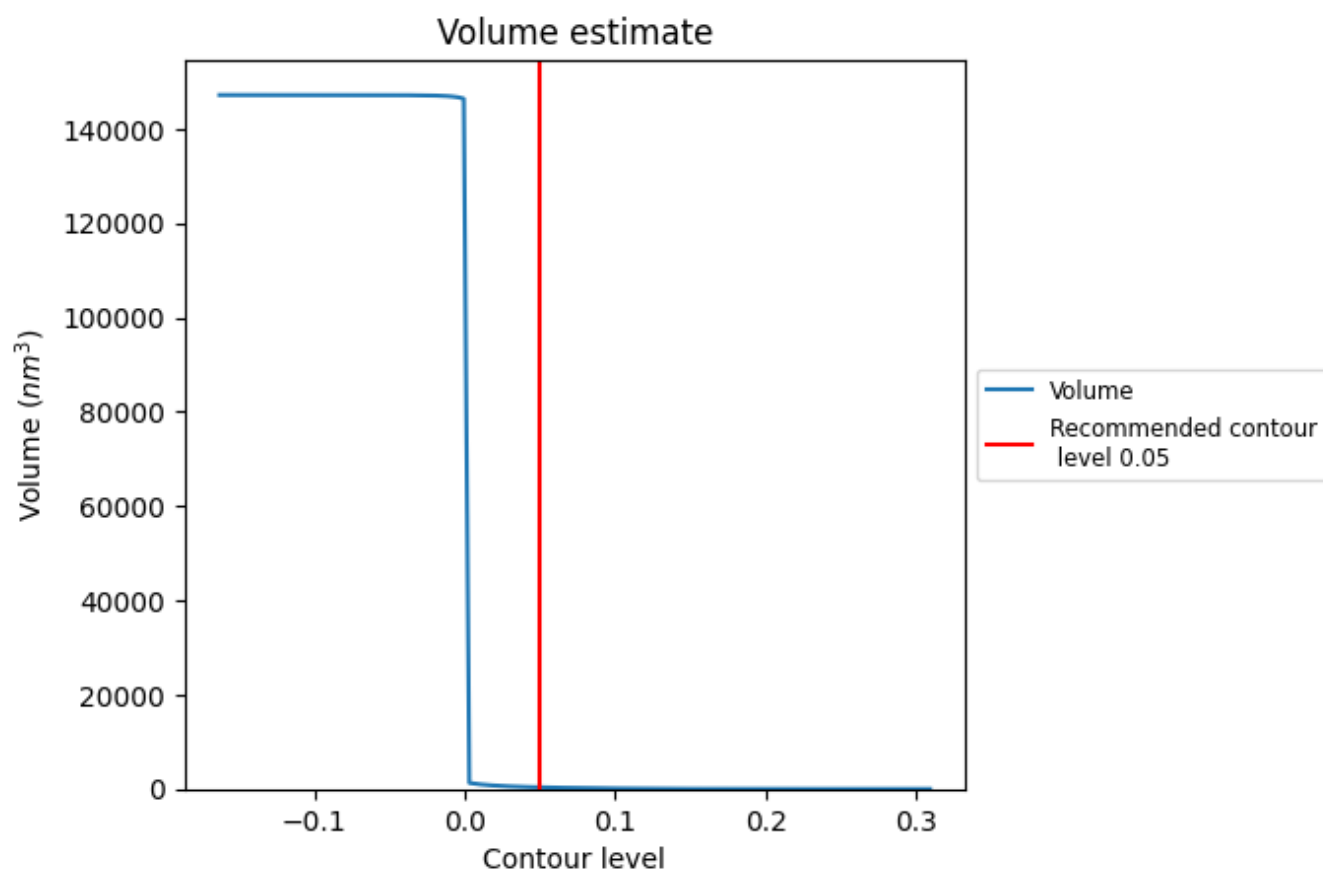
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

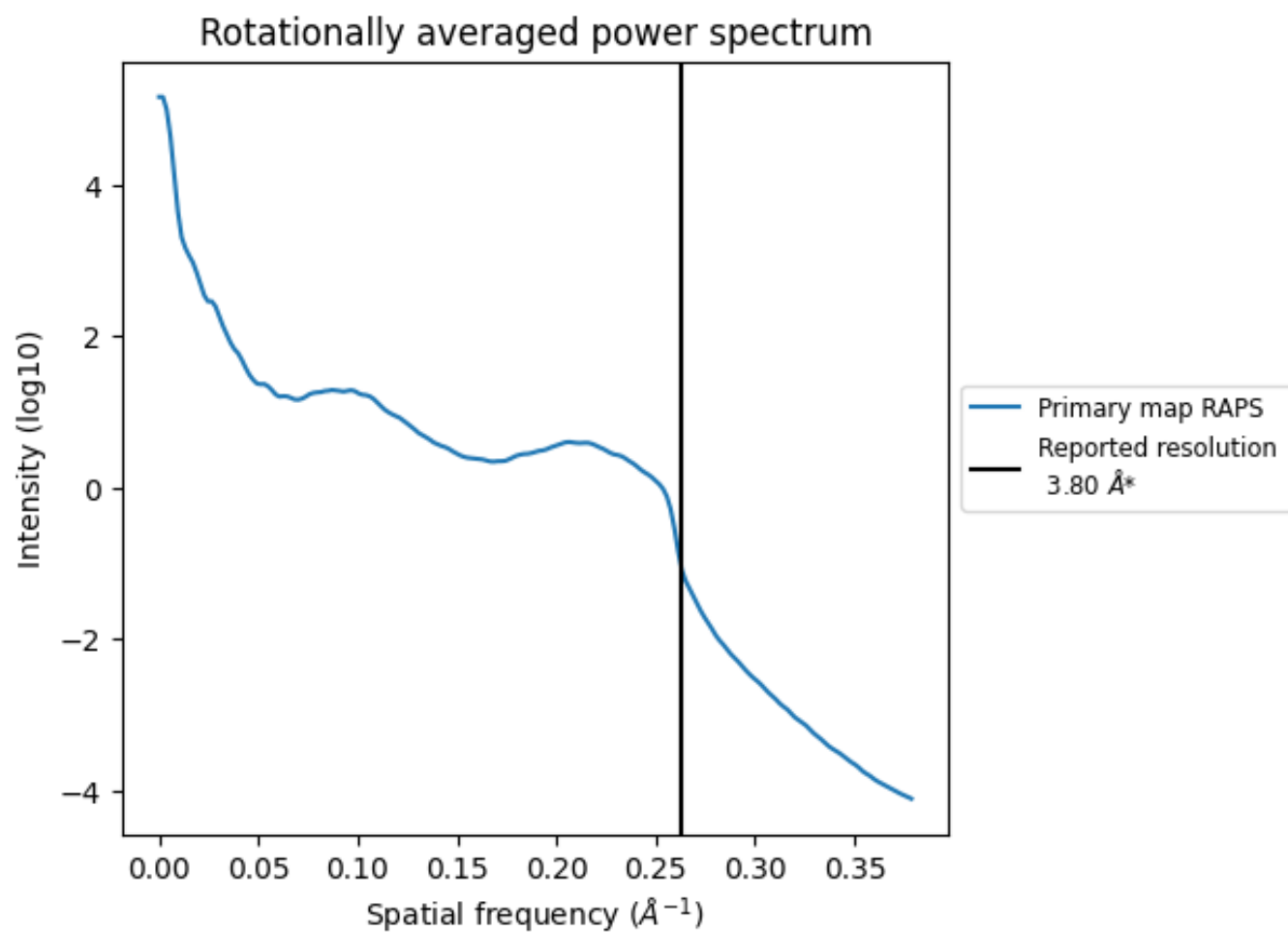
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 344 nm³; this corresponds to an approximate mass of 311 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

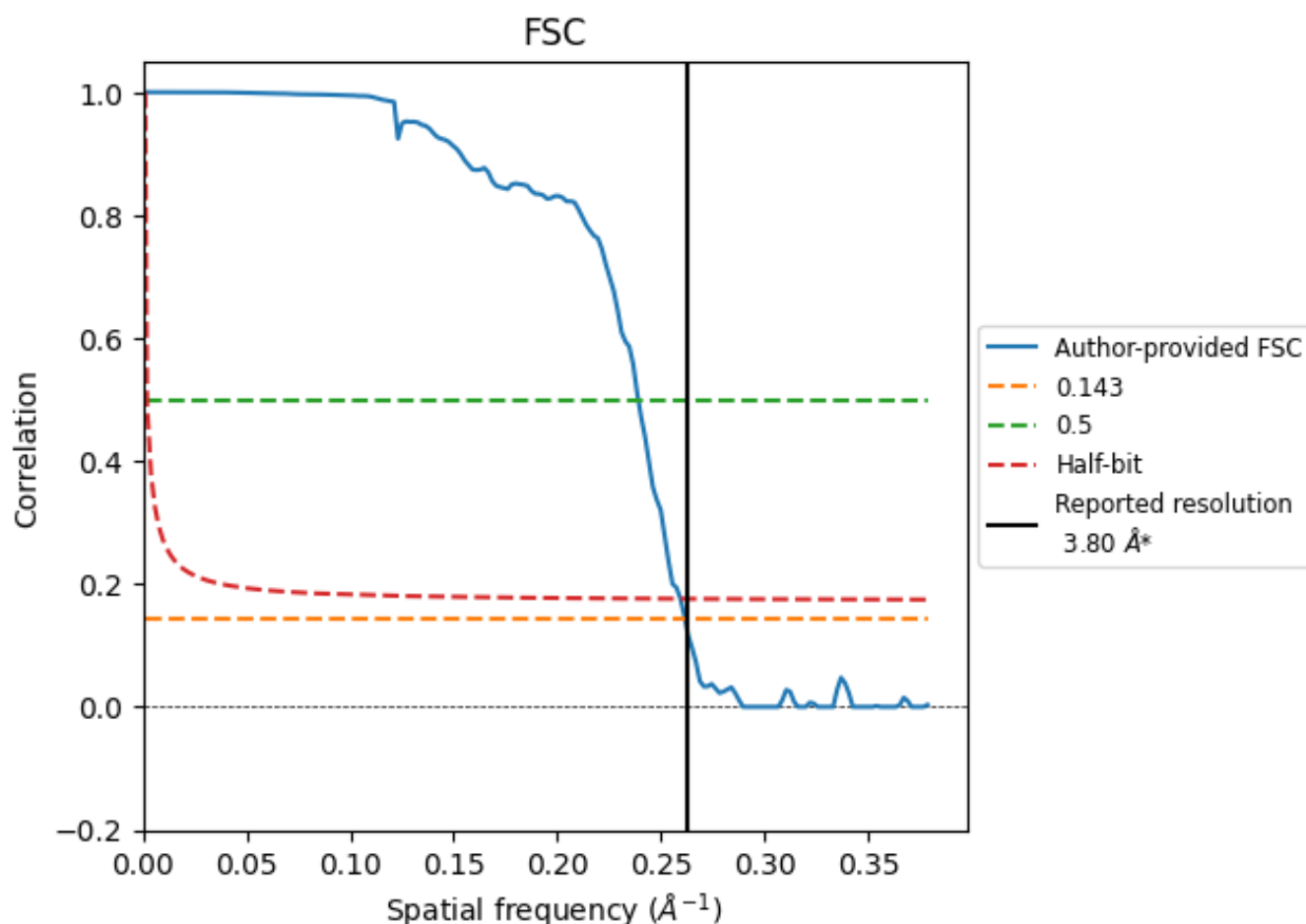


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

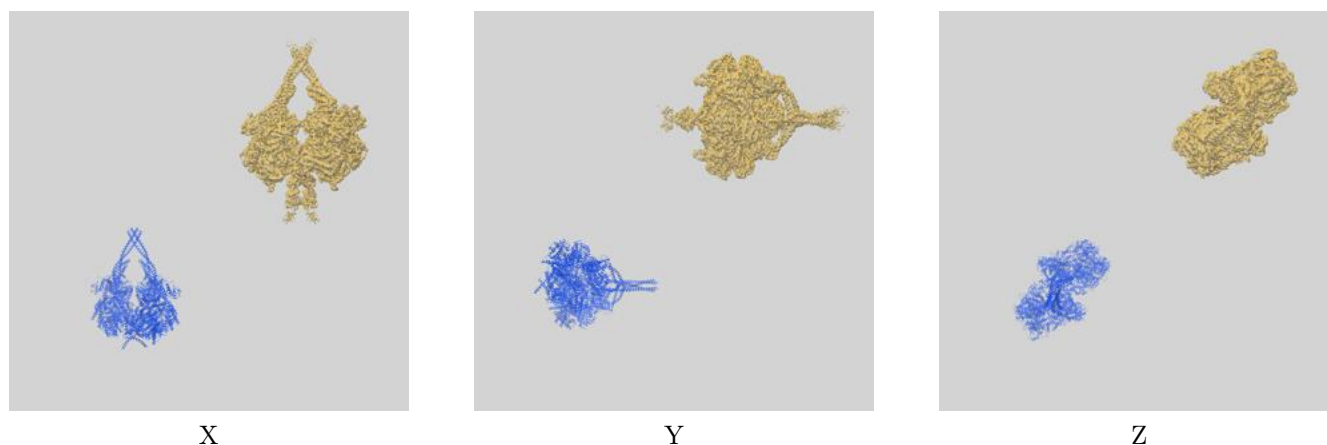
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.18	3.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

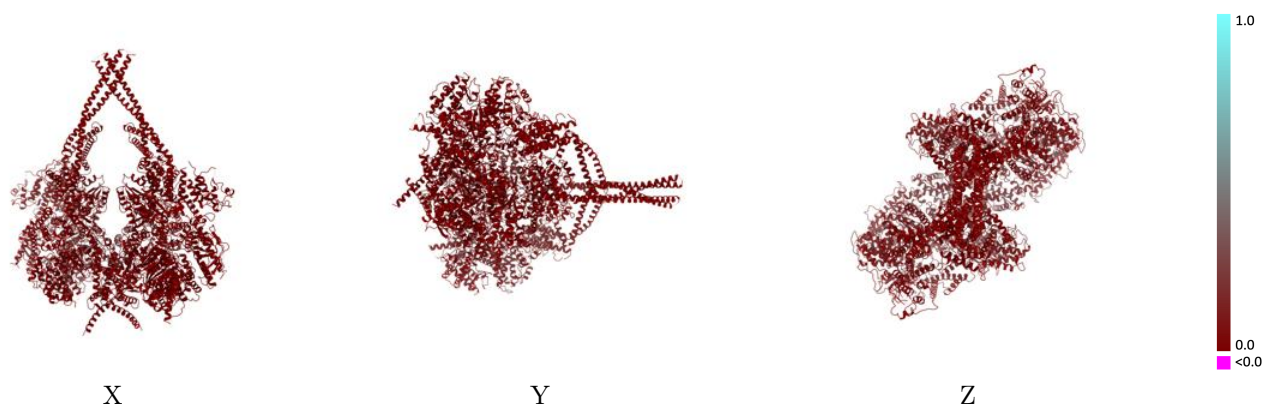
This section contains information regarding the fit between EMDB map EMD-3698 and PDB model 5NUG. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

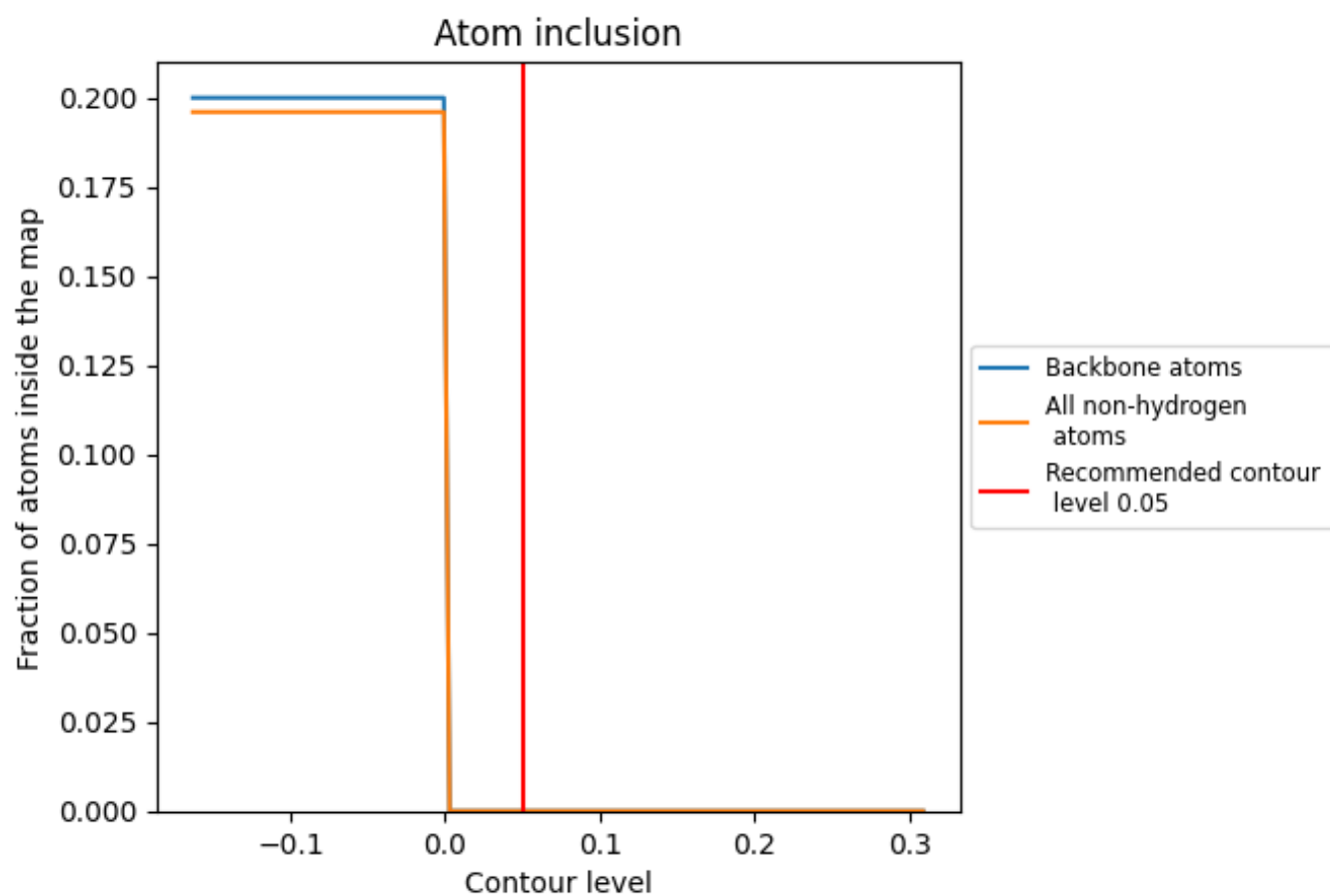


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0000
B	0.0000	0.0000

