



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2023 – 05:59 AM EDT

PDB ID : 3VKH
Title : X-ray structure of a functional full-length dynein motor domain
Authors : Kon, T.; Oyama, T.; Shimo-Kon, R.; Suto, K.; Kurisu, G.
Deposited on : 2011-11-16
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

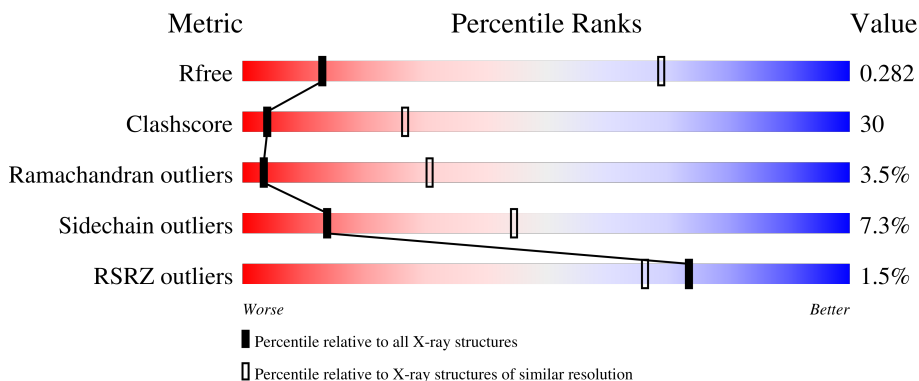
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3367	
1	B	3367	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 45974 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	3042	23374	14951	3955	4368	100	0	0	0
1	B	2908	22384	14307	3792	4190	95	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

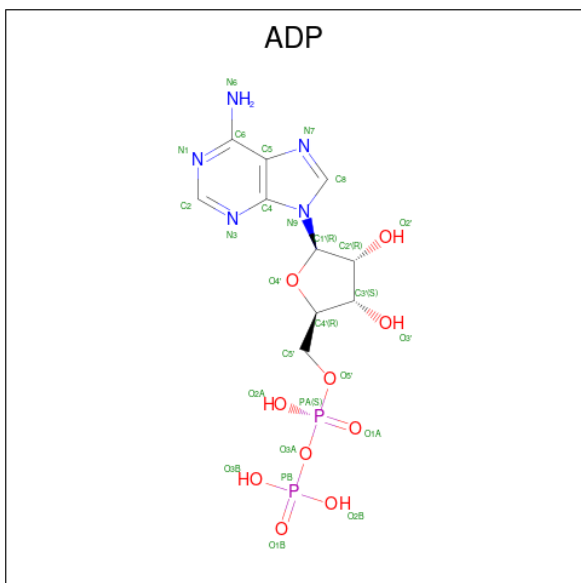
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	expression tag	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression tag	UNP P34036
A	1371	HIS	-	expression tag	UNP P34036
A	1372	HIS	-	expression tag	UNP P34036
A	1373	GLY	-	expression tag	UNP P34036
A	1374	GLY	-	expression tag	UNP P34036
A	1375	GLY	-	expression tag	UNP P34036
A	1376	ASP	-	expression tag	UNP P34036
A	1377	TYR	-	expression tag	UNP P34036
A	1378	LYS	-	expression tag	UNP P34036
A	1379	ASP	-	expression tag	UNP P34036
A	1380	ASP	-	expression tag	UNP P34036
A	1381	ASP	-	expression tag	UNP P34036
A	1382	ASP	-	expression tag	UNP P34036
A	1383	LYS	-	expression tag	UNP P34036
A	1384	GLY	-	expression tag	UNP P34036
A	1385	GLY	-	expression tag	UNP P34036
A	1386	GLY	-	expression tag	UNP P34036
A	1387	LYS	-	expression tag	UNP P34036
B	1364	MET	-	expression tag	UNP P34036

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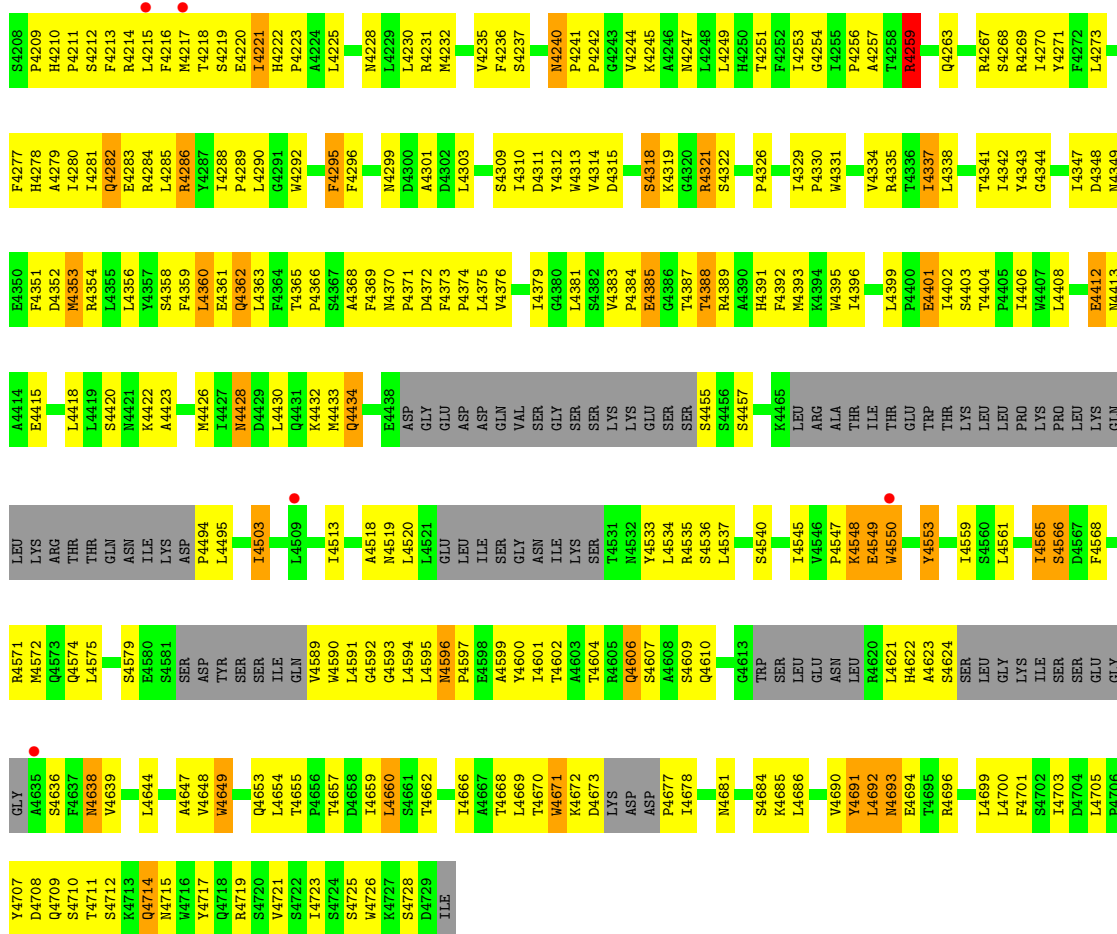
Chain	Residue	Modelled	Actual	Comment	Reference
B	1365	THR	-	expression tag	UNP P34036
B	1366	ARG	-	expression tag	UNP P34036
B	1367	HIS	-	expression tag	UNP P34036
B	1368	HIS	-	expression tag	UNP P34036
B	1369	HIS	-	expression tag	UNP P34036
B	1370	HIS	-	expression tag	UNP P34036
B	1371	HIS	-	expression tag	UNP P34036
B	1372	HIS	-	expression tag	UNP P34036
B	1373	GLY	-	expression tag	UNP P34036
B	1374	GLY	-	expression tag	UNP P34036
B	1375	GLY	-	expression tag	UNP P34036
B	1376	ASP	-	expression tag	UNP P34036
B	1377	TYR	-	expression tag	UNP P34036
B	1378	LYS	-	expression tag	UNP P34036
B	1379	ASP	-	expression tag	UNP P34036
B	1380	ASP	-	expression tag	UNP P34036
B	1381	ASP	-	expression tag	UNP P34036
B	1382	ASP	-	expression tag	UNP P34036
B	1383	LYS	-	expression tag	UNP P34036
B	1384	GLY	-	expression tag	UNP P34036
B	1385	GLY	-	expression tag	UNP P34036
B	1386	GLY	-	expression tag	UNP P34036
B	1387	LYS	-	expression tag	UNP P34036

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

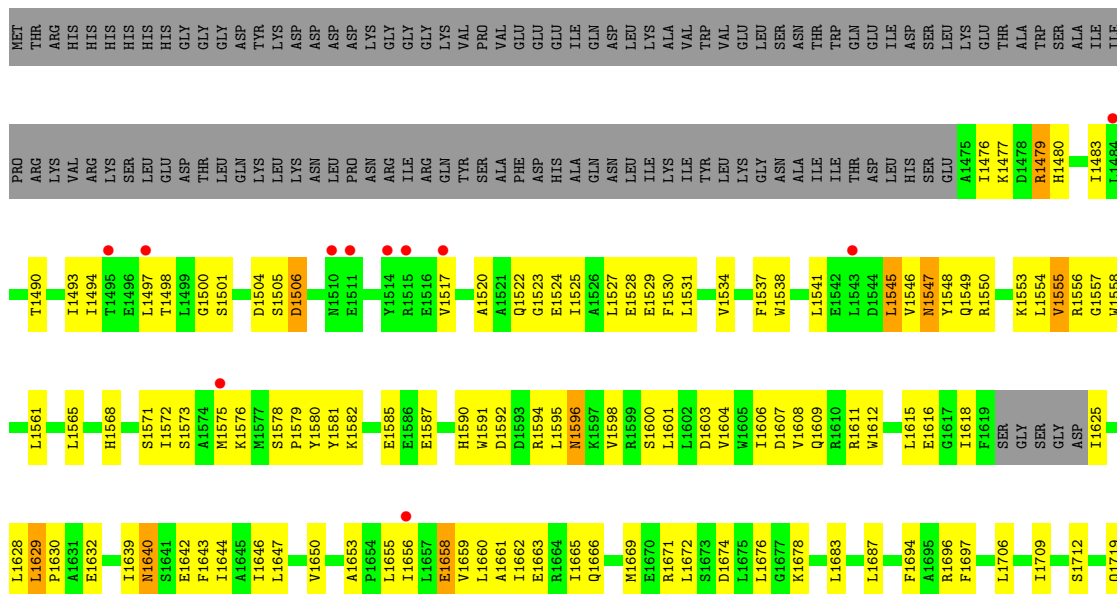


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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

L3108	M3109	C9112	K3113	E3114	T3115	A3116	Q3117	R3118	F3119	L3121	L3122	L3123	F3133	Q3136	K3140	H3141	H3142	V3143	V3144	F3145	T3146	N3147	K3148	P3149	A3150	S3151	F3152	F3154	H3155	K3156	R3157	S3158	L3164	F3165	N3166	R3167	C3168	V3169	L3170	D3171	K3172	F3173	G3174	E3175	E3179	A3180	V3184	Q3185	S3186					
R3027	F3028	M3032	N3033	G3034	L3035	S3036	L3037	F3038	T3039	I3040	K3041	V3042	M3043	S3048	Q2970	D3052	L3055	L3058	L3059	K3060	R3061	A3062	G3063	E3066	G3067	K3068	L3069	F3071	D3074	E3075	S3076	N3077	V3078	L3079	E3080	S3081	S3082	F3083	L3084	E3085	R3086	M3087	L3090	G3093	G3094	E3095	V3096	L3099						
R2948	F2949	L2950	L2951	N2952	S2953	N2954	W2955	L2956	P2962	S2966	D2967	L2968	R2969	E2970	Y2971	V2972	R2975	L2976	F2979	Y2980	D2985	T2986	P2987	L2988	V2989	L2990	D2995	G3002	N2992	M2993	F2994	L2995	L2998	Q3007	P3008	Q3009	Q3010	H3011	A3012	L3013	L3014	L3015	G3016	V3017	S3018	G3019	G3020	G3021	K3022	S3023	V3024	L3025	S3026	
H2871	Y2872	I2873	P2876	R2877	S2880	R2881	W2882	D2883	L2886	L2887	I2890	Q2891	T2892	M2893	D2894	G2895	C2896	T2897	L2898	V2899	R2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	L2899	
V2789	G2790	A2791	C2792	N2793	P2794	A2798	G2799	R2800	R2806	L2808	R2809	L2813	L2814	L2815	L2816	D2817	F2818	P2819	L2824	T2825	Q2826	L2827	Y2828	R2829	T2830	F2831	R2832	L2833	L2835	L2838	L2839	L2842	F2845	A2846	D2847	M2848	L2849	T2850	D2851	E2855	F2856	Y2857	R2863	F2864	L2868	Q2869	A2870							
L2710	L2711	K2712	T2713	Y2720	E2727	T2728	V2729	L2730	R2731	P2732	W2738	L2739	V2740	V2741	F2742	G2743	D2744	E2745	I2746	N2747	L2748	P2749	S2750	G2751	T2752	K2753	Y2754	G2755	T2756	V2759	I2760	F2762	Q2765	M2766	R2669	A2690	F2691	F2694	E2695	T2696	R2697	T2697	L2781	L2783	D2784	K2785	Q2786	E2708	L2709					
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N2547	V2548	I2549	E2550	T2551	M2560	S2561	P2562	E2563	Q2564	Q2565	T2570	N2571	L2572	L2573	L2574	L2575	M2578	W2579	G2580	L2581	G2582	E2583	G2584	E2585	L2586	L2587	R2590	E2591	K2595	Q2598	A2601	I2602	T2603	P2604	V2605	P2606	L2610	P2611	L2612	L2613	D2614	L2615	S2616	V2617	F2638	S2618	L2619	W2624	S2625	L2626	L2626			
K2323	T2324	W2327	T2328	D2329	F2332	T2335	R2338	L2339	I2340	D2341	N2342	V2343	E2346	K2349	R2350	D2351	V2352	I2353	G2357	D2358	V2359	D2360	T2361	E2362	W2363	V2364	N2366	L2367	N2368	S2369	L2370	L2371	N2374	K2375	L2376	L2377	T2378	L2379	P2380	N2381	G2382	E2383	R2384	L2385	A2386	L2387	V2391	R2392	V2393					
M2394	F2395	E2396	V2397	Q2398	D2399	L2400	K2401	Y2402	A2403	I2408	S2409	R2410	C2411	M2413	V2414	W2415	Q2424	M2425	I2426	L2431	D2432	T2433	S2435	R2436	E2437	F2438	F2439	Q2442	E2443	Q2446	Q2447	N2450	E2451	N2452	ALA	GLN	LEU	GLN	GLN	GLN	GLN	GLN	THR	THR	ILE	L2388	THR	PRU	ILE	LEU	THR			
S2169	GLN	LEU	PRO	PRO	ILE	THR	D2176	A2177	E2178	S2179	Y2190	V2194	L2195	L2196	L2197	S2198	L2199	N2200	D2201	E2202	M2203	L2204	P2205	K2206	L2207	T2208	D2211	L2212	P2213	L2214	I2215	L2218	L2219	L2220	D2221	V2222	F2223	P2224	L2228	Q2229	P2230	F2234	Q2236	P2308	K2239	L2243	R2247	H2248	L2249					
V2250	T2251	K2252	W2255	V2256	E2257	K2258	L2259	Q2260	Q2261	L2262	H2263	Q2264	L2266	N2269	H2270	G2271	D2272	M2273	M2274	V2275	S2278	K2282	T2283	T2284	S2285	W2286	E2287	V2288	Y2289	L2290	E2291	A2292	I2293	E2294	D2295	V2296	D2297	W2298	L2299	K2300	S2301	E2302	P2304	V2305	P2309	K2309	K2313	D2314	Q2315	L2316				
W2098	A2099	W2100	I2101	K2102	P2103	D2104	R2105	E2106	M2107	L2108	E2109	Q2110	V2111	M2112	L2113	S2114	W2115	F2118	K2119	T2120	A2121	E2122	M2123	L2124	A2125	L2126	L2127	L2128	V2129	F2130	K2133	L2134	C2135	Q2136	E2137	Q2138	L2139	S2140	A2141	Q2142	Q2143	H2144	Y2145	D2146	F2147	G2148	L2149	L2150	K2151	S2154	L2155	L2156	V2157	K2163



● Molecule 1: Dynein heavy chain, cytoplasmic



V2759	H2667	F2596	G2520	P2380	K2300	G2225	R2150	W2071	P1972	G1900	M1809	K1720
R2764	R2668	I2597	Q2521	M2381	S2301	SER	A2151	F2074	P1975	N1901	Y1810	H1721
Q2765	P2669	Q2598	R2522	G2382	H2304	GLN	L2152	V2075	P1976	K1902	P1811	F1722
M2766	T2670	T2599	E2383	E2384	V2305	L2228	K2153	T2076	G1978	D1903	T1812	M1725
	L2672	I2600	I2525	R2384	L2308	P2230	V2155	G2080	K1980	W1906	L1814	F1726
	D2676	T2603	D2527	L2387	F2308	I2231	L2156	Y2081	T1981	L1907	V1815	A1727
	P2676	P2604	F2528	V2391	K2309	Q2285	K2163	E2082	E1982	Y1908	L1816	G1728
	G2677	V2605	T2529	R2392	A2310	L2236	R2164	G2083	E1983	H1909	T1818	L1734
	L2684	L2610	R2530	V2393	T2312	R2237	K2165	R2084	T1984	O1911	S1819	D1735
	T2687	L2612	R2532	M2394	K2313	K2238	C2166	S2085	K1985	Y1914	Q1820	D1736
	L2688	L2613	V2533	F2395	R2314	K2239	GLN	W2086	Q1990	Y1914	I1821	D1736
	F2694	D2614	L2540	E2396	Q2315	I2240	PRO	L2091	L1991	E1919	T1739	
	E2695	V2615	M2541	V2397	E2241	E2241	PRO	L2091	G1992	N1920	T1740	
	V2696	S2616	N2542	Q2398	E2242	Q2243	GLN	F2095	R1992	N1920	I1741	
	L2699	V2617	V2546	L2400	A2244	A2244	PRO	R2096	R1993	V1921	I1741	
	W2700	D2620	M2547	K2401	W2327	V2280	PRO	S2097	V1997	H1923	I1742	
	F2701	A2622	V2548	Y2402	L2331	K2288	THR	M2098	C2000	I1925	L1831	
	A2704	N2623	I2549	T2407	L2331	K2288	ASP	M2100	D2001	V1926	I1841	
	T2705	E2624	E2550	S2409	T2335	Q2252	ALA	I2101	E2002	I1927	G1743	
	T2706	Q2553	Q2553	R2410	W2327	E2254	GLU	K2102	C2017	H1928	M1744	
	L2711	S2556	M2413	M2413	R2338	R2288	LYS	D2104	A2021	M1929	Q1844	
	F2714	F2558	V2415	V2414	I2339	I2289	THR	D2104	R2105	A1930	L1845	
	V2720	M2560	F2416	F2415	N2342	Q2261	LYS	E2106	F1938	N1932	Q1846	
	E2724	V2635	I2426	S2417	E2346	H2263	D2184	A2109	C2024	F1934	I1848	
	T2724	E2636	V2494	I2420	R2350	I2284	Q2185	W2112	R2029	Y1935	Q1850	
	T2724	T2638	V2494	L2421	R2350	I2284	Q2185	L2113	R2030	G1937	P1764	
	E2727	V2641	L2492	T2423	W2352	H2270	Q2271	W2114	L2031	F1938	I1765	
	V2728	A2642	M2495	Q2494	I2354	G2271	G2271	S2115	L2036	E1939	I1766	
	L2729	S2643	F2427	M2495	I2354	V2272	V2194	Q2116	L2036	Y1940	H1767	
	L2730	A2642	V2575	I2426	D2368	M2273	L2195	F2118	S2040	L1941	E1768	
	L2731	P2644	L2574	F2427	V2359	R2274	L2196	R2119	Q2044	G1942	W1769	
	L2732	D2644	V2576	L2431	D2360	G2276	S2198	T2120	Q2044	I1943	L1770	
	L2732	L2645	L2577	D2432	P2361	P2277	T2199	L2124	T2046	R1946	V1773	
	L2738	V2647	M2578	D2432	E2362	S2278	N2200	A2125	Q2047	V1948	M1777	
	L2739	G2560	G2579	D2440	V2364	G2280	M2203	G2126	V2048	Q1949	T1780	
	V2740	L2581	L2581	P2441	V2364	G2280	I2204	K2127	A2048	T1950	L1781	
	V2741	G2582	Q2504	Q2442	E2366	G2281	P2205	I2128	L2050	P1951	A1782	
	E2745	G2583	V2505	E2443	L2367	T2283	K2206	V2130	V2057	L1952	T1783	
	L2748	M2585	F2506	LYS	N2368	W2286	V2208	C2135	GLU	R1955	L1784	
	P2749	G2586	E2507	GLN	L2370	W2286	A2209	L2139	LEU	C1956	L1785	
	S2750	V2588	V2512	GLN	L2371	Y2289	D2210	L2139	LEU	Y1957	H1884	
	T2751	V2589	H2513	LYS	D2372	L2290	D2210	S2140	GLY	L1958	L1789	
	A2752	R2590	R2514	ARG	D2373	E2291	D2210	S2140	GLY	T1959	V1888	
	V2754	E2591	V2515	ASN	N2374	A2292	I2212	A2141	LYS	L1960	V1889	
	G2755	M2592	L2516	GLU	K2375	A2292	P2213	Q2142	N2064	T1961	M1793	
	L2756	W2663	E2517	ASN	L2376	V2286	L2219	H2144	L2067	Q1962	D1799	
	Q2757	L2664	E2518	ALA	T2377	M2298	F2223	Y2145	H2068	R1967	H1801	
	R2758	E2666	A2519	LEU	L2379	I2299	P2224	L2149	D2070	N1971	S1800	

K4082	L3947	M3585	L3170	S3082	L2999	F2913	L2838
L4033	F3948	S3586	D3171	F3083	R3000	Q2914	L2839
V4034	S3949	S3587	F3172	L3084	R3001	L2915	L2850
D4035	A3681	V3588	F3173	E3085	D3002	R2916	P2840
H4036	S3682	S3683	G3174	R3086	R3003	L2917	N2841
S4041	E3683	V3592	E3175	M3087	V3004	V2918	L2842
S4042	F3684	A3595	L3181	M3088	G3010	E2921	R2843
L4043	L3685	F3598	F3182	F3089	H3011	L2849	L2849
V4044	M3686	S3687	Q3183	L3090	H3012	T2850	T2850
K4045	M3687	F3598	Q3184	L3091	A3012	W2925	W2925
K4046	Q3688	V3601	S3184	A3092	L3013	D2926	D2926
F4047	F3689	Y3602	G3185	G3093	L3014	D2927	W2853
D4051	A3690	K3291	G3186	G3094	L3015	K2928	W2854
Q4052	D3691	L3292	E3187	E3095	G3016	K2929	E2855
V4053	K3692	R3293	L3192	VAL	S3017	L2930	F2856
P4056	K3693	D3294	L3193	PRO	S3018	D2931	F2856
I4057	K3694	L3295	E3195	GLY	S3023	E2932	Q2861
L4058	Q3607	T3295	N3196	LEU	V3024	V2933	R2863
P4059	Q3608	V3299	Y3199	PHE	L3025	A2934	R2864
E4060	M3614	L3302	P3202	GLY	S3026	L2935	T2865
I4063	M3617	L3306	P3202	E3103	R3027	H2937	T2866
V4064	M3618	L3309	M3212	E3104	F3028	F2938	D2867
A4067	R3620	K3313	GLY	F3105	V3029	P2939	L2868
Q4068	S3623	K3316	ASN	M3109	A3030	S2940	Q2869
L4069	F3628	L3318	ASN	C3112	L3035	V2941	Y2872
S4070	F3628	M3217	LEU	R3118	L3036	L2946	L2873
K4071	V3642	A3218	GLY	R3118	L3037	K2947	L2874
Q4072	E3544	I3219	LEU	ASN	Y3038	S2875	S2875
S4073	E3545	P3220	LEU	GLY	T3039	P2876	P2876
T4075	R3545	P3221	LEU	LEU	K3041	R2877	R2877
I4076	L3525	F3228	ASP	LEU	Y3042	S2880	S2880
M4079	Y3536	S3228	ASP	ASP	N3043	R2881	R2881
F4080	R3637	S3230	VAL	S3125	Y3046	W2882	W2882
K4081	L3638	L3231	VAL	L3129	D3050	D2883	D2883
L4082	S3639	L3232	ALA	L3129	M3057	L2886	L2886
L4084	V3647	Y3233	LEU	S3135	L3058	L2890	L2890
L4085	M3650	H3235	LEU	Q3136	L3059	Q2891	Q2891
M4086	L3652	Q3236	GLY	V3137	K3060	L2976	L2976
K4087	P3653	L3237	LYS	R3138	R3061	K2977	K2977
S4091	L3657	I3238	LYS	R3139	A3062	L2984	L2984
D4092	L3663	R3248	LYS	M3140	K3065	D2985	D2985
R4093	M3664	Y3254	TRP	F3145	C3064	E2986	E2986
L4094	M3667	V3255	ALA	S3151	K3066	C2990	C2990
L4095	F3668	T3257	ALA	A3159	E3066	L2901	L2901
Q4096	G3572	P3257	ALA	A3159	E3067	V2902	V2902
Q4097	R3573	R3258	LYS	T3160	K3068	R2990	R2990
S4098	V3574	G3259	LYS	T3161	L3069	L2991	L2991
P4028	E3575	Y3260	LYS	S3161	L3072	N2992	N2992
S4031	F3672	F3263	GLU	A3163	V3078	E2993	E2993
F4101	L3673	L3263	LYS	L3164	L3079	A2907	A2907
V4102	I3675	Q3584	ASN	M3165	E3080	E2968	E2968
						A2909	A2909
						H2997	H2997
						L2998	L2998

S4710	T4711	Q4714	N4715	W4716	Y4717	Q4718	W4721	S4722	I4723	S4724	S4725	S4728	D4729	ILE																																								
E4645	G4646	V4647	V4648	W4649	N4650	Q4653	T4657	D4658	I4659	L4660	S4661	T4662	P4663	I4664	S4665	I4666	A4667	T4668	L4669	W4671	K4672	D4673	K4674	D4675	ASP	PRO	I4685	L4686	S4687	V4688	P4689	V4690	Y4691	L4692	N4693	R4696	S4697	E4698	F4701	S4702	I4703	D4704	L4705	P4706	Y4707	D4708	A4643	Q4709						
M4572	Q4573	Q4574	L4575	S4576	S4581	SER	ASP	TYR	SER	SER	ILE	Q4588	V4589	L4590	L4591	G4592	G4593	M4596	P4597	I4601	T4604	S4607	L4611	L4614	SER	SER	LEU	L4621	H4622	A4623	S4624	LEU	GLY	LYS	ILE	SER	SER	GLY	ALA	S4636	F4637	M4638	V4639	M4642	A4643	L4644								
GLN	ASN	ILE	K4492	D4493	P4494	F4499	E4500	R4501	E4502	I4503	G4506	L4509	V4510	I4513	L4517	L4523	ILE	SER	GLY	ASN	I4529	S4530	T4531	R4535	S4536	L4537	S4540	I4541	S4542	K4543	G4544	I4545	K4548	E4549	W4550	K4551	W4552	Y4553	S4554	V4555	P4556	T4558	L4561	F4568	R4571									
R4424	K4425	M4426	I4427	N4428	D4429	L4430	Q4431	K4432	M4433	Q4434	E4437	GLU	ASP	GLY	ASP	ASP	GLN	VAL	SER	GLY	SER	SER	LYS	GLU	SER	SER	SER	S4486	E4459	A4464	K4465	LEU	ARG	ALA	THR	THR	GLU	TRP	THR	THR	LYS	LEU	LEU	PRO	LYS	PRO	L4410	P4411	E4412	M4413	N4414	E4415	K4422	A4423
T4341	I4342	Y4343	R4346	N4349	E4350	F4351	D4352	L4355	L4356	Y4357	S4358	F4359	L4360	E4361	Q4362	L4363	T4365	F4369	P4371	D4372	F4373	P4374	P4377	S4378	I4379	Q4380	L4381	T4388	R4389	A4390	H4391	P4400	I4401	S4403	T4404	P4405	I4406	W4407	L4408	G4409	L4410	P4411	E4412	M4413	N4414	E4415	K4422	A4423						
W4292	T4293	K4294	F4295	W4296	E4297	L4303	R4304	G4305	A4306	L4307	D4308	S4309	T4310	D4311	V4312	Y4313	W4314	D4315	S4318	S4322	M4323	I4324	D4327	I4328	I4329	P4330	W4331	T4332	A4333	V4334	M4335	T4336	I4337	L4338	G4339	S4340																		
L4192	A4193	P4194	L4197	L4200	E4201	S4206	A4207	L4208	I4211	S4208	P4209	F4213	R4214	L4215	F4216	M4217	T4218	S4219	E4220	L4221	H4222	W4223	A4224	L4225	P4226	A4227	N4228	L4229	L4230	R4231	M4232	V4235	F4236	S4237	Y4238	E4239	V4244	T4251	F4252	I4253	G4254	I4255	P4256	A4257	T4258	R4259	N4260	Q4263	P4264	A4265	E4266	R4267		
V4105	D4109	F4110	L4111	N4112	T4113	N4118	A4119	N4120	L4121	V4122	E4125	K4124	E4125	S4128	P4131	L4132	L4133	L4134	C4135	S4136	V4137	P4138	D4141	A4142	S4143	S4144	K4145	W4146	D4147	L4148	L4149	L4153	K4155	Q4156	H4154	Y4157	L4162	G4163	G4167	L4170	A4171	T4183	W4184	V4185	K4188	N4189	L4190	H4191						

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	195.73Å 228.96Å 201.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.80 48.78 – 3.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.79-3.80) 99.0 (48.78-3.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 3.77Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.292 0.211 , 0.282	Depositor DCC
R_{free} test set	4469 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	125.1	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 112.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.001 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	45974	wwPDB-VP
Average B, all atoms (Å ²)	138.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.24	0/23866	0.44	1/32482 (0.0%)
1	B	0.24	0/22846	0.43	0/31076
All	All	0.24	0/46712	0.44	1/63558 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3371	PRO	N-CA-CB	5.32	109.68	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23374	0	22545	1559	0
1	B	22384	0	21550	1149	0
2	A	108	0	48	7	0
2	B	108	0	48	3	0
All	All	45974	0	44191	2704	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 30.

All (2704) 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:3689:TYR:HB2	1:A:3694:ILE:HD11	1.29	1.14
1:A:3337:LYS:HB3	1:A:3525:LEU:HD13	1.35	1.07
1:B:3841:ALA:O	1:B:3842:SER:HB2	1.54	1.04
1:A:4242:PRO:HA	1:A:4286:ARG:HH12	1.22	1.03
1:A:4109:ASP:HA	1:A:4112:ASN:HD22	1.22	1.00
1:A:3373:ILE:HD13	1:A:3373:ILE:H	1.29	0.98
1:A:3673:LEU:HB2	1:A:3781:VAL:HG11	1.45	0.97
1:B:1959:THR:HG22	1:B:4341:THR:HA	1.46	0.96
1:B:1554:LEU:HB3	1:B:1609:GLN:HE22	1.29	0.95
1:B:4251:THR:HG23	1:B:4303:LEU:HD21	1.46	0.95
1:B:1928:HIS:CD2	1:B:1933:THR:HG22	2.02	0.95
1:A:4375:LEU:HD11	1:A:4383:VAL:HG23	1.48	0.95
1:B:3673:LEU:HB2	1:B:3781:VAL:HG11	1.44	0.95
1:A:3425:LYS:HD2	1:A:3428:GLU:HG3	1.49	0.94
1:B:2533:VAL:HB	1:B:2581:LEU:HD22	1.51	0.93
1:B:1655:LEU:HB2	1:B:1658:GLU:HB2	1.45	0.93
1:B:4574:GLN:HE22	1:B:4590:TRP:H	1.15	0.93
1:B:4121:ILE:HA	1:B:4125:GLU:HG3	1.48	0.93
1:A:2274:MET:HE3	1:A:2286:TRP:HB3	1.50	0.92
1:B:1972:PRO:HG2	1:B:2076:THR:HG22	1.52	0.92
1:A:4270:ILE:HA	1:A:4273:LEU:HD12	1.52	0.90
1:B:1789:LEU:HD23	1:B:1818:THR:HG23	1.50	0.90
1:A:3837:ALA:HB1	1:A:3850:SER:HB3	1.53	0.89
1:A:1639:ILE:HG23	1:A:1672:LEU:HD22	1.53	0.89
1:A:2313:LYS:HE3	1:A:2366:ASN:HD21	1.36	0.89
1:A:3018:SER:HB2	1:A:3256:THR:HG21	1.52	0.89
1:A:4495:LEU:H	1:A:4495:LEU:HD12	1.38	0.89
1:A:2890:ILE:HA	1:A:2893:MET:HE2	1.55	0.89
1:B:3930:LEU:HB3	1:B:3939:ARG:HH21	1.37	0.89
1:A:2200:ASN:HD22	1:A:2228:LEU:HD13	1.36	0.88
1:B:1813:GLN:HE22	1:B:1940:TYR:HA	1.37	0.88
1:B:2603:THR:HG22	1:B:2604:PRO:HD2	1.54	0.88
1:A:1690:GLN:HE22	1:A:1766:ILE:HG21	1.38	0.88
1:A:4046:GLN:HE22	1:A:4057:ILE:H	1.19	0.88
1:A:2447:GLN:HA	1:A:2450:ASN:HD22	1.39	0.88
1:B:4270:ILE:HG22	1:B:4310:ILE:HD13	1.55	0.88
1:B:1524:GLU:HG2	1:B:1580:TYR:HB3	1.57	0.87
1:A:3552:LYS:HA	1:A:3555:ASN:HD22	1.40	0.87
1:A:2570:THR:HG21	1:A:2603:THR:HG21	1.57	0.86
1:A:2914:GLN:HB2	1:A:2926:THR:HG21	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2381:ASN:HD21	1:B:2383:GLU:HB2	1.40	0.86
1:A:2200:ASN:HB2	1:A:2228:LEU:HD22	1.56	0.86
1:B:4604:THR:HG23	1:B:4671:TRP:HE1	1.40	0.86
1:A:4621:LEU:HD21	1:A:4669:LEU:HD23	1.55	0.86
1:B:3271:ILE:HG13	1:B:3592:VAL:HG11	1.57	0.86
1:A:2293:ILE:HG22	1:A:2350:ARG:HH22	1.41	0.85
1:B:4109:ASP:HA	1:B:4112:ASN:ND2	1.92	0.85
1:A:4686:LEU:HD21	1:A:4721:VAL:HG11	1.59	0.85
1:A:3809:THR:HA	1:A:3812:LYS:HE2	1.59	0.84
1:A:2560:MET:HG3	1:A:2561:SER:H	1.42	0.84
1:A:4251:THR:HG23	1:A:4303:LEU:HD21	1.58	0.84
1:B:2525:ILE:HD11	1:B:2815:LEU:HB2	1.58	0.84
1:A:4648:VAL:HG12	1:A:4662:THR:HG21	1.60	0.83
1:B:2841:ASN:ND2	1:B:2842:LEU:H	1.75	0.83
1:A:2910:LEU:HD23	1:A:2930:ILE:HD12	1.59	0.83
1:B:3930:LEU:HD11	1:B:3943:LEU:HD21	1.59	0.83
1:B:4548:LYS:HD2	1:B:4549:GLU:N	1.93	0.83
1:A:3718:LEU:HG	1:A:3719:LEU:H	1.42	0.83
1:B:4402:ILE:H	1:B:4402:ILE:HD12	1.42	0.83
1:A:4109:ASP:HA	1:A:4112:ASN:ND2	1.95	0.82
1:A:4190:ILE:HG12	1:A:4219:SER:HB3	1.61	0.82
1:A:3981:ASN:HD22	1:A:4076:ILE:HB	1.44	0.82
1:B:3785:ASN:HD21	1:B:3787:THR:HG23	1.43	0.82
1:B:2250:VAL:HB	1:B:2425:MET:HG3	1.60	0.82
1:B:1926:VAL:HG22	1:B:1935:TYR:CE2	2.15	0.82
1:A:3652:LEU:HD12	1:A:3653:PRO:HD2	1.62	0.82
1:B:1781:LEU:HG	1:B:1814:LEU:HD11	1.61	0.81
1:A:2651:VAL:HG13	1:A:2652:ASP:H	1.44	0.81
1:B:4657:THR:HG22	1:B:4659:ILE:H	1.45	0.81
1:A:3788:VAL:HG21	1:A:3913:LEU:HD22	1.61	0.81
1:A:4185:VAL:HG12	1:A:4186:LEU:H	1.44	0.81
1:B:2129:VAL:HG22	1:B:2130:PRO:HD3	1.62	0.81
1:B:4335:ARG:HH21	1:B:4365:THR:HG22	1.46	0.81
1:A:2371:LEU:CB	1:A:2410:ARG:HG3	2.10	0.81
1:A:3238:ILE:HG12	1:A:3601:TYR:CD2	2.16	0.81
1:A:3700:LEU:HD22	1:A:3701:ASP:H	1.43	0.80
1:A:3789:THR:HB	1:A:3790:PRO:HD2	1.63	0.80
1:A:2140:SER:HB2	1:A:2142:GLN:HE22	1.45	0.80
1:A:2857:TYR:HA	1:A:2913:PHE:HE1	1.46	0.80
1:A:2370:LEU:HD21	1:A:2387:LEU:HD13	1.64	0.80
1:A:4654:LEU:HD11	1:A:4705:LEU:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1660:LEU:HA	1:B:1665:ILE:HD11	1.63	0.80
1:A:2236:LEU:HD21	1:A:2293:ILE:HD13	1.63	0.80
1:A:3694:ILE:HG12	1:A:3717:PRO:HB2	1.63	0.80
1:A:4654:LEU:HD13	1:A:4686:LEU:HD23	1.62	0.79
1:A:2110:GLN:HG3	1:A:2122:GLU:HA	1.64	0.79
1:B:3607:GLN:HG2	1:B:3657:LEU:HD22	1.65	0.79
1:B:4270:ILE:HD11	1:B:4329:ILE:HD13	1.65	0.79
1:A:4086:MET:HG3	1:A:4093:ARG:HB2	1.65	0.79
1:A:4349:ASN:HD21	1:A:4351:PHE:HB2	1.46	0.79
1:A:2300:LYS:O	1:A:2349:LYS:HB2	1.81	0.79
1:B:4189:ASN:H	1:B:4218:THR:HG22	1.47	0.79
1:B:3844:ASN:O	1:B:3848:ASP:HB3	1.81	0.79
1:A:4353:MET:HE3	1:A:4356:LEU:HD23	1.64	0.78
1:A:2283:THR:HA	1:A:2286:TRP:HE1	1.48	0.78
1:A:2706:THR:HB	1:A:2707:PRO:HD2	1.65	0.78
1:A:2886:LEU:O	1:A:2890:ILE:HG12	1.84	0.78
1:B:2106:GLU:OE1	1:B:2129:VAL:HG21	1.82	0.78
1:B:4264:PRO:HB3	1:B:4323:ASN:HA	1.64	0.78
1:A:3673:LEU:HB2	1:A:3781:VAL:CG1	2.14	0.78
1:B:2657:VAL:HG13	1:B:2687:THR:HG23	1.64	0.78
1:B:3338:GLN:HG2	1:B:3525:LEU:HD13	1.65	0.78
1:A:1823:TRP:O	1:A:1827:VAL:HG23	1.84	0.78
1:A:2204:ILE:HA	1:A:2207:LEU:HD12	1.65	0.78
1:A:2705:THR:HA	1:A:2709:LEU:HD12	1.66	0.78
1:A:1796:ASP:HB3	1:A:1799:ASP:HB3	1.65	0.77
1:A:4575:LEU:H	1:A:4575:LEU:HD12	1.49	0.77
1:B:2578:MET:HB3	1:B:2597:ILE:HD12	1.65	0.77
1:B:4332:ILE:HD12	1:B:4332:ILE:H	1.48	0.77
1:B:4121:ILE:O	1:B:4125:GLU:HB2	1.85	0.77
1:B:3219:ILE:CB	1:B:3220:PRO:HD3	2.15	0.77
1:A:2766:MET:HB3	1:A:2783:LEU:HD11	1.67	0.76
1:A:4318:SER:HA	1:A:4321:ARG:HH21	1.50	0.76
1:A:3058:LEU:HD21	1:A:3141:LEU:HD11	1.67	0.76
1:A:3384:LYS:HD3	1:A:3386:LYS:HD3	1.66	0.76
1:B:3230:SER:HA	1:B:3620:ARG:HE	1.51	0.76
1:B:3313:LEU:HD13	1:B:3550:SER:HA	1.65	0.76
1:A:2505:TYR:O	1:A:2512:VAL:HG23	1.85	0.76
1:A:1959:THR:HA	1:A:4341:THR:OG1	1.85	0.76
1:B:3671:TYR:O	1:B:3781:VAL:HG13	1.86	0.76
1:B:4046:GLN:HG3	1:B:4047:PHE:N	2.00	0.76
1:B:4531:THR:O	1:B:4535:ARG:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2863:ARG:O	1:A:2863:ARG:HD3	1.84	0.76
1:B:4067:ALA:HB1	1:B:4073:GLN:HG3	1.65	0.76
1:B:3639:SER:HB3	1:B:3663:ILE:HD11	1.68	0.76
1:A:1813:GLN:HE22	1:A:1940:TYR:HA	1.50	0.75
1:A:3927:ASN:HB3	1:A:3930:LEU:HB2	1.68	0.75
1:B:1822:VAL:HG22	1:B:1826:GLN:HE21	1.50	0.75
1:A:3731:ASN:HD22	1:A:3731:ASN:H	1.35	0.75
1:A:4122:VAL:HG21	1:A:4216:PHE:CZ	2.20	0.75
1:B:4011:LEU:HD11	1:B:4041:SER:HB2	1.68	0.75
1:A:2273:MET:HB2	1:A:2395:PHE:HB2	1.68	0.75
1:B:3027:ARG:HA	1:B:3037:ILE:HD11	1.68	0.75
1:B:3966:THR:HG22	1:B:4426:MET:HG3	1.68	0.75
1:B:2426:ILE:H	1:B:2426:ILE:HD12	1.51	0.75
1:A:3358:GLN:HA	1:A:3361:LYS:HE2	1.69	0.75
1:A:3443:MET:HG3	1:A:3449:ARG:HG3	1.68	0.75
1:A:3039:THR:HG22	1:A:3040:ILE:H	1.50	0.75
1:A:4622:HIS:HE2	1:A:4678:ILE:HG21	1.50	0.75
1:A:4648:VAL:HG13	1:A:4657:THR:HG21	1.68	0.75
1:B:3766:THR:HG22	1:B:3768:ASP:H	1.52	0.75
1:B:3035:LEU:HD22	1:B:3068:LYS:HB3	1.68	0.75
1:A:2586:GLY:HA2	1:A:2815:LEU:HD13	1.67	0.75
1:B:1950:THR:HB	1:B:1951:PRO:HD2	1.68	0.75
1:A:3015:ILE:HD13	1:A:3147:MET:HG3	1.68	0.74
1:B:2315:GLN:HB3	1:B:2775:THR:HG21	1.69	0.74
1:A:2397:VAL:HG21	1:A:2400:LEU:HD21	1.68	0.74
1:A:3696:LYS:HZ2	1:A:4206:SER:HB3	1.52	0.74
1:B:2638:THR:HG21	1:B:2838:LEU:HD21	1.68	0.74
1:A:1547:ASN:HA	1:A:1553:LYS:HG2	1.70	0.74
1:B:1476:ILE:HG23	1:B:1480:HIS:HB2	1.68	0.74
1:A:2105:ARG:HG2	1:A:2105:ARG:HH11	1.53	0.74
1:A:3774:THR:HB	1:A:3775:PRO:HD2	1.70	0.73
1:A:4122:VAL:HG21	1:A:4216:PHE:HZ	1.53	0.73
1:B:4278:HIS:HD2	1:B:4343:TYR:OH	1.71	0.73
1:A:2309:LYS:HE2	1:A:2756:THR:HG21	1.68	0.73
1:A:4053:VAL:O	1:A:4053:VAL:HG12	1.86	0.73
1:A:3388:LEU:HD23	1:A:3473:ALA:HB1	1.68	0.73
1:A:2793:ASN:HD22	1:A:2793:ASN:N	1.85	0.73
1:A:3725:ASN:HD22	1:A:3725:ASN:H	1.35	0.73
1:A:3281:GLU:HB3	1:A:3581:PHE:HE1	1.54	0.73
1:A:1886:ARG:HG3	1:A:1887:ASP:N	2.04	0.73
1:B:3700:LEU:HD13	1:B:3701:ASP:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3202:PRO:HD2	1:A:3624:VAL:O	1.88	0.73
1:B:3602:ILE:HG23	1:B:3610:ARG:HG2	1.70	0.73
1:A:2675:PRO:HD2	1:A:2816:VAL:O	1.88	0.73
1:A:3453:THR:HA	1:A:3457:LEU:HB2	1.70	0.73
1:B:2309:LYS:NZ	1:B:2756:THR:HG21	2.04	0.73
1:B:2572:ARG:HG2	1:B:2617:VAL:HG11	1.69	0.73
1:B:4157:TYR:HB3	1:B:4184:TRP:HB2	1.71	0.73
1:A:2080:GLY:HA3	1:A:2084:ARG:O	1.89	0.73
1:B:3789:THR:HB	1:B:3790:PRO:HD2	1.70	0.73
1:B:4189:ASN:N	1:B:4189:ASN:HD22	1.85	0.73
1:A:3475:GLY:O	1:A:3478:VAL:HG12	1.88	0.73
1:A:4024:ARG:HD3	1:A:4034:VAL:HG21	1.71	0.73
1:B:3584:GLN:O	1:B:3588:VAL:HG23	1.87	0.73
1:B:2514:LYS:HE2	1:B:2600:ILE:HD11	1.71	0.72
1:A:1655:LEU:HB2	1:A:1658:GLU:HB2	1.69	0.72
1:A:1883:VAL:HG11	1:A:2111:VAL:HG22	1.70	0.72
1:A:3281:GLU:HB3	1:A:3581:PHE:CE1	2.24	0.72
1:A:3724:GLU:OE2	1:A:3766:THR:HG23	1.88	0.72
1:B:4136:SER:HB3	1:B:4238:TYR:HB2	1.72	0.72
1:B:1899:THR:HB	1:B:1903:ASP:HB2	1.72	0.72
1:B:2938:PHE:O	1:B:2941:VAL:HG12	1.88	0.72
1:B:4005:ILE:HD13	1:B:4020:LEU:HD23	1.70	0.72
1:A:2042:GLN:HE21	1:A:2059:LEU:HD11	1.54	0.72
1:B:2841:ASN:HD22	1:B:2842:LEU:H	1.37	0.72
1:A:1763:GLY:N	1:A:1764:PRO:HD3	2.04	0.72
1:A:2587:LEU:HG	1:A:2817:ASP:HB2	1.72	0.71
1:A:2626:LEU:H	1:A:2626:LEU:HD12	1.55	0.71
1:A:3700:LEU:HD13	1:A:3701:ASP:N	2.04	0.71
1:B:3292:LEU:HD13	1:B:3571:ARG:HA	1.72	0.71
1:B:4601:ILE:O	1:B:4604:THR:HG22	1.90	0.71
1:A:2042:GLN:NE2	1:A:2059:LEU:HD11	2.06	0.71
1:A:1742:ILE:HG22	1:A:1753:THR:HG22	1.71	0.71
1:A:3555:ASN:HB3	1:A:3559:ARG:NH1	2.04	0.71
1:A:4347:ILE:HG21	1:A:4353:MET:HG2	1.72	0.71
1:B:2839:LEU:HD13	1:B:2842:LEU:HD12	1.70	0.71
1:B:4506:GLY:O	1:B:4510:VAL:HG23	1.91	0.71
1:A:2371:LEU:HB3	1:A:2410:ARG:HG3	1.71	0.71
1:B:3700:LEU:HD22	1:B:3701:ASP:H	1.54	0.71
1:A:1807:VAL:HG13	1:A:1815:VAL:HG11	1.73	0.71
1:A:2208:VAL:HA	1:A:2415:TRP:CD1	2.24	0.71
1:A:2283:THR:HA	1:A:2286:TRP:NE1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3674:VAL:HG22	1:B:3784:VAL:HB	1.71	0.71
1:A:4242:PRO:HA	1:A:4286:ARG:NH1	2.01	0.71
1:A:4553:TYR:HD1	1:A:4553:TYR:H	1.38	0.71
1:B:3234:ILE:HG23	1:B:3617:TRP:NE1	2.06	0.71
1:A:2176:ASP:N	1:A:2179:SER:HG	1.87	0.71
1:A:2258:LYS:HA	1:A:2261:GLN:HG3	1.71	0.71
1:A:3859:LYS:O	1:A:3862:THR:HG22	1.90	0.71
1:A:4533:TYR:O	1:A:4537:LEU:HG	1.90	0.71
1:B:4157:TYR:CB	1:B:4184:TRP:HB2	2.21	0.71
1:A:3037:ILE:HD13	1:A:3037:ILE:H	1.56	0.71
1:A:4591:LEU:HD21	1:A:4601:ILE:HD11	1.72	0.71
1:A:2942:ASN:O	1:A:2944:ASP:N	2.24	0.71
1:A:4029:SER:HB2	1:A:4081:ARG:HH12	1.56	0.71
1:B:4703:ILE:HD12	1:B:4705:LEU:HD21	1.71	0.71
1:B:2282:LYS:HA	1:B:2416:PHE:CD1	2.26	0.71
1:A:4494:PRO:HG2	1:A:4607:SER:HA	1.73	0.70
1:B:2124:LEU:HD22	1:B:2195:LEU:HD22	1.71	0.70
1:B:4574:GLN:HE22	1:B:4590:TRP:N	1.89	0.70
1:B:1823:TRP:CD1	1:B:1885:GLN:HB3	2.26	0.70
1:A:1879:ILE:O	1:A:1883:VAL:HG23	1.91	0.70
1:A:2006:LEU:HD23	1:A:2035:ILE:HG23	1.73	0.70
1:A:2371:LEU:HB2	1:A:2410:ARG:HG3	1.71	0.70
1:A:4540:SER:HB2	1:A:4545:ILE:O	1.91	0.70
1:B:1879:ILE:O	1:B:1883:VAL:HG23	1.91	0.70
1:B:3238:ILE:CG2	1:B:3255:VAL:HG11	2.20	0.70
1:A:2113:LEU:HD21	1:A:2156:LEU:HD22	1.74	0.70
1:A:2788:PHE:O	1:A:2789:VAL:HG23	1.90	0.70
1:A:3153:ASP:HA	1:A:3156:ASN:ND2	2.06	0.70
1:A:3677:PRO:HG3	1:A:3787:THR:HG22	1.72	0.70
1:A:4095:LEU:HD11	1:A:4422:LYS:HB3	1.73	0.70
1:A:4649:TRP:HA	1:A:4649:TRP:CE3	2.27	0.70
1:A:2106:GLU:H	1:A:2106:GLU:CD	1.95	0.70
1:A:2954:ASN:H	1:A:2954:ASN:HD22	1.39	0.70
1:A:2308:PRO:HD2	1:A:2357:GLY:HA3	1.74	0.70
1:A:4179:ALA:HB1	1:A:4209:PRO:HB3	1.73	0.70
1:A:3380:VAL:HG11	1:A:3435:ILE:HG21	1.72	0.70
1:A:3812:LYS:O	1:A:3816:LEU:HB3	1.91	0.70
1:B:1928:HIS:NE2	1:B:1933:THR:HG22	2.06	0.70
1:A:3331:GLN:HE22	1:A:3533:LYS:HG3	1.56	0.69
1:A:4086:MET:CG	1:A:4093:ARG:HB2	2.21	0.69
1:B:2850:THR:O	1:B:2854:VAL:HG23	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3433:THR:HG22	1:A:3437:ASN:ND2	2.06	0.69
1:B:1687:LEU:HD21	1:B:1706:LEU:HD23	1.74	0.69
1:B:2540:LEU:HD23	1:B:2576:SER:HA	1.72	0.69
1:A:1846:GLN:HA	1:A:1893:GLN:NE2	2.08	0.69
1:A:4128:SER:HB2	1:A:4213:PHE:HB3	1.74	0.69
1:B:1739:THR:HB	1:B:1761:ALA:HB2	1.74	0.69
1:B:3700:LEU:H	1:B:3700:LEU:HD12	1.58	0.69
1:B:2235:GLN:NE2	1:B:2296:VAL:HG13	2.06	0.69
1:A:3912:SER:HB3	1:A:4231:ARG:HG2	1.75	0.69
1:B:1846:GLN:O	1:B:1850:GLN:HG2	1.92	0.69
1:B:3238:ILE:HG12	1:B:3601:TYR:CG	2.28	0.69
1:A:2028:PHE:HB3	1:A:2075:VAL:HG13	1.72	0.69
1:B:1534:VAL:HG13	1:B:1568:HIS:HD2	1.58	0.69
1:B:3238:ILE:HG21	1:B:3255:VAL:HG11	1.73	0.69
1:B:3256:THR:HB	1:B:3257:PRO:HD2	1.74	0.69
1:B:3768:ASP:HB3	1:B:3771:ALA:HB2	1.73	0.69
1:A:1746:SER:OG	1:A:1750:GLU:HB3	1.93	0.69
1:A:2202:THR:HG22	1:A:2265:ILE:HG12	1.74	0.69
1:B:2200:ASN:HB2	1:B:2228:LEU:HD22	1.75	0.69
1:B:2282:LYS:HA	1:B:2416:PHE:HD1	1.57	0.69
1:A:4623:ALA:HB2	1:A:4703:ILE:HD11	1.75	0.69
1:A:1770:LEU:O	1:A:1773:VAL:HG22	1.93	0.69
1:B:4005:ILE:CD1	1:B:4020:LEU:HD23	2.24	0.68
1:A:2748:LEU:HD21	1:A:2800:ARG:NH1	2.09	0.68
1:B:3724:GLU:OE2	1:B:3766:THR:HG23	1.93	0.68
1:B:4362:GLN:HB2	1:B:4714:GLN:NE2	2.08	0.68
1:B:2865:THR:H	1:B:2868:ILE:HD12	1.58	0.68
1:B:4574:GLN:NE2	1:B:4590:TRP:H	1.87	0.68
1:A:1886:ARG:NH1	1:A:1890:ARG:HH22	1.91	0.68
1:B:3652:LEU:HD12	1:B:3653:PRO:HD2	1.74	0.68
1:A:3210:GLU:HG3	1:A:3211:ILE:H	1.57	0.68
1:B:1545:LEU:HD12	1:B:1545:LEU:H	1.57	0.68
1:B:3043:ASN:ND2	1:B:3046:TYR:HB2	2.07	0.68
1:A:1554:LEU:HB3	1:A:1609:GLN:HE21	1.59	0.68
1:A:2010:SER:HB3	1:A:2060:LEU:HD21	1.75	0.68
1:B:1743:GLY:HA2	1:B:1754:PHE:CD1	2.29	0.68
1:B:2320:LEU:O	1:B:2320:LEU:HD23	1.93	0.68
1:A:4200:LEU:HD22	1:A:4204:LEU:HD11	1.75	0.68
1:A:1715:ILE:HD11	1:A:1760:ILE:HD13	1.74	0.68
1:A:1931:ASN:OD1	1:A:1962:GLN:NE2	2.25	0.68
1:A:2293:ILE:CG2	1:A:2350:ARG:HH22	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2400:LEU:HD13	1:B:2408:ILE:HD11	1.76	0.68
1:A:1846:GLN:HA	1:A:1893:GLN:HE22	1.59	0.67
1:A:2742:PHE:HA	1:A:2789:VAL:O	1.94	0.67
1:A:3961:ASN:O	1:A:3964:LYS:HB2	1.94	0.67
1:A:2699:LEU:HD11	1:A:2713:THR:HG21	1.77	0.67
1:A:3013:LEU:HD12	1:A:3145:PHE:HB3	1.74	0.67
1:B:2231:ILE:HG21	1:B:2264:GLN:NE2	2.09	0.67
1:A:2212:ILE:HG22	1:A:2213:PRO:HD3	1.77	0.67
1:B:4251:THR:HG23	1:B:4303:LEU:CD2	2.23	0.67
1:A:3563:LEU:HD11	1:A:3851:VAL:HG22	1.77	0.67
1:B:2793:ASN:HB3	1:B:2794:PRO:HD2	1.76	0.67
1:A:1963:ALA:HB1	1:A:2096:ARG:HG3	1.76	0.67
1:A:2447:GLN:HE22	1:A:2492:LEU:HD23	1.58	0.67
1:A:3397:PRO:HG2	1:A:3419:TRP:CZ2	2.29	0.67
1:B:4189:ASN:H	1:B:4218:THR:CG2	2.08	0.67
1:B:2815:LEU:HD23	1:B:2816:VAL:N	2.09	0.67
1:B:4184:TRP:CD1	1:B:4214:ARG:HB2	2.30	0.67
1:B:4189:ASN:H	1:B:4189:ASN:HD22	1.40	0.67
1:A:4210:HIS:ND1	1:A:4211:PRO:HD2	2.09	0.67
1:A:4259:ARG:HD3	1:A:4271:TYR:OH	1.95	0.67
1:A:2014:VAL:HG13	1:A:2065:ILE:HG21	1.78	0.66
1:A:4548:LYS:HG3	1:A:4549:GLU:H	1.60	0.66
1:B:1719:GLN:HA	1:B:1722:PHE:CD2	2.29	0.66
1:B:3078:VAL:HG23	1:B:3083:PHE:HB2	1.76	0.66
1:B:3958:THR:HG23	1:B:4235:VAL:HB	1.76	0.66
1:B:2297:ASP:O	1:B:2299:ILE:HG13	1.94	0.66
1:B:2361:PRO:HD3	1:B:2402:TYR:O	1.96	0.66
1:A:2595:LYS:HE3	1:A:2611:PRO:HG3	1.75	0.66
1:A:4270:ILE:HD13	1:A:4314:VAL:HG21	1.78	0.66
1:B:2423:THR:HG23	1:B:2530:ARG:HD2	1.76	0.66
1:B:2766:MET:HB3	1:B:2783:LEU:HD11	1.75	0.66
1:A:2108:ILE:O	1:A:2112:MET:HB2	1.96	0.66
1:A:3875:VAL:O	1:A:3879:ILE:HG12	1.95	0.66
1:A:3925:ASN:HD22	1:A:3925:ASN:N	1.93	0.66
1:B:2861:GLN:HG3	1:B:2874:TYR:HB2	1.75	0.66
1:A:3245:LEU:HD12	1:A:3249:GLN:HB2	1.78	0.66
1:A:4572:MET:HE1	1:A:4575:LEU:HD11	1.77	0.66
1:A:2124:LEU:HD22	1:A:2195:LEU:HD22	1.78	0.66
1:A:2125:ALA:HA	1:A:2128:ILE:HG22	1.78	0.66
1:B:2113:LEU:HD21	1:B:2156:LEU:HD22	1.78	0.66
1:A:2315:GLN:HB3	1:A:2775:THR:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2910:LEU:CD2	1:A:2930:ILE:HD12	2.25	0.66
1:A:3309:LYS:O	1:A:3313:LEU:HG	1.96	0.66
1:B:1769:TRP:O	1:B:1773:VAL:HG23	1.96	0.66
1:B:2984:LEU:HD22	1:B:2986:VAL:HG22	1.78	0.66
1:A:3989:ASP:O	1:A:3993:LYS:HB2	1.96	0.66
1:B:1885:GLN:O	1:B:1889:VAL:HG23	1.96	0.66
1:B:3785:ASN:ND2	1:B:3787:THR:HG23	2.11	0.66
1:A:3410:LEU:HD22	1:A:3452:ILE:HD11	1.78	0.65
1:A:3647:TRP:HB3	1:A:3652:LEU:HD23	1.78	0.65
1:A:3965:LEU:HG	1:A:4426:MET:HE3	1.77	0.65
1:A:4230:LEU:H	1:A:4230:LEU:HD12	1.61	0.65
1:A:2289:TYR:O	1:A:2293:ILE:HG12	1.95	0.65
1:A:3285:LEU:HD13	1:A:3578:SER:HA	1.78	0.65
1:A:2535:ASN:HD22	1:A:2668:ARG:HH12	1.45	0.65
1:A:3271:ILE:HG13	1:A:3592:VAL:HG11	1.78	0.65
1:A:4186:LEU:C	1:A:4187:LEU:HD12	2.17	0.65
1:B:1901:ASN:H	1:B:1901:ASN:HD22	1.43	0.65
1:B:2498:CYS:HA	1:B:2501:ILE:HD12	1.77	0.65
1:B:3639:SER:HB3	1:B:3663:ILE:CD1	2.25	0.65
1:A:2552:ASN:HD21	1:A:2560:MET:HB2	1.59	0.65
1:A:3700:LEU:CD2	1:A:3701:ASP:H	2.09	0.65
1:A:4054:GLY:O	1:A:4055:GLU:C	2.34	0.65
1:B:2359:VAL:HG13	1:B:2364:VAL:HG21	1.79	0.65
1:B:3813:ARG:O	1:B:3817:LEU:HD13	1.97	0.65
1:A:2975:ARG:HE	1:A:2975:ARG:HA	1.61	0.65
1:B:2339:ILE:HA	1:B:2346:GLU:HG2	1.76	0.65
1:A:1537:PHE:O	1:A:1541:LEU:HB2	1.97	0.65
1:A:2948:ARG:HG2	1:A:2948:ARG:HH11	1.62	0.65
1:A:3015:ILE:HG22	1:A:3149:PRO:HG3	1.77	0.65
1:A:3242:ASN:OD1	1:A:3253:ASN:HB3	1.96	0.65
1:A:4024:ARG:HG3	1:A:4031:SER:HA	1.78	0.65
1:A:4622:HIS:ND1	1:A:4623:ALA:N	2.45	0.65
1:A:2120:THR:O	1:A:2121:ALA:C	2.33	0.65
1:A:3255:VAL:HA	1:A:3259:HIS:HD2	1.61	0.65
1:B:1920:ASN:HD22	1:B:1921:VAL:H	1.44	0.65
1:B:3949:SER:HA	1:B:4110:PHE:HE1	1.62	0.65
1:A:1748:GLU:HG2	1:A:1943:ILE:HB	1.79	0.65
1:A:2305:VAL:HG21	1:A:2769:LYS:HE2	1.79	0.65
1:A:4553:TYR:HB3	1:A:4595:LEU:HD23	1.79	0.65
1:A:4649:TRP:HA	1:A:4649:TRP:HE3	1.60	0.65
1:B:3109:MET:HB3	1:B:3129:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4389:ARG:HG2	1:B:4389:ARG:HH11	1.62	0.65
1:A:2127:LYS:C	1:A:2130:PRO:HD2	2.17	0.64
1:A:2129:VAL:HB	1:A:2130:PRO:HD3	1.78	0.64
1:A:2968:LEU:O	1:A:2972:VAL:HG23	1.97	0.64
1:A:3270:LEU:HB2	1:A:3592:VAL:HG13	1.77	0.64
1:A:4221:ILE:H	1:A:4221:ILE:HD12	1.62	0.64
1:B:1931:ASN:HB2	1:B:4312:TYR:CZ	2.32	0.64
1:B:3063:GLY:HA2	1:B:3136:GLN:HB3	1.78	0.64
1:B:4063:ILE:HD12	1:B:4063:ILE:H	1.62	0.64
1:A:2704:ALA:HB3	1:A:3085:GLU:HG3	1.77	0.64
1:B:4288:ILE:HG23	1:B:4292:TRP:O	1.97	0.64
1:A:2606:PRO:HD3	1:A:2624:TRP:CD1	2.32	0.64
1:A:3700:LEU:H	1:A:3700:LEU:HD12	1.62	0.64
1:A:1921:VAL:HG23	1:A:1922:LEU:HD22	1.79	0.64
1:A:2525:ILE:HG13	1:A:2584:SER:O	1.98	0.64
1:A:2651:VAL:HG13	1:A:2652:ASP:N	2.12	0.64
1:A:3387:HIS:CB	1:A:3473:ALA:HB2	2.27	0.64
1:B:1811:PRO:O	1:B:1815:VAL:HG23	1.98	0.64
1:B:2866:PRO:HG3	1:B:2873:ILE:HG22	1.78	0.64
1:A:1811:PRO:HD2	1:A:1814:LEU:HD12	1.78	0.64
1:A:3528:SER:O	1:A:3531:THR:HG22	1.98	0.64
1:B:4188:LYS:HA	1:B:4218:THR:HG22	1.80	0.64
1:A:3602:ILE:HG23	1:A:3610:ARG:HG2	1.80	0.64
1:A:4349:ASN:HD22	1:A:4352:ASP:N	1.95	0.64
1:A:2199:ILE:O	1:A:2203:MET:HB2	1.98	0.64
1:A:2273:MET:CB	1:A:2395:PHE:HB2	2.27	0.64
1:A:2506:PHE:CD1	1:A:2512:VAL:HG21	2.33	0.64
1:A:4050:LYS:O	1:A:4052:GLN:N	2.30	0.64
1:B:3991:LEU:O	1:B:4427:ILE:HD12	1.98	0.64
1:A:1545:LEU:HB3	1:A:1553:LYS:HE2	1.80	0.64
1:A:2979:PHE:CE2	1:A:3028:PHE:HA	2.33	0.64
1:A:3696:LYS:NZ	1:A:4206:SER:HB3	2.13	0.64
1:A:3897:TYR:HE1	1:A:3913:LEU:HA	1.63	0.64
1:A:4296:PHE:CE2	1:A:4347:ILE:HD13	2.33	0.64
1:B:3299:VAL:HG11	1:B:3564:LEU:HG	1.78	0.64
1:A:3114:GLU:HG2	1:A:3118:ARG:NH1	2.13	0.64
1:A:4693:ASN:HD22	1:A:4693:ASN:N	1.95	0.64
1:B:1554:LEU:HD12	1:B:2323:THR:HG22	1.79	0.64
1:B:1694:PHE:HB3	1:B:1697:PHE:CD2	2.33	0.64
1:B:4548:LYS:HD2	1:B:4549:GLU:H	1.59	0.64
1:A:1611:ARG:HH11	1:A:1611:ARG:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2051:LYS:O	1:A:2051:LYS:HD3	1.96	0.64
1:A:2163:LYS:HB2	1:A:2194:VAL:HG11	1.79	0.64
1:A:2207:LEU:HD13	1:A:2215:ILE:HG21	1.79	0.64
1:A:3293:ARG:HH11	1:A:3293:ARG:HG3	1.63	0.64
1:A:3785:ASN:HD22	1:A:3786:PHE:N	1.95	0.64
1:A:3804:THR:O	1:A:3807:PRO:HD3	1.98	0.64
1:A:4362:GLN:HG3	1:A:4714:GLN:OE1	1.97	0.64
1:B:1557:GLY:O	1:B:1561:LEU:HD23	1.98	0.64
1:B:4351:PHE:CE2	1:B:4689:PRO:HG3	2.32	0.64
1:A:2490:ALA:O	1:A:2494:VAL:HG23	1.97	0.63
1:A:4296:PHE:CE2	1:A:4347:ILE:HA	2.33	0.63
1:A:4396:ILE:O	1:A:4399:LEU:HB2	1.98	0.63
1:B:3043:ASN:HD22	1:B:3046:TYR:HB2	1.63	0.63
1:B:3087:MET:CE	1:B:3090:LEU:HD23	2.28	0.63
1:A:3387:HIS:HB3	1:A:3473:ALA:HB2	1.80	0.63
1:B:4607:SER:O	1:B:4611:LEU:HG	1.98	0.63
1:A:1811:PRO:O	1:A:1815:VAL:HG23	1.98	0.63
1:A:3416:LYS:HE3	1:A:3418:GLU:HB3	1.80	0.63
1:A:3711:ALA:HA	1:A:3716:CYS:SG	2.39	0.63
1:A:4277:PHE:HB2	1:A:4363:LEU:HD12	1.79	0.63
1:B:1525:ILE:HA	1:B:1528:GLU:HB3	1.80	0.63
1:B:1607:ASP:O	1:B:1611:ARG:HG2	1.97	0.63
1:B:1780:THR:HG22	1:B:1784:LEU:HD12	1.80	0.63
1:B:3563:LEU:HD11	1:B:3845:ILE:HD11	1.79	0.63
1:A:3985:GLU:O	1:A:3989:ASP:HB2	1.97	0.63
1:A:4571:ARG:HA	1:A:4590:TRP:HZ3	1.63	0.63
1:A:2995:LEU:HA	1:A:2998:ILE:HD11	1.80	0.63
1:B:1523:GLY:HA3	1:B:1580:TYR:CE2	2.33	0.63
1:B:3238:ILE:HD11	1:B:3617:TRP:HZ2	1.63	0.63
1:A:2938:PHE:HB3	1:A:2941:VAL:HG23	1.80	0.63
1:A:2972:VAL:O	1:A:2976:LEU:HB2	1.98	0.63
1:A:3482:THR:O	1:A:3486:TYR:HB2	1.99	0.63
1:A:3994:GLY:HA3	1:A:4087:LYS:CE	2.29	0.63
1:A:4310:ILE:O	1:A:4314:VAL:HB	1.99	0.63
1:A:2995:LEU:HD23	1:A:2998:ILE:HD11	1.80	0.63
1:A:3063:GLY:HA2	1:A:3136:GLN:HB3	1.81	0.63
1:B:3841:ALA:O	1:B:3842:SER:CB	2.35	0.63
1:A:2000:CYS:SG	1:A:2031:LEU:HD11	2.37	0.63
1:A:3255:VAL:HA	1:A:3259:HIS:CD2	2.33	0.63
1:A:3445:THR:HG23	1:A:3449:ARG:NH1	2.14	0.63
1:A:4269:ARG:CZ	1:A:4383:VAL:HG11	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1592:ASP:O	1:B:1596:ASN:HB2	1.99	0.63
1:B:3035:LEU:CD2	1:B:3068:LYS:HB3	2.28	0.63
1:B:4133:LEU:HD23	1:B:4230:LEU:HD23	1.79	0.63
1:B:2711:LEU:HD12	1:B:2714:PHE:HD2	1.63	0.63
1:B:2751:THR:HB	1:B:2756:THR:H	1.63	0.63
1:A:2250:VAL:HB	1:A:2425:MET:HE2	1.80	0.62
1:A:3300:LYS:HA	1:A:3564:LEU:HD11	1.81	0.62
1:A:3647:TRP:CH2	1:A:3663:ILE:HD12	2.34	0.62
1:A:3725:ASN:H	1:A:3725:ASN:ND2	1.96	0.62
1:A:4049:GLY:O	1:A:4050:LYS:O	2.17	0.62
1:B:2841:ASN:HD22	1:B:2841:ASN:N	1.97	0.62
1:A:1922:LEU:HD13	1:A:1938:PHE:HD1	1.63	0.62
1:B:3865:ILE:O	1:B:3869:VAL:HG23	1.98	0.62
1:B:4194:PRO:O	1:B:4197:LEU:HB2	1.99	0.62
1:A:2247:ARG:HB2	1:A:2249:LEU:HG	1.81	0.62
1:A:2542:ASN:O	1:A:2546:VAL:HG23	1.99	0.62
1:A:3599:LEU:HD11	1:A:3638:LEU:HD13	1.80	0.62
1:B:2877:ARG:HB3	1:B:2881:ARG:HH12	1.63	0.62
1:A:1695:ALA:HB1	1:A:2019:CYS:SG	2.39	0.62
1:A:2205:PRO:HG2	1:A:2265:ILE:HD11	1.81	0.62
1:A:1743:GLY:HA3	1:A:1753:THR:HA	1.81	0.62
1:A:1975:PRO:HD2	1:A:2101:ILE:HA	1.80	0.62
1:A:2546:VAL:HA	1:A:2549:ILE:HD12	1.80	0.62
1:A:2793:ASN:N	1:A:2793:ASN:ND2	2.44	0.62
1:B:2080:GLY:HA2	1:B:2086:ASN:ND2	2.14	0.62
1:A:1927:ILE:HD13	1:A:1991:LEU:HD22	1.79	0.62
1:A:3011:HIS:ND1	1:A:3143:VAL:HG23	2.15	0.62
1:B:2277:PRO:HA	1:B:2398:GLN:HG3	1.81	0.62
1:B:3844:ASN:O	1:B:3848:ASP:CB	2.47	0.62
1:B:2584:SER:HB3	1:B:2813:ILE:HB	1.82	0.62
1:A:1957:TYR:CD2	1:A:1987:LEU:HD13	2.35	0.62
1:A:2645:ASP:O	1:A:2647:VAL:HG23	1.98	0.62
1:A:3557:VAL:O	1:A:3561:ILE:HG13	2.00	0.62
1:B:2199:ILE:HG23	1:B:2203:MET:HG3	1.81	0.62
1:B:2206:LYS:HB3	1:B:2413:MET:HB3	1.81	0.62
1:A:3408:VAL:HG11	1:A:3477:LEU:HG	1.82	0.62
1:A:3452:ILE:HG21	1:A:3485:THR:HG21	1.82	0.62
1:A:3634:VAL:HB	1:A:3635:PRO:HD3	1.82	0.62
1:A:3812:LYS:HB3	1:A:3875:VAL:HG22	1.81	0.62
1:A:4389:ARG:HG2	1:A:4389:ARG:HH11	1.65	0.62
1:A:3566:ASN:HB3	1:A:3855:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4568:PHE:O	1:A:4572:MET:HG2	2.00	0.62
1:B:1726:PHE:CD2	1:B:1729:LEU:HD22	2.35	0.62
1:B:4410:LEU:HD22	1:B:4411:PRO:HD2	1.81	0.62
1:A:1967:ARG:HH22	1:A:2069:GLN:HG3	1.63	0.61
1:A:2151:ALA:O	1:A:2155:VAL:HG12	1.99	0.61
1:A:4402:ILE:H	1:A:4402:ILE:HD12	1.65	0.61
1:A:2357:GLY:O	1:A:2397:VAL:HG12	2.00	0.61
1:A:2954:ASN:H	1:A:2954:ASN:ND2	1.97	0.61
1:A:3445:THR:N	1:A:3446:PRO:HD2	2.16	0.61
1:B:2275:VAL:HG13	1:B:2397:VAL:HG13	1.82	0.61
1:A:2090:ASN:C	1:A:2090:ASN:HD22	2.02	0.61
1:A:2912:LEU:C	1:A:2913:PHE:HD2	2.04	0.61
1:A:3909:TYR:CE1	1:A:3959:LEU:HA	2.35	0.61
1:B:2212:ILE:N	1:B:2213:PRO:HD2	2.15	0.61
1:A:2239:LYS:HA	1:A:2239:LYS:HE3	1.81	0.61
1:A:2243:ILE:HD12	1:A:2292:ALA:HB2	1.82	0.61
1:A:2670:LEU:HG	1:A:2789:VAL:HG22	1.83	0.61
1:A:3271:ILE:O	1:A:3275:ARG:HB2	2.00	0.61
1:B:2208:VAL:HG23	1:B:2211:ASP:HB2	1.81	0.61
1:B:2704:ALA:HB2	1:B:3085:GLU:OE2	1.98	0.61
1:B:3664:MET:O	1:B:3668:PHE:HB3	1.99	0.61
1:B:4402:ILE:HD12	1:B:4402:ILE:N	2.14	0.61
1:A:3260:TYR:O	1:A:3264:ILE:HG12	2.01	0.61
1:A:3731:ASN:HD22	1:A:3731:ASN:N	1.97	0.61
1:A:2258:LYS:HD3	1:A:2261:GLN:HG3	1.83	0.61
1:A:2262:LEU:HD11	1:A:2274:MET:HE2	1.81	0.61
1:A:2272:VAL:O	1:A:2394:MET:HA	2.00	0.61
1:A:2791:ALA:O	1:A:2792:CYS:HB3	2.00	0.61
1:A:2869:GLN:HB3	1:A:2872:TYR:CD1	2.36	0.61
1:A:4329:ILE:HD12	1:A:4331:TRP:CZ2	2.35	0.61
1:B:2140:SER:O	1:B:2142:GLN:HG2	1.99	0.61
1:B:3673:LEU:HB2	1:B:3781:VAL:CG1	2.26	0.61
1:A:2948:ARG:HD3	1:A:2950:ILE:HG13	1.82	0.61
1:A:4076:ILE:HD11	1:A:4104:SER:O	2.00	0.61
1:A:4589:VAL:HG12	1:A:4638:ASN:O	2.01	0.61
1:A:2088:PRO:HB2	1:A:2090:ASN:ND2	2.15	0.61
1:A:3474:CYS:HA	1:A:3477:LEU:HD22	1.83	0.61
1:A:3686:MET:HE2	1:A:3696:LYS:HD2	1.81	0.61
1:A:4600:TYR:O	1:A:4604:THR:HG23	2.01	0.61
1:B:2305:VAL:HG22	1:B:2354:ILE:HB	1.83	0.61
1:B:2732:PRO:HG3	1:B:2739:LEU:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3587:THR:HB	1:A:3628:PHE:HA	1.82	0.61
1:B:2586:GLY:HA2	1:B:2815:LEU:HD13	1.81	0.61
1:B:3291:LYS:HD2	1:B:3835:LEU:HG	1.81	0.61
1:B:4189:ASN:N	1:B:4218:THR:HG22	2.14	0.61
1:A:2190:TYR:O	1:A:2194:VAL:HG23	2.01	0.61
1:A:2985:ASP:O	1:A:2987:PRO:HD3	2.01	0.61
1:A:4624:SER:HB2	1:A:4668:THR:HB	1.83	0.61
1:B:3650:ASN:OD1	1:B:3688:GLN:HA	2.00	0.61
1:A:2152:LEU:O	1:A:2156:LEU:HG	2.01	0.60
1:A:3385:LYS:O	1:A:3389:ASP:HB2	2.00	0.60
1:A:4396:ILE:HA	1:A:4399:LEU:HD12	1.83	0.60
1:A:4503:ILE:HG23	1:A:4575:LEU:HB3	1.82	0.60
1:B:2582:GLY:HA2	1:B:2585:MET:HE3	1.81	0.60
1:B:2869:GLN:HB2	1:B:2872:TYR:CG	2.36	0.60
1:B:4135:CYS:HA	1:B:4219:SER:O	2.00	0.60
1:A:1687:LEU:HD22	1:A:1705:LEU:HD23	1.83	0.60
1:A:3137:VAL:HG13	1:A:3141:LEU:HD23	1.82	0.60
1:A:3994:GLY:HA3	1:A:4087:LYS:HE2	1.83	0.60
1:A:4590:TRP:CE3	1:A:4593:GLY:HA3	2.36	0.60
1:B:3559:ARG:NE	1:B:3846:LEU:O	2.35	0.60
1:A:3239:GLY:O	1:A:3243:ILE:HG13	2.00	0.60
1:A:4536:SER:HB2	1:A:4548:LYS:NZ	2.16	0.60
1:A:4636:SER:HB3	1:A:4670:THR:HA	1.83	0.60
1:A:2144:HIS:HB2	1:A:2413:MET:SD	2.40	0.60
1:A:2408:ILE:O	1:A:2409:SER:C	2.38	0.60
1:A:2903:ARG:NH2	1:A:2950:ILE:HA	2.16	0.60
1:B:2231:ILE:HG21	1:B:2264:GLN:HE22	1.64	0.60
1:B:2364:VAL:HB	1:B:2407:THR:HG21	1.82	0.60
1:B:3219:ILE:O	1:B:3221:PRO:HD3	2.00	0.60
1:A:2118:PHE:CE1	1:A:2163:LYS:HD2	2.37	0.60
1:A:2309:LYS:HG3	1:A:2358:ASP:HB2	1.84	0.60
1:A:3345:GLN:O	1:A:3349:ASP:HB2	2.01	0.60
1:A:4690:VAL:O	1:A:4700:LEU:HB2	2.01	0.60
1:A:1763:GLY:H	1:A:1764:PRO:HD3	1.65	0.60
1:A:2250:VAL:HB	1:A:2425:MET:CE	2.31	0.60
1:A:2532:ARG:HG3	1:A:2808:LEU:O	2.01	0.60
1:A:2917:LEU:HD12	1:A:2923:LYS:HA	1.84	0.60
1:A:3075:GLU:O	1:A:3078:VAL:HG12	2.01	0.60
1:A:3562:ALA:O	1:A:3566:ASN:HB2	2.02	0.60
1:A:3718:LEU:HD23	1:A:3762:ILE:HG13	1.84	0.60
1:A:4092:ASP:OD2	1:A:4093:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4182:GLY:HA3	1:A:4212:SER:OG	2.02	0.60
1:B:1820:GLN:HE22	1:B:1990:GLN:NE2	1.99	0.60
1:B:2976:LEU:HD12	1:B:2990:LEU:HD11	1.84	0.60
1:B:3813:ARG:HB3	1:B:3879:ILE:HD13	1.83	0.60
1:A:3598:PHE:CD2	1:A:3634:VAL:HG11	2.36	0.60
1:A:3994:GLY:HA3	1:A:4087:LYS:NZ	2.17	0.60
1:A:4503:ILE:HA	1:A:4575:LEU:HD23	1.84	0.60
1:B:1752:VAL:HG22	1:B:1811:PRO:HG3	1.84	0.60
1:B:1908:TYR:CE1	1:B:1958:LEU:HD22	2.37	0.60
1:A:2239:LYS:HD3	1:A:2295:GLN:NE2	2.16	0.60
1:A:2730:LEU:HD23	1:A:2783:LEU:HD23	1.83	0.60
1:A:4574:GLN:NE2	1:A:4590:TRP:HB3	2.17	0.60
1:B:2129:VAL:HG22	1:B:2130:PRO:CD	2.30	0.60
1:B:2522:ARG:HD3	1:B:2585:MET:SD	2.42	0.60
1:B:4153:LEU:HB2	1:B:4155:LYS:HG2	1.83	0.60
1:B:4541:ILE:HA	1:B:4561:LEU:HD11	1.83	0.60
1:A:1921:VAL:HG23	1:A:1922:LEU:CD2	2.32	0.60
1:A:3040:ILE:HG22	1:A:3042:VAL:HG13	1.82	0.60
1:A:3803:LYS:HE3	1:A:3810:HIS:NE2	2.17	0.60
1:B:1608:VAL:HG21	1:B:1669:MET:HG3	1.83	0.60
1:B:3559:ARG:O	1:B:3563:LEU:HB2	2.02	0.60
1:B:4060:GLU:O	1:B:4064:VAL:HG23	2.02	0.60
1:A:2091:LEU:HD22	1:A:2095:PHE:CE1	2.37	0.60
1:A:2439:PHE:H	1:A:2495:GLN:HE22	1.48	0.60
1:A:3262:ASP:HB2	1:A:3670:ARG:HE	1.67	0.60
1:A:1604:VAL:HG11	1:A:1670:GLU:HA	1.84	0.59
1:A:3922:ASN:HD22	1:A:3922:ASN:N	2.00	0.59
1:A:3969:LEU:HD12	1:A:4426:MET:HE2	1.82	0.59
1:A:4004:THR:OG1	1:A:4006:PRO:HD3	2.01	0.59
1:B:3017:VAL:HG13	1:B:3174:GLY:O	2.02	0.59
1:A:4691:TYR:CD2	1:A:4696:ARG:HG2	2.36	0.59
1:B:1948:VAL:O	1:B:1950:THR:HG23	2.02	0.59
1:B:3671:TYR:HD2	1:B:3734:LEU:HA	1.67	0.59
1:B:4499:PHE:O	1:B:4503:ILE:HB	2.01	0.59
1:A:2864:PHE:HB3	1:A:2872:TYR:CD2	2.38	0.59
1:A:3785:ASN:HD22	1:A:3786:PHE:H	1.49	0.59
1:A:4644:LEU:HD12	1:A:4723:ILE:HG12	1.85	0.59
1:B:2494:VAL:HG11	1:B:2548:VAL:HB	1.84	0.59
1:A:2273:MET:SD	1:A:2408:ILE:HG22	2.42	0.59
1:A:3923:LEU:HD22	1:A:3947:ILE:HG12	1.83	0.59
1:A:4545:ILE:O	1:A:4561:LEU:HD21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4715:ASN:O	1:A:4719:ARG:HB2	2.02	0.59
1:B:2377:LEU:O	1:B:2384:ARG:HA	2.02	0.59
1:B:2616:SER:HB3	1:B:2627:TRP:CE2	2.37	0.59
1:B:3673:LEU:HD22	1:B:3783:PHE:HE1	1.66	0.59
1:B:4124:LYS:O	1:B:4125:GLU:HG2	2.01	0.59
1:B:4131:PRO:HD2	1:B:4232:MET:O	2.03	0.59
1:B:4137:VAL:HB	1:B:4138:PRO:HD2	1.85	0.59
1:A:3672:PRO:HA	1:A:3782:THR:HG23	1.84	0.59
1:A:4190:ILE:HB	1:A:4197:LEU:HD11	1.83	0.59
1:A:4371:PRO:HA	1:A:4385:GLU:OE1	2.03	0.59
1:B:1612:TRP:O	1:B:1616:GLU:HB2	2.02	0.59
1:B:2000:CYS:HB3	1:B:2031:LEU:HD13	1.83	0.59
1:A:2528:PHE:CE1	1:A:2533:VAL:HG11	2.38	0.59
1:A:3730:LEU:HD11	1:A:3762:ILE:CD1	2.33	0.59
1:A:3731:ASN:HB2	1:A:3732:PRO:HD3	1.84	0.59
1:A:4157:TYR:OH	1:A:4186:LEU:HD22	2.03	0.59
1:A:4597:PRO:HB2	1:A:4700:LEU:HD21	1.85	0.59
1:B:3024:VAL:HG11	2:B:9010:ADP:H3'	1.83	0.59
1:B:3809:THR:HG21	1:B:3882:VAL:HG11	1.84	0.59
1:B:3897:TYR:HE1	1:B:3913:LEU:HA	1.67	0.59
1:B:4273:LEU:HD13	1:B:4363:LEU:O	2.02	0.59
1:A:2293:ILE:HG22	1:A:2350:ARG:NH2	2.12	0.59
1:A:2648:ILE:HG21	1:A:2827:ILE:HA	1.84	0.59
1:A:2938:PHE:HB3	1:A:2941:VAL:CG2	2.33	0.59
1:A:3924:LEU:HD23	1:A:3943:LEU:CD2	2.32	0.59
1:A:3951:THR:O	1:A:3955:VAL:HG23	2.02	0.59
1:B:1625:ILE:HD12	1:B:1628:LEU:HB2	1.83	0.59
1:B:2863:ARG:O	1:B:2863:ARG:HD3	2.02	0.59
1:A:3190:ARG:HA	1:A:3224:ARG:HH12	1.66	0.59
1:A:4494:PRO:HD3	1:A:4610:GLN:HE22	1.67	0.59
1:B:1546:VAL:HG22	1:B:1556:ARG:CZ	2.33	0.59
1:B:4207:LEU:O	1:B:4209:PRO:HD3	2.02	0.59
1:B:4424:ARG:NH2	1:B:4558:THR:HG21	2.17	0.59
1:A:2863:ARG:HD2	1:A:2864:PHE:CE1	2.36	0.59
1:A:3313:LEU:HD13	1:A:3550:SER:OG	2.03	0.59
1:A:4136:SER:O	1:A:4221:ILE:HD12	2.03	0.59
1:B:1477:LYS:H	1:B:1480:HIS:HD2	1.50	0.59
1:B:2273:MET:HG2	1:B:2395:PHE:HB2	1.84	0.59
1:B:2598:GLN:HG2	1:B:2612:LEU:HD23	1.85	0.59
1:B:4332:ILE:O	1:B:4336:THR:HG23	2.02	0.59
1:A:1538:TRP:HZ3	1:A:1656:ILE:HD13	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1978:THR:CG2	1:A:2103:PRO:HD3	2.33	0.59
1:A:2598:GLN:CG	1:A:2612:LEU:HB2	2.33	0.59
1:A:2991:PHE:HE1	1:A:2993:GLU:HB2	1.67	0.59
1:A:4572:MET:HA	1:A:4575:LEU:HD13	1.85	0.59
1:B:3788:VAL:HG11	1:B:3913:LEU:HD22	1.85	0.59
1:A:1763:GLY:N	1:A:1764:PRO:CD	2.65	0.58
1:A:1797:VAL:CG1	1:A:1855:ILE:HD11	2.33	0.58
1:A:1973:PHE:CE1	1:A:2099:ALA:HA	2.38	0.58
1:A:2278:SER:HA	1:A:2806:ARG:HH11	1.68	0.58
1:A:4066:GLN:NE2	1:A:4081:ARG:HD3	2.18	0.58
1:B:3233:TYR:CD2	1:B:3620:ARG:HG3	2.38	0.58
1:B:4109:ASP:HA	1:B:4112:ASN:HD22	1.67	0.58
1:A:1735:ASP:OD2	1:A:1737:GLU:HB2	2.03	0.58
1:B:2375:LYS:HB3	1:B:2387:LEU:HB3	1.84	0.58
1:B:4349:ASN:HB3	1:B:4352:ASP:OD2	2.03	0.58
1:B:4351:PHE:CD2	1:B:4689:PRO:HG3	2.38	0.58
1:A:2043:ILE:HG23	1:A:2073:ILE:HD12	1.84	0.58
1:A:3331:GLN:NE2	1:A:3533:LYS:HG3	2.18	0.58
1:A:3723:VAL:HG12	1:A:3766:THR:OG1	2.03	0.58
1:A:4193:ALA:O	1:A:4197:LEU:HD23	2.03	0.58
1:B:3027:ARG:HG2	1:B:3037:ILE:HD12	1.85	0.58
1:B:3170:LEU:HD21	1:B:3172:TRP:HE3	1.67	0.58
1:B:4030:PHE:HD1	1:B:4033:LEU:HD22	1.68	0.58
1:A:2153:LYS:O	1:A:2157:VAL:HG23	2.03	0.58
1:A:3830:LEU:HB3	1:A:3858:LEU:HD13	1.86	0.58
1:A:4251:THR:HG23	1:A:4303:LEU:CD2	2.30	0.58
1:A:4349:ASN:HD22	1:A:4352:ASP:H	1.51	0.58
1:A:4368:ALA:HA	1:A:4373:PHE:CE1	2.38	0.58
1:B:1901:ASN:HD22	1:B:1901:ASN:N	2.01	0.58
1:B:2166:CYS:HA	1:B:2190:TYR:OH	2.03	0.58
1:B:3182:PHE:O	1:B:3186:SER:HB2	2.03	0.58
1:A:2087:LEU:HB2	1:A:2092:LYS:HG3	1.86	0.58
1:A:2361:PRO:HD3	1:A:2402:TYR:O	2.03	0.58
1:A:3803:LYS:HG3	1:A:3810:HIS:CD2	2.39	0.58
1:A:4003:GLU:HG3	1:B:2842:LEU:CD2	2.34	0.58
1:A:4032:LYS:HG3	1:A:4069:LEU:HD11	1.83	0.58
1:B:1884:HIS:O	1:B:1888:VAL:HG23	2.03	0.58
1:B:3620:ARG:HG2	1:B:3620:ARG:HH11	1.69	0.58
1:A:1950:THR:HB	1:A:1951:PRO:HD2	1.84	0.58
1:A:2212:ILE:N	1:A:2213:PRO:HD2	2.18	0.58
1:B:1821:ILE:HG21	1:B:1914:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2338:ARG:HD2	1:B:2346:GLU:OE1	2.04	0.58
1:A:1849:GLU:HG3	1:A:1893:GLN:OE1	2.03	0.58
1:B:1719:GLN:HA	1:B:1722:PHE:CE2	2.38	0.58
1:B:2997:HIS:O	1:B:3001:ILE:HG13	2.03	0.58
1:B:3013:LEU:HD22	1:B:3164:LEU:HD12	1.85	0.58
1:B:4388:THR:HG23	1:B:4391:HIS:HD2	1.68	0.58
1:A:3615:ARG:O	1:A:3619:ILE:HG13	2.03	0.58
1:A:4572:MET:HA	1:A:4575:LEU:CD1	2.34	0.58
1:B:1855:ILE:HG22	1:B:1859:LEU:HD12	1.85	0.58
1:B:3923:LEU:HD22	1:B:3947:ILE:HG23	1.85	0.58
1:A:1863:VAL:HG21	1:A:2115:SER:O	2.04	0.58
1:A:2135:CYS:HB3	1:A:2147:PHE:CZ	2.38	0.58
1:B:1748:GLU:HB3	1:B:1943:ILE:HD12	1.85	0.58
1:A:1995:VAL:HA	1:A:2022:TRP:HB2	1.84	0.58
1:B:1643:PHE:CE2	1:B:1647:LEU:HD11	2.39	0.58
1:B:1926:VAL:HG12	1:B:1928:HIS:CD2	2.39	0.58
1:B:3192:LEU:HD11	1:B:3268:VAL:HA	1.84	0.58
1:B:3263:PHE:O	1:B:3267:VAL:HG23	2.03	0.58
1:B:4648:VAL:HA	1:B:4662:THR:HG21	1.85	0.58
1:A:2838:LEU:O	1:A:2839:LEU:HD23	2.04	0.57
1:A:3255:VAL:O	1:A:3255:VAL:HG13	2.03	0.57
1:A:3337:LYS:HA	1:A:3341:ALA:HB3	1.86	0.57
1:A:3595:ALA:HB1	1:A:3638:LEU:HD11	1.85	0.57
1:A:4559:ILE:O	1:A:4559:ILE:HG23	2.04	0.57
1:B:1813:GLN:NE2	1:B:1941:LEU:H	2.02	0.57
1:B:1939:GLU:O	1:B:1941:LEU:HG	2.03	0.57
1:B:2863:ARG:HG3	1:B:2925:TRP:CE2	2.39	0.57
1:B:3785:ASN:HD21	1:B:3787:THR:CG2	2.16	0.57
1:A:1982:GLU:HG3	2:A:9001:ADP:H3'	1.86	0.57
1:A:3274:LYS:O	1:A:3278:LEU:HD23	2.04	0.57
1:A:3487:TYR:O	1:A:3490:ILE:HG12	2.04	0.57
1:A:4284:ARG:HG3	1:A:4408:LEU:HB3	1.86	0.57
1:B:1554:LEU:HD22	1:B:1609:GLN:OE1	2.03	0.57
1:B:4189:ASN:N	1:B:4189:ASN:ND2	2.53	0.57
1:A:2739:LEU:HD23	1:A:2740:VAL:N	2.19	0.57
1:B:2869:GLN:HB2	1:B:2872:TYR:CD2	2.39	0.57
1:B:3674:VAL:HG13	1:B:3786:PHE:HD2	1.68	0.57
1:B:3897:TYR:CE1	1:B:3913:LEU:HA	2.38	0.57
1:B:4255:ILE:HD11	1:B:4307:LEU:HD11	1.85	0.57
1:A:2560:MET:HG3	1:A:2561:SER:N	2.16	0.57
1:A:2839:LEU:HD11	1:A:2890:ILE:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3668:PHE:CD1	1:A:3672:PRO:HD3	2.39	0.57
1:A:4277:PHE:HB2	1:A:4363:LEU:CD1	2.34	0.57
1:B:1888:VAL:O	1:B:1892:LEU:HD12	2.04	0.57
1:B:2533:VAL:HB	1:B:2581:LEU:CD2	2.30	0.57
1:A:3909:TYR:OH	1:A:3960:LEU:HG	2.04	0.57
1:A:4313:TRP:HB3	1:A:4330:PRO:HG2	1.86	0.57
1:B:1687:LEU:HD21	1:B:1706:LEU:CD2	2.33	0.57
1:B:1889:VAL:HA	1:B:1892:LEU:HD13	1.86	0.57
1:B:2219:LEU:CD1	1:B:2228:LEU:HD11	2.35	0.57
1:B:2235:GLN:HE22	1:B:2296:VAL:HG13	1.68	0.57
1:B:2417:SER:O	1:B:2420:ILE:HG12	2.03	0.57
1:B:2578:MET:HE1	1:B:2612:LEU:HD12	1.86	0.57
1:B:4379:ILE:O	1:B:4379:ILE:HG13	2.05	0.57
1:A:2053:ASN:O	1:A:2054:SER:C	2.42	0.57
1:A:2195:LEU:O	1:A:2199:ILE:HG12	2.04	0.57
1:A:2252:LYS:O	1:A:2256:VAL:HG23	2.05	0.57
1:A:2873:ILE:H	1:A:2873:ILE:HD12	1.68	0.57
1:A:3863:THR:O	1:A:3867:LEU:HB3	2.04	0.57
1:B:2835:LEU:HD11	1:B:2890:ILE:HD12	1.85	0.57
1:B:2841:ASN:HD22	1:B:2842:LEU:N	2.02	0.57
1:B:3638:LEU:HD12	1:B:3663:ILE:HG21	1.86	0.57
1:B:4318:SER:HB3	1:B:4324:ILE:HD11	1.85	0.57
1:A:2616:SER:HB3	1:A:2627:TRP:CE2	2.40	0.57
1:A:4288:ILE:HG23	1:A:4292:TRP:O	2.04	0.57
1:B:2270:HIS:HA	1:B:2392:ARG:HH11	1.70	0.57
1:B:1591:TRP:O	1:B:1595:LEU:HB2	2.05	0.57
1:A:1718:ILE:HG22	1:A:1722:PHE:CE2	2.40	0.57
1:A:4245:LYS:HD2	1:A:4399:LEU:O	2.04	0.57
1:B:2540:LEU:HD12	1:B:2662:ALA:HB3	1.85	0.57
1:B:3238:ILE:HG12	1:B:3601:TYR:CD2	2.40	0.57
1:B:3793:LEU:HD23	1:B:3894:SER:HA	1.86	0.57
1:A:1681:LYS:O	1:A:1685:GLU:HG3	2.04	0.57
1:A:1978:THR:HG22	1:A:2103:PRO:HD3	1.87	0.57
1:A:4050:LYS:O	1:A:4051:ASP:C	2.42	0.57
1:A:4415:GLU:HA	1:A:4415:GLU:OE2	2.05	0.57
1:B:2586:GLY:HA2	1:B:2815:LEU:CD1	2.34	0.57
1:B:3912:SER:HB3	1:B:4231:ARG:HG2	1.86	0.57
1:B:4313:TRP:HB3	1:B:4330:PRO:HG2	1.87	0.57
1:A:2989:VAL:HG13	1:A:3187:GLU:CD	2.25	0.56
1:A:3266:GLN:HE21	1:A:3270:LEU:CD2	2.18	0.56
1:A:3291:LYS:HG3	1:A:3835:LEU:HD22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3439:ASP:HB3	1:A:3442:LYS:HG2	1.87	0.56
1:A:3571:ARG:HB3	1:A:3571:ARG:HH11	1.69	0.56
1:A:4132:LEU:HD23	1:A:4236:PHE:HE2	1.70	0.56
1:A:4375:LEU:HD11	1:A:4383:VAL:CG2	2.30	0.56
1:B:1537:PHE:O	1:B:1541:LEU:HB2	2.05	0.56
1:B:3274:LYS:HE3	1:B:3637:PHE:CE2	2.39	0.56
1:B:3614:MET:O	1:B:3618:MET:HG3	2.04	0.56
1:B:4043:ASP:HB3	1:B:4059:PRO:HB3	1.87	0.56
1:B:4543:LYS:HD2	1:B:4545:ILE:HD13	1.87	0.56
1:A:1927:ILE:HD13	1:A:1991:LEU:CD2	2.35	0.56
1:A:1978:THR:HG21	1:A:2101:ILE:O	2.05	0.56
1:A:2121:ALA:O	1:A:2122:GLU:C	2.43	0.56
1:A:4132:LEU:HD13	1:A:4216:PHE:CE1	2.40	0.56
1:A:4432:LYS:C	1:A:4434:GLN:H	2.08	0.56
1:B:4618:ASN:HD22	1:B:4618:ASN:N	2.02	0.56
1:A:2560:MET:CE	1:A:2564:ASN:HD22	2.18	0.56
1:A:2675:PRO:HG2	1:A:2678:SER:HB3	1.88	0.56
1:A:2979:PHE:HE2	1:A:3028:PHE:HA	1.70	0.56
1:A:3195:GLU:OE1	1:A:3224:ARG:HB2	2.04	0.56
1:A:3299:VAL:HG21	1:A:3563:LEU:HD23	1.87	0.56
1:A:3567:LEU:CD2	1:A:3855:LEU:HD11	2.36	0.56
1:A:3813:ARG:HB2	1:A:3813:ARG:CZ	2.34	0.56
1:A:3813:ARG:HB3	1:A:3879:ILE:HD11	1.88	0.56
1:B:1531:LEU:HD13	1:B:1587:GLU:OE2	2.05	0.56
1:B:1554:LEU:HB3	1:B:1609:GLN:NE2	2.09	0.56
1:B:1956:CYS:SG	1:B:1983:THR:HG21	2.45	0.56
1:B:3893:CYS:SG	1:B:3947:ILE:HG21	2.44	0.56
1:A:2229:GLN:HB3	1:A:2230:PRO:HD2	1.86	0.56
1:A:2806:ARG:HH12	2:A:9002:ADP:PB	2.28	0.56
1:A:3584:GLN:O	1:A:3588:VAL:HG23	2.06	0.56
1:A:3598:PHE:HA	1:A:3602:ILE:HG12	1.88	0.56
1:A:3682:MET:SD	1:A:3696:LYS:HE2	2.46	0.56
1:A:4277:PHE:O	1:A:4281:ILE:HG12	2.06	0.56
1:B:2660:LEU:HD21	1:B:2672:LEU:HD21	1.87	0.56
1:B:4213:PHE:CZ	1:B:4215:LEU:HB2	2.40	0.56
1:A:1752:VAL:HG22	1:A:1811:PRO:HG3	1.86	0.56
1:A:1947:LEU:HD11	1:A:1982:GLU:HB3	1.87	0.56
1:A:4117:ASP:OD1	1:A:4119:ALA:HB3	2.06	0.56
1:B:2144:HIS:HB3	1:B:2400:LEU:HD12	1.86	0.56
1:B:2739:LEU:HB3	1:B:2786:ILE:HG12	1.87	0.56
1:A:2087:LEU:O	1:A:2092:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1948:VAL:O	1:A:1950:THR:HG23	2.06	0.56
1:A:2284:THR:O	1:A:2288:VAL:HG23	2.06	0.56
1:A:4534:LEU:HA	1:A:4537:LEU:HD12	1.88	0.56
1:B:2560:MET:HG3	1:B:2564:ASN:HB2	1.88	0.56
1:B:2670:LEU:HD11	1:B:2789:VAL:HG13	1.88	0.56
1:B:2841:ASN:ND2	1:B:2841:ASN:N	2.54	0.56
1:A:2954:ASN:ND2	1:A:2954:ASN:N	2.53	0.56
1:A:3445:THR:HA	1:A:3449:ARG:HD3	1.87	0.56
1:A:3848:ASP:HB3	1:A:3851:VAL:HG12	1.88	0.56
1:A:3887:ASN:HB3	1:A:3888:PRO:HD3	1.88	0.56
1:B:2841:ASN:ND2	1:B:2842:LEU:N	2.52	0.56
1:B:3043:ASN:HD22	1:B:3043:ASN:H	1.54	0.56
1:B:3758:PRO:HG2	1:B:3759:SER:H	1.71	0.56
1:A:1687:LEU:HD21	1:A:1706:LEU:HD23	1.88	0.56
1:A:1862:SER:O	1:A:1865:GLN:HG2	2.06	0.56
1:A:2748:LEU:N	1:A:2749:PRO:CD	2.69	0.56
1:A:2906:ALA:O	1:A:2910:LEU:HG	2.05	0.56
1:A:2941:VAL:HG12	1:A:2942:ASN:N	2.20	0.56
1:A:3376:ALA:O	1:A:3380:VAL:HG23	2.06	0.56
1:A:3813:ARG:HH22	1:A:3817:LEU:CD1	2.18	0.56
1:A:4622:HIS:HE2	1:A:4678:ILE:CG2	2.16	0.56
1:B:1479:ARG:CZ	1:B:1479:ARG:HB2	2.35	0.56
1:B:2081:TYR:O	1:B:2084:ARG:HD2	2.06	0.56
1:B:2163:LYS:HB2	1:B:2194:VAL:HG11	1.87	0.56
1:A:2381:ASN:OD1	1:A:2383:GLU:HB2	2.06	0.56
1:A:3404:ALA:HA	1:A:3462:PHE:HE1	1.71	0.56
1:A:4589:VAL:HG12	1:A:4639:VAL:HA	1.88	0.56
1:B:2276:GLY:O	1:B:2398:GLN:HA	2.06	0.56
1:B:3729:VAL:O	1:B:3729:VAL:HG22	2.05	0.56
1:A:1957:TYR:O	1:A:1961:THR:HG23	2.07	0.55
1:A:3292:LEU:HD22	1:A:3567:LEU:HD22	1.89	0.55
1:B:3908:LEU:HD22	1:B:4221:ILE:HG23	1.87	0.55
1:B:4147:ASP:HA	1:B:4157:TYR:OH	2.06	0.55
1:B:4190:ILE:HG12	1:B:4219:SER:HB2	1.86	0.55
1:B:4389:ARG:HG2	1:B:4389:ARG:NH1	2.21	0.55
1:B:4535:ARG:HG2	1:B:4535:ARG:HH11	1.71	0.55
1:A:1800:HIS:HB2	1:A:1858:ASN:HD22	1.71	0.55
1:A:2910:LEU:HD23	1:A:2930:ILE:CD1	2.33	0.55
1:A:3673:LEU:HD13	1:A:3783:PHE:CE1	2.40	0.55
1:A:4005:ILE:HG22	1:A:4008:LEU:HB2	1.87	0.55
1:B:2829:GLY:HA2	1:B:2850:THR:OG1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3700:LEU:CD2	1:B:3701:ASP:H	2.18	0.55
1:B:4388:THR:O	1:B:4391:HIS:HB2	2.07	0.55
1:A:1699:PHE:HE1	1:A:2015:GLY:HA3	1.71	0.55
1:A:1926:VAL:HG12	1:A:1928:HIS:CD2	2.41	0.55
1:A:2615:TYR:HD1	1:A:2624:TRP:HB3	1.72	0.55
1:A:2650:THR:H	1:A:2653:THR:HB	1.71	0.55
1:A:2991:PHE:CE1	1:A:2993:GLU:HB2	2.40	0.55
1:A:4590:TRP:CD2	1:A:4593:GLY:HA3	2.42	0.55
1:B:2101:ILE:O	1:B:2103:PRO:HD3	2.07	0.55
1:B:2440:ASP:OD1	1:B:2441:PRO:HD2	2.06	0.55
1:B:2603:THR:O	1:B:2605:VAL:HG13	2.06	0.55
1:A:3066:GLU:HG2	1:A:3136:GLN:HE21	1.71	0.55
1:A:3368:LYS:C	1:A:3374:ILE:HD11	2.26	0.55
1:A:3419:TRP:CE3	1:A:3422:ILE:HD11	2.42	0.55
1:B:2369:SER:HA	1:B:2372:ASP:OD2	2.07	0.55
1:A:1625:ILE:HG23	1:A:1626:ASN:H	1.70	0.55
1:A:2606:PRO:HG2	1:A:2615:TYR:CE1	2.42	0.55
1:A:3555:ASN:HB3	1:A:3559:ARG:HH11	1.71	0.55
1:B:2774:ARG:HB2	1:B:2781:ILE:CD1	2.37	0.55
1:A:1763:GLY:H	1:A:1764:PRO:CD	2.19	0.55
1:A:1875:PHE:O	1:A:1879:ILE:HG12	2.07	0.55
1:A:3471:SER:HB3	1:A:3474:CYS:SG	2.47	0.55
1:A:3930:LEU:HG	1:A:3939:ARG:NH1	2.21	0.55
1:A:3991:LEU:O	1:A:3991:LEU:HD12	2.07	0.55
1:A:4094:VAL:HB	1:A:4423:ALA:HB1	1.88	0.55
1:B:1872:ARG:HH12	1:B:2164:ARG:HD3	1.71	0.55
1:A:1608:VAL:HG13	1:A:1676:LEU:CD1	2.37	0.55
1:A:1797:VAL:HG13	1:A:1855:ILE:HD11	1.89	0.55
1:A:2274:MET:CE	1:A:2286:TRP:HB3	2.30	0.55
1:A:2765:GLN:O	1:A:2769:LYS:HB2	2.07	0.55
1:A:3453:THR:O	1:A:3458:GLU:HG2	2.06	0.55
1:A:4319:LYS:H	1:A:4321:ARG:NH2	2.04	0.55
1:B:1555:VAL:HG23	1:B:1609:GLN:HE21	1.70	0.55
1:B:3018:SER:O	1:B:3256:THR:HB	2.06	0.55
1:B:3306:LEU:HD22	1:B:3553:VAL:HG13	1.89	0.55
1:B:4132:LEU:HD13	1:B:4216:PHE:CE1	2.42	0.55
1:B:4624:SER:HB2	1:B:4668:THR:HB	1.87	0.55
1:B:4644:LEU:HG	1:B:4664:ILE:HD11	1.88	0.55
1:B:4685:LYS:HE2	1:B:4706:PRO:HD3	1.88	0.55
1:A:2262:LEU:HD11	1:A:2274:MET:CE	2.37	0.55
1:A:2446:GLN:O	1:A:2450:ASN:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4571:ARG:O	1:A:4574:GLN:HB3	2.07	0.55
1:A:1907:LEU:HA	1:A:1911:ARG:NH1	2.21	0.55
1:A:2439:PHE:H	1:A:2495:GLN:NE2	2.05	0.55
1:A:3647:TRP:HH2	1:A:3663:ILE:HD12	1.71	0.55
1:B:2000:CYS:C	1:B:2002:GLU:H	2.10	0.55
1:B:2612:LEU:HD11	1:B:2624:TRP:CH2	2.42	0.55
1:B:2779:THR:O	1:B:2781:ILE:HD12	2.06	0.55
1:B:2863:ARG:HD2	1:B:2864:PHE:CE1	2.42	0.55
1:B:2918:VAL:HG13	1:B:3172:TRP:NE1	2.22	0.55
1:B:4095:LEU:HD11	1:B:4422:LYS:CB	2.37	0.55
1:A:3965:LEU:HG	1:A:4426:MET:CE	2.37	0.55
1:A:4495:LEU:H	1:A:4495:LEU:CD1	2.16	0.55
1:B:4024:ARG:HA	1:B:4030:PHE:O	2.07	0.55
1:A:1755:LYS:HG2	1:A:1780:THR:HG23	1.89	0.54
1:A:2648:ILE:HD13	1:A:2831:PHE:CZ	2.42	0.54
1:A:3253:ASN:HB2	1:A:3604:PHE:CE2	2.42	0.54
1:A:3373:ILE:H	1:A:3373:ILE:CD1	2.06	0.54
1:B:2898:LEU:O	1:B:2902:VAL:HG23	2.06	0.54
1:B:4101:PHE:O	1:B:4105:VAL:HG23	2.07	0.54
1:B:4571:ARG:HD3	1:B:4593:GLY:O	2.06	0.54
1:A:1908:TYR:CE1	1:A:1958:LEU:HD13	2.42	0.54
1:A:2196:LEU:HD21	1:A:2219:LEU:HD22	1.89	0.54
1:A:2204:ILE:N	1:A:2205:PRO:CD	2.69	0.54
1:A:2275:VAL:HG13	1:A:2415:TRP:CE3	2.42	0.54
1:A:3266:GLN:HE21	1:A:3270:LEU:HD21	1.71	0.54
1:A:3390:GLU:O	1:A:3394:LEU:HG	2.07	0.54
1:A:4413:ASN:ND2	1:A:4660:LEU:HG	2.22	0.54
1:B:1694:PHE:CE1	1:B:1770:LEU:HD13	2.42	0.54
1:B:2832:ASN:HA	1:B:2835:LEU:HB3	1.89	0.54
1:B:3652:LEU:HB2	1:B:3684:PHE:CD1	2.43	0.54
1:A:1890:ARG:O	1:A:1894:LYS:HG3	2.07	0.54
1:A:2431:LEU:HD11	1:A:2506:PHE:CD2	2.42	0.54
1:A:3647:TRP:HB3	1:A:3652:LEU:CD2	2.37	0.54
1:A:3830:LEU:HB3	1:A:3858:LEU:CD1	2.37	0.54
1:B:2200:ASN:HA	1:B:2204:ILE:HG12	1.89	0.54
1:B:2968:LEU:O	1:B:2972:VAL:HG23	2.07	0.54
1:A:3086:ARG:HH11	1:A:3096:VAL:CG1	2.20	0.54
1:A:4319:LYS:N	1:A:4321:ARG:NH2	2.55	0.54
1:B:2283:THR:HA	1:B:2286:TRP:NE1	2.22	0.54
1:B:2331:LEU:HD21	1:B:2773:TRP:CD1	2.43	0.54
1:B:4013:SER:H	1:B:4016:GLN:HE21	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1691:ARG:HD3	1:A:1698:TYR:CD1	2.41	0.54
1:A:3336:ILE:O	1:A:3340:ASP:HB3	2.08	0.54
1:A:3700:LEU:CG	1:A:3701:ASP:H	2.20	0.54
1:A:4121:ILE:O	1:A:4126:VAL:HG12	2.06	0.54
1:A:4553:TYR:N	1:A:4553:TYR:CD1	2.75	0.54
1:B:1548:TYR:CD1	1:B:1549:GLN:HG2	2.43	0.54
1:B:1655:LEU:H	1:B:1655:LEU:HD22	1.72	0.54
1:B:2024:CYS:HA	1:B:2074:PHE:O	2.06	0.54
1:B:2498:CYS:SG	1:B:2569:ILE:HG13	2.47	0.54
1:B:2803:LEU:HD12	1:B:2808:LEU:HD21	1.90	0.54
1:B:2990:LEU:HD23	1:B:2994:VAL:HG11	1.90	0.54
1:B:4323:ASN:N	1:B:4323:ASN:ND2	2.54	0.54
1:A:1951:PRO:HG2	1:A:2104:ASP:OD1	2.08	0.54
1:A:2014:VAL:HG22	1:A:2065:ILE:HD13	1.90	0.54
1:A:2766:MET:HB3	1:A:2783:LEU:CD1	2.36	0.54
1:A:3602:ILE:O	1:A:3604:PHE:N	2.40	0.54
1:A:4122:VAL:HG23	1:A:4214:ARG:HD2	1.89	0.54
1:B:1782:ALA:HA	1:B:1938:PHE:CE1	2.42	0.54
1:B:2603:THR:CG2	1:B:2604:PRO:HD2	2.31	0.54
1:B:2874:TYR:OH	1:B:2916:ARG:HD2	2.08	0.54
1:A:2121:ALA:O	1:A:2124:LEU:N	2.41	0.54
1:A:3423:ARG:O	1:A:3426:ILE:HG22	2.07	0.54
1:A:4254:GLY:O	1:A:4256:PRO:HD3	2.07	0.54
1:B:2516:LEU:HD12	1:B:2581:LEU:HD13	1.90	0.54
1:B:2519:ALA:HB2	1:B:2593:PHE:CZ	2.43	0.54
1:B:4080:PHE:HB2	1:B:4101:PHE:CE1	2.43	0.54
1:A:2031:LEU:HD23	1:A:2035:ILE:HG22	1.89	0.54
1:A:2751:THR:HB	1:A:2755:GLY:HA2	1.90	0.54
1:A:3263:PHE:O	1:A:3267:VAL:HG23	2.07	0.54
1:A:3399:THR:N	1:A:3400:PRO:HD2	2.23	0.54
1:A:4013:SER:H	1:A:4016:GLN:HB3	1.73	0.54
1:A:4348:ASP:OD2	1:A:4349:ASN:N	2.40	0.54
1:B:2641:VAL:HG12	1:B:2642:ALA:N	2.23	0.54
1:B:4058:ILE:HD12	1:B:4082:LYS:HG2	1.89	0.54
1:A:1724:LYS:HD3	1:A:2382:GLY:O	2.07	0.54
1:A:2266:LEU:HD21	1:A:2394:MET:HE3	1.89	0.54
1:A:2447:GLN:HE22	1:A:2492:LEU:CD2	2.21	0.54
1:A:3043:ASN:HD22	1:A:3043:ASN:N	2.05	0.54
1:A:4547:PRO:HB2	1:A:4550:TRP:CE3	2.43	0.54
1:B:1975:PRO:HD2	1:B:2100:MET:O	2.07	0.54
1:B:1982:GLU:OE1	1:B:1982:GLU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2500:ALA:HA	1:B:2503:SER:OG	2.08	0.54
1:B:2636:VAL:HG21	1:B:2648:ILE:HD11	1.89	0.54
1:B:2929:LYS:O	1:B:2933:VAL:HG23	2.07	0.54
1:B:4336:THR:O	1:B:4340:SER:HB3	2.08	0.54
1:A:1822:VAL:HG12	1:A:1826:GLN:OE1	2.07	0.54
1:A:2128:ILE:HG13	1:A:2152:LEU:HD21	1.90	0.54
1:A:2689:ARG:C	1:A:2691:PHE:H	2.12	0.54
1:A:2819:PRO:HD2	1:A:2876:PRO:HG2	1.89	0.54
1:A:3109:MET:O	1:A:3112:CYS:HB2	2.08	0.54
1:A:3373:ILE:HD13	1:A:3373:ILE:N	2.12	0.54
1:A:3760:PHE:CG	1:A:3761:MET:N	2.75	0.54
1:A:3827:LEU:O	1:A:3831:GLU:HG3	2.08	0.54
1:A:4318:SER:CA	1:A:4321:ARG:HH21	2.19	0.54
1:B:2653:THR:O	1:B:2657:VAL:HG23	2.08	0.54
1:B:3255:VAL:HA	1:B:3259:HIS:CD2	2.43	0.54
1:B:3677:PRO:CD	1:B:3787:THR:HG22	2.38	0.54
1:B:4257:ALA:HB2	1:B:4389:ARG:HD3	1.90	0.54
1:A:2653:THR:O	1:A:2657:VAL:HG23	2.07	0.53
1:B:1910:MET:CA	1:B:1929:MET:HG3	2.39	0.53
1:B:4639:VAL:O	1:B:4666:ILE:HD12	2.08	0.53
1:A:2969:ARG:HG3	1:A:2970:GLU:N	2.23	0.53
1:A:3218:ALA:O	1:A:3219:ILE:C	2.47	0.53
1:A:3698:SER:HB2	1:A:3721:GLN:HB2	1.90	0.53
1:A:4375:LEU:CD1	1:A:4383:VAL:HG23	2.32	0.53
1:A:4553:TYR:HD1	1:A:4553:TYR:N	2.05	0.53
1:B:1581:TYR:O	1:B:1585:GLU:HB2	2.08	0.53
1:B:1646:ILE:O	1:B:1650:VAL:HG23	2.08	0.53
1:B:1831:LEU:HD13	1:B:1900:GLY:O	2.07	0.53
1:B:2863:ARG:HG3	1:B:2925:TRP:CZ2	2.44	0.53
1:B:3342:ARG:O	1:B:3345:GLN:HB3	2.07	0.53
1:A:2825:THR:O	1:A:2829:GLY:HA3	2.08	0.53
1:A:3418:GLU:O	1:A:3422:ILE:HG23	2.08	0.53
1:A:4012:LEU:HD12	1:A:4012:LEU:N	2.23	0.53
1:B:1655:LEU:HB2	1:B:1658:GLU:CB	2.31	0.53
1:B:1920:ASN:HD22	1:B:1921:VAL:N	2.06	0.53
1:B:2050:LEU:HG	1:B:2067:LEU:HD21	1.89	0.53
1:A:1699:PHE:N	1:A:1699:PHE:HD1	2.06	0.53
1:A:1803:TYR:HE1	1:A:1855:ILE:HD13	1.74	0.53
1:A:1827:VAL:O	1:A:1831:LEU:HG	2.08	0.53
1:A:4376:VAL:HG12	1:A:4379:ILE:HG22	1.90	0.53
1:A:4596:ASN:HD22	1:A:4596:ASN:C	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2118:PHE:CE1	1:B:2163:LYS:HG3	2.44	0.53
1:B:2309:LYS:CE	1:B:2756:THR:HG21	2.39	0.53
1:B:3677:PRO:HG3	1:B:3787:THR:HG22	1.89	0.53
1:B:3700:LEU:HD13	1:B:3701:ASP:H	1.71	0.53
1:A:1650:VAL:HG13	1:A:1659:VAL:HG11	1.91	0.53
1:A:2704:ALA:O	1:A:2706:THR:HG23	2.08	0.53
1:A:2994:VAL:O	1:A:2998:ILE:HG12	2.08	0.53
1:B:4671:TRP:C	1:B:4672:LYS:HG2	2.29	0.53
1:A:2016:LEU:HD21	1:A:2023:GLY:HA3	1.89	0.53
1:A:2274:MET:HE1	1:A:2286:TRP:HD1	1.73	0.53
1:A:2341:ASP:O	1:A:2343:VAL:N	2.40	0.53
1:B:2515:VAL:HG11	1:B:2577:LEU:HD13	1.90	0.53
1:B:2540:LEU:HD12	1:B:2662:ALA:CB	2.39	0.53
1:B:3067:GLU:O	1:B:3069:ILE:HG13	2.08	0.53
1:B:3109:MET:O	1:B:3129:LEU:HD21	2.09	0.53
1:B:4098:SER:O	1:B:4102:VAL:HG23	2.09	0.53
1:A:1709:ILE:HA	1:A:1766:ILE:HG12	1.90	0.53
1:A:1820:GLN:HB3	1:A:1912:TYR:CD2	2.44	0.53
1:A:2397:VAL:HG21	1:A:2400:LEU:CD2	2.38	0.53
1:A:2745:GLU:HB3	1:A:2748:LEU:HD12	1.91	0.53
1:A:2863:ARG:HD3	1:A:2863:ARG:C	2.29	0.53
1:B:1948:VAL:O	1:B:1950:THR:N	2.41	0.53
1:B:4260:MET:HG3	1:B:4271:TYR:CD1	2.43	0.53
1:B:4693:ASN:H	1:B:4693:ASN:ND2	2.06	0.53
1:A:2274:MET:HE1	1:A:2286:TRP:CD1	2.44	0.53
1:A:2548:VAL:HG11	1:A:2565:GLN:HE21	1.73	0.53
1:A:3700:LEU:HD13	1:A:3701:ASP:H	1.73	0.53
1:A:4036:HIS:HD2	1:A:4044:TRP:HE1	1.56	0.53
1:B:1541:LEU:HD23	1:B:1656:ILE:HG21	1.91	0.53
1:B:1558:TRP:CZ3	1:B:1606:ILE:HB	2.44	0.53
1:B:1932:ALA:HB1	1:B:1934:PHE:CE2	2.44	0.53
1:B:4278:HIS:CD2	1:B:4303:LEU:HB2	2.44	0.53
1:B:4597:PRO:HG2	1:B:4692:LEU:HD13	1.90	0.53
1:A:2701:PHE:CG	1:A:2705:THR:HG21	2.43	0.53
1:A:3821:GLY:O	1:A:3825:VAL:HG23	2.08	0.53
1:A:4207:LEU:O	1:A:4209:PRO:HD3	2.08	0.53
1:B:2280:GLY:O	1:B:2420:ILE:HD11	2.08	0.53
1:B:2497:GLU:O	1:B:2501:ILE:HG13	2.08	0.53
1:A:1538:TRP:CH2	1:A:1565:LEU:HG	2.44	0.53
1:A:2142:GLN:HE21	1:A:2208:VAL:HG11	1.75	0.53
1:A:2359:VAL:CG2	1:A:2397:VAL:HG11	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3802:LEU:CD2	1:A:3882:VAL:HG12	2.39	0.53
1:A:4122:VAL:O	1:A:4122:VAL:HG22	2.08	0.53
1:A:4188:LYS:HA	1:A:4218:THR:HB	1.90	0.53
1:B:1538:TRP:HZ3	1:B:1656:ILE:HD13	1.73	0.53
1:B:3895:ARG:HH12	1:B:3977:LYS:HG2	1.73	0.53
1:A:2598:GLN:HG2	1:A:2612:LEU:HD22	1.90	0.52
1:A:3956:THR:OG1	1:A:3964:LYS:HE3	2.08	0.52
1:A:2017:CYS:HB3	1:A:2067:LEU:HD12	1.90	0.52
1:A:3555:ASN:O	1:A:3559:ARG:HD3	2.09	0.52
1:A:3776:ASP:O	1:A:3780:ARG:HG2	2.09	0.52
1:A:3927:ASN:HB3	1:A:3930:LEU:CB	2.39	0.52
1:B:1525:ILE:HG13	1:B:1529:GLU:HG2	1.91	0.52
1:B:1612:TRP:CZ2	1:B:1644:ILE:HD11	2.44	0.52
1:B:1863:VAL:HG21	1:B:2115:SER:O	2.09	0.52
1:B:2205:PRO:HA	1:B:2261:GLN:OE1	2.09	0.52
1:B:2661:HIS:O	1:B:2665:SER:HB3	2.09	0.52
1:B:2704:ALA:HB2	1:B:3085:GLU:CD	2.29	0.52
1:B:2818:PHE:HD1	1:B:2876:PRO:HD3	1.74	0.52
1:A:2142:GLN:HE21	1:A:2208:VAL:CG1	2.22	0.52
1:A:2275:VAL:HB	1:A:2413:MET:HE2	1.90	0.52
1:A:2297:ASP:C	1:A:2299:ILE:H	2.12	0.52
1:A:2431:LEU:HD21	1:A:2506:PHE:CE2	2.44	0.52
1:A:2578:MET:CE	1:A:2613:LEU:HA	2.39	0.52
1:A:3233:TYR:O	1:A:3237:THR:HG23	2.10	0.52
1:A:3878:GLU:O	1:A:3882:VAL:HG23	2.10	0.52
1:A:4693:ASN:N	1:A:4693:ASN:ND2	2.57	0.52
1:B:3023:SER:HB2	2:B:9010:ADP:O1A	2.09	0.52
1:B:3059:LEU:HD23	1:B:3137:VAL:HG11	1.92	0.52
1:B:4118:MET:O	1:B:4122:VAL:HG22	2.08	0.52
1:A:2956:LEU:HD21	1:A:2971:TYR:CG	2.44	0.52
1:B:2838:LEU:O	1:B:2840:PRO:HD3	2.10	0.52
1:A:3439:ASP:C	1:A:3441:LYS:H	2.13	0.52
1:A:4048:PHE:HD1	1:A:4048:PHE:H	1.58	0.52
1:B:1930:ALA:HB2	1:B:1958:LEU:HD11	1.91	0.52
1:B:2036:LEU:HD23	1:B:2040:SER:HB3	1.90	0.52
1:B:2532:ARG:HG2	1:B:2532:ARG:HH11	1.74	0.52
1:B:3017:VAL:HG11	1:B:3175:GLU:CD	2.30	0.52
1:B:3082:SER:HA	1:B:3085:GLU:OE1	2.09	0.52
1:B:3681:ALA:HB2	1:B:3786:PHE:CG	2.45	0.52
1:A:1690:GLN:HE22	1:A:1766:ILE:CG2	2.17	0.52
1:A:2258:LYS:HE3	1:A:2415:TRP:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2857:TYR:HA	1:A:2913:PHE:CE1	2.36	0.52
1:A:3225:ASP:O	1:A:3229:SER:HB3	2.08	0.52
1:A:3415:LYS:O	1:A:3417:LEU:HD12	2.09	0.52
1:A:4103:CYS:SG	1:A:4108:GLU:HA	2.50	0.52
1:A:4371:PRO:O	1:A:4372:ASP:HB2	2.09	0.52
1:B:2144:HIS:HB3	1:B:2400:LEU:CD1	2.40	0.52
1:B:2907:HIS:HA	1:B:2910:LEU:HD12	1.92	0.52
1:B:4323:ASN:N	1:B:4323:ASN:HD22	2.06	0.52
1:A:2139:LEU:O	1:A:2140:SER:C	2.48	0.52
1:A:2142:GLN:HG2	1:A:2208:VAL:HG11	1.91	0.52
1:A:2531:LEU:HD12	1:A:2809:ARG:HD2	1.91	0.52
1:A:2708:GLU:O	1:A:2711:LEU:HB2	2.10	0.52
1:A:2793:ASN:HD22	1:A:2793:ASN:H	1.57	0.52
1:A:4006:PRO:C	1:A:4008:LEU:H	2.11	0.52
1:A:4413:ASN:HD21	1:A:4660:LEU:HG	1.74	0.52
1:B:1600:SER:O	1:B:1604:VAL:HG23	2.10	0.52
1:B:2282:LYS:HB2	1:B:2282:LYS:NZ	2.25	0.52
1:B:2748:LEU:N	1:B:2749:PRO:CD	2.73	0.52
1:B:4156:GLN:O	1:B:4183:THR:HB	2.10	0.52
1:A:1629:LEU:HD11	1:A:1686:TYR:CD2	2.44	0.52
1:A:2003:GLY:O	1:A:2004:PHE:C	2.49	0.52
1:A:2105:ARG:HG2	1:A:2105:ARG:NH1	2.23	0.52
1:A:2528:PHE:HE1	1:A:2533:VAL:HG11	1.73	0.52
1:A:3373:ILE:HG12	1:A:3374:ILE:H	1.74	0.52
1:A:3653:PRO:HB2	1:A:3658:CYS:SG	2.50	0.52
1:A:4288:ILE:CG2	1:A:4289:PRO:HA	2.40	0.52
1:B:1565:LEU:HD23	1:B:1595:LEU:CD1	2.39	0.52
1:B:1873:LYS:HB3	1:B:1943:ILE:HG21	1.90	0.52
1:B:2231:ILE:HD11	1:B:2260:LEU:HG	1.91	0.52
1:B:2506:PHE:CE1	1:B:2512:VAL:HG21	2.43	0.52
1:B:2531:LEU:HD13	1:B:2809:ARG:NH2	2.24	0.52
1:B:3233:TYR:O	1:B:3237:THR:HG23	2.09	0.52
1:B:4270:ILE:CG2	1:B:4310:ILE:HD13	2.34	0.52
1:A:2408:ILE:O	1:A:2410:ARG:N	2.43	0.52
1:A:3256:THR:OG1	1:A:3779:SER:HB3	2.09	0.52
1:A:3698:SER:C	1:A:3700:LEU:H	2.13	0.52
1:A:3924:LEU:HD23	1:A:3943:LEU:HD21	1.91	0.52
1:A:3988:TRP:NE1	1:A:3992:LEU:HD11	2.25	0.52
1:B:2741:VAL:HB	1:B:2788:PHE:CD2	2.44	0.52
1:B:2906:ALA:O	1:B:2909:ALA:HB3	2.10	0.52
1:B:4157:TYR:HB2	1:B:4184:TRP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1964:LEU:HD12	1:A:2074:PHE:HZ	1.75	0.52
1:A:2641:VAL:HG12	1:A:2831:PHE:HB3	1.92	0.52
1:A:2893:MET:HE3	1:A:2896:CYS:HB2	1.92	0.52
1:A:3813:ARG:HG3	1:A:3814:SER:N	2.24	0.52
1:A:4033:LEU:HD13	1:A:4062:TRP:CE2	2.45	0.52
1:B:4423:ALA:O	1:B:4427:ILE:HG12	2.10	0.52
1:A:1715:ILE:HD11	1:A:1760:ILE:HG21	1.92	0.51
1:A:2561:SER:OG	1:A:2564:ASN:HB3	2.09	0.51
1:B:1957:TYR:O	1:B:1961:THR:HG23	2.10	0.51
1:B:2820:SER:OG	1:B:2823:SER:HB2	2.09	0.51
1:B:2910:LEU:O	1:B:2914:GLN:HB3	2.10	0.51
1:B:3563:LEU:HD11	1:B:3845:ILE:CD1	2.40	0.51
1:B:3843:GLY:O	1:B:3845:ILE:N	2.35	0.51
1:A:2898:LEU:CD1	1:A:2941:VAL:HG22	2.40	0.51
1:A:4213:PHE:CZ	1:A:4215:LEU:HB2	2.45	0.51
1:A:4269:ARG:HG2	1:A:4369:PHE:CE1	2.45	0.51
1:B:1817:LEU:O	1:B:1821:ILE:HG13	2.10	0.51
1:B:2764:ARG:HD2	1:B:2806:ARG:O	2.10	0.51
1:B:4690:VAL:HG21	1:B:4701:PHE:CE1	2.45	0.51
1:A:2271:GLY:O	1:A:2411:CYS:HA	2.10	0.51
1:A:2535:ASN:ND2	1:A:2668:ARG:HH12	2.08	0.51
1:A:3567:LEU:HD23	1:A:3855:LEU:HD11	1.92	0.51
1:A:4136:SER:O	1:A:4220:GLU:HA	2.10	0.51
1:B:1937:GLY:HA3	1:B:1992:GLY:O	2.10	0.51
1:B:1975:PRO:HG2	1:B:1978:THR:HG21	1.91	0.51
1:B:2549:ILE:O	1:B:2553:GLN:HB2	2.09	0.51
1:B:3595:ALA:O	1:B:3598:PHE:HB3	2.11	0.51
1:B:3682:MET:SD	1:B:3696:LYS:HE2	2.49	0.51
1:B:4671:TRP:O	1:B:4672:LYS:HG2	2.11	0.51
1:B:4690:VAL:HG11	1:B:4701:PHE:CZ	2.44	0.51
1:A:1959:THR:HG21	1:A:2098:MET:HB2	1.92	0.51
1:A:2144:HIS:O	1:A:2413:MET:HG2	2.10	0.51
1:A:2732:PRO:CG	1:A:2739:LEU:HB2	2.40	0.51
1:A:2918:VAL:HG13	1:A:3172:TRP:NE1	2.26	0.51
1:A:3366:LEU:HD12	1:A:3366:LEU:O	2.10	0.51
1:A:3730:LEU:HD13	1:A:3734:LEU:HD21	1.91	0.51
1:A:3969:LEU:HD12	1:A:4426:MET:CE	2.41	0.51
1:B:2311:ILE:HB	1:B:2315:GLN:HE21	1.76	0.51
1:B:3902:GLU:C	1:B:3904:SER:H	2.13	0.51
1:B:4592:GLY:HA3	1:B:4725:SER:O	2.10	0.51
1:B:4636:SER:HA	1:B:4670:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1611:ARG:HG3	1:A:1611:ARG:NH1	2.23	0.51
1:A:2370:LEU:HD12	1:A:2377:LEU:CB	2.41	0.51
1:A:2586:GLY:HA2	1:A:2815:LEU:CD1	2.37	0.51
1:A:3114:GLU:HG2	1:A:3118:ARG:HH12	1.74	0.51
1:A:3353:LYS:O	1:A:3357:VAL:HG23	2.10	0.51
1:A:3452:ILE:CG2	1:A:3485:THR:HG21	2.39	0.51
1:A:3670:ARG:O	1:A:3782:THR:HG22	2.10	0.51
1:A:3768:ASP:HB3	1:A:3771:ALA:HB2	1.93	0.51
1:A:4025:GLN:HG3	1:B:2899:GLU:OE2	2.10	0.51
1:A:4240:ASN:OD1	1:A:4240:ASN:N	2.38	0.51
1:B:1920:ASN:ND2	1:B:1921:VAL:H	2.09	0.51
1:B:2238:LYS:HA	1:B:2241:GLN:HE21	1.74	0.51
1:B:3843:GLY:C	1:B:3845:ILE:H	2.13	0.51
1:A:1625:ILE:HG23	1:A:1626:ASN:OD1	2.11	0.51
1:A:2738:TRP:CE2	1:A:2785:LYS:HG2	2.46	0.51
1:A:4200:LEU:HD22	1:A:4204:LEU:CD1	2.41	0.51
1:B:1662:ILE:HB	1:B:1665:ILE:CG2	2.40	0.51
1:B:1971:ASN:O	1:B:2097:SER:HA	2.11	0.51
1:B:2815:LEU:HD23	1:B:2815:LEU:C	2.31	0.51
1:B:3889:MET:CE	1:B:3943:LEU:HB3	2.41	0.51
1:B:4086:MET:HG3	1:B:4097:TYR:CD2	2.45	0.51
1:B:4222:HIS:CG	1:B:4223:PRO:HD2	2.45	0.51
1:B:4340:SER:HB2	1:B:4357:TYR:OH	2.10	0.51
1:B:2638:THR:O	1:B:2641:VAL:HG23	2.10	0.51
1:B:3306:LEU:HD13	1:B:3557:VAL:HG22	1.92	0.51
1:A:2732:PRO:HG3	1:A:2739:LEU:HB2	1.93	0.51
1:A:3289:LEU:HD13	1:A:3293:ARG:NH2	2.25	0.51
1:A:3721:GLN:NE2	1:A:4205:HIS:NE2	2.58	0.51
1:A:4384:PRO:HB3	1:A:4395:TRP:CD1	2.45	0.51
1:B:1556:ARG:HG2	1:B:1557:GLY:N	2.25	0.51
1:B:2219:LEU:HD13	1:B:2228:LEU:HD11	1.93	0.51
1:B:2643:SER:HB3	1:B:2646:VAL:HG23	1.93	0.51
1:B:2801:VAL:HG12	1:B:2802:GLN:N	2.25	0.51
1:B:2877:ARG:HB3	1:B:2881:ARG:NH1	2.26	0.51
1:B:2931:ASP:O	1:B:2935:LEU:HG	2.11	0.51
1:B:3063:GLY:HA2	1:B:3136:GLN:CB	2.41	0.51
1:B:3566:ASN:ND2	1:B:3859:LYS:NZ	2.59	0.51
1:B:4121:ILE:HA	1:B:4125:GLU:CG	2.32	0.51
1:B:4550:TRP:O	1:B:4552:TRP:N	2.40	0.51
1:A:1713:LYS:O	1:A:1715:ILE:N	2.44	0.51
1:A:2138:GLN:NE2	1:A:2218:LEU:HD21	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2327:TRP:CZ3	1:A:2380:PRO:HD2	2.46	0.51
1:A:2540:LEU:HD23	1:A:2662:ALA:HB3	1.92	0.51
1:A:2619:ILE:HG13	1:A:2619:ILE:O	2.11	0.51
1:A:4299:ASN:OD1	1:A:4301:ALA:HB3	2.11	0.51
1:A:4389:ARG:HH12	1:A:4393:MET:CE	2.24	0.51
1:A:4428:ASN:O	1:A:4432:LYS:HG2	2.10	0.51
1:B:1520:ALA:HA	1:B:1580:TYR:CE1	2.46	0.51
1:B:1639:ILE:HG21	1:B:1676:LEU:HG	1.93	0.51
1:B:2283:THR:HA	1:B:2286:TRP:HE1	1.76	0.51
1:B:2542:ASN:O	1:B:2546:VAL:HG23	2.10	0.51
1:B:2849:LEU:HD21	1:B:2886:LEU:HD13	1.93	0.51
1:B:2921:GLU:CD	1:B:2921:GLU:H	2.13	0.51
1:B:2968:LEU:CD2	1:B:2999:LEU:HD11	2.41	0.51
1:B:3219:ILE:CB	1:B:3220:PRO:CD	2.89	0.51
1:A:2204:ILE:HG13	1:A:2205:PRO:HD3	1.92	0.51
1:A:3032:MET:C	1:A:3034:GLY:H	2.15	0.51
1:A:3425:LYS:HA	1:A:3428:GLU:CG	2.41	0.51
1:A:4222:HIS:ND1	1:A:4223:PRO:HD2	2.26	0.51
1:B:1578:SER:C	1:B:1580:TYR:H	2.14	0.51
1:B:1823:TRP:O	1:B:1827:VAL:HG23	2.10	0.51
1:B:1892:LEU:HA	1:B:1895:CYS:SG	2.51	0.51
1:B:2199:ILE:O	1:B:2203:MET:HB2	2.11	0.51
1:B:3583:THR:O	1:B:3587:THR:HG23	2.11	0.51
1:B:3618:MET:HB3	1:B:3628:PHE:CZ	2.46	0.51
1:B:3790:PRO:HA	1:B:3898:PHE:CE2	2.46	0.51
1:A:2582:GLY:O	1:A:2585:MET:HB2	2.11	0.50
1:A:2839:LEU:HD22	1:A:2896:CYS:HB3	1.93	0.50
1:A:3116:ALA:HB1	1:A:3121:LEU:O	2.12	0.50
1:B:1527:LEU:HD22	1:B:1575:MET:HB2	1.92	0.50
1:B:1573:SER:HA	1:B:1576:LYS:HE2	1.93	0.50
1:B:1687:LEU:HD11	1:B:1706:LEU:HD21	1.93	0.50
1:B:4288:ILE:HG23	1:B:4289:PRO:HA	1.92	0.50
1:B:4644:LEU:HD13	1:B:4647:ALA:HB3	1.92	0.50
1:A:1776:GLU:HA	1:A:1779:SER:HB3	1.93	0.50
1:A:1963:ALA:HB1	1:A:2096:ARG:CG	2.41	0.50
1:A:2212:ILE:N	1:A:2213:PRO:CD	2.75	0.50
1:A:2856:PHE:CE1	1:A:2930:ILE:HG12	2.46	0.50
1:A:3923:LEU:HD11	1:A:3943:LEU:HA	1.94	0.50
1:B:1479:ARG:O	1:B:1483:ILE:HG13	2.11	0.50
1:B:1534:VAL:HG13	1:B:1568:HIS:CD2	2.42	0.50
1:B:2729:VAL:HG12	1:B:2782:LYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3038:TYR:CD2	1:B:3058:LEU:HD13	2.46	0.50
1:B:4267:ARG:NH2	1:B:4315:ASP:OD1	2.43	0.50
1:A:1719:GLN:HA	1:A:1722:PHE:CD2	2.46	0.50
1:A:4285:LEU:O	1:A:4288:ILE:HG13	2.10	0.50
1:B:1951:PRO:HG2	1:B:2104:ASP:OD2	2.10	0.50
1:B:4170:LEU:HD12	1:B:4171:ALA:N	2.26	0.50
1:B:4686:LEU:HD12	1:B:4687:SER:N	2.27	0.50
1:A:2049:ALA:O	1:A:2054:SER:HB3	2.12	0.50
1:A:2586:GLY:O	1:A:2590:ARG:HB2	2.10	0.50
1:A:3067:GLU:O	1:A:3069:ILE:HD12	2.12	0.50
1:A:4044:TRP:CE3	1:A:4048:PHE:HE1	2.29	0.50
1:A:4122:VAL:HA	1:A:4126:VAL:HG11	1.91	0.50
1:A:4326:PRO:HB3	1:A:4369:PHE:CD2	2.46	0.50
1:B:1907:LEU:HA	1:B:1911:ARG:NH1	2.26	0.50
1:B:1967:ARG:HG2	1:B:1967:ARG:HH11	1.75	0.50
1:B:2135:CYS:HB3	1:B:2139:LEU:HD12	1.92	0.50
1:B:2142:GLN:HB2	1:B:2145:TYR:CD1	2.46	0.50
1:A:2533:VAL:HB	1:A:2581:LEU:HA	1.94	0.50
1:A:2954:ASN:HD22	1:A:2954:ASN:N	2.02	0.50
1:A:3380:VAL:HG11	1:A:3435:ILE:CG2	2.41	0.50
1:A:3834:LEU:HA	1:A:3854:THR:HG21	1.93	0.50
1:A:4028:PRO:C	1:A:4030:PHE:H	2.15	0.50
1:A:4118:MET:HB3	1:A:4149:LEU:HD22	1.94	0.50
1:B:2865:THR:N	1:B:2868:ILE:HD12	2.26	0.50
1:A:2720:TYR:HE1	1:A:2781:ILE:HG21	1.76	0.50
1:A:4052:GLN:C	1:A:4054:GLY:H	2.14	0.50
1:B:1862:SER:O	1:B:1867:LEU:HD21	2.12	0.50
1:B:1926:VAL:HG22	1:B:1935:TYR:HE2	1.75	0.50
1:B:2367:LEU:HD12	1:B:2367:LEU:N	2.26	0.50
1:B:3691:ASP:C	1:B:3693:LYS:H	2.15	0.50
1:B:4111:LEU:N	1:B:4111:LEU:HD12	2.26	0.50
1:A:1971:ASN:ND2	1:A:2087:LEU:HD11	2.26	0.50
1:A:2197:ASN:O	1:A:2201:ASP:HB2	2.12	0.50
1:A:2627:TRP:O	1:A:2629:ASN:N	2.45	0.50
1:A:2913:PHE:N	1:A:2913:PHE:CD2	2.79	0.50
1:A:4388:THR:O	1:A:4391:HIS:HB2	2.12	0.50
1:A:4518:ALA:C	1:A:4520:LEU:H	2.15	0.50
1:B:1662:ILE:HB	1:B:1665:ILE:HG23	1.93	0.50
1:B:2723:THR:CG2	1:B:2727:GLU:HB2	2.42	0.50
1:B:4020:LEU:HD11	1:B:4033:LEU:HG	1.93	0.50
1:B:2918:VAL:HG22	1:B:3172:TRP:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3105:PHE:O	1:B:3109:MET:HG3	2.12	0.50
1:A:1639:ILE:HD11	1:A:1675:LEU:HB3	1.94	0.50
1:A:1889:VAL:HA	1:A:1892:LEU:HD12	1.94	0.50
1:A:3410:LEU:HA	1:A:3414:GLY:O	2.12	0.50
1:A:3433:THR:HG22	1:A:3437:ASN:HD22	1.75	0.50
1:A:3583:THR:O	1:A:3587:THR:HG23	2.11	0.50
1:A:3977:LYS:O	1:A:3979:THR:HG23	2.12	0.50
1:A:4078:SER:HA	1:A:4081:ARG:HD2	1.94	0.50
1:A:4185:VAL:HG12	1:A:4186:LEU:N	2.19	0.50
1:B:2989:VAL:HG13	1:B:3187:GLU:OE2	2.12	0.50
1:B:4644:LEU:O	1:B:4661:SER:HB2	2.11	0.50
1:A:1926:VAL:HG12	1:A:1928:HIS:NE2	2.26	0.49
1:A:2798:ALA:C	1:A:2800:ARG:H	2.14	0.49
1:A:3992:LEU:HD22	1:A:4430:LEU:CB	2.41	0.49
1:A:4278:HIS:CD2	1:A:4343:TYR:OH	2.64	0.49
1:B:1522:GLN:O	1:B:1525:ILE:HG22	2.11	0.49
1:B:1781:LEU:O	1:B:1814:LEU:HD21	2.12	0.49
1:B:2504:GLN:HA	1:B:2507:GLU:OE2	2.12	0.49
1:B:2976:LEU:HD11	1:B:2990:LEU:HD21	1.94	0.49
1:B:3061:ARG:HB3	1:B:3067:GLU:OE2	2.12	0.49
1:B:3181:LEU:CB	1:B:3232:VAL:HG13	2.42	0.49
1:B:4132:LEU:HD13	1:B:4216:PHE:CZ	2.47	0.49
1:B:4259:ARG:NH2	1:B:4307:LEU:HB3	2.27	0.49
1:B:4339:GLY:HA3	1:B:4360:LEU:HD11	1.93	0.49
1:A:2511:LEU:HD11	1:A:2574:LEU:HD21	1.94	0.49
1:A:3011:HIS:CE1	1:A:3143:VAL:HG23	2.47	0.49
1:A:3059:LEU:HD21	1:A:3090:LEU:HD13	1.94	0.49
1:A:3337:LYS:CB	1:A:3525:LEU:HD13	2.24	0.49
1:A:3919:ILE:HG21	1:A:3951:THR:HA	1.94	0.49
1:A:4054:GLY:O	1:A:4055:GLU:O	2.30	0.49
1:A:4055:GLU:HG3	1:A:4093:ARG:NH1	2.27	0.49
1:B:1494:ILE:HA	1:B:1497:LEU:HD12	1.93	0.49
1:B:2877:ARG:HG2	2:B:9009:ADP:H4'	1.94	0.49
1:B:3935:ASP:O	1:B:3939:ARG:HG3	2.12	0.49
1:B:4060:GLU:HA	1:B:4063:ILE:HD13	1.94	0.49
1:B:4402:ILE:H	1:B:4402:ILE:CD1	2.21	0.49
1:B:4596:ASN:C	1:B:4596:ASN:HD22	2.15	0.49
1:B:4642:MET:HG2	1:B:4725:SER:HA	1.94	0.49
1:A:1739:THR:O	1:A:1760:ILE:HG12	2.12	0.49
1:A:2018:GLN:HE21	1:A:2066:SER:HB3	1.77	0.49
1:A:2057:VAL:HG22	1:A:2058:GLU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2133:LYS:O	1:A:2133:LYS:HD3	2.12	0.49
1:A:2869:GLN:HG2	1:A:2871:HIS:CE1	2.47	0.49
1:A:3192:LEU:O	1:A:3224:ARG:NH2	2.46	0.49
1:A:3398:PRO:C	1:A:3400:PRO:HD2	2.33	0.49
1:A:3723:VAL:HG23	1:A:3764:LEU:HD22	1.94	0.49
1:A:4068:GLN:C	1:A:4070:SER:H	2.15	0.49
1:A:4365:THR:HB	1:A:4366:PRO:HD2	1.93	0.49
1:A:4574:GLN:HE22	1:A:4590:TRP:H	1.60	0.49
1:B:3135:SER:HA	1:B:3138:ARG:HG2	1.95	0.49
1:B:3700:LEU:CG	1:B:3701:ASP:H	2.23	0.49
1:A:1887:ASP:O	1:A:1891:GLN:HG3	2.12	0.49
1:A:2029:ASN:HD22	1:A:2030:ARG:N	2.11	0.49
1:A:2302:GLU:HG2	1:A:2304:HIS:CE1	2.46	0.49
1:A:2374:ASN:O	1:A:2375:LYS:HB2	2.11	0.49
1:A:3338:GLN:HA	1:A:3342:ARG:CB	2.42	0.49
1:A:3725:ASN:ND2	1:A:3725:ASN:N	2.58	0.49
1:A:4075:THR:HG23	1:A:4076:ILE:N	2.27	0.49
1:A:4122:VAL:HA	1:A:4126:VAL:CG1	2.42	0.49
1:A:4244:VAL:HG23	1:A:4403:SER:CB	2.42	0.49
1:B:3192:LEU:HD11	1:B:3268:VAL:HG22	1.94	0.49
1:A:1934:PHE:CD2	1:A:1934:PHE:N	2.81	0.49
1:A:2370:LEU:HD23	1:A:2387:LEU:HD22	1.95	0.49
1:A:3116:ALA:HB1	1:A:3123:LEU:HD12	1.94	0.49
1:A:3947:ILE:CG2	1:A:3948:PHE:N	2.76	0.49
1:B:2021:ALA:O	1:B:2071:MET:HA	2.13	0.49
1:B:3316:LYS:HD2	1:B:3546:ILE:HD12	1.94	0.49
1:A:1629:LEU:N	1:A:1630:PRO:HD3	2.28	0.49
1:A:1699:PHE:N	1:A:1699:PHE:CD1	2.77	0.49
1:A:1907:LEU:HA	1:A:1911:ARG:HH11	1.77	0.49
1:A:2029:ASN:HD22	1:A:2029:ASN:N	2.10	0.49
1:A:3217:MET:O	1:A:3218:ALA:C	2.50	0.49
1:A:3655:ASP:O	1:A:3659:ILE:HG13	2.13	0.49
1:A:3674:VAL:HG13	1:A:3786:PHE:HD2	1.78	0.49
1:B:2315:GLN:HB3	1:B:2775:THR:CG2	2.41	0.49
1:B:2832:ASN:HD22	1:B:2835:LEU:HD23	1.77	0.49
1:B:2839:LEU:HD22	1:B:2896:CYS:HB3	1.95	0.49
1:B:4012:LEU:N	1:B:4012:LEU:HD23	2.27	0.49
1:B:4313:TRP:HB3	1:B:4330:PRO:CG	2.42	0.49
1:A:2272:VAL:HA	1:A:2412:GLY:H	1.77	0.49
1:A:2848:ASN:HB3	1:A:2938:PHE:HE1	1.77	0.49
1:A:3039:THR:HG22	1:A:3040:ILE:N	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2612:LEU:HD11	1:B:2624:TRP:CZ3	2.48	0.49
1:B:4167:GLY:HA2	1:B:4170:LEU:HD11	1.93	0.49
1:A:2941:VAL:CG1	1:A:2942:ASN:N	2.76	0.49
1:A:2948:ARG:HG2	1:A:2948:ARG:NH1	2.28	0.49
1:A:3262:ASP:CB	1:A:3670:ARG:HE	2.25	0.49
1:A:3997:ASN:HD21	1:A:4001:ILE:HD11	1.77	0.49
1:A:4068:GLN:N	1:A:4073:GLN:HE21	2.11	0.49
1:A:4072:GLN:OE1	1:A:4077:VAL:HG21	2.11	0.49
1:A:4295:PHE:C	1:A:4295:PHE:CD2	2.86	0.49
1:B:2000:CYS:CB	1:B:2031:LEU:HD13	2.42	0.49
1:B:2517:GLU:O	1:B:2521:GLN:HG2	2.13	0.49
1:B:2677:GLY:HA3	1:B:2875:SER:OG	2.12	0.49
1:B:3991:LEU:HG	1:B:3992:LEU:HD23	1.94	0.49
1:B:4109:ASP:HA	1:B:4112:ASN:HD21	1.72	0.49
1:A:2208:VAL:HG22	1:A:2211:ASP:HB2	1.95	0.49
1:A:2610:ILE:HD12	1:A:2615:TYR:OH	2.13	0.49
1:A:3069:ILE:O	1:A:3141:LEU:O	2.30	0.49
1:A:3981:ASN:HD22	1:A:4076:ILE:CB	2.20	0.49
1:A:4230:LEU:HB3	1:A:4235:VAL:HG21	1.94	0.49
1:A:4536:SER:HB2	1:A:4548:LYS:HZ1	1.77	0.49
1:A:4548:LYS:O	1:A:4550:TRP:N	2.46	0.49
1:A:4596:ASN:ND2	1:A:4599:ALA:H	2.11	0.49
1:B:2723:THR:OG1	1:B:2724:PRO:HD2	2.13	0.49
1:B:4618:ASN:ND2	1:B:4618:ASN:H	2.11	0.49
1:A:1565:LEU:HD11	1:A:1598:VAL:HG12	1.94	0.49
1:A:1603:ASP:O	1:A:1606:ILE:HG22	2.13	0.49
1:A:1639:ILE:HG21	1:A:1676:LEU:HG	1.94	0.49
1:A:1800:HIS:HB2	1:A:1858:ASN:ND2	2.28	0.49
1:A:3180:ALA:O	1:A:3184:VAL:HG23	2.12	0.49
1:A:3370:GLU:O	1:A:3372:ALA:N	2.46	0.49
1:A:3689:TYR:CB	1:A:3694:ILE:HD11	2.21	0.49
1:A:4402:ILE:HD12	1:A:4402:ILE:N	2.26	0.49
1:B:1823:TRP:NE1	1:B:1885:GLN:HB3	2.27	0.49
1:B:1934:PHE:CD2	1:B:1934:PHE:N	2.81	0.49
1:B:1959:THR:HG21	1:B:2098:MET:SD	2.53	0.49
1:B:2241:GLN:HA	1:B:2244:ALA:HB3	1.93	0.49
1:B:2655:ARG:O	1:B:2659:VAL:HG23	2.13	0.49
1:B:3929:ASN:HB3	1:B:3942:TYR:CD1	2.47	0.49
1:B:4693:ASN:HD22	1:B:4693:ASN:N	2.09	0.49
1:A:1820:GLN:HE22	1:A:1990:GLN:HE22	1.60	0.48
1:A:2572:ARG:O	1:A:2575:TYR:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3017:VAL:HG22	1:A:3018:SER:N	2.27	0.48
1:A:3048:SER:HB2	1:A:3080:GLU:OE1	2.13	0.48
1:A:3457:LEU:HD11	1:A:3482:THR:HA	1.95	0.48
1:A:3598:PHE:O	1:A:3602:ILE:HB	2.11	0.48
1:B:1926:VAL:HG12	1:B:1928:HIS:NE2	2.28	0.48
1:B:2616:SER:HB3	1:B:2627:TRP:CD2	2.47	0.48
1:B:3540:ILE:O	1:B:3544:GLU:HG3	2.13	0.48
1:A:2720:TYR:CE1	1:A:2781:ILE:HG21	2.48	0.48
1:A:3150:ALA:O	1:A:3151:SER:C	2.51	0.48
1:A:3238:ILE:HG12	1:A:3601:TYR:HD2	1.69	0.48
1:A:4003:GLU:HG3	1:B:2842:LEU:HD23	1.95	0.48
1:A:4043:ASP:HB3	1:A:4059:PRO:HB3	1.95	0.48
1:A:4083:ILE:HD11	1:A:4098:SER:HA	1.94	0.48
1:A:4589:VAL:CG1	1:A:4639:VAL:HA	2.43	0.48
1:B:1813:GLN:NE2	1:B:1940:TYR:HA	2.17	0.48
1:B:1934:PHE:HB3	1:B:1993:ARG:HH22	1.78	0.48
1:B:2229:GLN:O	1:B:2230:PRO:O	2.30	0.48
1:B:2276:GLY:O	1:B:2282:LYS:HE2	2.13	0.48
1:B:2968:LEU:HG	1:B:2995:LEU:HD22	1.95	0.48
1:B:3295:THR:O	1:B:3299:VAL:HG23	2.12	0.48
1:B:4263:GLN:HA	1:B:4264:PRO:C	2.34	0.48
1:B:4513:ILE:HD12	1:B:4568:PHE:CE2	2.47	0.48
1:A:2088:PRO:C	1:A:2090:ASN:H	2.16	0.48
1:A:3007:GLN:NE2	1:A:3008:PRO:HD2	2.29	0.48
1:A:4133:LEU:HD21	1:A:4225:LEU:HD13	1.94	0.48
1:A:4604:THR:OG1	1:A:4671:TRP:HZ3	1.96	0.48
1:B:2604:PRO:O	1:B:2624:TRP:NE1	2.46	0.48
1:B:2720:TYR:CE1	1:B:2730:LEU:HD13	2.48	0.48
1:B:4306:ALA:HB1	1:B:4338:LEU:HD13	1.94	0.48
1:A:3145:PHE:CE2	1:A:3164:LEU:HD21	2.48	0.48
1:A:3920:PHE:O	1:A:3923:LEU:HB3	2.13	0.48
1:A:4133:LEU:HA	1:A:4217:MET:HB2	1.94	0.48
1:A:4335:ARG:HD3	1:A:4361:GLU:HA	1.96	0.48
1:B:1910:MET:HA	1:B:1929:MET:HG3	1.95	0.48
1:B:2080:GLY:HA3	1:B:2084:ARG:O	2.13	0.48
1:B:2621:ASP:C	1:B:2623:ASN:H	2.16	0.48
1:B:2782:LYS:HB2	1:B:2782:LYS:NZ	2.28	0.48
1:B:3673:LEU:HD13	1:B:3783:PHE:CE1	2.48	0.48
1:A:2273:MET:HG3	1:A:2413:MET:CE	2.44	0.48
1:A:2752:ASP:C	1:A:2754:TYR:H	2.17	0.48
1:A:3042:VAL:HB	1:A:3079:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3289:LEU:HD13	1:A:3293:ARG:HH22	1.77	0.48
1:A:3425:LYS:HA	1:A:3428:GLU:HG2	1.95	0.48
1:A:4047:PHE:HD2	1:A:4048:PHE:CD1	2.32	0.48
1:A:4190:ILE:HB	1:A:4197:LEU:HD21	1.94	0.48
1:A:4684:SER:O	1:A:4707:TYR:CE2	2.67	0.48
1:B:2025:PHE:HB2	1:B:2075:VAL:HG22	1.94	0.48
1:B:2641:VAL:CG2	1:B:2887:LEU:HD22	2.43	0.48
1:B:2774:ARG:HB2	1:B:2781:ILE:HD13	1.94	0.48
1:B:3677:PRO:HG3	1:B:3769:PRO:HB3	1.94	0.48
1:B:4024:ARG:HG3	1:B:4031:SER:O	2.14	0.48
1:A:2204:ILE:CG1	1:A:2205:PRO:HD3	2.44	0.48
1:A:2902:VAL:HG21	1:A:2941:VAL:HG21	1.95	0.48
1:A:2952:TYR:CE1	1:A:2962:PRO:HG3	2.48	0.48
1:A:3238:ILE:N	1:A:3238:ILE:HD12	2.28	0.48
1:A:3371:PRO:O	1:A:3372:ALA:C	2.52	0.48
1:A:3408:VAL:HG11	1:A:3477:LEU:CG	2.43	0.48
1:A:3487:TYR:O	1:A:3489:GLU:N	2.47	0.48
1:A:3664:MET:O	1:A:3668:PHE:HB3	2.13	0.48
1:A:3924:LEU:C	1:A:3925:ASN:HD22	2.15	0.48
1:A:4029:SER:CB	1:A:4081:ARG:HH12	2.25	0.48
1:A:4384:PRO:HB3	1:A:4395:TRP:CG	2.48	0.48
1:B:3196:ASN:ND2	1:B:3199:TYR:HB2	2.28	0.48
1:B:3911:PHE:CZ	1:B:3955:VAL:HG13	2.49	0.48
1:B:3990:PHE:CE2	1:B:4023:LEU:HD13	2.48	0.48
1:B:4410:LEU:CD2	1:B:4411:PRO:HD2	2.43	0.48
1:B:4653:GLN:OE1	1:B:4708:ASP:HA	2.14	0.48
1:A:1960:LEU:O	1:A:1964:LEU:N	2.39	0.48
1:A:1973:PHE:HE1	1:A:2099:ALA:CB	2.27	0.48
1:A:1974:GLY:C	1:A:2079:PRO:HD3	2.34	0.48
1:A:3323:LYS:HE3	1:A:3539:LEU:HG	1.95	0.48
1:A:3865:ILE:HA	1:A:3869:VAL:HG23	1.94	0.48
1:A:3891:LEU:HD21	1:A:3895:ARG:NH2	2.28	0.48
1:B:1525:ILE:HD12	1:B:1528:GLU:HB3	1.96	0.48
1:B:1694:PHE:CE1	1:B:1770:LEU:HB3	2.48	0.48
1:B:3011:HIS:ND1	1:B:3091:LEU:HD22	2.28	0.48
1:B:3677:PRO:HB3	1:B:3769:PRO:HD3	1.94	0.48
1:B:3887:ASN:N	1:B:3888:PRO:CD	2.77	0.48
1:B:4400:PRO:HG2	1:B:4407:TRP:CH2	2.49	0.48
1:B:4540:SER:HB2	1:B:4545:ILE:O	2.13	0.48
1:A:1974:GLY:CA	1:A:2079:PRO:HD3	2.44	0.48
1:A:3863:THR:O	1:A:3863:THR:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3987:GLU:HG3	1:A:4027:VAL:CG1	2.44	0.48
1:A:4184:TRP:N	1:A:4184:TRP:CD1	2.82	0.48
1:A:4406:ILE:HB	1:A:4412:GLU:OE2	2.14	0.48
1:A:4591:LEU:CD2	1:A:4601:ILE:HD11	2.42	0.48
1:B:2084:ARG:HG2	1:B:2084:ARG:HH11	1.79	0.48
1:B:3955:VAL:HG12	1:B:3959:LEU:HG	1.96	0.48
1:B:4070:SER:O	1:B:4071:ASN:C	2.52	0.48
1:A:1701:GLY:HA2	1:A:2011:ARG:NH1	2.29	0.48
1:A:1800:HIS:CB	1:A:1858:ASN:HD22	2.26	0.48
1:A:3397:PRO:HG2	1:A:3419:TRP:CE2	2.48	0.48
1:A:3473:ALA:O	1:A:3476:PRO:HD2	2.13	0.48
1:A:4132:LEU:HB2	1:A:4216:PHE:HD1	1.79	0.48
1:A:4655:THR:HG22	1:A:4708:ASP:HB2	1.96	0.48
1:B:1962:GLN:HB3	1:B:4341:THR:HG21	1.96	0.48
1:B:3273:GLU:OE1	1:B:3667:ARG:NH2	2.47	0.48
1:B:3585:MET:HA	1:B:3588:VAL:HG23	1.96	0.48
1:B:3638:LEU:HB2	1:B:3663:ILE:HD12	1.96	0.48
1:B:3731:ASN:HB2	1:B:3732:PRO:HD3	1.94	0.48
1:B:4407:TRP:CD1	1:B:4407:TRP:N	2.82	0.48
1:A:1535:ARG:HA	1:A:1591:TRP:CZ2	2.49	0.48
1:A:2208:VAL:HA	1:A:2415:TRP:HD1	1.74	0.48
1:A:2299:ILE:CG2	1:A:2349:LYS:HA	2.44	0.48
1:A:2375:LYS:HG2	1:A:2387:LEU:HD23	1.95	0.48
1:A:2704:ALA:HB3	1:A:3085:GLU:CG	2.44	0.48
1:A:2813:ILE:HG22	1:A:2814:LEU:N	2.28	0.48
1:A:3145:PHE:CD1	1:A:3164:LEU:HD11	2.48	0.48
1:A:3695:THR:HG21	1:A:3707:ASN:OD1	2.14	0.48
1:A:4201:GLU:HG3	1:A:4228:ASN:HB2	1.94	0.48
1:B:2532:ARG:HG2	1:B:2532:ARG:NH1	2.29	0.48
1:B:3232:VAL:O	1:B:3236:GLN:HG3	2.14	0.48
1:B:3350:VAL:HG12	1:B:3354:GLU:OE2	2.13	0.48
1:B:4083:ILE:CD1	1:B:4098:SER:HA	2.44	0.48
1:B:4288:ILE:CG2	1:B:4289:PRO:HA	2.44	0.48
1:B:4360:LEU:C	1:B:4362:GLN:H	2.17	0.48
1:A:3078:VAL:O	1:A:3078:VAL:HG13	2.13	0.47
1:A:3699:PHE:CZ	1:A:3726:ILE:HG13	2.49	0.47
1:A:4048:PHE:CD1	1:A:4048:PHE:N	2.82	0.47
1:A:4296:PHE:CZ	1:A:4347:ILE:HD13	2.49	0.47
1:B:2397:VAL:HG22	1:B:2398:GLN:N	2.29	0.47
1:B:2613:LEU:HD22	1:B:2655:ARG:NH1	2.29	0.47
1:B:2886:LEU:HD23	1:B:2904:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3960:LEU:HD23	1:B:4237:SER:HB2	1.96	0.47
1:A:2128:ILE:HG23	1:A:2129:VAL:N	2.29	0.47
1:A:2207:LEU:CD1	1:A:2215:ILE:HG21	2.43	0.47
1:A:2497:GLU:O	1:A:2501:ILE:HG13	2.13	0.47
1:A:3074:ASP:H	1:A:3077:ASN:HD22	1.62	0.47
1:A:3408:VAL:HG23	1:A:3409:CYS:H	1.80	0.47
1:A:3903:LEU:HD23	1:A:4433:MET:SD	2.54	0.47
1:A:3930:LEU:HD11	1:A:3939:ARG:HG2	1.95	0.47
1:A:3992:LEU:HD22	1:A:4430:LEU:HB2	1.96	0.47
1:A:4268:SER:OG	1:A:4387:THR:HA	2.14	0.47
1:A:4335:ARG:HD3	1:A:4360:LEU:C	2.35	0.47
1:B:1568:HIS:O	1:B:1572:ILE:HG13	2.14	0.47
1:B:1910:MET:HB2	1:B:1929:MET:HG3	1.95	0.47
1:B:2212:ILE:N	1:B:2213:PRO:CD	2.77	0.47
1:B:2918:VAL:HG22	1:B:3172:TRP:CE2	2.49	0.47
1:B:4568:PHE:O	1:B:4572:MET:HG2	2.14	0.47
1:A:1639:ILE:CD1	1:A:1675:LEU:HB3	2.44	0.47
1:A:1934:PHE:HE1	1:A:1964:LEU:HD22	1.78	0.47
1:A:2313:LYS:CE	1:A:2366:ASN:HD21	2.17	0.47
1:A:3781:VAL:HG12	1:A:3782:THR:N	2.29	0.47
1:A:3897:TYR:CE1	1:A:3913:LEU:HA	2.47	0.47
1:A:3997:ASN:O	1:A:3999:THR:N	2.47	0.47
1:A:3997:ASN:ND2	1:A:4001:ILE:HD11	2.27	0.47
1:B:1628:LEU:HD13	1:B:1709:ILE:HG22	1.95	0.47
1:B:1659:VAL:C	1:B:1661:ALA:H	2.18	0.47
1:B:3013:LEU:HG	1:B:3013:LEU:O	2.13	0.47
1:A:2368:ASN:HB3	1:A:2410:ARG:NH1	2.29	0.47
1:A:2598:GLN:HG3	1:A:2612:LEU:HB2	1.96	0.47
1:A:2616:SER:OG	1:A:2617:VAL:N	2.47	0.47
1:A:3219:ILE:CB	1:A:3220:PRO:CD	2.93	0.47
1:A:3338:GLN:HG3	1:A:3529:ILE:HD12	1.96	0.47
1:A:3480:TRP:HE1	1:A:3484:GLN:HE21	1.62	0.47
1:A:3804:THR:C	1:A:3806:ARG:H	2.18	0.47
1:B:1591:TRP:HA	1:B:1591:TRP:CE3	2.49	0.47
1:B:1811:PRO:HB2	1:B:1814:LEU:HD12	1.95	0.47
1:B:1971:ASN:HA	1:B:2075:VAL:O	2.14	0.47
1:B:2309:LYS:O	1:B:2758:ARG:HD2	2.14	0.47
1:B:2363:TRP:CH2	1:B:2395:PHE:HE1	2.32	0.47
1:B:2427:PHE:O	1:B:2431:LEU:HG	2.14	0.47
1:B:2595:LYS:HE3	1:B:2611:PRO:HG3	1.96	0.47
1:B:2754:TYR:O	1:B:2755:GLY:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3966:THR:N	1:B:4426:MET:HE2	2.29	0.47
1:A:1592:ASP:O	1:A:1596:ASN:HB2	2.14	0.47
1:A:1628:LEU:C	1:A:1630:PRO:HD3	2.35	0.47
1:A:2010:SER:O	1:A:2060:LEU:HD11	2.14	0.47
1:A:2282:LYS:HB2	2:A:9002:ADP:O3B	2.15	0.47
1:A:3648:HIS:CE1	1:A:3654:SER:HA	2.49	0.47
1:A:3730:LEU:CD2	1:A:3733:VAL:HB	2.44	0.47
1:A:4200:LEU:HD22	1:A:4204:LEU:CG	2.45	0.47
1:A:4313:TRP:HB3	1:A:4330:PRO:CG	2.45	0.47
1:B:1603:ASP:O	1:B:1606:ILE:HG22	2.15	0.47
1:B:1920:ASN:ND2	1:B:1921:VAL:N	2.62	0.47
1:B:3605:PHE:HB3	1:B:3609:PHE:HB3	1.95	0.47
1:A:1831:LEU:HD23	1:A:1841:ILE:CG2	2.45	0.47
1:A:1831:LEU:HD23	1:A:1841:ILE:HG23	1.96	0.47
1:A:2204:ILE:HA	1:A:2207:LEU:CD1	2.42	0.47
1:A:2250:VAL:HG21	1:A:2425:MET:HA	1.97	0.47
1:A:3794:GLN:HG3	1:A:3891:LEU:HA	1.96	0.47
1:A:4326:PRO:HB3	1:A:4369:PHE:HD2	1.79	0.47
1:B:1766:ILE:HG23	1:B:1767:HIS:N	2.30	0.47
1:B:2532:ARG:CZ	1:B:2813:ILE:HD12	2.45	0.47
1:B:2667:HIS:HA	1:B:2787:GLN:OE1	2.14	0.47
1:B:4596:ASN:C	1:B:4596:ASN:ND2	2.68	0.47
1:B:4618:ASN:HD22	1:B:4618:ASN:H	1.60	0.47
1:A:1927:ILE:C	1:A:1928:HIS:HD2	2.18	0.47
1:A:2088:PRO:HB2	1:A:2090:ASN:HD21	1.80	0.47
1:A:2196:LEU:HA	1:A:2199:ILE:HG12	1.97	0.47
1:A:2273:MET:HB3	1:A:2395:PHE:CD1	2.50	0.47
1:A:2990:LEU:HD23	1:A:2994:VAL:HG11	1.97	0.47
1:A:3032:MET:O	1:A:3034:GLY:N	2.47	0.47
1:A:3036:SER:N	1:A:3068:LYS:O	2.48	0.47
1:A:3074:ASP:H	1:A:3077:ASN:ND2	2.13	0.47
1:A:3370:GLU:O	1:A:3371:PRO:C	2.51	0.47
1:A:4043:ASP:OD2	1:A:4043:ASP:N	2.45	0.47
1:A:4109:ASP:O	1:A:4112:ASN:HB2	2.15	0.47
1:A:4344:GLY:HA2	1:A:4347:ILE:HG13	1.95	0.47
1:A:4430:LEU:O	1:A:4434:GLN:HB2	2.15	0.47
1:A:4690:VAL:HG21	1:A:4701:PHE:CE1	2.50	0.47
1:B:1547:ASN:HD21	1:B:1550:ARG:H	1.63	0.47
1:B:1611:ARG:O	1:B:1615:LEU:HD23	2.14	0.47
1:B:1782:ALA:HB2	1:B:1922:LEU:HD23	1.96	0.47
1:B:2125:ALA:O	1:B:2129:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2231:ILE:HG12	1:B:2260:LEU:HD23	1.96	0.47
1:B:2335:THR:O	1:B:2339:ILE:HG13	2.14	0.47
1:B:2512:VAL:HA	1:B:2515:VAL:HG12	1.95	0.47
1:B:2540:LEU:HB3	1:B:2576:SER:OG	2.14	0.47
1:B:2676:PRO:HG3	1:B:2873:ILE:HD12	1.96	0.47
1:B:2882:TRP:CZ2	1:B:2909:ALA:HB2	2.48	0.47
1:B:3650:ASN:O	1:B:3651:SER:HB2	2.15	0.47
1:B:3698:SER:HB3	1:B:3700:LEU:CD1	2.44	0.47
1:B:4059:PRO:O	1:B:4063:ILE:HD12	2.15	0.47
1:B:4119:ALA:HA	1:B:4149:LEU:HD11	1.96	0.47
1:B:4359:PHE:O	1:B:4362:GLN:HB3	2.15	0.47
1:B:4429:ASP:O	1:B:4433:MET:HG3	2.15	0.47
1:B:4673:ASP:C	1:B:4675:ASP:H	2.18	0.47
1:A:2127:LYS:HB3	1:A:2222:VAL:HG13	1.97	0.47
1:A:2641:VAL:O	1:A:2646:VAL:HG11	2.15	0.47
1:A:2766:MET:CB	1:A:2783:LEU:HD11	2.42	0.47
1:A:3563:LEU:O	1:A:3567:LEU:HG	2.14	0.47
1:A:3988:TRP:O	1:A:3992:LEU:HG	2.14	0.47
1:A:4162:ILE:HG13	1:A:4187:LEU:HD23	1.97	0.47
1:A:4244:VAL:HG23	1:A:4403:SER:HB3	1.96	0.47
1:A:4269:ARG:HA	1:A:4392:PHE:CZ	2.50	0.47
1:A:4331:TRP:CD1	1:A:4366:PRO:HD3	2.49	0.47
1:B:3043:ASN:HD22	1:B:3043:ASN:N	2.10	0.47
1:B:3849:ASP:HA	1:B:3852:ILE:HG22	1.97	0.47
1:A:1868:SER:O	1:A:1872:ARG:HB2	2.15	0.47
1:A:2370:LEU:CD2	1:A:2387:LEU:HD22	2.45	0.47
1:A:3776:ASP:HB3	1:A:3780:ARG:HH12	1.80	0.47
1:A:4295:PHE:C	1:A:4295:PHE:HD2	2.18	0.47
1:B:2252:LYS:HE2	1:B:2254:GLU:HG2	1.96	0.47
1:B:2556:SER:C	1:B:2558:PHE:H	2.17	0.47
1:B:2587:LEU:HD12	1:B:2817:ASP:HB3	1.96	0.47
1:B:3601:TYR:O	1:B:3602:ILE:C	2.53	0.47
1:B:4005:ILE:HG21	1:B:4008:LEU:HD12	1.96	0.47
1:A:2316:LEU:HD23	1:A:2363:TRP:HB2	1.97	0.47
1:A:2424:GLN:HG3	1:A:2508:PRO:HG3	1.97	0.47
1:A:2905:TRP:CZ3	1:A:2934:ALA:HB2	2.50	0.47
1:A:4376:VAL:HB	1:A:4381:LEU:HB2	1.97	0.47
1:B:2309:LYS:HE2	1:B:2756:THR:HG21	1.96	0.47
1:B:2660:LEU:O	1:B:2664:LEU:HB2	2.15	0.47
1:B:2669:PRO:HG2	1:B:2810:HIS:O	2.14	0.47
1:B:2701:PHE:CE2	1:B:2759:VAL:HG11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3677:PRO:CG	1:B:3787:THR:HG22	2.45	0.47
1:B:3930:LEU:O	1:B:3931:VAL:C	2.53	0.47
1:B:4136:SER:O	1:B:4220:GLU:HA	2.15	0.47
1:B:4157:TYR:HB2	1:B:4184:TRP:C	2.35	0.47
1:B:4650:ASN:O	1:B:4653:GLN:HG3	2.15	0.47
1:A:2065:ILE:HG22	1:A:2066:SER:N	2.30	0.46
1:A:2651:VAL:CG1	1:A:2652:ASP:H	2.23	0.46
1:A:3040:ILE:HG22	1:A:3040:ILE:O	2.14	0.46
1:A:3270:LEU:CB	1:A:3592:VAL:HG13	2.44	0.46
1:A:3285:LEU:HD22	1:A:3578:SER:HB2	1.97	0.46
1:A:3452:ILE:O	1:A:3457:LEU:HD23	2.15	0.46
1:A:3639:SER:HB2	1:A:3643:GLU:OE1	2.15	0.46
1:A:4099:HIS:ND1	1:A:4111:LEU:HD12	2.30	0.46
1:A:4537:LEU:HD23	1:A:4548:LYS:HE3	1.97	0.46
1:A:4599:ALA:O	1:A:4602:THR:HG22	2.15	0.46
1:B:1576:LYS:HG2	1:B:1585:GLU:OE2	2.14	0.46
1:B:1642:GLU:O	1:B:1646:ILE:HG12	2.16	0.46
1:B:1788:SER:HA	1:B:1810:TYR:CZ	2.49	0.46
1:B:2270:HIS:HB3	1:B:2392:ARG:NH1	2.29	0.46
1:B:2774:ARG:HG2	1:B:2776:SER:OG	2.15	0.46
1:B:3973:ILE:HG13	1:B:3988:TRP:CZ3	2.50	0.46
1:A:1886:ARG:CZ	1:A:1890:ARG:HH22	2.28	0.46
1:A:1969:GLY:N	1:A:2047:GLN:NE2	2.64	0.46
1:A:2101:ILE:HD13	1:A:2101:ILE:N	2.30	0.46
1:A:4067:ALA:C	1:A:4073:GLN:HE21	2.19	0.46
1:B:1555:VAL:H	1:B:1609:GLN:NE2	2.12	0.46
1:B:1788:SER:HA	1:B:1810:TYR:CE2	2.50	0.46
1:B:2532:ARG:HG3	1:B:2808:LEU:O	2.14	0.46
1:B:3027:ARG:HA	1:B:3037:ILE:CD1	2.43	0.46
1:B:4128:SER:HB2	1:B:4213:PHE:HB3	1.96	0.46
1:B:4604:THR:HG23	1:B:4671:TRP:NE1	2.21	0.46
1:A:1809:ASN:HD22	1:A:1809:ASN:HA	1.60	0.46
1:A:2415:TRP:CE3	1:A:2415:TRP:HA	2.51	0.46
1:A:2720:TYR:CE1	1:A:2730:LEU:HD13	2.50	0.46
1:A:2956:LEU:HD21	1:A:2971:TYR:CD2	2.50	0.46
1:A:3021:GLY:O	1:A:3025:LEU:HB2	2.14	0.46
1:A:3283:LEU:C	1:A:3283:LEU:HD23	2.36	0.46
1:A:3975:SER:C	1:A:3977:LYS:H	2.18	0.46
1:A:4220:GLU:O	1:A:4222:HIS:N	2.49	0.46
1:B:1601:LEU:HA	1:B:1666:GLN:OE1	2.16	0.46
1:B:4030:PHE:HE1	1:B:4085:LEU:HG	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4190:ILE:HG12	1:B:4219:SER:CB	2.44	0.46
1:A:1630:PRO:O	1:A:1634:THR:HG23	2.15	0.46
1:A:2492:LEU:HG	1:A:2496:LYS:NZ	2.31	0.46
1:A:2882:TRP:CZ2	1:A:2905:TRP:NE1	2.83	0.46
1:A:2903:ARG:HB2	1:A:2945:ALA:O	2.15	0.46
1:A:3071:PHE:HE2	1:A:3087:MET:HE3	1.79	0.46
1:A:3219:ILE:CB	1:A:3220:PRO:HD3	2.46	0.46
1:A:4087:LYS:O	1:A:4087:LYS:HG2	2.15	0.46
1:A:4589:VAL:HG22	1:A:4590:TRP:N	2.29	0.46
1:B:2191:GLU:HA	1:B:2194:VAL:HG23	1.98	0.46
1:B:2529:THR:OG1	1:B:2532:ARG:HB2	2.15	0.46
1:B:2937:HIS:C	1:B:2939:PRO:HD3	2.35	0.46
1:B:3288:GLY:HA3	1:B:3574:TRP:CZ3	2.49	0.46
1:B:3773:PHE:HB3	1:B:3777:LEU:HD23	1.98	0.46
1:A:1948:VAL:O	1:A:1950:THR:N	2.49	0.46
1:A:2257:GLU:O	1:A:2261:GLN:HG2	2.16	0.46
1:A:2856:PHE:CZ	1:A:2930:ILE:HG12	2.49	0.46
1:A:3324:LEU:HD12	1:A:3539:LEU:CD2	2.46	0.46
1:A:3733:VAL:C	1:A:3735:ASN:H	2.19	0.46
1:A:3998:LEU:O	1:A:3998:LEU:HD13	2.15	0.46
1:B:1555:VAL:H	1:B:1609:GLN:HE22	1.64	0.46
1:B:1846:GLN:O	1:B:1849:GLU:HB3	2.16	0.46
1:B:2127:LYS:C	1:B:2130:PRO:HD2	2.35	0.46
1:B:2907:HIS:HB2	1:B:2950:ILE:HG21	1.96	0.46
1:A:1786:SER:HB2	1:A:1914:TYR:OH	2.16	0.46
1:A:2101:ILE:HG13	1:A:4348:ASP:HB2	1.98	0.46
1:A:2376:LEU:HA	1:A:2385:LEU:O	2.15	0.46
1:A:2435:SER:HB3	1:A:2496:LYS:HG2	1.97	0.46
1:A:2832:ASN:ND2	1:A:2883:ASP:OD2	2.49	0.46
1:A:3007:GLN:O	1:A:3142:HIS:HE1	1.99	0.46
1:A:3113:LYS:HG3	1:A:3123:LEU:O	2.15	0.46
1:A:3387:HIS:HB2	1:A:3473:ALA:HB2	1.95	0.46
1:A:3725:ASN:HD22	1:A:3725:ASN:N	1.99	0.46
1:A:4044:TRP:HE3	1:A:4048:PHE:HE1	1.62	0.46
1:A:4044:TRP:CE2	1:A:4059:PRO:HG3	2.51	0.46
1:B:1721:HIS:C	1:B:1725:MET:HE2	2.36	0.46
1:B:1799:ASP:OD1	1:B:1801:SER:HB3	2.15	0.46
1:B:2748:LEU:HD11	1:B:3162:PRO:HG2	1.97	0.46
1:B:3891:LEU:HD21	1:B:3895:ARG:NH2	2.31	0.46
1:B:4296:PHE:HB3	1:B:4346:ARG:HD2	1.98	0.46
1:A:2243:ILE:HG21	1:A:2288:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2578:MET:HE1	1:A:2613:LEU:HA	1.96	0.46
1:A:3830:LEU:HD12	1:A:3858:LEU:HD13	1.96	0.46
1:A:3990:PHE:HD2	1:A:4084:LEU:HD22	1.81	0.46
1:A:4318:SER:HA	1:A:4321:ARG:NH2	2.23	0.46
1:B:1962:GLN:CB	1:B:4341:THR:HG21	2.46	0.46
1:B:2532:ARG:NH1	1:B:2813:ILE:HD12	2.31	0.46
1:B:2749:PRO:O	1:B:2757:GLN:HG2	2.16	0.46
1:B:2841:ASN:ND2	1:B:2842:LEU:HG	2.31	0.46
1:B:3788:VAL:HG11	1:B:3913:LEU:CD2	2.46	0.46
1:B:4020:LEU:HG	1:B:4034:VAL:HG22	1.98	0.46
1:B:4222:HIS:ND1	1:B:4223:PRO:HD2	2.31	0.46
1:B:4281:ILE:HG13	1:B:4282:GLN:N	2.31	0.46
1:B:4645:GLU:HG3	1:B:4722:SER:OG	2.15	0.46
1:A:1904:PHE:C	1:A:1906:TRP:H	2.17	0.46
1:A:2059:LEU:HG	1:A:2060:LEU:HG	1.97	0.46
1:A:2205:PRO:HG3	1:A:2261:GLN:OE1	2.16	0.46
1:A:2360:ASP:HB2	1:A:2361:PRO:HD2	1.96	0.46
1:A:2443:GLU:OE2	1:A:2489:PRO:HB2	2.15	0.46
1:A:2603:THR:HG22	1:A:2604:PRO:HD2	1.97	0.46
1:A:2829:GLY:HA2	1:A:2850:THR:OG1	2.16	0.46
1:A:4022:CYS:O	1:A:4026:GLN:HB2	2.16	0.46
1:A:4681:ASN:ND2	1:A:4685:LYS:HE3	2.30	0.46
1:A:4719:ARG:HH11	1:A:4719:ARG:HG3	1.81	0.46
1:B:3993:LYS:O	1:B:3994:GLY:C	2.54	0.46
1:B:4597:PRO:HG2	1:B:4692:LEU:CD1	2.46	0.46
1:A:1530:PHE:CZ	1:A:1571:SER:HB2	2.51	0.46
1:A:1745:SER:OG	1:A:1751:THR:HG22	2.16	0.46
1:A:3925:ASN:N	1:A:3925:ASN:ND2	2.63	0.46
1:A:4395:TRP:CZ3	1:A:4399:LEU:HD11	2.51	0.46
1:A:4596:ASN:C	1:A:4596:ASN:ND2	2.69	0.46
1:B:1683:LEU:HD12	1:B:1683:LEU:O	2.16	0.46
1:B:3715:GLY:HA3	1:B:3758:PRO:HG2	1.98	0.46
1:B:4284:ARG:NH2	1:B:4355:LEU:HD21	2.31	0.46
1:B:4331:TRP:CZ2	1:B:4369:PHE:HE2	2.34	0.46
1:A:1662:ILE:HG22	1:A:1663:GLU:N	2.32	0.46
1:A:1911:ARG:H	1:A:1911:ARG:HD3	1.81	0.46
1:A:2641:VAL:O	1:A:2643:SER:N	2.49	0.46
1:A:2864:PHE:HB3	1:A:2872:TYR:HD2	1.81	0.46
1:A:2952:TYR:CZ	1:A:2962:PRO:HG3	2.51	0.46
1:A:3017:VAL:HG21	1:A:3257:PRO:HD3	1.98	0.46
1:A:4263:GLN:NE2	1:A:4322:SER:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4278:HIS:HD2	1:A:4343:TYR:OH	1.99	0.46
1:A:4402:ILE:H	1:A:4402:ILE:CD1	2.28	0.46
1:B:2044:GLN:O	1:B:2048:VAL:HG23	2.16	0.46
1:B:3789:THR:H	1:B:3792:SER:HB3	1.81	0.46
1:B:4095:LEU:HD11	1:B:4422:LYS:HB3	1.97	0.46
1:B:4274:LEU:HD11	1:B:4306:ALA:HB1	1.98	0.46
1:B:4400:PRO:HG2	1:B:4407:TRP:HH2	1.81	0.46
1:A:1642:GLU:O	1:A:1646:ILE:HG13	2.16	0.45
1:A:2249:LEU:HB3	2:A:9002:ADP:N6	2.30	0.45
1:A:2338:ARG:HH11	1:A:2338:ARG:HG2	1.81	0.45
1:A:2851:ASP:HB3	1:A:2937:HIS:CE1	2.51	0.45
1:A:2980:TYR:OH	1:A:2987:PRO:HA	2.15	0.45
1:A:4726:TRP:CH2	1:A:4728:SER:HB2	2.51	0.45
1:B:1534:VAL:HG22	1:B:1568:HIS:CD2	2.50	0.45
1:B:1604:VAL:O	1:B:1608:VAL:HG23	2.16	0.45
1:B:1822:VAL:HG13	1:B:1823:TRP:N	2.31	0.45
1:B:1985:LYS:HD3	1:B:1997:VAL:HG21	1.98	0.45
1:B:2275:VAL:HG11	1:B:2400:LEU:HG	1.97	0.45
1:B:2873:ILE:O	1:B:2873:ILE:HG13	2.14	0.45
1:B:3912:SER:HB3	1:B:4231:ARG:CG	2.45	0.45
1:B:4122:VAL:HG11	1:B:4216:PHE:HZ	1.81	0.45
1:B:4434:GLN:HE21	1:B:4434:GLN:HB3	1.55	0.45
1:B:4574:GLN:NE2	1:B:4590:TRP:HB3	2.31	0.45
1:A:3015:ILE:CG2	1:A:3149:PRO:HG3	2.45	0.45
1:A:3023:SER:HB2	2:A:9004:ADP:O1A	2.16	0.45
1:A:3271:ILE:HG12	1:A:3592:VAL:HG21	1.97	0.45
1:A:3551:SER:O	1:A:3554:LYS:HB2	2.16	0.45
1:A:4039:GLN:HB3	1:A:4040:ASN:H	1.57	0.45
1:A:4309:SER:O	1:A:4312:TYR:HB3	2.16	0.45
1:B:1931:ASN:HD21	1:B:1962:GLN:HE22	1.64	0.45
1:B:2309:LYS:HZ3	1:B:2756:THR:HG21	1.77	0.45
1:B:2331:LEU:HD21	1:B:2773:TRP:CG	2.51	0.45
1:B:2723:THR:HG22	1:B:2727:GLU:O	2.16	0.45
1:B:4379:ILE:HG23	1:B:4381:LEU:HG	1.98	0.45
1:A:3190:ARG:C	1:A:3192:LEU:H	2.20	0.45
1:A:3481:ALA:O	1:A:3485:THR:HG23	2.16	0.45
1:A:3798:LEU:O	1:A:3802:LEU:HG	2.17	0.45
1:A:3814:SER:C	1:A:3818:LYS:HD3	2.37	0.45
1:A:4026:GLN:HB3	1:A:4027:VAL:H	1.60	0.45
1:A:4281:ILE:HG13	1:A:4282:GLN:N	2.31	0.45
1:A:4337:ILE:O	1:A:4341:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4653:GLN:O	1:A:4655:THR:HG23	2.17	0.45
1:B:2745:GLU:HG2	1:B:2748:LEU:HD11	1.98	0.45
1:B:4431:GLN:O	1:B:4431:GLN:HG2	2.16	0.45
1:A:2323:THR:O	1:A:2324:THR:HG23	2.16	0.45
1:A:2398:GLN:NE2	1:A:2806:ARG:HG2	2.31	0.45
1:A:2738:TRP:CZ3	1:A:2785:LYS:HA	2.51	0.45
1:A:2845:PHE:O	1:A:2848:ASN:HB2	2.16	0.45
1:A:2896:CYS:SG	1:A:2897:THR:N	2.90	0.45
1:A:2976:LEU:HD12	1:A:3028:PHE:CE1	2.51	0.45
1:A:3792:SER:OG	1:A:3793:LEU:N	2.50	0.45
1:A:3893:CYS:HB3	1:A:3916:PHE:HZ	1.81	0.45
1:B:2849:LEU:HD13	1:B:2901:LEU:HD11	1.99	0.45
1:B:3015:ILE:HD12	1:B:3170:LEU:HD11	1.98	0.45
1:B:3306:LEU:HD13	1:B:3557:VAL:CG2	2.46	0.45
1:B:3536:TYR:O	1:B:3540:ILE:HD13	2.16	0.45
1:B:3990:PHE:HD2	1:B:4084:LEU:HD22	1.82	0.45
1:B:4047:PHE:HE1	1:B:4086:MET:HE1	1.81	0.45
1:B:4335:ARG:NH2	1:B:4365:THR:HG22	2.22	0.45
1:A:3459:ASP:HB3	1:A:3462:PHE:CB	2.47	0.45
1:A:3549:GLU:O	1:A:3553:VAL:HG23	2.17	0.45
1:A:3686:MET:CE	1:A:3696:LYS:HB2	2.46	0.45
1:A:4279:ALA:O	1:A:4283:GLU:HB2	2.17	0.45
1:A:4349:ASN:O	1:A:4352:ASP:HB2	2.16	0.45
1:A:4648:VAL:HG23	1:A:4655:THR:OG1	2.16	0.45
1:B:2630:LYS:CB	1:B:2654:THR:HG21	2.47	0.45
1:B:3930:LEU:HD22	1:B:3939:ARG:HE	1.81	0.45
1:B:4012:LEU:HA	1:B:4016:GLN:NE2	2.31	0.45
1:A:1726:PHE:HB2	1:A:1729:LEU:HB3	1.98	0.45
1:A:1784:LEU:HB3	1:A:1814:LEU:HD13	1.99	0.45
1:A:1842:GLN:OE1	1:A:1893:GLN:HG2	2.17	0.45
1:A:1964:LEU:HD12	1:A:2074:PHE:CZ	2.51	0.45
1:A:1968:MET:HB3	1:A:2094:LEU:O	2.16	0.45
1:A:1973:PHE:C	1:A:1973:PHE:CD1	2.89	0.45
1:A:2603:THR:CB	1:A:2604:PRO:HD2	2.46	0.45
1:A:3011:HIS:C	1:A:3168:CYS:HB3	2.36	0.45
1:A:3350:VAL:HG12	1:A:3350:VAL:O	2.15	0.45
1:A:3897:TYR:HD2	1:A:3898:PHE:CD2	2.34	0.45
1:A:3919:ILE:HD13	1:A:3951:THR:HA	1.98	0.45
1:B:2819:PRO:HB2	1:B:2824:LEU:CD2	2.46	0.45
1:B:3673:LEU:HD22	1:B:3783:PHE:CE1	2.48	0.45
1:B:4404:THR:HB	1:B:4405:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4693:ASN:ND2	1:B:4693:ASN:N	2.64	0.45
1:B:4714:GLN:O	1:B:4718:GLN:HG3	2.16	0.45
1:A:1907:LEU:HD22	1:A:1911:ARG:NH1	2.31	0.45
1:A:2124:LEU:HD22	1:A:2195:LEU:CD2	2.46	0.45
1:A:2435:SER:CB	1:A:2496:LYS:HG2	2.47	0.45
1:A:3022:LYS:HA	1:A:3173:PHE:CE1	2.52	0.45
1:A:3234:ILE:O	1:A:3238:ILE:HD13	2.17	0.45
1:A:3388:LEU:CD2	1:A:3473:ALA:HB1	2.44	0.45
1:A:3463:ASP:O	1:A:3467:VAL:HG23	2.17	0.45
1:A:4249:LEU:O	1:A:4253:ILE:HG13	2.17	0.45
1:B:2825:THR:HG23	1:B:2854:VAL:HG21	1.98	0.45
1:B:3004:VAL:O	1:B:3010:GLY:HA3	2.17	0.45
1:B:3542:GLU:O	1:B:3546:ILE:HG12	2.16	0.45
1:B:3696:LYS:HG3	1:B:3719:LEU:HD23	1.99	0.45
1:B:4666:ILE:HG13	1:B:4667:ALA:N	2.32	0.45
1:A:1800:HIS:CD2	1:A:1858:ASN:HB3	2.52	0.45
1:A:1922:LEU:HD13	1:A:1938:PHE:CD1	2.48	0.45
1:A:2902:VAL:HG21	1:A:2941:VAL:CG2	2.47	0.45
1:A:3911:PHE:CZ	1:A:3955:VAL:HG13	2.52	0.45
1:A:4329:ILE:HB	1:A:4331:TRP:CE2	2.51	0.45
1:A:4384:PRO:HG2	1:A:4392:PHE:CD1	2.51	0.45
1:A:4668:THR:C	1:A:4669:LEU:HD12	2.37	0.45
1:B:1618:ILE:HD13	1:B:1683:LEU:HD21	1.99	0.45
1:B:1740:THR:HG22	1:B:1759:SER:HA	1.98	0.45
1:B:2091:LEU:HD22	1:B:2095:PHE:CE2	2.51	0.45
1:B:3990:PHE:CZ	1:B:4023:LEU:HD13	2.52	0.45
1:B:4197:LEU:HB3	1:B:4226:PRO:HG2	1.98	0.45
1:B:4618:ASN:N	1:B:4618:ASN:ND2	2.65	0.45
1:A:1925:LEU:HD23	1:A:1936:TYR:HB2	1.98	0.45
1:A:2052:GLU:O	1:A:2053:ASN:CB	2.64	0.45
1:A:2140:SER:HB2	1:A:2211:ASP:OD2	2.15	0.45
1:A:2196:LEU:HA	1:A:2199:ILE:CG1	2.46	0.45
1:A:2526:MET:O	1:A:2527:ASP:C	2.55	0.45
1:A:3145:PHE:CG	1:A:3164:LEU:HD11	2.52	0.45
1:A:3218:ALA:O	1:A:3220:PRO:N	2.49	0.45
1:A:3602:ILE:O	1:A:3603:GLY:C	2.54	0.45
1:A:3639:SER:OG	1:A:3663:ILE:HD11	2.17	0.45
1:A:4032:LYS:HE2	1:A:4032:LYS:HA	1.97	0.45
1:A:4046:GLN:NE2	1:A:4057:ILE:HG22	2.32	0.45
1:A:4311:ASP:O	1:A:4315:ASP:HB3	2.17	0.45
1:A:4347:ILE:CG2	1:A:4353:MET:HG2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2204:ILE:N	1:B:2205:PRO:CD	2.80	0.45
1:B:2270:HIS:HB3	1:B:2392:ARG:HH11	1.82	0.45
1:B:3254:TYR:CD2	1:B:3775:PRO:HA	2.52	0.45
1:B:3992:LEU:HD12	1:B:4434:GLN:NE2	2.31	0.45
1:B:4095:LEU:HD11	1:B:4422:LYS:HB2	1.99	0.45
1:B:4621:LEU:HG	1:B:4622:HIS:H	1.82	0.45
1:B:4657:THR:HG22	1:B:4658:ASP:N	2.32	0.45
1:A:2272:VAL:HB	1:A:2394:MET:HE2	1.97	0.45
1:A:3027:ARG:HH11	1:A:3027:ARG:HB2	1.81	0.45
1:A:3540:ILE:HD12	1:A:3540:ILE:N	2.32	0.45
1:A:3542:GLU:O	1:A:3546:ILE:HG13	2.17	0.45
1:A:3696:LYS:HZ3	1:A:3721:GLN:CD	2.21	0.45
1:A:3813:ARG:HA	1:A:3875:VAL:HG11	1.99	0.45
1:A:3903:LEU:HD13	1:A:3959:LEU:HD21	1.99	0.45
1:A:3908:LEU:HD21	1:A:4237:SER:OG	2.16	0.45
1:A:3912:SER:HB3	1:A:4231:ARG:CG	2.45	0.45
1:A:4116:LEU:HB3	1:A:4117:ASP:H	1.52	0.45
1:A:4455:SER:C	1:A:4457:SER:H	2.20	0.45
1:B:1548:TYR:HD2	1:B:1554:LEU:HD11	1.82	0.45
1:B:1764:PRO:HB2	1:B:1768:GLU:CB	2.47	0.45
1:B:2641:VAL:HG13	1:B:2831:PHE:HB3	1.98	0.45
1:B:2998:ILE:CG2	1:B:3025:LEU:HD22	2.47	0.45
1:B:3078:VAL:O	1:B:3078:VAL:HG13	2.16	0.45
1:B:4197:LEU:HD13	1:B:4226:PRO:HD3	1.99	0.45
1:B:4220:GLU:O	1:B:4222:HIS:N	2.50	0.45
1:B:4253:ILE:O	1:B:4253:ILE:HG22	2.17	0.45
1:A:1777:MET:CE	1:A:1939:GLU:HA	2.48	0.44
1:A:1958:LEU:O	1:A:1962:GLN:HB2	2.16	0.44
1:A:2730:LEU:HD22	1:A:2772:PHE:CZ	2.52	0.44
1:A:3682:MET:CE	1:A:3721:GLN:HE21	2.31	0.44
1:A:3776:ASP:HB3	1:A:3780:ARG:NH1	2.31	0.44
1:A:3825:VAL:HA	1:A:3828:ARG:HD3	1.99	0.44
1:A:4076:ILE:HD12	1:A:4105:VAL:HG22	1.99	0.44
1:B:1629:LEU:HD22	1:B:1632:GLU:HG2	1.98	0.44
1:B:1869:ALA:HA	1:B:1872:ARG:HB3	1.99	0.44
1:B:2381:ASN:ND2	1:B:2383:GLU:HB2	2.20	0.44
1:B:2705:THR:HG22	1:B:2759:VAL:HG21	1.98	0.44
1:B:2774:ARG:C	1:B:2776:SER:H	2.20	0.44
1:A:1609:GLN:O	1:A:1613:VAL:HG23	2.17	0.44
1:A:1748:GLU:HB3	1:A:1943:ILE:HD12	1.99	0.44
1:A:2142:GLN:NE2	1:A:2208:VAL:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2302:GLU:HG2	1:A:2304:HIS:HE1	1.81	0.44
1:A:2359:VAL:HG11	1:A:2400:LEU:HD22	1.99	0.44
1:A:2433:THR:HG23	1:A:2437:GLU:HG3	1.99	0.44
1:A:2898:LEU:O	1:A:2898:LEU:HD13	2.17	0.44
1:A:3408:VAL:HG23	1:A:3409:CYS:N	2.32	0.44
1:A:3490:ILE:O	1:A:3490:ILE:HG13	2.18	0.44
1:A:3974:ILE:O	1:A:3977:LYS:HB2	2.17	0.44
1:A:4121:ILE:HG22	1:A:4122:VAL:N	2.32	0.44
1:B:2263:HIS:HB2	1:B:2289:TYR:CE1	2.52	0.44
1:B:2955:TRP:HZ2	1:B:3002:ASP:OD1	2.00	0.44
1:B:3088:ASN:OD1	1:B:3163:ALA:HB3	2.17	0.44
1:B:3233:TYR:CG	1:B:3620:ARG:HG3	2.52	0.44
1:B:4192:LEU:C	1:B:4194:PRO:HD3	2.38	0.44
1:A:2016:LEU:HD21	1:A:2023:GLY:CA	2.47	0.44
1:A:2056:GLU:O	1:A:2056:GLU:HG3	2.17	0.44
1:A:2340:ILE:HD11	1:A:2386:ALA:O	2.17	0.44
1:A:2502:ILE:HD12	1:A:2506:PHE:HE2	1.82	0.44
1:A:3055:LEU:O	1:A:3059:LEU:HD23	2.17	0.44
1:A:3361:LYS:HE2	1:A:3361:LYS:HB3	1.84	0.44
1:A:3809:THR:HG22	1:A:3812:LYS:NZ	2.32	0.44
1:A:4691:TYR:HA	1:A:4699:LEU:HA	1.99	0.44
1:B:2660:LEU:HD21	1:B:2672:LEU:CD2	2.48	0.44
1:B:4266:GLU:HG3	1:B:4369:PHE:CE1	2.52	0.44
1:B:4686:LEU:HD12	1:B:4687:SER:H	1.83	0.44
1:A:2046:ILE:HD11	1:A:2059:LEU:HD22	2.00	0.44
1:A:2399:ASP:O	1:A:2400:LEU:HD23	2.16	0.44
1:A:2641:VAL:HG21	1:A:2887:LEU:HD13	1.99	0.44
1:A:2742:PHE:HD1	1:A:2789:VAL:HG12	1.83	0.44
1:A:2902:VAL:HG22	1:A:2938:PHE:CD2	2.53	0.44
1:A:3670:ARG:NH1	1:A:3781:VAL:O	2.51	0.44
1:A:3675:ILE:O	1:A:3675:ILE:HG22	2.17	0.44
1:A:3731:ASN:H	1:A:3731:ASN:ND2	2.09	0.44
1:A:3805:GLU:HB3	1:A:3886:TYR:OH	2.17	0.44
1:B:1640:ASN:ND2	1:B:1644:ILE:HG12	2.32	0.44
1:B:2381:ASN:ND2	1:B:2381:ASN:C	2.71	0.44
1:B:3011:HIS:CE1	1:B:3091:LEU:HA	2.53	0.44
1:B:3316:LYS:HD2	1:B:3546:ILE:CD1	2.47	0.44
1:B:3601:TYR:O	1:B:3603:GLY:N	2.50	0.44
1:B:3958:THR:CG2	1:B:4235:VAL:HB	2.47	0.44
1:B:4087:LYS:HG2	1:B:4087:LYS:O	2.17	0.44
1:B:4244:VAL:HG23	1:B:4403:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4405:PRO:HD3	1:B:4415:GLU:HG2	1.98	0.44
1:B:4693:ASN:H	1:B:4693:ASN:HD22	1.64	0.44
1:A:1719:GLN:OE1	1:A:1732:LEU:N	2.50	0.44
1:A:2200:ASN:O	1:A:2204:ILE:HG12	2.18	0.44
1:A:2200:ASN:ND2	1:A:2228:LEU:HD13	2.18	0.44
1:A:2339:ILE:HG21	1:A:2391:VAL:CG2	2.48	0.44
1:A:3154:PHE:C	1:A:3156:ASN:H	2.21	0.44
1:A:3274:LYS:HD3	1:A:3274:LYS:HA	1.77	0.44
1:A:3293:ARG:HG3	1:A:3293:ARG:NH1	2.27	0.44
1:A:3338:GLN:NE2	1:A:3525:LEU:HB2	2.32	0.44
1:A:3727:ASP:CB	1:A:3729:VAL:HG12	2.48	0.44
1:A:3902:GLU:O	1:A:3905:GLN:HG2	2.17	0.44
1:A:4513:ILE:HA	1:A:4550:TRP:HE1	1.82	0.44
1:A:4673:ASP:O	1:A:4677:PRO:HD2	2.18	0.44
1:B:1828:ASP:OD2	1:B:1901:ASN:HB2	2.17	0.44
1:B:2301:SER:HA	1:B:2350:ARG:O	2.18	0.44
1:B:2886:LEU:O	1:B:2890:ILE:HG13	2.18	0.44
1:B:2976:LEU:CD1	1:B:2990:LEU:HD11	2.48	0.44
1:B:3602:ILE:HG23	1:B:3610:ARG:CG	2.43	0.44
1:A:1628:LEU:HD23	1:A:1628:LEU:O	2.18	0.44
1:A:2125:ALA:HA	1:A:2128:ILE:CG2	2.46	0.44
1:A:2152:LEU:O	1:A:2152:LEU:HD13	2.18	0.44
1:A:3410:LEU:HD23	1:A:3410:LEU:C	2.38	0.44
1:A:4075:THR:HG23	1:A:4076:ILE:H	1.82	0.44
1:A:4296:PHE:HE2	1:A:4347:ILE:HA	1.77	0.44
1:B:2986:VAL:O	1:B:2988:LEU:HG	2.17	0.44
1:B:4265:ALA:H	1:B:4323:ASN:HB3	1.83	0.44
1:B:4304:ARG:HA	1:B:4307:LEU:HD12	1.99	0.44
1:B:4330:PRO:O	1:B:4333:ALA:HB3	2.17	0.44
1:A:1674:ASP:OD1	1:A:1678:LYS:HE2	2.17	0.44
1:A:1904:PHE:C	1:A:1906:TRP:N	2.71	0.44
1:A:2056:GLU:HB2	1:A:2065:ILE:O	2.18	0.44
1:A:2077:MET:HB3	1:A:2077:MET:HE2	1.81	0.44
1:A:2991:PHE:O	1:A:2992:ASN:C	2.55	0.44
1:A:3521:THR:O	1:A:3525:LEU:HD12	2.18	0.44
1:A:3603:GLY:HA2	1:A:3664:MET:CE	2.48	0.44
1:B:1530:PHE:CZ	1:B:1571:SER:HB2	2.53	0.44
1:B:2694:PHE:HA	1:B:2738:TRP:O	2.18	0.44
1:B:3013:LEU:HD13	1:B:3145:PHE:HB3	2.00	0.44
1:B:3164:LEU:C	1:B:3166:ASN:H	2.22	0.44
1:B:3715:GLY:HA2	1:B:3760:PHE:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4374:PRO:HB3	1:B:4377:PRO:HG3	1.98	0.44
1:B:4686:LEU:HD22	1:B:4716:TRP:HB3	2.00	0.44
1:A:1535:ARG:HA	1:A:1591:TRP:HZ2	1.83	0.44
1:A:1695:ALA:CB	1:A:2019:CYS:SG	3.06	0.44
1:A:1973:PHE:HE1	1:A:2099:ALA:HA	1.81	0.44
1:A:2289:TYR:CE1	1:A:2293:ILE:HD11	2.53	0.44
1:A:2376:LEU:HD12	1:A:2385:LEU:C	2.38	0.44
1:A:2903:ARG:HD2	1:A:2945:ALA:O	2.18	0.44
1:A:2926:THR:O	1:A:2930:ILE:HG13	2.18	0.44
1:A:3205:PHE:CE2	1:A:3221:PRO:HB3	2.52	0.44
1:A:3812:LYS:HB3	1:A:3875:VAL:CG2	2.47	0.44
1:A:3813:ARG:HH22	1:A:3817:LEU:HD13	1.83	0.44
1:A:3869:VAL:O	1:A:3869:VAL:HG12	2.18	0.44
1:B:2612:LEU:O	1:B:2612:LEU:HD13	2.18	0.44
1:B:2766:MET:HB3	1:B:2783:LEU:CD1	2.43	0.44
1:B:2828:TYR:HE1	1:B:2880:SER:HA	1.83	0.44
1:B:3552:LYS:HB2	1:B:3552:LYS:NZ	2.33	0.44
1:B:3553:VAL:O	1:B:3557:VAL:HG23	2.18	0.44
1:B:3872:THR:O	1:B:3876:MET:HG2	2.18	0.44
1:B:4289:PRO:HB2	1:B:4696:ARG:HD2	2.00	0.44
1:B:4689:PRO:HD2	1:B:4721:VAL:O	2.18	0.44
1:A:1973:PHE:HE1	1:A:2099:ALA:HB2	1.83	0.44
1:A:2361:PRO:HD2	1:A:2754:TYR:CE1	2.53	0.44
1:A:2903:ARG:HH22	1:A:2950:ILE:HA	1.82	0.44
1:A:2913:PHE:HD2	1:A:2913:PHE:N	2.15	0.44
1:A:3190:ARG:HA	1:A:3224:ARG:NH1	2.32	0.44
1:A:3700:LEU:CD1	1:A:3701:ASP:H	2.31	0.44
1:A:4257:ALA:C	1:A:4259:ARG:H	2.21	0.44
1:B:1869:ALA:O	1:B:1872:ARG:HB3	2.17	0.44
1:B:2112:MET:O	1:B:2116:GLN:HG2	2.17	0.44
1:B:2839:LEU:CD2	1:B:2896:CYS:HB3	2.48	0.44
1:B:2965:ARG:HG3	1:B:2965:ARG:HH11	1.82	0.44
1:B:3903:LEU:HD11	1:B:3967:PHE:CD1	2.53	0.44
1:A:1591:TRP:HA	1:A:1591:TRP:CE3	2.53	0.43
1:A:1756:LYS:HB2	1:A:1756:LYS:NZ	2.32	0.43
1:A:2091:LEU:HD22	1:A:2095:PHE:HE1	1.80	0.43
1:A:2249:LEU:HD22	2:A:9002:ADP:C5	2.53	0.43
1:A:2255:TRP:CH2	1:A:2259:ILE:HD11	2.53	0.43
1:A:2560:MET:HE3	1:A:2564:ASN:HD22	1.81	0.43
1:A:2617:VAL:HG13	1:A:2617:VAL:O	2.18	0.43
1:A:3585:MET:HA	1:A:3588:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3652:LEU:HD12	1:A:3653:PRO:CD	2.41	0.43
1:A:4690:VAL:HG11	1:A:4701:PHE:CE2	2.53	0.43
1:B:2426:ILE:H	1:B:2426:ILE:CD1	2.27	0.43
1:B:2714:PHE:HE1	1:B:2741:VAL:HG21	1.83	0.43
1:B:2902:VAL:HG21	1:B:2941:VAL:HG21	2.00	0.43
1:B:3038:TYR:HE2	1:B:3058:LEU:HD22	1.82	0.43
1:B:3046:TYR:CE1	1:B:3050:ASP:HB2	2.53	0.43
1:B:3961:ASN:HA	1:B:3964:LYS:HE2	2.00	0.43
1:A:2547:ASN:O	1:A:2551:TYR:HB2	2.17	0.43
1:A:2650:THR:OG1	1:A:2651:VAL:N	2.50	0.43
1:A:3462:PHE:CE2	1:A:3478:VAL:HG23	2.53	0.43
1:B:1674:ASP:O	1:B:1678:LYS:HG3	2.18	0.43
1:B:2265:ILE:HD12	1:B:2414:VAL:HG22	1.99	0.43
1:B:2522:ARG:NH1	1:B:2593:PHE:HD1	2.16	0.43
1:B:4024:ARG:O	1:B:4024:ARG:HG2	2.17	0.43
1:B:4153:LEU:HB2	1:B:4155:LYS:CG	2.46	0.43
1:B:4691:TYR:HA	1:B:4698:GLU:O	2.18	0.43
1:A:1755:LYS:HA	1:A:1755:LYS:HD2	1.80	0.43
1:A:1922:LEU:CD1	1:A:1938:PHE:HD1	2.31	0.43
1:A:1958:LEU:HD23	1:A:4341:THR:HB	1.99	0.43
1:A:2053:ASN:N	1:A:2053:ASN:ND2	2.65	0.43
1:A:2400:LEU:HB3	1:A:2403:ALA:HB3	2.00	0.43
1:A:2408:ILE:HG13	1:A:2409:SER:H	1.83	0.43
1:A:3019:GLY:HA2	2:A:9004:ADP:H5'2	2.00	0.43
1:A:3470:ALA:O	1:A:3471:SER:HB2	2.17	0.43
1:A:4091:SER:O	1:A:4420:SER:HA	2.18	0.43
1:A:4319:LYS:O	1:A:4321:ARG:NH1	2.52	0.43
1:B:1497:LEU:HD22	1:B:1501:SER:HB2	1.99	0.43
1:B:2282:LYS:HB2	1:B:2282:LYS:HZ2	1.83	0.43
1:B:2773:TRP:CZ3	1:B:2780:TRP:HB2	2.53	0.43
1:B:3686:MET:HA	1:B:3694:ILE:HG21	2.00	0.43
1:B:4225:LEU:HD23	1:B:4230:LEU:HD21	2.00	0.43
1:A:1604:VAL:O	1:A:1608:VAL:HG23	2.18	0.43
1:A:1835:THR:O	1:A:1836:LEU:CB	2.67	0.43
1:A:2359:VAL:HB	1:A:2397:VAL:HG11	2.00	0.43
1:A:3062:ALA:HB2	1:A:3069:ILE:HD13	1.99	0.43
1:A:3681:ALA:HB2	1:A:3786:PHE:CD2	2.53	0.43
1:A:3933:LYS:HZ3	1:A:3933:LYS:HB3	1.84	0.43
1:A:3990:PHE:CE2	1:A:4023:LEU:HG	2.54	0.43
1:A:4052:GLN:O	1:A:4054:GLY:N	2.43	0.43
1:A:4182:GLY:HA3	1:A:4212:SER:HG	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1831:LEU:HA	1:B:1841:ILE:HG23	1.99	0.43
1:B:1975:PRO:HG2	1:B:1978:THR:CG2	2.48	0.43
1:B:2964:ASN:HD21	1:B:2967:ASP:CG	2.22	0.43
1:B:3041:LYS:N	1:B:3041:LYS:HD2	2.33	0.43
1:B:3192:LEU:HD22	1:B:3271:ILE:HG21	2.00	0.43
1:B:3634:VAL:HB	1:B:3635:PRO:HD3	1.99	0.43
1:B:3635:PRO:C	1:B:3637:PHE:H	2.21	0.43
1:B:4012:LEU:HD11	1:B:4020:LEU:HD22	2.01	0.43
1:B:4022:CYS:HB3	1:B:4026:GLN:HE21	1.84	0.43
1:A:1830:ALA:O	1:A:1841:ILE:HG23	2.18	0.43
1:A:3096:VAL:HB	1:A:3099:LEU:HB2	2.00	0.43
1:A:3445:THR:HA	1:A:3449:ARG:HB2	2.00	0.43
1:A:4132:LEU:HB2	1:A:4216:PHE:CD1	2.52	0.43
1:B:1639:ILE:HG23	1:B:1672:LEU:HD22	2.01	0.43
1:B:2352:TRP:CD1	1:B:2392:ARG:HB2	2.54	0.43
1:B:3234:ILE:HG23	1:B:3617:TRP:CD1	2.54	0.43
1:B:3289:LEU:HA	1:B:3292:LEU:HD12	1.99	0.43
1:B:4574:GLN:HE22	1:B:4590:TRP:HB3	1.82	0.43
1:A:1955:ARG:NH1	1:A:1955:ARG:HB2	2.33	0.43
1:A:2012:ILE:HG22	1:A:2016:LEU:CD1	2.49	0.43
1:A:2057:VAL:HG22	1:A:2058:GLU:N	2.34	0.43
1:A:2200:ASN:ND2	1:A:2228:LEU:HB3	2.33	0.43
1:A:3015:ILE:HG21	1:A:3172:TRP:CH2	2.54	0.43
1:A:3078:VAL:O	1:A:3078:VAL:HG22	2.19	0.43
1:A:3357:VAL:O	1:A:3357:VAL:HG12	2.18	0.43
1:A:3638:LEU:HD22	1:A:3667:ARG:HD3	2.01	0.43
1:A:4066:GLN:HE22	1:A:4081:ARG:HD3	1.81	0.43
1:A:4337:ILE:HG22	1:A:4338:LEU:HD12	1.99	0.43
1:B:1653:ALA:HB1	1:B:1658:GLU:HG2	2.01	0.43
1:B:1744:MET:SD	1:B:1777:MET:HG3	2.59	0.43
1:B:2882:TRP:O	1:B:2886:LEU:HG	2.18	0.43
1:B:3160:THR:O	1:B:3162:PRO:HD3	2.18	0.43
1:B:3181:LEU:HB3	1:B:3232:VAL:HG13	2.00	0.43
1:B:3902:GLU:C	1:B:3904:SER:N	2.71	0.43
1:B:3993:LYS:HG3	1:B:4431:GLN:HG3	1.99	0.43
1:B:4407:TRP:HD1	1:B:4407:TRP:H	1.64	0.43
1:B:4728:SER:OG	1:B:4729:ASP:N	2.51	0.43
1:A:1906:TRP:CZ2	1:A:1911:ARG:HG2	2.54	0.43
1:A:2145:TYR:OH	1:A:2207:LEU:HA	2.18	0.43
1:A:2263:HIS:HB2	1:A:2289:TYR:CE1	2.54	0.43
1:A:2270:HIS:ND1	1:A:2270:HIS:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2678:SER:HB2	1:A:2817:ASP:O	2.18	0.43
1:A:2748:LEU:HD21	1:A:2800:ARG:CZ	2.48	0.43
1:A:3451:ALA:O	1:A:3455:GLY:N	2.51	0.43
1:A:4179:ALA:HA	1:A:4213:PHE:CD1	2.53	0.43
1:A:4280:ILE:HG21	1:A:4359:PHE:CE1	2.53	0.43
1:A:4288:ILE:HG23	1:A:4289:PRO:HA	2.01	0.43
1:A:4389:ARG:HG2	1:A:4389:ARG:NH1	2.32	0.43
1:A:4648:VAL:HG13	1:A:4657:THR:CG2	2.44	0.43
1:B:1546:VAL:O	1:B:1553:LYS:HA	2.19	0.43
1:B:1766:ILE:HD12	1:B:1769:TRP:HE1	1.84	0.43
1:B:2968:LEU:HD22	1:B:2999:LEU:HD11	2.00	0.43
1:B:3238:ILE:HD11	1:B:3617:TRP:CZ2	2.48	0.43
1:B:4293:THR:HG23	1:B:4352:ASP:OD1	2.19	0.43
1:A:1658:GLU:O	1:A:1661:ALA:HB3	2.19	0.43
1:A:2290:LEU:HD23	1:A:2301:SER:O	2.19	0.43
1:A:2304:HIS:N	1:A:2352:TRP:O	2.51	0.43
1:A:2327:TRP:CZ2	1:A:2379:LEU:HD22	2.54	0.43
1:A:3197:PRO:HG2	1:A:3198:GLN:OE1	2.18	0.43
1:A:3324:LEU:HD12	1:A:3539:LEU:HD23	2.00	0.43
1:A:3416:LYS:HE3	1:A:3418:GLU:CB	2.48	0.43
1:A:3681:ALA:HB2	1:A:3786:PHE:CG	2.54	0.43
1:A:3862:THR:C	1:A:3864:GLU:H	2.22	0.43
1:A:4379:ILE:HG23	1:A:4381:LEU:HD13	2.00	0.43
1:B:1606:ILE:HG23	1:B:1607:ASP:N	2.33	0.43
1:B:1780:THR:HG22	1:B:1784:LEU:CD1	2.48	0.43
1:B:2840:PRO:O	1:B:2843:ARG:HB2	2.19	0.43
1:B:3065:LYS:O	1:B:3066:GLU:C	2.57	0.43
1:B:3139:ARG:HG3	1:B:3139:ARG:HH11	1.84	0.43
1:B:3289:LEU:O	1:B:3293:ARG:HG3	2.19	0.43
1:B:3675:ILE:O	1:B:3675:ILE:HG22	2.19	0.43
1:B:3725:ASN:ND2	1:B:3725:ASN:N	2.67	0.43
1:B:4028:PRO:O	1:B:4031:SER:N	2.52	0.43
1:B:4058:ILE:CD1	1:B:4082:LYS:HG2	2.48	0.43
1:B:4331:TRP:HZ2	1:B:4369:PHE:CE2	2.37	0.43
1:A:1578:SER:HA	1:A:1579:PRO:HD3	1.92	0.43
1:A:1892:LEU:C	1:A:1894:LYS:H	2.22	0.43
1:A:2269:ASN:O	1:A:2272:VAL:HG23	2.19	0.43
1:A:2645:ASP:O	1:A:2646:VAL:C	2.57	0.43
1:A:2774:ARG:CZ	1:A:2781:ILE:HD11	2.48	0.43
1:A:3588:VAL:O	1:A:3592:VAL:HG23	2.18	0.43
1:A:3859:LYS:C	1:A:3859:LYS:HD3	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3902:GLU:HB3	1:A:4433:MET:HG2	2.00	0.43
1:A:4565:ILE:HG22	1:A:4566:SER:N	2.34	0.43
1:B:2304:HIS:NE2	1:B:2351:HIS:HD2	2.17	0.43
1:B:2339:ILE:HG21	1:B:2391:VAL:CG2	2.49	0.43
1:B:3202:PRO:HG3	1:B:3623:SER:O	2.19	0.43
1:B:3272:ASN:HD22	1:B:3272:ASN:HA	1.61	0.43
1:B:3620:ARG:HG2	1:B:3620:ARG:NH1	2.34	0.43
1:B:3895:ARG:NH1	1:B:3977:LYS:HG2	2.34	0.43
1:B:4023:LEU:O	1:B:4027:VAL:HB	2.18	0.43
1:B:4079:ASN:O	1:B:4082:LYS:HB2	2.18	0.43
1:B:4185:VAL:O	1:B:4215:LEU:HD12	2.19	0.43
1:B:4282:GLN:O	1:B:4285:LEU:HB2	2.19	0.43
1:A:1927:ILE:O	1:A:1928:HIS:HD2	2.01	0.43
1:A:2211:ASP:C	1:A:2213:PRO:HD2	2.38	0.43
1:A:2362:GLU:C	1:A:2364:VAL:H	2.22	0.43
1:A:3391:ILE:HD11	1:A:3471:SER:OG	2.19	0.43
1:A:3953:ASN:O	1:A:3956:THR:HG22	2.19	0.43
1:A:4335:ARG:HG2	1:A:4360:LEU:HG	2.01	0.43
1:A:4432:LYS:C	1:A:4434:GLN:N	2.72	0.43
1:A:4659:ILE:N	1:A:4659:ILE:HD12	2.34	0.43
1:A:4708:ASP:C	1:A:4710:SER:H	2.22	0.43
1:B:4075:THR:HG23	1:B:4076:ILE:N	2.34	0.43
1:B:4324:ILE:H	1:B:4324:ILE:HG13	1.52	0.43
1:B:4617:GLU:HG2	1:B:4618:ASN:N	2.34	0.43
1:B:4638:ASN:HB3	1:B:4666:ILE:HD11	2.00	0.43
1:A:1963:ALA:HA	1:A:2096:ARG:HH11	1.83	0.42
1:A:1967:ARG:NH1	1:A:2053:ASN:HA	2.34	0.42
1:A:3716:CYS:H	1:A:3760:PHE:HB2	1.84	0.42
1:A:4024:ARG:HA	1:A:4030:PHE:O	2.19	0.42
1:A:4354:ARG:HD3	1:A:4717:TYR:CD2	2.53	0.42
1:B:2196:LEU:HD11	1:B:2223:PHE:CD2	2.54	0.42
1:B:2271:GLY:HA2	1:B:2393:VAL:O	2.19	0.42
1:B:2368:ASN:O	1:B:2410:ARG:NH1	2.52	0.42
1:B:2849:LEU:CD1	1:B:2901:LEU:HD11	2.49	0.42
1:B:3722:ASP:HA	1:B:3724:GLU:OE1	2.19	0.42
1:B:3723:VAL:HG23	1:B:3764:LEU:HD22	2.01	0.42
1:A:1554:LEU:HD22	1:A:1609:GLN:HG3	2.00	0.42
1:A:1907:LEU:HD22	1:A:1911:ARG:CZ	2.49	0.42
1:A:2425:MET:HE2	1:A:2425:MET:HB3	1.81	0.42
1:A:2560:MET:CG	1:A:2565:GLN:HB2	2.49	0.42
1:A:3782:THR:HG23	1:A:3782:THR:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3992:LEU:CD1	1:A:4434:GLN:HG3	2.48	0.42
1:A:4358:SER:O	1:A:4362:GLN:HB2	2.19	0.42
1:A:4596:ASN:OD1	1:A:4599:ALA:HB2	2.18	0.42
1:A:4678:ILE:HG22	1:A:4678:ILE:O	2.19	0.42
1:B:2109:ALA:HA	1:B:2156:LEU:CD1	2.49	0.42
1:B:2423:THR:HA	1:B:2426:ILE:HD13	2.00	0.42
1:B:2886:LEU:HD23	1:B:2904:LEU:HD22	2.01	0.42
1:B:2991:PHE:CE1	1:B:2993:GLU:HB2	2.54	0.42
1:B:3234:ILE:HG23	1:B:3617:TRP:CE2	2.54	0.42
1:B:3598:PHE:CD2	1:B:3634:VAL:HG11	2.55	0.42
1:B:3647:TRP:HB3	1:B:3652:LEU:CD2	2.49	0.42
1:B:3676:ASP:CB	1:B:3681:ALA:HB3	2.49	0.42
1:B:4673:ASP:OD1	1:B:4674:LYS:N	2.52	0.42
1:A:1816:LEU:HD23	1:A:1878:LEU:CD1	2.49	0.42
1:A:2259:ILE:HG23	1:A:2289:TYR:HB2	2.02	0.42
1:A:2525:ILE:HD12	1:A:2526:MET:N	2.33	0.42
1:A:2832:ASN:CG	1:A:2849:LEU:HD23	2.39	0.42
1:A:2870:ALA:C	1:A:2872:TYR:H	2.21	0.42
1:A:3067:GLU:HG2	1:A:3068:LYS:N	2.34	0.42
1:A:3096:VAL:HB	1:A:3099:LEU:HD22	2.01	0.42
1:A:3156:ASN:C	1:A:3158:SER:H	2.21	0.42
1:A:3718:LEU:HG	1:A:3719:LEU:N	2.21	0.42
1:A:4000:SER:O	1:B:2940:SER:HB3	2.19	0.42
1:B:1505:SER:O	1:B:1506:ASP:C	2.57	0.42
1:B:1960:LEU:HD13	1:B:2074:PHE:CE1	2.54	0.42
1:B:2017:CYS:SG	1:B:2046:ILE:HD13	2.59	0.42
1:B:2129:VAL:N	1:B:2130:PRO:CD	2.82	0.42
1:B:2669:PRO:HA	1:B:2788:PHE:O	2.19	0.42
1:B:3030:ALA:HB3	1:B:3037:ILE:HD11	2.00	0.42
1:B:3078:VAL:O	1:B:3078:VAL:HG22	2.18	0.42
1:B:3698:SER:HB3	1:B:3700:LEU:HD12	2.00	0.42
1:B:3962:ASP:C	1:B:3964:LYS:H	2.23	0.42
1:A:1639:ILE:HG12	1:A:1675:LEU:HD23	2.01	0.42
1:A:1732:LEU:HD13	1:A:1741:ILE:HD12	2.01	0.42
1:A:1752:VAL:CG2	1:A:1811:PRO:HG3	2.48	0.42
1:A:1816:LEU:O	1:A:1820:GLN:HG3	2.19	0.42
1:A:1973:PHE:O	1:A:1973:PHE:HD1	2.02	0.42
1:A:2142:GLN:HB2	1:A:2145:TYR:CD1	2.54	0.42
1:A:2266:LEU:HD21	1:A:2394:MET:CE	2.49	0.42
1:A:2615:TYR:CD2	1:A:2615:TYR:N	2.87	0.42
1:A:2819:PRO:HB2	1:A:2824:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3018:SER:O	1:A:3257:PRO:HD2	2.18	0.42
1:A:3209:ALA:CB	1:A:3221:PRO:HG3	2.49	0.42
1:A:3700:LEU:CD1	1:A:3701:ASP:N	2.80	0.42
1:A:3993:LYS:O	1:A:3995:GLY:N	2.53	0.42
1:A:4109:ASP:CA	1:A:4112:ASN:HD22	2.11	0.42
1:A:4134:LEU:HD23	1:A:4236:PHE:HB2	2.01	0.42
1:A:4168:PHE:O	1:A:4172:GLU:HG3	2.19	0.42
1:A:4289:PRO:HA	1:A:4292:TRP:O	2.20	0.42
1:B:1811:PRO:HB2	1:B:1814:LEU:CD1	2.49	0.42
1:B:2125:ALA:C	1:B:2127:LYS:H	2.21	0.42
1:B:2272:VAL:HG12	1:B:2273:MET:N	2.34	0.42
1:B:2591:GLU:HA	1:B:2613:LEU:HD12	2.01	0.42
1:B:3039:THR:HG22	1:B:3072:ILE:HB	2.01	0.42
1:B:3057:MET:O	1:B:3061:ARG:HG3	2.19	0.42
1:B:3181:LEU:HB2	1:B:3232:VAL:HG13	2.01	0.42
1:B:3960:LEU:CD2	1:B:4237:SER:HB2	2.50	0.42
1:A:1708:ILE:HD11	1:A:1721:HIS:HB3	2.01	0.42
1:A:1967:ARG:CB	1:A:2051:LYS:HA	2.50	0.42
1:A:2051:LYS:HD3	1:A:2051:LYS:C	2.39	0.42
1:A:2408:ILE:O	1:A:2411:CYS:HB2	2.20	0.42
1:A:2502:ILE:CG2	1:A:2573:LEU:HD12	2.48	0.42
1:A:2534:LEU:HB3	1:A:2538:PHE:CE2	2.55	0.42
1:A:2587:LEU:CG	1:A:2817:ASP:HB2	2.45	0.42
1:A:2905:TRP:HZ3	1:A:2934:ALA:HB2	1.83	0.42
1:A:3192:LEU:HD11	1:A:3271:ILE:HG22	2.01	0.42
1:A:3262:ASP:OD2	1:A:3670:ARG:NE	2.52	0.42
1:A:3536:TYR:O	1:A:3540:ILE:HD13	2.20	0.42
1:A:4373:PHE:CD1	1:A:4374:PRO:HD2	2.54	0.42
1:B:2112:MET:SD	1:B:2153:LYS:HG2	2.59	0.42
1:B:2528:PHE:HE1	1:B:2533:VAL:HG11	1.85	0.42
1:B:2706:THR:HA	1:B:2759:VAL:HG22	2.01	0.42
1:B:3084:LEU:O	1:B:3087:MET:N	2.52	0.42
1:B:3598:PHE:O	1:B:3602:ILE:HB	2.20	0.42
1:A:1766:ILE:HG23	1:A:1767:HIS:N	2.35	0.42
1:A:1777:MET:HE3	1:A:1939:GLU:HA	2.02	0.42
1:A:1979:GLY:O	1:A:1980:LYS:C	2.58	0.42
1:A:2106:GLU:CD	1:A:2106:GLU:N	2.69	0.42
1:A:2370:LEU:HD23	1:A:2370:LEU:O	2.19	0.42
1:A:2415:TRP:HA	1:A:2415:TRP:HE3	1.83	0.42
1:A:2910:LEU:HB3	1:A:2911:ARG:HH12	1.85	0.42
1:A:3009:GLN:HG2	1:A:3138:ARG:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3061:ARG:O	1:A:3067:GLU:HB3	2.18	0.42
1:A:3108:LEU:HD11	1:A:3133:PHE:CZ	2.54	0.42
1:A:3915:ALA:O	1:A:3918:ASP:HB2	2.19	0.42
1:A:3954:ARG:O	1:A:3954:ARG:HD3	2.19	0.42
1:A:4128:SER:CB	1:A:4213:PHE:HB3	2.48	0.42
1:A:4178:ALA:HA	1:A:4183:THR:OG1	2.20	0.42
1:B:1598:VAL:HG22	1:B:1660:LEU:HD22	2.01	0.42
1:B:1914:TYR:CZ	1:B:1924:LYS:HB3	2.54	0.42
1:B:2230:PRO:HB3	1:B:2237:ARG:HH22	1.84	0.42
1:B:2327:TRP:CH2	1:B:2380:PRO:HD2	2.55	0.42
1:B:2610:ILE:HD12	1:B:2615:TYR:OH	2.20	0.42
1:B:3043:ASN:ND2	1:B:3043:ASN:N	2.68	0.42
1:B:3160:THR:C	1:B:3162:PRO:HD3	2.40	0.42
1:A:2126:GLY:O	1:A:2130:PRO:HG2	2.19	0.42
1:A:2269:ASN:O	1:A:2271:GLY:N	2.53	0.42
1:A:2270:HIS:HB2	1:A:2392:ARG:HD2	2.02	0.42
1:A:2426:ILE:CD1	1:A:2530:ARG:HD3	2.50	0.42
1:A:2573:LEU:HD23	1:A:2573:LEU:C	2.40	0.42
1:A:2701:PHE:HB2	1:A:2745:GLU:O	2.20	0.42
1:A:3457:LEU:HD12	1:A:3486:TYR:CE1	2.55	0.42
1:B:2290:LEU:HD22	1:B:2352:TRP:CZ3	2.55	0.42
1:B:2588:VAL:HG23	1:B:2589:GLU:N	2.34	0.42
1:B:2773:TRP:CH2	1:B:2780:TRP:HB2	2.54	0.42
1:B:3061:ARG:O	1:B:3067:GLU:HB3	2.19	0.42
1:B:3990:PHE:CD2	1:B:4084:LEU:HD22	2.55	0.42
1:A:1791:HIS:HD2	1:A:1806:TRP:HD1	1.66	0.42
1:A:1952:LEU:HD22	1:A:2103:PRO:HA	2.01	0.42
1:A:2057:VAL:HB	1:A:2067:LEU:HD13	2.01	0.42
1:A:2561:SER:HA	1:A:2562:PRO:HD3	1.95	0.42
1:A:2849:LEU:HA	1:A:2938:PHE:HZ	1.85	0.42
1:A:3268:VAL:HG13	1:A:3269:LEU:N	2.35	0.42
1:A:3602:ILE:HG22	1:A:3603:GLY:N	2.34	0.42
1:A:4313:TRP:CD1	1:A:4334:VAL:HG22	2.55	0.42
1:B:1608:VAL:HG13	1:B:1676:LEU:CD1	2.50	0.42
1:B:1907:LEU:HD22	1:B:1911:ARG:NH2	2.34	0.42
1:B:2084:ARG:CZ	1:B:4295:PHE:CD2	3.03	0.42
1:B:2513:HIS:O	1:B:2517:GLU:HG3	2.19	0.42
1:B:2528:PHE:CE1	1:B:2533:VAL:HG11	2.54	0.42
1:B:2825:THR:CG2	1:B:2854:VAL:HG21	2.50	0.42
1:B:3259:HIS:NE2	1:B:3779:SER:HA	2.34	0.42
1:B:4036:HIS:CD2	1:B:4044:TRP:HE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4280:ILE:HG23	1:B:4408:LEU:HA	2.01	0.42
1:B:4284:ARG:CG	1:B:4408:LEU:HB3	2.49	0.42
1:A:1792:PHE:C	1:A:1792:PHE:CD2	2.92	0.42
1:A:2009:MET:HE3	1:A:2012:ILE:HB	2.02	0.42
1:A:2071:MET:O	1:A:2071:MET:HG3	2.20	0.42
1:A:2585:MET:O	1:A:2815:LEU:HD13	2.19	0.42
1:A:2842:LEU:HD11	1:A:2897:THR:C	2.40	0.42
1:A:2989:VAL:HG13	1:A:3187:GLU:OE2	2.20	0.42
1:A:3075:GLU:C	1:A:3077:ASN:H	2.23	0.42
1:A:3224:ARG:HB2	1:A:3224:ARG:HE	1.73	0.42
1:A:3449:ARG:NH1	1:A:3449:ARG:HB3	2.35	0.42
1:B:2540:LEU:HB3	1:B:2576:SER:CB	2.49	0.42
1:B:2856:PHE:HE2	1:B:2913:PHE:CD2	2.37	0.42
1:B:2989:VAL:HG21	1:B:3184:VAL:HA	2.02	0.42
1:B:3039:THR:CG2	1:B:3072:ILE:HB	2.50	0.42
1:B:3235:HIS:CE1	1:B:3260:TYR:HB2	2.55	0.42
1:B:3256:THR:CG2	1:B:3779:SER:HB3	2.50	0.42
1:B:3976:VAL:O	1:B:3979:THR:HG23	2.20	0.42
1:A:1556:ARG:HG2	1:A:1557:GLY:N	2.35	0.42
1:A:1746:SER:HB3	1:A:1940:TYR:CZ	2.55	0.42
1:A:1818:THR:O	1:A:1822:VAL:HG23	2.20	0.42
1:A:1929:MET:O	1:A:1930:ALA:HB3	2.20	0.42
1:A:1973:PHE:HE1	1:A:2099:ALA:CA	2.33	0.42
1:A:2833:ARG:HA	1:A:2846:ALA:HB1	2.02	0.42
1:A:3148:ASN:HA	1:A:3149:PRO:HD3	1.93	0.42
1:A:3315:VAL:O	1:A:3319:GLN:HB2	2.19	0.42
1:A:4065:ALA:O	1:A:4069:LEU:HB2	2.20	0.42
1:A:4070:SER:C	1:A:4072:GLN:N	2.72	0.42
1:A:4418:LEU:HD11	1:A:4422:LYS:HZ3	1.84	0.42
1:A:4575:LEU:H	1:A:4575:LEU:CD1	2.26	0.42
1:B:1615:LEU:HD13	1:B:1618:ILE:HD12	2.01	0.42
1:B:1952:LEU:HA	1:B:1955:ARG:NH2	2.35	0.42
1:B:2684:LEU:HD13	1:B:2684:LEU:C	2.40	0.42
1:B:3017:VAL:HG11	1:B:3175:GLU:HA	2.01	0.42
1:B:4070:SER:O	1:B:4072:GLN:N	2.53	0.42
1:B:4434:GLN:O	1:B:4434:GLN:HG2	2.19	0.42
1:A:2140:SER:HB2	1:A:2142:GLN:NE2	2.23	0.41
1:A:2204:ILE:HG13	1:A:2205:PRO:CD	2.50	0.41
1:A:2898:LEU:HD11	1:A:2941:VAL:HG22	2.01	0.41
1:A:3889:MET:SD	1:A:3889:MET:C	2.99	0.41
1:A:4370:ASN:N	1:A:4370:ASN:HD22	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1565:LEU:HD23	1:B:1595:LEU:HD12	2.00	0.41
1:B:2272:VAL:O	1:B:2394:MET:HA	2.20	0.41
1:B:2292:ALA:O	1:B:2296:VAL:HG23	2.20	0.41
1:B:2370:LEU:HD12	1:B:2377:LEU:HB2	2.02	0.41
1:B:2579:TRP:HZ2	1:B:2655:ARG:HD2	1.84	0.41
1:B:3923:LEU:HD22	1:B:3947:ILE:CG2	2.47	0.41
1:B:4191:HIS:CD2	1:B:4220:GLU:HG2	2.54	0.41
1:A:1831:LEU:HA	1:A:1841:ILE:HG12	2.02	0.41
1:A:1973:PHE:C	1:A:1973:PHE:HD1	2.23	0.41
1:A:2258:LYS:HA	1:A:2261:GLN:CG	2.44	0.41
1:A:2370:LEU:HA	1:A:2375:LYS:HA	2.02	0.41
1:A:2745:GLU:CB	1:A:2748:LEU:HD12	2.50	0.41
1:A:2783:LEU:HD22	1:A:2786:ILE:HB	2.01	0.41
1:A:3256:THR:HB	1:A:3257:PRO:HD2	2.01	0.41
1:A:3808:ASP:CG	1:A:3809:THR:N	2.73	0.41
1:A:3990:PHE:O	1:A:3994:GLY:HA2	2.20	0.41
1:A:4337:ILE:O	1:A:4341:THR:CG2	2.68	0.41
1:A:4623:ALA:HB2	1:A:4703:ILE:CD1	2.48	0.41
1:A:4684:SER:O	1:A:4707:TYR:HE2	2.02	0.41
1:B:1785:LEU:HB2	1:B:1814:LEU:HD23	2.00	0.41
1:B:1960:LEU:HD13	1:B:2074:PHE:HE1	1.85	0.41
1:B:3573:ARG:HG2	1:B:3573:ARG:HH11	1.84	0.41
1:B:3700:LEU:CD1	1:B:3701:ASP:H	2.30	0.41
1:B:3877:GLN:O	1:B:3881:GLU:HB2	2.20	0.41
1:B:4277:PHE:HZ	1:B:4356:LEU:HD21	1.84	0.41
1:A:1625:ILE:HG23	1:A:1626:ASN:N	2.33	0.41
1:A:1719:GLN:HA	1:A:1722:PHE:CE2	2.56	0.41
1:A:1959:THR:O	1:A:1963:ALA:CB	2.69	0.41
1:A:2893:MET:O	1:A:2895:GLY:N	2.46	0.41
1:A:3148:ASN:OD1	1:A:3150:ALA:N	2.45	0.41
1:A:3206:ILE:HA	1:A:3221:PRO:HG2	2.03	0.41
1:A:3443:MET:HE3	1:A:3449:ARG:HA	2.02	0.41
1:A:3994:GLY:O	1:A:3995:GLY:C	2.58	0.41
1:A:4278:HIS:O	1:A:4282:GLN:HB2	2.20	0.41
1:B:1590:HIS:NE2	1:B:1594:ARG:NH1	2.68	0.41
1:B:1872:ARG:NH2	1:B:2164:ARG:NE	2.68	0.41
1:B:2208:VAL:HG12	1:B:2415:TRP:NE1	2.36	0.41
1:B:2231:ILE:CG2	1:B:2264:GLN:HE22	2.31	0.41
1:B:2578:MET:O	1:B:2582:GLY:HA3	2.19	0.41
1:B:2670:LEU:HD12	1:B:2670:LEU:O	2.20	0.41
1:B:3563:LEU:CD1	1:B:3845:ILE:HD11	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3566:ASN:HD21	1:B:3859:LYS:HZ2	1.69	0.41
1:B:3886:TYR:CE2	1:B:3940:LEU:HD23	2.56	0.41
1:B:3910:GLN:HB3	1:B:4231:ARG:HD3	2.03	0.41
1:B:3960:LEU:HB3	1:B:4239:GLU:OE2	2.21	0.41
1:B:4201:GLU:HG3	1:B:4228:ASN:HB2	2.03	0.41
1:B:4284:ARG:HG2	1:B:4408:LEU:HB3	2.02	0.41
1:A:1697:PHE:CD2	1:A:1705:LEU:HD11	2.55	0.41
1:A:1701:GLY:HA2	1:A:2011:ARG:CZ	2.50	0.41
1:A:2127:LYS:O	1:A:2130:PRO:HD2	2.20	0.41
1:A:2376:LEU:HD12	1:A:2386:ALA:N	2.35	0.41
1:A:2586:GLY:CA	1:A:2815:LEU:HD13	2.43	0.41
1:A:2612:LEU:O	1:A:2612:LEU:HD12	2.21	0.41
1:A:2749:PRO:HG2	1:A:2759:VAL:HG11	2.01	0.41
1:A:2774:ARG:HH21	1:A:2779:THR:HB	1.85	0.41
1:A:2868:ILE:HG21	1:A:2922:GLU:OE2	2.21	0.41
1:A:3013:LEU:HD23	1:A:3170:LEU:HD12	2.01	0.41
1:A:3164:LEU:HD12	1:A:3164:LEU:HA	1.81	0.41
1:A:3553:VAL:O	1:A:3557:VAL:HG23	2.21	0.41
1:A:3652:LEU:HD21	1:A:3662:ALA:HB2	2.02	0.41
1:A:3819:ILE:C	1:A:3821:GLY:H	2.23	0.41
1:A:4012:LEU:HD12	1:A:4012:LEU:H	1.84	0.41
1:A:4270:ILE:HG22	1:A:4310:ILE:HD13	2.01	0.41
1:A:4314:VAL:O	1:A:4314:VAL:CG1	2.68	0.41
1:A:4349:ASN:ND2	1:A:4352:ASP:N	2.65	0.41
1:A:4648:VAL:CG1	1:A:4662:THR:HG21	2.41	0.41
1:A:4692:LEU:HD12	1:A:4700:LEU:HD21	2.02	0.41
1:B:2036:LEU:HD23	1:B:2036:LEU:O	2.20	0.41
1:B:2556:SER:C	1:B:2558:PHE:N	2.73	0.41
1:B:3602:ILE:O	1:B:3603:GLY:C	2.59	0.41
1:B:4068:GLN:C	1:B:4070:SER:H	2.24	0.41
1:B:4371:PRO:O	1:B:4372:ASP:HB2	2.20	0.41
1:A:1782:ALA:HA	1:A:1938:PHE:CZ	2.55	0.41
1:A:2204:ILE:CA	1:A:2207:LEU:HD12	2.44	0.41
1:A:2222:VAL:C	1:A:2224:PRO:HD3	2.40	0.41
1:A:2376:LEU:HD21	1:A:2384:ARG:HB3	2.02	0.41
1:A:2606:PRO:HG2	1:A:2615:TYR:CD1	2.56	0.41
1:A:2832:ASN:HA	1:A:2835:LEU:HB3	2.01	0.41
1:A:4012:LEU:HD21	1:A:4020:LEU:HD22	2.02	0.41
1:A:4283:GLU:OE2	1:A:4286:ARG:NH1	2.54	0.41
1:A:4289:PRO:HB2	1:A:4696:ARG:HD2	2.01	0.41
1:A:4401:GLU:HB2	1:A:4402:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1493:ILE:O	1:B:1497:LEU:HG	2.21	0.41
1:B:1817:LEU:HD11	1:B:1936:TYR:CD2	2.55	0.41
1:B:2223:PHE:C	1:B:2225:GLY:H	2.23	0.41
1:B:3606:ASP:O	1:B:3610:ARG:HG3	2.21	0.41
1:B:4006:PRO:C	1:B:4008:LEU:H	2.24	0.41
1:B:4553:TYR:O	1:B:4555:VAL:HG22	2.20	0.41
1:A:1766:ILE:HG23	1:A:1767:HIS:H	1.84	0.41
1:A:1888:VAL:HG22	1:A:1909:HIS:CE1	2.56	0.41
1:A:2275:VAL:HG23	1:A:2397:VAL:HG23	2.03	0.41
1:A:2579:TRP:HZ2	1:A:2655:ARG:HD2	1.85	0.41
1:A:2694:PHE:CD2	1:A:2738:TRP:HB2	2.56	0.41
1:A:2748:LEU:CD2	1:A:2800:ARG:HD3	2.51	0.41
1:A:3439:ASP:OD2	1:A:3442:LYS:HE2	2.21	0.41
1:A:3571:ARG:HB3	1:A:3571:ARG:NH1	2.35	0.41
1:A:4001:ILE:HB	1:A:4018:LYS:HD3	2.02	0.41
1:A:4006:PRO:O	1:A:4008:LEU:N	2.52	0.41
1:A:4240:ASN:HA	1:A:4241:PRO:HD2	1.89	0.41
1:A:4247:ASN:HD21	1:A:4282:GLN:HE21	1.67	0.41
1:A:4278:HIS:HD2	1:A:4343:TYR:CE1	2.39	0.41
1:A:4535:ARG:HH11	1:A:4535:ARG:HG2	1.84	0.41
1:A:4537:LEU:CD2	1:A:4548:LYS:HE3	2.50	0.41
1:A:4670:THR:HG22	1:A:4671:TRP:N	2.36	0.41
1:B:1910:MET:CB	1:B:1929:MET:HG3	2.50	0.41
1:B:2670:LEU:HD12	1:B:2670:LEU:C	2.41	0.41
1:B:2711:LEU:HD12	1:B:2711:LEU:HA	1.89	0.41
1:B:3087:MET:HE2	1:B:3090:LEU:HD23	2.03	0.41
1:B:4184:TRP:NE1	1:B:4214:ARG:HB2	2.35	0.41
1:A:2057:VAL:HG13	1:A:2059:LEU:H	1.86	0.41
1:A:2615:TYR:N	1:A:2615:TYR:HD2	2.18	0.41
1:A:2696:VAL:HG22	1:A:2697:VAL:N	2.36	0.41
1:A:2855:GLU:OE2	1:A:2933:VAL:HG22	2.21	0.41
1:B:1483:ILE:HG22	1:B:1517:VAL:HG22	2.02	0.41
1:B:1497:LEU:HB3	1:B:1501:SER:CB	2.51	0.41
1:B:1500:GLY:O	1:B:1504:ASP:N	2.50	0.41
1:B:2239:LYS:O	1:B:2243:ILE:HG13	2.21	0.41
1:B:2278:SER:H	1:B:2398:GLN:NE2	2.17	0.41
1:B:2363:TRP:C	1:B:2365:GLU:H	2.24	0.41
1:B:2400:LEU:HD13	1:B:2408:ILE:CD1	2.48	0.41
1:B:2853:MET:HA	1:B:2882:TRP:CZ3	2.56	0.41
1:B:3567:LEU:HD23	1:B:3567:LEU:HA	1.94	0.41
1:B:3903:LEU:O	1:B:3909:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4023:LEU:HG	1:B:4030:PHE:CD1	2.56	0.41
1:B:4509:LEU:HD23	1:B:4568:PHE:CE1	2.55	0.41
1:B:4535:ARG:HG2	1:B:4535:ARG:NH1	2.34	0.41
1:B:4644:LEU:HD23	1:B:4723:ILE:HG12	2.02	0.41
1:A:2000:CYS:O	1:A:2001:ASP:C	2.58	0.41
1:A:2028:PHE:CB	1:A:2075:VAL:HG13	2.44	0.41
1:A:2269:ASN:C	1:A:2271:GLY:H	2.24	0.41
1:A:2579:TRP:CE3	1:A:2659:VAL:HG21	2.56	0.41
1:A:3567:LEU:HD23	1:A:3567:LEU:HA	1.91	0.41
1:A:3652:LEU:HB2	1:A:3684:PHE:CD1	2.55	0.41
1:A:4033:LEU:HD13	1:A:4062:TRP:CZ2	2.55	0.41
1:A:4426:MET:O	1:A:4430:LEU:HG	2.21	0.41
1:B:3258:ARG:HD2	1:B:3779:SER:HB2	2.01	0.41
1:B:3781:VAL:HG12	1:B:3782:THR:N	2.34	0.41
1:B:3930:LEU:O	1:B:3932:ASP:N	2.54	0.41
1:A:1712:SER:HB3	1:A:1766:ILE:HB	2.03	0.41
1:A:1726:PHE:CD2	1:A:1729:LEU:HD22	2.55	0.41
1:A:1886:ARG:HG3	1:A:1887:ASP:H	1.81	0.41
1:A:2088:PRO:C	1:A:2090:ASN:N	2.75	0.41
1:A:2848:ASN:HB3	1:A:2938:PHE:CE1	2.55	0.41
1:A:2890:ILE:HD13	1:A:2893:MET:CE	2.51	0.41
1:A:3078:VAL:HG23	1:A:3083:PHE:HB2	2.02	0.41
1:A:3093:GLY:O	1:A:3095:GLU:N	2.54	0.41
1:A:3230:SER:HA	1:A:3620:ARG:HE	1.86	0.41
1:A:3597:ALA:O	1:A:3601:TYR:HD1	2.04	0.41
1:A:3844:ASN:O	1:A:3848:ASP:HB2	2.20	0.41
1:A:4024:ARG:CG	1:A:4031:SER:HA	2.49	0.41
1:A:4060:GLU:O	1:A:4064:VAL:HG23	2.21	0.41
1:A:4592:GLY:CA	1:A:4725:SER:HB2	2.50	0.41
1:B:1734:LEU:HA	1:B:1742:ILE:HG12	2.03	0.41
1:B:1739:THR:O	1:B:1760:ILE:N	2.54	0.41
1:B:1831:LEU:HB3	1:B:1900:GLY:HA2	2.02	0.41
1:B:1844:GLN:O	1:B:1847:SER:HB2	2.21	0.41
1:B:2029:ASN:N	1:B:2029:ASN:HD22	2.18	0.41
1:B:2084:ARG:HG2	1:B:2084:ARG:NH1	2.36	0.41
1:B:2151:ALA:O	1:B:2154:SER:N	2.52	0.41
1:B:2236:LEU:O	1:B:2240:ILE:HG13	2.21	0.41
1:B:2270:HIS:CA	1:B:2392:ARG:HH11	2.33	0.41
1:B:2381:ASN:C	1:B:2381:ASN:HD22	2.25	0.41
1:B:2420:ILE:HG13	1:B:2421:LEU:N	2.36	0.41
1:B:2492:LEU:O	1:B:2493:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2578:MET:HB3	1:B:2597:ILE:CD1	2.43	0.41
1:B:2887:LEU:O	1:B:2891:GLN:HG3	2.21	0.41
1:B:3228:VAL:HA	1:B:3231:LEU:HD12	2.03	0.41
1:B:3539:LEU:HD12	1:B:3539:LEU:HA	1.92	0.41
1:B:3571:ARG:O	1:B:3575:GLU:HG3	2.19	0.41
1:B:3647:TRP:HB3	1:B:3652:LEU:HD22	2.02	0.41
1:B:4022:CYS:HB3	1:B:4026:GLN:NE2	2.36	0.41
1:B:4056:PRO:HD2	1:B:4093:ARG:NH2	2.36	0.41
1:B:4094:VAL:HB	1:B:4423:ALA:HB1	2.02	0.41
1:B:4141:ASP:OD2	1:B:4143:SER:HB2	2.21	0.41
1:B:4145:LYS:HE2	1:B:4238:TYR:CE1	2.55	0.41
1:B:4157:TYR:HB2	1:B:4184:TRP:CB	2.50	0.41
1:B:4162:ILE:HG22	1:B:4163:GLY:N	2.35	0.41
1:B:4277:PHE:HB2	1:B:4363:LEU:HD12	2.03	0.41
1:B:4306:ALA:HA	1:B:4338:LEU:HD22	2.03	0.41
1:B:4413:ASN:ND2	1:B:4660:LEU:HD23	2.36	0.41
1:B:4503:ILE:HD11	1:B:4575:LEU:O	2.21	0.41
1:B:4509:LEU:O	1:B:4513:ILE:HG13	2.20	0.41
1:B:4649:TRP:CE3	1:B:4649:TRP:HA	2.55	0.41
1:A:1939:GLU:O	1:A:1941:LEU:HG	2.21	0.41
1:A:2332:PHE:HA	1:A:2335:THR:OG1	2.20	0.41
1:A:2359:VAL:HG23	1:A:2397:VAL:HG11	2.03	0.41
1:A:3606:ASP:O	1:A:3610:ARG:HG3	2.21	0.41
1:A:3698:SER:C	1:A:3700:LEU:HD12	2.41	0.41
1:A:4063:ILE:HD13	1:A:4082:LYS:NZ	2.36	0.41
1:A:4122:VAL:HB	1:A:4132:LEU:CD2	2.51	0.41
1:A:4606:GLN:HA	1:A:4609:SER:OG	2.21	0.41
1:B:1909:HIS:O	1:B:1911:ARG:HD3	2.22	0.41
1:B:1947:LEU:HD21	1:B:1982:GLU:CG	2.51	0.41
1:B:2260:LEU:O	1:B:2263:HIS:HB3	2.21	0.41
1:B:3015:ILE:O	1:B:3173:PHE:N	2.51	0.41
1:B:3017:VAL:HG13	1:B:3174:GLY:C	2.41	0.41
1:B:3685:LEU:O	1:B:3689:TYR:HB2	2.20	0.41
1:B:4711:THR:OG1	1:B:4716:TRP:NE1	2.54	0.41
1:A:1633:SER:O	1:A:1637:LYS:HG2	2.21	0.40
1:A:2269:ASN:C	1:A:2271:GLY:N	2.74	0.40
1:A:2439:PHE:HZ	1:A:2542:ASN:OD1	2.03	0.40
1:A:2877:ARG:HD2	1:A:2881:ARG:NH2	2.36	0.40
1:A:2935:LEU:HD23	1:A:2935:LEU:C	2.41	0.40
1:A:3022:LYS:HB2	1:A:3022:LYS:NZ	2.36	0.40
1:A:3025:LEU:HD23	1:A:3025:LEU:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3199:TYR:OH	1:A:3226:ALA:HB2	2.21	0.40
1:A:3237:THR:OG1	1:A:3238:ILE:HD12	2.21	0.40
1:A:3720:VAL:HG21	1:A:3762:ILE:HD11	2.03	0.40
1:A:4086:MET:HG2	1:A:4093:ARG:HB2	1.99	0.40
1:A:4090:HIS:C	1:A:4092:ASP:H	2.24	0.40
1:A:4647:ALA:HA	1:A:4657:THR:HG22	2.02	0.40
1:B:2120:THR:HB	1:B:2124:LEU:HG	2.03	0.40
1:B:2754:TYR:O	1:B:2756:THR:HG22	2.21	0.40
1:B:3046:TYR:CZ	1:B:3050:ASP:HB2	2.55	0.40
1:B:3234:ILE:O	1:B:3238:ILE:HD13	2.21	0.40
1:B:3976:VAL:HG13	1:B:4105:VAL:HG11	2.01	0.40
1:B:4499:PHE:HA	1:B:4502:GLU:HB2	2.03	0.40
1:A:2005:ASP:OD1	1:A:2006:LEU:N	2.55	0.40
1:A:2212:ILE:O	1:A:2215:ILE:HG22	2.22	0.40
1:A:3225:ASP:O	1:A:3229:SER:CB	2.69	0.40
1:A:3698:SER:O	1:A:3704:PHE:HB2	2.22	0.40
1:A:3727:ASP:C	1:A:3729:VAL:H	2.25	0.40
1:A:3997:ASN:O	1:A:3998:LEU:C	2.60	0.40
1:A:4117:ASP:C	1:A:4119:ALA:H	2.25	0.40
1:B:1546:VAL:HG12	1:B:1547:ASN:N	2.36	0.40
1:B:1820:GLN:NE2	1:B:1990:GLN:NE2	2.66	0.40
1:B:1928:HIS:CG	1:B:1933:THR:HG22	2.52	0.40
1:B:2081:TYR:O	1:B:2082:ALA:HB3	2.21	0.40
1:B:3218:ALA:O	1:B:3219:ILE:C	2.60	0.40
1:B:4083:ILE:HD11	1:B:4098:SER:HA	2.03	0.40
1:B:4264:PRO:HA	1:B:4322:SER:O	2.21	0.40
1:B:4493:ASP:OD1	1:B:4494:PRO:HD2	2.21	0.40
1:A:1726:PHE:CB	1:A:1729:LEU:HB3	2.51	0.40
1:A:2793:ASN:HB3	1:A:2794:PRO:HD2	2.04	0.40
1:A:2986:VAL:O	1:A:2988:LEU:HG	2.20	0.40
1:A:2995:LEU:CD2	1:A:2998:ILE:HD11	2.48	0.40
1:A:3256:THR:HB	1:A:3257:PRO:CD	2.51	0.40
1:A:4130:SER:HA	1:A:4131:PRO:HD3	1.88	0.40
1:A:4189:ASN:HA	1:A:4191:HIS:CD2	2.57	0.40
1:A:4245:LYS:HE2	1:A:4249:LEU:HD11	2.03	0.40
1:A:4418:LEU:HD11	1:A:4422:LYS:NZ	2.36	0.40
1:B:1696:ARG:HH21	1:B:1726:PHE:HA	1.86	0.40
1:B:2379:LEU:HD12	1:B:2383:GLU:HG2	2.03	0.40
1:B:3256:THR:N	1:B:3259:HIS:HD2	2.19	0.40
1:B:3700:LEU:CD1	1:B:3701:ASP:N	2.80	0.40
1:B:3966:THR:HG23	1:B:4426:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4402:ILE:N	1:B:4402:ILE:CD1	2.81	0.40
1:B:4403:SER:HB2	1:B:4407:TRP:CD2	2.56	0.40
1:B:4428:ASN:O	1:B:4432:LYS:HG3	2.21	0.40
1:B:4703:ILE:CD1	1:B:4705:LEU:HD21	2.45	0.40
1:A:1853:GLN:HE22	1:A:1886:ARG:HH11	1.68	0.40
1:A:1898:LEU:HD23	1:A:1898:LEU:HA	1.89	0.40
1:A:2529:THR:O	1:A:2530:ARG:C	2.60	0.40
1:A:2536:SER:HB2	1:A:2580:GLY:O	2.21	0.40
1:A:3947:ILE:O	1:A:3947:ILE:HD13	2.21	0.40
1:A:4247:ASN:HD21	1:A:4282:GLN:NE2	2.19	0.40
1:B:1867:LEU:H	1:B:1867:LEU:HD12	1.86	0.40
1:B:2029:ASN:HD22	1:B:2030:ARG:N	2.20	0.40
1:B:2135:CYS:O	1:B:2139:LEU:HB2	2.21	0.40
1:B:2258:LYS:HD3	1:B:2261:GLN:OE1	2.21	0.40
1:B:2688:LEU:HD13	1:B:2696:VAL:HB	2.04	0.40
1:B:3002:ASP:HA	1:B:3029:VAL:HG11	2.04	0.40
1:A:1778:LYS:HB3	1:A:1922:LEU:HD11	2.04	0.40
1:A:1831:LEU:HD22	1:A:1898:LEU:HD13	2.04	0.40
1:A:2036:LEU:HD12	1:A:2036:LEU:O	2.21	0.40
1:A:2236:LEU:HD21	1:A:2293:ILE:CD1	2.44	0.40
1:A:2591:GLU:OE1	1:A:2611:PRO:HG2	2.22	0.40
1:A:2710:LEU:HD23	1:A:2762:PHE:CE2	2.57	0.40
1:A:3066:GLU:HG2	1:A:3136:GLN:NE2	2.36	0.40
1:A:3296:GLU:HG3	1:A:3567:LEU:HD13	2.04	0.40
1:A:3459:ASP:HA	1:A:3460:PRO:HD3	1.97	0.40
1:A:3845:ILE:H	1:A:3845:ILE:HG13	1.57	0.40
1:A:4057:ILE:HD12	1:A:4057:ILE:HA	1.96	0.40
1:A:4284:ARG:CG	1:A:4408:LEU:HB3	2.49	0.40
1:B:1813:GLN:HE22	1:B:1941:LEU:H	1.69	0.40
1:B:1906:TRP:CZ2	1:B:1911:ARG:HG2	2.57	0.40
1:B:1928:HIS:NE2	1:B:1933:THR:CG2	2.81	0.40
1:B:2270:HIS:CB	1:B:2392:ARG:HH11	2.34	0.40
1:B:2309:LYS:HG3	1:B:2358:ASP:HB2	2.02	0.40
1:B:2519:ALA:HB2	1:B:2593:PHE:CE1	2.57	0.40
1:B:2645:ASP:OD2	1:B:2645:ASP:N	2.54	0.40
1:B:2745:GLU:HG2	1:B:2748:LEU:CD1	2.51	0.40
1:B:2799:GLY:HA3	1:B:3159:ALA:HB1	2.04	0.40
1:B:3271:ILE:HA	1:B:3592:VAL:HG21	2.03	0.40
1:B:3927:ASN:HB3	1:B:3930:LEU:HD12	2.02	0.40
1:B:4432:LYS:C	1:B:4434:GLN:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3010/3367 (89%)	2424 (80%)	448 (15%)	138 (5%)	2	24
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	6	38
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	3	31

All (205) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1836	LEU
1	A	2121	ALA
1	A	2409	SER
1	A	2560	MET
1	A	2617	VAL
1	A	2641	VAL
1	A	2646	VAL
1	A	2943	LEU
1	A	2992	ASN
1	A	3033	ASN
1	A	3219	ILE
1	A	3370	GLU
1	A	3371	PRO
1	A	3372	ALA
1	A	3603	GLY
1	A	4050	LYS
1	A	4051	ASP
1	A	4117	ASP
1	A	4121	ILE
1	A	4207	LEU
1	A	4548	LYS
1	A	4549	GLU
1	A	4660	LEU
1	B	1949	GLN
1	B	1975	PRO

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Mol	Chain	Res	Type
1	B	1980	LYS
1	B	2071	MET
1	B	3602	ILE
1	B	3931	VAL
1	B	4207	LEU
1	A	1714	ASP
1	A	1949	GLN
1	A	2004	PHE
1	A	2080	GLY
1	A	2101	ILE
1	A	2342	ASN
1	A	2527	ASP
1	A	2530	ARG
1	A	2628	LYS
1	A	2642	ALA
1	A	2645	ASP
1	A	2727	GLU
1	A	2776	SER
1	A	2789	VAL
1	A	2792	CYS
1	A	3218	ALA
1	A	3430	ASN
1	A	3440	THR
1	A	3488	SER
1	A	3715	GLY
1	A	3719	LEU
1	A	3841	ALA
1	A	3926	ASN
1	A	3994	GLY
1	A	3998	LEU
1	A	4000	SER
1	A	4014	THR
1	A	4053	VAL
1	A	4116	LEU
1	A	4123	GLU
1	A	4125	GLU
1	A	4158	LYS
1	A	4221	ILE
1	A	4342	ILE
1	A	4594	LEU
1	A	4666	ILE
1	A	4672	LYS

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Mol	Chain	Res	Type
1	A	4709	GLN
1	B	1919	GLU
1	B	2141	ALA
1	B	2230	PRO
1	B	2384	ARG
1	B	2600	ILE
1	B	2641	VAL
1	B	2755	GLY
1	B	2775	THR
1	B	3092	ALA
1	B	3603	GLY
1	B	3842	SER
1	B	3844	ASN
1	B	4113	THR
1	B	4221	ILE
1	B	4297	GLU
1	B	4340	SER
1	B	4464	ALA
1	B	4551	LYS
1	A	1663	GLU
1	A	1697	PHE
1	A	1703	GLU
1	A	1727	ALA
1	A	1923	HIS
1	A	2001	ASP
1	A	2089	ASP
1	A	2140	SER
1	A	2282	LYS
1	A	2329	ASP
1	A	2374	ASN
1	A	2705	THR
1	A	2871	HIS
1	A	2990	LEU
1	A	3082	SER
1	A	3671	TYR
1	A	3693	LYS
1	A	3843	GLY
1	A	3933	LYS
1	A	4007	GLN
1	A	4055	GLU
1	A	4118	MET
1	A	4131	PRO

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Mol	Chain	Res	Type
1	A	4163	GLY
1	A	4168	PHE
1	A	4318	SER
1	A	4401	GLU
1	A	4412	GLU
1	B	1663	GLU
1	B	2001	ASP
1	B	2527	ASP
1	B	2915	ASP
1	B	3080	GLU
1	B	3094	GLY
1	B	3248	ARG
1	B	3692	LYS
1	B	4071	ASN
1	B	4692	LEU
1	A	1799	ASP
1	A	1837	GLN
1	A	2002	GLU
1	A	2054	SER
1	A	2122	GLU
1	A	2177	ALA
1	A	2270	HIS
1	A	2370	LEU
1	A	2653	THR
1	A	2690	ALA
1	A	2744	ASP
1	A	2891	GLN
1	A	3094	GLY
1	A	3166	ASN
1	A	3444	MET
1	A	3699	PHE
1	A	3907	HIS
1	A	4026	GLN
1	A	4029	SER
1	A	4259	ARG
1	A	4519	ASN
1	B	1506	ASP
1	B	2165	LYS
1	B	2308	PRO
1	B	2401	LYS
1	B	2749	PRO
1	B	2947	LYS

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Mol	Chain	Res	Type
1	B	3932	ASP
1	B	4003	GLU
1	B	4051	ASP
1	B	4053	VAL
1	B	4189	ASN
1	B	4674	LYS
1	A	2363	TRP
1	A	2601	ALA
1	A	2987	PRO
1	A	3140	ASN
1	A	3142	HIS
1	A	3471	SER
1	A	3712	LEU
1	A	3999	THR
1	A	4011	LEU
1	A	4169	GLU
1	A	4579	SER
1	A	4691	TYR
1	A	4712	SER
1	B	1498	THR
1	B	2069	GLN
1	B	2140	SER
1	B	2210	ASP
1	B	2558	PHE
1	B	3693	LYS
1	B	3849	ASP
1	B	3963	ASP
1	B	4412	GLU
1	A	1868	SER
1	A	1944	GLY
1	A	2966	SER
1	A	3164	LEU
1	A	3716	CYS
1	A	3845	ILE
1	B	1582	LYS
1	B	1630	PRO
1	B	1727	ALA
1	B	4459	GLU
1	B	4621	LEU
1	A	3395	PRO
1	A	3806	ARG
1	A	3976	VAL

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Mol	Chain	Res	Type
1	B	4131	PRO
1	A	4056	PRO
1	B	3093	GLY
1	B	4556	PRO
1	A	2644	PRO
1	A	2755	GLY
1	A	3602	ILE
1	A	3677	PRO
1	B	1579	PRO
1	B	2380	PRO
1	A	2208	VAL
1	B	4094	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2457/3028 (81%)	2249 (92%)	208 (8%)	10	40
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	18	50
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	14	45

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1516	GLU
1	A	1559	ASP
1	A	1593	ASP
1	A	1594	ARG
1	A	1665	ILE
1	A	1699	PHE
1	A	1719	GLN
1	A	1744	MET
1	A	1753	THR
1	A	1756	LYS
1	A	1803	TYR

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Mol	Chain	Res	Type
1	A	1809	ASN
1	A	1844	GLN
1	A	1849	GLU
1	A	1865	GLN
1	A	1874	LYS
1	A	1882	LEU
1	A	1911	ARG
1	A	1922	LEU
1	A	1934	PHE
1	A	1962	GLN
1	A	1973	PHE
1	A	1978	THR
1	A	2006	LEU
1	A	2029	ASN
1	A	2051	LYS
1	A	2053	ASN
1	A	2069	GLN
1	A	2071	MET
1	A	2073	ILE
1	A	2090	ASN
1	A	2096	ARG
1	A	2105	ARG
1	A	2107	MET
1	A	2120	THR
1	A	2136	GLN
1	A	2142	GLN
1	A	2149	LEU
1	A	2152	LEU
1	A	2221	ASP
1	A	2234	ASP
1	A	2239	LYS
1	A	2274	MET
1	A	2297	ASP
1	A	2324	THR
1	A	2329	ASP
1	A	2346	GLU
1	A	2350	ARG
1	A	2359	VAL
1	A	2369	SER
1	A	2384	ARG
1	A	2392	ARG
1	A	2408	ILE

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Mol	Chain	Res	Type
1	A	2409	SER
1	A	2415	TRP
1	A	2424	GLN
1	A	2435	SER
1	A	2442	GLN
1	A	2450	ASN
1	A	2511	LEU
1	A	2512	VAL
1	A	2527	ASP
1	A	2529	THR
1	A	2572	ARG
1	A	2587	LEU
1	A	2603	THR
1	A	2613	LEU
1	A	2614	ASP
1	A	2615	TYR
1	A	2626	LEU
1	A	2645	ASP
1	A	2650	THR
1	A	2685	THR
1	A	2694	PHE
1	A	2728	THR
1	A	2747	ASN
1	A	2761	THR
1	A	2793	ASN
1	A	2809	ARG
1	A	2817	ASP
1	A	2863	ARG
1	A	2873	ILE
1	A	2880	SER
1	A	2883	ASP
1	A	2897	THR
1	A	2926	THR
1	A	2944	ASP
1	A	2954	ASN
1	A	2998	ILE
1	A	3007	GLN
1	A	3026	SER
1	A	3027	ARG
1	A	3037	ILE
1	A	3043	ASN
1	A	3052	ASP

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Mol	Chain	Res	Type
1	A	3084	LEU
1	A	3123	LEU
1	A	3141	LEU
1	A	3143	VAL
1	A	3145	PHE
1	A	3158	SER
1	A	3168	CYS
1	A	3175	GLU
1	A	3179	GLU
1	A	3186	SER
1	A	3195	GLU
1	A	3200	ILE
1	A	3216	LEU
1	A	3240	GLU
1	A	3269	LEU
1	A	3278	LEU
1	A	3330	ASP
1	A	3337	LYS
1	A	3365	ASP
1	A	3366	LEU
1	A	3373	ILE
1	A	3381	SER
1	A	3399	THR
1	A	3405	MET
1	A	3432	ILE
1	A	3457	LEU
1	A	3468	ASN
1	A	3516	ASP
1	A	3536	TYR
1	A	3564	LEU
1	A	3566	ASN
1	A	3569	SER
1	A	3571	ARG
1	A	3583	THR
1	A	3584	GLN
1	A	3612	ASP
1	A	3623	SER
1	A	3630	SER
1	A	3663	ILE
1	A	3676	ASP
1	A	3678	SER
1	A	3691	ASP

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Mol	Chain	Res	Type
1	A	3695	THR
1	A	3700	LEU
1	A	3707	ASN
1	A	3719	LEU
1	A	3725	ASN
1	A	3730	LEU
1	A	3731	ASN
1	A	3759	SER
1	A	3760	PHE
1	A	3776	ASP
1	A	3785	ASN
1	A	3791	SER
1	A	3799	HIS
1	A	3806	ARG
1	A	3813	ARG
1	A	3817	LEU
1	A	3830	LEU
1	A	3865	ILE
1	A	3867	LEU
1	A	3887	ASN
1	A	3922	ASN
1	A	3925	ASN
1	A	3947	ILE
1	A	3974	ILE
1	A	3998	LEU
1	A	4007	GLN
1	A	4023	LEU
1	A	4026	GLN
1	A	4034	VAL
1	A	4039	GLN
1	A	4043	ASP
1	A	4048	PHE
1	A	4055	GLU
1	A	4069	LEU
1	A	4079	ASN
1	A	4100	SER
1	A	4200	LEU
1	A	4206	SER
1	A	4232	MET
1	A	4240	ASN
1	A	4259	ARG
1	A	4267	ARG

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Mol	Chain	Res	Type
1	A	4282	GLN
1	A	4286	ARG
1	A	4290	LEU
1	A	4295	PHE
1	A	4321	ARG
1	A	4337	ILE
1	A	4353	MET
1	A	4360	LEU
1	A	4362	GLN
1	A	4385	GLU
1	A	4388	THR
1	A	4404	THR
1	A	4428	ASN
1	A	4434	GLN
1	A	4503	ILE
1	A	4550	TRP
1	A	4553	TYR
1	A	4565	ILE
1	A	4566	SER
1	A	4596	ASN
1	A	4606	GLN
1	A	4638	ASN
1	A	4649	TRP
1	A	4671	TRP
1	A	4692	LEU
1	A	4693	ASN
1	A	4694	GLU
1	A	4711	THR
1	A	4714	GLN
1	B	1479	ARG
1	B	1490	THR
1	B	1545	LEU
1	B	1547	ASN
1	B	1555	VAL
1	B	1596	ASN
1	B	1629	LEU
1	B	1640	ASN
1	B	1658	GLU
1	B	1671	ARG
1	B	1712	SER
1	B	1734	LEU
1	B	1736	ASP

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Mol	Chain	Res	Type
1	B	1762	ASN
1	B	1793	ASN
1	B	1809	ASN
1	B	1817	LEU
1	B	1828	ASP
1	B	1867	LEU
1	B	1901	ASN
1	B	1911	ARG
1	B	1920	ASN
1	B	1946	ARG
1	B	2029	ASN
1	B	2071	MET
1	B	2106	GLU
1	B	2129	VAL
1	B	2149	LEU
1	B	2166	CYS
1	B	2185	GLN
1	B	2189	GLN
1	B	2197	ASN
1	B	2211	ASP
1	B	2235	GLN
1	B	2236	LEU
1	B	2239	LYS
1	B	2253	GLN
1	B	2254	GLU
1	B	2260	LEU
1	B	2290	LEU
1	B	2313	LYS
1	B	2320	LEU
1	B	2342	ASN
1	B	2352	TRP
1	B	2374	ASN
1	B	2381	ASN
1	B	2423	THR
1	B	2425	MET
1	B	2432	ASP
1	B	2504	GLN
1	B	2541	MET
1	B	2550	GLU
1	B	2581	LEU
1	B	2587	LEU
1	B	2603	THR

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Mol	Chain	Res	Type
1	B	2612	LEU
1	B	2613	LEU
1	B	2699	LEU
1	B	2745	GLU
1	B	2797	ASP
1	B	2821	THR
1	B	2825	THR
1	B	2841	ASN
1	B	2843	ARG
1	B	2883	ASP
1	B	2897	THR
1	B	2899	GLU
1	B	2927	ASP
1	B	2928	LYS
1	B	2929	LYS
1	B	2946	LEU
1	B	2966	SER
1	B	2977	LYS
1	B	2984	LEU
1	B	2996	ASP
1	B	3018	SER
1	B	3026	SER
1	B	3043	ASN
1	B	3050	ASP
1	B	3059	LEU
1	B	3087	MET
1	B	3140	ASN
1	B	3151	SER
1	B	3164	LEU
1	B	3195	GLU
1	B	3284	HIS
1	B	3302	LEU
1	B	3322	GLN
1	B	3560	SER
1	B	3563	LEU
1	B	3566	ASN
1	B	3619	ILE
1	B	3620	ARG
1	B	3623	SER
1	B	3676	ASP
1	B	3700	LEU
1	B	3725	ASN

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Mol	Chain	Res	Type
1	B	3780	ARG
1	B	3833	SER
1	B	3867	LEU
1	B	3954	ARG
1	B	3998	LEU
1	B	4005	ILE
1	B	4012	LEU
1	B	4029	SER
1	B	4046	GLN
1	B	4091	SER
1	B	4105	VAL
1	B	4157	TYR
1	B	4185	VAL
1	B	4189	ASN
1	B	4200	LEU
1	B	4206	SER
1	B	4218	THR
1	B	4219	SER
1	B	4232	MET
1	B	4258	THR
1	B	4309	SER
1	B	4318	SER
1	B	4323	ASN
1	B	4324	ILE
1	B	4327	ASP
1	B	4334	VAL
1	B	4356	LEU
1	B	4402	ILE
1	B	4413	ASN
1	B	4425	LYS
1	B	4434	GLN
1	B	4500	GLU
1	B	4503	ILE
1	B	4548	LYS
1	B	4555	VAL
1	B	4558	THR
1	B	4573	GLN
1	B	4576	SER
1	B	4596	ASN
1	B	4607	SER
1	B	4618	ASN
1	B	4644	LEU

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Mol	Chain	Res	Type
1	B	4693	ASN
1	B	4698	GLU
1	B	4709	GLN
1	B	4715	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1512	ASN
1	A	1522	GLN
1	A	1549	GLN
1	A	1563	ASN
1	A	1609	GLN
1	A	1690	GLN
1	A	1791	HIS
1	A	1798	ASN
1	A	1809	ASN
1	A	1813	GLN
1	A	1844	GLN
1	A	1853	GLN
1	A	1857	ASN
1	A	1858	ASN
1	A	1865	GLN
1	A	1877	HIS
1	A	1971	ASN
1	A	1990	GLN
1	A	2018	GLN
1	A	2029	ASN
1	A	2042	GLN
1	A	2044	GLN
1	A	2047	GLN
1	A	2053	ASN
1	A	2086	ASN
1	A	2090	ASN
1	A	2136	GLN
1	A	2138	GLN
1	A	2142	GLN
1	A	2167	GLN
1	A	2197	ASN
1	A	2200	ASN
1	A	2295	GLN
1	A	2351	HIS

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Mol	Chain	Res	Type
1	A	2366	ASN
1	A	2368	ASN
1	A	2428	GLN
1	A	2436	ASN
1	A	2447	GLN
1	A	2450	ASN
1	A	2495	GLN
1	A	2535	ASN
1	A	2552	ASN
1	A	2553	GLN
1	A	2564	ASN
1	A	2565	GLN
1	A	2598	GLN
1	A	2656	HIS
1	A	2747	ASN
1	A	2787	GLN
1	A	2793	ASN
1	A	2810	HIS
1	A	2826	GLN
1	A	2869	GLN
1	A	2907	HIS
1	A	2942	ASN
1	A	2954	ASN
1	A	2961	GLN
1	A	3007	GLN
1	A	3009	GLN
1	A	3033	ASN
1	A	3043	ASN
1	A	3077	ASN
1	A	3156	ASN
1	A	3223	HIS
1	A	3253	ASN
1	A	3266	GLN
1	A	3277	GLN
1	A	3286	ASN
1	A	3331	GLN
1	A	3338	GLN
1	A	3377	GLN
1	A	3437	ASN
1	A	3555	ASN
1	A	3566	ASN
1	A	3607	GLN

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Mol	Chain	Res	Type
1	A	3646	ASN
1	A	3687	ASN
1	A	3721	GLN
1	A	3725	ASN
1	A	3731	ASN
1	A	3785	ASN
1	A	3794	GLN
1	A	3820	GLN
1	A	3887	ASN
1	A	3922	ASN
1	A	3925	ASN
1	A	3981	ASN
1	A	4017	GLN
1	A	4046	GLN
1	A	4066	GLN
1	A	4073	GLN
1	A	4079	ASN
1	A	4112	ASN
1	A	4191	HIS
1	A	4210	HIS
1	A	4234	ASN
1	A	4263	GLN
1	A	4278	HIS
1	A	4282	GLN
1	A	4349	ASN
1	A	4362	GLN
1	A	4370	ASN
1	A	4413	ASN
1	A	4573	GLN
1	A	4574	GLN
1	A	4596	ASN
1	A	4610	GLN
1	A	4653	GLN
1	A	4693	ASN
1	A	4715	ASN
1	A	4718	GLN
1	B	1480	HIS
1	B	1522	GLN
1	B	1547	ASN
1	B	1568	HIS
1	B	1589	ASN
1	B	1609	GLN

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Mol	Chain	Res	Type
1	B	1640	ASN
1	B	1690	GLN
1	B	1793	ASN
1	B	1813	GLN
1	B	1820	GLN
1	B	1826	GLN
1	B	1857	ASN
1	B	1891	GLN
1	B	1901	ASN
1	B	1920	ASN
1	B	1931	ASN
1	B	1990	GLN
1	B	2029	ASN
1	B	2044	GLN
1	B	2086	ASN
1	B	2110	GLN
1	B	2235	GLN
1	B	2241	GLN
1	B	2264	GLN
1	B	2315	GLN
1	B	2342	ASN
1	B	2351	HIS
1	B	2368	ASN
1	B	2381	ASN
1	B	2398	GLN
1	B	2504	GLN
1	B	2542	ASN
1	B	2547	ASN
1	B	2564	ASN
1	B	2571	ASN
1	B	2793	ASN
1	B	2826	GLN
1	B	2832	ASN
1	B	2841	ASN
1	B	2861	GLN
1	B	2937	HIS
1	B	2992	ASN
1	B	3043	ASN
1	B	3196	ASN
1	B	3223	HIS
1	B	3235	HIS
1	B	3272	ASN

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Mol	Chain	Res	Type
1	B	3322	GLN
1	B	3338	GLN
1	B	3555	ASN
1	B	3566	ASN
1	B	3577	GLN
1	B	3687	ASN
1	B	3725	ASN
1	B	3731	ASN
1	B	3785	ASN
1	B	3794	GLN
1	B	3799	HIS
1	B	3925	ASN
1	B	3926	ASN
1	B	3953	ASN
1	B	3981	ASN
1	B	4016	GLN
1	B	4026	GLN
1	B	4036	HIS
1	B	4038	GLN
1	B	4040	ASN
1	B	4052	GLN
1	B	4112	ASN
1	B	4152	GLN
1	B	4189	ASN
1	B	4199	GLN
1	B	4263	GLN
1	B	4278	HIS
1	B	4323	ASN
1	B	4391	HIS
1	B	4413	ASN
1	B	4434	GLN
1	B	4573	GLN
1	B	4574	GLN
1	B	4596	ASN
1	B	4618	ASN
1	B	4651	ASN
1	B	4693	ASN
1	B	4709	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	9001	-	24,29,29	1.26	3 (12%)	29,45,45	1.57	5 (17%)
2	ADP	B	9010	-	24,29,29	1.24	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	B	9007	-	24,29,29	1.23	3 (12%)	29,45,45	1.54	5 (17%)
2	ADP	B	9008	-	24,29,29	1.23	3 (12%)	29,45,45	1.55	5 (17%)
2	ADP	A	9003	-	24,29,29	1.26	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	A	9002	-	24,29,29	1.23	2 (8%)	29,45,45	1.56	5 (17%)
2	ADP	B	9009	-	24,29,29	1.25	3 (12%)	29,45,45	1.56	5 (17%)
2	ADP	A	9004	-	24,29,29	1.23	3 (12%)	29,45,45	1.56	5 (17%)

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	9001	-	-	5/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	6/12/32/32	0/3/3/3
2	ADP	B	9007	-	-	4/12/32/32	0/3/3/3
2	ADP	B	9008	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	9003	-	-	5/12/32/32	0/3/3/3
2	ADP	A	9002	-	-	3/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	5/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	3/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9002	ADP	C5-C4	2.99	1.48	1.40
2	B	9008	ADP	C5-C4	2.95	1.48	1.40
2	B	9009	ADP	C5-C4	2.93	1.48	1.40
2	A	9003	ADP	C5-C4	2.93	1.48	1.40
2	A	9004	ADP	C5-C4	2.91	1.48	1.40
2	B	9010	ADP	C5-C4	2.91	1.48	1.40
2	B	9007	ADP	C5-C4	2.90	1.48	1.40
2	A	9001	ADP	C5-C4	2.90	1.48	1.40
2	A	9001	ADP	C2-N3	2.85	1.36	1.32
2	B	9008	ADP	C2-N3	2.79	1.36	1.32
2	A	9002	ADP	C2-N3	2.78	1.36	1.32
2	B	9010	ADP	C2-N3	2.78	1.36	1.32
2	B	9009	ADP	C2-N3	2.78	1.36	1.32
2	A	9003	ADP	C2-N3	2.77	1.36	1.32
2	B	9007	ADP	C2-N3	2.74	1.36	1.32
2	A	9004	ADP	C2-N3	2.71	1.36	1.32
2	A	9001	ADP	O4'-C1'	2.34	1.44	1.41
2	A	9003	ADP	O4'-C1'	2.25	1.44	1.41
2	B	9009	ADP	O4'-C1'	2.22	1.44	1.41
2	B	9010	ADP	O4'-C1'	2.11	1.44	1.41
2	A	9004	ADP	O4'-C1'	2.06	1.44	1.41
2	B	9007	ADP	O4'-C1'	2.03	1.43	1.41
2	B	9008	ADP	O4'-C1'	2.00	1.43	1.41

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9004	ADP	N3-C2-N1	-4.33	121.91	128.68
2	A	9003	ADP	N3-C2-N1	-4.30	121.96	128.68
2	B	9007	ADP	N3-C2-N1	-4.29	121.97	128.68
2	B	9010	ADP	N3-C2-N1	-4.27	122.00	128.68
2	A	9001	ADP	N3-C2-N1	-4.27	122.00	128.68
2	B	9009	ADP	N3-C2-N1	-4.25	122.03	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9002	ADP	N3-C2-N1	-4.20	122.11	128.68
2	B	9008	ADP	N3-C2-N1	-4.18	122.14	128.68
2	A	9003	ADP	C3'-C2'-C1'	3.70	106.55	100.98
2	A	9001	ADP	C3'-C2'-C1'	3.68	106.52	100.98
2	B	9009	ADP	C3'-C2'-C1'	3.67	106.50	100.98
2	B	9007	ADP	C3'-C2'-C1'	3.60	106.40	100.98
2	B	9008	ADP	C3'-C2'-C1'	3.57	106.36	100.98
2	A	9002	ADP	C3'-C2'-C1'	3.54	106.31	100.98
2	B	9010	ADP	C3'-C2'-C1'	3.54	106.31	100.98
2	A	9004	ADP	C3'-C2'-C1'	3.52	106.28	100.98
2	A	9002	ADP	PA-O3A-PB	-3.22	121.77	132.83
2	B	9008	ADP	PA-O3A-PB	-3.15	122.01	132.83
2	A	9001	ADP	PA-O3A-PB	-3.12	122.11	132.83
2	B	9009	ADP	PA-O3A-PB	-3.01	122.49	132.83
2	A	9003	ADP	PA-O3A-PB	-2.98	122.61	132.83
2	B	9010	ADP	PA-O3A-PB	-2.98	122.61	132.83
2	A	9004	ADP	PA-O3A-PB	-2.94	122.73	132.83
2	B	9007	ADP	PA-O3A-PB	-2.84	123.08	132.83
2	B	9007	ADP	C4-C5-N7	-2.61	106.68	109.40
2	B	9010	ADP	C4-C5-N7	-2.60	106.69	109.40
2	A	9001	ADP	C4-C5-N7	-2.58	106.71	109.40
2	A	9004	ADP	C4-C5-N7	-2.58	106.71	109.40
2	A	9002	ADP	C4-C5-N7	-2.58	106.71	109.40
2	B	9009	ADP	C4-C5-N7	-2.58	106.71	109.40
2	A	9003	ADP	C4-C5-N7	-2.57	106.72	109.40
2	B	9008	ADP	C4-C5-N7	-2.57	106.72	109.40
2	A	9004	ADP	C2-N1-C6	2.28	122.66	118.75
2	B	9007	ADP	C2-N1-C6	2.24	122.58	118.75
2	A	9001	ADP	C2-N1-C6	2.23	122.57	118.75
2	A	9003	ADP	C2-N1-C6	2.22	122.56	118.75
2	B	9010	ADP	C2-N1-C6	2.22	122.56	118.75
2	B	9009	ADP	C2-N1-C6	2.21	122.54	118.75
2	B	9008	ADP	C2-N1-C6	2.21	122.53	118.75
2	A	9002	ADP	C2-N1-C6	2.18	122.49	118.75

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	9001	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	C5'-O5'-PA-O2A
2	A	9003	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	9003	ADP	C5'-O5'-PA-O2A
2	B	9007	ADP	C5'-O5'-PA-O3A
2	B	9009	ADP	C5'-O5'-PA-O1A
2	B	9009	ADP	C5'-O5'-PA-O2A
2	B	9010	ADP	C5'-O5'-PA-O2A
2	B	9010	ADP	C5'-O5'-PA-O3A
2	A	9001	ADP	PB-O3A-PA-O2A
2	A	9002	ADP	PB-O3A-PA-O2A
2	A	9003	ADP	PB-O3A-PA-O2A
2	A	9004	ADP	PB-O3A-PA-O2A
2	B	9007	ADP	PB-O3A-PA-O2A
2	B	9008	ADP	PB-O3A-PA-O2A
2	B	9009	ADP	PB-O3A-PA-O2A
2	B	9010	ADP	PB-O3A-PA-O2A
2	B	9007	ADP	C5'-O5'-PA-O1A
2	B	9010	ADP	C5'-O5'-PA-O1A
2	A	9001	ADP	O4'-C4'-C5'-O5'
2	A	9002	ADP	O4'-C4'-C5'-O5'
2	B	9008	ADP	O4'-C4'-C5'-O5'
2	A	9003	ADP	O4'-C4'-C5'-O5'
2	A	9004	ADP	O4'-C4'-C5'-O5'
2	B	9007	ADP	O4'-C4'-C5'-O5'
2	B	9009	ADP	O4'-C4'-C5'-O5'
2	B	9010	ADP	O4'-C4'-C5'-O5'
2	A	9001	ADP	C5'-O5'-PA-O3A
2	A	9003	ADP	C5'-O5'-PA-O3A
2	B	9009	ADP	C5'-O5'-PA-O3A
2	A	9004	ADP	PB-O3A-PA-O1A
2	B	9010	ADP	PB-O3A-PA-O1A
2	A	9002	ADP	C5'-O5'-PA-O1A

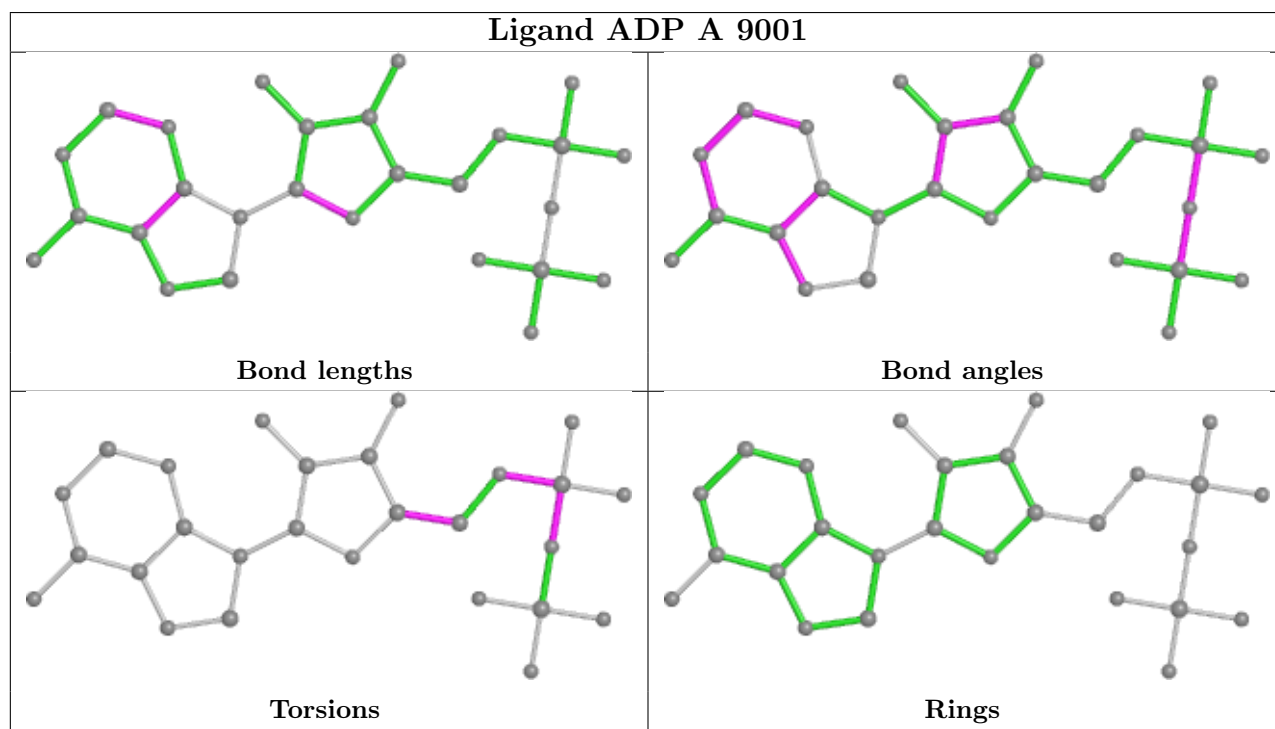
There are no ring outliers.

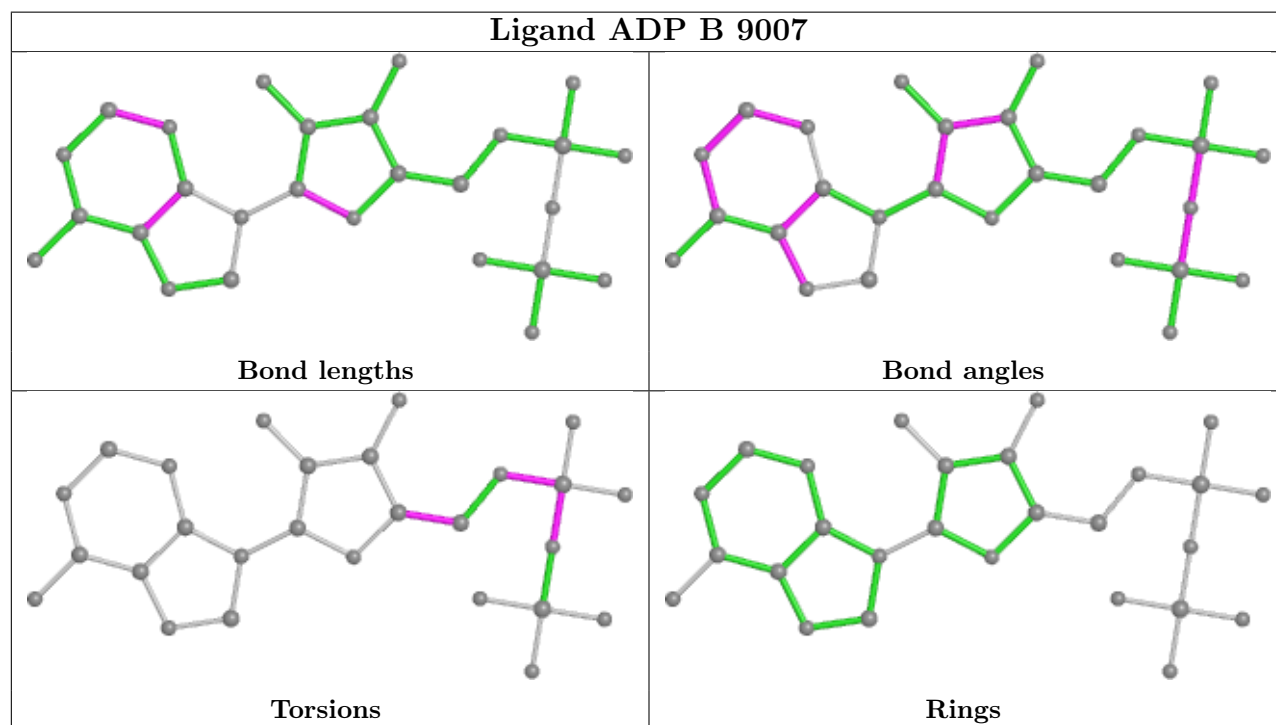
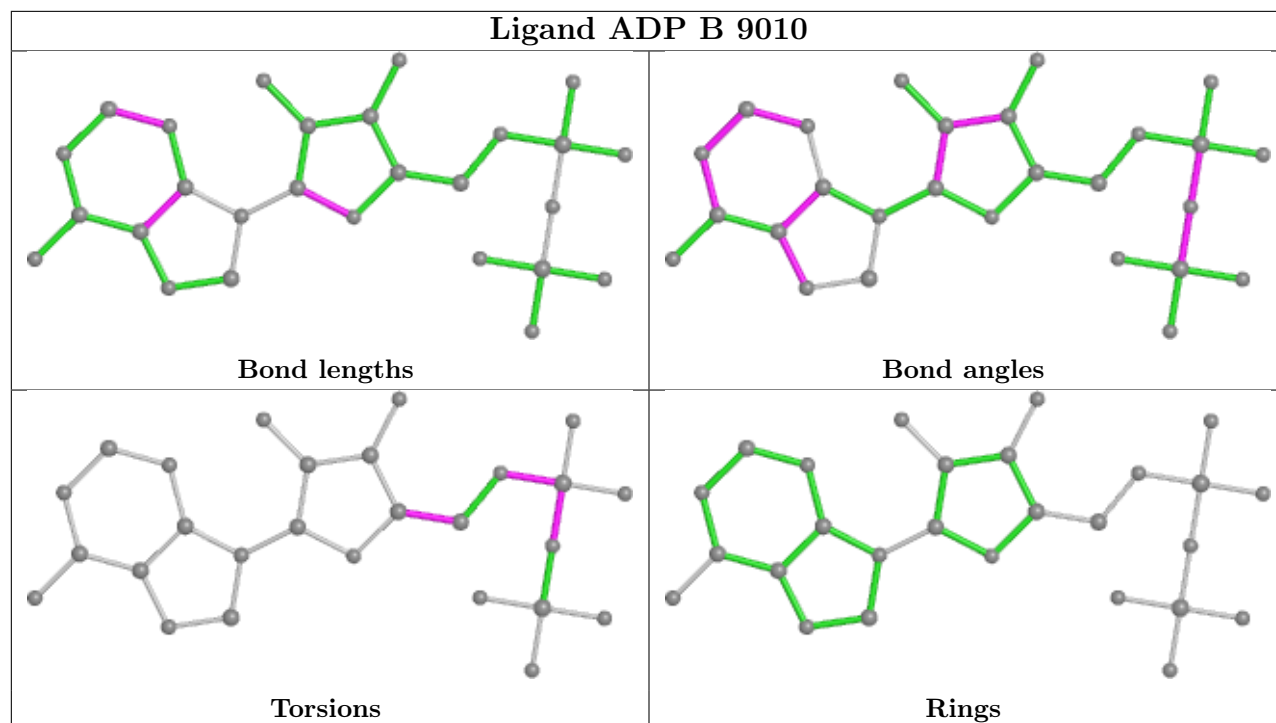
5 monomers are involved in 10 short contacts:

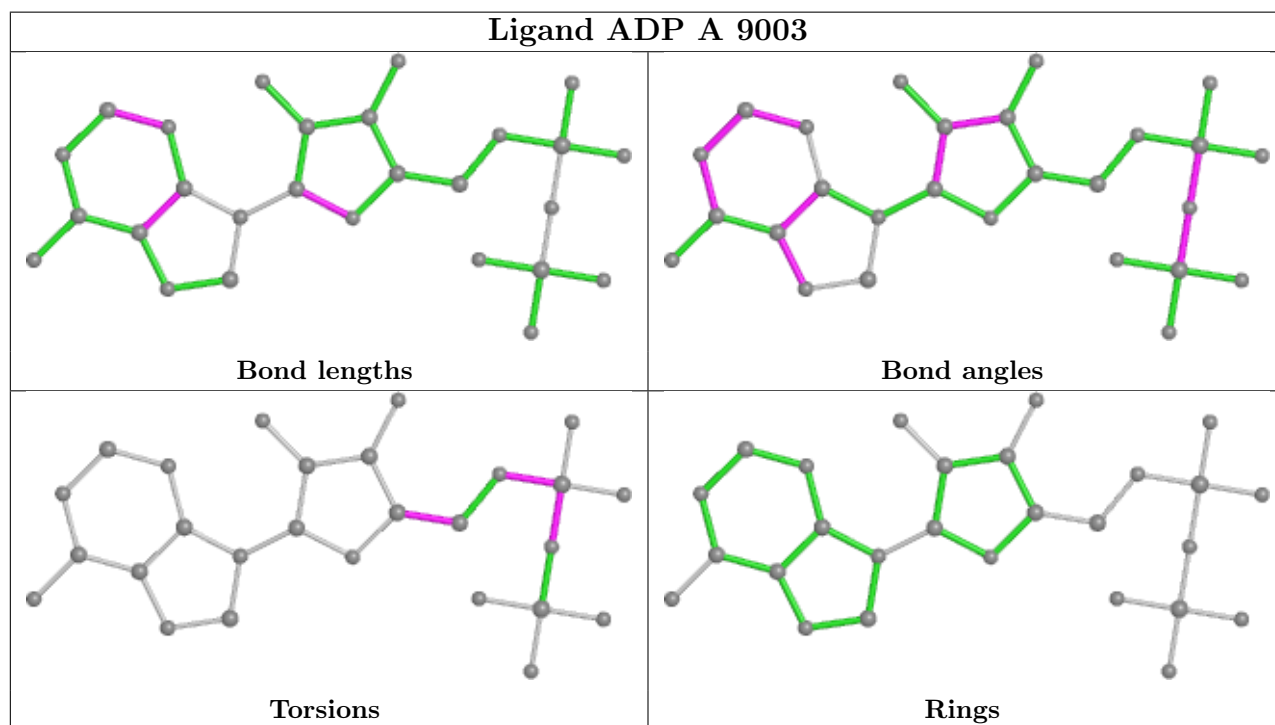
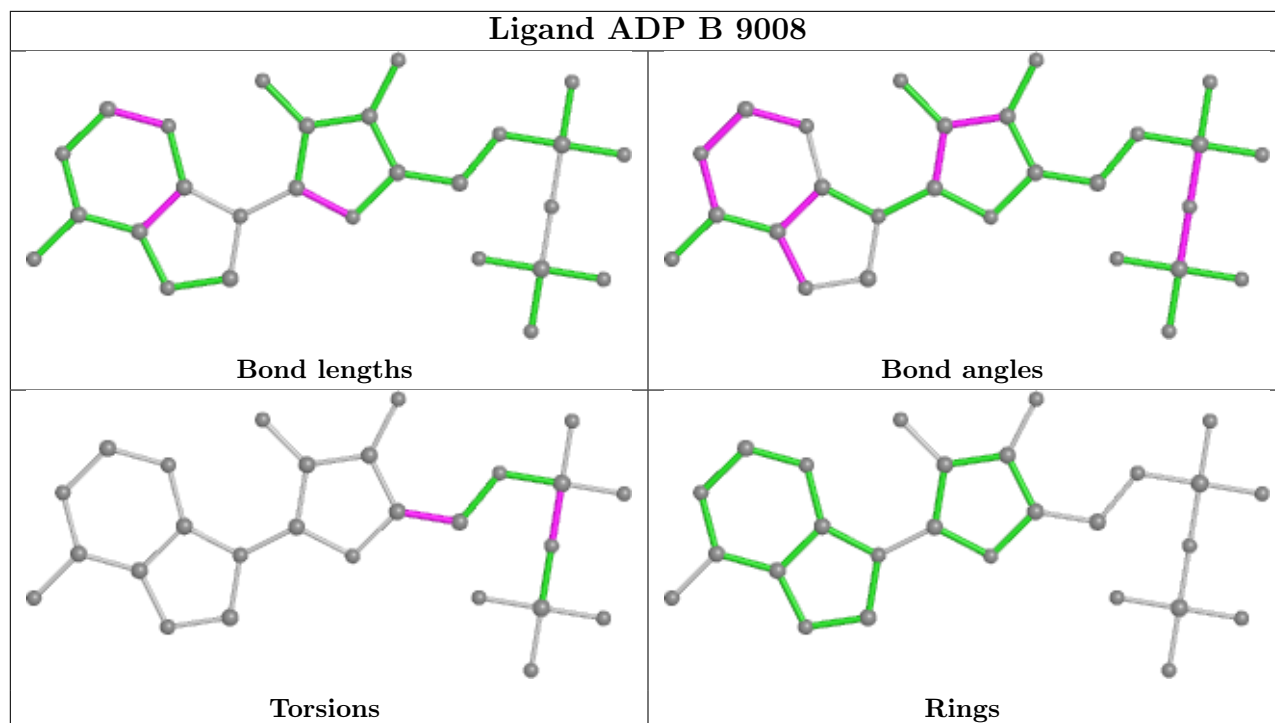
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9001	ADP	1	0
2	B	9010	ADP	2	0
2	A	9002	ADP	4	0
2	B	9009	ADP	1	0
2	A	9004	ADP	2	0

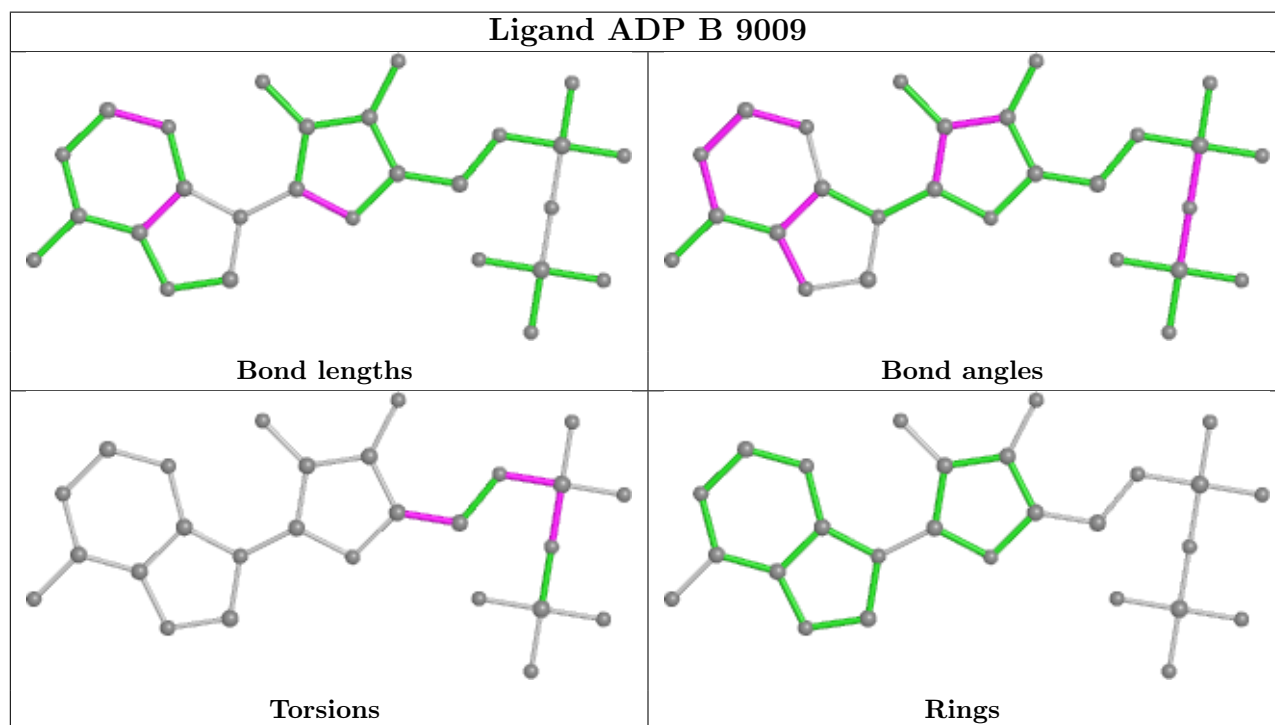
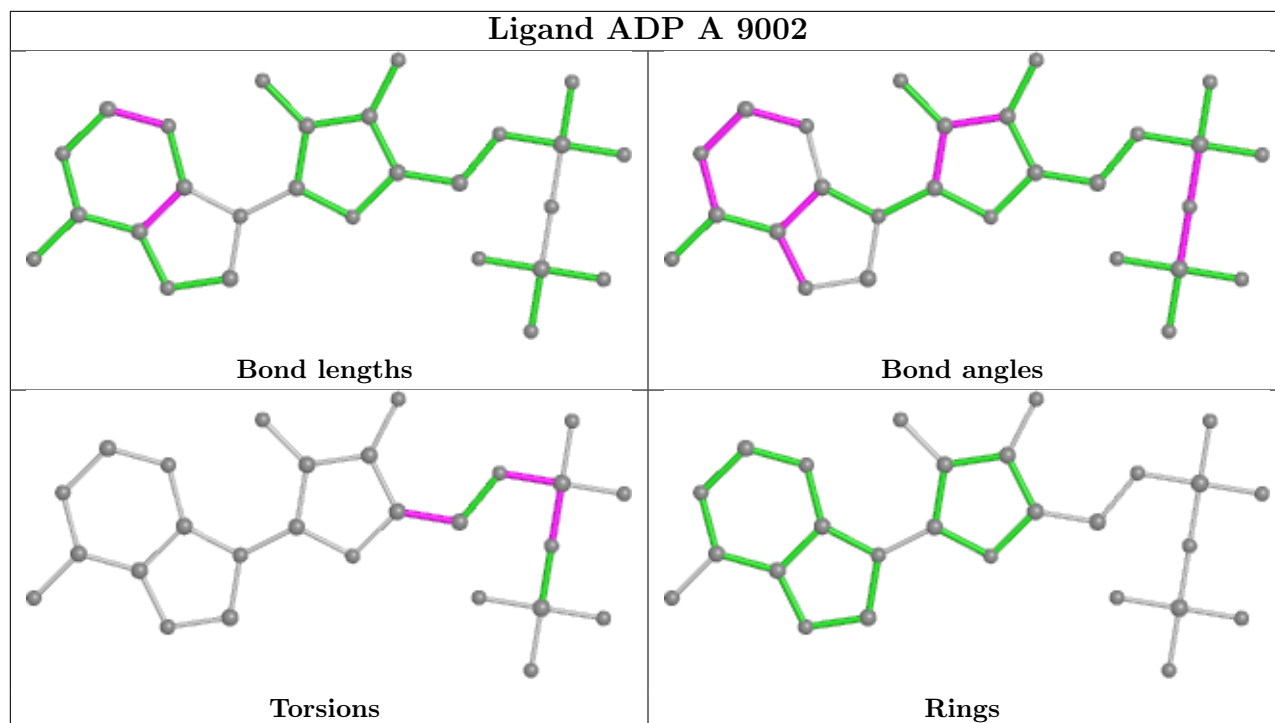
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

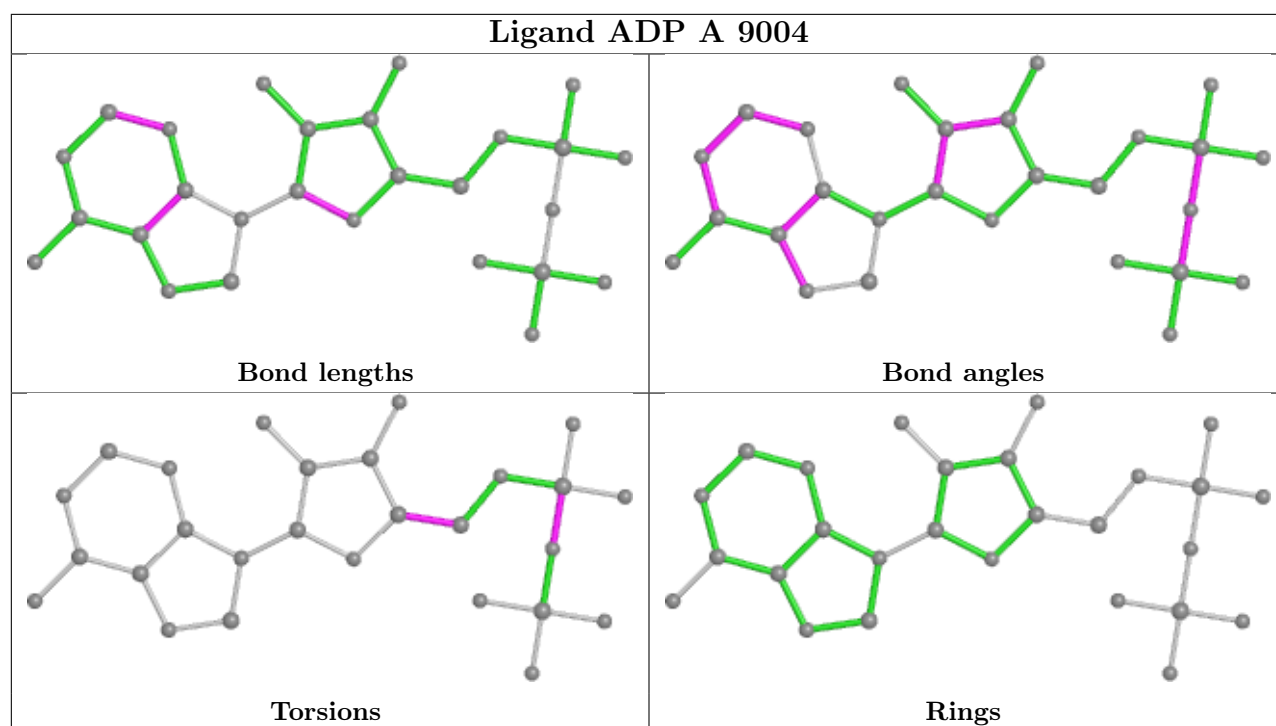
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	3042/3367 (90%)	-0.14	61 (2%) 65 58	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.18	29 (0%) 82 76	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.16	90 (1%) 73 66	64, 133, 209, 335	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	5.7
1	B	1517	VAL	4.8
1	A	1652	GLY	4.7
1	A	4187	LEU	4.5
1	A	1651	SER	4.1
1	A	3516	ASP	4.0
1	A	1555	VAL	4.0
1	A	3718	LEU	3.8
1	A	4122	VAL	3.8
1	A	4550	TRP	3.7
1	A	1545	LEU	3.6
1	B	1484	LEU	3.6
1	A	1650	VAL	3.6
1	A	4165	PRO	3.4
1	A	4509	LEU	3.4
1	A	3512	LYS	3.4
1	A	4217	MET	3.4
1	A	4162	ILE	3.3
1	A	3842	SER	3.3
1	A	3515	GLN	3.2
1	A	3518	ILE	3.2
1	A	1657	LEU	3.1
1	B	3356	ALA	3.0
1	A	3328	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	3334	ALA	3.0
1	B	2304	HIS	3.0
1	B	2720	TYR	2.9
1	B	2335	THR	2.9
1	A	4215	LEU	2.9
1	B	4517	LEU	2.9
1	A	4185	VAL	2.9
1	A	4168	PHE	2.9
1	A	3513	LEU	2.8
1	A	1575	MET	2.8
1	A	3846	LEU	2.8
1	A	1554	LEU	2.8
1	A	1656	ILE	2.7
1	A	1538	TRP	2.7
1	B	4541	ILE	2.7
1	A	1584	PHE	2.7
1	A	3866	ALA	2.6
1	B	1495	THR	2.6
1	A	3536	TYR	2.6
1	A	3360	VAL	2.6
1	A	1639	ILE	2.5
1	B	1575	MET	2.5
1	A	4118	MET	2.5
1	A	3359	LYS	2.5
1	B	2620	ASP	2.4
1	B	1543	LEU	2.4
1	B	2574	LEU	2.4
1	A	1527	LEU	2.4
1	A	3330	ASP	2.4
1	A	4131	PRO	2.3
1	A	1565	LEU	2.3
1	A	3762	ILE	2.3
1	A	3764	LEU	2.3
1	B	1656	ILE	2.3
1	A	4186	LEU	2.3
1	A	2060	LEU	2.3
1	B	1511	GLU	2.3
1	A	4192	LEU	2.3
1	A	1549	GLN	2.3
1	B	1514	TYR	2.3
1	A	1551	LYS	2.3
1	A	2353	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	4635	ALA	2.2
1	A	1544	ASP	2.2
1	A	3341	ALA	2.2
1	A	4142	ALA	2.2
1	B	3112	CYS	2.2
1	B	4550	TRP	2.2
1	A	2452	ASN	2.2
1	B	4215	LEU	2.2
1	B	1497	LEU	2.2
1	A	3319	GLN	2.2
1	A	3346	VAL	2.2
1	A	3533	LYS	2.2
1	B	1515	ARG	2.1
1	B	3341	ALA	2.1
1	A	3388	LEU	2.1
1	B	3544	GLU	2.1
1	B	3324	LEU	2.1
1	B	3842	SER	2.1
1	B	1510	ASN	2.1
1	A	3763	PHE	2.0
1	B	4537	LEU	2.0
1	B	3309	LYS	2.0
1	A	4183	THR	2.0
1	B	2597	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

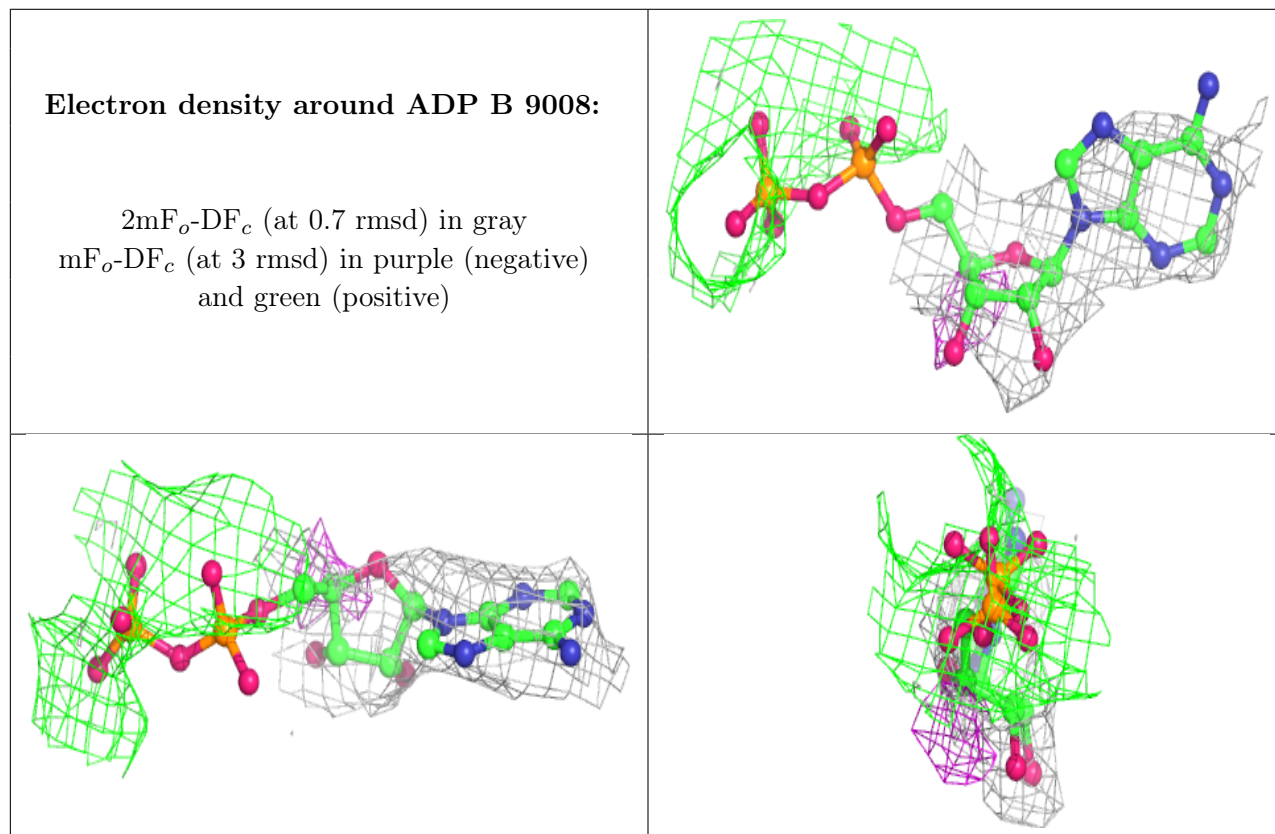
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

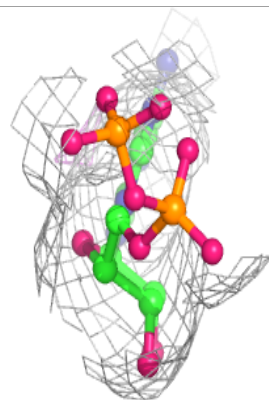
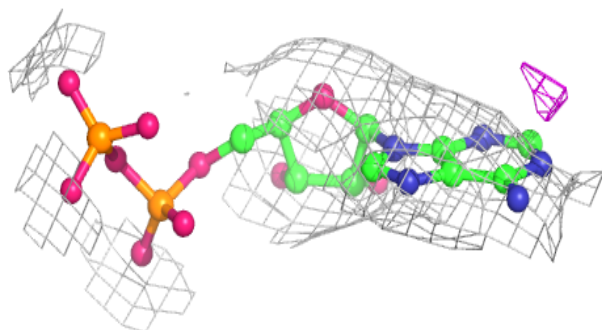
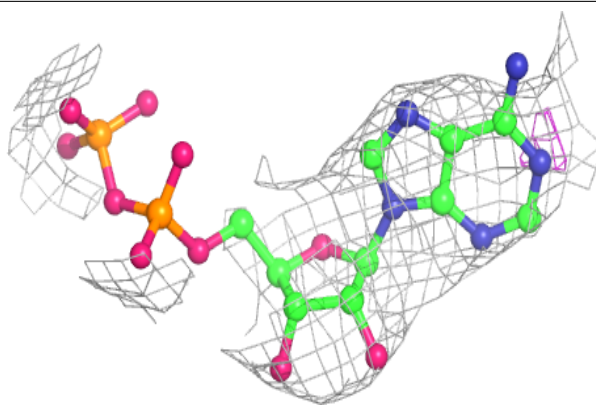
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	B	9008	27/27	0.85	0.40	129,129,129,129	0
2	ADP	B	9010	27/27	0.86	0.31	129,129,129,129	0
2	ADP	A	9002	27/27	0.90	0.30	129,129,129,129	0
2	ADP	B	9007	27/27	0.90	0.37	129,129,129,129	0
2	ADP	A	9004	27/27	0.91	0.30	129,129,129,129	0
2	ADP	A	9003	27/27	0.91	0.33	129,129,129,129	0
2	ADP	A	9001	27/27	0.94	0.38	129,129,129,129	0
2	ADP	B	9009	27/27	0.95	0.31	129,129,129,129	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

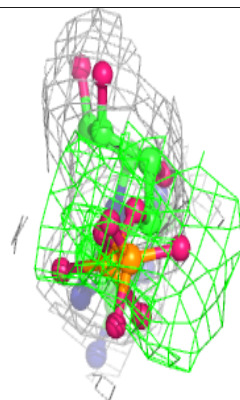
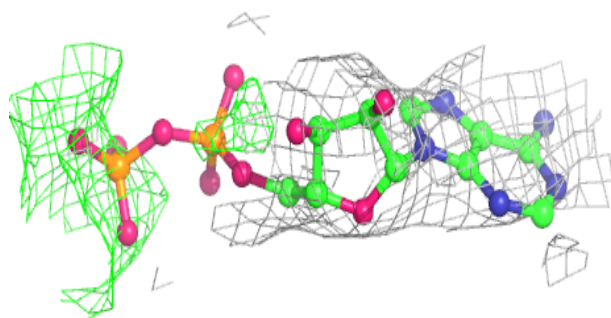
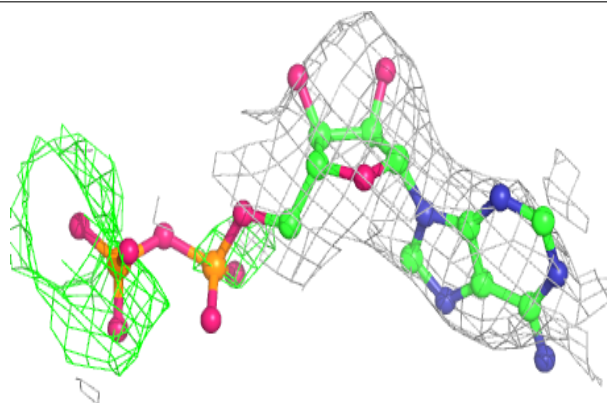


Electron density around ADP B 9010:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

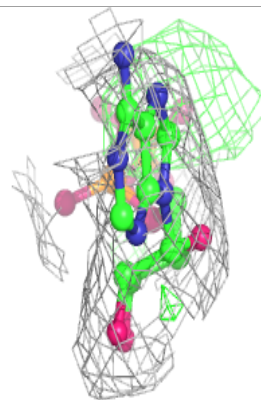
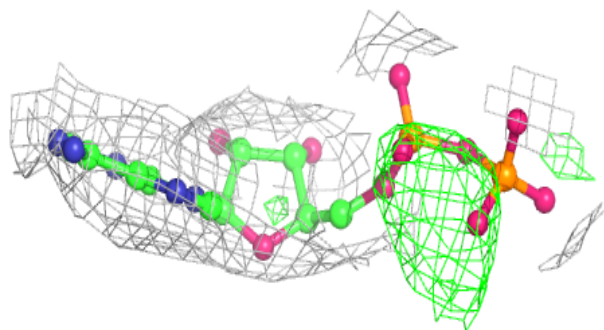
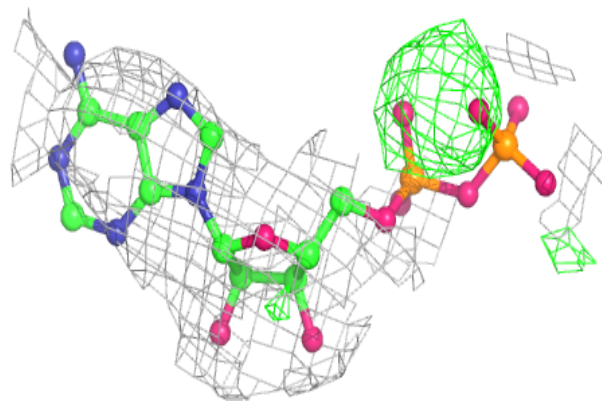
**Electron density around ADP A 9002:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

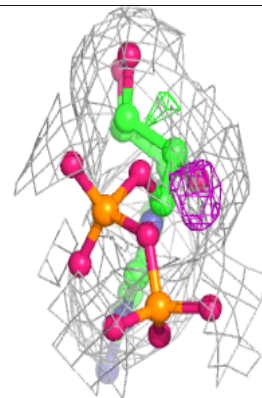
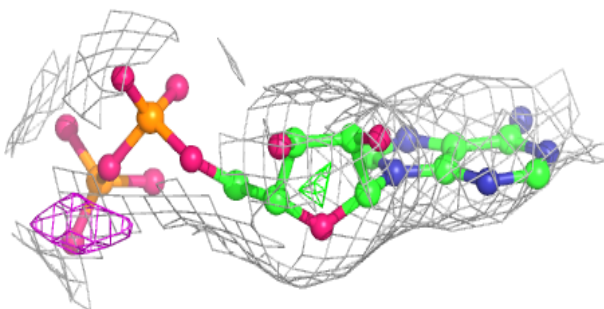
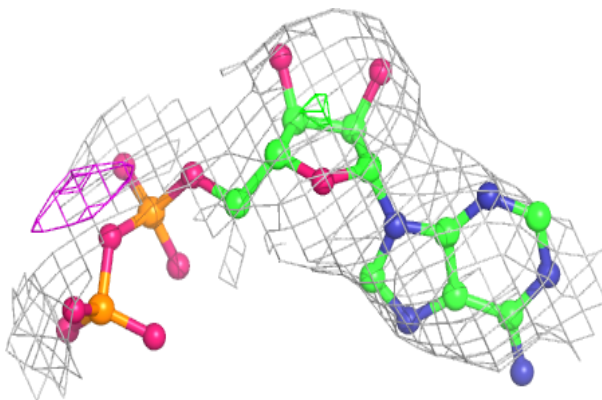


Electron density around ADP B 9007:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

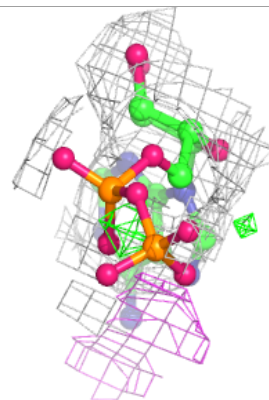
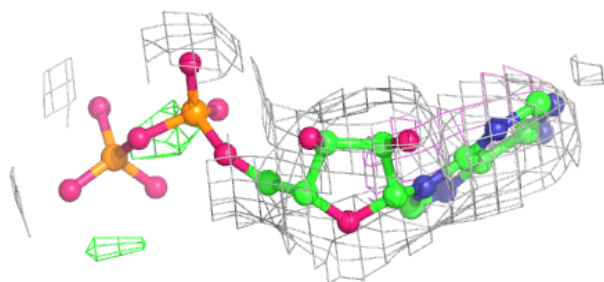
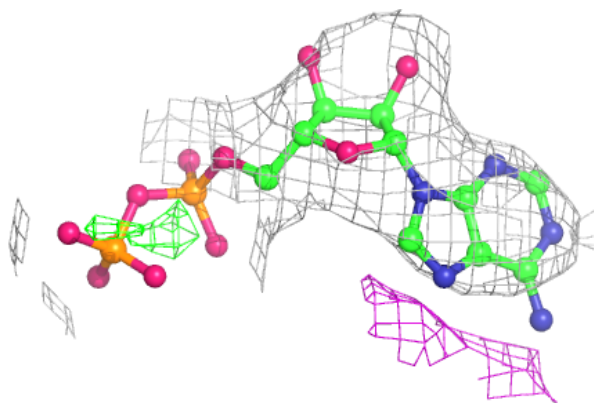
**Electron density around ADP A 9004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

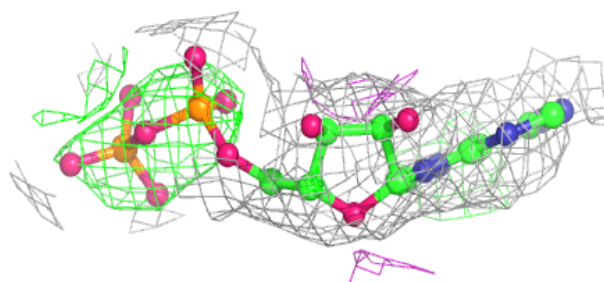
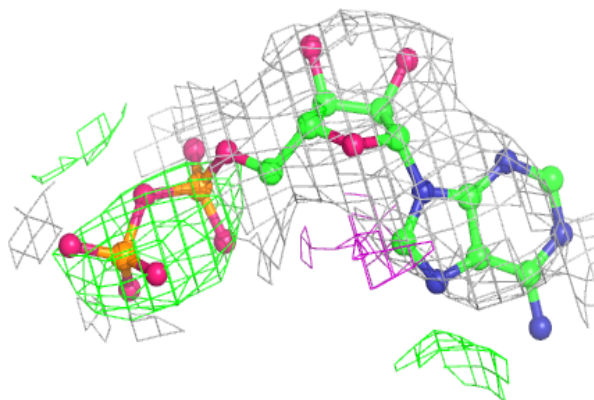


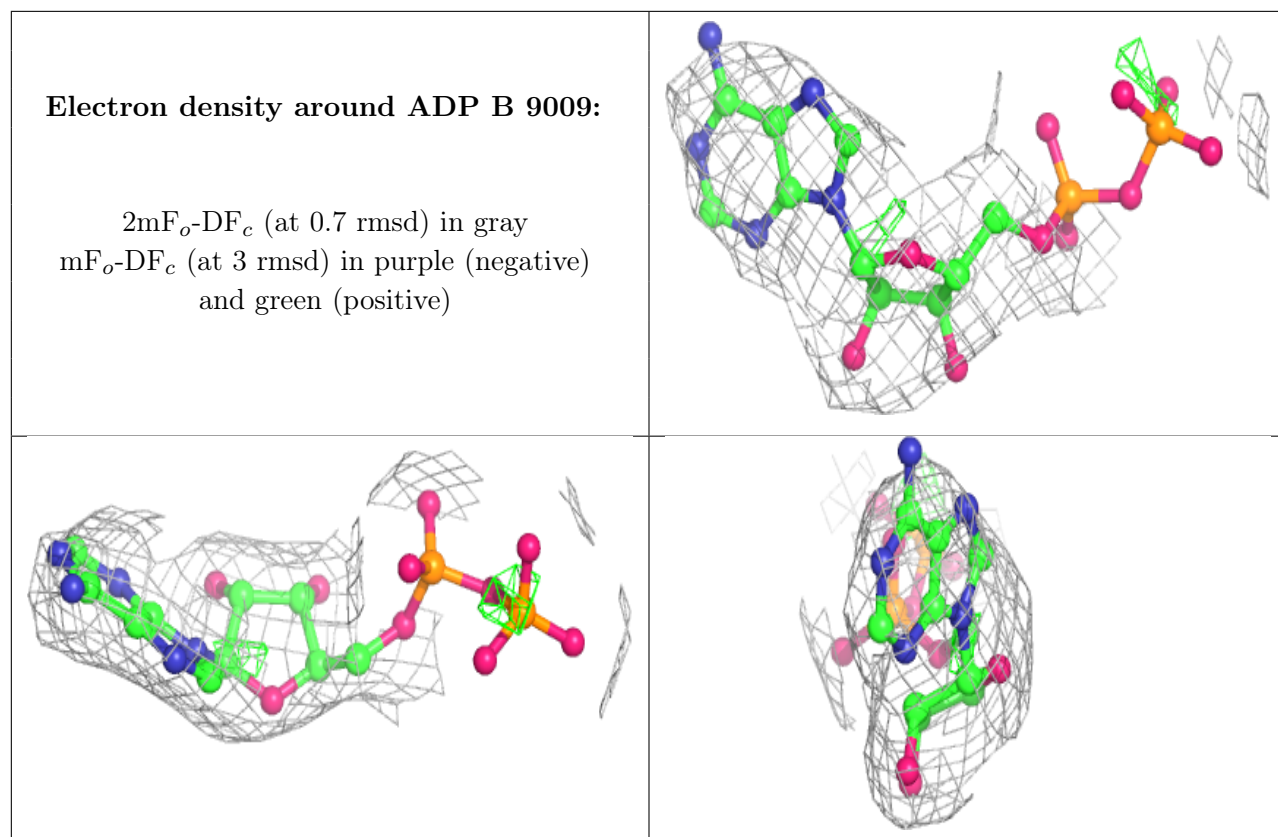
Electron density around ADP A 9003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP A 9001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.