



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:01 am GMT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

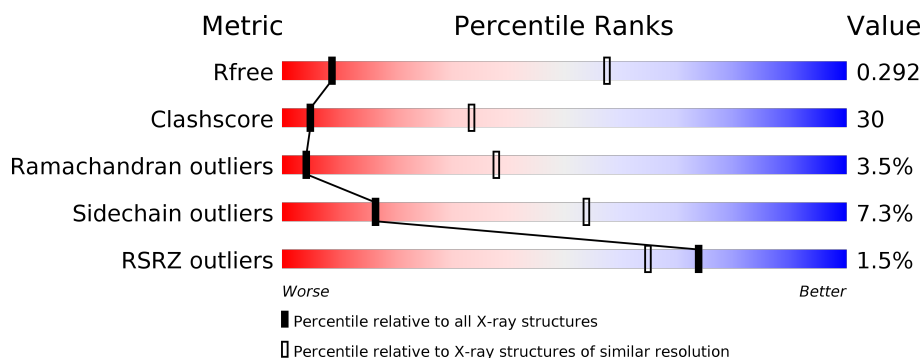
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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

Mol	Chain	Length	Quality of chain
1	A	3367	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>42%</div> <div>6%</div> <div>10%</div> </div> </div>
1	B	3367	<div> <div>%</div> <div> <div></div> <div>46%</div> <div>37%</div> <div>•</div> <div>14%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	9001	-	-	-	X
2	ADP	B	9007	-	-	-	X

## 2 Entry composition

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
1	A	3042	Total	C	N	O	S	0	0	0
			23374	14951	3955	4368	100			
1	B	2908	Total	C	N	O	S	0	0	0
			22384	14307	3792	4190	95			

There are 48 discrepancies between the modelled and reference sequences:

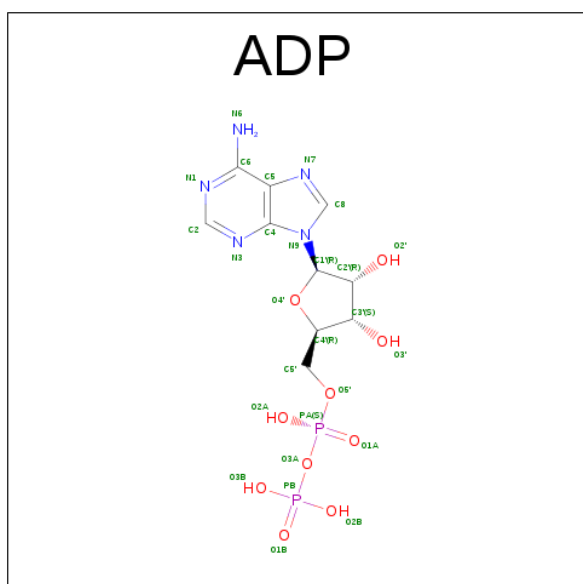
Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	EXPRESSION TAG	UNP P34036
A	1365	THR	-	EXPRESSION TAG	UNP P34036
A	1366	ARG	-	EXPRESSION TAG	UNP P34036
A	1367	HIS	-	EXPRESSION TAG	UNP P34036
A	1368	HIS	-	EXPRESSION TAG	UNP P34036
A	1369	HIS	-	EXPRESSION TAG	UNP P34036
A	1370	HIS	-	EXPRESSION 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:  $C_{10}H_{15}N_5O_{10}P_2$ ).



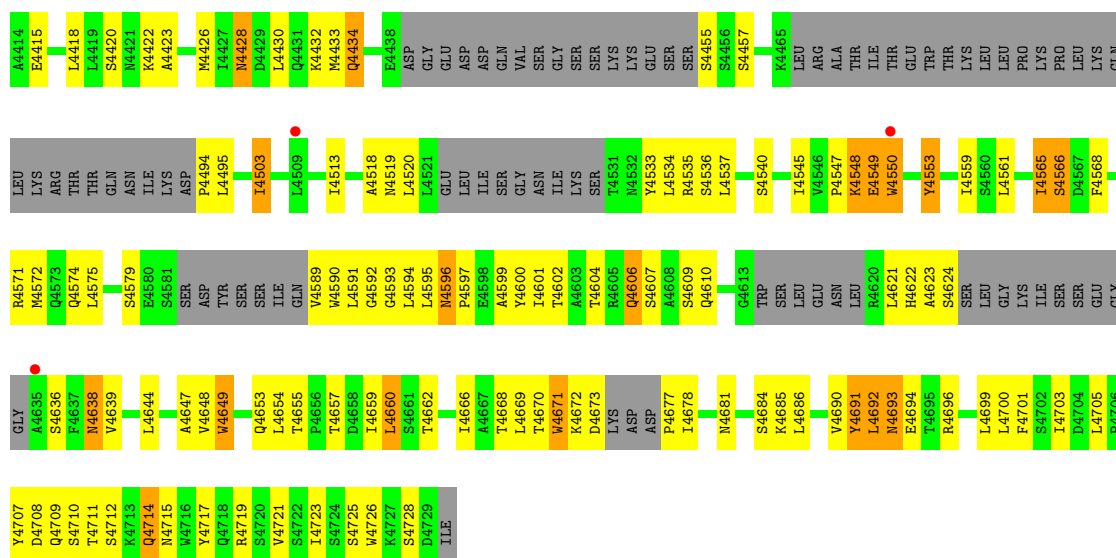
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B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



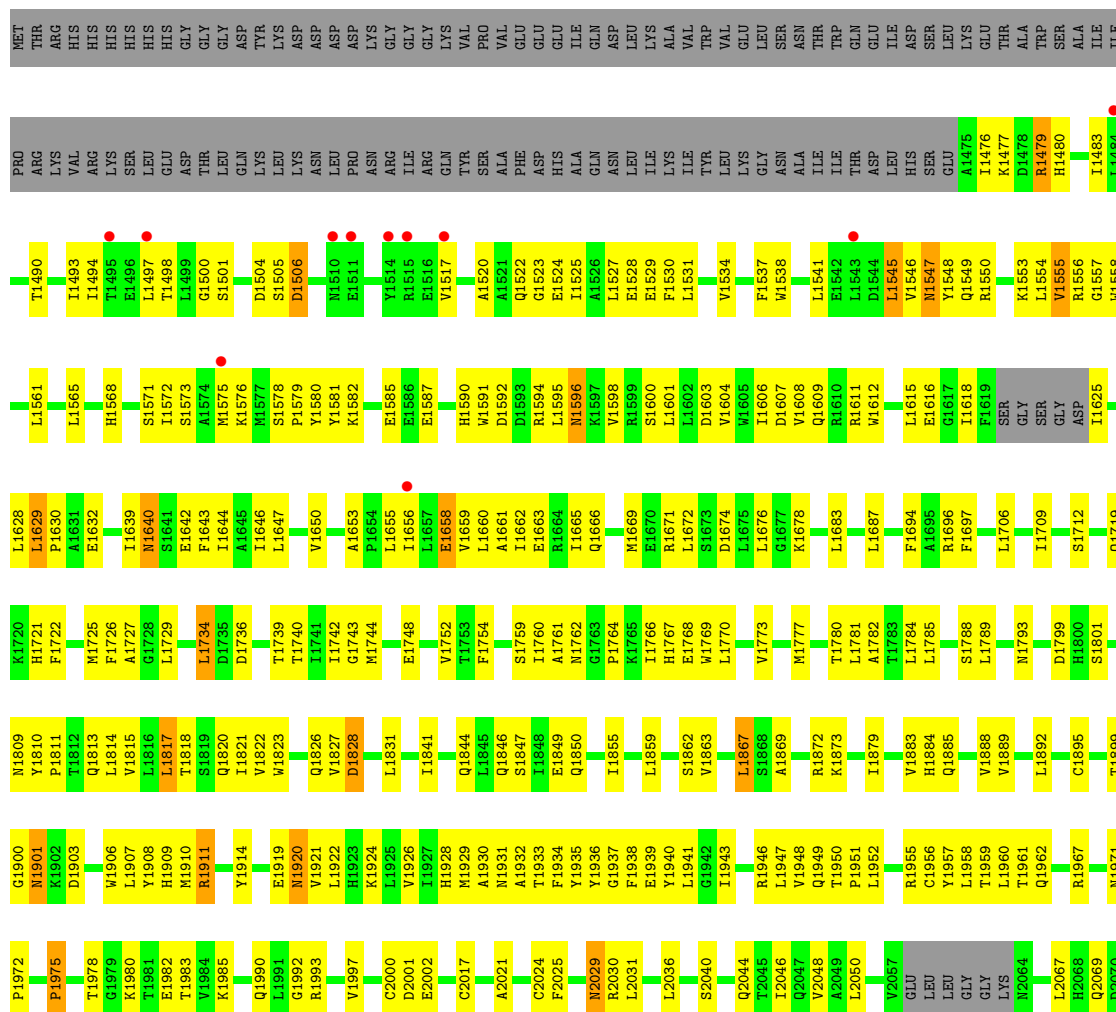
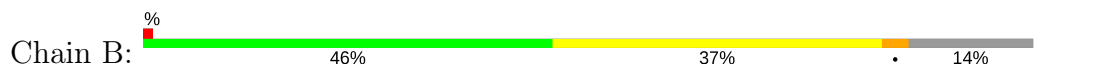
H3259	E3187	L3108	R3027	R2948	H2871	V2789	L2710	V2627	N2547	H2394	T3223	V2250	P2169
V3260	R3109	R3109	F3028	P2949	Y2872	G2790	L2711	K2628	V2548	F2395	T3224	T2251	GLN
D3262	L3261	L3261	L2950	L2950	L2873	A2791	T2712	N2629	L2549	E2396	W2327	K2252	LEU
L3264	L3192	C3112	N3032	Y2952	P2876	C2792	T2713	K2630	E2550	T2397	W2328	W2255	PRO
V3265	L3195	E3114	G3034	S2953	R2877	N2793	Y2720	VAL	N2551	Q2399	D2329	E2257	PRO
Q3266	V3196	L3115	L3035	N2954	R2877	P2794		PRO	N2552	L2400	F2332	K2258	ILE
V3267	F3197	A3116	S3036	Y2955	S2880	A2798	E2727	SER	K2560	K2401	F2332	L2259	THR
V3268	R3198	R3117	L3037	L2956	R2881	G2799	T2728	V2634	S2561	T2402		Q2261	
L3269	W3199	R3118	Y3038	L2956	R2882	R2800	T2729	V2641	S2562	ARG	T2335	Q2261	A2177
L3270	L3200	L3121	T3039	P2962	D2883	R2806	L2730	A2642	E2563	SER		Q2261	E2178
L3271	A3201	L3122	L3040	S2966	L2886	R2807	R2731	S2643	N2564	THR	R2338	L2266	S2179
	P3202	L3123	V3042	D2867	L2887	L2808	P2732	P2644	Q2565	THR	I2339	Q2264	
K3274	F3205	F3133	R3043	L2867	L2887	R2809		R2645		SER	I2340	Q2264	Y2190
K3275	L3206		S3048	L2968	T2890	L2813	W2739	V2646	T2570	THR	D2341	L2266	
L3278	A3209	Q3136	D3052	L2969	Q2891	L2814	L2739	V2647	N2571	THR	N2342	L2266	
E3281	E3210	V3137		E2970	T2892	L2815	V2741	T2649	L2573	MET	V2343	N2269	
Q3282	L3211	R3138	L3055	Y2971	D2894	L2816	F2742	T2650	L2574		E2346	H2270	
L3283	MET	R3139	L3058	R2975	D2894	D2817	G2743	V2651	L2575			G2271	
H3284	GLY	N3140	L3059	L2976	C2896	D2818	D2744	D2652	M2578	Q2424	K2349	V2272	
L3285	ASN	H3142	L3059	F2979	T2897	P2819	E2745	T2653	W2579	N2425	R2350	M2273	
		V3143	X3060	Y2980	L2898		L2746	T2654	Q2580	N2426	H2351	M2274	
L3289	L3216	V3144	R3061	V2985	L2824	L2824	N2747	R2655	L2581	L2431	W2352	V2275	
K3290	K3217	F3145	A3062	V2986	T2825	T2825	L2748	R2656	L2581	Q2432	G2357	S2278	
K3291	A3218	T3146	G3063	V2987	L2904	L2827	D2750	D2658	Q2583	L2433	D2358	K2282	
L3292	L3219	N3147	P2987	Y2988	L2905	T2828	D2751	V2659	S2584	L2434	T2359	T2283	
K3293	P3220	N3148	E3066	V2989	A2906	Q2829	D2752	L2670	M2585	S2435	D2360	T2284	
	P3221	P3149	E3067	V2989	L2930	T2830	D2753	A2662	Q2586	E2437	P2361	S2285	
E3296		A3150	K3068	L2990	L2910	F2831	Q2754		L2501	T2438	E2362	W2286	
V3299	R3224	S3151	K3068	L2991	R2911	N2832	Q2755	R2668	Y2505	F2439	W2363	E2287	
K3300	D3225	P3152	E2993	N2992	L2912	R2833	T2756	P2669	E2506	Q2442	E2365	Y2289	
	A3226	D3153	E2994	V2994	F2913	A2834	V2759	L2670	E2507	E2443	N2366	L2290	
K3309	S3229	H3155	D3074	L2995	Q2914	L2835	T2760	P2675	K2595		L2367	E2291	
L3313	S3230	N3156	E3075	L2998	L2917	L2838	T2761	S2678	Q2598	Q2446	N2368	A2292	
D3314	R3167	R3167	S3076	T2998	V2918	L2839	F2762		V2512	Q2447	S2369	L2293	
V3315	S3077	V3078	L3079	Q3007	E2922	L2842	Q2765	T2685	A2801	N2450	L2370	E2294	
Q3319	R3165	F3165	E3080	Q3007	K2923	F2845	M2766	R2689	T2603	E2451	L2371	Q2295	
K3323	L3164	R3166	S3081	Q3010	T2926	A2846	K2769	F2691	P2604	N2452		D2297	
L3324	R3167	S3082	S3081	H3011	T2930	S2847	F2772	P2694	V2605	ALA	K2375	N2298	
V3328	F3168	F3083	F3083	H3012	L2930	N2848	W2773	E2695	T2610	GLN	L2376	L2299	
Q3329	A3241	L3084	L3014	L3013	L2849	L2849	R2774	E2696	L2531	GLN	T2377	K2300	
Q3330	N3242	E3085	L3014	L3015	T2850	T2850	T2775	V2697	P2611	GLN	T2379	S2301	
Q3331	L3243	R3086	L3016	L3016	D2851	D2851	S2776	S2698	L2612	GLN	P2380	E2302	
	L3245	H3087	V3017	V3017	L2935	L2935		S2698	L2613	GLN	N2381	A2303	
A3334	Q3249	E3174	S3018	S3018	K2836	E2855	T2779	L2699	D2614	GLN	Q2382	H2304	
E3335	E3175	E3175	G3019	G3019	H2937	F2856	W2780	W2700	T2615	THR	E2383	V2305	
L3336	R3179	G3094	Q3020	Q3020	F2938	Y2857	L2781	F2701	Y2617	THR	R2384	P2308	
K3337	A3180	N2942	K3022	K3022	V2941	R2863	L2783	A2704	S2618	ILE	L2385	K2239	
Q3338	V3255	F3095	S3023	S3023	L2943	F2864	T2705	T2705	L2619	THR	A2386	P2309	
K3339	T3256	V3184	V3024	V3024	L2943	T2868	K2785	T2706	W2541	PRO	L2387	K2313	
D3340	P3257	D3185	L3025	L3025	D2944	Q2869	Q2786	T2708	N2542	ILE		D2314	
R3258	R3258	S3186	S3026	S3026	A2945	Q2870	F2788	L2709	L2626	THR	V2391	Q2316	







• Molecule 1: Dynein heavy chain, cytoplasmic



L3170	S3082	L2999	F2913	V2759	H2687	G2520	GLN	P2380	K2300	G2225	R2150	K2071
D3171	F3063	R3000	Q2914	R2764	R2688	Q2521	GLN	M2381	S2301	SER	A2151	F2074
F3172	L3084	I3001	D2915	R2765	P2669	R2522	GLN	G2382	H2304	GLN	L2152	V2075
F3173	E3085	D3002	R2916	L2670	L2671	I2525	GLN	E2383	V2305	L2228	K2153	T2076
G3174	R3086	K3003	L2917	M2766	L2672	I2526	THR	R2384	P2308	P2230	S2154	
E3175	M3087	V3004	V2918	L2673	L2674	I2527	THR	L2387	K2309	I2231	V2155	
	N3088				T2603	D2527	THR				L2156	G2080
L3181	T3089	G3010	E2921	R2773	P2604	F2528	THR				Y2081	
F3182	L3090	H3011	R2774	R2775	P2605	F2529	ILE	V2391	A2310	Q2235	K2163	A2082
Q3183	A3012	W2925	S2776	G2677	V2605	R2530	THR	R2392	K2311	L2236	R2164	G2083
V3184	A3092	L2926		L2684	I2610	R2531	SER	V2393	T2312	R2237	K2165	R2084
G3185	G3093	D2927	M2853	T2687	P2611	R2532	PRO	R2394	K2313	K2238	C2166	S2085
S3186	G3094	K2928	V2854	T2688	L2613	R2533	ILE	M2394	D2314	K2239	GLN	N2086
E3187	K2929	G3016	V2855	L2689	D2614	L2540	LEU	F2395	Q2315	I2240	PRO	
	V2856	K2782	F2866	F2694	V2615	M2541	THR	E2396		Q2241	GLN	L2091
L3192	VAL	D2931	L2783	F2695	S2616	N2542	PRO	V2397	L2320	E2242	LEU	F2095
E3195	GLY	E2932	Q2861	E2696	V2617	V2546	THR	D2398	T2323	A2244	PRO	R2096
L3196	LEU	S2933	K2862	V2697	D2620	V2547	THR	L2400		V2250	PRO	S2097
N3196	PHE	A2934	Q2787	L2699	D2621	N2548	THR	K2401	W2327	T2251	ILE	M2098
Y3199	GLU	L2935	F2788	M2700	E2622	T2549	SER	T2407	L2331	K2252	THR	A2099
	GLY	S2936	V2789	F2701	A2623	E2550	SER	T2408		Q2253	ASP	M2100
E3103	GLY	H2937	D2867	N2793	N2623		ARG	S2409	T2335	E2254	ALA	I2101
E3104	F3028	P2938	L2868	A2704	W2624	Q2553	SER	R2410			GLU	K2102
F3105	V3029	P2794	Q2869	T2705			THR		R2338	K2258	SER	P2103
	A3030	D2797		T2706	W2627	S2556	THR	M2413	I2339	L2259	LYS	D2104
	L3035	A2798	Y2872	L2711	K2630	D2557	THR	W2414		L2260	THR	R2105
ASN	S3036	R2807	L2873	R2714	V2631	P2558	THR	W2415	N2342	Q2261	ALA	E2106
GLY	I3037	R2801	S2875	F2714	PRO	P2559	THR	F2416		L2262	ALA	A2109
I3219	T3038	Q2802	P2876	L2803	SER	M2560	MET	S2417	E2346	H2263	Q2185	
P3220	L3040	L2803	R2877		VAL	N2564	ILE			Q2264		M2112
P3221	K3041				E2635		PRO	L2420	R2350	L2265	Q2189	L2113
LEU	N3042	R2806	S2880	T2723	P2636	T2569	THR	L2421	H2351		Y2190	S2115
ASP	Y3043	L2807	R2881	P2724	E2637		THR	T2422	W2352	H2270	G2271	Q2116
	Y3046	R2808	D2882	F2724	T2638		THR	T2423	I2353	G2271	G2117	
S3229	S3057	H2810	L2886	E2727	V2641	R2572	THR	Q2424	I2354	V2272	V2194	
S3230	D3050		L2887	T2728	A2642	L2573		M2425		M2273	L2195	
L3231	K3057	L2814	L2887	V2729	S2643	L2574		I2426	D2358	P2274	L2196	
Y3233	L3058	L2815	L2887	R2730	P2644	Y2575		F2427	V2359	G2275	S2198	
I3234	F3059	V2816	Q2891	R2731	D2645	S2576		L2431	P2361	G2276	T2199	
H3235	R3060	D2817	L2886	P2732	V2646	M2578		D2432	G2362	G2277	G2125	
Q3236	R3061	F2818	C2886	W2738	W2647	V2579		D2440	E2363	S2278	A2125	
T3237		L2739	T2887	L2739	L2648	G2580		P2441	V2364	G2279	K2127	
I3238		P2819	T2887	V2740		L2581		Q2442	E2365	G2281	L2128	
		S2820	L2887	T2821	T2653	G2582		E2443	K2366	K2282	V2129	
R3248		T2821		E2745	T2654	G2583		LYS	L2367	T2283	K2206	
Y3254		S2822			R2655	S2584		GLY	N2368		L2207	
V3255		L2823		L2748	W2656	M2585		GLN	S2369	W2286	V2208	
T3256		L2824		P2749	V2657	G2586		GLN	L2370		A2209	
P3257		T2825		S2750	D2658	L2587		LYS	Y2289	Y2289	D2210	
R3258		W2905		L2751	V2659	L2588		ARG	L2372	L2290	D2211	
H3259		A2906		G2751	L2660	E2589		ASN	D2373	E2291	T2121	
Y3260		H2907		Y2754	H2661	R2590		GLY	N2374	A2292	P2213	
		Q2908		G2755	A2662	E2591		ASN	K2375		S2143	
F3263		A2909		T2756	W2663	N2592		ASN	L2376	V2296	H2144	
N3166		E2907		Q2757	L2664	F2593		ALA	D2297	D2297	Y2145	
V3267		L2910		R2758	S2665	K2595		LEU	T2378	T2299	F2223	
		L2835			E2666				L2379		P2224	





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.52 (at 3.77Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.219 , 0.292 0.220 , 0.292	Depositor DCC
$R_{free}$ test set	4442 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	125.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 112.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	45974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	138.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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:HD12	1:B:4402:ILE:H	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:H	1:A:3731:ASN:HD22	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:HD12	1:B:2426:ILE:H	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:2572:ARG:HG2	1:B:2617:VAL:HG11	1.69	0.73
1:B:2309:LYS:NZ	1:B:2756:THR:HG21	2.04	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:HD22	1:B:4189:ASN:N	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:2626:LEU:HD12	1:A:2626:LEU:H	1.55	0.71
1:A:2587:LEU:HG	1:A:2817:ASP:HB2	1.72	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:H	1:A:4553:TYR:HD1	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:H	1:A:3037:ILE:HD13	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:CD	1:A:2106:GLU:H	1.95	0.70
1:A:2954:ASN:HD22	1:A:2954:ASN:H	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:HD12	1:B:3700:LEU:H	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:H	1:B:1545:LEU:HD12	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:HD23	1:B:2320:LEU:O	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:4189:ASN:H	1:B:4189:ASN:HD22	1.40	0.67
1:B:4184:TRP:CD1	1:B:4214:ARG:HB2	2.30	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:N	1:A:3925:ASN:HD22	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:HD22	1:B:1901:ASN:H	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:3063:GLY:HA2	1:B:3136:GLN:HB3	1.78	0.64
1:B:4063:ILE:H	1:B:4063:ILE:HD12	1.62	0.64
1:B:1931:ASN:HB2	1:B:4312:TYR:CZ	2.32	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:N	1:A:4693:ASN:HD22	1.95	0.64
1:B:1694:PHE:HB3	1:B:1697:PHE:CD2	2.33	0.64
1:B:1554:LEU:HD12	1:B:2323:THR:HG22	1.79	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:HG3	1:A:3293:ARG:HH11	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:ND2	1:A:2793:ASN:N	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:HD12	1:A:4402:ILE:H	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:HD22	1:A:2090:ASN:C	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:N	1:A:3731:ASN:HD22	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:4004:THR:OG1	1:A:4006:PRO:HD3	2.01	0.59
1:A:3969:LEU:HD12	1:A:4426:MET:HE2	1.82	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:4137:VAL:HB	1:B:4138:PRO:HD2	1.85	0.59
1:B:4131:PRO:HD2	1:B:4232:MET:O	2.03	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: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:B:3024:VAL:HG11	2:B:9010:ADP:H3'	1.83	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:HH11	1:B:3620:ARG:HG2	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:HG23	1:A:4559:ILE:O	2.04	0.57
1:B:1939:GLU:O	1:B:1941:LEU:HG	2.03	0.57
1:B:1813:GLN:NE2	1:B:1941:LEU:H	2.02	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: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:A:1982:GLU:HG3	2:A:9001:ADP:H3'	1.86	0.57
1:B:1554:LEU:HD22	1:B:1609:GLN:OE1	2.03	0.57
1:B:4189:ASN:ND2	1:B:4189:ASN:N	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:HD12	1:A:2873:ILE:H	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:OE2	1:A:4415:GLU:HA	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:3439:ASP:HB3	1:A:3442:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3571:ARG:HB3	1:A:3571:ARG:HH11	1.69	0.56
1:A:3291:LYS:HG3	1:A:3835:LEU:HD22	1.86	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:1978:THR:HG21	1:A:2101:ILE:O	2.05	0.56
1:A:1927:ILE:HD13	1:A:1991:LEU:CD2	2.35	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:N	1:B:4618:ASN:HD22	2.02	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:B:1554:LEU:HB3	1:B:1609:GLN:NE2	2.09	0.56
1:B:3893:CYS:SG	1:B:3947:ILE:HG21	2.44	0.56
1:A:2560:MET:CE	1:A:2564:ASN:HD22	2.18	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:1956:CYS:SG	1:B:1983:THR:HG21	2.45	0.56
1:A:2229:GLN:HB3	1:A:2230:PRO:HD2	1.86	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:A:2806:ARG:HH12	2:A:9002:ADP:PB	2.28	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:N	1:A:2954:ASN:ND2	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:H	1:B:3043:ASN:HD22	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:HB2	1:B:1479:ARG:CZ	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:HG22	1:B:3729:VAL:O	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:4644:LEU:HG	1:B:4664:ILE:HD11	1.88	0.55
1:B:4624:SER:HB2	1:B:4668:THR:HB	1.87	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:CD1	1:A:4495:LEU:H	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:CD1	1:A:3373:ILE:H	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:2204:ILE:N	1:A:2205:PRO:CD	2.69	0.54
1:A:2196:LEU:HD21	1:A:2219:LEU:HD22	1.89	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:CD1	1:A:4553:TYR:N	2.75	0.54
1:B:1548:TYR:CD1	1:B:1549:GLN:HG2	2.43	0.54
1:B:1655:LEU:HD22	1:B:1655:LEU:H	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:ND2	1:B:4323:ASN:N	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:2519:ALA:HB2	1:B:2593:PHE:CZ	2.43	0.54
1:B:2516:LEU:HD12	1:B:2581:LEU:HD13	1.90	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:N	1:A:3043:ASN:HD22	2.05	0.54
1:A:4547:PRO:HB2	1:A:4550:TRP:CE3	2.43	0.54
1:B:1982:GLU:HA	1:B:1982:GLU:OE1	2.08	0.54
1:B:1975:PRO:HD2	1:B:2100:MET:O	2.07	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:N	1:A:4553:TYR:HD1	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:N	1:A:4012:LEU:HD12	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:HD1	1:A:1699:PHE:N	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:C	1:A:4596:ASN:HD22	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:ND2	1:B:4693:ASN:H	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:1558:TRP:CZ3	1:B:1606:ILE:HB	2.44	0.53
1:B:1541:LEU:HD23	1:B:1656:ILE:HG21	1.91	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:HG22	1:A:4122:VAL:O	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:2818:PHE:HD1	1:B:2876:PRO:HD3	1.74	0.52
1:B:2704:ALA:HB2	1:B:3085:GLU:CD	2.29	0.52
1:A:2142:GLN:HE21	1:A:2208:VAL:CG1	2.22	0.52
1:A:2297:ASP:C	1:A:2299:ILE:H	2.12	0.52
1:A:2275:VAL:HB	1:A:2413:MET:HE2	1.90	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:HH11	1:B:2532:ARG:HG2	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:HD22	1:B:4323:ASN:N	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:NZ	1:B:2282:LYS:HB2	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:3698:SER:C	1:A:3700:LEU:H	2.13	0.52
1:A:3256:THR:OG1	1:A:3779:SER:HB3	2.09	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:3843:GLY:O	1:B:3845:ILE:N	2.35	0.51
1:B:3563:LEU:HD11	1:B:3845:ILE:CD1	2.40	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:O	1:A:3366:LEU:HD12	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:4636:SER:HA	1:B:4670:THR:HG22	1.91	0.51
1:B:4592:GLY:HA3	1:B:4725:SER:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1611:ARG:NH1	1:A:1611:ARG:HG3	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:2619:ILE:O	1:A:2619:ILE:HG13	2.11	0.51
1:A:2540:LEU:HD23	1:A:2662:ALA:HB3	1.92	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:H	1:B:2921:GLU:CD	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:1573:SER:HA	1:B:1576:LYS:HE2	1.93	0.50
1:B:1527:LEU:HD22	1:B:1575:MET:HB2	1.92	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:CD2	1:A:2913:PHE:N	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:3105:PHE:O	1:B:3109:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2918:VAL:HG22	1:B:3172:TRP:CD2	2.47	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:4278:HIS:CD2	1:A:4343:TYR:OH	2.64	0.49
1:A:3992:LEU:HD22	1:A:4430:LEU:CB	2.41	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:4055:GLU:HG3	1:A:4093:ARG:NH1	2.27	0.49
1:A:4054:GLY:O	1:A:4055:GLU:O	2.30	0.49
1:B:1494:ILE:HA	1:B:1497:LEU:HD12	1.93	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:CD1	1:B:4402:ILE:H	2.21	0.49
1:B:4596:ASN:HD22	1:B:4596:ASN:C	2.15	0.49
1:B:4642:MET:HG2	1:B:4725:SER:HA	1.94	0.49
1:B:2877:ARG:HG2	2:B:9009:ADP:H4'	1.94	0.49
1:A:1739:THR:O	1:A:1760:ILE:HG12	2.12	0.49
1:A:2057:VAL:HG22	1:A:2058:GLU:H	1.78	0.49
1:A:2018:GLN:HE21	1:A:2066:SER:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2133:LYS:HD3	1:A:2133:LYS:O	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:N	1:A:3725:ASN:ND2	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:N	1:A:1934:PHE:CD2	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:NH1	1:A:2948:ARG:HG2	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:H	1:B:4618:ASN:ND2	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: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:1934:PHE:HB3	1:B:1993:ARG:HH22	1.78	0.48
1:B:1813:GLN:NE2	1:B:1940:TYR:HA	2.17	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:A:4003:GLU:HG3	1:B:2842:LEU:HD23	1.95	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:HD12	1:A:3238:ILE:N	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:1974:GLY:C	1:A:2079:PRO:HD3	2.34	0.48
1:A:1973:PHE:HE1	1:A:2099:ALA:CB	2.27	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:CD1	1:A:4184:TRP:N	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:HH11	1:B:2084:ARG:HG2	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:1800:HIS:CB	1:A:1858:ASN:HD22	2.26	0.48
1:A:1701:GLY:HA2	1:A:2011:ARG:NH1	2.29	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: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:1962:GLN:HB3	1:B:4341:THR:HG21	1.96	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: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:2208:VAL:HA	1:A:2415:TRP:HD1	1.74	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:NH1	1:B:2532:ARG:HG2	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:N	1:A:4048:PHE:CD1	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:3930:LEU:HD11	1:A:3939:ARG:HG2	1.95	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:A:3992:LEU:HD22	1:A:4430:LEU:HB2	1.96	0.47
1:A:3903:LEU:HD23	1:A:4433:MET:SD	2.54	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:O	1:B:3013:LEU:HG	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:3480:TRP:HE1	1:A:3484:GLN:HE21	1.62	0.47
1:A:3338:GLN:HG3	1:A:3529:ILE:HD12	1.96	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:2667:HIS:HA	1:B:2787:GLN:OE1	2.14	0.47
1:B:2532:ARG:CZ	1:B:2813:ILE:HD12	2.45	0.47
1:B:4596:ASN:ND2	1:B:4596:ASN:C	2.68	0.47
1:B:4618:ASN:H	1:B:4618:ASN:HD22	1.60	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:3370:GLU:O	1:A:3371:PRO:C	2.51	0.47
1:A:4043:ASP:N	1:A:4043:ASP:OD2	2.45	0.47
1:A:4430:LEU:O	1:A:4434:GLN:HB2	2.15	0.47
1:B:1611:ARG:O	1:B:1615:LEU:HD23	2.14	0.47
1:B:2125:ALA:O	1:B:2129:VAL:HG13	2.14	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: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: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:3074:ASP:H	1:A:3077:ASN:ND2	2.13	0.47
1:A:4109:ASP:O	1:A:4112:ASN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4344:GLY:HA2	1:A:4347:ILE:HG13	1.95	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:1782:ALA:HB2	1:B:1922:LEU:HD23	1.96	0.47
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: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: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: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
1:B:2309:LYS:HE2	1:B:2756:THR:HG21	1.96	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:4157:TYR:HB2	1:B:4184:TRP:C	2.35	0.47
1:B:4136:SER:O	1:B:4220:GLU:HA	2.15	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: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:3270:LEU:CB	1:A:3592:VAL:HG13	2.44	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:HA	1:A:2415:TRP:CE3	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:HG2	1:A:4087:LYS:O	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:3113:LYS:HG3	1:A:3123:LEU:O	2.15	0.46
1:A:3007:GLN:O	1:A:3142:HIS:HE1	1.99	0.46
1:A:3387:HIS:HB2	1:A:3473:ALA:HB2	1.95	0.46
1:A:3725:ASN:N	1:A:3725:ASN:HD22	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:2749:PRO:O	1:B:2757:GLN:HG2	2.16	0.46
1:B:2532:ARG:NH1	1:B:2813:ILE:HD12	2.31	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:1962:GLN:CB	1:B:4341:THR:HG21	2.46	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:HG3	1:A:4719:ARG:HH11	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:ND2	1:A:4596:ASN:C	2.69	0.46
1:B:1683:LEU:O	1:B:1683:LEU:HD12	2.16	0.46
1:B:3715:GLY:HA3	1:B:3758:PRO:HG2	1.98	0.46
1:B:4331:TRP:CZ2	1:B:4369:PHE:HE2	2.34	0.46
1:B:4284:ARG:NH2	1:B:4355:LEU:HD21	2.31	0.46
1:A:1662:ILE:HG22	1:A:1663:GLU:N	2.32	0.46
1:A:1911:ARG:HD3	1:A:1911:ARG:H	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:CD1	1:A:4402:ILE:H	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: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:A:2249:LEU:HB3	2:A:9002:ADP:N6	2.30	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: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:A:3023:SER:HB2	2:A:9004:ADP:O1A	2.16	0.45
1:B:1931:ASN:HD21	1:B:1962:GLN:HE22	1.64	0.45
1:B:2723:THR:HG22	1:B:2727:GLU:O	2.16	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: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:HG2	1:B:4431:GLN:O	2.16	0.45
1:A:2323:THR:O	1:A:2324:THR:HG23	2.16	0.45
1:A:2738:TRP:CZ3	1:A:2785:LYS:HA	2.51	0.45
1:A:2398:GLN:NE2	1:A:2806:ARG:HG2	2.31	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:3536:TYR:O	1:B:3540:ILE:HD13	2.16	0.45
1:B:3306:LEU:HD13	1:B:3557:VAL:CG2	2.46	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: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:1964:LEU:HD12	1:A:2074:PHE:CZ	2.51	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:O	1:A:3350:VAL:HG12	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:3463:ASP:O	1:A:3467:VAL:HG23	2.17	0.45
1:A:3388:LEU:CD2	1:A:3473:ALA:HB1	2.44	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:HA	1:A:4032:LYS:HE2	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:4095:LEU:HD11	1:B:4422:LYS:HB2	1.99	0.45
1:B:3992:LEU:HD12	1:B:4434:GLN:NE2	2.31	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:N	1:A:3540:ILE:HD12	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: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:3903:LEU:HD13	1:A:3959:LEU:HD21	1.99	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:4220:GLU:O	1:B:4222:HIS:N	2.50	0.45
1:B:4197:LEU:HD13	1:B:4226:PRO:HD3	1.99	0.45
1:B:4253:ILE:HG22	1:B:4253:ILE:O	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:HD13	1:A:2898:LEU:O	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:4087:LYS:HG2	1:B:4087:LYS:O	2.17	0.44
1:B:3958:THR:CG2	1:B:4235:VAL:HB	2.47	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:HD22	1:B:4693:ASN:H	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:4304:ARG:HA	1:B:4307:LEU:HD12	1.99	0.44
1:B:4265:ALA:H	1:B:4323:ASN:HB3	1.83	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:HE2	1:A:2077:MET:HB3	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:1973:PHE:HE1	1:A:2099:ALA:HA	1.81	0.44
1:A:1695:ALA:CB	1:A:2019:CYS:SG	3.06	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:NZ	1:B:3552:LYS:HB2	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:2913:PHE:HD2	1:A:2913:PHE:N	2.15	0.44
1:A:2903:ARG:HH22	1:A:2950:ILE:HA	1.82	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:CE3	1:A:1591:TRP:HA	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: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
1:A:3652:LEU:HD12	1:A:3653:PRO:CD	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4690:VAL:HG11	1:A:4701:PHE:CE2	2.53	0.43
1:A:2249:LEU:HD22	2:A:9002:ADP:C5	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:3046:TYR:CE1	1:B:3050:ASP:HB2	2.53	0.43
1:B:3038:TYR:HE2	1:B:3058:LEU:HD22	1.82	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: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:4319:LYS:O	1:A:4321:ARG:NH1	2.52	0.43
1:A:1958:LEU:HD23	1:A:4341:THR:HB	1.99	0.43
1:A:4091:SER:O	1:A:4420:SER:HA	2.18	0.43
1:B:1497:LEU:HD22	1:B:1501:SER:HB2	1.99	0.43
1:B:2282:LYS:HZ2	1:B:2282:LYS:HB2	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:HB3	1:A:3933:LYS:HZ3	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:3635:PRO:C	1:B:3637:PHE:H	2.21	0.43
1:B:3634:VAL:HB	1:B:3635:PRO:HD3	1.99	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:HB2	1:A:1955:ARG:NH1	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:4407:TRP:H	1:B:4407:TRP:HD1	1.64	0.43
1:B:3993:LYS:HG3	1:B:4431:GLN:HG3	1.99	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:2270:HIS:ND1	1:A:2270:HIS:N	2.66	0.43
1:A:2263:HIS:HB2	1:A:2289:TYR:CE1	2.54	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:NH1	1:A:4389:ARG:HG2	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:2327:TRP:CZ2	1:A:2379:LEU:HD22	2.54	0.43
1:A:2304:HIS:N	1:A:2352:TRP:O	2.51	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:HH11	1:B:3139:ARG:HG3	1.84	0.43
1:B:3289:LEU:O	1:B:3293:ARG:HG3	2.19	0.43
1:B:3675:ILE:HG22	1:B:3675:ILE:O	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:NH1	1:B:3620:ARG:HG2	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:HD12	1:A:4659:ILE:N	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:HG13	1:B:4324:ILE:H	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:2368:ASN:O	1:B:2410:ARG:NH1	2.52	0.42
1:B:2271:GLY:HA2	1:B:2393:VAL:O	2.19	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:4358:SER:O	1:A:4362:GLN:HB2	2.19	0.42
1:A:3992:LEU:CD1	1:A:4434:GLN:HG3	2.48	0.42
1:A:4596:ASN:OD1	1:A:4599:ALA:HB2	2.18	0.42
1:A:4678:ILE:O	1:A:4678:ILE:HG22	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: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:A:4000:SER:O	1:B:2940:SER:HB3	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:HD1	1:A:1973:PHE:O	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:3057:MET:O	1:B:3061:ARG:HG3	2.19	0.42
1:B:3039:THR:HG22	1:B:3072:ILE:HB	2.01	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:2051:LYS:C	1:A:2051:LYS:HD3	2.39	0.42
1:A:1967:ARG:CB	1:A:2051:LYS:HA	2.50	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:3262:ASP:OD2	1:A:3670:ARG:NE	2.52	0.42
1:A:3192:LEU:HD11	1:A:3271:ILE:HG22	2.01	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:HD3	1:A:3954:ARG:O	2.19	0.42
1:A:4178:ALA:HA	1:A:4183:THR:OG1	2.20	0.42
1:A:4128:SER:CB	1:A:4213:PHE:HB3	2.48	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:N	1:B:3043:ASN:ND2	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:C	1:A:2573:LEU:HD23	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:2057:VAL:HB	1:A:2067:LEU:HD13	2.01	0.42
1:A:1952:LEU:HD22	1:A:2103:PRO:HA	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:CD2	1:A:1792:PHE:C	2.92	0.42
1:A:2009:MET:HE3	1:A:2012:ILE:HB	2.02	0.42
1:A:2071:MET:HG3	1:A:2071:MET:O	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:3039:THR:CG2	1:B:3072:ILE:HB	2.50	0.42
1:B:2989:VAL:HG21	1:B:3184:VAL:HA	2.02	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:HD1	1:A:1973:PHE:C	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:HH11	1:B:3573:ARG:HG2	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:3910:GLN:HB3	1:B:4231:ARG:HD3	2.03	0.41
1:B:3886:TYR:CE2	1:B:3940:LEU:HD23	2.56	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:2612:LEU:HD12	1:A:2612:LEU:O	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:2586:GLY:CA	1:A:2815:LEU:HD13	2.43	0.41
1:A:2868:ILE:HG21	1:A:2922:GLU:OE2	2.21	0.41
1:A:3164:LEU:HA	1:A:3164:LEU:HD12	1.81	0.41
1:A:3013:LEU:HD23	1:A:3170:LEU:HD12	2.01	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:H	1:A:4012:LEU:HD12	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:O	1:B:2036:LEU:HD23	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:NH1	1:A:3571:ARG:HB3	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:4278:HIS:HD2	1:A:4343:TYR:CE1	2.39	0.41
1:A:4247:ASN:HD21	1:A:4282:GLN:HE21	1.67	0.41
1:A:4535:ARG:HG2	1:A:4535:ARG:HH11	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:C	1:B:2670:LEU:HD12	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:HD2	1:A:2615:TYR:N	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: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:1483:ILE:HG22	1:B:1517:VAL:HG22	2.02	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: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:3597:ALA:O	1:A:3601:TYR:HD1	2.04	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: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: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: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
1:B:2578:MET:HB3	1:B:2597:ILE:CD1	2.43	0.41
1:B:3228:VAL:HA	1:B:3231:LEU:HD12	2.03	0.41
1:B:3647:TRP:HB3	1:B:3652:LEU:HD22	2.02	0.41
1:B:4056:PRO:HD2	1:B:4093:ARG:NH2	2.36	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:4306:ALA:HA	1:B:4338:LEU:HD22	2.03	0.41
1:B:4277:PHE:HB2	1:B:4363:LEU:HD12	2.03	0.41
1:B:4094:VAL:HB	1:B:4423:ALA:HB1	2.02	0.41
1:B:4503:ILE:HD11	1:B:4575:LEU:O	2.21	0.41
1:A:1886:ARG:HG3	1:A:1887:ASP:H	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2088:PRO:C	1:A:2090:ASN:N	2.75	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: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:B:1739:THR:O	1:B:1760:ILE:N	2.54	0.41
1:B:1734:LEU:HA	1:B:1742:ILE:HG12	2.03	0.41
1:B:1831:LEU:HB3	1:B:1900:GLY:HA2	2.02	0.41
1:B:2084:ARG:HG2	1:B:2084:ARG:NH1	2.36	0.41
1:B:2381:ASN:HD22	1:B:2381:ASN:C	2.25	0.41
1:B:2887:LEU:O	1:B:2891:GLN:HG3	2.21	0.41
1:B:3539:LEU:HA	1:B:3539:LEU:HD12	1.92	0.41
1:B:3571:ARG:O	1:B:3575:GLU:HG3	2.19	0.41
1:B:4022:CYS:HB3	1:B:4026:GLN:NE2	2.36	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:4509:LEU:O	1:B:4513:ILE:HG13	2.20	0.41
1:B:4649:TRP:HA	1:B:4649:TRP:CE3	2.55	0.41
1:B:4413:ASN:ND2	1:B:4660:LEU:HD23	2.36	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:C	1:A:2935:LEU:HD23	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:4090:HIS:C	1:A:4092:ASP:H	2.24	0.40
1:A:4086:MET:HG2	1:A:4093:ARG:HB2	1.99	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:1928:HIS:CG	1:B:1933:THR:HG22	2.52	0.40
1:B:1820:GLN:NE2	1:B:1990:GLN:NE2	2.66	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:4402:ILE:N	1:B:4402:ILE:CD1	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4403:SER:HB2	1:B:4407:TRP:CD2	2.56	0.40
1:B:3966:THR:HG23	1:B:4426:MET:HE3	2.02	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:HA	1:A:1898:LEU:HD23	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:3459:ASP:HA	1:A:3460:PRO:HD3	1.97	0.40
1:A:3296:GLU:HG3	1:A:3567:LEU:HD13	2.04	0.40
1:A:3845:ILE:HG13	1:A:3845:ILE:H	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: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:1813:GLN:HE22	1:B:1941:LEU:H	1.69	0.40
1:B:2309:LYS:HG3	1:B:2358:ASP:HB2	2.02	0.40
1:B:2270:HIS:CB	1:B:2392:ARG:HH11	2.34	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%)	3	31
1	B	2870/3367 (85%)	2476 (86%)	327 (11%)	67 (2%)	7	46
All	All	5880/6734 (87%)	4900 (83%)	775 (13%)	205 (4%)	4	38

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 ⓘ

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%)	12	48
1	B	2353/3028 (78%)	2210 (94%)	143 (6%)	22	60
All	All	4810/6056 (79%)	4459 (93%)	351 (7%)	16	54

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

Some 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 carbohydrates 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	-	25,29,29	1.28	3 (12%)	24,45,45	1.99	4 (16%)
2	ADP	A	9002	-	25,29,29	1.24	2 (8%)	24,45,45	1.98	4 (16%)
2	ADP	A	9003	-	25,29,29	1.28	3 (12%)	24,45,45	2.00	4 (16%)
2	ADP	A	9004	-	25,29,29	1.26	2 (8%)	24,45,45	2.02	4 (16%)
2	ADP	B	9007	-	25,29,29	1.26	2 (8%)	24,45,45	2.00	4 (16%)
2	ADP	B	9008	-	25,29,29	1.25	2 (8%)	24,45,45	1.97	4 (16%)
2	ADP	B	9009	-	25,29,29	1.27	3 (12%)	24,45,45	1.99	4 (16%)
2	ADP	B	9010	-	25,29,29	1.26	2 (8%)	24,45,45	2.00	4 (16%)

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	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9002	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9003	-	-	0/12/32/32	0/3/3/3
2	ADP	A	9004	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9007	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	B	9008	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9009	-	-	0/12/32/32	0/3/3/3
2	ADP	B	9010	-	-	0/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9009	ADP	O4'-C1'	2.10	1.44	1.41
2	A	9003	ADP	O4'-C1'	2.14	1.44	1.41
2	A	9001	ADP	O4'-C1'	2.23	1.44	1.41
2	A	9004	ADP	C2-N3	2.56	1.36	1.32
2	B	9007	ADP	C2-N3	2.59	1.36	1.32
2	A	9003	ADP	C2-N3	2.62	1.36	1.32
2	B	9009	ADP	C2-N3	2.63	1.36	1.32
2	B	9010	ADP	C2-N3	2.63	1.36	1.32
2	A	9002	ADP	C2-N3	2.63	1.36	1.32
2	B	9008	ADP	C2-N3	2.64	1.36	1.32
2	A	9001	ADP	C2-N3	2.70	1.36	1.32
2	A	9001	ADP	C5-C4	3.59	1.48	1.40
2	B	9007	ADP	C5-C4	3.60	1.48	1.40
2	B	9010	ADP	C5-C4	3.61	1.48	1.40
2	A	9004	ADP	C5-C4	3.61	1.48	1.40
2	A	9003	ADP	C5-C4	3.62	1.48	1.40
2	B	9009	ADP	C5-C4	3.63	1.48	1.40
2	B	9008	ADP	C5-C4	3.65	1.48	1.40
2	A	9002	ADP	C5-C4	3.70	1.48	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9004	ADP	N3-C2-N1	-7.98	121.91	128.86
2	A	9003	ADP	N3-C2-N1	-7.92	121.96	128.86
2	B	9007	ADP	N3-C2-N1	-7.91	121.97	128.86
2	B	9010	ADP	N3-C2-N1	-7.88	122.00	128.86
2	A	9001	ADP	N3-C2-N1	-7.88	122.00	128.86
2	B	9009	ADP	N3-C2-N1	-7.84	122.03	128.86
2	A	9002	ADP	N3-C2-N1	-7.74	122.11	128.86
2	B	9008	ADP	N3-C2-N1	-7.71	122.14	128.86
2	B	9007	ADP	C4-C5-N7	-2.82	106.68	109.41
2	B	9010	ADP	C4-C5-N7	-2.82	106.69	109.41
2	A	9001	ADP	C4-C5-N7	-2.80	106.71	109.41
2	A	9004	ADP	C4-C5-N7	-2.79	106.71	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	9002	ADP	C4-C5-N7	-2.79	106.71	109.41
2	B	9009	ADP	C4-C5-N7	-2.79	106.71	109.41
2	A	9003	ADP	C4-C5-N7	-2.79	106.72	109.41
2	B	9008	ADP	C4-C5-N7	-2.79	106.72	109.41
2	A	9001	ADP	C4'-O4'-C1'	2.06	111.96	109.77
2	A	9004	ADP	C4'-O4'-C1'	2.09	112.00	109.77
2	B	9008	ADP	C4'-O4'-C1'	2.11	112.02	109.77
2	A	9002	ADP	C2-N1-C6	2.12	122.49	118.77
2	B	9010	ADP	C4'-O4'-C1'	2.12	112.03	109.77
2	B	9008	ADP	C2-N1-C6	2.15	122.53	118.77
2	B	9009	ADP	C2-N1-C6	2.16	122.54	118.77
2	B	9010	ADP	C2-N1-C6	2.16	122.56	118.77
2	A	9003	ADP	C2-N1-C6	2.17	122.56	118.77
2	A	9001	ADP	C2-N1-C6	2.17	122.57	118.77
2	B	9007	ADP	C2-N1-C6	2.18	122.58	118.77
2	A	9002	ADP	C4'-O4'-C1'	2.21	112.13	109.77
2	B	9007	ADP	C4'-O4'-C1'	2.22	112.13	109.77
2	A	9004	ADP	C2-N1-C6	2.22	122.66	118.77
2	A	9003	ADP	C4'-O4'-C1'	2.22	112.14	109.77
2	B	9009	ADP	C4'-O4'-C1'	2.29	112.20	109.77

There are no chirality outliers.

There are no torsion outliers.

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	A	9002	ADP	4	0
2	A	9004	ADP	2	0
2	B	9009	ADP	1	0
2	B	9010	ADP	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	3042/3367 (90%)	-0.14	62 (2%) 65 56	64, 130, 209, 322	0
1	B	2908/3367 (86%)	-0.18	30 (1%) 82 75	72, 136, 208, 335	0
All	All	5950/6734 (88%)	-0.16	92 (1%) 74 65	64, 133, 209, 335	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1543	LEU	5.7
1	A	1652	GLY	4.9
1	B	1517	VAL	4.9
1	A	4187	LEU	4.5
1	A	1651	SER	4.3
1	A	1555	VAL	4.0
1	A	3516	ASP	4.0
1	A	3718	LEU	3.8
1	A	4122	VAL	3.7
1	A	4550	TRP	3.7
1	A	1545	LEU	3.7
1	B	1484	LEU	3.6
1	A	1650	VAL	3.6
1	A	4165	PRO	3.5
1	A	4509	LEU	3.4
1	A	4217	MET	3.4
1	A	3512	LYS	3.4
1	A	4162	ILE	3.4
1	A	3515	GLN	3.2
1	A	3842	SER	3.2
1	A	3518	ILE	3.2
1	B	3356	ALA	3.1
1	A	1657	LEU	3.1
1	A	3334	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	2304	HIS	2.9
1	A	3328	VAL	2.9
1	A	3513	LEU	2.9
1	B	2335	THR	2.9
1	B	2720	TYR	2.9
1	B	4517	LEU	2.9
1	A	4168	PHE	2.9
1	A	4215	LEU	2.9
1	A	4185	VAL	2.8
1	A	1575	MET	2.8
1	A	3846	LEU	2.8
1	A	1554	LEU	2.7
1	B	4541	ILE	2.7
1	A	1584	PHE	2.7
1	A	1656	ILE	2.7
1	A	1538	TRP	2.7
1	B	1495	THR	2.6
1	A	3866	ALA	2.6
1	A	3360	VAL	2.6
1	B	1575	MET	2.5
1	A	1639	ILE	2.5
1	A	3536	TYR	2.5
1	A	3359	LYS	2.5
1	A	4118	MET	2.5
1	A	1527	LEU	2.5
1	B	1543	LEU	2.4
1	B	2620	ASP	2.4
1	A	3330	ASP	2.4
1	B	2574	LEU	2.4
1	A	4131	PRO	2.4
1	A	2060	LEU	2.3
1	A	3762	ILE	2.3
1	A	1544	ASP	2.3
1	A	4186	LEU	2.3
1	A	3764	LEU	2.3
1	B	1656	ILE	2.3
1	A	1565	LEU	2.3
1	A	1549	GLN	2.3
1	B	1514	TYR	2.3
1	B	3112	CYS	2.3
1	A	2353	ILE	2.2
1	A	4192	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	4635	ALA	2.2
1	A	3341	ALA	2.2
1	B	1511	GLU	2.2
1	B	1497	LEU	2.2
1	A	1551	LYS	2.2
1	A	3319	GLN	2.2
1	A	4142	ALA	2.2
1	B	4215	LEU	2.2
1	A	3346	VAL	2.2
1	B	3341	ALA	2.1
1	B	4550	TRP	2.1
1	A	2452	ASN	2.1
1	A	3533	LYS	2.1
1	B	1515	ARG	2.1
1	B	1510	ASN	2.1
1	A	3388	LEU	2.1
1	B	3842	SER	2.1
1	B	3544	GLU	2.1
1	B	3324	LEU	2.1
1	A	3763	PHE	2.0
1	B	4537	LEU	2.0
1	B	3332	GLN	2.0
1	A	2990	LEU	2.0
1	B	3328	VAL	2.0
1	B	2597	ILE	2.0
1	A	4030	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	A	9001	27/27	0.94	0.39	2.68	129,129,129,129	0
2	ADP	B	9007	27/27	0.90	0.37	2.40	129,129,129,129	0
2	ADP	B	9009	27/27	0.95	0.31	1.90	129,129,129,129	0
2	ADP	A	9003	27/27	0.91	0.33	1.86	129,129,129,129	0
2	ADP	B	9008	27/27	0.85	0.40	1.80	129,129,129,129	0
2	ADP	A	9002	27/27	0.90	0.30	1.31	129,129,129,129	0
2	ADP	B	9010	27/27	0.86	0.30	0.79	129,129,129,129	0
2	ADP	A	9004	27/27	0.91	0.30	0.07	129,129,129,129	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.