



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:12 AM UTC

PDB ID : 8UQ3 / pdb_00008uq3
EMDB ID : EMD-42459
Title : Structure of human RyR2-S2808D in the closed state in the presence of ARM210
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-10-23
Resolution : 3.18 Å(reported)
Based on initial model : 7UA5

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

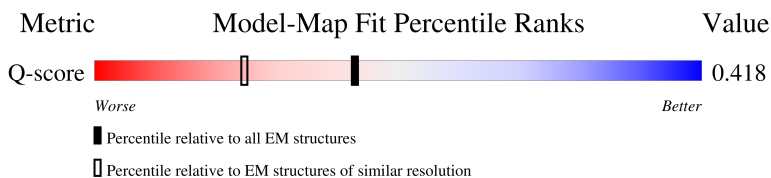
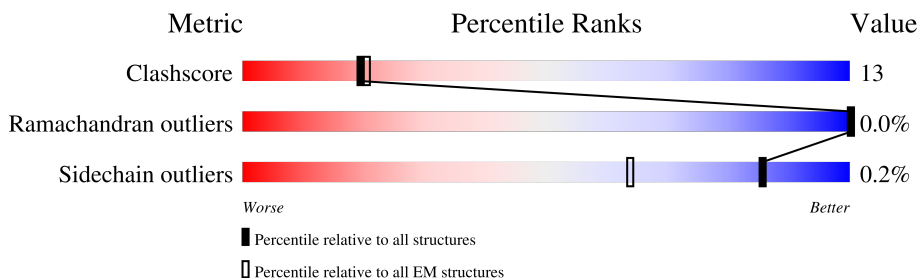
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



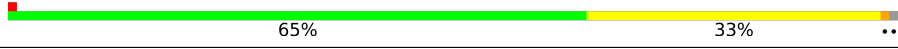
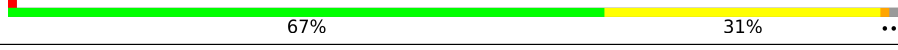
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14470 (2.68 - 3.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4967	10% 62% 23% 15%
1	B	4967	10% 62% 23% 15%
1	C	4967	10% 62% 23% 15%
1	D	4967	10% 62% 23% 15%

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Mol	Chain	Length	Quality of chain
2	E	108	 67% 31% ..
2	F	108	 68% 31% ..
2	G	108	 65% 33% ..
2	H	108	 67% 31% ..

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
4	ATP	A	5003	-	-	X	-
4	ATP	B	5003	-	-	X	-
4	ATP	C	5003	-	-	X	-
4	ATP	D	5003	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 138700 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2808	ASP	SER	engineered mutation	UNP Q92736
B	2808	ASP	SER	engineered mutation	UNP Q92736
C	2808	ASP	SER	engineered mutation	UNP Q92736
D	2808	ASP	SER	engineered mutation	UNP Q92736

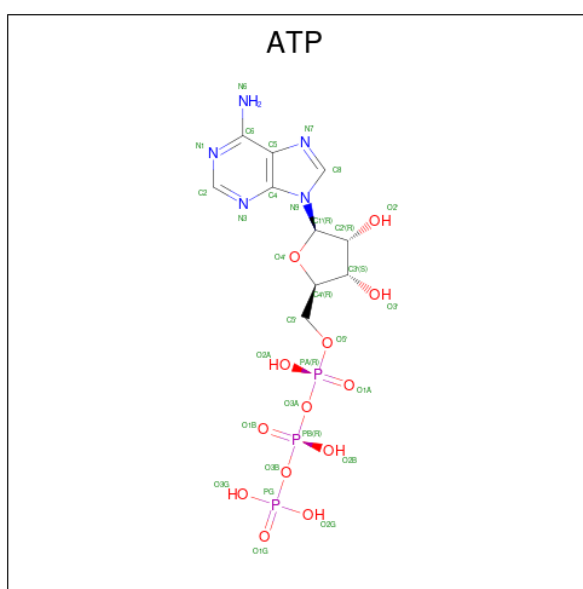
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



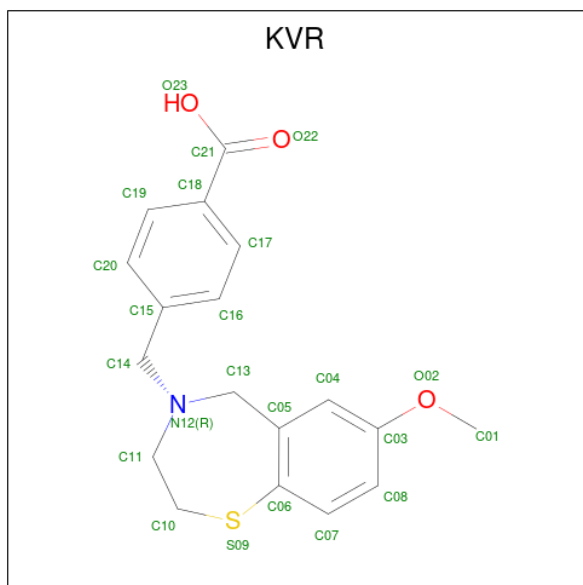
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10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

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

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (CCD ID: KVR) (formula: C₁₈H₁₉NO₃S).

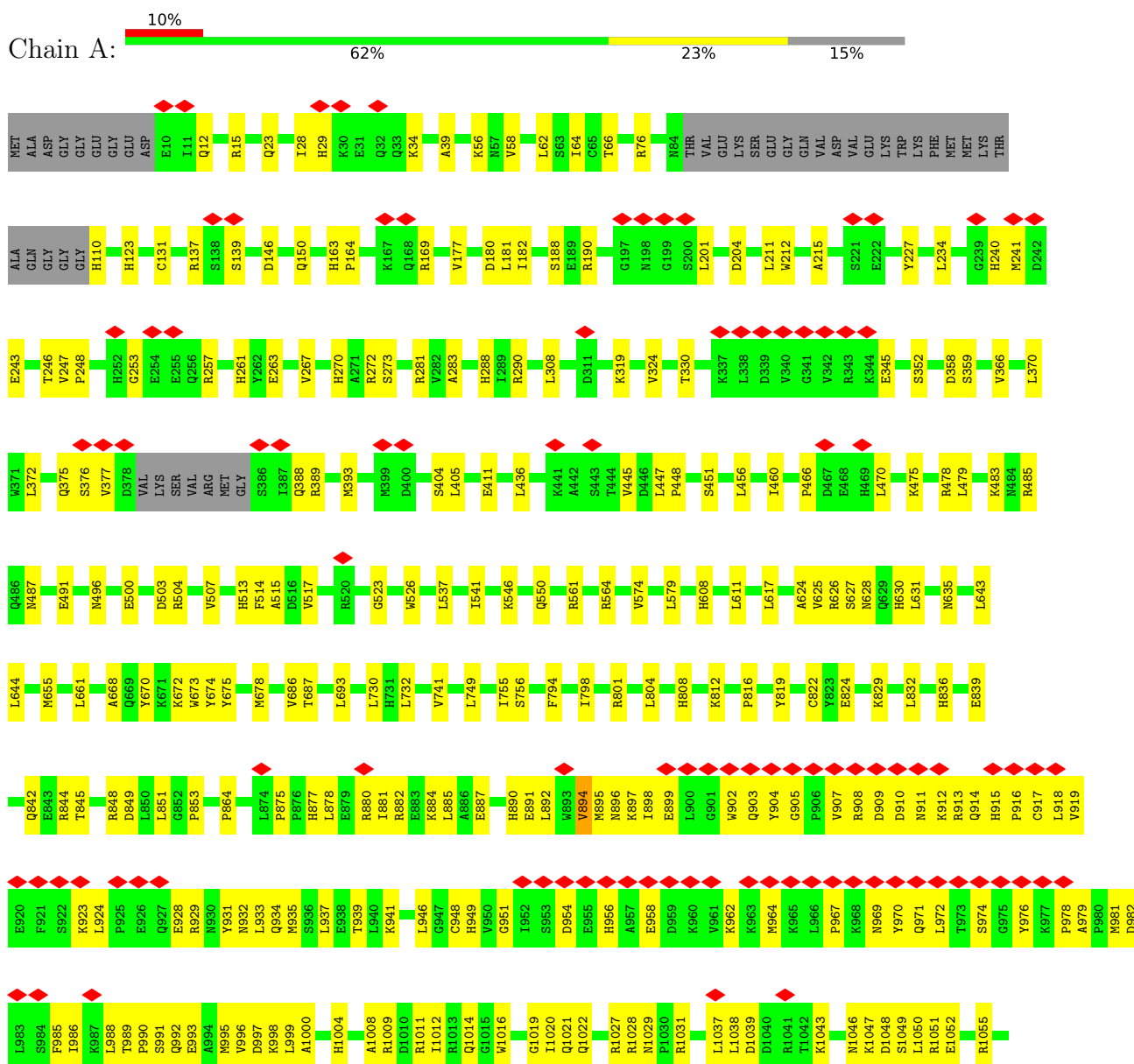


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	C	1	Total	C	N	O	S	0
			23	18	1	3	1	
5	D	1	Total	C	N	O	S	0
			23	18	1	3	1	

3 Residue-property plots

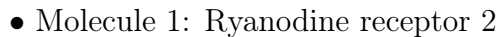
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ryanodine receptor 2





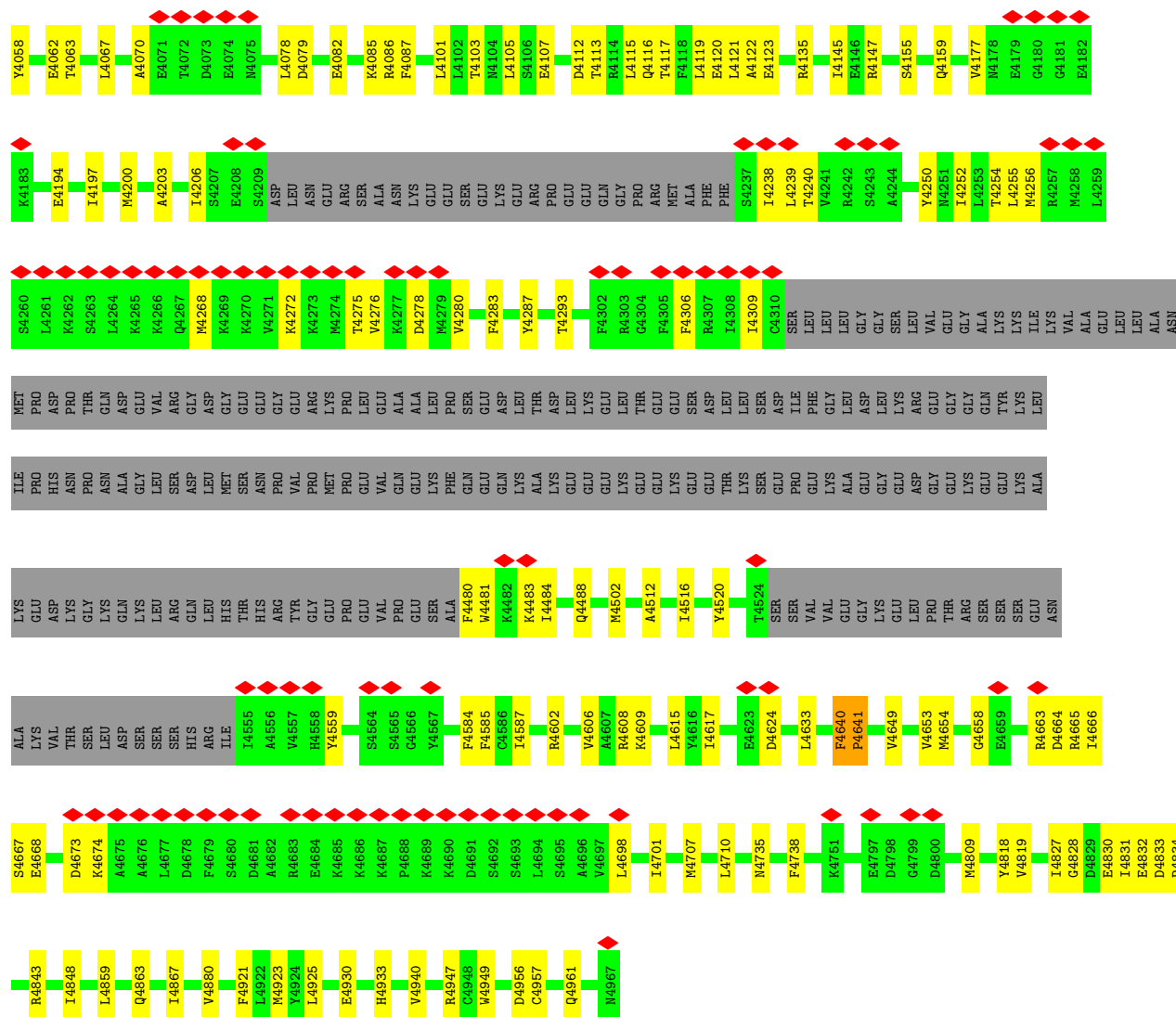
ASN	GLU	TYR	L3306	M3241	L3175	F3109	A3042	F2975	G2906	T2832	L2763	G2699	K2619
LEU	LEU	ALA	I3307	Y3245	D3176	E3110	R3043	K2976	F2907	S2764	S2764	N2700	T2620
ALA	ALA	PHE	K3308	K3246	K3177	H3111	T3044	N2977	K2908	K2833	E2765	F2701	C2621
LEU	LEU	PRO	K3309	S3247	H3178	I3112	V3045	N2978	D2909	S2834	E2767	L2623	L2623
ALA	ALA	LEU	P3312	R3248	N3179	G3113	M3046	R2979	L2910	R2835	E2768	G2626	G2626
LYS	LYS	THR	G3113	W3249	I3180	Q3114	T3048	Y2981	E2911	L2837	E2769	W2627	W2627
ASN	ASN	ILE	I3183	W3250	I3183	F3117	G3049	F2982	L2912	A2841	I2770	D2707	G2628
ARG	ARG	THR	Y3184	K3250	Y3184	G3118	L3050	L2983	D2913	E2842	R2772	T2708	G2629
THR	THR	LYS	N3185	K3252	H3185	E3119	E3061	S2984	D2914	M2843	W2773	S2709	N2629
PHE	PHE	VAL	T3186	H3252	T3186	G3120	S3052	A2985	T2915	M2844	P2774	N2710	F2630
LYS	LYS	ASP	T3187	K3255	K3187	D3120	V3053	A2986	S2916	M2847	I2711	I2711	E2635
MET	MET	TYR	S3188	E3255	S3188	I3121	K3054	S2987	L2917	N2847	T2712	T2712	E2636
ASN	ASN	ASN	S3189	N3256	S3189	L3122	L3057	R2988	E2918	K2779	I2713	I2713	E2637
ALA	ALA	ALA	R3190	K3257	R3190	L3123	R3058	R2989	K2919	P2714	P2714	P2714	L2638
LYS	LYS	LYS	E3191	P3258	E3191	E3124	G3058	L2990	R2920	E2715	E2715	E2715	W2639
VAL	VAL	TRP	R3192	R3260	R3192	D3125	L3061	L2990	R2921	W2785	K2716	K2716	L2640
LEU	LEU	LEU	A3193	A3261	A3193	D3062	D3062	C2991	F2922	G2786	L2717	L2717	S2641
GLY	GLY	ASP	A3194	E3262	A3194	V3126	N3063	S2992	Y2923	W2787	E2718	E2718	E2657
PRO	PRO	LYS	L3195	M3263	M3263	Q3127	E3066	G2993	L2929	R2788	Y2719	Y2719	Q2659
ASN	ASN	GLU	L3196	C3264	L3196	Y3131	D3067	G2994	I2930	E2861	W2791	D2730	F2662
PRO	PRO	PRO	L3197	C3265	L3197	L3134	L3068	H2995	L2930	S2862	T2792	K2723	K2663
LYS	LYS	LYS	P3198	T3266	P3198	T3135	E3069	S2997	V2933	K2863	R2793	A2725	L2664
ALA	ALA	ALA	T3199	A3267	T3199	S3136	K3070	N2998	W2833	G2864	E2794	A2726	K2656
MET	MET	GLU	N3200	L3268	N3200	G3140	T3071	K2999	H2937	G2865	G2795	E2726	Y2657
LYS	LYS	GLU	V3201	S3270	V3201	M3072	M3072	E3000	Y2938	G2866	D2796	H2727	E2658
GLY	GLY	PHE	E3202	E3271	E3202	E3073	E3073	K3001	Y2939	G2867	S2797	H2728	Q2659
ARG	ARG	ARG	D3203	K3272	D3203	T3142	N3074	E3002	F2943	N2867	W2798	H2729	F2662
MET	MET	VAL	V3204	L3271	V3204	S3143	Q3077	K3003	D2944	H2868	A2799	K2731	K2663
TYR	TYR	ALA	P3209	K3274	P3209	K3144	G3078	V3004	G2945	P2869	N2802	W2734	L2664
ALA	ALA	GLU	T3275	T3275	S3210	S3145	Q3078	T3005	G2946	L2870	THR	D2735	A2665
GLU	GLU	VAL	L3276	L3276	L3211	I3146	Q3079	S3006	S2947	L2871	ARG	K2736	L2666
VAL	VAL	PHE	L3277	L3277	E3212	Y3147	F3080	K3017	G2948	P2872	ARG	L2737	P2667
THR	THR	ILE	L3218	L3218	K3213	V3148	T3081	L3010	R2949	P2873	ILE	A2738	S2670
LEU	LEU	LEU	M3215	M3215	L3214	E3149	THR	L3014	K2950	Y2874	ASP	N2739	P2677
TRP	TRP	TRP	E3216	E3216	M3216	Q3150	ARG	V3015	G2951	D2875	ASP	N2741	Y2680
ALA	ALA	LYS	E3217	E3217	I3218	Q3151	GLN	R3016	E2952	T2876	GLN	W2741	E2681
LYS	LYS	LYS	I3218	I3218	L3221	S3153	ASN	R3017	H2953	L2877	VAL	G2744	E2682
ASP	ASP	ASP	L3221	L3221	S3224	A3154	PRO	L3019	F2954	E2881	SER	E2745	S2683
GLY	GLY	GLY	G3225	G3225	G3225	E3157	G3089	S3020	P2955	K2884	VAL	I2746	N2684
LEU	LEU	GLU	I3226	I3226	I3226	G3158	V3090	D3025	P2956	D2885	ASP	I2747	Y2685
LEU	LEU	GLU	R3227	R3227	R3227	L3159	T3091	A3026	E2957	R2886	ALA	S2748	V2686
LEU	LEU	GLN	Y3228	Y3228	Y3228	Q3092	Q3092	I3026	Q2958	E2887	ALA	D2749	S2687
ASN	ASN	ASN	T3229	T3229	T3229	I3093	I3093	I3029	E2959	Q2890	HIS	S2750	M2688
ASP	ASP	ASP	Q3230	Q3230	Q3230	Q3094	M3095	V3030	I2960	D2891	Y2821	S2751	M2689
VAL	VAL	VAL	M3231	M3231	M3231	A3163	A3096	F2962	K2961	L2892	Y2822	K2752	E2690
VAL	VAL	VAL	P3232	P3232	P3232	G3164	T3097	F2963	F2963	L2893	S2822	P2753	K2691
THR	THR	THR	H3233	H3233	H3233	A3165	T3097	A2964	K2964	L2894	P2823	Q2754	K2691
ASN	ASN	ASN	V3234	V3234	V3234	L3033	A3100	K2965	K2965	F2895	R2824	P2755	Q2692
PRO	PRO	PRO	E3235	E3235	E3235	H3034	L3101	R2896	V2966	L2896	A2825	L2756	Q2693
GLY	GLY	GLY	M3235	M3235	M3235	I3035	L3101	F2897	V2967	Q2897	I2826	M2757	S2694
ILE	ILE	ILE	E3236	E3236	E3236	G3037	L3102	V2967	V2967	L2898	T2827	K2758	M2695
ASP	ASP	ASP	V3237	V3237	V3237	Q3038	P3103	Q3038	P2969	N2899	L2827	P2759	D2696
ASP	ASP	ASP	F3302	F3302	F3302	M3104	M3104	T3039	L2970	A2902	M2828	Y2760	S2697
GLN	GLN	GLN	Q3303	Q3303	Q3303	L3108	L3108	L3040	I2971	K2902	S2829	K2761	E2698
LEU	LEU	LEU	Q3304	Q3304	Q3304	T3170	T3170	L3041	D2972	L2762			





L2763	S2764	L2633	S2834	R2835	D2836	L2837	A2841	E2842	M2843	M2844	A2845	E2846	N2847	W2852	K2855	K2856	R2768	R2791	T2792	R2793	E2794	G2795	D2796	S2797	H2798	A2799	N2802	ARG	THR	ARG	ARG	ILE	ASP	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	I2826	D2827	M2828	S2829	
E2698	Q2699	L2633	E2766	K2767	K2768	E2769	L2770	T2771	R2772	T2773	P2774	L2775	L2779	K2780	W2785	E2786	L2787	R2768	R2791	T2792	R2793	E2794	G2795	D2796	S2797	H2798	A2799	N2802	ARG	THR	ARG	ARG	ILE	ASP	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	I2826	D2827	M2828	S2829
H2486	L2487	L2488	E2489	V2490	G2491	F2492	L2496	D2497	A2498	W2512	L2525	P2526	L2527	E2539	L2544	I2545	L2548	L2549	S2556	K2557	R2566	I2569	E2570	V2571	C2572	L2573	I2576	L2580	R2581	P2582	S2583	M2584	L2589	R2590	R2591	L2592	V2593	M2605	P2606	L2607	L2610	T2611	N2612	H2613	Y2614									
L2619	Y2620	Y2621	G2622	L2623	G2626	W2627	G2628	N2629	F2630	E2635	E2636	E2637	L2638	H2639	L2640	R2642	L2644	F2645	K2655	K2656	Y2657	E2658	Q2659	F2662	K2663	L2664	A2665	L2666	P2667	S2670	P2677	Y2680	M2681	E2682	S2683	N2684	Y2685	V2686	S2687	M2688	M2689	E2690	K2691	Q2692	S2693	S2694	M2695	D2696	S2697					
E2698	Q2699	N2700	F2701	Q2704	D2707	T2708	S2709	N2710	L2711	L2712	L2713	P2714	E2715	K2716	L2717	E2718	Y2719	F2720	K2723	Y2724	A2725	E2726	H2727	S2728	H2729	D2730	K2731	N2734	D2735	K2736	L2737	A2738	N2739	G2740	W2741	L2742	Y2743	G2744	E2745	L2746	Y2747	S2750	S2751	K2752	V2753	Q2754	P2755	L2756	H2757	K2758	P2759	Y2760	K2761	L2762
L2763	S2764	E2765	K2766	E2767	K2768	E2769	L2770	Y2771	R2772	T2773	P2774	L2775	L2779	K2780	W2785	E2786	L2787	R2768	R2791	T2792	R2793	E2794	G2795	D2796	S2797	H2798	A2799	N2802	ARG	THR	ARG	ARG	ILE	ASP	GLN	THR	SER	GLN	VAL	SER	VAL	ASP	ALA	HIS	G2820	Y2821	S2822	P2823	R2824	A2825	I2826	D2827	M2828	S2829
T2832	L2833	S2834	R2835	D2836	L2837	A2841	E2842	M2843	M2844	A2845	E2846	N2847	W2852	K2855	K2856	E2857	K2858	E2861	S2862	K2863	E2864	G2865	E2866	N2867	K2868	F2869	L2870	L2871	V2872	D2873	L2874	D2875	T2876	L2877	E2881	K2884	D2885	R2886	E2887	Q2890	D2891	L2892	L2893	K2894	R2895	L2896	Q2897	N2899	A2902					
Q1684	L1685	I1689	Y1693	Y1703	L1706	T1716	A1717	R1718	L1719	M1720	M1721	E1724	M1729	L1748	P1749	G1750	I1751	L1757	L1784	D1785	I1786	L1787	M1831	G1832	I1833	F1834	L1839	I1842	V1850	E1853	A1854	ALA	THR	PRO	GLU	GLU	GLU	ASP	THR	THR	LEU	LEU	LYS											
GLU	LEU	SER	VAL	ASP	ALA	LYS	GLN	GLY	ALA	GLY	GLU	LYS	GLY	LYS	P1889	K1890	G1891	G1895	L1898	Q2059	Q2060	P1989	E1990	E1991	I1992	R1993	L1996	H2000	R2004	I2009	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	SER	ASP	LEU	THR	I1E	ARG	GLY	ARG					
S1954	A1955	A1956	L1957	T1958	A1959	R1960	TYR	K1961	L1962	K1963	R1966	S1967	Q1972	I1973	M1974	M1975	L1976	F1979	D1982	K2054	S2055	S2056	L2057	L2058	Q2059	Q2060	A2070	Q2071	I2075	E2076	D2077	V2081	L2087	R2090	Q2091	I2095	G2096	V2099	I2117	L2120	A2121	S2122	I2126	R2127										
K2053	K2054	S2055	S2056	L2057	Q2058	Q2059	Q2060	A2070	Q2071	I2075	E2076	D2077	V2081	L2087	R2090	Q2091	I2095	G2096	V2099	I2117	L2120	A2121	S2122	I2126	R2127																													
N2142	L2143	L2146	F2155	P2159	N2162	R2163	N2172	E2173	V2174	N2175	N2176	N2177	V2178	Q2180	Q2181	E2183	S2184	R2185	L2187	N2192	V2193	A2194	L2200	E2201	Y2202	L2206	Q2209	K2212	F2215	Y2220	L2221	L2222	V2227	P2232	K2233	N2234	S2237	A2243																
V2247	E2252	L2253	L2257	R2258	E2259	D2261	L2262	E2263	K2264	V2265	V2266	Y2268	L2274	M2279	K2283	G2284	Y2285	E2296	R2297	Y2298	V2319	L2323	R2327	P2328	E2329	G2332	P2333	R2336	G2337	E2338	L2344	E2348	I2351	K2352	E2355	P2364	ASN	SER	GLY	SER														
LYS	THR	ASP	THR	GLU	E2377	E2378	D2379	D2380	T2381	L2382	G2385	M2389	T2390	T2396	D2397	R2401	E2402	A2403	I2409	R2420	G2434	F2440	Q2441	M2442	P2443	T2444	A2446	K2447	D2448	D2455	M2456	S2457	K2465	M2468	V2475	I2478	E2479	V2480	Q2481	D2482	F2483	L2484	L2485											
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M3956	E3815	E3632	K3316	H3252	T3186	D3120	A2985	A2986	P2915
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H4055	F3603	E3710	VAL	K3297	T3229	A3158	T3091	D3025	E2957
	R3604	V3711	GLY	L3298	M3231	K3161	I3092	A3026	Q2958
		Q3728	ALA	K3300	H3233	F3162	I3093	I3029	E2959
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				S3303	E3236	F3166	T3097	F3030	F2962
					V3237	V3168	A3100	H3034	K2964
					I3238	A3169	L3101	L3035	K2965
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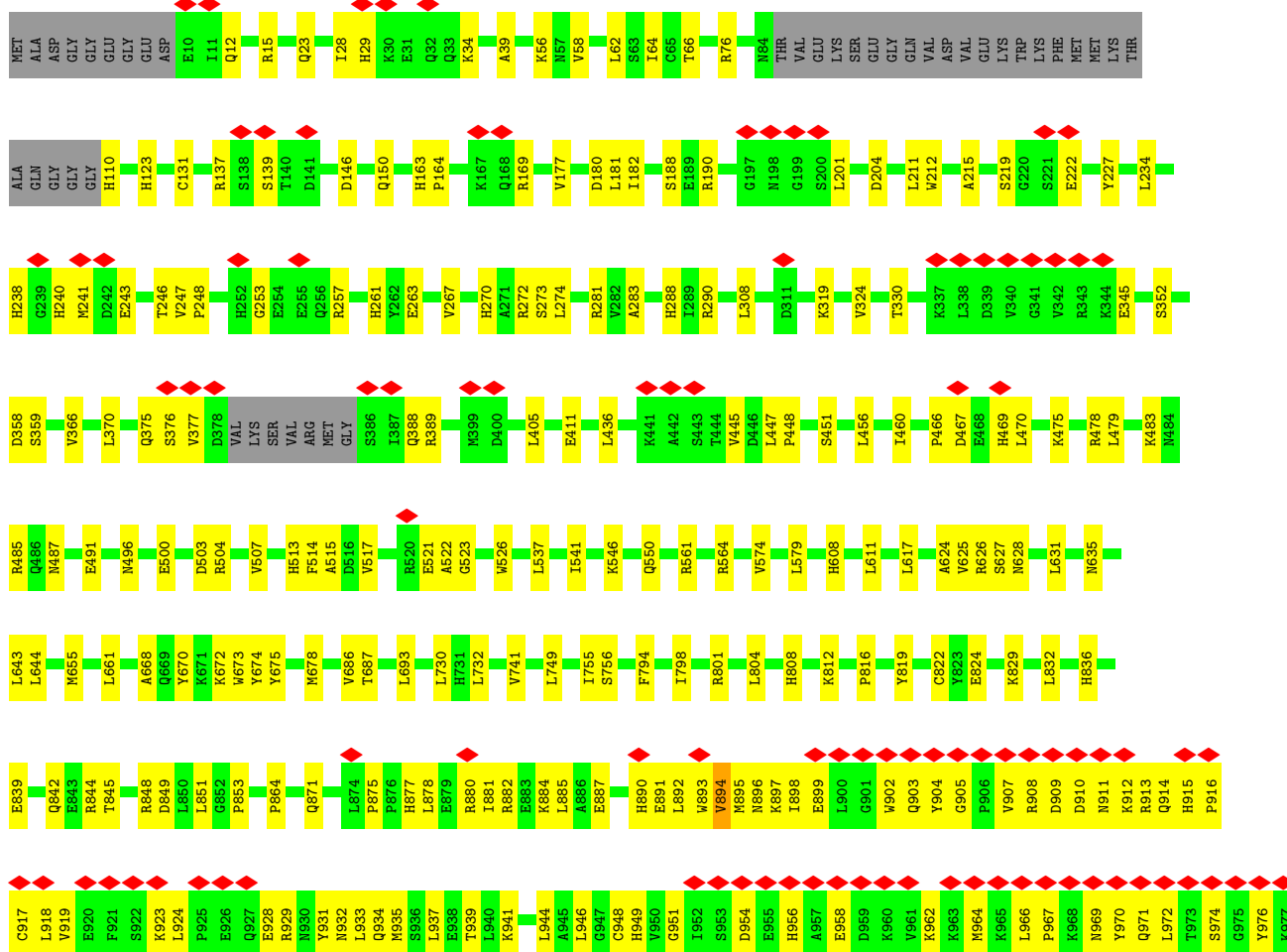




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A3042	A3042	L2833	S2834	S2764	L2623	L2623	L2489	GLU	LEU
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F2982	F2982	L2833	S2834	L2774	L2712	L2712	L2498	D2384	GLN
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C2991	C2991	L2833	S2834	L2778	L2716	L2716	L2502	D2388	PRO
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G2993	G2993	L2833	S2834	L2780	L2718	L2718	L2504	D2390	GLU
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L3007	L3007	L2833	S2834	L2793	L2731	L2731	L2517	D2403	SER
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R3016	R3016	L2833	S2834	L2798	L2736	L2736	L2522	D2408	SER
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		L2833	S2834	L2875	L2813	L2813	L2599	D2485	SER
		L2833	S2834	L2876	L2814	L2814	L2600	D2486	SER
		L2833	S2834	L2877	L2815	L2815	L2601	D2487	SER
		L2833	S2834	L2878	L2816	L2816	L2602	D2488	SER
		L2833	S2834	L2879	L2817	L2817	L2603	D2489	SER
		L2833	S2834	L2880	L2818	L2818	L2604	D2490	SER
		L2833	S2834	L2881	L2819	L2819	L2605	D2491	SER
		L2833	S2834	L2882	L2820	L2820	L2606	D2492	SER
		L2833	S2834	L2883	L2821	L2821	L2607	D2493	SER
		L2833	S2834	L2884	L2822	L2822	L2608	D2494	SER
		L2833	S2834	L2885	L2823	L2823	L2609	D2495	SER
		L2833	S2834	L2886	L2824	L2824	L2610	D2496	SER
		L2833	S2834	L2887	L2825	L2825	L2611	D2497	SER
		L2833	S2834	L2888	L2826	L2826	L2612	D2498	SER
		L2833	S2834	L2889	L2827	L2827	L2613	D2499	SER
		L2833	S2834	L2890	L2828	L2828	L2614	D2500	SER
		L2833	S2834	L2891	L2829	L2829	L2615	D2501	SER
		L2833	S2834	L2892	L2830	L2830	L2616	D2502	SER
		L2833	S2834	L2893	L2831	L2831	L2617	D2503	SER
		L2833	S2834	L2894	L2832	L2832	L2618	D2504	SER
		L2833	S2834	L2895	L2833	L2833	L2619	D2505	SER
		L2833	S2834	L2896	L2834	L2834	L2620	D2506	SER
		L2833	S2834	L2897	L2835	L2835	L2621	D2507	SER
		L2833	S2834	L2898	L2836	L2836	L2622	D2508	SER
		L2833	S2834	L2899	L2837	L2837	L2623	D25	



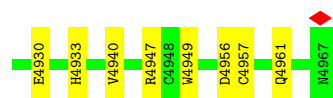
- Molecule 1: Ryanodine receptor 2



P978	A979	F980	G981	D982	L983	S984	F985	G986	K987	L988	T989	P990	S991	Q992	E993	I994	K995	V996	D997	K998	L999	A1000	H1004	A1008	R1009	D1010	R1011	I1012	R1013	Q1014	G1015	W1016	G1019	I1020	Q1021	Q1022	R1027	R1028	M1029	P1030	R1031	L1037	L1038	D1039	D1040	R1041	T1042	K1043	K1047	D1048	S1049	L1050	R1051
E1052	A1053	V1054	R1055	T1056	L1057	L1058	G1059	Y1060	G1061	Y1062	H1063	L1064	E1065	A1066	P1067	D1068	Q1069	D1070	H1071	A1072	A1073	R1074	A1075	E1076	V1077	C1078	S1079	G1080	T1081	Q1014	G1082	E1083	E1091	Y1094	R1100	V1108	G1111	D1112	M1113	S1118	P1124	G1129	F1140	K1141	W1145	W1156	V1161						
V1166	D1167	M1173	G1179	D1184	D1185	S1186	G1187	S1188	V1204	V1212	G1213	R1214	F1217	G1218	K1219	K1225	I1229	E1234	A1240	T1243	D1246	I1247	T1249	P1256	I1268	E1269	R1272	T1276	I1277	D1278	L1283	K1284	T1286	Q1287	K1288	G1291	S1292	Q1293	M1294														
S1295	N1296	M1300	R1303	L1304	E1312	K1316	THR	VAL	ALA	GLY	GLY	PRO	LEU	ARG	GLY	ALA	GLY	PHE	LEU	GLY	PRO	LYS	ASN	ASP	GLU	ASP	TYR	ASP	ALA	ASP	SER	PHE	GLU	VAL	LEU	GLY	LEU	VAL	PRO	ASP	ARG	VAL	ASP	LYS	ASP	LYS	GLU	ALA					
THR	LYS	PRO	GLU	PHE	ASN	ASN	HIS	LYS	ASP	TYR	ALA	GLN	GLU	PRO	LYS	ARG	LEU	LYS	GLN	ARG	PHE	LEU	LEU	ARG	ARG	THR	LYS	PRO	ASP	GLU	TYR	SER	HIS	SER	ALA	ARG	THR	GLU	VAL	ASP	VAL	LEU	ALA	ASP	R1414	D1415	Y1417	D1418	F1419	L1420	M1421	I1432	G1444
G1456	R1461	T1464	D1471	E1472	K1473	G1474	K1475	V1476	H1477	E1478	S1483	M1487	M1494	G1497	Q1498	G1499	R1500	N1501	N1502	G1504	L1505	T1548	F1555	R1559	M1564	K1576	C1582	L1586	H1593	V1594	M1599	F1603	V1608	I1611	Q1615	L1618																	
L1630	E1635	L1644	E1649	L1650	H1656	T1657	L1660	L1667	R1671	E1682	P1683	Q1684	L1685	I1689	Y1693	L1697	N1697	Y1703	L1706	T1716	A1717	R1718	L1719	M1720	E1724	M1729	L1748	P1749	G1750	I1751	L1757	I1771	L1784	D1785	I1786	K1788																	
M1831	G1832	F1834	L1839	T1842	V1850	E1853	A1854	THR	PRO	GLU	GLU	GLU	GLY	LYS	GLY	LEU	SER	THR	LEU	LYS	GLN	GLY	ALA	GLY	GLU	GLU	ALA	LYS	ARG	P1859	K1890	E1891	G1892	Q1895	L1898	V1902	Q1911																
C1914	V1918	I1922	V1926	D1930	D1931	F1932	L1936	Q1937	R1941	F1942	E1946	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1956	L1957	T1958	A1959	R1960	K1961	T1962	K1963	R1966	S1967	Q1972	I1973	R1974	M1975	L1976	F1979	D1982	K1983	S1984	E1985	C1986	P1989	E1990	E1991	I1992	R1993								
L1996	H2000	K2004	L2009	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	SER	ASP	THR	ILE	ARG	GLY	ARG	GLY	ARG	LEU	LEU	SER	VAL	GLU	LYS	THR	TYR	LEU	LYS	LYS	GLN	ALA	GLU	LYS	PRO	VAL	GLU	SER	ASP	SER	K2053	K2054	S2055	Z2056	T2057	L2058	Q2059	Q2060	Q2071
D2077	V2081	L2087	R2090	Q2091	L2095	G2096	V2099	I2117	L2120	A2121	S2122	I2126	R2127	L2130	M2142	I2143	L2146	F2155	P2159	R2162	M2163	M2172	E2173	V2174	M2175	V2176	M2177	V2178	L2179	G2180	G2181	G2182	E2183	S2184	K2185	E2186	I2187	M2192	V2193	A2194	L2200												
C2201	Y2202	I2206	Q2209	K2212	F2215	Y2220	L2221	L2222	V2227	P2230	A2233	N2234	S2237	A2243	V2247	E2252	L2253	L2257	R2258	E2259	P2260	D2261	E2262	E2263	K2264	V2265	R2266	R2267	L2274	M2279	K2283	G2284	Y2285	E2296	R2297	Y2298	V2319	L2323	R2327														
P2328	E2329	G2332	P2333	R2336	E2337	E2338	L2344	M2347	E2348	I2351	K2352	E2355	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLU	GLU	E2377	E2378	D2379	D2380	T2381	L2382	G2385	M2389	T2390	L2396	D2397	R2401	C2402	A2403	T2409	R2420	G2434	F2440	Q2441									

GLU	K3282	K3215	R3152	THR	L3014	E2952	L2877	GLN	M2739	S2870	L2580	M2442
ALA	I3283	E3216	S3153	ARG	V3015	H2953	E2981	THR	G2740	P2677	L2581	P2443
ARG	I3284	E3217	A3154	ASN	R3016	F2954	E2981	GLN	W2741	G2740	P2582	T2444
GLY	Y3285	I3218	L3155	GLN	H3017	F2955	E2981	VAL	I2742	Y2680	S2583	T2445
ASP	N3286	L3221	G3156	PRO	R3018	Y2956	K2884	SER	Y2743	M2681	M2584	A2446
MET	N3287	L3221	E3157	K3088	I3019	E2957	D2885	ASP	G2744	E2682	K2447	K2448
SER	K3288	S3224	C3158	V3090	S3020	Q2958	E2887	ALA	E2745	S2683	L2589	D2448
GLU	G3289	G3225	L3159	T3091	D3025	Q2959	Q2890	ALA	E2746	M2684	R2590	D2455
ALA	K3290	I3226	A3161	T3092	A3026	I2960	D2891	HIS	Y2747	Y2685	R2591	D2456
LEU	D3291	R3227	F3162	Q3092	I3029	K2961	L2892	HIS	D2748	Y2686	L2592	S2457
LEU	E3292	Y3228	A3163	I3093	V3030	F2962	D2893	ASP	S2749	M2687	V2593	
TLE	G3293	Y3229	A3164	N3095	I3033	F2963	K2894	ASP	Y2750	M2688	M2605	
LEU	A3294	Q3230	G3164	T3096	V3030	A2964	L2895	ALA	S2751	M2689	P2606	
LEU	W3295	M3231	F3166	Y3096	I3033	V2967	L2896	ALA	K2752	E2690	L2607	
ASP	M3296	P3232	P3167	P3097	H3034	Q2967	Q2897	ASP	Q2753	K2691	V2475	
GLU	K3297	H3233	P3168	T3097	I3035	L2968	Q2897	ASP	Q2754	Q2692	L2610	
PHE	R3298	W3234	V3168	A3100	L3036	L2898	Q2897	ASP	P2755	S2692	T2611	
THR	K3299	M3235	L3171	L3101	G3037	P2969	N2899	THR	Q2756	Q2693	N2612	
THR	A3300	E3236	A3169	L3102	P3038	L2970		THR	L2757	S2694	H2613	
LEU	V3301	V3237	F3170	P3103	T3039	I2971		LEU	K2758	M2695	Y2614	
ALA	F3302	V3238	L3171	M3104	L3040	D2972	A2902	ALA	P2759	D2696		
ARG	S3303	I3239	T3173	L3108	D3041	Y2974	G2906	ARG	Y2760	S2697	K2619	
ASP	Q3304	P3240	E3172	F3109	A3042	F2975	F2907	ASP	K2761	S2697	Y2620	
LEU	P3305	M3241	H3174	E3110	R3043	Q2976	K2908	LEU	L2762	E2698	Y2621	
TYR	I3306		L3175	H3111	T3044	N2977		TYR	L2763	C2622	C2622	
ALA	I3307		D3176	H3112	V3045	H2978	D2909	ALA	L2763	E2699	L2623	
PHE	N3308		K3177	G3113	M3046	R2979	L2910	PHE	S2764	G2699		
TYR	K3309		H3178	G3114	K3047	L2980	E2911	TYR	E2765	N2700	G2626	
PRO	K3309		I3179	Q3114	T3048	Y2981		PRO	K2766	F2701	G2627	
LEU	I3180		I3180					LEU			G2628	
TLE								TLE		Q2704	N2629	
ARG	Q3312		I3183	F3117	G3049	F2982	D2913	ARG	K2768	D2707	F2630	
ARG	L3314		I3184	G3118	L3050	L2983	T2914	ARG	E2769	T2708		
PHE	L3315		N3184	E3051	E3051	S2984	P2915	PHE	L2770	S2709	E2635	
VAL	K3316		N3185	G3119	V3052	A2985	S2916	VAL	L2771	N2710	E2636	
ASP	T3317		K3186	D3120	V3053	A2986	L2917	ASP	K2772	L2711	P2637	
TYR	F3319		K3187	L3121	K3054	S2987	E2918	TYR	P2773	L2712	L2638	
ASN	F3320		S3188	L3122	L3057	R2988	K2919	ASN	L2774	L2713	H2639	
ARG	L3321		S3189	L3123	R3058	P2989	L2920	ARG	L2775	T2713	L2640	
LYS	M3322		R3190	D3125	L3061	L2990	F2921	LYS	L2779	T2714	S2641	
TRP	E3324		K3192	E3124	D3062	C2991	Y2923	TRP	K2780	E2715	R2642	
LEU	K3325		E3191	E3124	N3063	S2992	L2929	LEU	W2785	K2716	L2644	
LYS	L3326		A3193	V3126	M3063	G2993	L2930	LYS	G2786	L2717	F2645	
GLU	K3327		A3194	Q3127	E3066	G2994		GLU	W2787	E2718	K2655	
PRO	K3328		L3195	Y3131	D3067	H2995	V2933	PRO	R2788	F2720	K2656	
PRO	K3329		L3196	L3134	L3068	A2996	D2934	PRO	Y2719	K2723	Y2657	
GLU	A3330		L3197	T3135	E3069	S2997	D2934	GLU	K2791	Y2724	E2658	
ALA	A3331		P3198	S3136	K3070	N2998	H2937	ALA	T2792	A2725	Q2659	
GLU	T3332		T3199	K3140	M3072	K2999	Q2938	GLU	E2794	H2726	F2662	
LEU	V3333		N3200	G3141	E3073	E3000	Y2939	LEU	K2799	K2737	K2663	
PHE	V3334		E3202	T3142	H3074	K3001	F2943	PHE	S2728	S2728	E2570	
ARG	S3335		D3203	K3144	Q3077	E3002	D2944	ARG	D2729	D2730	A2665	
MET	E3336		V3204	S3145	G3078	M3003	G2945	MET	H2737	H2737	L2666	
VAL	K3337		V3205	T3146	G3079	T3005	G2946	VAL	K2731	D2730	A2667	
ALA	ASP		I3208	Y3147	Q3079	S3006	S2947	ALA	W2732	K2731	P2667	
GLU	HIS		P3209	T3148	F3080	L3007	R2948	GLU	ARG	W2733		
LEU	LEU		S3210	V3148	T3081	K3010	K2948	LEU	THR	S2734		
LYS	LYS		L3211	E3149	F3081	L3011	G2949	LYS	ARG	D2735		
ALA	ALA		K3212	R3150	Q3151	L3011	G2950	ALA	ASP	K2736		
VAL	VAL		L3214	Q3151			G2951	VAL	ASP	A2738		





- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	83460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.550	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/34511	0.43	4/46614 (0.0%)
1	B	0.16	0/34511	0.43	4/46614 (0.0%)
1	C	0.16	0/34511	0.43	4/46614 (0.0%)
1	D	0.16	0/34511	0.43	4/46614 (0.0%)
2	E	0.16	0/834	0.45	0/1123
2	F	0.16	0/834	0.45	0/1123
2	G	0.16	0/834	0.44	0/1123
2	H	0.16	0/834	0.44	0/1123
All	All	0.16	0/141380	0.43	16/190948 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2004	MET	CB-CG-SD	5.52	129.27	112.70
1	A	2004	MET	CB-CG-SD	5.51	129.24	112.70
1	C	2004	MET	CB-CG-SD	5.51	129.22	112.70
1	D	2004	MET	CB-CG-SD	5.51	129.22	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	894	VAL	CA-C-N	-5.28	113.86	122.26
1	A	894	VAL	C-N-CA	-5.28	113.86	122.26
1	D	894	VAL	CA-C-N	-5.27	113.87	122.26
1	D	894	VAL	C-N-CA	-5.27	113.87	122.26
1	D	3277	LEU	CA-CB-CG	5.26	134.73	116.30
1	C	894	VAL	CA-C-N	-5.26	113.89	122.26
1	C	894	VAL	C-N-CA	-5.26	113.89	122.26
1	A	3277	LEU	CA-CB-CG	5.25	134.69	116.30
1	C	3277	LEU	CA-CB-CG	5.25	134.67	116.30
1	B	894	VAL	CA-C-N	-5.25	113.92	122.26
1	B	894	VAL	C-N-CA	-5.25	113.92	122.26
1	B	3277	LEU	CA-CB-CG	5.25	134.66	116.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3192	ARG	Sidechain
1	A	3926	GLY	Peptide
1	A	4640	PHE	Peptide
1	B	3192	ARG	Sidechain
1	B	3926	GLY	Peptide
1	B	4640	PHE	Peptide
1	C	3192	ARG	Sidechain
1	C	3926	GLY	Peptide
1	C	4640	PHE	Peptide
1	D	3192	ARG	Sidechain
1	D	3926	GLY	Peptide
1	D	4640	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33771	0	33455	839	0
1	B	33771	0	33455	840	0
1	C	33771	0	33455	844	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	33771	0	33455	854	0
2	E	818	0	821	25	0
2	F	818	0	821	23	0
2	G	818	0	821	26	0
2	H	818	0	821	27	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	9	0
4	B	62	0	24	9	0
4	C	62	0	24	9	0
4	D	62	0	24	10	0
5	A	23	0	0	7	0
5	B	23	0	0	7	0
5	C	23	0	0	7	0
5	D	23	0	0	7	0
All	All	138700	0	137200	3462	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (3462) 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:C:2142:MET:HE1	1:C:2174:VAL:HG11	1.44	0.98
1:B:2142:MET:HE1	1:B:2174:VAL:HG11	1.44	0.97
1:D:2142:MET:HE1	1:D:2174:VAL:HG11	1.44	0.97
1:A:2142:MET:HE1	1:A:2174:VAL:HG11	1.43	0.97
1:C:3227:ARG:HE	1:C:3228:TYR:H	1.13	0.92
1:B:4834:PRO:HB3	1:B:4843:ARG:HD3	1.51	0.92
1:D:4834:PRO:HB3	1:D:4843:ARG:HD3	1.51	0.92
1:A:3227:ARG:HE	1:A:3228:TYR:H	1.13	0.91
1:A:4834:PRO:HB3	1:A:4843:ARG:HD3	1.51	0.91
1:C:4834:PRO:HB3	1:C:4843:ARG:HD3	1.51	0.90
1:B:3260:ARG:NH1	1:B:3264:CYS:SG	2.47	0.88
1:D:3227:ARG:HE	1:D:3228:TYR:H	1.13	0.88
1:A:3260:ARG:NH1	1:A:3264:CYS:SG	2.47	0.88
1:C:3260:ARG:NH1	1:C:3264:CYS:SG	2.47	0.88
1:D:3260:ARG:NH1	1:D:3264:CYS:SG	2.47	0.88
1:B:3227:ARG:HE	1:B:3228:TYR:H	1.13	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2004:MET:HE2	1:C:2009:ILE:HG13	1.58	0.86
1:B:2004:MET:HE2	1:B:2009:ILE:HG13	1.58	0.85
1:B:3227:ARG:HH11	1:B:3290:ILE:HG13	1.41	0.84
1:D:3218:ILE:HD11	1:D:3276:LEU:HD22	1.60	0.84
1:D:2004:MET:HE2	1:D:2009:ILE:HG13	1.58	0.84
1:D:3227:ARG:HH11	1:D:3290:ILE:HG13	1.41	0.84
2:E:51:ILE:O	2:E:53:LYS:NZ	2.11	0.84
1:A:3227:ARG:HH11	1:A:3290:ILE:HG13	1.41	0.84
2:H:51:ILE:O	2:H:53:LYS:NZ	2.11	0.84
1:B:3270:SER:HA	1:B:3273:MET:HE2	1.60	0.84
1:C:3218:ILE:HD11	1:C:3276:LEU:HD22	1.60	0.84
1:A:3218:ILE:HD11	1:A:3276:LEU:HD22	1.60	0.83
1:A:3270:SER:HA	1:A:3273:MET:HE2	1.60	0.83
1:B:3218:ILE:HD11	1:B:3276:LEU:HD22	1.60	0.83
1:A:2004:MET:HE2	1:A:2009:ILE:HG13	1.58	0.83
1:C:3270:SER:HA	1:C:3273:MET:HE2	1.60	0.82
2:F:51:ILE:O	2:F:53:LYS:NZ	2.11	0.82
1:C:3227:ARG:HH11	1:C:3290:ILE:HG13	1.41	0.82
2:G:51:ILE:O	2:G:53:LYS:NZ	2.11	0.82
1:D:3270:SER:HA	1:D:3273:MET:HE2	1.60	0.81
1:B:1611:ILE:HD11	1:B:1618:LEU:HB2	1.62	0.81
1:C:1611:ILE:HD11	1:C:1618:LEU:HB2	1.62	0.81
1:B:891:GLU:HA	1:B:894:VAL:HG22	1.63	0.81
1:C:3127:GLN:HG3	1:C:3183:ILE:HB	1.63	0.80
1:A:891:GLU:HA	1:A:894:VAL:HG22	1.63	0.80
1:A:1611:ILE:HD11	1:A:1618:LEU:HB2	1.62	0.80
1:D:2719:TYR:HE2	1:D:2799:ALA:HB2	1.47	0.80
1:C:891:GLU:HA	1:C:894:VAL:HG22	1.63	0.80
1:C:2719:TYR:HE2	1:C:2799:ALA:HB2	1.47	0.80
1:D:891:GLU:HA	1:D:894:VAL:HG22	1.63	0.80
1:B:3292:GLU:HG2	1:B:3334:VAL:HG21	1.65	0.79
1:B:3127:GLN:HG3	1:B:3183:ILE:HB	1.63	0.79
1:A:2719:TYR:HE2	1:A:2799:ALA:HB2	1.47	0.79
1:D:1611:ILE:HD11	1:D:1618:LEU:HB2	1.62	0.79
1:A:3292:GLU:HG2	1:A:3334:VAL:HG21	1.65	0.79
1:D:3292:GLU:HG2	1:D:3334:VAL:HG21	1.64	0.79
1:D:3127:GLN:HG3	1:D:3183:ILE:HB	1.63	0.79
1:A:3127:GLN:HG3	1:A:3183:ILE:HB	1.63	0.79
1:C:3292:GLU:HG2	1:C:3334:VAL:HG21	1.65	0.78
1:B:2719:TYR:HE2	1:B:2799:ALA:HB2	1.47	0.78
4:B:5003:ATP:O2A	5:B:5004:KVR:C14	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1031:ARG:NH1	5:B:5004:KVR:O22	2.18	0.77
1:A:2998:ASN:ND2	1:A:3048:THR:OG1	2.18	0.77
1:D:2998:ASN:ND2	1:D:3048:THR:OG1	2.18	0.77
1:B:2998:ASN:ND2	1:B:3048:THR:OG1	2.18	0.77
1:C:1031:ARG:NH1	5:C:5004:KVR:O22	2.18	0.77
4:D:5003:ATP:O2A	5:D:5004:KVR:C14	2.32	0.77
1:A:3227:ARG:NH1	1:A:3290:ILE:O	2.18	0.77
4:A:5003:ATP:O2A	5:A:5004:KVR:C14	2.33	0.77
4:C:5003:ATP:O2A	5:C:5004:KVR:C14	2.33	0.76
1:A:1031:ARG:NH1	5:A:5004:KVR:O22	2.18	0.76
1:C:2998:ASN:ND2	1:C:3048:THR:OG1	2.18	0.76
1:C:3227:ARG:NH1	1:C:3290:ILE:O	2.18	0.76
1:C:1947:VAL:HG22	1:C:1961:LYS:HE2	1.68	0.75
1:D:1031:ARG:NH1	5:D:5004:KVR:O22	2.18	0.75
1:B:3227:ARG:NH1	1:B:3290:ILE:O	2.18	0.75
1:D:3227:ARG:NH1	1:D:3290:ILE:O	2.18	0.75
1:B:1947:VAL:HG22	1:B:1961:LYS:HE2	1.68	0.75
1:A:76:ARG:HD2	1:D:3890:TRP:HB3	1.67	0.74
1:B:3945:VAL:HG23	1:B:4006:SER:HB3	1.70	0.74
1:D:1947:VAL:HG22	1:D:1961:LYS:HE2	1.68	0.74
1:B:3674:THR:O	1:B:3679:LYS:NZ	2.21	0.74
1:C:3945:VAL:HG23	1:C:4006:SER:HB3	1.70	0.74
1:A:3674:THR:O	1:A:3679:LYS:NZ	2.21	0.74
1:B:2895:PHE:O	1:B:2899:ASN:ND2	2.21	0.74
1:D:2895:PHE:O	1:D:2899:ASN:ND2	2.21	0.74
1:A:1548:THR:O	1:D:2832:THR:OG1	2.05	0.73
1:A:1947:VAL:HG22	1:A:1961:LYS:HE2	1.68	0.73
1:C:3149:GLU:O	1:C:3152:ARG:NH1	2.21	0.73
1:A:3149:GLU:O	1:A:3152:ARG:NH1	2.21	0.73
1:C:483:LYS:O	1:C:487:ASN:ND2	2.21	0.73
4:C:5003:ATP:H5'2	5:C:5004:KVR:C20	2.19	0.73
1:A:3192:ARG:HH22	1:A:3197:LEU:HD23	1.54	0.73
1:C:2895:PHE:O	1:C:2899:ASN:ND2	2.21	0.73
1:C:3674:THR:O	1:C:3679:LYS:NZ	2.21	0.73
1:B:3149:GLU:O	1:B:3152:ARG:NH1	2.21	0.73
1:C:2929:LEU:HD11	1:C:2971:ILE:HG12	1.70	0.73
1:D:3192:ARG:HH22	1:D:3197:LEU:HD23	1.54	0.73
1:D:3674:THR:O	1:D:3679:LYS:NZ	2.21	0.73
1:A:483:LYS:O	1:A:487:ASN:ND2	2.21	0.73
1:A:2657:TYR:HA	1:A:2662:PHE:CE1	2.24	0.73
1:D:3042:ALA:HB3	1:D:3117:PHE:HE1	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3149:GLU:O	1:D:3152:ARG:NH1	2.21	0.73
4:D:5003:ATP:H5'2	5:D:5004:KVR:C20	2.19	0.73
1:C:3817:LEU:HD23	1:C:3819:MET:HE2	1.71	0.73
1:D:2657:TYR:HA	1:D:2662:PHE:CE1	2.24	0.73
1:A:2711:ILE:O	1:A:2780:LYS:NZ	2.21	0.72
1:A:2799:ALA:O	1:A:2802:ASN:ND2	2.22	0.72
1:B:2711:ILE:O	1:B:2780:LYS:NZ	2.22	0.72
1:C:2799:ALA:O	1:C:2802:ASN:ND2	2.22	0.72
1:A:2895:PHE:O	1:A:2899:ASN:ND2	2.21	0.72
1:A:3945:VAL:HG23	1:A:4006:SER:HB3	1.70	0.72
1:A:4640:PHE:CD2	1:A:4641:PRO:HD3	2.24	0.72
1:B:2657:TYR:HA	1:B:2662:PHE:CE1	2.24	0.72
4:B:5003:ATP:H5'2	5:B:5004:KVR:C20	2.19	0.72
1:C:4640:PHE:CD2	1:C:4641:PRO:HD3	2.24	0.72
1:B:1268:ILE:HD11	1:B:1300:MET:HE2	1.71	0.72
1:B:3817:LEU:HD23	1:B:3819:MET:HE2	1.71	0.72
1:B:4640:PHE:CD2	1:B:4641:PRO:HD3	2.24	0.72
1:C:3042:ALA:HB3	1:C:3117:PHE:HE1	1.54	0.72
1:B:3890:TRP:HB3	1:C:76:ARG:HD2	1.71	0.72
1:D:483:LYS:O	1:D:487:ASN:ND2	2.21	0.72
1:D:3945:VAL:HG23	1:D:4006:SER:HB3	1.70	0.72
1:B:958:GLU:HG2	1:B:1061:GLY:HA3	1.72	0.72
1:C:2657:TYR:HA	1:C:2662:PHE:CE1	2.24	0.72
1:D:958:GLU:HG2	1:D:1061:GLY:HA3	1.72	0.72
1:A:3042:ALA:HB3	1:A:3117:PHE:HE1	1.54	0.72
1:B:678:MET:SD	1:B:801:ARG:NH2	2.63	0.72
1:B:2929:LEU:HD11	1:B:2971:ILE:HG12	1.70	0.72
1:C:3192:ARG:HH22	1:C:3197:LEU:HD23	1.54	0.72
1:D:678:MET:SD	1:D:801:ARG:NH2	2.63	0.72
1:A:3817:LEU:HD23	1:A:3819:MET:HE2	1.71	0.72
4:A:5003:ATP:H5'2	5:A:5004:KVR:C20	2.19	0.72
1:B:2799:ALA:O	1:B:2802:ASN:ND2	2.22	0.72
1:B:3042:ALA:HB3	1:B:3117:PHE:HE1	1.54	0.72
1:C:2711:ILE:O	1:C:2780:LYS:NZ	2.22	0.71
1:A:1268:ILE:HD11	1:A:1300:MET:HE2	1.71	0.71
1:B:3192:ARG:HH22	1:B:3197:LEU:HD23	1.54	0.71
1:C:3890:TRP:HB3	1:D:76:ARG:HD2	1.71	0.71
1:D:2799:ALA:O	1:D:2802:ASN:ND2	2.22	0.71
1:D:2929:LEU:HD11	1:D:2971:ILE:HG12	1.70	0.71
1:A:2929:LEU:HD11	1:A:2971:ILE:HG12	1.70	0.71
1:A:678:MET:SD	1:A:801:ARG:NH2	2.63	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:LYS:O	1:B:487:ASN:ND2	2.21	0.71
1:C:678:MET:SD	1:C:801:ARG:NH2	2.63	0.71
1:C:1268:ILE:HD11	1:C:1300:MET:HE2	1.71	0.71
1:D:4640:PHE:CD2	1:D:4641:PRO:HD3	2.24	0.71
1:B:2743:TYR:HD1	1:B:2757:MET:HB2	1.56	0.71
1:D:3817:LEU:HD23	1:D:3819:MET:HE2	1.71	0.71
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.72	0.71
1:D:1268:ILE:HD11	1:D:1300:MET:HE2	1.71	0.71
1:C:882:ARG:NH2	1:C:933:LEU:O	2.24	0.71
1:C:2832:THR:OG1	1:D:1548:THR:O	2.09	0.71
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.72	0.70
1:C:958:GLU:HG2	1:C:1061:GLY:HA3	1.72	0.70
1:C:2743:TYR:HD1	1:C:2757:MET:HB2	1.56	0.70
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.72	0.70
1:A:882:ARG:NH2	1:A:933:LEU:O	2.24	0.70
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.72	0.70
1:B:2004:MET:HE1	1:B:2095:ILE:HD13	1.74	0.70
1:B:882:ARG:NH2	1:B:933:LEU:O	2.24	0.70
1:A:2832:THR:OG1	1:B:1548:THR:O	2.09	0.70
1:A:2996:ALA:O	1:A:3001:LYS:NZ	2.25	0.70
1:C:2004:MET:HE1	1:C:2095:ILE:HD13	1.74	0.70
1:C:2996:ALA:O	1:C:3001:LYS:NZ	2.25	0.70
1:D:882:ARG:NH2	1:D:933:LEU:O	2.24	0.70
1:A:958:GLU:HG2	1:A:1061:GLY:HA3	1.72	0.70
1:A:2743:TYR:HD1	1:A:2757:MET:HB2	1.56	0.70
1:D:2890:GLN:HB3	1:D:2894:LYS:HE2	1.72	0.70
1:D:2996:ALA:O	1:D:3001:LYS:NZ	2.25	0.70
1:B:2890:GLN:HB3	1:B:2894:LYS:HE2	1.72	0.70
1:A:2890:GLN:HB3	1:A:2894:LYS:HE2	1.72	0.69
1:D:2729:HIS:N	1:D:2771:TYR:OH	2.25	0.69
1:A:2004:MET:HE1	1:A:2095:ILE:HD13	1.74	0.69
1:D:2743:TYR:HD1	1:D:2757:MET:HB2	1.56	0.69
1:A:2744:GLY:HA3	1:A:2753:VAL:HB	1.75	0.69
1:C:2729:HIS:N	1:C:2771:TYR:OH	2.26	0.69
1:C:2890:GLN:HB3	1:C:2894:LYS:HE2	1.72	0.69
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.75	0.69
1:D:2004:MET:HE1	1:D:2095:ILE:HD13	1.74	0.69
1:A:2607:LEU:HD11	1:A:2664:LEU:HG	1.75	0.69
1:A:2729:HIS:N	1:A:2771:TYR:OH	2.26	0.69
1:B:2979:ARG:HH22	1:B:3035:ILE:HB	1.58	0.69
1:B:2996:ALA:O	1:B:3001:LYS:NZ	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3097:THR:HA	1:B:3101:LEU:HD12	1.75	0.69
1:C:2744:GLY:HA3	1:C:2753:VAL:HB	1.75	0.69
1:D:2979:ARG:HH22	1:D:3035:ILE:HB	1.58	0.69
1:A:2979:ARG:HH22	1:A:3035:ILE:HB	1.58	0.69
1:D:2711:ILE:O	1:D:2780:LYS:NZ	2.22	0.69
1:B:2729:HIS:N	1:B:2771:TYR:OH	2.26	0.69
1:C:2979:ARG:HH22	1:C:3035:ILE:HB	1.58	0.69
1:B:1972:GLN:HA	1:B:1975:MET:HE2	1.76	0.68
1:B:2832:THR:OG1	1:C:1548:THR:O	2.11	0.68
1:B:3016:ARG:NH2	1:B:3066:GLU:OE2	2.26	0.68
1:C:1972:GLN:HA	1:C:1975:MET:HE2	1.75	0.68
1:A:3097:THR:HA	1:A:3101:LEU:HD12	1.75	0.68
1:C:3016:ARG:NH2	1:C:3066:GLU:OE2	2.26	0.68
1:D:1972:GLN:HA	1:D:1975:MET:HE2	1.75	0.68
1:D:3097:THR:HA	1:D:3101:LEU:HD12	1.75	0.68
1:B:2744:GLY:HA3	1:B:2753:VAL:HB	1.74	0.68
1:C:2607:LEU:HD11	1:C:2664:LEU:HG	1.75	0.68
1:B:2607:LEU:HD11	1:B:2664:LEU:HG	1.75	0.68
1:C:3097:THR:HA	1:C:3101:LEU:HD12	1.75	0.68
1:D:2920:ARG:NH1	1:D:2981:TYR:OH	2.27	0.68
1:D:2744:GLY:HA3	1:D:2753:VAL:HB	1.75	0.68
2:E:24:VAL:HG22	2:E:48:LYS:HG2	1.75	0.68
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.75	0.68
1:D:2607:LEU:HD11	1:D:2664:LEU:HG	1.75	0.67
1:A:3016:ARG:NH2	1:A:3066:GLU:OE2	2.26	0.67
1:A:1972:GLN:HA	1:A:1975:MET:HE2	1.76	0.67
2:F:24:VAL:HG22	2:F:48:LYS:HG2	1.75	0.67
1:D:3016:ARG:NH2	1:D:3066:GLU:OE2	2.26	0.67
1:C:1788:LYS:HD3	1:C:1833:ILE:HG22	1.77	0.67
1:A:2920:ARG:NH1	1:A:2981:TYR:OH	2.27	0.67
1:B:3166:PHE:O	1:B:3248:ARG:NH2	2.28	0.67
1:C:2891:ASP:OD1	1:C:2892:ILE:N	2.28	0.67
1:A:2891:ASP:OD1	1:A:2892:ILE:N	2.28	0.67
1:B:2920:ARG:NH1	1:B:2981:TYR:OH	2.27	0.67
1:D:3166:PHE:O	1:D:3248:ARG:NH2	2.28	0.67
1:A:1074:ARG:HH22	1:A:1078:CYS:HB3	1.58	0.67
1:B:1788:LYS:HD3	1:B:1833:ILE:HG22	1.77	0.67
1:C:2920:ARG:NH1	1:C:2981:TYR:OH	2.27	0.67
1:A:3890:TRP:HB3	1:B:76:ARG:HD2	1.76	0.66
1:D:2891:ASP:OD1	1:D:2892:ILE:N	2.28	0.66
1:B:4031:THR:OG1	1:B:4055:HIS:NE2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1074:ARG:HH22	1:C:1078:CYS:HB3	1.58	0.66
1:D:1074:ARG:HH22	1:D:1078:CYS:HB3	1.58	0.66
1:D:3314:LEU:O	1:D:3318:HIS:HB2	1.96	0.66
1:B:1498:GLN:HG2	1:B:1499:GLY:H	1.61	0.66
1:A:1788:LYS:HD3	1:A:1833:ILE:HG22	1.77	0.66
1:D:1788:LYS:HD3	1:D:1833:ILE:HG22	1.77	0.66
1:D:1986:CYS:SG	1:D:1993:ARG:NH2	2.69	0.66
1:A:3314:LEU:O	1:A:3318:HIS:HB2	1.96	0.66
1:D:1498:GLN:HG2	1:D:1499:GLY:H	1.61	0.66
1:A:1498:GLN:HG2	1:A:1499:GLY:H	1.61	0.66
1:A:2943:PHE:HZ	1:A:2956:TYR:HB2	1.61	0.66
1:C:3314:LEU:O	1:C:3318:HIS:HB2	1.96	0.66
1:C:4031:THR:OG1	1:C:4055:HIS:NE2	2.29	0.66
1:A:895:MET:HB3	1:A:972:LEU:HB3	1.78	0.66
1:B:895:MET:HB3	1:B:972:LEU:HB3	1.78	0.66
1:B:2891:ASP:OD1	1:B:2892:ILE:N	2.28	0.66
1:C:875:PRO:HD2	1:C:878:LEU:HD12	1.78	0.66
1:C:1986:CYS:SG	1:C:1993:ARG:NH2	2.69	0.65
1:B:3314:LEU:O	1:B:3318:HIS:HB2	1.96	0.65
1:C:895:MET:HB3	1:C:972:LEU:HB3	1.78	0.65
1:D:2943:PHE:HZ	1:D:2956:TYR:HB2	1.61	0.65
1:A:875:PRO:HD2	1:A:878:LEU:HD12	1.78	0.65
1:B:875:PRO:HD2	1:B:878:LEU:HD12	1.78	0.65
1:B:2769:GLU:O	1:B:2771:TYR:N	2.27	0.65
1:B:2972:ASP:HA	1:B:3035:ILE:HD11	1.78	0.65
1:D:981:MET:HE1	1:D:1055:ARG:HG3	1.79	0.65
1:A:2769:GLU:O	1:A:2771:TYR:N	2.27	0.65
1:A:3166:PHE:O	1:A:3248:ARG:NH2	2.28	0.65
1:B:844:ARG:NH1	1:B:845:THR:OG1	2.30	0.65
1:D:1911:GLN:OE1	1:D:2090:ARG:NH1	2.30	0.65
1:D:2916:SER:HB3	1:D:2919:LYS:HB2	1.79	0.65
1:A:1986:CYS:SG	1:A:1993:ARG:NH2	2.69	0.65
1:A:2916:SER:HB3	1:A:2919:LYS:HB2	1.79	0.65
1:B:2057:THR:HB	1:B:2060:GLN:HG3	1.79	0.65
1:C:1498:GLN:HG2	1:C:1499:GLY:H	1.61	0.65
1:C:2972:ASP:HA	1:C:3035:ILE:HD11	1.78	0.65
1:B:2916:SER:HB3	1:B:2919:LYS:HB2	1.79	0.65
1:C:919:VAL:HG21	1:C:923:LYS:HZ2	1.61	0.65
1:C:3166:PHE:O	1:C:3248:ARG:NH2	2.28	0.65
1:B:1074:ARG:HH22	1:B:1078:CYS:HB3	1.58	0.65
1:C:2570:GLU:HG2	1:C:2605:MET:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2937:HIS:HA	1:D:3014:LEU:HD11	1.79	0.65
1:A:2057:THR:HB	1:A:2060:GLN:HG3	1.79	0.65
1:B:1986:CYS:SG	1:B:1993:ARG:NH2	2.69	0.65
1:C:844:ARG:NH1	1:C:845:THR:OG1	2.30	0.65
1:C:1456:GLY:O	1:C:1461:ARG:NH2	2.30	0.65
1:C:2159:PRO:HA	1:C:2162:MET:HE2	1.79	0.65
1:D:895:MET:HB3	1:D:972:LEU:HB3	1.78	0.65
1:D:4667:SER:HB2	1:D:4674:LYS:HE2	1.79	0.65
1:A:844:ARG:NH1	1:A:845:THR:OG1	2.30	0.65
1:D:844:ARG:NH1	1:D:845:THR:OG1	2.30	0.65
1:A:981:MET:HE1	1:A:1055:ARG:HG3	1.78	0.64
1:C:3231:MET:HE3	1:C:3233:HIS:HB2	1.80	0.64
1:C:2057:THR:HB	1:C:2060:GLN:HG3	1.79	0.64
1:D:875:PRO:HD2	1:D:878:LEU:HD12	1.78	0.64
1:B:1911:GLN:OE1	1:B:2090:ARG:NH1	2.30	0.64
1:C:2916:SER:HB3	1:C:2919:LYS:HB2	1.79	0.64
1:D:4031:THR:OG1	1:D:4055:HIS:NE2	2.29	0.64
1:A:4031:THR:OG1	1:A:4055:HIS:NE2	2.29	0.64
1:B:2570:GLU:HG2	1:B:2605:MET:HB2	1.79	0.64
1:A:1911:GLN:OE1	1:A:2090:ARG:NH1	2.30	0.64
1:B:2159:PRO:HA	1:B:2162:MET:HE2	1.79	0.64
1:C:1911:GLN:OE1	1:C:2090:ARG:NH1	2.30	0.64
1:C:2937:HIS:HA	1:C:3014:LEU:HD11	1.79	0.64
1:C:2943:PHE:HZ	1:C:2956:TYR:HB2	1.61	0.64
1:C:4667:SER:HB2	1:C:4674:LYS:HE2	1.79	0.64
1:D:1456:GLY:O	1:D:1461:ARG:NH2	2.30	0.64
1:B:919:VAL:HG21	1:B:923:LYS:HZ1	1.62	0.64
1:A:2159:PRO:HA	1:A:2162:MET:HE2	1.79	0.64
1:B:864:PRO:HB2	1:B:1009:ARG:HG2	1.80	0.64
1:C:864:PRO:HB2	1:C:1009:ARG:HG2	1.80	0.64
1:D:2057:THR:HB	1:D:2060:GLN:HG3	1.79	0.64
1:D:2570:GLU:HG2	1:D:2605:MET:HB2	1.79	0.64
1:A:864:PRO:HB2	1:A:1009:ARG:HG2	1.80	0.64
1:B:2943:PHE:HZ	1:B:2956:TYR:HB2	1.61	0.64
1:A:4667:SER:HB2	1:A:4674:LYS:HE2	1.79	0.64
1:C:981:MET:HE1	1:C:1055:ARG:HG3	1.79	0.64
1:C:3261:ALA:O	1:C:3262:GLU:HG3	1.98	0.64
1:D:2972:ASP:HA	1:D:3035:ILE:HD11	1.79	0.64
1:A:247:VAL:O	1:A:272:ARG:NH2	2.31	0.64
1:B:247:VAL:O	1:B:272:ARG:NH2	2.31	0.64
1:B:981:MET:HE1	1:B:1055:ARG:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3231:MET:HE3	1:B:3233:HIS:HB2	1.80	0.64
1:D:2670:SER:HB2	1:D:2973:GLN:HG2	1.79	0.64
1:D:864:PRO:HB2	1:D:1009:ARG:HG2	1.80	0.63
1:D:986:ILE:O	1:D:1055:ARG:NH2	2.32	0.63
1:D:3004:VAL:HA	1:D:3007:LEU:HD13	1.80	0.63
1:B:2670:SER:HB2	1:B:2973:GLN:HG2	1.79	0.63
1:A:2670:SER:HB2	1:A:2973:GLN:HG2	1.79	0.63
1:A:2972:ASP:HA	1:A:3035:ILE:HD11	1.79	0.63
1:A:3004:VAL:HA	1:A:3007:LEU:HD13	1.80	0.63
1:B:3261:ALA:O	1:B:3262:GLU:HG3	1.98	0.63
1:A:2478:ILE:HG21	1:A:2527:LEU:HD11	1.81	0.63
1:A:3231:MET:HE3	1:A:3233:HIS:HB2	1.80	0.63
1:C:2478:ILE:HG21	1:C:2527:LEU:HD11	1.81	0.63
1:C:3227:ARG:NH1	1:C:3287:ASN:HB2	2.14	0.63
1:A:986:ILE:O	1:A:1055:ARG:NH2	2.32	0.63
1:A:2570:GLU:HG2	1:A:2605:MET:HB2	1.79	0.63
1:B:904:TYR:HB2	1:B:918:LEU:HD23	1.81	0.63
1:C:839:GLU:HB3	1:C:851:LEU:HD12	1.80	0.63
1:B:2787:TRP:CZ2	1:B:2843:MET:HE3	2.34	0.63
1:B:2937:HIS:HA	1:B:3014:LEU:HD11	1.79	0.63
1:C:247:VAL:O	1:C:272:ARG:NH2	2.31	0.63
1:C:986:ILE:O	1:C:1055:ARG:NH2	2.32	0.63
1:D:3033:LEU:HD13	1:D:3104:MET:HB3	1.81	0.63
1:A:904:TYR:HB2	1:A:918:LEU:HD23	1.81	0.63
1:A:1456:GLY:O	1:A:1461:ARG:NH2	2.30	0.63
1:A:2787:TRP:CZ2	1:A:2843:MET:HE3	2.34	0.63
1:A:2937:HIS:HA	1:A:3014:LEU:HD11	1.79	0.63
1:C:2892:ILE:HG23	1:C:2893:LEU:HD12	1.81	0.63
1:D:247:VAL:O	1:D:272:ARG:NH2	2.31	0.63
1:D:932:ASN:HA	1:D:935:MET:HE2	1.81	0.63
1:B:4667:SER:HB2	1:B:4674:LYS:HE2	1.79	0.63
1:B:986:ILE:O	1:B:1055:ARG:NH2	2.32	0.62
1:B:2478:ILE:HG21	1:B:2527:LEU:HD11	1.81	0.62
1:B:2892:ILE:HG23	1:B:2893:LEU:HD12	1.81	0.62
1:B:3227:ARG:NH1	1:B:3287:ASN:HB2	2.13	0.62
1:C:964:MET:HB3	1:C:979:ALA:HB3	1.81	0.62
1:C:2670:SER:HB2	1:C:2973:GLN:HG2	1.79	0.62
1:D:839:GLU:HB3	1:D:851:LEU:HD12	1.80	0.62
1:D:919:VAL:HG21	1:D:923:LYS:HZ2	1.62	0.62
1:D:2478:ILE:HG21	1:D:2527:LEU:HD11	1.81	0.62
1:D:3227:ARG:NH1	1:D:3287:ASN:HB2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4200:MET:HE2	1:D:4923:MET:HE1	1.81	0.62
1:A:3261:ALA:O	1:A:3262:GLU:HG3	1.98	0.62
1:C:1464:THR:HG22	1:C:1483:SER:HB2	1.81	0.62
1:C:2787:TRP:CZ2	1:C:2843:MET:HE3	2.34	0.62
1:C:4609:LYS:HD2	1:C:4615:LEU:HD13	1.82	0.62
1:D:2787:TRP:CZ2	1:D:2843:MET:HE3	2.34	0.62
1:D:2892:ILE:HG23	1:D:2893:LEU:HD12	1.81	0.62
1:D:3261:ALA:O	1:D:3262:GLU:HG3	1.98	0.62
1:A:4930:GLU:HA	1:A:4933:HIS:CD2	2.35	0.62
1:B:964:MET:HB3	1:B:979:ALA:HB3	1.81	0.62
1:C:932:ASN:HA	1:C:935:MET:HE2	1.81	0.62
1:C:3033:LEU:HD13	1:C:3104:MET:HB3	1.81	0.62
1:D:3250:TRP:CE3	1:D:3273:MET:HE3	2.34	0.62
1:B:1464:THR:HG22	1:B:1483:SER:HB2	1.81	0.62
1:B:4930:GLU:HA	1:B:4933:HIS:CD2	2.35	0.62
1:C:4930:GLU:HA	1:C:4933:HIS:CD2	2.35	0.62
1:D:2159:PRO:HA	1:D:2162:MET:HE2	1.79	0.62
1:A:3033:LEU:HD13	1:A:3104:MET:HB3	1.81	0.62
1:A:4609:LYS:HD2	1:A:4615:LEU:HD13	1.82	0.62
1:B:891:GLU:OE1	1:B:895:MET:HE1	2.00	0.62
1:B:3033:LEU:HD13	1:B:3104:MET:HB3	1.81	0.62
1:B:3250:TRP:CE3	1:B:3273:MET:HE3	2.34	0.62
1:A:954:ASP:OD2	1:A:956:HIS:NE2	2.33	0.62
1:A:3037:GLY:HA2	1:A:3040:LEU:HD23	1.81	0.62
1:A:3227:ARG:NH1	1:A:3287:ASN:HB2	2.14	0.62
1:A:3259:GLU:O	1:A:3260:ARG:HD3	2.00	0.62
1:A:4082:GLU:HA	1:A:4085:LYS:HE2	1.82	0.62
1:B:3259:GLU:O	1:B:3260:ARG:HD3	2.00	0.62
1:B:4609:LYS:HD2	1:B:4615:LEU:HD13	1.82	0.62
1:D:4930:GLU:HA	1:D:4933:HIS:CD2	2.35	0.62
1:A:3250:TRP:CE3	1:A:3273:MET:HE3	2.34	0.62
1:C:4200:MET:HE2	1:C:4923:MET:HE1	1.81	0.62
1:D:4082:GLU:HA	1:D:4085:LYS:HE2	1.82	0.62
1:A:964:MET:HB3	1:A:979:ALA:HB3	1.82	0.62
2:F:22:THR:HA	2:F:50:ARG:HA	1.81	0.62
1:B:839:GLU:HB3	1:B:851:LEU:HD12	1.80	0.62
1:C:1303:ARG:NH2	1:C:1635:GLU:OE1	2.33	0.62
1:C:2769:GLU:O	1:C:2771:TYR:N	2.27	0.62
1:D:2769:GLU:O	1:D:2771:TYR:N	2.27	0.62
1:D:3231:MET:HE3	1:D:3233:HIS:HB2	1.80	0.62
1:D:4609:LYS:HD2	1:D:4615:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2717:LEU:HD23	1:A:2779:LEU:HD23	1.82	0.62
1:B:1303:ARG:NH2	1:B:1635:GLU:OE1	2.33	0.62
1:C:3004:VAL:HA	1:C:3007:LEU:HD13	1.80	0.62
1:C:3259:GLU:O	1:C:3260:ARG:HD3	2.00	0.62
1:A:2892:ILE:HG23	1:A:2893:LEU:HD12	1.81	0.62
1:A:4200:MET:HE2	1:A:4923:MET:HE1	1.81	0.62
2:E:22:THR:HA	2:E:50:ARG:HA	1.81	0.62
1:D:964:MET:HB3	1:D:979:ALA:HB3	1.81	0.62
1:A:3042:ALA:HB3	1:A:3117:PHE:CE1	2.35	0.61
4:A:5003:ATP:H5'1	5:A:5004:KVR:C14	2.30	0.61
1:B:932:ASN:HA	1:B:935:MET:HE2	1.81	0.61
1:C:954:ASP:OD2	1:C:956:HIS:NE2	2.33	0.61
1:D:891:GLU:OE1	1:D:895:MET:HE1	2.00	0.61
1:A:839:GLU:HB3	1:A:851:LEU:HD12	1.80	0.61
1:B:1456:GLY:O	1:B:1461:ARG:NH2	2.30	0.61
1:B:3004:VAL:HA	1:B:3007:LEU:HD13	1.80	0.61
4:B:5003:ATP:H5'1	5:B:5004:KVR:C14	2.30	0.61
1:C:3250:TRP:CE3	1:C:3273:MET:HE3	2.34	0.61
4:C:5003:ATP:H5'1	5:C:5004:KVR:C14	2.30	0.61
1:B:466:PRO:HG2	1:B:479:LEU:HG	1.82	0.61
1:C:904:TYR:HB2	1:C:918:LEU:HD23	1.81	0.61
2:H:22:THR:HA	2:H:50:ARG:HA	1.81	0.61
1:B:3037:GLY:HA2	1:B:3040:LEU:HD23	1.81	0.61
1:B:4082:GLU:HA	1:B:4085:LYS:HE2	1.82	0.61
1:C:891:GLU:OE1	1:C:895:MET:HE1	2.00	0.61
1:D:3037:GLY:HA2	1:D:3040:LEU:HD23	1.81	0.61
1:A:928:GLU:OE2	1:A:932:ASN:ND2	2.34	0.61
2:G:22:THR:HA	2:G:50:ARG:HA	1.81	0.61
1:C:466:PRO:HG2	1:C:479:LEU:HG	1.82	0.61
1:C:3037:GLY:HA2	1:C:3040:LEU:HD23	1.81	0.61
1:A:891:GLU:OE1	1:A:895:MET:HE1	2.00	0.61
1:A:1464:THR:HG22	1:A:1483:SER:HB2	1.81	0.61
1:C:4082:GLU:HA	1:C:4085:LYS:HE2	1.82	0.61
1:D:1464:THR:HG22	1:D:1483:SER:HB2	1.81	0.61
1:A:2691:LYS:HZ1	1:A:2874:TYR:HB3	1.65	0.61
1:D:3259:GLU:O	1:D:3260:ARG:HD3	2.00	0.61
4:D:5003:ATP:H5'1	5:D:5004:KVR:C14	2.30	0.61
1:C:288:HIS:O	1:C:290:ARG:NH1	2.34	0.61
1:D:954:ASP:OD2	1:D:956:HIS:NE2	2.33	0.61
1:A:932:ASN:HA	1:A:935:MET:HE2	1.81	0.61
1:B:954:ASP:OD2	1:B:956:HIS:NE2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2717:LEU:HD23	1:B:2779:LEU:HD23	1.82	0.61
1:D:928:GLU:OE2	1:D:932:ASN:ND2	2.34	0.61
1:A:1303:ARG:NH2	1:A:1635:GLU:OE1	2.33	0.61
1:B:4200:MET:HE2	1:B:4923:MET:HE1	1.81	0.61
1:C:951:GLY:H	1:C:1064:LEU:HD23	1.66	0.61
1:D:904:TYR:HB2	1:D:918:LEU:HD23	1.81	0.61
1:C:2717:LEU:HD23	1:C:2779:LEU:HD23	1.82	0.60
1:B:1420:LEU:O	1:B:1564:MET:HE3	2.02	0.60
1:D:1303:ARG:NH2	1:D:1635:GLU:OE1	2.33	0.60
1:D:2717:LEU:HD23	1:D:2779:LEU:HD23	1.82	0.60
1:A:288:HIS:O	1:A:290:ARG:NH1	2.34	0.60
1:B:928:GLU:OE2	1:B:932:ASN:ND2	2.34	0.60
1:A:1420:LEU:O	1:A:1564:MET:HE3	2.02	0.60
1:B:949:HIS:HB2	1:B:1065:GLU:HB2	1.84	0.60
1:B:3606:ALA:HB1	1:B:3610:ASN:HB2	1.84	0.60
1:B:3042:ALA:HB3	1:B:3117:PHE:CE1	2.35	0.60
1:B:4107:GLU:OE1	1:B:4147:ARG:NH1	2.33	0.60
1:C:3606:ALA:HB1	1:C:3610:ASN:HB2	1.84	0.60
1:D:466:PRO:HG2	1:D:479:LEU:HG	1.82	0.60
1:D:3269:ASN:HB2	1:D:3272:HIS:ND1	2.16	0.60
1:A:466:PRO:HG2	1:A:479:LEU:HG	1.82	0.60
1:B:2930:ILE:O	1:B:3010:LYS:NZ	2.35	0.60
1:D:2096:GLY:HA2	1:D:2099:VAL:HG22	1.84	0.60
1:A:919:VAL:HG21	1:A:923:LYS:HZ1	1.65	0.60
1:A:2096:GLY:HA2	1:A:2099:VAL:HG22	1.84	0.60
1:A:3606:ALA:HB1	1:A:3610:ASN:HB2	1.84	0.60
1:B:1630:LEU:HD22	1:B:1644:LEU:HD11	1.84	0.60
1:C:1630:LEU:HD22	1:C:1644:LEU:HD11	1.84	0.60
1:C:3269:ASN:HB2	1:C:3272:HIS:ND1	2.16	0.60
1:C:949:HIS:HB2	1:C:1065:GLU:HB2	1.84	0.60
1:D:995:MET:O	1:D:998:LYS:HG3	2.02	0.60
1:A:3269:ASN:HB2	1:A:3272:HIS:ND1	2.16	0.60
1:C:928:GLU:OE2	1:C:932:ASN:ND2	2.34	0.60
1:C:995:MET:O	1:C:998:LYS:HG3	2.02	0.60
1:C:2692:GLN:HA	1:C:2695:MET:HE2	1.84	0.60
1:A:2723:LYS:HA	1:A:2726:GLU:HB2	1.83	0.59
1:D:288:HIS:O	1:D:290:ARG:NH1	2.34	0.59
1:D:951:GLY:H	1:D:1064:LEU:HD23	1.66	0.59
1:D:4107:GLU:OE1	1:D:4147:ARG:NH1	2.33	0.59
1:A:2930:ILE:O	1:A:3010:LYS:NZ	2.35	0.59
1:B:2692:GLN:HA	1:B:2695:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3160:ALA:HB2	1:B:3240:PRO:HB3	1.84	0.59
1:C:3257:ASN:ND2	1:C:3259:GLU:OE2	2.36	0.59
1:D:15:ARG:HD3	1:D:110:HIS:HB3	1.84	0.59
1:D:1420:LEU:O	1:D:1564:MET:HE3	2.02	0.59
1:A:995:MET:O	1:A:998:LYS:HG3	2.02	0.59
1:A:1630:LEU:HD22	1:A:1644:LEU:HD11	1.84	0.59
1:A:2973:GLN:NE2	1:A:2977:ASN:OD1	2.36	0.59
1:B:288:HIS:O	1:B:290:ARG:NH1	2.34	0.59
1:B:3269:ASN:HB2	1:B:3272:HIS:ND1	2.16	0.59
1:D:1630:LEU:HD22	1:D:1644:LEU:HD11	1.84	0.59
1:D:3001:LYS:HE3	1:D:3044:THR:HG21	1.84	0.59
1:D:3160:ALA:HB2	1:D:3240:PRO:HB3	1.84	0.59
1:C:2590:ARG:NH2	1:C:2875:ASP:OD2	2.35	0.59
1:C:3246:MET:HE3	1:C:3268:LEU:HD11	1.85	0.59
1:D:2692:GLN:HA	1:D:2695:MET:HE2	1.84	0.59
1:D:3606:ALA:HB1	1:D:3610:ASN:HB2	1.84	0.59
1:B:1757:LEU:HD22	1:B:2117:ILE:HD11	1.84	0.59
1:B:2096:GLY:HA2	1:B:2099:VAL:HG22	1.84	0.59
1:C:15:ARG:HD3	1:C:110:HIS:HB3	1.84	0.59
1:D:905:GLY:HA3	1:D:914:GLN:HB3	1.83	0.59
1:A:905:GLY:HA3	1:A:914:GLN:HB3	1.83	0.59
1:A:3920:LEU:HD22	1:A:3935:LEU:HD11	1.85	0.59
1:B:644:LEU:HD13	1:B:1630:LEU:HD21	1.84	0.59
1:B:3257:ASN:ND2	1:B:3259:GLU:OE2	2.36	0.59
1:C:2930:ILE:O	1:C:3010:LYS:NZ	2.35	0.59
1:D:644:LEU:HD13	1:D:1630:LEU:HD21	1.84	0.59
1:A:2590:ARG:NH2	1:A:2875:ASP:OD2	2.34	0.59
1:A:3209:PRO:HB3	1:A:3213:LYS:HD2	1.84	0.59
1:B:905:GLY:HA3	1:B:914:GLN:HB3	1.83	0.59
1:B:951:GLY:H	1:B:1064:LEU:HD23	1.66	0.59
1:C:1420:LEU:O	1:C:1564:MET:HE3	2.02	0.59
1:C:3042:ALA:HB3	1:C:3117:PHE:CE1	2.35	0.59
1:C:3209:PRO:HB3	1:C:3213:LYS:HD2	1.84	0.59
1:A:625:VAL:HG23	1:A:628:ASN:HB2	1.85	0.59
1:A:951:GLY:H	1:A:1064:LEU:HD23	1.66	0.59
1:C:2096:GLY:HA2	1:C:2099:VAL:HG22	1.84	0.59
1:C:3109:PHE:CE2	1:C:3162:PHE:HD1	2.20	0.59
1:D:625:VAL:HG23	1:D:628:ASN:HB2	1.85	0.59
1:D:2973:GLN:NE2	1:D:2977:ASN:OD1	2.36	0.59
1:D:3209:PRO:HB3	1:D:3213:LYS:HD2	1.84	0.59
1:A:3160:ALA:HB2	1:A:3240:PRO:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3257:ASN:ND2	1:A:3259:GLU:OE2	2.36	0.59
1:A:4238:ILE:HG13	1:B:4624:ASP:HB3	1.85	0.59
1:B:3001:LYS:HE3	1:B:3044:THR:HG21	1.84	0.59
1:B:3109:PHE:CE2	1:B:3162:PHE:HD1	2.21	0.59
1:B:3246:MET:HE3	1:B:3268:LEU:HD11	1.85	0.59
1:B:3920:LEU:HD22	1:B:3935:LEU:HD11	1.85	0.59
1:B:4030:ASP:HA	1:B:4033:LYS:HE2	1.85	0.59
4:B:5003:ATP:C5'	5:B:5004:KVR:C20	2.81	0.59
1:D:3257:ASN:ND2	1:D:3259:GLU:OE2	2.36	0.59
1:C:3160:ALA:HB2	1:C:3240:PRO:HB3	1.84	0.59
1:D:949:HIS:HB2	1:D:1065:GLU:HB2	1.84	0.59
1:D:2723:LYS:HA	1:D:2726:GLU:HB2	1.83	0.59
4:D:5003:ATP:C5'	5:D:5004:KVR:C20	2.81	0.59
1:B:3209:PRO:HB3	1:B:3213:LYS:HD2	1.84	0.58
1:D:2930:ILE:O	1:D:3010:LYS:NZ	2.35	0.58
1:A:626:ARG:NH2	1:A:1667:LEU:O	2.36	0.58
1:B:995:MET:O	1:B:998:LYS:HG3	2.02	0.58
1:B:2723:LYS:HA	1:B:2726:GLU:HB2	1.83	0.58
1:C:905:GLY:HA3	1:C:914:GLN:HB3	1.83	0.58
1:C:1757:LEU:HD22	1:C:2117:ILE:HD11	1.84	0.58
1:C:3016:ARG:NH1	1:C:3067:ASP:OD2	2.36	0.58
1:C:3649:ALA:HB1	1:C:3652:PRO:HB2	1.85	0.58
1:D:1757:LEU:HD22	1:D:2117:ILE:HD11	1.84	0.58
1:D:4481:TRP:HA	1:D:4484:ILE:HG12	1.86	0.58
1:A:2692:GLN:HA	1:A:2695:MET:HE2	1.84	0.58
1:A:2760:TYR:HA	1:A:2763:LEU:HD12	1.85	0.58
1:A:3109:PHE:CE2	1:A:3162:PHE:HD1	2.20	0.58
4:A:5003:ATP:C5'	5:A:5004:KVR:C20	2.81	0.58
1:B:880:ARG:O	1:B:884:LYS:NZ	2.36	0.58
1:B:2612:ASN:OD1	1:B:2613:HIS:N	2.37	0.58
1:B:3649:ALA:HB1	1:B:3652:PRO:HB2	1.85	0.58
1:D:3016:ARG:NH1	1:D:3067:ASP:OD2	2.37	0.58
1:A:4481:TRP:HA	1:A:4484:ILE:HG12	1.86	0.58
1:B:3227:ARG:HD3	1:B:3291:ASP:HB2	1.84	0.58
1:C:2723:LYS:HA	1:C:2726:GLU:HB2	1.83	0.58
1:C:3797:MET:HE1	1:C:3870:ILE:HG23	1.86	0.58
1:C:4030:ASP:HA	1:C:4033:LYS:HE2	1.85	0.58
1:D:28:ILE:HG22	1:D:29:HIS:CD2	2.38	0.58
1:D:3109:PHE:CE2	1:D:3162:PHE:HD1	2.21	0.58
1:A:4520:TYR:CE2	1:A:4559:TYR:HB3	2.39	0.58
1:B:15:ARG:HD3	1:B:110:HIS:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:VAL:HG23	1:C:628:ASN:HB2	1.85	0.58
1:C:2612:ASN:OD1	1:C:2613:HIS:N	2.37	0.58
4:C:5003:ATP:C5'	5:C:5004:KVR:C20	2.81	0.58
1:D:3042:ALA:HB3	1:D:3117:PHE:CE1	2.35	0.58
1:D:3246:MET:HE3	1:D:3268:LEU:HD11	1.85	0.58
1:A:880:ARG:O	1:A:884:LYS:NZ	2.36	0.58
1:A:2742:ILE:O	1:A:2754:GLN:N	2.20	0.58
1:B:28:ILE:HG22	1:B:29:HIS:CD2	2.38	0.58
1:B:625:VAL:HG23	1:B:628:ASN:HB2	1.85	0.58
1:B:2760:TYR:HA	1:B:2763:LEU:HD12	1.85	0.58
1:B:2973:GLN:NE2	1:B:2977:ASN:OD1	2.36	0.58
1:C:28:ILE:HG22	1:C:29:HIS:CD2	2.38	0.58
1:D:1269:GLU:HB2	1:D:1288:LYS:HG2	1.85	0.58
1:D:3920:LEU:HD22	1:D:3935:LEU:HD11	1.85	0.58
1:A:949:HIS:HB2	1:A:1065:GLU:HB2	1.84	0.58
1:C:3920:LEU:HD22	1:C:3935:LEU:HD11	1.85	0.58
1:D:2760:TYR:HA	1:D:2763:LEU:HD12	1.85	0.58
1:D:4520:TYR:CE2	1:D:4559:TYR:HB3	2.39	0.58
1:A:2333:PRO:HA	1:A:2336:ARG:HE	1.69	0.58
1:A:3227:ARG:HD3	1:A:3291:ASP:HB2	1.85	0.58
1:A:4832:GLU:O	1:A:4843:ARG:NH2	2.37	0.58
1:B:3235:MET:HA	1:B:3239:LEU:HD13	1.86	0.58
1:C:880:ARG:O	1:C:884:LYS:NZ	2.36	0.58
1:D:880:ARG:O	1:D:884:LYS:NZ	2.36	0.58
1:D:3227:ARG:HD3	1:D:3291:ASP:HB2	1.84	0.58
1:A:3001:LYS:HE3	1:A:3044:THR:HG21	1.84	0.58
1:A:3235:MET:HA	1:A:3239:LEU:HD13	1.86	0.58
1:B:4832:GLU:O	1:B:4843:ARG:NH2	2.37	0.58
1:C:2973:GLN:NE2	1:C:2977:ASN:OD1	2.36	0.58
1:D:2742:ILE:O	1:D:2754:GLN:N	2.20	0.58
1:A:15:ARG:HD3	1:A:110:HIS:HB3	1.84	0.58
1:A:644:LEU:HD13	1:A:1630:LEU:HD21	1.84	0.58
1:A:2612:ASN:OD1	1:A:2613:HIS:N	2.37	0.58
1:A:4030:ASP:HA	1:A:4033:LYS:HE2	1.85	0.58
1:C:1269:GLU:HB2	1:C:1288:LYS:HG2	1.85	0.58
1:C:2760:TYR:HA	1:C:2763:LEU:HD12	1.85	0.58
1:C:3001:LYS:HE3	1:C:3044:THR:HG21	1.84	0.58
1:D:436:LEU:HD11	1:D:447:LEU:HD11	1.86	0.58
1:D:2612:ASN:OD1	1:D:2613:HIS:N	2.37	0.58
1:D:2691:LYS:HZ1	1:D:2874:TYR:HB3	1.69	0.58
1:D:4832:GLU:O	1:D:4843:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2622:CYS:SG	1:A:2623:LEU:N	2.77	0.57
1:C:3227:ARG:HD3	1:C:3291:ASP:HB2	1.85	0.57
1:C:3235:MET:HA	1:C:3239:LEU:HD13	1.86	0.57
1:C:4481:TRP:HA	1:C:4484:ILE:HG12	1.86	0.57
1:D:3043:ARG:N	1:D:3117:PHE:HZ	2.02	0.57
1:C:644:LEU:HD13	1:C:1630:LEU:HD21	1.84	0.57
1:C:2742:ILE:O	1:C:2754:GLN:N	2.20	0.57
1:A:1269:GLU:HB2	1:A:1288:LYS:HG2	1.85	0.57
1:A:1757:LEU:HD22	1:A:2117:ILE:HD11	1.84	0.57
1:A:3246:MET:HE3	1:A:3268:LEU:HD11	1.85	0.57
4:A:5003:ATP:H5'2	5:A:5004:KVR:C15	2.35	0.57
1:B:1269:GLU:HB2	1:B:1288:LYS:HG2	1.85	0.57
1:B:4520:TYR:CE2	1:B:4559:TYR:HB3	2.39	0.57
1:D:3649:ALA:HB1	1:D:3652:PRO:HB2	1.86	0.57
1:D:3797:MET:HE1	1:D:3870:ILE:HG23	1.86	0.57
1:B:3069:GLU:HG3	1:B:3072:MET:HE2	1.87	0.57
4:B:5003:ATP:H5'2	5:B:5004:KVR:C15	2.35	0.57
1:C:4832:GLU:O	1:C:4843:ARG:NH2	2.37	0.57
1:D:4030:ASP:HA	1:D:4033:LYS:HE2	1.85	0.57
1:A:3649:ALA:HB1	1:A:3652:PRO:HB2	1.85	0.57
1:B:1785:ASP:OD2	1:B:1786:ILE:N	2.38	0.57
1:B:3016:ARG:NH1	1:B:3067:ASP:OD2	2.37	0.57
1:C:1611:ILE:HB	1:C:1615:GLN:HB2	1.86	0.57
1:C:2333:PRO:HA	1:C:2336:ARG:HE	1.69	0.57
1:C:2622:CYS:SG	1:C:2623:LEU:N	2.77	0.57
1:C:3043:ARG:N	1:C:3117:PHE:HZ	2.02	0.57
1:C:4520:TYR:CE2	1:C:4559:TYR:HB3	2.39	0.57
1:D:3235:MET:HA	1:D:3239:LEU:HD13	1.86	0.57
1:B:2742:ILE:O	1:B:2754:GLN:N	2.20	0.57
1:B:3797:MET:HE1	1:B:3870:ILE:HG23	1.86	0.57
1:C:3069:GLU:HG3	1:C:3072:MET:HE2	1.87	0.57
1:A:3016:ARG:NH1	1:A:3067:ASP:OD2	2.36	0.57
1:B:3043:ARG:N	1:B:3117:PHE:HZ	2.02	0.57
1:C:1914:CYS:SG	1:C:2091:GLN:NE2	2.77	0.57
1:D:1975:MET:HG3	1:D:1976:LEU:HD12	1.87	0.57
1:D:2333:PRO:HA	1:D:2336:ARG:HE	1.69	0.57
1:D:2622:CYS:SG	1:D:2623:LEU:N	2.77	0.57
1:A:436:LEU:HD11	1:A:447:LEU:HD11	1.86	0.57
1:A:1785:ASP:OD2	1:A:1786:ILE:N	2.38	0.57
1:B:263:GLU:OE2	1:B:388:GLN:NE2	2.38	0.57
1:B:2333:PRO:HA	1:B:2336:ARG:HE	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2622:CYS:SG	1:B:2623:LEU:N	2.77	0.57
1:B:4481:TRP:HA	1:B:4484:ILE:HG12	1.86	0.57
1:C:436:LEU:HD11	1:C:447:LEU:HD11	1.86	0.57
1:C:3192:ARG:NH1	1:C:3199:THR:HA	2.20	0.57
4:C:5003:ATP:H5'2	5:C:5004:KVR:C15	2.35	0.57
1:D:3015:VAL:HG11	1:D:3029:ILE:HG21	1.87	0.57
1:A:546:LYS:O	1:A:550:GLN:HG2	2.05	0.57
1:A:3043:ARG:N	1:A:3117:PHE:HZ	2.02	0.57
1:A:3069:GLU:HG3	1:A:3072:MET:HE2	1.87	0.57
1:A:3797:MET:HE1	1:A:3870:ILE:HG23	1.86	0.57
1:D:3002:GLU:O	1:D:3005:THR:OG1	2.22	0.57
1:B:1611:ILE:HB	1:B:1615:GLN:HB2	1.86	0.57
1:B:1989:PRO:HD2	1:B:1992:ILE:HD12	1.87	0.57
1:C:948:CYS:HA	1:C:1067:PRO:HD3	1.87	0.57
1:C:1989:PRO:HD2	1:C:1992:ILE:HD12	1.87	0.57
1:D:263:GLU:OE2	1:D:388:GLN:NE2	2.38	0.57
1:D:1611:ILE:HB	1:D:1615:GLN:HB2	1.86	0.57
1:D:3171:LEU:HG	1:D:3211:LEU:HB3	1.87	0.57
1:A:794:PHE:HB2	1:A:798:ILE:HG13	1.86	0.56
1:A:3002:GLU:O	1:A:3005:THR:OG1	2.22	0.56
1:B:948:CYS:HA	1:B:1067:PRO:HD3	1.87	0.56
1:C:794:PHE:HB2	1:C:798:ILE:HG13	1.87	0.56
1:C:3015:VAL:HG11	1:C:3029:ILE:HG21	1.87	0.56
1:A:28:ILE:HG22	1:A:29:HIS:CD2	2.38	0.56
1:A:3171:LEU:HG	1:A:3211:LEU:HB3	1.87	0.56
1:D:546:LYS:O	1:D:550:GLN:HG2	2.05	0.56
1:D:3069:GLU:HG3	1:D:3072:MET:HE2	1.87	0.56
1:D:3192:ARG:NH1	1:D:3199:THR:HA	2.20	0.56
1:A:263:GLU:OE2	1:A:388:GLN:NE2	2.38	0.56
1:A:1611:ILE:HB	1:A:1615:GLN:HB2	1.86	0.56
1:A:1989:PRO:HD2	1:A:1992:ILE:HD12	1.87	0.56
1:A:2403:ALA:HB2	1:A:2475:VAL:HG22	1.88	0.56
1:A:3192:ARG:NH1	1:A:3199:THR:HA	2.20	0.56
1:A:4107:GLU:OE1	1:A:4147:ARG:NH1	2.33	0.56
2:H:8:ILE:HA	1:D:730:LEU:HD11	1.86	0.56
1:B:436:LEU:HD11	1:B:447:LEU:HD11	1.86	0.56
1:B:3192:ARG:NH1	1:B:3199:THR:HA	2.20	0.56
1:C:1975:MET:HG3	1:C:1976:LEU:HD12	1.87	0.56
1:A:3227:ARG:NH1	1:A:3290:ILE:HG13	2.18	0.56
1:D:3209:PRO:HG2	1:D:3214:LEU:HD21	1.87	0.56
1:A:948:CYS:HA	1:A:1067:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1785:ASP:OD2	1:C:1786:ILE:N	2.38	0.56
1:C:3171:LEU:HG	1:C:3211:LEU:HB3	1.87	0.56
1:A:1975:MET:HG3	1:A:1976:LEU:HD12	1.87	0.56
1:B:3015:VAL:HG11	1:B:3029:ILE:HG21	1.87	0.56
1:B:3209:PRO:HG2	1:B:3214:LEU:HD21	1.87	0.56
1:C:263:GLU:OE2	1:C:388:GLN:NE2	2.38	0.56
1:C:2259:GLU:OE2	1:C:3806:ASN:ND2	2.39	0.56
1:D:1914:CYS:SG	1:D:2091:GLN:NE2	2.77	0.56
1:D:2403:ALA:HB2	1:D:2475:VAL:HG22	1.88	0.56
1:B:2403:ALA:HB2	1:B:2475:VAL:HG22	1.88	0.56
1:C:626:ARG:NH2	1:C:1667:LEU:O	2.36	0.56
1:C:2403:ALA:HB2	1:C:2475:VAL:HG22	1.88	0.56
1:A:515:ALA:HB2	1:A:523:GLY:HA3	1.88	0.56
1:A:2259:GLU:OE2	1:A:3806:ASN:ND2	2.39	0.56
1:A:2263:GLU:HG3	1:A:2267:ARG:NH1	2.21	0.56
1:B:515:ALA:HB2	1:B:523:GLY:HA3	1.88	0.56
1:D:794:PHE:HB2	1:D:798:ILE:HG13	1.87	0.56
1:D:948:CYS:HA	1:D:1067:PRO:HD3	1.86	0.56
1:D:1785:ASP:OD2	1:D:1786:ILE:N	2.38	0.56
1:D:1973:ILE:HG13	1:D:3619:LEU:HB3	1.87	0.56
1:D:1989:PRO:HD2	1:D:1992:ILE:HD12	1.87	0.56
4:D:5003:ATP:H5'2	5:D:5004:KVR:C15	2.35	0.56
1:A:3783:GLU:OE2	1:A:3784:LYS:NZ	2.39	0.56
1:B:794:PHE:HB2	1:B:798:ILE:HG13	1.86	0.56
1:B:3783:GLU:OE2	1:B:3784:LYS:NZ	2.39	0.56
1:C:3209:PRO:HG2	1:C:3214:LEU:HD21	1.87	0.56
1:C:4107:GLU:OE1	1:C:4147:ARG:NH1	2.33	0.56
1:D:2194:ALA:HA	1:D:2237:SER:HB3	1.88	0.56
1:D:2263:GLU:HG3	1:D:2267:ARG:NH1	2.21	0.56
2:H:88:HIS:H	2:H:92:ILE:HB	1.71	0.56
1:B:1914:CYS:SG	1:B:2091:GLN:NE2	2.77	0.56
1:B:2351:ILE:O	1:B:2355:GLU:HG2	2.06	0.56
1:B:2627:TRP:HB2	1:B:2630:PHE:HB2	1.88	0.56
1:B:4194:GLU:CD	1:B:4608:ARG:HH22	2.14	0.56
1:C:3269:ASN:HB3	1:C:3271:GLU:HG3	1.88	0.56
1:D:2143:ILE:HG13	1:D:2192:MET:HE1	1.88	0.56
1:D:3171:LEU:HD11	1:D:3214:LEU:HD12	1.88	0.56
1:A:2754:GLN:HG3	1:A:2756:LEU:H	1.71	0.55
1:A:3171:LEU:HD11	1:A:3214:LEU:HD12	1.88	0.55
1:A:4624:ASP:HB3	1:D:4238:ILE:HG13	1.88	0.55
1:A:4633:LEU:HD13	1:A:4707:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1217:PHE:CE2	1:B:1249:MET:HE1	2.41	0.55
1:B:1721:MET:HE1	1:B:2120:LEU:O	2.07	0.55
1:B:3171:LEU:HG	1:B:3211:LEU:HB3	1.87	0.55
1:C:1217:PHE:CE2	1:C:1249:MET:HE1	2.41	0.55
1:C:2754:GLN:HG3	1:C:2756:LEU:H	1.71	0.55
1:D:1721:MET:HE1	1:D:2120:LEU:O	2.07	0.55
1:A:1721:MET:HE1	1:A:2120:LEU:O	2.07	0.55
1:A:3209:PRO:HG2	1:A:3214:LEU:HD21	1.87	0.55
1:A:3965:ILE:HD12	1:A:4086:ARG:HD2	1.88	0.55
2:E:88:HIS:H	2:E:92:ILE:HB	1.72	0.55
1:B:2259:GLU:OE2	1:B:3806:ASN:ND2	2.39	0.55
1:B:3965:ILE:HD12	1:B:4086:ARG:HD2	1.88	0.55
1:C:515:ALA:HB2	1:C:523:GLY:HA3	1.88	0.55
1:C:546:LYS:O	1:C:550:GLN:HG2	2.05	0.55
1:D:2259:GLU:OE2	1:D:3806:ASN:ND2	2.39	0.55
1:A:1217:PHE:CE2	1:A:1249:MET:HE1	2.41	0.55
1:A:2194:ALA:HA	1:A:2237:SER:HB3	1.88	0.55
1:A:3015:VAL:HG11	1:A:3029:ILE:HG21	1.87	0.55
1:B:546:LYS:O	1:B:550:GLN:HG2	2.05	0.55
1:B:3171:LEU:HD11	1:B:3214:LEU:HD12	1.88	0.55
1:B:3269:ASN:HB3	1:B:3271:GLU:HG3	1.88	0.55
1:B:4633:LEU:HD13	1:B:4707:MET:HE3	1.89	0.55
1:C:4633:LEU:HD13	1:C:4707:MET:HE3	1.88	0.55
1:D:2627:TRP:HB2	1:D:2630:PHE:HB2	1.88	0.55
1:D:4633:LEU:HD13	1:D:4707:MET:HE3	1.88	0.55
1:A:997:ASP:HA	1:A:1047:LYS:HE2	1.89	0.55
1:A:2143:ILE:HG13	1:A:2192:MET:HE1	1.88	0.55
1:A:2285:TYR:OH	1:A:2382:ILE:N	2.37	0.55
1:A:3315:LEU:HA	1:A:3319:PHE:CD2	2.42	0.55
2:F:8:ILE:HA	1:B:730:LEU:HD11	1.88	0.55
1:B:981:MET:HG3	1:B:1059:GLY:HA3	1.88	0.55
1:B:1975:MET:HG3	1:B:1976:LEU:HD12	1.87	0.55
1:B:2263:GLU:HG3	1:B:2267:ARG:NH1	2.21	0.55
1:C:986:ILE:HB	1:C:1055:ARG:HE	1.72	0.55
1:C:1850:VAL:HG22	1:C:2055:SER:HB3	1.89	0.55
1:C:2252:GLU:HG2	1:C:3819:MET:SD	2.46	0.55
1:C:2743:TYR:CD1	1:C:2757:MET:HB2	2.41	0.55
1:D:515:ALA:HB2	1:D:523:GLY:HA3	1.88	0.55
1:D:1000:ALA:HB2	1:D:1050:LEU:HD11	1.89	0.55
1:D:1850:VAL:HG22	1:D:2055:SER:HB3	1.89	0.55
1:A:1000:ALA:HB2	1:A:1050:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4194:GLU:CD	1:A:4608:ARG:HH22	2.14	0.55
1:B:909:ASP:HB3	1:B:912:LYS:HB2	1.89	0.55
1:B:992:GLN:O	1:B:996:VAL:HG23	2.06	0.55
1:B:2943:PHE:CZ	1:B:2956:TYR:HB2	2.41	0.55
1:C:2143:ILE:HG13	1:C:2192:MET:HE1	1.88	0.55
1:C:3171:LEU:HD11	1:C:3214:LEU:HD12	1.88	0.55
1:D:1217:PHE:CE2	1:D:1249:MET:HE1	2.41	0.55
1:D:2720:PHE:CE1	1:D:2896:LEU:HA	2.42	0.55
1:A:1217:PHE:HE2	1:A:1249:MET:HE1	1.72	0.55
1:A:1914:CYS:SG	1:A:2091:GLN:NE2	2.77	0.55
1:A:2252:GLU:HG2	1:A:3819:MET:SD	2.46	0.55
1:A:2351:ILE:O	1:A:2355:GLU:HG2	2.07	0.55
1:B:2720:PHE:CE1	1:B:2896:LEU:HA	2.41	0.55
1:B:2754:GLN:HG3	1:B:2756:LEU:H	1.71	0.55
1:C:908:ARG:HG3	1:C:915:HIS:HD2	1.72	0.55
1:C:997:ASP:HA	1:C:1047:LYS:HE2	1.89	0.55
1:C:2351:ILE:O	1:C:2355:GLU:HG2	2.07	0.55
1:C:2658:GLU:H	1:C:2662:PHE:HE1	1.54	0.55
1:C:4194:GLU:CD	1:C:4608:ARG:HH22	2.14	0.55
1:D:962:LYS:HZ3	1:D:982:ASP:CG	2.13	0.55
1:D:981:MET:HG3	1:D:1059:GLY:HA3	1.88	0.55
1:D:1219:LYS:NZ	1:D:1243:THR:O	2.40	0.55
1:D:2351:ILE:O	1:D:2355:GLU:HG2	2.07	0.55
1:D:2743:TYR:CD1	1:D:2757:MET:HB2	2.41	0.55
1:D:2754:GLN:HG3	1:D:2756:LEU:H	1.71	0.55
1:D:4194:GLU:CD	1:D:4608:ARG:HH22	2.14	0.55
1:A:64:ILE:HA	1:A:123:HIS:HE2	1.72	0.55
1:A:246:THR:HG21	1:A:267:VAL:HG21	1.89	0.55
1:B:626:ARG:NH2	1:B:1667:LEU:O	2.36	0.55
1:B:1973:ILE:HG13	1:B:3619:LEU:HB3	1.87	0.55
1:B:4654:MET:O	1:B:4663:ARG:NH1	2.40	0.55
1:C:246:THR:HG21	1:C:267:VAL:HG21	1.89	0.55
1:C:992:GLN:O	1:C:996:VAL:HG23	2.06	0.55
1:C:4046:ARG:HG3	1:C:4050:LYS:NZ	2.22	0.55
1:D:4654:MET:O	1:D:4663:ARG:NH1	2.40	0.55
1:A:908:ARG:HG3	1:A:915:HIS:HD2	1.72	0.55
1:A:1850:VAL:HG22	1:A:2055:SER:HB3	1.89	0.55
1:A:2720:PHE:CE1	1:A:2896:LEU:HA	2.41	0.55
2:F:88:HIS:H	2:F:92:ILE:HB	1.72	0.55
2:G:88:HIS:H	2:G:92:ILE:HB	1.72	0.55
1:B:908:ARG:HG3	1:B:915:HIS:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:997:ASP:HA	1:B:1047:LYS:HE2	1.89	0.55
1:B:2252:GLU:HG2	1:B:3819:MET:SD	2.46	0.55
1:B:2590:ARG:NH2	1:B:2875:ASP:OD2	2.34	0.55
1:B:4238:ILE:HG13	1:C:4624:ASP:HB3	1.89	0.55
1:C:1721:MET:HE1	1:C:2120:LEU:O	2.06	0.55
1:C:2263:GLU:HG3	1:C:2267:ARG:NH1	2.21	0.55
1:D:2589:LEU:HD23	1:D:2592:LEU:HD12	1.89	0.55
1:D:3965:ILE:HD12	1:D:4086:ARG:HD2	1.89	0.55
1:A:1219:LYS:NZ	1:A:1243:THR:O	2.40	0.55
1:A:2589:LEU:HD23	1:A:2592:LEU:HD12	1.89	0.55
1:B:2194:ALA:HA	1:B:2237:SER:HB3	1.88	0.55
1:B:2658:GLU:H	1:B:2662:PHE:HE1	1.54	0.55
1:C:909:ASP:HB3	1:C:912:LYS:HB2	1.89	0.55
1:C:2627:TRP:HB2	1:C:2630:PHE:HB2	1.88	0.55
1:C:2691:LYS:HZ1	1:C:2874:TYR:HB3	1.72	0.55
1:D:3315:LEU:HA	1:D:3319:PHE:CD2	2.42	0.55
1:A:909:ASP:HB3	1:A:912:LYS:HB2	1.89	0.55
1:B:986:ILE:HB	1:B:1055:ARG:HE	1.72	0.55
1:B:1217:PHE:HE2	1:B:1249:MET:HE1	1.72	0.55
1:B:2143:ILE:HG13	1:B:2192:MET:HE1	1.88	0.55
1:B:3315:LEU:HA	1:B:3319:PHE:CD2	2.42	0.55
1:C:3026:ALA:O	1:C:3030:VAL:HG23	2.07	0.55
1:D:908:ARG:HG3	1:D:915:HIS:HD2	1.72	0.55
1:D:992:GLN:O	1:D:996:VAL:HG23	2.06	0.55
1:D:2590:ARG:NH2	1:D:2875:ASP:OD2	2.34	0.55
1:A:895:MET:HE2	1:A:978:PRO:HA	1.89	0.54
1:A:981:MET:HG3	1:A:1059:GLY:HA3	1.88	0.54
1:A:992:GLN:O	1:A:996:VAL:HG23	2.06	0.54
1:A:1973:ILE:HG13	1:A:3619:LEU:HB3	1.87	0.54
1:A:2627:TRP:HB2	1:A:2630:PHE:HB2	1.88	0.54
1:B:2979:ARG:NH2	1:B:3035:ILE:HB	2.22	0.54
1:C:1217:PHE:HE2	1:C:1249:MET:HE1	1.71	0.54
1:C:2589:LEU:HD23	1:C:2592:LEU:HD12	1.89	0.54
1:C:3965:ILE:HD12	1:C:4086:ARG:HD2	1.89	0.54
1:D:895:MET:HE2	1:D:978:PRO:HA	1.89	0.54
1:D:1217:PHE:HE2	1:D:1249:MET:HE1	1.71	0.54
1:D:2734:MET:HE1	1:D:2823:PRO:HA	1.89	0.54
1:D:4046:ARG:HG3	1:D:4050:LYS:NZ	2.22	0.54
1:A:2943:PHE:CZ	1:A:2956:TYR:HB2	2.41	0.54
1:A:3016:ARG:NH1	1:A:3063:ASN:HB3	2.23	0.54
1:A:4046:ARG:HG3	1:A:4050:LYS:NZ	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2619:LYS:HZ1	1:B:2627:TRP:CG	2.25	0.54
1:B:4046:ARG:HG3	1:B:4050:LYS:NZ	2.22	0.54
1:C:2619:LYS:HZ1	1:C:2627:TRP:CG	2.25	0.54
1:D:997:ASP:HA	1:D:1047:LYS:HE2	1.89	0.54
1:D:2252:GLU:HG2	1:D:3819:MET:SD	2.46	0.54
1:D:3250:TRP:CZ3	1:D:3273:MET:HE3	2.43	0.54
1:A:3026:ALA:O	1:A:3030:VAL:HG23	2.07	0.54
1:A:4116:GLN:HA	1:A:4119:LEU:HD12	1.90	0.54
1:C:2720:PHE:CE1	1:C:2896:LEU:HA	2.41	0.54
1:C:3002:GLU:O	1:C:3005:THR:OG1	2.22	0.54
1:C:3233:HIS:O	1:C:3237:VAL:HG22	2.08	0.54
1:D:627:SER:O	1:D:631:LEU:HG	2.08	0.54
1:D:986:ILE:HB	1:D:1055:ARG:HE	1.72	0.54
1:D:3026:ALA:O	1:D:3030:VAL:HG23	2.07	0.54
1:D:3269:ASN:HB3	1:D:3271:GLU:HG3	1.88	0.54
1:A:4654:MET:O	1:A:4663:ARG:NH1	2.40	0.54
1:B:1850:VAL:HG22	1:B:2055:SER:HB3	1.89	0.54
1:C:3003:MET:O	1:C:3006:SER:OG	2.18	0.54
1:C:3315:LEU:HA	1:C:3319:PHE:CD2	2.42	0.54
1:C:4238:ILE:HG13	1:D:4624:ASP:HB3	1.89	0.54
1:D:3016:ARG:NH1	1:D:3063:ASN:HB3	2.23	0.54
1:A:908:ARG:HG3	1:A:915:HIS:CD2	2.43	0.54
1:A:986:ILE:HB	1:A:1055:ARG:HE	1.72	0.54
1:B:908:ARG:HG3	1:B:915:HIS:CD2	2.43	0.54
1:B:1219:LYS:NZ	1:B:1243:THR:O	2.40	0.54
1:B:2589:LEU:HD23	1:B:2592:LEU:HD12	1.89	0.54
1:B:3002:GLU:O	1:B:3005:THR:OG1	2.22	0.54
1:C:644:LEU:HD11	1:C:1650:LEU:HD22	1.90	0.54
1:C:895:MET:HE2	1:C:978:PRO:HA	1.89	0.54
1:C:2194:ALA:HA	1:C:2237:SER:HB3	1.88	0.54
1:C:3159:LEU:HD13	1:C:3241:MET:HE3	1.90	0.54
1:C:4654:MET:O	1:C:4663:ARG:NH1	2.40	0.54
1:D:4116:GLN:HA	1:D:4119:LEU:HD12	1.90	0.54
1:A:2933:VAL:HG22	1:A:2963:PHE:HE1	1.73	0.54
1:A:3246:MET:SD	1:A:3276:LEU:HD12	2.48	0.54
2:G:8:ILE:HA	1:C:730:LEU:HD11	1.89	0.54
1:B:895:MET:HE2	1:B:978:PRO:HA	1.89	0.54
1:B:1979:PHE:HZ	1:B:1996:LEU:HB3	1.73	0.54
1:B:3233:HIS:O	1:B:3237:VAL:HG22	2.08	0.54
1:B:3250:TRP:CZ3	1:B:3273:MET:HE3	2.42	0.54
1:C:2455:ASP:OD2	1:C:2457:SER:OG	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3246:MET:SD	1:D:3276:LEU:HD12	2.48	0.54
1:A:962:LYS:HZ3	1:A:982:ASP:CG	2.12	0.54
1:A:3269:ASN:HB3	1:A:3271:GLU:HG3	1.88	0.54
1:B:246:THR:HG21	1:B:267:VAL:HG21	1.89	0.54
1:B:1100:ARG:NH1	1:B:1167:ASP:OD1	2.40	0.54
1:C:908:ARG:HG3	1:C:915:HIS:CD2	2.43	0.54
1:C:1100:ARG:NH1	1:C:1167:ASP:OD1	2.40	0.54
1:C:1973:ILE:HG13	1:C:3619:LEU:HB3	1.87	0.54
1:C:2979:ARG:NH2	1:C:3035:ILE:HB	2.22	0.54
1:D:909:ASP:HB3	1:D:912:LYS:HB2	1.89	0.54
1:D:3164:GLY:O	1:D:3248:ARG:NE	2.41	0.54
1:D:3233:HIS:O	1:D:3237:VAL:HG22	2.08	0.54
1:A:308:LEU:HD21	1:A:370:LEU:HD12	1.90	0.54
1:A:3250:TRP:CZ3	1:A:3273:MET:HE3	2.42	0.54
1:B:2285:TYR:OH	1:B:2382:ILE:N	2.37	0.54
1:B:3016:ARG:NH1	1:B:3063:ASN:HB3	2.23	0.54
1:B:3159:LEU:HD13	1:B:3241:MET:HE3	1.90	0.54
1:B:4252:ILE:HG21	1:C:4707:MET:HG3	1.89	0.54
1:D:2485:LEU:HD12	1:D:2544:LEU:HD23	1.89	0.54
1:D:3783:GLU:OE2	1:D:3784:LYS:NZ	2.39	0.54
1:A:4120:GLU:HA	1:A:4123:GLU:HG2	1.90	0.54
1:C:1000:ALA:HB2	1:C:1050:LEU:HD11	1.89	0.54
1:C:1219:LYS:NZ	1:C:1243:THR:O	2.40	0.54
1:C:2943:PHE:CZ	1:C:2956:TYR:HB2	2.41	0.54
1:C:3016:ARG:NH1	1:C:3063:ASN:HB3	2.23	0.54
1:C:3227:ARG:NH1	1:C:3290:ILE:HG13	2.18	0.54
1:D:541:ILE:HD11	1:D:574:VAL:HG13	1.90	0.54
1:D:3089:GLY:O	1:D:3093:ILE:HG12	2.08	0.54
1:D:3227:ARG:NH1	1:D:3290:ILE:HG13	2.18	0.54
1:A:1100:ARG:NH1	1:A:1167:ASP:OD1	2.40	0.54
1:B:644:LEU:HD11	1:B:1650:LEU:HD22	1.90	0.54
1:B:1941:ARG:NH2	1:B:3609:TYR:O	2.41	0.54
1:C:981:MET:HG3	1:C:1059:GLY:HA3	1.88	0.54
1:D:64:ILE:HA	1:D:123:HIS:HE2	1.72	0.54
1:D:1100:ARG:NH1	1:D:1167:ASP:OD1	2.40	0.54
1:D:1941:ARG:NH2	1:D:3609:TYR:O	2.41	0.54
1:A:541:ILE:HD11	1:A:574:VAL:HG13	1.90	0.53
1:A:2621:TYR:OH	1:A:2637:GLU:OE2	2.17	0.53
1:A:3089:GLY:O	1:A:3093:ILE:HG12	2.08	0.53
1:A:3285:TYR:CE1	1:A:3325:LYS:HD2	2.44	0.53
1:B:1000:ALA:HB2	1:B:1050:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2348:GLU:OE2	1:B:2352:LYS:NZ	2.42	0.53
1:B:2734:MET:HE1	1:B:2823:PRO:HA	1.89	0.53
1:C:308:LEU:HD21	1:C:370:LEU:HD12	1.90	0.53
1:C:1941:ARG:NH2	1:C:3609:TYR:O	2.41	0.53
1:D:644:LEU:HD11	1:D:1650:LEU:HD22	1.90	0.53
1:A:2348:GLU:OE2	1:A:2352:LYS:NZ	2.42	0.53
1:B:180:ASP:HB3	1:B:211:LEU:HD12	1.91	0.53
1:B:627:SER:O	1:B:631:LEU:HG	2.08	0.53
1:B:2296:GLU:HG3	1:B:2390:THR:HG22	1.91	0.53
1:B:3246:MET:SD	1:B:3276:LEU:HD12	2.48	0.53
1:B:3285:TYR:CE1	1:B:3325:LYS:HD2	2.44	0.53
1:B:3805:LEU:HD21	1:B:3888:PHE:HA	1.90	0.53
1:C:3154:ALA:O	1:C:3157:GLU:HG3	2.09	0.53
1:C:3250:TRP:CZ3	1:C:3273:MET:HE3	2.43	0.53
1:C:4252:ILE:HG21	1:D:4707:MET:HG3	1.90	0.53
1:D:2933:VAL:HG22	1:D:2963:PHE:HE1	1.73	0.53
1:D:3180:ILE:HA	1:D:3185:ASN:HD22	1.73	0.53
1:A:2545:ILE:HD12	1:A:2580:LEU:HD11	1.90	0.53
1:A:4819:VAL:HG12	1:A:4830:GLU:HG3	1.91	0.53
1:B:2545:ILE:HD12	1:B:2580:LEU:HD11	1.90	0.53
1:C:436:LEU:HG	1:C:445:VAL:HG11	1.90	0.53
1:C:1048:ASP:HA	1:C:1051:ARG:HE	1.74	0.53
1:C:2348:GLU:OE2	1:C:2352:LYS:NZ	2.42	0.53
1:C:3071:THR:HG23	1:C:3094:ILE:HG12	1.90	0.53
1:C:4116:GLN:HA	1:C:4119:LEU:HD12	1.90	0.53
1:D:308:LEU:HD21	1:D:370:LEU:HD12	1.90	0.53
1:D:2348:GLU:OE2	1:D:2352:LYS:NZ	2.42	0.53
1:D:2658:GLU:H	1:D:2662:PHE:HE1	1.54	0.53
1:D:3154:ALA:O	1:D:3157:GLU:HG3	2.09	0.53
1:A:1941:ARG:NH2	1:A:3609:TYR:O	2.41	0.53
1:A:2979:ARG:NH2	1:A:3035:ILE:HB	2.22	0.53
1:A:4250:TYR:O	1:A:4254:THR:HG23	2.09	0.53
1:C:180:ASP:HB3	1:C:211:LEU:HD12	1.91	0.53
1:C:3805:LEU:HD21	1:C:3888:PHE:HA	1.91	0.53
1:D:3285:TYR:CE1	1:D:3325:LYS:HD2	2.44	0.53
1:A:1048:ASP:HA	1:A:1051:ARG:HE	1.74	0.53
1:A:3233:HIS:O	1:A:3237:VAL:HG22	2.08	0.53
1:A:3805:LEU:HD21	1:A:3888:PHE:HA	1.91	0.53
1:B:308:LEU:HD21	1:B:370:LEU:HD12	1.90	0.53
1:B:990:PRO:HA	1:B:993:GLU:HB2	1.91	0.53
1:B:3026:ALA:O	1:B:3030:VAL:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3154:ALA:O	1:B:3157:GLU:HG3	2.09	0.53
1:B:4116:GLN:HA	1:B:4119:LEU:HD12	1.90	0.53
1:B:4120:GLU:HA	1:B:4123:GLU:HG2	1.90	0.53
1:C:1979:PHE:HZ	1:C:1996:LEU:HB3	1.73	0.53
1:C:3246:MET:SD	1:C:3276:LEU:HD12	2.48	0.53
1:C:4819:VAL:HG12	1:C:4830:GLU:HG3	1.91	0.53
1:D:436:LEU:HG	1:D:445:VAL:HG11	1.90	0.53
1:D:3071:THR:HG23	1:D:3094:ILE:HG12	1.90	0.53
1:D:3159:LEU:HD13	1:D:3241:MET:HE3	1.90	0.53
1:D:3805:LEU:HD21	1:D:3888:PHE:HA	1.91	0.53
1:A:2296:GLU:HG3	1:A:2390:THR:HG22	1.91	0.53
1:A:2734:MET:HE1	1:A:2823:PRO:HA	1.89	0.53
1:A:2943:PHE:CE1	1:A:2954:PHE:HB3	2.44	0.53
1:A:3071:THR:HG23	1:A:3094:ILE:HG12	1.90	0.53
1:A:3154:ALA:O	1:A:3157:GLU:HG3	2.09	0.53
1:A:3198:PRO:HD2	1:A:3204:VAL:HG22	1.91	0.53
1:B:2629:ASN:OD1	1:B:2630:PHE:N	2.42	0.53
1:B:3030:VAL:HG12	1:B:3034:HIS:NE2	2.24	0.53
1:B:3071:THR:HG23	1:B:3094:ILE:HG12	1.90	0.53
1:B:3285:TYR:HE1	1:B:3328:LYS:HE3	1.74	0.53
1:C:962:LYS:HZ3	1:C:982:ASP:CG	2.16	0.53
1:C:2296:GLU:HG3	1:C:2390:THR:HG22	1.91	0.53
1:D:246:THR:HG21	1:D:267:VAL:HG21	1.89	0.53
1:D:626:ARG:NH2	1:D:1667:LEU:O	2.36	0.53
1:D:2285:TYR:OH	1:D:2382:ILE:N	2.37	0.53
1:D:2296:GLU:HG3	1:D:2390:THR:HG22	1.91	0.53
1:A:627:SER:O	1:A:631:LEU:HG	2.08	0.53
1:A:2485:LEU:HD12	1:A:2544:LEU:HD23	1.89	0.53
1:A:2619:LYS:HZ1	1:A:2627:TRP:CG	2.26	0.53
1:A:3164:GLY:O	1:A:3248:ARG:NE	2.41	0.53
1:A:4113:THR:O	1:A:4117:THR:HG23	2.09	0.53
1:B:892:LEU:HA	1:B:895:MET:SD	2.49	0.53
1:B:2691:LYS:HZ1	1:B:2874:TYR:HB3	1.73	0.53
1:B:2769:GLU:C	1:B:2771:TYR:H	2.16	0.53
1:B:3198:PRO:HD2	1:B:3204:VAL:HG22	1.91	0.53
1:C:627:SER:O	1:C:631:LEU:HG	2.08	0.53
1:C:896:ASN:OD1	1:C:897:LYS:N	2.42	0.53
1:C:1972:GLN:HG2	1:C:1975:MET:HE2	1.91	0.53
1:C:3030:VAL:HG12	1:C:3034:HIS:NE2	2.24	0.53
1:C:4250:TYR:O	1:C:4254:THR:HG23	2.09	0.53
1:D:892:LEU:HA	1:D:895:MET:SD	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:908:ARG:HG3	1:D:915:HIS:CD2	2.43	0.53
1:D:2943:PHE:CE1	1:D:2954:PHE:HB3	2.44	0.53
1:D:2943:PHE:CZ	1:D:2956:TYR:HB2	2.42	0.53
1:D:2968:LEU:HB3	1:D:2969:PRO:HD3	1.91	0.53
1:A:644:LEU:HD11	1:A:1650:LEU:HD22	1.90	0.53
1:A:881:ILE:HG13	1:A:885:LEU:HD23	1.91	0.53
1:A:892:LEU:HA	1:A:895:MET:SD	2.49	0.53
1:A:2968:LEU:HB3	1:A:2969:PRO:HD3	1.91	0.53
1:A:3285:TYR:HE1	1:A:3328:LYS:HE3	1.74	0.53
1:B:3180:ILE:HA	1:B:3185:ASN:HD22	1.74	0.53
1:C:2485:LEU:HD12	1:C:2544:LEU:HD23	1.89	0.53
1:C:2629:ASN:OD1	1:C:2630:PHE:N	2.42	0.53
1:C:2716:LYS:HG3	1:C:2717:LEU:HD12	1.90	0.53
1:D:849:ASP:OD1	1:D:1214:ARG:NE	2.42	0.53
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.26	0.53
1:D:1972:GLN:HG2	1:D:1975:MET:HE2	1.91	0.53
1:D:2787:TRP:HZ2	1:D:2843:MET:HE3	1.74	0.53
1:A:2684:ASN:ND2	1:A:2909:ASP:OD1	2.39	0.53
1:A:2787:TRP:HZ2	1:A:2843:MET:HE3	1.74	0.53
1:B:849:ASP:OD1	1:B:1214:ARG:NE	2.42	0.53
1:B:881:ILE:HG13	1:B:885:LEU:HD23	1.91	0.53
1:B:896:ASN:OD1	1:B:897:LYS:N	2.42	0.53
1:B:2968:LEU:HB3	1:B:2969:PRO:HD3	1.91	0.53
1:B:4819:VAL:HG12	1:B:4830:GLU:HG3	1.91	0.53
1:C:2787:TRP:HZ2	1:C:2843:MET:HE3	1.74	0.53
1:D:2619:LYS:HZ1	1:D:2627:TRP:CG	2.25	0.53
1:D:3285:TYR:HE1	1:D:3328:LYS:HE3	1.73	0.53
1:A:896:ASN:OD1	1:A:897:LYS:N	2.42	0.53
1:A:990:PRO:HA	1:A:993:GLU:HB2	1.91	0.53
1:A:2497:ARG:HH12	1:A:2877:LEU:HA	1.74	0.53
1:A:2658:GLU:H	1:A:2662:PHE:HE1	1.54	0.53
1:A:3030:VAL:HG12	1:A:3034:HIS:NE2	2.24	0.53
1:A:3134:LEU:HD12	1:A:3162:PHE:HE2	1.74	0.53
1:B:1184:ASP:OD2	1:B:1188:SER:OG	2.26	0.53
1:B:2485:LEU:HD12	1:B:2544:LEU:HD23	1.89	0.53
1:B:4113:THR:O	1:B:4117:THR:HG23	2.09	0.53
1:C:1284:LYS:NZ	1:C:1286:THR:OG1	2.41	0.53
1:C:2734:MET:HE1	1:C:2823:PRO:HA	1.89	0.53
1:C:2765:GLU:HA	1:C:2768:LYS:HD2	1.91	0.53
1:C:3285:TYR:CE1	1:C:3325:LYS:HD2	2.43	0.53
1:C:4045:LYS:HE2	1:C:4078:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2763:LEU:HB3	1:D:2767:GLU:OE2	2.10	0.53
1:D:4045:LYS:HE2	1:D:4078:LEU:HD22	1.91	0.53
1:A:180:ASP:HB3	1:A:211:LEU:HD12	1.91	0.52
1:A:972:LEU:HD11	1:A:976:TYR:HB2	1.91	0.52
1:A:4707:MET:HG3	1:D:4252:ILE:HG21	1.91	0.52
1:B:2716:LYS:HG3	1:B:2717:LEU:HD12	1.90	0.52
1:C:881:ILE:HG13	1:C:885:LEU:HD23	1.91	0.52
1:C:3089:GLY:O	1:C:3093:ILE:HG12	2.08	0.52
1:D:180:ASP:HB3	1:D:211:LEU:HD12	1.91	0.52
1:D:1048:ASP:HA	1:D:1051:ARG:HE	1.74	0.52
1:D:3030:VAL:HG12	1:D:3034:HIS:NE2	2.24	0.52
1:D:4113:THR:O	1:D:4117:THR:HG23	2.09	0.52
1:D:4250:TYR:O	1:D:4254:THR:HG23	2.09	0.52
1:A:2629:ASN:OD1	1:A:2630:PHE:N	2.42	0.52
1:A:3159:LEU:HD13	1:A:3241:MET:HE3	1.90	0.52
1:B:2765:GLU:HA	1:B:2768:LYS:HD2	1.91	0.52
1:B:2933:VAL:HG22	1:B:2963:PHE:HE1	1.73	0.52
1:C:541:ILE:HD11	1:C:574:VAL:HG13	1.90	0.52
1:D:881:ILE:HG13	1:D:885:LEU:HD23	1.91	0.52
1:D:990:PRO:HA	1:D:993:GLU:HB2	1.91	0.52
1:D:1979:PHE:HZ	1:D:1996:LEU:HB3	1.73	0.52
1:D:2716:LYS:HG3	1:D:2717:LEU:HD12	1.90	0.52
1:A:655:MET:HE2	1:A:1608:VAL:HG21	1.92	0.52
1:A:2095:ILE:HD11	1:A:3629:ILE:HG23	1.91	0.52
1:A:2763:LEU:HB3	1:A:2767:GLU:OE2	2.10	0.52
1:B:1685:LEU:O	1:B:1689:ILE:HG12	2.09	0.52
1:B:2623:LEU:HD23	1:B:2626:GLY:H	1.74	0.52
1:B:3089:GLY:O	1:B:3093:ILE:HG12	2.08	0.52
1:B:3134:LEU:HD12	1:B:3162:PHE:HE2	1.74	0.52
1:B:3778:LEU:HB2	1:B:3854:PHE:CE1	2.44	0.52
1:C:2623:LEU:HD23	1:C:2626:GLY:H	1.74	0.52
1:C:4120:GLU:HA	1:C:4123:GLU:HG2	1.90	0.52
1:D:4120:GLU:HA	1:D:4123:GLU:HG2	1.90	0.52
1:A:2736:LYS:HB3	1:A:2741:TRP:HB2	1.92	0.52
1:A:2937:HIS:HB2	1:A:3014:LEU:HD21	1.92	0.52
1:A:3180:ILE:HA	1:A:3185:ASN:HD22	1.74	0.52
1:B:1048:ASP:HA	1:B:1051:ARG:HE	1.74	0.52
1:B:4250:TYR:O	1:B:4254:THR:HG23	2.09	0.52
1:C:1685:LEU:O	1:C:1689:ILE:HG12	2.10	0.52
1:C:2874:TYR:HA	1:C:2877:LEU:HD13	1.91	0.52
1:C:2923:TYR:HE2	1:C:2999:LYS:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2497:ARG:HH12	1:D:2877:LEU:HA	1.74	0.52
1:A:436:LEU:HG	1:A:445:VAL:HG11	1.90	0.52
1:A:881:ILE:O	1:A:885:LEU:HD23	2.10	0.52
1:A:1685:LEU:O	1:A:1689:ILE:HG12	2.10	0.52
1:A:4256:MET:HE2	1:A:4256:MET:HA	1.92	0.52
1:B:4045:LYS:HE2	1:B:4078:LEU:HD22	1.91	0.52
1:C:375:GLN:HG2	1:C:377:VAL:HG13	1.92	0.52
1:C:2000:HIS:O	1:C:2004:MET:HG2	2.10	0.52
1:C:2968:LEU:HB3	1:C:2969:PRO:HD3	1.91	0.52
1:C:3180:ILE:HA	1:C:3185:ASN:HD22	1.74	0.52
1:C:3218:ILE:HA	1:C:3221:LEU:HG	1.92	0.52
1:C:3778:LEU:HB2	1:C:3854:PHE:CE1	2.44	0.52
1:C:4113:THR:O	1:C:4117:THR:HG23	2.09	0.52
1:D:896:ASN:OD1	1:D:897:LYS:N	2.42	0.52
1:D:4819:VAL:HG12	1:D:4830:GLU:HG3	1.91	0.52
1:A:2765:GLU:HA	1:A:2768:LYS:HD2	1.91	0.52
1:A:3778:LEU:HB2	1:A:3854:PHE:CE1	2.44	0.52
1:A:4921:PHE:HE2	1:A:4940:VAL:HG11	1.74	0.52
1:B:972:LEU:HD11	1:B:976:TYR:HB2	1.90	0.52
1:B:4256:MET:HA	1:B:4256:MET:HE2	1.92	0.52
1:C:655:MET:HE2	1:C:1608:VAL:HG21	1.92	0.52
1:C:849:ASP:OD1	1:C:1214:ARG:NE	2.42	0.52
1:C:892:LEU:HA	1:C:895:MET:SD	2.49	0.52
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.26	0.52
1:C:2497:ARG:HH12	1:C:2877:LEU:HA	1.74	0.52
1:C:3198:PRO:HD2	1:C:3204:VAL:HG22	1.91	0.52
1:C:4921:PHE:HE2	1:C:4940:VAL:HG11	1.74	0.52
1:D:972:LEU:HD11	1:D:976:TYR:HB2	1.91	0.52
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.26	0.52
1:A:2623:LEU:HD23	1:A:2626:GLY:H	1.74	0.52
1:A:2769:GLU:C	1:A:2771:TYR:H	2.16	0.52
1:A:3245:TYR:O	1:A:3249:TRP:HE3	1.93	0.52
1:A:4045:LYS:HE2	1:A:4078:LEU:HD22	1.91	0.52
1:B:1972:GLN:HG2	1:B:1975:MET:HE2	1.91	0.52
1:B:2497:ARG:HH12	1:B:2877:LEU:HA	1.74	0.52
1:B:2937:HIS:HB2	1:B:3014:LEU:HD21	1.92	0.52
1:C:882:ARG:HH22	1:C:933:LEU:C	2.18	0.52
1:C:2937:HIS:HB2	1:C:3014:LEU:HD21	1.92	0.52
1:C:2943:PHE:CE1	1:C:2954:PHE:HB3	2.44	0.52
1:C:3285:TYR:HE1	1:C:3328:LYS:HE3	1.74	0.52
1:D:2095:ILE:HD11	1:D:3629:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2979:ARG:NH2	1:D:3035:ILE:HB	2.22	0.52
1:D:3198:PRO:HD2	1:D:3204:VAL:HG22	1.91	0.52
1:A:1979:PHE:HZ	1:A:1996:LEU:HB3	1.73	0.52
1:A:2455:ASP:OD2	1:A:2457:SER:OG	2.21	0.52
1:A:2657:TYR:HA	1:A:2662:PHE:HE1	1.75	0.52
1:B:436:LEU:HG	1:B:445:VAL:HG11	1.90	0.52
1:B:541:ILE:HD11	1:B:574:VAL:HG13	1.90	0.52
1:B:1074:ARG:HH12	1:B:1078:CYS:H	1.58	0.52
1:B:2736:LYS:HB3	1:B:2741:TRP:HB2	1.92	0.52
1:B:2763:LEU:HB3	1:B:2767:GLU:OE2	2.10	0.52
1:B:3164:GLY:O	1:B:3248:ARG:NE	2.41	0.52
1:B:3218:ILE:HA	1:B:3221:LEU:HG	1.92	0.52
1:B:3245:TYR:O	1:B:3249:TRP:HE3	1.93	0.52
1:B:4306:PHE:HA	1:B:4309:ILE:HG12	1.92	0.52
1:C:3011:LEU:HD21	1:C:3036:LEU:CD1	2.40	0.52
1:C:3164:GLY:O	1:C:3248:ARG:NE	2.41	0.52
1:D:881:ILE:O	1:D:885:LEU:HD23	2.10	0.52
1:D:2202:TYR:O	1:D:2206:ILE:HG12	2.10	0.52
1:D:2629:ASN:OD1	1:D:2630:PHE:N	2.42	0.52
1:D:3003:MET:O	1:D:3006:SER:OG	2.18	0.52
1:D:3011:LEU:HD21	1:D:3036:LEU:CD1	2.40	0.52
1:D:3879:LEU:O	1:D:3882:GLN:HG3	2.10	0.52
1:A:988:LEU:HD12	1:A:992:GLN:HE21	1.75	0.52
1:A:2716:LYS:HG3	1:A:2717:LEU:HD12	1.90	0.52
1:A:2874:TYR:HA	1:A:2877:LEU:HD13	1.91	0.52
1:A:3011:LEU:HD21	1:A:3036:LEU:CD1	2.40	0.52
1:B:2943:PHE:CE1	1:B:2954:PHE:HB3	2.44	0.52
1:B:3011:LEU:HD21	1:B:3036:LEU:CD1	2.40	0.52
1:C:988:LEU:HD12	1:C:992:GLN:HE21	1.75	0.52
1:C:2763:LEU:HB3	1:C:2767:GLU:OE2	2.10	0.52
1:D:988:LEU:HD12	1:D:992:GLN:HE21	1.75	0.52
1:D:2937:HIS:HB2	1:D:3014:LEU:HD21	1.92	0.52
1:A:2923:TYR:HE2	1:A:2999:LYS:HB3	1.74	0.52
1:A:3277:LEU:HD13	1:A:3306:ILE:HG22	1.92	0.52
1:B:882:ARG:HH22	1:B:933:LEU:C	2.18	0.52
1:B:1048:ASP:OD1	1:B:1049:SER:N	2.43	0.52
1:B:3277:LEU:HD13	1:B:3306:ILE:HG22	1.92	0.52
1:C:1724:GLU:OE2	1:C:2127:ARG:NH2	2.42	0.52
1:C:2545:ILE:HD12	1:C:2580:LEU:HD11	1.90	0.52
1:C:2933:VAL:HG22	1:C:2963:PHE:HE1	1.73	0.52
1:C:3134:LEU:HD12	1:C:3162:PHE:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2545:ILE:HD12	1:D:2580:LEU:HD11	1.90	0.52
1:D:3134:LEU:HD12	1:D:3162:PHE:HE2	1.74	0.52
1:D:3277:LEU:HD13	1:D:3306:ILE:HG22	1.92	0.52
1:D:3315:LEU:HA	1:D:3319:PHE:HD2	1.75	0.52
1:D:4256:MET:HE2	1:D:4256:MET:HA	1.92	0.52
1:A:1972:GLN:HG2	1:A:1975:MET:HE2	1.91	0.51
1:A:3218:ILE:HA	1:A:3221:LEU:HG	1.92	0.51
1:B:2202:TYR:O	1:B:2206:ILE:HG12	2.10	0.51
1:B:3250:TRP:CD1	1:B:3256:ASN:HD21	2.28	0.51
1:B:4921:PHE:HE2	1:B:4940:VAL:HG11	1.74	0.51
1:C:990:PRO:HA	1:C:993:GLU:HB2	1.91	0.51
1:C:2285:TYR:OH	1:C:2382:ILE:N	2.37	0.51
1:C:3229:THR:HG23	1:C:3291:ASP:OD2	2.10	0.51
1:C:3277:LEU:HD13	1:C:3306:ILE:HG22	1.92	0.51
1:D:675:TYR:HB3	1:D:822:CYS:SG	2.51	0.51
1:D:882:ARG:HH22	1:D:933:LEU:C	2.18	0.51
1:D:1014:GLN:O	1:D:1027:ARG:NH2	2.43	0.51
1:D:2447:LYS:HA	1:D:2447:LYS:HE3	1.92	0.51
1:D:2874:TYR:HA	1:D:2877:LEU:HD13	1.91	0.51
1:D:3134:LEU:HB2	1:D:3162:PHE:CE2	2.46	0.51
1:D:3136:SER:O	1:D:3140:LEU:HD22	2.10	0.51
1:D:3778:LEU:HB2	1:D:3854:PHE:CE1	2.44	0.51
1:D:4921:PHE:HE2	1:D:4940:VAL:HG11	1.74	0.51
1:A:675:TYR:HB3	1:A:822:CYS:SG	2.50	0.51
1:B:2000:HIS:O	1:B:2004:MET:HG2	2.10	0.51
1:B:2447:LYS:HE3	1:B:2447:LYS:HA	1.93	0.51
1:B:2787:TRP:HZ2	1:B:2843:MET:HE3	1.74	0.51
1:B:3314:LEU:HD12	1:B:3318:HIS:ND1	2.25	0.51
1:C:881:ILE:O	1:C:885:LEU:HD23	2.10	0.51
1:C:1014:GLN:O	1:C:1027:ARG:NH2	2.43	0.51
1:C:2943:PHE:HE1	1:C:2954:PHE:HB3	1.75	0.51
1:D:2736:LYS:HB3	1:D:2741:TRP:HB2	1.92	0.51
1:D:3229:THR:HG23	1:D:3291:ASP:OD2	2.10	0.51
1:D:3314:LEU:HD12	1:D:3318:HIS:ND1	2.25	0.51
1:D:4105:LEU:HB3	1:D:4115:LEU:HD21	1.92	0.51
1:A:2635:GLU:HA	1:A:2638:LEU:HB2	1.93	0.51
1:A:3136:SER:O	1:A:3140:LEU:HD22	2.10	0.51
1:A:3274:ASN:HA	1:A:3277:LEU:HD23	1.93	0.51
1:B:675:TYR:HB3	1:B:822:CYS:SG	2.51	0.51
1:B:2657:TYR:HA	1:B:2662:PHE:HE1	1.75	0.51
1:B:2923:TYR:HE2	1:B:2999:LYS:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:LEU:HD11	1:C:976:TYR:HB2	1.90	0.51
1:C:1074:ARG:HH12	1:C:1078:CYS:H	1.58	0.51
1:D:2623:LEU:HD23	1:D:2626:GLY:H	1.74	0.51
1:D:2769:GLU:C	1:D:2771:TYR:N	2.69	0.51
1:D:3274:ASN:HA	1:D:3277:LEU:HD23	1.93	0.51
1:A:2202:TYR:O	1:A:2206:ILE:HG12	2.10	0.51
1:B:655:MET:HE2	1:B:1608:VAL:HG21	1.92	0.51
1:B:2095:ILE:HD11	1:B:3629:ILE:HG23	1.91	0.51
1:B:3108:LEU:HD12	1:B:3109:PHE:CD1	2.46	0.51
1:C:675:TYR:HB3	1:C:822:CYS:SG	2.50	0.51
1:C:3227:ARG:HB3	1:C:3230:GLN:OE1	2.11	0.51
1:C:3783:GLU:OE2	1:C:3784:LYS:NZ	2.39	0.51
1:D:375:GLN:HG2	1:D:377:VAL:HG13	1.92	0.51
1:D:1246:ASP:OD1	1:D:1693:TYR:OH	2.29	0.51
1:D:3250:TRP:CD1	1:D:3256:ASN:HD21	2.28	0.51
1:A:849:ASP:OD1	1:A:1214:ARG:NE	2.42	0.51
1:A:2000:HIS:O	1:A:2004:MET:HG2	2.10	0.51
1:A:3314:LEU:HD12	1:A:3318:HIS:ND1	2.25	0.51
2:G:83:TYR:HB3	2:G:87:GLY:HA2	1.93	0.51
1:B:988:LEU:HD12	1:B:992:GLN:HE21	1.75	0.51
1:B:2635:GLU:HA	1:B:2638:LEU:HB2	1.93	0.51
1:B:3134:LEU:HB2	1:B:3162:PHE:CE2	2.45	0.51
1:B:4105:LEU:HB3	1:B:4115:LEU:HD21	1.92	0.51
1:C:2447:LYS:HA	1:C:2447:LYS:HE3	1.92	0.51
1:C:3245:TYR:O	1:C:3249:TRP:HE3	1.93	0.51
1:C:3314:LEU:HD12	1:C:3318:HIS:CE1	2.46	0.51
1:C:3879:LEU:O	1:C:3882:GLN:HG3	2.10	0.51
1:D:1048:ASP:OD1	1:D:1049:SER:N	2.43	0.51
1:D:2488:LEU:HD11	1:D:2548:LEU:HD13	1.93	0.51
1:D:2765:GLU:HA	1:D:2768:LYS:HD2	1.91	0.51
1:D:3314:LEU:HD12	1:D:3318:HIS:CE1	2.46	0.51
1:D:3729:ALA:HA	1:D:3732:HIS:CD2	2.46	0.51
1:D:4306:PHE:HA	1:D:4309:ILE:HG12	1.92	0.51
1:A:1048:ASP:OD1	1:A:1049:SER:N	2.43	0.51
1:A:1246:ASP:OD1	1:A:1693:TYR:OH	2.29	0.51
1:A:1963:LYS:HA	1:A:1966:ARG:HE	1.76	0.51
1:A:2835:ARG:NH1	1:A:2836:ASP:HB2	2.26	0.51
1:A:3227:ARG:HE	1:A:3228:TYR:N	1.96	0.51
1:B:123:HIS:HD1	1:B:149:LEU:HD11	1.76	0.51
1:B:1014:GLN:O	1:B:1027:ARG:NH2	2.43	0.51
1:B:2714:PRO:HD2	1:B:2717:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2874:TYR:HA	1:B:2877:LEU:HD13	1.92	0.51
1:B:3003:MET:O	1:B:3006:SER:OG	2.18	0.51
1:C:2635:GLU:HA	1:C:2638:LEU:HB2	1.93	0.51
1:C:3134:LEU:HB2	1:C:3162:PHE:CE2	2.46	0.51
1:C:3227:ARG:NE	1:C:3228:TYR:H	1.96	0.51
1:D:219:SER:OG	1:D:222:GLU:OE1	2.23	0.51
1:D:1685:LEU:O	1:D:1689:ILE:HG12	2.10	0.51
1:D:2769:GLU:C	1:D:2771:TYR:H	2.16	0.51
1:D:3227:ARG:HB3	1:D:3230:GLN:OE1	2.11	0.51
1:A:882:ARG:HH22	1:A:933:LEU:C	2.18	0.51
1:A:2447:LYS:HA	1:A:2447:LYS:HE3	1.92	0.51
1:A:2939:TYR:HB3	1:A:2943:PHE:HE2	1.76	0.51
1:A:2973:GLN:HA	1:A:2976:LYS:HG2	1.93	0.51
1:A:3003:MET:O	1:A:3006:SER:OG	2.18	0.51
1:A:3250:TRP:CD1	1:A:3256:ASN:HD21	2.28	0.51
1:A:3314:LEU:HD12	1:A:3318:HIS:CE1	2.46	0.51
1:A:4255:LEU:HB2	1:A:4293:THR:HG21	1.93	0.51
2:H:32:GLN:NE2	1:D:1312:GLU:HB3	2.25	0.51
2:H:83:TYR:HB3	2:H:87:GLY:HA2	1.93	0.51
1:C:928:GLU:OE1	4:C:5003:ATP:H8	1.94	0.51
1:C:2095:ILE:HD11	1:C:3629:ILE:HG23	1.91	0.51
1:C:3250:TRP:CD1	1:C:3256:ASN:HD21	2.28	0.51
1:C:4256:MET:HE2	1:C:4256:MET:HA	1.92	0.51
1:D:2000:HIS:O	1:D:2004:MET:HG2	2.10	0.51
1:D:2635:GLU:HA	1:D:2638:LEU:HB2	1.93	0.51
1:D:2835:ARG:NH1	1:D:2836:ASP:HB2	2.26	0.51
1:D:2923:TYR:HE2	1:D:2999:LYS:HB3	1.74	0.51
1:A:131:CYS:SG	1:A:150:GLN:HB2	2.51	0.51
1:A:1014:GLN:O	1:A:1027:ARG:NH2	2.43	0.51
1:A:2264:LYS:HG2	1:A:2267:ARG:NH2	2.26	0.51
1:A:2794:GLU:HB2	1:B:1498:GLN:OE1	2.11	0.51
1:A:3072:MET:HB3	1:A:3140:LEU:HD21	1.93	0.51
1:A:3134:LEU:HB2	1:A:3162:PHE:CE2	2.46	0.51
1:A:3315:LEU:HA	1:A:3319:PHE:HD2	1.75	0.51
1:A:3879:LEU:O	1:A:3882:GLN:HG3	2.10	0.51
1:B:3879:LEU:O	1:B:3882:GLN:HG3	2.10	0.51
1:B:4255:LEU:HB2	1:B:4293:THR:HG21	1.93	0.51
1:C:2488:LEU:HD11	1:C:2548:LEU:HD13	1.93	0.51
1:C:2973:GLN:HA	1:C:2976:LYS:HG2	1.93	0.51
1:C:3314:LEU:HD12	1:C:3318:HIS:ND1	2.25	0.51
1:D:928:GLU:OE1	4:D:5003:ATP:H8	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3187:LYS:NZ	1:D:3195:LEU:HD13	2.26	0.51
1:A:2714:PRO:HD2	1:A:2717:LEU:HD13	1.93	0.51
1:B:131:CYS:SG	1:B:150:GLN:HB2	2.51	0.51
1:B:1963:LYS:HA	1:B:1966:ARG:HE	1.76	0.51
1:B:2488:LEU:HD11	1:B:2548:LEU:HD13	1.93	0.51
1:B:2696:ASP:OD2	1:B:2701:PHE:N	2.43	0.51
1:B:4103:THR:O	1:B:4107:GLU:HG3	2.11	0.51
1:B:4275:THR:HG22	1:B:4278:ASP:H	1.76	0.51
1:C:1008:ALA:O	1:C:1012:ILE:HG12	2.11	0.51
1:C:1048:ASP:OD1	1:C:1049:SER:N	2.43	0.51
1:C:2264:LYS:HG2	1:C:2267:ARG:NH2	2.26	0.51
1:C:3108:LEU:HD12	1:C:3109:PHE:CD1	2.46	0.51
1:C:3187:LYS:NZ	1:C:3195:LEU:HD13	2.26	0.51
1:C:3315:LEU:HA	1:C:3319:PHE:HD2	1.75	0.51
1:C:4306:PHE:HA	1:C:4309:ILE:HG12	1.92	0.51
1:D:2972:ASP:HA	1:D:3035:ILE:CD1	2.41	0.51
1:A:3729:ALA:HA	1:A:3732:HIS:CD2	2.46	0.51
1:A:4103:THR:O	1:A:4107:GLU:HG3	2.11	0.51
1:B:2835:ARG:NH1	1:B:2836:ASP:HB2	2.26	0.51
1:B:2943:PHE:HE1	1:B:2954:PHE:HB3	1.75	0.51
1:C:2696:ASP:OD2	1:C:2701:PHE:N	2.43	0.51
1:C:2714:PRO:HD2	1:C:2717:LEU:HD13	1.93	0.51
1:C:2736:LYS:HB3	1:C:2741:TRP:HB2	1.92	0.51
1:C:2769:GLU:C	1:C:2771:TYR:N	2.69	0.51
1:C:3274:ASN:HA	1:C:3277:LEU:HD23	1.93	0.51
1:C:4255:LEU:HB2	1:C:4293:THR:HG21	1.93	0.51
1:A:375:GLN:HG2	1:A:377:VAL:HG13	1.92	0.50
1:A:2972:ASP:HA	1:A:3035:ILE:CD1	2.41	0.50
1:A:3187:LYS:NZ	1:A:3195:LEU:HD13	2.26	0.50
1:A:4135:ARG:HD3	1:A:4147:ARG:HD3	1.94	0.50
1:A:4848:ILE:HD11	1:D:4818:TYR:HA	1.92	0.50
1:B:1008:ALA:O	1:B:1012:ILE:HG12	2.11	0.50
1:B:2590:ARG:HA	1:B:2640:LEU:HD11	1.93	0.50
1:B:2973:GLN:HA	1:B:2976:LYS:HG2	1.93	0.50
1:B:3227:ARG:CZ	1:B:3287:ASN:HB2	2.41	0.50
1:B:3729:ALA:HA	1:B:3732:HIS:CD2	2.46	0.50
1:C:1049:SER:O	1:C:1052:GLU:HG3	2.11	0.50
1:C:3072:MET:HB3	1:C:3140:LEU:HD21	1.93	0.50
1:D:1049:SER:O	1:D:1052:GLU:HG3	2.11	0.50
1:D:3218:ILE:HA	1:D:3221:LEU:HG	1.92	0.50
1:D:3227:ARG:CZ	1:D:3287:ASN:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:GLU:OE1	4:A:5003:ATP:H8	1.94	0.50
1:A:4306:PHE:HA	1:A:4309:ILE:HG12	1.92	0.50
2:E:83:TYR:HB3	2:E:87:GLY:HA2	1.93	0.50
1:B:375:GLN:HG2	1:B:377:VAL:HG13	1.92	0.50
1:B:881:ILE:O	1:B:885:LEU:HD23	2.10	0.50
1:B:1724:GLU:OE2	1:B:2127:ARG:NH2	2.42	0.50
1:B:3314:LEU:HD12	1:B:3318:HIS:CE1	2.46	0.50
1:C:2202:TYR:O	1:C:2206:ILE:HG12	2.10	0.50
1:C:3102:LEU:HD22	1:C:3154:ALA:HB1	1.93	0.50
1:C:4103:THR:O	1:C:4107:GLU:HG3	2.11	0.50
1:D:2264:LYS:HG2	1:D:2267:ARG:NH2	2.26	0.50
1:D:2708:THR:HG21	1:D:2780:LYS:C	2.37	0.50
1:D:2939:TYR:HB3	1:D:2943:PHE:HE2	1.76	0.50
1:D:3245:TYR:O	1:D:3249:TRP:HE3	1.93	0.50
1:D:3315:LEU:HD23	1:D:3319:PHE:CE2	2.46	0.50
1:A:878:LEU:O	1:A:881:ILE:HG22	2.11	0.50
1:A:967:PRO:O	1:A:971:GLN:HB2	2.12	0.50
1:A:969:ASN:OD1	1:A:970:TYR:N	2.45	0.50
1:A:1074:ARG:HH12	1:A:1078:CYS:H	1.58	0.50
1:A:2488:LEU:HD11	1:A:2548:LEU:HD13	1.93	0.50
1:A:2590:ARG:HA	1:A:2640:LEU:HD11	1.93	0.50
1:B:967:PRO:O	1:B:971:GLN:HB2	2.12	0.50
1:B:1049:SER:O	1:B:1052:GLU:HG3	2.11	0.50
1:B:2972:ASP:HA	1:B:3035:ILE:CD1	2.41	0.50
1:B:3072:MET:HB3	1:B:3140:LEU:HD21	1.93	0.50
1:B:4480:PHE:HA	1:B:4483:LYS:HZ3	1.77	0.50
1:C:1963:LYS:HA	1:C:1966:ARG:HE	1.76	0.50
1:C:2590:ARG:HA	1:C:2640:LEU:HD11	1.93	0.50
1:C:3044:THR:HA	1:C:3047:LYS:HG2	1.94	0.50
1:C:3058:ARG:HE	1:C:3061:LEU:HD21	1.77	0.50
1:C:3227:ARG:CZ	1:C:3287:ASN:HB2	2.42	0.50
1:D:131:CYS:SG	1:D:150:GLN:HB2	2.51	0.50
1:A:3058:ARG:HE	1:A:3061:LEU:HD21	1.77	0.50
1:A:3187:LYS:HG2	1:A:3191:GLU:CD	2.37	0.50
1:A:3227:ARG:CZ	1:A:3287:ASN:HB2	2.42	0.50
1:A:3229:THR:HG23	1:A:3291:ASP:OD2	2.10	0.50
1:A:4105:LEU:HB3	1:A:4115:LEU:HD21	1.92	0.50
1:B:969:ASN:OD1	1:B:970:TYR:N	2.45	0.50
1:B:2593:VAL:HG12	1:B:2644:LEU:HB2	1.94	0.50
1:B:3102:LEU:HD22	1:B:3154:ALA:HB1	1.93	0.50
1:B:3187:LYS:HG2	1:B:3191:GLU:CD	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3227:ARG:HB3	1:B:3230:GLN:OE1	2.11	0.50
1:B:3274:ASN:HA	1:B:3277:LEU:HD23	1.93	0.50
1:C:131:CYS:SG	1:C:150:GLN:HB2	2.51	0.50
1:C:878:LEU:O	1:C:881:ILE:HG22	2.11	0.50
1:C:2708:THR:HG21	1:C:2780:LYS:C	2.37	0.50
1:C:3136:SER:O	1:C:3140:LEU:HD22	2.10	0.50
1:C:3315:LEU:HD23	1:C:3319:PHE:CE2	2.47	0.50
1:D:270:HIS:ND1	1:D:491:GLU:HG3	2.27	0.50
1:D:2590:ARG:HA	1:D:2640:LEU:HD11	1.93	0.50
1:D:2708:THR:O	1:D:2708:THR:HG22	2.12	0.50
1:D:2973:GLN:HA	1:D:2976:LYS:HG2	1.93	0.50
1:D:3227:ARG:NE	1:D:3228:TYR:H	1.96	0.50
1:D:4103:THR:O	1:D:4107:GLU:HG3	2.11	0.50
1:A:270:HIS:ND1	1:A:491:GLU:HG3	2.27	0.50
1:A:1284:LYS:NZ	1:A:1286:THR:OG1	2.41	0.50
1:A:2943:PHE:HE1	1:A:2954:PHE:HB3	1.75	0.50
1:B:878:LEU:O	1:B:881:ILE:HG22	2.11	0.50
1:B:962:LYS:HZ3	1:B:982:ASP:CG	2.17	0.50
1:B:3044:THR:HA	1:B:3047:LYS:HG2	1.94	0.50
1:B:3229:THR:HG23	1:B:3291:ASP:OD2	2.10	0.50
1:C:2657:TYR:HA	1:C:2662:PHE:HE1	1.75	0.50
1:D:3072:MET:HB3	1:D:3140:LEU:HD21	1.93	0.50
1:A:2708:THR:HG21	1:A:2780:LYS:C	2.37	0.50
1:A:2719:TYR:O	1:A:2719:TYR:HD1	1.94	0.50
2:F:83:TYR:HB3	2:F:87:GLY:HA2	1.93	0.50
1:B:270:HIS:ND1	1:B:491:GLU:HG3	2.27	0.50
1:B:2377:GLU:OE2	1:B:2457:SER:OG	2.30	0.50
1:B:2455:ASP:OD2	1:B:2457:SER:OG	2.21	0.50
1:C:270:HIS:ND1	1:C:491:GLU:HG3	2.27	0.50
1:C:2377:GLU:OE2	1:C:2457:SER:OG	2.30	0.50
1:D:3044:THR:HA	1:D:3047:LYS:HG2	1.94	0.50
1:A:2377:GLU:OE2	1:A:2457:SER:OG	2.30	0.50
1:A:3108:LEU:HD12	1:A:3109:PHE:CD1	2.46	0.50
1:B:2719:TYR:O	1:B:2719:TYR:HD1	1.94	0.50
1:B:2720:PHE:HE1	1:B:2896:LEU:HA	1.77	0.50
1:B:2743:TYR:CD1	1:B:2757:MET:HB2	2.41	0.50
1:B:3315:LEU:HA	1:B:3319:PHE:HD2	1.75	0.50
1:C:2835:ARG:NH1	1:C:2836:ASP:HB2	2.26	0.50
1:C:4105:LEU:HB3	1:C:4115:LEU:HD21	1.92	0.50
1:D:655:MET:HE2	1:D:1608:VAL:HG21	1.92	0.50
1:D:878:LEU:O	1:D:881:ILE:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1074:ARG:HH12	1:D:1078:CYS:H	1.58	0.50
1:D:3102:LEU:HD22	1:D:3154:ALA:HB1	1.93	0.50
1:A:537:LEU:O	1:A:541:ILE:HG12	2.12	0.50
1:A:730:LEU:HD11	2:E:8:ILE:HA	1.93	0.50
1:A:1049:SER:O	1:A:1052:GLU:HG3	2.11	0.50
1:A:2696:ASP:OD2	1:A:2701:PHE:N	2.43	0.50
1:B:2264:LYS:HG2	1:B:2267:ARG:NH2	2.26	0.50
1:B:2939:TYR:HB3	1:B:2943:PHE:HE2	1.76	0.50
1:B:3058:ARG:HE	1:B:3061:LEU:HD21	1.77	0.50
1:C:1839:LEU:HD12	1:C:1842:ILE:HD11	1.94	0.50
1:C:2719:TYR:HD1	1:C:2719:TYR:O	1.94	0.50
1:C:3729:ALA:HA	1:C:3732:HIS:CD2	2.46	0.50
1:C:4275:THR:HG22	1:C:4278:ASP:H	1.76	0.50
1:D:686:VAL:HG13	1:D:687:THR:HG23	1.94	0.50
1:D:2174:VAL:O	1:D:2178:VAL:HG23	2.12	0.50
1:D:2593:VAL:HG12	1:D:2644:LEU:HB2	1.94	0.50
1:D:3108:LEU:HD12	1:D:3109:PHE:CD1	2.46	0.50
1:D:4052:MET:HE3	1:D:4063:THR:HG23	1.94	0.50
1:D:4275:THR:HG22	1:D:4278:ASP:H	1.76	0.50
1:B:537:LEU:O	1:B:541:ILE:HG12	2.12	0.50
1:B:3227:ARG:HE	1:B:3228:TYR:N	1.96	0.50
1:C:4029:SER:HG	1:C:4055:HIS:CD2	2.29	0.50
1:D:967:PRO:O	1:D:971:GLN:HB2	2.12	0.50
1:D:2714:PRO:HD2	1:D:2717:LEU:HD13	1.93	0.50
1:D:4135:ARG:HD3	1:D:4147:ARG:HD3	1.94	0.50
1:A:992:GLN:HB2	1:A:995:MET:HE2	1.95	0.49
1:A:2833:LEU:HD13	1:A:2837:LEU:HB3	1.94	0.49
2:F:50:ARG:HG2	2:F:53:LYS:HE3	1.94	0.49
2:H:50:ARG:HG2	2:H:53:LYS:HE3	1.93	0.49
1:B:928:GLU:OE1	4:B:5003:ATP:H8	1.94	0.49
1:B:3184:TYR:HE2	1:B:3201:VAL:HB	1.77	0.49
1:C:163:HIS:HB2	1:C:182:ILE:HG13	1.94	0.49
1:C:2593:VAL:HG12	1:C:2644:LEU:HB2	1.94	0.49
1:D:1008:ALA:O	1:D:1012:ILE:HG12	2.11	0.49
1:D:1611:ILE:HD12	1:D:1611:ILE:H	1.77	0.49
1:D:2720:PHE:HE1	1:D:2896:LEU:HA	1.77	0.49
1:D:2943:PHE:HE1	1:D:2954:PHE:HB3	1.75	0.49
1:A:137:ARG:HH22	1:A:204:ASP:HB3	1.77	0.49
2:G:50:ARG:HG2	2:G:53:LYS:HE3	1.94	0.49
1:B:137:ARG:HH22	1:B:204:ASP:HB3	1.77	0.49
1:B:163:HIS:HB2	1:B:182:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1839:LEU:HD12	1:B:1842:ILE:HD11	1.94	0.49
1:B:3136:SER:O	1:B:3140:LEU:HD22	2.10	0.49
1:B:3187:LYS:NZ	1:B:3195:LEU:HD13	2.26	0.49
1:C:123:HIS:HD1	1:C:149:LEU:HD11	1.76	0.49
1:C:2720:PHE:HE1	1:C:2896:LEU:HA	1.77	0.49
1:D:504:ARG:O	1:D:507:VAL:HG22	2.13	0.49
1:D:2719:TYR:O	1:D:2719:TYR:HD1	1.94	0.49
1:A:686:VAL:HG13	1:A:687:THR:HG23	1.94	0.49
1:A:2589:LEU:O	1:A:2593:VAL:HG13	2.13	0.49
2:H:54:GLN:O	1:D:1771:ILE:HD11	2.11	0.49
1:B:253:GLY:O	1:B:257:ARG:HG2	2.13	0.49
1:B:2708:THR:O	1:B:2708:THR:HG22	2.12	0.49
1:C:2708:THR:HG22	1:C:2708:THR:O	2.12	0.49
1:D:4255:LEU:HB2	1:D:4293:THR:HG21	1.93	0.49
1:A:1420:LEU:HD11	1:A:1559:ARG:HH21	1.77	0.49
1:A:2174:VAL:O	1:A:2178:VAL:HG23	2.12	0.49
1:A:3044:THR:HA	1:A:3047:LYS:HG2	1.94	0.49
1:A:3192:ARG:NH2	1:A:3197:LEU:HD23	2.26	0.49
1:C:1685:LEU:HD13	1:C:1706:LEU:HD13	1.94	0.49
1:C:3187:LYS:HG2	1:C:3191:GLU:CD	2.37	0.49
1:C:4135:ARG:HD3	1:C:4147:ARG:HD3	1.94	0.49
1:C:4818:TYR:HA	1:D:4848:ILE:HD11	1.94	0.49
1:D:227:TYR:CG	1:D:352:SER:HB2	2.48	0.49
1:D:969:ASN:OD1	1:D:970:TYR:N	2.45	0.49
1:D:1304:LEU:HB3	1:D:1586:LEU:HD11	1.95	0.49
1:D:3187:LYS:HG2	1:D:3191:GLU:CD	2.37	0.49
1:D:4079:ASP:O	1:D:4082:GLU:HG3	2.13	0.49
1:A:4052:MET:HE3	1:A:4063:THR:HG23	1.94	0.49
1:A:4480:PHE:HA	1:A:4483:LYS:HZ3	1.77	0.49
2:F:79:PRO:HD3	2:F:97:THR:OG1	2.13	0.49
1:B:3315:LEU:HD23	1:B:3319:PHE:CE2	2.46	0.49
1:B:4177:VAL:HG11	1:B:4880:VAL:HA	1.94	0.49
1:C:969:ASN:OD1	1:C:970:TYR:N	2.45	0.49
1:C:4177:VAL:HG11	1:C:4880:VAL:HA	1.94	0.49
1:D:1963:LYS:HA	1:D:1966:ARG:HE	1.76	0.49
1:D:2589:LEU:O	1:D:2593:VAL:HG13	2.13	0.49
1:D:2696:ASP:OD2	1:D:2701:PHE:N	2.43	0.49
1:A:163:HIS:HB2	1:A:182:ILE:HG13	1.94	0.49
1:A:253:GLY:O	1:A:257:ARG:HG2	2.13	0.49
1:A:829:LYS:NZ	1:A:1037:LEU:O	2.39	0.49
1:A:3227:ARG:HB3	1:A:3230:GLN:OE1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3315:LEU:HD23	1:A:3319:PHE:CE2	2.47	0.49
1:A:3823:GLU:OE1	1:A:3826:GLY:N	2.41	0.49
1:A:4275:THR:HG22	1:A:4278:ASP:H	1.76	0.49
1:B:234:LEU:HD13	1:B:405:LEU:HD22	1.95	0.49
1:B:2589:LEU:O	1:B:2593:VAL:HG13	2.13	0.49
1:B:3187:LYS:HD2	1:B:3192:ARG:HH21	1.78	0.49
1:C:686:VAL:HG13	1:C:687:THR:HG23	1.94	0.49
1:C:1246:ASP:OD1	1:C:1693:TYR:OH	2.29	0.49
1:C:2939:TYR:HB3	1:C:2943:PHE:HE2	1.76	0.49
1:D:992:GLN:HB2	1:D:995:MET:HE2	1.95	0.49
1:D:2377:GLU:OE2	1:D:2457:SER:OG	2.30	0.49
1:A:2743:TYR:CD1	1:A:2757:MET:HB2	2.41	0.49
2:F:8:ILE:HD11	2:F:74:LYS:HB2	1.95	0.49
2:H:79:PRO:HD3	2:H:97:THR:OG1	2.13	0.49
1:B:4052:MET:HE3	1:B:4063:THR:HG23	1.94	0.49
1:B:4818:TYR:HA	1:C:4848:ILE:HD11	1.94	0.49
1:C:2972:ASP:HA	1:C:3035:ILE:CD1	2.41	0.49
1:C:3043:ARG:C	1:C:3047:LYS:HZ2	2.21	0.49
1:C:3215:MET:HA	1:C:3218:ILE:HG12	1.94	0.49
1:C:4052:MET:HE3	1:C:4063:THR:HG23	1.94	0.49
1:C:4079:ASP:O	1:C:4082:GLU:HG3	2.13	0.49
1:C:4086:ARG:HH21	1:C:4087:PHE:HE2	1.61	0.49
1:D:3058:ARG:HE	1:D:3061:LEU:HD21	1.77	0.49
1:A:1611:ILE:H	1:A:1611:ILE:HD12	1.77	0.49
1:A:3102:LEU:HD22	1:A:3154:ALA:HB1	1.93	0.49
1:A:4079:ASP:O	1:A:4082:GLU:HG3	2.13	0.49
1:A:4956:ASP:OD1	1:A:4957:CYS:N	2.46	0.49
1:B:1246:ASP:OD1	1:B:1693:TYR:OH	2.29	0.49
1:B:2344:LEU:HD22	1:B:2434:GLY:HA3	1.95	0.49
1:B:3304:GLN:HA	1:B:3307:ILE:HG12	1.95	0.49
1:C:227:TYR:CG	1:C:352:SER:HB2	2.48	0.49
1:C:503:ASP:O	1:C:507:VAL:HG13	2.13	0.49
1:C:3184:TYR:HE2	1:C:3201:VAL:HB	1.78	0.49
1:C:3227:ARG:HE	1:C:3228:TYR:N	1.96	0.49
1:D:537:LEU:O	1:D:541:ILE:HG12	2.12	0.49
1:D:2455:ASP:OD2	1:D:2457:SER:OG	2.22	0.49
1:A:181:LEU:N	1:A:212:TRP:O	2.36	0.49
1:A:4058:TYR:HB3	1:A:4062:GLU:HB2	1.95	0.49
2:H:58:LYS:O	2:H:62:GLU:OE1	2.31	0.49
1:B:504:ARG:O	1:B:507:VAL:HG22	2.13	0.49
1:B:992:GLN:HB2	1:B:995:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:ARG:NH1	1:B:1078:CYS:H	2.11	0.49
1:B:2621:TYR:OH	1:B:2637:GLU:OE2	2.17	0.49
1:B:2708:THR:HG21	1:B:2780:LYS:C	2.37	0.49
1:C:137:ARG:HH22	1:C:204:ASP:HB3	1.77	0.49
1:C:504:ARG:O	1:C:507:VAL:HG22	2.13	0.49
1:C:967:PRO:O	1:C:971:GLN:HB2	2.12	0.49
1:D:1420:LEU:HD11	1:D:1559:ARG:HH21	1.77	0.49
1:D:1716:THR:O	1:D:1720:MET:HG3	2.13	0.49
1:D:3184:TYR:HE2	1:D:3201:VAL:HB	1.78	0.49
1:D:3695:MET:HB3	1:D:3731:LEU:HD11	1.95	0.49
1:D:4058:TYR:HB3	1:D:4062:GLU:HB2	1.95	0.49
1:D:4086:ARG:HH21	1:D:4087:PHE:HE2	1.61	0.49
1:A:1304:LEU:HB3	1:A:1586:LEU:HD11	1.95	0.49
1:A:2344:LEU:HD22	1:A:2434:GLY:HA3	1.95	0.49
1:A:2592:LEU:HD13	1:A:2610:LEU:CD2	2.43	0.49
1:C:234:LEU:HD13	1:C:405:LEU:HD22	1.95	0.49
1:C:2971:ILE:HG23	1:C:2975:PHE:CE2	2.48	0.49
1:C:4480:PHE:HA	1:C:4483:LYS:HZ3	1.78	0.49
1:D:2957:GLU:HB2	1:D:2961:LYS:NZ	2.28	0.49
1:A:3112:ILE:HG23	1:A:3117:PHE:HB3	1.95	0.48
2:E:50:ARG:HG2	2:E:53:LYS:HE3	1.93	0.48
2:E:79:PRO:HD3	2:E:97:THR:OG1	2.13	0.48
2:H:12:ASP:OD2	2:H:13:GLY:N	2.46	0.48
1:B:3695:MET:HB3	1:B:3731:LEU:HD11	1.95	0.48
1:C:537:LEU:O	1:C:541:ILE:HG12	2.12	0.48
1:C:1611:ILE:H	1:C:1611:ILE:HD12	1.77	0.48
1:C:3112:ILE:HG23	1:C:3117:PHE:HB3	1.95	0.48
1:D:4145:ILE:HB	1:D:4961:GLN:HG3	1.95	0.48
1:A:1008:ALA:O	1:A:1012:ILE:HG12	2.11	0.48
1:A:3043:ARG:C	1:A:3047:LYS:HZ2	2.22	0.48
2:E:58:LYS:O	2:E:62:GLU:OE1	2.31	0.48
2:G:51:ILE:C	2:G:53:LYS:HZ1	2.11	0.48
2:G:58:LYS:O	2:G:62:GLU:OE1	2.31	0.48
1:B:227:TYR:CG	1:B:352:SER:HB2	2.48	0.48
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.95	0.48
1:B:1420:LEU:HD11	1:B:1559:ARG:HH21	1.77	0.48
1:B:2684:ASN:ND2	1:B:2909:ASP:OD1	2.39	0.48
1:B:3112:ILE:HG23	1:B:3117:PHE:HB3	1.95	0.48
1:B:3215:MET:HA	1:B:3218:ILE:HG12	1.94	0.48
1:C:56:LYS:HA	1:C:324:VAL:HG23	1.95	0.48
1:C:253:GLY:O	1:C:257:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2258:ARG:HB3	1:C:2260:PRO:HD2	1.95	0.48
1:C:2592:LEU:HD13	1:C:2610:LEU:CD2	2.43	0.48
1:C:4145:ILE:HB	1:C:4961:GLN:HG3	1.95	0.48
1:D:1685:LEU:HD13	1:D:1706:LEU:HD13	1.94	0.48
1:D:1839:LEU:HD12	1:D:1842:ILE:HD11	1.94	0.48
1:D:3215:MET:HA	1:D:3218:ILE:HG12	1.94	0.48
1:D:4177:VAL:HG11	1:D:4880:VAL:HA	1.94	0.48
1:A:504:ARG:O	1:A:507:VAL:HG22	2.13	0.48
1:A:982:ASP:H	1:A:985:PHE:HE1	1.62	0.48
1:A:2708:THR:HG22	1:A:2708:THR:O	2.12	0.48
1:A:2720:PHE:HE1	1:A:2896:LEU:HA	1.77	0.48
1:A:3227:ARG:NE	1:A:3228:TYR:H	1.96	0.48
2:E:12:ASP:OD2	2:E:13:GLY:N	2.46	0.48
1:B:686:VAL:HG13	1:B:687:THR:HG23	1.94	0.48
1:B:1979:PHE:CG	1:B:1993:ARG:HG2	2.49	0.48
1:B:2833:LEU:HD13	1:B:2837:LEU:HB3	1.94	0.48
1:B:3227:ARG:NH1	1:B:3290:ILE:HG13	2.18	0.48
1:B:4145:ILE:HB	1:B:4961:GLN:HG3	1.95	0.48
1:C:466:PRO:HG3	1:C:478:ARG:HD2	1.96	0.48
1:C:1074:ARG:NH1	1:C:1078:CYS:H	2.11	0.48
1:D:137:ARG:HH22	1:D:204:ASP:HB3	1.78	0.48
1:D:902:TRP:CZ2	1:D:913:ARG:HA	2.48	0.48
1:A:234:LEU:HD13	1:A:405:LEU:HD22	1.95	0.48
1:A:503:ASP:O	1:A:507:VAL:HG13	2.13	0.48
1:A:1979:PHE:CG	1:A:1993:ARG:HG2	2.49	0.48
1:A:3184:TYR:HE2	1:A:3201:VAL:HB	1.78	0.48
1:A:3653:GLU:OE2	1:A:3660:ARG:NH2	2.46	0.48
1:A:4145:ILE:HB	1:A:4961:GLN:HG3	1.95	0.48
2:E:8:ILE:HD11	2:E:74:LYS:HB2	1.95	0.48
2:F:12:ASP:OD2	2:F:13:GLY:N	2.46	0.48
2:G:12:ASP:OD2	2:G:13:GLY:N	2.46	0.48
2:H:8:ILE:HD11	2:H:74:LYS:HB2	1.95	0.48
1:B:56:LYS:HA	1:B:324:VAL:HG23	1.95	0.48
1:B:887:GLU:O	1:B:890:HIS:ND1	2.46	0.48
1:B:2163:ARG:NH1	1:B:2209:GLN:HB3	2.29	0.48
1:C:902:TRP:CD1	1:C:903:GLN:H	2.32	0.48
1:C:1898:LEU:HD13	1:C:1902:VAL:HG12	1.96	0.48
1:C:1937:GLN:NE2	1:C:3608:LEU:O	2.32	0.48
1:C:2174:VAL:O	1:C:2178:VAL:HG23	2.12	0.48
1:C:2719:TYR:HD1	1:C:2723:LYS:HZ2	1.60	0.48
1:C:3697:LYS:HA	1:C:3700:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3187:LYS:HD2	1:D:3192:ARG:HH21	1.78	0.48
1:A:1682:GLU:HB3	1:A:1683:PRO:HD3	1.95	0.48
1:A:2258:ARG:HB3	1:A:2260:PRO:HD2	1.95	0.48
1:A:2593:VAL:HG12	1:A:2644:LEU:HB2	1.94	0.48
1:A:3956:MET:HE2	1:A:4016:PHE:HB2	1.96	0.48
1:B:1898:LEU:HD13	1:B:1902:VAL:HG12	1.96	0.48
1:B:2971:ILE:HG23	1:B:2975:PHE:CE2	2.48	0.48
1:B:3227:ARG:HH12	1:B:3287:ASN:HB2	1.78	0.48
1:B:4079:ASP:O	1:B:4082:GLU:HG3	2.13	0.48
1:B:4135:ARG:HD3	1:B:4147:ARG:HD3	1.94	0.48
1:C:992:GLN:HB2	1:C:995:MET:HE2	1.95	0.48
1:C:3653:GLU:OE2	1:C:3660:ARG:NH2	2.46	0.48
1:D:466:PRO:HG3	1:D:478:ARG:HD2	1.96	0.48
1:D:1979:PHE:CG	1:D:1993:ARG:HG2	2.49	0.48
1:D:2971:ILE:HG23	1:D:2975:PHE:CE2	2.48	0.48
1:A:227:TYR:CG	1:A:352:SER:HB2	2.47	0.48
1:A:887:GLU:O	1:A:890:HIS:ND1	2.46	0.48
1:A:1724:GLU:OE2	1:A:2127:ARG:NH2	2.42	0.48
1:A:2163:ARG:NH1	1:A:2209:GLN:HB3	2.29	0.48
1:A:2274:LEU:HG	1:A:2329:GLU:HG3	1.96	0.48
2:G:8:ILE:HD11	2:G:74:LYS:HB2	1.95	0.48
2:G:79:PRO:HD3	2:G:97:THR:OG1	2.13	0.48
1:B:674:TYR:CE1	1:B:756:SER:HB2	2.49	0.48
1:B:902:TRP:CZ2	1:B:913:ARG:HA	2.48	0.48
1:B:4086:ARG:HH21	1:B:4087:PHE:HE2	1.61	0.48
1:C:1420:LEU:HD11	1:C:1559:ARG:HH21	1.77	0.48
1:C:2163:ARG:NH1	1:C:2209:GLN:HB3	2.29	0.48
1:C:2589:LEU:O	1:C:2593:VAL:HG13	2.13	0.48
1:C:2957:GLU:HB2	1:C:2961:LYS:NZ	2.28	0.48
1:D:253:GLY:O	1:D:257:ARG:HG2	2.13	0.48
1:D:2163:ARG:NH1	1:D:2209:GLN:HB3	2.29	0.48
1:D:2258:ARG:HB3	1:D:2260:PRO:HD2	1.95	0.48
1:D:2274:LEU:HG	1:D:2329:GLU:HG3	1.96	0.48
1:D:3653:GLU:OE2	1:D:3660:ARG:NH2	2.46	0.48
1:D:4268:MET:O	1:D:4272:LYS:HG2	2.14	0.48
1:A:2971:ILE:HG23	1:A:2975:PHE:CE2	2.48	0.48
1:A:3304:GLN:HA	1:A:3307:ILE:HG12	1.95	0.48
1:A:3336:GLU:OE2	1:A:3337:GLU:HG3	2.13	0.48
1:A:4086:ARG:HH21	1:A:4087:PHE:HE2	1.61	0.48
1:A:4177:VAL:HG11	1:A:4880:VAL:HA	1.94	0.48
1:B:972:LEU:HD12	1:B:974:SER:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:982:ASP:H	1:B:985:PHE:HE1	1.62	0.48
1:B:2174:VAL:O	1:B:2178:VAL:HG23	2.12	0.48
1:B:4058:TYR:HB3	1:B:4062:GLU:HB2	1.95	0.48
1:C:674:TYR:CE1	1:C:756:SER:HB2	2.48	0.48
1:C:824:GLU:HA	1:C:1020:ILE:HD12	1.96	0.48
1:C:902:TRP:CZ2	1:C:913:ARG:HA	2.48	0.48
1:C:946:LEU:HG	1:C:998:LYS:HD3	1.96	0.48
1:C:2833:LEU:HD13	1:C:2837:LEU:HB3	1.94	0.48
1:C:3227:ARG:HH12	1:C:3287:ASN:HB2	1.78	0.48
1:C:3336:GLU:OE2	1:C:3337:GLU:HG3	2.13	0.48
1:C:4956:ASP:OD1	1:C:4957:CYS:N	2.46	0.48
1:D:163:HIS:HB2	1:D:182:ILE:HG13	1.94	0.48
1:D:1276:THR:OG1	1:D:1278:ASP:OD1	2.32	0.48
1:D:2833:LEU:HD13	1:D:2837:LEU:HB3	1.94	0.48
1:A:1685:LEU:HD13	1:A:1706:LEU:HD13	1.94	0.48
1:A:3187:LYS:HD2	1:A:3192:ARG:HH21	1.78	0.48
1:A:3250:TRP:NE1	1:A:3256:ASN:HD21	2.12	0.48
1:B:137:ARG:HH12	1:B:204:ASP:HB3	1.79	0.48
1:B:503:ASP:O	1:B:507:VAL:HG13	2.13	0.48
1:B:910:ASP:OD2	1:B:911:ASN:N	2.47	0.48
1:B:1047:LYS:HG3	1:B:1051:ARG:CZ	2.44	0.48
1:B:1304:LEU:HB3	1:B:1586:LEU:HD11	1.95	0.48
1:B:3303:SER:HA	1:B:3306:ILE:HD13	1.96	0.48
1:B:3697:LYS:HA	1:B:3700:HIS:CD2	2.49	0.48
1:B:4051:ALA:O	1:B:4055:HIS:ND1	2.19	0.48
1:C:887:GLU:O	1:C:890:HIS:ND1	2.46	0.48
1:C:3304:GLN:HA	1:C:3307:ILE:HG12	1.95	0.48
1:D:887:GLU:O	1:D:890:HIS:ND1	2.46	0.48
1:D:2344:LEU:HD22	1:D:2434:GLY:HA3	1.95	0.48
1:A:674:TYR:CE1	1:A:756:SER:HB2	2.48	0.48
1:A:902:TRP:CZ2	1:A:913:ARG:HA	2.48	0.48
1:A:2059:GLN:NE2	1:A:2091:GLN:O	2.47	0.48
1:A:2768:LYS:HB3	1:A:2772:ARG:NH1	2.29	0.48
1:A:2957:GLU:HA	1:A:2960:ILE:HG12	1.96	0.48
1:A:3215:MET:HA	1:A:3218:ILE:HG12	1.94	0.48
1:B:824:GLU:HA	1:B:1020:ILE:HD12	1.96	0.48
1:B:1685:LEU:HD13	1:B:1706:LEU:HD13	1.94	0.48
1:B:1716:THR:O	1:B:1720:MET:HG3	2.13	0.48
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.95	0.48
1:C:1304:LEU:HB3	1:C:1586:LEU:HD11	1.95	0.48
1:C:1716:THR:O	1:C:1720:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1979:PHE:CG	1:C:1993:ARG:HG2	2.49	0.48
1:C:2920:ARG:HH22	1:C:3000:GLU:HG2	1.79	0.48
1:C:2957:GLU:HA	1:C:2960:ILE:HG12	1.96	0.48
1:C:4058:TYR:HB3	1:C:4062:GLU:HB2	1.95	0.48
1:D:503:ASP:O	1:D:507:VAL:HG13	2.13	0.48
1:D:902:TRP:CD1	1:D:903:GLN:H	2.32	0.48
1:D:982:ASP:H	1:D:985:PHE:HE1	1.61	0.48
1:D:2997:SER:O	1:D:3000:GLU:HB2	2.14	0.48
1:D:4480:PHE:HA	1:D:4483:LYS:HZ3	1.78	0.48
1:A:972:LEU:HD12	1:A:974:SER:HB2	1.96	0.48
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.95	0.48
1:A:3277:LEU:O	1:A:3281:LEU:HG	2.14	0.48
1:A:3296:MET:HA	1:A:3299:LEU:HG	1.96	0.48
1:B:1611:ILE:H	1:B:1611:ILE:HD12	1.77	0.48
1:B:2274:LEU:HG	1:B:2329:GLU:HG3	1.96	0.48
1:B:2572:CYS:O	1:B:2576:ILE:HG13	2.14	0.48
1:B:2769:GLU:C	1:B:2771:TYR:N	2.69	0.48
1:C:2059:GLN:NE2	1:C:2091:GLN:O	2.47	0.48
1:C:2344:LEU:HD22	1:C:2434:GLY:HA3	1.95	0.48
1:C:2724:TYR:CD1	1:C:2895:PHE:CD2	3.02	0.48
1:C:3250:TRP:NE1	1:C:3256:ASN:HD21	2.12	0.48
1:C:3296:MET:HA	1:C:3299:LEU:HG	1.96	0.48
1:C:3303:SER:HA	1:C:3306:ILE:HD13	1.96	0.48
1:C:3316:LYS:O	1:C:3317:THR:OG1	2.30	0.48
1:C:3695:MET:HB3	1:C:3731:LEU:HD11	1.95	0.48
1:D:181:LEU:N	1:D:212:TRP:O	2.36	0.48
1:D:1724:GLU:OE2	1:D:2127:ARG:NH2	2.42	0.48
1:D:3025:ASP:O	1:D:3029:ILE:HD12	2.14	0.48
1:D:3324:GLU:OE2	1:D:3325:LYS:HE3	2.14	0.48
1:A:56:LYS:HA	1:A:324:VAL:HG23	1.95	0.47
1:A:137:ARG:HH12	1:A:204:ASP:HB3	1.79	0.47
1:A:470:LEU:HB2	1:A:475:LYS:HG3	1.96	0.47
1:A:1716:THR:O	1:A:1720:MET:HG3	2.13	0.47
1:A:1839:LEU:HD12	1:A:1842:ILE:HD11	1.94	0.47
2:G:38:ASP:OD1	2:G:43:ARG:NH1	2.47	0.47
1:B:643:LEU:HD13	1:B:1657:THR:HG23	1.96	0.47
1:B:902:TRP:CD1	1:B:903:GLN:H	2.32	0.47
1:B:1416:ASP:O	1:B:1420:LEU:HB2	2.14	0.47
1:B:2957:GLU:HB2	1:B:2961:LYS:NZ	2.28	0.47
1:B:3336:GLU:OE2	1:B:3337:GLU:HG3	2.13	0.47
1:C:611:LEU:HD22	1:C:1660:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2274:LEU:HG	1:C:2329:GLU:HG3	1.96	0.47
1:D:234:LEU:HD13	1:D:405:LEU:HD22	1.95	0.47
1:D:674:TYR:CE1	1:D:756:SER:HB2	2.48	0.47
1:D:1682:GLU:HB3	1:D:1683:PRO:HD3	1.95	0.47
1:D:2592:LEU:HD13	1:D:2610:LEU:CD2	2.43	0.47
1:D:2957:GLU:HA	1:D:2960:ILE:HG12	1.96	0.47
1:D:3697:LYS:HA	1:D:3700:HIS:CD2	2.49	0.47
1:A:902:TRP:CD1	1:A:903:GLN:H	2.32	0.47
1:A:4252:ILE:HG21	1:B:4707:MET:HG3	1.95	0.47
4:A:5003:ATP:C5'	5:A:5004:KVR:C15	2.92	0.47
2:E:38:ASP:OD1	2:E:43:ARG:NH1	2.47	0.47
2:F:58:LYS:O	2:F:62:GLU:OE1	2.31	0.47
1:B:466:PRO:HG3	1:B:478:ARG:HD2	1.96	0.47
1:B:2592:LEU:HD13	1:B:2610:LEU:CD2	2.43	0.47
1:B:2724:TYR:CD1	1:B:2895:PHE:CD2	3.02	0.47
1:B:2957:GLU:HA	1:B:2960:ILE:HG12	1.96	0.47
1:C:982:ASP:H	1:C:985:PHE:HE1	1.61	0.47
1:C:3324:GLU:OE2	1:C:3325:LYS:HE3	2.14	0.47
1:D:3112:ILE:HG23	1:D:3117:PHE:HB3	1.95	0.47
1:D:3336:GLU:OE2	1:D:3337:GLU:HG3	2.13	0.47
1:D:4956:ASP:OD1	1:D:4957:CYS:N	2.46	0.47
1:A:2997:SER:O	1:A:3000:GLU:HB2	2.14	0.47
1:B:1284:LYS:NZ	1:B:1286:THR:OG1	2.41	0.47
1:B:2768:LYS:HB3	1:B:2772:ARG:NH1	2.29	0.47
1:B:2920:ARG:HH22	1:B:3000:GLU:HG2	1.79	0.47
1:B:3296:MET:HA	1:B:3299:LEU:HG	1.96	0.47
1:B:3844:GLN:O	1:B:3848:GLU:HG3	2.15	0.47
1:C:137:ARG:HH12	1:C:204:ASP:HB3	1.79	0.47
1:C:910:ASP:OD2	1:C:911:ASN:N	2.47	0.47
1:C:1416:ASP:O	1:C:1420:LEU:HB2	2.14	0.47
1:C:4026:LEU:HD11	1:C:4052:MET:HA	1.96	0.47
1:D:1047:LYS:HG3	1:D:1051:ARG:CZ	2.44	0.47
1:D:1284:LYS:NZ	1:D:1286:THR:OG1	2.41	0.47
1:D:2719:TYR:CE2	1:D:2799:ALA:HB2	2.38	0.47
1:D:2724:TYR:CD1	1:D:2895:PHE:CD2	3.02	0.47
1:D:3187:LYS:O	1:D:3191:GLU:HB3	2.15	0.47
1:D:3304:GLN:HA	1:D:3307:ILE:HG12	1.95	0.47
1:A:2920:ARG:HH22	1:A:3000:GLU:HG2	1.79	0.47
2:G:54:GLN:O	1:C:1771:ILE:HD11	2.14	0.47
1:B:137:ARG:NH1	1:B:146:ASP:OD1	2.48	0.47
1:B:470:LEU:HB2	1:B:475:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1788:LYS:HG3	1:B:1834:PHE:CE1	2.50	0.47
1:B:3250:TRP:NE1	1:B:3256:ASN:HD21	2.12	0.47
1:B:3653:GLU:OE2	1:B:3660:ARG:NH2	2.46	0.47
1:B:4026:LEU:HD11	1:B:4052:MET:HA	1.96	0.47
4:B:5003:ATP:C5'	5:B:5004:KVR:C15	2.93	0.47
1:C:643:LEU:HD13	1:C:1657:THR:HG23	1.96	0.47
1:C:972:LEU:HD12	1:C:974:SER:HB2	1.96	0.47
1:C:2918:GLU:HA	1:C:2923:TYR:HB3	1.96	0.47
1:C:2920:ARG:NH1	1:C:2981:TYR:HH	2.12	0.47
1:C:2997:SER:O	1:C:3000:GLU:HB2	2.14	0.47
1:C:4203:ALA:HA	1:C:4206:ILE:HG12	1.97	0.47
1:D:470:LEU:HB2	1:D:475:LYS:HG3	1.96	0.47
1:D:1471:ASP:OD1	1:D:1475:LYS:N	2.47	0.47
1:D:3296:MET:HA	1:D:3299:LEU:HG	1.96	0.47
1:D:4203:ALA:HA	1:D:4206:ILE:HG12	1.97	0.47
1:A:1047:LYS:HG3	1:A:1051:ARG:CZ	2.44	0.47
1:A:2724:TYR:CD1	1:A:2895:PHE:CD2	3.02	0.47
1:A:3187:LYS:HD2	1:A:3192:ARG:NH2	2.30	0.47
1:A:4268:MET:O	1:A:4272:LYS:HG2	2.14	0.47
1:B:2655:LYS:O	1:B:2958:GLN:NE2	2.48	0.47
1:C:514:PHE:CD2	1:C:526:TRP:HB2	2.50	0.47
1:C:3025:ASP:O	1:C:3029:ILE:HD12	2.14	0.47
1:D:56:LYS:HA	1:D:324:VAL:HG23	1.95	0.47
1:D:137:ARG:HH12	1:D:204:ASP:HB3	1.79	0.47
1:D:946:LEU:HG	1:D:998:LYS:HD3	1.96	0.47
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.95	0.47
1:D:2768:LYS:HB3	1:D:2772:ARG:NH1	2.29	0.47
1:D:3303:SER:HA	1:D:3306:ILE:HD13	1.96	0.47
1:D:3956:MET:HE2	1:D:4016:PHE:HB2	1.96	0.47
1:A:466:PRO:HG3	1:A:478:ARG:HD2	1.96	0.47
1:A:910:ASP:OD2	1:A:911:ASN:N	2.47	0.47
1:A:1074:ARG:NH1	1:A:1078:CYS:H	2.11	0.47
1:A:1124:PRO:HD2	1:A:1594:VAL:HG23	1.97	0.47
1:A:2572:CYS:O	1:A:2576:ILE:HG13	2.14	0.47
1:A:3025:ASP:O	1:A:3029:ILE:HD12	2.14	0.47
1:A:3187:LYS:O	1:A:3191:GLU:HB3	2.15	0.47
1:A:3697:LYS:HA	1:A:3700:HIS:CD2	2.49	0.47
1:A:3844:GLN:O	1:A:3848:GLU:HG3	2.15	0.47
2:H:38:ASP:OD1	2:H:43:ARG:NH1	2.47	0.47
1:B:939:THR:HG23	1:B:999:LEU:HD21	1.96	0.47
1:B:1276:THR:OG1	1:B:1278:ASP:OD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1682:GLU:HB3	1:B:1683:PRO:HD3	1.95	0.47
1:C:1047:LYS:HG3	1:C:1051:ARG:CZ	2.44	0.47
1:C:2572:CYS:O	1:C:2576:ILE:HG13	2.14	0.47
1:C:2768:LYS:HB3	1:C:2772:ARG:NH1	2.29	0.47
1:C:4268:MET:O	1:C:4272:LYS:HG2	2.14	0.47
1:D:939:THR:HG23	1:D:999:LEU:HD21	1.97	0.47
1:D:1074:ARG:NH1	1:D:1078:CYS:H	2.11	0.47
1:D:1416:ASP:O	1:D:1420:LEU:HB2	2.14	0.47
1:D:2059:GLN:NE2	1:D:2091:GLN:O	2.47	0.47
1:D:2445:ILE:HG23	1:D:2865:GLY:HA2	1.97	0.47
1:D:3187:LYS:HD2	1:D:3192:ARG:NH2	2.30	0.47
1:D:3277:LEU:O	1:D:3281:LEU:HG	2.14	0.47
1:A:939:THR:HG23	1:A:999:LEU:HD21	1.96	0.47
1:A:946:LEU:HG	1:A:998:LYS:HD3	1.96	0.47
1:A:1416:ASP:O	1:A:1420:LEU:HB2	2.14	0.47
1:A:1898:LEU:HD13	1:A:1902:VAL:HG12	1.96	0.47
1:A:1937:GLN:NE2	1:A:3608:LEU:O	2.31	0.47
1:A:2215:PHE:CD2	1:A:2253:LEU:HD22	2.50	0.47
1:A:2445:ILE:HG23	1:A:2865:GLY:HA2	1.97	0.47
1:A:2730:ASP:O	1:A:2734:MET:HG2	2.15	0.47
1:A:3005:THR:HG21	1:A:3045:VAL:HG21	1.97	0.47
1:A:3324:GLU:OE2	1:A:3325:LYS:HE3	2.14	0.47
1:A:3677:THR:HB	1:A:3679:LYS:NZ	2.30	0.47
1:B:164:PRO:HB3	1:B:169:ARG:HB2	1.97	0.47
1:B:1185:ASP:OD1	1:B:1186:SER:N	2.48	0.47
1:B:2059:GLN:NE2	1:B:2091:GLN:O	2.47	0.47
1:B:2215:PHE:CD2	1:B:2253:LEU:HD22	2.50	0.47
1:B:2445:ILE:HG23	1:B:2865:GLY:HA2	1.97	0.47
1:B:3005:THR:HG21	1:B:3045:VAL:HG21	1.97	0.47
1:B:3025:ASP:O	1:B:3029:ILE:HD12	2.14	0.47
1:B:3192:ARG:NH2	1:B:3197:LEU:HD23	2.26	0.47
1:B:3277:LEU:O	1:B:3281:LEU:HG	2.14	0.47
1:B:3324:GLU:OE2	1:B:3325:LYS:HE3	2.14	0.47
1:C:1682:GLU:HB3	1:C:1683:PRO:HD3	1.95	0.47
1:C:2655:LYS:O	1:C:2958:GLN:NE2	2.48	0.47
1:C:3005:THR:HG21	1:C:3045:VAL:HG21	1.97	0.47
1:C:3187:LYS:HD2	1:C:3192:ARG:NH2	2.30	0.47
1:C:3187:LYS:HD2	1:C:3192:ARG:HH21	1.78	0.47
1:C:4011:GLU:HB2	1:C:4121:LEU:HD23	1.97	0.47
1:C:4043:ILE:O	1:C:4078:LEU:HD23	2.15	0.47
1:D:829:LYS:NZ	1:D:1037:LEU:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2566:ARG:HA	1:D:2569:ILE:HG12	1.97	0.47
1:D:2655:LYS:O	1:D:2958:GLN:NE2	2.48	0.47
1:D:2920:ARG:HH22	1:D:3000:GLU:HG2	1.79	0.47
1:D:4283:PHE:CE1	1:D:4287:TYR:HE2	2.33	0.47
1:A:514:PHE:CD2	1:A:526:TRP:HB2	2.50	0.47
1:A:1471:ASP:OD1	1:A:1475:LYS:N	2.47	0.47
1:A:2957:GLU:HB2	1:A:2961:LYS:NZ	2.28	0.47
1:A:3227:ARG:HH12	1:A:3287:ASN:HB2	1.78	0.47
1:A:3695:MET:HB3	1:A:3731:LEU:HD11	1.95	0.47
1:B:1272:ARG:NH2	1:B:1582:CYS:SG	2.88	0.47
1:B:2176:VAL:HG22	1:B:2220:TYR:HE2	1.80	0.47
1:C:470:LEU:HB2	1:C:475:LYS:HG3	1.96	0.47
1:C:732:LEU:HG	1:C:741:VAL:HG11	1.97	0.47
1:C:3017:HIS:CD2	1:C:3093:ILE:HD12	2.50	0.47
1:C:3250:TRP:CE3	1:C:3309:LYS:HE3	2.50	0.47
1:D:1898:LEU:HD13	1:D:1902:VAL:HG12	1.96	0.47
1:D:2572:CYS:O	1:D:2576:ILE:HG13	2.14	0.47
1:D:3250:TRP:NE1	1:D:3256:ASN:HD21	2.12	0.47
4:D:5003:ATP:C5'	5:D:5004:KVR:C15	2.92	0.47
1:A:164:PRO:HB3	1:A:169:ARG:HB2	1.97	0.47
1:A:611:LEU:HD22	1:A:1660:LEU:HD22	1.96	0.47
1:A:643:LEU:HD13	1:A:1657:THR:HG23	1.96	0.47
1:A:1048:ASP:HA	1:A:1051:ARG:NE	2.30	0.47
1:A:1788:LYS:HG3	1:A:1834:PHE:CE1	2.50	0.47
1:A:4283:PHE:CE1	1:A:4287:TYR:HE2	2.33	0.47
1:B:181:LEU:N	1:B:212:TRP:O	2.36	0.47
1:B:2258:ARG:HB3	1:B:2260:PRO:HD2	1.95	0.47
1:B:4203:ALA:HA	1:B:4206:ILE:HG12	1.97	0.47
1:B:4956:ASP:OD1	1:B:4957:CYS:N	2.46	0.47
1:C:1471:ASP:OD1	1:C:1475:LYS:N	2.47	0.47
1:C:2566:ARG:HA	1:C:2569:ILE:HG12	1.97	0.47
1:A:1100:ARG:NH2	1:A:1234:GLU:O	2.48	0.47
1:A:1185:ASP:OD1	1:A:1186:SER:N	2.48	0.47
1:A:2785:TRP:HH2	1:A:2847:ASN:ND2	2.13	0.47
1:A:2918:GLU:HA	1:A:2923:TYR:HB3	1.96	0.47
1:A:3811:GLN:NE2	1:A:3815:GLU:OE2	2.47	0.47
1:A:4203:ALA:HA	1:A:4206:ILE:HG12	1.97	0.47
2:F:38:ASP:OD1	2:F:43:ARG:NH1	2.47	0.47
1:B:514:PHE:CD2	1:B:526:TRP:HB2	2.50	0.47
1:B:1048:ASP:HA	1:B:1051:ARG:NE	2.30	0.47
1:B:1471:ASP:OD1	1:B:1475:LYS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:PRO:HB2	1:C:451:SER:OG	2.15	0.47
1:C:3187:LYS:O	1:C:3191:GLU:HB3	2.15	0.47
1:C:3622:GLN:HB3	1:C:3626:LYS:NZ	2.30	0.47
1:C:3956:MET:HE2	1:C:4016:PHE:HB2	1.96	0.47
1:D:2215:PHE:CD2	1:D:2253:LEU:HD22	2.50	0.47
1:D:2730:ASP:O	1:D:2734:MET:HG2	2.15	0.47
1:D:2785:TRP:HH2	1:D:2847:ASN:ND2	2.13	0.47
1:D:4026:LEU:HD11	1:D:4052:MET:HA	1.96	0.47
1:A:824:GLU:HA	1:A:1020:ILE:HD12	1.96	0.46
1:A:904:TYR:CE1	1:A:916:PRO:HA	2.51	0.46
1:A:928:GLU:OE2	4:A:5003:ATP:C8	2.69	0.46
1:A:1272:ARG:NH2	1:A:1582:CYS:SG	2.88	0.46
1:A:2566:ARG:HA	1:A:2569:ILE:HG12	1.97	0.46
1:A:3017:HIS:CD2	1:A:3093:ILE:HD12	2.50	0.46
1:A:3622:GLN:HB3	1:A:3626:LYS:NZ	2.30	0.46
1:B:2769:GLU:OE2	1:B:2772:ARG:NH2	2.48	0.46
1:B:2785:TRP:HH2	1:B:2847:ASN:ND2	2.13	0.46
1:B:2997:SER:O	1:B:3000:GLU:HB2	2.14	0.46
1:B:4011:GLU:HB2	1:B:4121:LEU:HD23	1.96	0.46
1:C:164:PRO:HB3	1:C:169:ARG:HB2	1.97	0.46
4:C:5003:ATP:C5'	5:C:5004:KVR:C15	2.92	0.46
1:D:514:PHE:CD2	1:D:526:TRP:HB2	2.50	0.46
1:D:643:LEU:HD13	1:D:1657:THR:HG23	1.96	0.46
1:D:972:LEU:HD12	1:D:974:SER:HB2	1.96	0.46
1:D:3288:LEU:HD21	1:D:3336:GLU:HG3	1.97	0.46
1:D:3823:GLU:OE1	1:D:3826:GLY:N	2.41	0.46
1:A:281:ARG:NE	1:A:283:ALA:O	2.41	0.46
1:A:732:LEU:HG	1:A:741:VAL:HG11	1.97	0.46
1:A:2692:GLN:HG2	1:A:2704:GLN:HG3	1.97	0.46
1:A:2701:PHE:HD1	1:A:2873:PRO:HG3	1.80	0.46
1:A:3288:LEU:HD21	1:A:3336:GLU:HG3	1.97	0.46
1:A:3303:SER:HA	1:A:3306:ILE:HD13	1.96	0.46
1:B:829:LYS:NZ	1:B:1037:LEU:O	2.39	0.46
1:B:2719:TYR:HE2	1:B:2799:ALA:CB	2.24	0.46
1:B:2730:ASP:O	1:B:2734:MET:HG2	2.15	0.46
1:B:3187:LYS:O	1:B:3191:GLU:HB3	2.15	0.46
1:C:2215:PHE:CD2	1:C:2253:LEU:HD22	2.50	0.46
1:C:3677:THR:HB	1:C:3679:LYS:NZ	2.30	0.46
1:C:4283:PHE:CE1	1:C:4287:TYR:HE2	2.33	0.46
1:D:910:ASP:OD2	1:D:911:ASN:N	2.47	0.46
1:D:1979:PHE:HB3	1:D:1986:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2266:VAL:HG12	1:D:2327:ARG:HD2	1.96	0.46
1:D:2788:ARG:NH2	1:D:2906:GLY:O	2.45	0.46
1:D:3005:THR:HG21	1:D:3045:VAL:HG21	1.97	0.46
1:D:3101:LEU:HD23	1:D:3104:MET:HE2	1.97	0.46
1:D:3227:ARG:HH12	1:D:3287:ASN:HB2	1.78	0.46
1:D:4664:ASP:OD1	1:D:4665:ARG:N	2.49	0.46
1:A:902:TRP:CZ2	1:A:915:HIS:CE1	3.04	0.46
1:A:4827:ILE:O	1:A:4831:ILE:HG12	2.15	0.46
1:B:23:GLN:HB2	1:B:34:LYS:HD2	1.97	0.46
1:B:1100:ARG:NH2	1:B:1234:GLU:O	2.48	0.46
1:B:3017:HIS:CD2	1:B:3093:ILE:HD12	2.50	0.46
1:B:3288:LEU:HD21	1:B:3336:GLU:HG3	1.97	0.46
1:B:3956:MET:HE2	1:B:4016:PHE:HB2	1.96	0.46
1:B:4268:MET:O	1:B:4272:LYS:HG2	2.14	0.46
1:C:270:HIS:CE1	1:C:491:GLU:HG3	2.50	0.46
1:C:1124:PRO:HD2	1:C:1594:VAL:HG23	1.97	0.46
1:C:1979:PHE:HB3	1:C:1986:CYS:SG	2.55	0.46
1:C:2266:VAL:HG12	1:C:2327:ARG:HD2	1.97	0.46
1:C:2730:ASP:O	1:C:2734:MET:HG2	2.15	0.46
1:D:448:PRO:HB2	1:D:451:SER:OG	2.15	0.46
1:D:1048:ASP:HA	1:D:1051:ARG:NE	2.30	0.46
1:D:2581:ARG:HD3	1:D:2582:PRO:HD2	1.98	0.46
1:D:2920:ARG:NH1	1:D:2981:TYR:HH	2.13	0.46
1:D:4011:GLU:HB2	1:D:4121:LEU:HD23	1.97	0.46
1:A:668:ALA:HB2	1:A:1012:ILE:HD11	1.98	0.46
1:A:1936:LEU:HD11	1:A:1976:LEU:HD23	1.97	0.46
1:A:1979:PHE:HB3	1:A:1986:CYS:SG	2.55	0.46
1:B:1979:PHE:HB3	1:B:1986:CYS:SG	2.55	0.46
1:B:2566:ARG:HA	1:B:2569:ILE:HG12	1.97	0.46
1:B:3316:LYS:O	1:B:3317:THR:OG1	2.30	0.46
1:C:2443:PRO:HD3	1:C:2512:MET:HG2	1.97	0.46
1:C:2573:LEU:HD23	1:C:2605:MET:SD	2.56	0.46
1:C:2581:ARG:HD3	1:C:2582:PRO:HD2	1.97	0.46
1:C:3846:LEU:HD22	1:C:3854:PHE:CE2	2.51	0.46
1:C:4602:ARG:O	1:C:4606:VAL:HG23	2.16	0.46
1:D:611:LEU:HD22	1:D:1660:LEU:HD22	1.96	0.46
1:D:732:LEU:HG	1:D:741:VAL:HG11	1.97	0.46
1:D:824:GLU:HA	1:D:1020:ILE:HD12	1.96	0.46
1:D:2396:ILE:HG13	1:D:2468:MET:HE1	1.97	0.46
1:D:2443:PRO:HD3	1:D:2512:MET:HG2	1.97	0.46
1:D:2769:GLU:OE2	1:D:2772:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3622:GLN:HB3	1:D:3626:LYS:NZ	2.30	0.46
1:D:3844:GLN:O	1:D:3848:GLU:HG3	2.15	0.46
1:D:3846:LEU:HD22	1:D:3854:PHE:CE2	2.51	0.46
1:A:1276:THR:OG1	1:A:1278:ASP:OD1	2.32	0.46
1:A:2266:VAL:HG12	1:A:2327:ARG:HD2	1.96	0.46
1:A:2920:ARG:NH1	1:A:2981:TYR:HH	2.13	0.46
1:A:3101:LEU:HD23	1:A:3104:MET:HE2	1.97	0.46
1:B:611:LEU:HD22	1:B:1660:LEU:HD22	1.96	0.46
1:B:928:GLU:OE2	4:B:5003:ATP:C8	2.68	0.46
1:B:3187:LYS:HD2	1:B:3192:ARG:NH2	2.30	0.46
1:B:3622:GLN:HB3	1:B:3626:LYS:NZ	2.30	0.46
1:C:939:THR:HG23	1:C:999:LEU:HD21	1.96	0.46
1:C:1185:ASP:OD1	1:C:1186:SER:N	2.48	0.46
1:C:2592:LEU:HD13	1:C:2610:LEU:HD21	1.98	0.46
1:C:2719:TYR:HE2	1:C:2799:ALA:CB	2.24	0.46
1:C:2785:TRP:HH2	1:C:2847:ASN:ND2	2.13	0.46
1:C:3277:LEU:O	1:C:3281:LEU:HG	2.14	0.46
1:C:3844:GLN:O	1:C:3848:GLU:HG3	2.15	0.46
1:C:4827:ILE:O	1:C:4831:ILE:HG12	2.15	0.46
1:D:1936:LEU:HD11	1:D:1976:LEU:HD23	1.97	0.46
1:D:2610:LEU:HD12	1:D:2614:TYR:HE2	1.80	0.46
1:D:3033:LEU:HD13	1:D:3104:MET:CB	2.44	0.46
1:D:3677:THR:HB	1:D:3679:LYS:NZ	2.30	0.46
1:A:2222:LEU:HD23	1:A:2222:LEU:HA	1.79	0.46
1:A:4011:GLU:HB2	1:A:4121:LEU:HD23	1.97	0.46
1:B:904:TYR:CE1	1:B:916:PRO:HA	2.51	0.46
1:B:2610:LEU:HD12	1:B:2614:TYR:HE2	1.80	0.46
1:B:2701:PHE:HD1	1:B:2873:PRO:HG3	1.81	0.46
1:B:3159:LEU:HB2	1:B:3241:MET:HE3	1.98	0.46
1:B:3245:TYR:HA	1:B:3249:TRP:CZ3	2.51	0.46
1:B:4827:ILE:O	1:B:4831:ILE:HG12	2.15	0.46
1:C:928:GLU:OE2	4:C:5003:ATP:C8	2.68	0.46
1:C:948:CYS:SG	1:C:1064:LEU:HB3	2.56	0.46
1:C:1100:ARG:NH2	1:C:1234:GLU:O	2.48	0.46
1:C:1272:ARG:NH2	1:C:1582:CYS:SG	2.88	0.46
1:C:2396:ILE:HG13	1:C:2468:MET:HE1	1.97	0.46
1:C:2445:ILE:HG23	1:C:2865:GLY:HA2	1.97	0.46
1:C:2852:TRP:HA	1:C:2855:LYS:HE3	1.98	0.46
1:C:3131:TYR:HE1	1:C:3166:PHE:CZ	2.33	0.46
1:D:164:PRO:HB3	1:D:169:ARG:HB2	1.97	0.46
1:D:2573:LEU:HD23	1:D:2605:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2918:GLU:HA	1:D:2923:TYR:HB3	1.96	0.46
1:D:3245:TYR:HA	1:D:3249:TRP:CZ3	2.51	0.46
1:A:2610:LEU:HD12	1:A:2614:TYR:HE2	1.80	0.46
1:A:2655:LYS:O	1:A:2958:GLN:NE2	2.48	0.46
1:A:2719:TYR:CE2	1:A:2799:ALA:HB2	2.38	0.46
1:A:3245:TYR:HA	1:A:3249:TRP:CZ3	2.51	0.46
1:A:4584:PHE:O	1:A:4587:ILE:HG22	2.16	0.46
2:H:75:LEU:HB2	2:H:100:PHE:HB2	1.98	0.46
1:B:4043:ILE:O	1:B:4078:LEU:HD23	2.15	0.46
1:B:4283:PHE:CE1	1:B:4287:TYR:HE2	2.33	0.46
1:C:1788:LYS:HG3	1:C:1834:PHE:CE1	2.50	0.46
1:C:2610:LEU:HD12	1:C:2614:TYR:HE2	1.80	0.46
1:C:3101:LEU:HD23	1:C:3104:MET:HE2	1.97	0.46
1:D:668:ALA:HB2	1:D:1012:ILE:HD11	1.98	0.46
1:D:693:LEU:HD22	1:D:798:ILE:HD12	1.98	0.46
1:D:902:TRP:CZ2	1:D:915:HIS:CE1	3.04	0.46
1:D:1788:LYS:HG3	1:D:1834:PHE:CE1	2.50	0.46
1:D:2592:LEU:HD13	1:D:2610:LEU:HD21	1.98	0.46
1:D:3159:LEU:HB2	1:D:3241:MET:HE3	1.98	0.46
1:D:3312:PRO:HA	1:D:3315:LEU:HD12	1.98	0.46
1:D:3969:LYS:HB2	1:D:3969:LYS:HE2	1.75	0.46
1:D:4051:ALA:O	1:D:4055:HIS:ND1	2.19	0.46
1:D:4827:ILE:O	1:D:4831:ILE:HG12	2.15	0.46
1:A:2573:LEU:HD23	1:A:2605:MET:SD	2.56	0.46
1:A:3033:LEU:HD13	1:A:3104:MET:CB	2.44	0.46
1:A:3250:TRP:CE3	1:A:3309:LYS:HE3	2.50	0.46
1:A:4051:ALA:O	1:A:4055:HIS:ND1	2.19	0.46
1:B:281:ARG:NE	1:B:283:ALA:O	2.41	0.46
1:B:561:ARG:O	1:B:564:ARG:HG2	2.16	0.46
1:B:1124:PRO:HD2	1:B:1594:VAL:HG23	1.97	0.46
1:B:2573:LEU:HD23	1:B:2605:MET:SD	2.56	0.46
1:B:3144:LYS:HB2	1:B:3233:HIS:CE1	2.51	0.46
1:B:3677:THR:HB	1:B:3679:LYS:NZ	2.30	0.46
1:B:4602:ARG:O	1:B:4606:VAL:HG23	2.16	0.46
1:C:561:ARG:O	1:C:564:ARG:HG2	2.16	0.46
1:C:842:GLN:HB2	1:C:1603:PHE:HB2	1.98	0.46
1:C:904:TYR:CE1	1:C:916:PRO:HA	2.51	0.46
1:C:2176:VAL:HG22	1:C:2220:TYR:HE2	1.80	0.46
1:C:2332:GLY:O	1:C:2336:ARG:HG3	2.16	0.46
1:C:2692:GLN:HG2	1:C:2704:GLN:HG3	1.97	0.46
1:C:4947:ARG:HD3	1:C:4949:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:HIS:CE1	1:D:491:GLU:HG3	2.50	0.46
1:D:904:TYR:CE1	1:D:916:PRO:HA	2.51	0.46
1:D:928:GLU:OE2	4:D:5003:ATP:C8	2.68	0.46
1:D:1124:PRO:HD2	1:D:1594:VAL:HG23	1.97	0.46
1:D:2176:VAL:HG22	1:D:2220:TYR:HE2	1.80	0.46
1:D:2852:TRP:HA	1:D:2855:LYS:HE3	1.98	0.46
1:D:4602:ARG:O	1:D:4606:VAL:HG23	2.16	0.46
1:D:4795:LYS:HA	1:D:4795:LYS:HD2	1.80	0.46
1:A:2769:GLU:C	1:A:2771:TYR:N	2.69	0.46
1:A:3316:LYS:O	1:A:3317:THR:OG1	2.30	0.46
1:B:270:HIS:CE1	1:B:491:GLU:HG3	2.51	0.46
1:B:948:CYS:SG	1:B:1064:LEU:HB3	2.56	0.46
1:B:1922:ILE:O	1:B:1926:VAL:HG23	2.16	0.46
1:B:2319:VAL:O	1:B:2323:LEU:HG	2.16	0.46
1:B:2332:GLY:O	1:B:2336:ARG:HG3	2.16	0.46
1:B:2821:TYR:O	1:B:2823:PRO:HD3	2.16	0.46
1:B:2918:GLU:HA	1:B:2923:TYR:HB3	1.96	0.46
1:B:2920:ARG:NH1	1:B:2981:TYR:HH	2.14	0.46
1:C:1048:ASP:HA	1:C:1051:ARG:NE	2.30	0.46
1:C:2004:MET:SD	1:C:3632:GLU:HG2	2.56	0.46
1:C:4480:PHE:HA	1:C:4483:LYS:NZ	2.31	0.46
1:D:842:GLN:HB2	1:D:1603:PHE:HB2	1.98	0.46
1:D:1185:ASP:OD1	1:D:1186:SER:N	2.48	0.46
1:D:2004:MET:SD	1:D:3632:GLU:HG2	2.56	0.46
1:D:3017:HIS:CD2	1:D:3093:ILE:HD12	2.50	0.46
1:D:3167:PRO:HA	1:D:3248:ARG:NH2	2.31	0.46
1:D:3250:TRP:CE3	1:D:3309:LYS:HE3	2.50	0.46
1:D:4043:ILE:O	1:D:4078:LEU:HD23	2.15	0.46
1:A:137:ARG:NH1	1:A:146:ASP:OD1	2.48	0.46
1:A:1498:GLN:OE1	1:D:2794:GLU:HB2	2.16	0.46
1:A:2212:LYS:HG3	1:A:2253:LEU:HD21	1.98	0.46
1:A:2443:PRO:HD3	1:A:2512:MET:HG2	1.97	0.46
1:A:3015:VAL:HG11	1:A:3029:ILE:CG2	2.46	0.46
1:A:3187:LYS:HZ2	1:A:3195:LEU:HD13	1.80	0.46
1:A:3846:LEU:HD22	1:A:3854:PHE:CE2	2.51	0.46
1:A:4026:LEU:HD11	1:A:4052:MET:HA	1.96	0.46
1:A:4602:ARG:O	1:A:4606:VAL:HG23	2.16	0.46
2:G:75:LEU:HB2	2:G:100:PHE:HB2	1.98	0.46
1:B:732:LEU:HG	1:B:741:VAL:HG11	1.97	0.46
1:B:946:LEU:HG	1:B:998:LYS:HD3	1.96	0.46
1:B:2443:PRO:HD3	1:B:2512:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2773:TRP:HB3	1:B:2774:PRO:HD3	1.98	0.46
1:B:3250:TRP:CE3	1:B:3309:LYS:HE3	2.50	0.46
1:B:3846:LEU:HD22	1:B:3854:PHE:CE2	2.51	0.46
1:B:4029:SER:OG	1:B:4055:HIS:NE2	2.49	0.46
1:C:808:HIS:CD2	1:C:832:LEU:HD23	2.51	0.46
1:C:902:TRP:CZ2	1:C:915:HIS:CE1	3.04	0.46
1:C:1276:THR:OG1	1:C:1278:ASP:OD1	2.32	0.46
1:C:2090:ARG:HE	1:C:2090:ARG:HB3	1.58	0.46
1:C:2212:LYS:HG3	1:C:2253:LEU:HD21	1.98	0.46
1:C:3320:LEU:O	1:C:3323:MET:HG2	2.16	0.46
1:C:4664:ASP:OD1	1:C:4665:ARG:N	2.49	0.46
1:D:1100:ARG:NH2	1:D:1234:GLU:O	2.48	0.46
1:D:1784:LEU:HD13	1:D:1833:ILE:HD11	1.98	0.46
1:D:3131:TYR:HE1	1:D:3166:PHE:CZ	2.33	0.46
1:D:4035:TYR:HE2	1:D:4051:ALA:HA	1.81	0.46
1:A:23:GLN:HB2	1:A:34:LYS:HD2	1.97	0.45
1:A:948:CYS:SG	1:A:1064:LEU:HB3	2.56	0.45
1:A:2176:VAL:HG22	1:A:2220:TYR:HE2	1.80	0.45
1:A:3312:PRO:HA	1:A:3315:LEU:HD12	1.98	0.45
1:A:4664:ASP:OD1	1:A:4665:ARG:N	2.49	0.45
1:A:4864:GLY:HA2	1:D:4867:ILE:HG12	1.97	0.45
2:F:36:LYS:HE3	2:F:36:LYS:HB3	1.80	0.45
1:B:3312:PRO:HA	1:B:3315:LEU:HD12	1.98	0.45
1:C:514:PHE:HD2	1:C:526:TRP:HB2	1.82	0.45
1:C:2319:VAL:O	1:C:2323:LEU:HG	2.16	0.45
1:C:2769:GLU:OE2	1:C:2772:ARG:NH2	2.48	0.45
1:D:1272:ARG:NH2	1:D:1582:CYS:SG	2.88	0.45
1:D:2332:GLY:O	1:D:2336:ARG:HG3	2.16	0.45
1:D:3043:ARG:C	1:D:3047:LYS:HZ2	2.24	0.45
1:D:3282:LYS:O	1:D:3285:TYR:HB3	2.17	0.45
1:D:4947:ARG:HD3	1:D:4949:TRP:CZ2	2.51	0.45
1:A:808:HIS:CD2	1:A:832:LEU:HD23	2.51	0.45
1:A:1839:LEU:HA	1:A:1842:ILE:HG12	1.99	0.45
1:A:1922:ILE:O	1:A:1926:VAL:HG23	2.16	0.45
1:A:2004:MET:SD	1:A:3632:GLU:HG2	2.56	0.45
1:A:2581:ARG:HD3	1:A:2582:PRO:HD2	1.97	0.45
1:A:2769:GLU:OE2	1:A:2772:ARG:NH2	2.48	0.45
1:A:2788:ARG:NH2	1:A:2906:GLY:O	2.45	0.45
1:A:3131:TYR:HE1	1:A:3166:PHE:CZ	2.33	0.45
1:A:4043:ILE:O	1:A:4078:LEU:HD23	2.15	0.45
1:A:4159:GLN:HB3	1:A:4200:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2004:MET:SD	1:B:3632:GLU:HG2	2.56	0.45
1:B:2710:ASN:OD1	1:B:2711:ILE:N	2.50	0.45
1:B:3325:LYS:HD2	1:B:3328:LYS:HZ2	1.82	0.45
1:B:3328:LYS:HG3	1:B:3329:LYS:HD3	1.98	0.45
1:C:137:ARG:NH1	1:C:146:ASP:OD1	2.48	0.45
1:C:693:LEU:HD22	1:C:798:ILE:HD12	1.98	0.45
1:C:2232:PRO:C	1:C:2234:MET:H	2.24	0.45
1:C:3159:LEU:HB2	1:C:3241:MET:HE3	1.98	0.45
1:C:3245:TYR:HA	1:C:3249:TRP:CZ3	2.51	0.45
1:C:4112:ASP:O	1:C:4116:GLN:HG2	2.17	0.45
1:D:23:GLN:HB2	1:D:34:LYS:HD2	1.97	0.45
1:D:561:ARG:O	1:D:564:ARG:HG2	2.16	0.45
1:D:1019:GLY:HA3	1:D:1028:ARG:HE	1.81	0.45
1:D:2701:PHE:HD1	1:D:2873:PRO:HG3	1.80	0.45
1:D:3320:LEU:O	1:D:3323:MET:HG2	2.16	0.45
1:D:3986:LEU:HD12	1:D:4101:LEU:HD12	1.98	0.45
1:A:2710:ASN:OD1	1:A:2711:ILE:N	2.50	0.45
1:A:4480:PHE:HA	1:A:4483:LYS:NZ	2.31	0.45
1:B:902:TRP:CZ2	1:B:915:HIS:CE1	3.04	0.45
1:B:2266:VAL:HG12	1:B:2327:ARG:HD2	1.97	0.45
1:B:2396:ILE:HG13	1:B:2468:MET:HE1	1.97	0.45
1:B:2397:ASP:O	1:B:2401:ARG:HG3	2.17	0.45
1:B:3033:LEU:HD13	1:B:3104:MET:CB	2.44	0.45
1:B:3131:TYR:HE1	1:B:3166:PHE:CZ	2.33	0.45
1:B:4664:ASP:OD1	1:B:4665:ARG:N	2.49	0.45
1:C:3144:LYS:HB2	1:C:3233:HIS:CE1	2.51	0.45
1:C:3167:PRO:HA	1:C:3248:ARG:NH2	2.31	0.45
1:C:3192:ARG:NH2	1:C:3197:LEU:HD23	2.26	0.45
1:C:4698:LEU:O	1:C:4701:ILE:HG22	2.17	0.45
1:D:137:ARG:NH1	1:D:146:ASP:OD1	2.48	0.45
1:D:982:ASP:HB2	1:D:985:PHE:CD1	2.52	0.45
1:D:2057:THR:HG22	1:D:2059:GLN:H	1.82	0.45
1:D:2710:ASN:OD1	1:D:2711:ILE:N	2.50	0.45
1:D:2723:LYS:N	1:D:2726:GLU:OE1	2.45	0.45
1:D:2821:TYR:O	1:D:2823:PRO:HD3	2.16	0.45
1:D:3284:ILE:HA	1:D:3287:ASN:OD1	2.16	0.45
1:A:448:PRO:HB2	1:A:451:SER:OG	2.15	0.45
1:A:1019:GLY:HA3	1:A:1028:ARG:HE	1.81	0.45
1:A:1106:GLU:OE1	1:A:1214:ARG:NH1	2.44	0.45
1:A:2057:THR:HG22	1:A:2059:GLN:H	1.82	0.45
1:A:2396:ILE:HG13	1:A:2468:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:PRO:HB2	1:B:451:SER:OG	2.15	0.45
1:B:1269:GLU:HB3	1:B:1286:THR:HB	1.98	0.45
1:B:3101:LEU:HD23	1:B:3104:MET:HE2	1.97	0.45
1:B:3282:LYS:O	1:B:3285:TYR:HB3	2.17	0.45
1:C:2397:ASP:O	1:C:2401:ARG:HG3	2.16	0.45
1:C:2710:ASN:OD1	1:C:2711:ILE:N	2.50	0.45
1:C:3033:LEU:HD13	1:C:3104:MET:CB	2.44	0.45
1:C:3312:PRO:HA	1:C:3315:LEU:HD12	1.98	0.45
1:C:3823:GLU:OE1	1:C:3826:GLY:N	2.41	0.45
1:D:808:HIS:CD2	1:D:832:LEU:HD23	2.51	0.45
1:D:948:CYS:SG	1:D:1064:LEU:HB3	2.56	0.45
1:D:2692:GLN:HG2	1:D:2704:GLN:HG3	1.97	0.45
1:D:3811:GLN:NE2	1:D:3815:GLU:OE2	2.47	0.45
1:D:4480:PHE:HA	1:D:4483:LYS:NZ	2.31	0.45
1:D:4502:MET:SD	1:D:4585:PHE:HB3	2.57	0.45
1:A:887:GLU:HA	1:A:890:HIS:ND1	2.31	0.45
1:A:2332:GLY:O	1:A:2336:ARG:HG3	2.16	0.45
1:A:3159:LEU:HB2	1:A:3241:MET:HE3	1.98	0.45
1:A:3282:LYS:O	1:A:3285:TYR:HB3	2.17	0.45
1:A:4947:ARG:HD3	1:A:4949:TRP:CZ2	2.51	0.45
2:F:57:ILE:HG13	2:F:60:PHE:HB2	1.98	0.45
2:H:57:ILE:HG13	2:H:60:PHE:HB2	1.98	0.45
1:B:693:LEU:HD22	1:B:798:ILE:HD12	1.98	0.45
1:B:2581:ARG:HD3	1:B:2582:PRO:HD2	1.97	0.45
1:B:2852:TRP:HA	1:B:2855:LYS:HE3	1.98	0.45
1:B:3649:ALA:C	1:B:3652:PRO:HD2	2.42	0.45
1:B:3986:LEU:HD12	1:B:4101:LEU:HD12	1.98	0.45
1:B:4947:ARG:HD3	1:B:4949:TRP:CZ2	2.51	0.45
1:C:1922:ILE:O	1:C:1926:VAL:HG23	2.16	0.45
1:C:3224:SER:OG	1:C:3226:ILE:HG12	2.17	0.45
1:C:3288:LEU:HD21	1:C:3336:GLU:HG3	1.97	0.45
1:C:3649:ALA:C	1:C:3652:PRO:HD2	2.42	0.45
1:D:1269:GLU:HB3	1:D:1286:THR:HB	1.98	0.45
1:D:2186:GLU:HG3	1:D:2187:ILE:H	1.82	0.45
1:D:3224:SER:OG	1:D:3226:ILE:HG12	2.17	0.45
1:D:3649:ALA:C	1:D:3652:PRO:HD2	2.42	0.45
1:D:4029:SER:OG	1:D:4055:HIS:NE2	2.49	0.45
1:A:1269:GLU:HB3	1:A:1286:THR:HB	1.98	0.45
1:A:2319:VAL:O	1:A:2323:LEU:HG	2.16	0.45
1:A:3144:LYS:HB2	1:A:3233:HIS:CE1	2.51	0.45
1:A:3224:SER:OG	1:A:3226:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4112:ASP:O	1:A:4116:GLN:HG2	2.17	0.45
1:B:514:PHE:HD2	1:B:526:TRP:HB2	1.82	0.45
1:B:808:HIS:CD2	1:B:832:LEU:HD23	2.51	0.45
1:B:2670:SER:HB2	1:B:2973:GLN:CG	2.47	0.45
1:B:4480:PHE:HA	1:B:4483:LYS:NZ	2.31	0.45
1:B:4698:LEU:O	1:B:4701:ILE:HG22	2.17	0.45
1:C:1936:LEU:HD11	1:C:1976:LEU:HD23	1.97	0.45
1:C:3015:VAL:HG11	1:C:3029:ILE:CG2	2.46	0.45
1:C:4584:PHE:O	1:C:4587:ILE:HG22	2.16	0.45
1:C:4735:ASN:HB3	1:C:4738:PHE:CD2	2.52	0.45
1:D:514:PHE:HD2	1:D:526:TRP:HB2	1.82	0.45
1:D:887:GLU:HA	1:D:890:HIS:ND1	2.31	0.45
1:D:2492:PHE:O	1:D:2496:LEU:HD12	2.17	0.45
1:D:3015:VAL:HG11	1:D:3029:ILE:CG2	2.47	0.45
1:D:3144:LYS:HB2	1:D:3233:HIS:CE1	2.51	0.45
1:D:4112:ASP:O	1:D:4116:GLN:HG2	2.17	0.45
1:A:270:HIS:CE1	1:A:491:GLU:HG3	2.50	0.45
1:A:1784:LEU:HD13	1:A:1833:ILE:HD11	1.98	0.45
1:A:3320:LEU:O	1:A:3323:MET:HG2	2.16	0.45
1:A:3986:LEU:HD12	1:A:4101:LEU:HD12	1.98	0.45
1:A:4029:SER:OG	1:A:4055:HIS:NE2	2.49	0.45
1:A:4035:TYR:HE2	1:A:4051:ALA:HA	1.81	0.45
1:A:4502:MET:SD	1:A:4585:PHE:HB3	2.57	0.45
1:B:668:ALA:HB2	1:B:1012:ILE:HD11	1.98	0.45
1:B:3043:ARG:C	1:B:3047:LYS:HZ2	2.24	0.45
1:B:4112:ASP:O	1:B:4116:GLN:HG2	2.17	0.45
1:B:4155:SER:O	1:B:4159:GLN:HG2	2.17	0.45
1:C:23:GLN:HB2	1:C:34:LYS:HD2	1.97	0.45
1:C:281:ARG:NE	1:C:283:ALA:O	2.41	0.45
1:C:2701:PHE:HD1	1:C:2873:PRO:HG3	1.80	0.45
1:C:2821:TYR:O	1:C:2823:PRO:HD3	2.16	0.45
1:C:3986:LEU:HD12	1:C:4101:LEU:HD12	1.99	0.45
1:D:1432:ILE:HB	1:D:1505:LEU:HB3	1.99	0.45
1:D:2728:SER:HA	1:D:2731:LYS:HG2	1.99	0.45
1:D:3050:LEU:HG	1:D:3052:SER:H	1.82	0.45
1:A:514:PHE:HD2	1:A:526:TRP:HB2	1.82	0.45
1:A:561:ARG:O	1:A:564:ARG:HG2	2.16	0.45
1:A:842:GLN:HB2	1:A:1603:PHE:HB2	1.98	0.45
1:A:989:THR:HB	1:A:992:GLN:OE1	2.17	0.45
1:A:2592:LEU:HD13	1:A:2610:LEU:HD21	1.98	0.45
1:A:2852:TRP:HA	1:A:2855:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3833:ASP:OD2	1:A:3908:LYS:HD2	2.17	0.45
1:A:4698:LEU:O	1:A:4701:ILE:HG22	2.17	0.45
1:B:261:HIS:CD2	1:B:263:GLU:HG3	2.52	0.45
1:B:887:GLU:HA	1:B:890:HIS:ND1	2.31	0.45
1:B:931:TYR:O	1:B:934:GLN:HG3	2.17	0.45
1:B:1047:LYS:C	1:B:1051:ARG:HE	2.25	0.45
1:B:2692:GLN:HG2	1:B:2704:GLN:HG3	1.97	0.45
1:B:3167:PRO:HA	1:B:3248:ARG:NH2	2.31	0.45
1:B:3284:ILE:HA	1:B:3287:ASN:OD1	2.16	0.45
1:B:3651:PRO:HB2	1:B:3652:PRO:HD3	1.99	0.45
1:C:982:ASP:HB2	1:C:985:PHE:CD1	2.52	0.45
1:C:1269:GLU:HB3	1:C:1286:THR:HB	1.98	0.45
1:C:2261:ASP:O	1:C:2265:VAL:HG23	2.17	0.45
1:C:2794:GLU:HB2	1:D:1498:GLN:OE1	2.16	0.45
1:C:3192:ARG:HH12	1:C:3197:LEU:HD23	1.82	0.45
1:C:3284:ILE:HA	1:C:3287:ASN:OD1	2.16	0.45
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	1.99	0.45
1:D:2397:ASP:O	1:D:2401:ARG:HG3	2.17	0.45
1:D:2773:TRP:HB3	1:D:2774:PRO:HD3	1.98	0.45
1:D:4584:PHE:O	1:D:4587:ILE:HG22	2.16	0.45
1:D:4698:LEU:O	1:D:4701:ILE:HG22	2.17	0.45
1:A:2232:PRO:C	1:A:2234:MET:H	2.24	0.45
1:A:2492:PHE:O	1:A:2496:LEU:HD12	2.17	0.45
1:A:2723:LYS:N	1:A:2726:GLU:OE1	2.45	0.45
1:A:3192:ARG:HH12	1:A:3197:LEU:HD23	1.82	0.45
1:A:3321:PRO:O	1:A:3325:LYS:HG2	2.17	0.45
1:A:4155:SER:O	1:A:4159:GLN:HG2	2.17	0.45
2:F:75:LEU:HB2	2:F:100:PHE:HB2	1.98	0.45
2:G:18:LYS:HE2	2:G:21:GLN:OE1	2.17	0.45
1:B:1936:LEU:HD11	1:B:1976:LEU:HD23	1.97	0.45
1:B:2592:LEU:HD13	1:B:2610:LEU:HD21	1.98	0.45
1:B:3015:VAL:HG11	1:B:3029:ILE:CG2	2.46	0.45
1:C:678:MET:HE1	1:C:812:LYS:NZ	2.32	0.45
1:C:2279:MET:SD	1:C:2283:LYS:HD3	2.57	0.45
1:C:2728:SER:HA	1:C:2731:LYS:HG2	1.98	0.45
1:C:2867:ASN:OD1	1:C:2868:HIS:N	2.50	0.45
1:D:3651:PRO:HB2	1:D:3652:PRO:HD3	1.99	0.45
1:D:4239:LEU:HD12	1:D:4240:THR:N	2.32	0.45
1:D:4735:ASN:HB3	1:D:4738:PHE:CD2	2.52	0.45
1:A:261:HIS:CD2	1:A:263:GLU:HG3	2.52	0.45
1:A:376:SER:HA	1:A:389:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:LEU:HD22	1:A:798:ILE:HD12	1.98	0.45
1:A:2397:ASP:O	1:A:2401:ARG:HG3	2.17	0.45
1:A:3167:PRO:HA	1:A:3248:ARG:NH2	2.31	0.45
2:G:57:ILE:HG13	2:G:60:PHE:HB2	1.98	0.45
1:B:2794:GLU:HB2	1:C:1498:GLN:OE1	2.16	0.45
1:B:3151:GLN:O	1:B:3155:LEU:HD12	2.17	0.45
1:B:3224:SER:OG	1:B:3226:ILE:HG12	2.17	0.45
1:B:3321:PRO:O	1:B:3325:LYS:HG2	2.17	0.45
1:B:4584:PHE:O	1:B:4587:ILE:HG22	2.16	0.45
1:C:895:MET:HA	1:C:898:ILE:HG22	1.99	0.45
1:C:2179:LEU:HD13	1:C:2227:VAL:HG21	1.99	0.45
1:C:2186:GLU:HG3	1:C:2187:ILE:H	1.82	0.45
1:C:2666:LEU:HB3	1:C:2667:PRO:HD3	1.99	0.45
1:C:3282:LYS:O	1:C:3285:TYR:HB3	2.17	0.45
1:C:3328:LYS:HG3	1:C:3329:LYS:HD3	1.98	0.45
1:C:4029:SER:OG	1:C:4055:HIS:NE2	2.49	0.45
1:C:4035:TYR:HE2	1:C:4051:ALA:HA	1.81	0.45
1:C:4239:LEU:HD12	1:C:4240:THR:N	2.32	0.45
1:C:4658:GLY:HA3	1:C:4663:ARG:HD3	1.99	0.45
1:D:895:MET:HA	1:D:898:ILE:HG22	1.99	0.45
1:D:1839:LEU:HA	1:D:1842:ILE:HG12	1.98	0.45
1:D:1922:ILE:O	1:D:1926:VAL:HG23	2.16	0.45
1:D:2867:ASN:OD1	1:D:2868:HIS:N	2.50	0.45
1:D:4159:GLN:HB3	1:D:4200:MET:HG2	1.98	0.45
1:A:1047:LYS:C	1:A:1051:ARG:HE	2.25	0.44
1:A:2497:ARG:NH1	1:A:2876:THR:O	2.51	0.44
1:A:4239:LEU:HD12	1:A:4240:THR:N	2.32	0.44
1:B:358:ASP:OD1	1:B:359:SER:N	2.50	0.44
1:B:1839:LEU:HA	1:B:1842:ILE:HG12	1.98	0.44
1:B:2279:MET:SD	1:B:2283:LYS:HD3	2.57	0.44
1:B:2593:VAL:HG12	1:B:2644:LEU:HD13	1.99	0.44
1:B:2867:ASN:OD1	1:B:2868:HIS:N	2.50	0.44
1:B:3811:GLN:NE2	1:B:3815:GLU:OE2	2.47	0.44
1:C:358:ASP:OD1	1:C:359:SER:N	2.50	0.44
1:C:376:SER:HA	1:C:389:ARG:HD2	1.99	0.44
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.99	0.44
1:C:989:THR:HB	1:C:992:GLN:OE1	2.17	0.44
1:C:2670:SER:HB2	1:C:2973:GLN:CG	2.46	0.44
1:C:2684:ASN:ND2	1:C:2909:ASP:OD1	2.39	0.44
1:C:2788:ARG:NH2	1:C:2906:GLY:O	2.45	0.44
1:D:1649:GLU:HG2	1:D:1650:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2232:PRO:C	1:D:2234:MET:H	2.24	0.44
1:D:3328:LYS:HG3	1:D:3329:LYS:HD3	1.98	0.44
1:D:3833:ASP:OD2	1:D:3908:LYS:HD2	2.17	0.44
1:A:2821:TYR:O	1:A:2823:PRO:HD3	2.16	0.44
1:A:3284:ILE:HA	1:A:3287:ASN:OD1	2.16	0.44
1:A:3649:ALA:C	1:A:3652:PRO:HD2	2.42	0.44
1:A:3651:PRO:HB2	1:A:3652:PRO:HD3	1.99	0.44
1:B:749:LEU:HD22	1:B:755:ILE:HD11	1.99	0.44
1:B:2212:LYS:HG3	1:B:2253:LEU:HD21	1.98	0.44
1:B:2492:PHE:O	1:B:2496:LEU:HD12	2.17	0.44
1:B:2719:TYR:HD1	1:B:2723:LYS:HZ2	1.62	0.44
1:B:3320:LEU:O	1:B:3323:MET:HG2	2.16	0.44
1:B:3833:ASP:OD2	1:B:3908:LYS:HD2	2.17	0.44
1:B:4502:MET:SD	1:B:4585:PHE:HB3	2.57	0.44
1:C:853:PRO:HB3	1:C:1083:GLU:OE2	2.18	0.44
1:C:887:GLU:HA	1:C:890:HIS:ND1	2.31	0.44
1:C:1039:ASP:O	1:C:1043:LYS:HB2	2.17	0.44
1:C:1784:LEU:HD13	1:C:1833:ILE:HD11	1.98	0.44
1:C:3651:PRO:HB2	1:C:3652:PRO:HD3	1.99	0.44
1:D:376:SER:HA	1:D:389:ARG:HD2	1.99	0.44
1:D:931:TYR:O	1:D:934:GLN:HG3	2.17	0.44
1:D:1140:PHE:CD2	1:D:1141:LYS:HE3	2.53	0.44
1:D:1697:LEU:HD23	1:D:1697:LEU:HA	1.88	0.44
1:D:1937:GLN:NE2	1:D:3608:LEU:O	2.31	0.44
1:D:3261:ALA:C	1:D:3263:MET:H	2.26	0.44
1:D:4155:SER:O	1:D:4159:GLN:HG2	2.17	0.44
1:D:4658:GLY:HA3	1:D:4663:ARG:HD3	2.00	0.44
1:A:931:TYR:O	1:A:934:GLN:HG3	2.17	0.44
1:A:1432:ILE:HB	1:A:1505:LEU:HB3	1.99	0.44
1:A:2261:ASP:O	1:A:2265:VAL:HG23	2.17	0.44
1:A:2773:TRP:HB3	1:A:2774:PRO:HD3	1.98	0.44
1:A:3016:ARG:HA	1:A:3096:TYR:OH	2.18	0.44
1:A:3050:LEU:HG	1:A:3052:SER:H	1.82	0.44
1:A:3151:GLN:O	1:A:3155:LEU:HD12	2.17	0.44
2:E:75:LEU:HB2	2:E:100:PHE:HB2	1.98	0.44
1:B:678:MET:HE1	1:B:812:LYS:NZ	2.32	0.44
1:B:842:GLN:HB2	1:B:1603:PHE:HB2	1.98	0.44
1:B:1140:PHE:CD2	1:B:1141:LYS:HE3	2.53	0.44
1:B:1937:GLN:NE2	1:B:3608:LEU:O	2.31	0.44
1:B:2057:THR:HG22	1:B:2059:GLN:H	1.82	0.44
1:B:2179:LEU:HD13	1:B:2227:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2232:PRO:C	1:B:2234:MET:H	2.24	0.44
1:B:4159:GLN:HB3	1:B:4200:MET:HG2	1.98	0.44
1:C:668:ALA:HB2	1:C:1012:ILE:HD11	1.98	0.44
1:C:1019:GLY:HA3	1:C:1028:ARG:HE	1.81	0.44
1:C:2773:TRP:HB3	1:C:2774:PRO:HD3	1.98	0.44
1:C:4155:SER:O	1:C:4159:GLN:HG2	2.17	0.44
1:D:1750:GLY:HA3	1:D:1839:LEU:HD21	2.00	0.44
1:D:2279:MET:SD	1:D:2283:LYS:HD3	2.57	0.44
1:D:2923:TYR:CE2	1:D:2999:LYS:HB3	2.52	0.44
1:D:3151:GLN:O	1:D:3155:LEU:HD12	2.17	0.44
1:A:358:ASP:OD1	1:A:359:SER:N	2.50	0.44
1:A:853:PRO:HB3	1:A:1083:GLU:OE2	2.18	0.44
1:A:2923:TYR:CE2	1:A:2999:LYS:HB3	2.52	0.44
1:A:3100:ALA:C	1:A:3103:PRO:HD2	2.43	0.44
1:A:3677:THR:HB	1:A:3679:LYS:HZ3	1.81	0.44
2:E:57:ILE:HG13	2:E:60:PHE:HB2	1.98	0.44
1:B:982:ASP:HB2	1:B:985:PHE:HD1	1.83	0.44
1:B:2247:VAL:HG11	1:B:2257:LEU:HD12	2.00	0.44
1:B:2497:ARG:NH1	1:B:2876:THR:O	2.51	0.44
1:B:3975:GLN:O	1:B:3979:VAL:HG23	2.18	0.44
1:B:4239:LEU:HD12	1:B:4240:THR:N	2.32	0.44
1:C:181:LEU:N	1:C:212:TRP:O	2.36	0.44
1:C:931:TYR:O	1:C:934:GLN:HG3	2.17	0.44
1:C:1043:LYS:O	1:C:1047:LYS:CB	2.66	0.44
1:C:2492:PHE:O	1:C:2496:LEU:HD12	2.17	0.44
1:C:2593:VAL:HG12	1:C:2644:LEU:HD13	1.99	0.44
1:C:3016:ARG:HA	1:C:3096:TYR:OH	2.17	0.44
1:C:3321:PRO:O	1:C:3325:LYS:HG2	2.17	0.44
1:D:261:HIS:CD2	1:D:263:GLU:HG3	2.52	0.44
1:D:2212:LYS:HG3	1:D:2253:LEU:HD21	1.98	0.44
1:D:3038:GLN:HA	1:D:3111:HIS:CD2	2.53	0.44
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.99	0.44
1:A:2728:SER:HA	1:A:2731:LYS:HG2	1.99	0.44
1:A:3328:LYS:HG3	1:A:3329:LYS:HD3	1.98	0.44
2:F:18:LYS:HE2	2:F:21:GLN:OE1	2.17	0.44
2:H:18:LYS:HE2	2:H:21:GLN:OE1	2.17	0.44
1:B:376:SER:HA	1:B:389:ARG:HD2	1.99	0.44
1:B:1019:GLY:HA3	1:B:1028:ARG:HE	1.81	0.44
1:B:1043:LYS:O	1:B:1047:LYS:CB	2.65	0.44
1:B:2172:MET:O	1:B:2176:VAL:HG23	2.18	0.44
1:B:2186:GLU:HG3	1:B:2187:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3016:ARG:HA	1:B:3096:TYR:OH	2.17	0.44
1:B:3016:ARG:HG2	1:B:3017:HIS:ND1	2.33	0.44
1:B:3038:GLN:HA	1:B:3111:HIS:CD2	2.53	0.44
1:B:3192:ARG:HH12	1:B:3197:LEU:HD23	1.82	0.44
1:B:4035:TYR:HE2	1:B:4051:ALA:HA	1.81	0.44
1:B:4735:ASN:HB3	1:B:4738:PHE:CD2	2.52	0.44
1:C:261:HIS:CD2	1:C:263:GLU:HG3	2.52	0.44
1:C:1140:PHE:CD2	1:C:1141:LYS:HE3	2.53	0.44
1:C:1839:LEU:HA	1:C:1842:ILE:HG12	1.99	0.44
1:C:2057:THR:HG22	1:C:2059:GLN:H	1.82	0.44
1:C:2593:VAL:HG11	1:C:2640:LEU:HG	2.00	0.44
1:C:3050:LEU:HG	1:C:3052:SER:H	1.82	0.44
1:C:3261:ALA:C	1:C:3263:MET:H	2.26	0.44
1:C:3833:ASP:OD2	1:C:3908:LYS:HD2	2.17	0.44
1:C:4051:ALA:O	1:C:4055:HIS:ND1	2.19	0.44
1:C:4502:MET:SD	1:C:4585:PHE:HB3	2.57	0.44
1:D:678:MET:HE1	1:D:812:LYS:NZ	2.32	0.44
1:D:1043:LYS:O	1:D:1047:LYS:CB	2.65	0.44
1:D:3325:LYS:HD2	1:D:3328:LYS:HZ2	1.82	0.44
1:D:4664:ASP:O	1:D:4668:GLU:OE1	2.35	0.44
1:A:982:ASP:HB2	1:A:985:PHE:CD1	2.52	0.44
1:A:982:ASP:HB2	1:A:985:PHE:HD1	1.83	0.44
1:A:2175:MET:HE2	1:A:2175:MET:HB3	1.88	0.44
1:A:2247:VAL:HG11	1:A:2257:LEU:HD12	2.00	0.44
1:A:2867:ASN:OD1	1:A:2868:HIS:N	2.50	0.44
1:A:3016:ARG:HG2	1:A:3017:HIS:ND1	2.33	0.44
1:A:3038:GLN:HA	1:A:3111:HIS:CD2	2.53	0.44
1:A:3237:VAL:C	1:A:3240:PRO:HD2	2.43	0.44
1:A:4735:ASN:HB3	1:A:4738:PHE:CD2	2.52	0.44
2:G:32:GLN:NE2	1:C:1312:GLU:HB3	2.33	0.44
1:B:219:SER:OG	1:B:222:GLU:OE1	2.24	0.44
1:B:895:MET:HA	1:B:898:ILE:HG22	1.99	0.44
1:B:982:ASP:HB2	1:B:985:PHE:CD1	2.52	0.44
1:B:1039:ASP:O	1:B:1043:LYS:HB2	2.17	0.44
1:B:2642:ARG:HD2	1:B:2680:TYR:HE2	1.83	0.44
1:B:2923:TYR:CE2	1:B:2999:LYS:HB3	2.52	0.44
1:B:3100:ALA:C	1:B:3103:PRO:HD2	2.43	0.44
1:B:3237:VAL:C	1:B:3240:PRO:HD2	2.43	0.44
1:B:4276:VAL:O	1:B:4280:VAL:HG23	2.18	0.44
1:C:749:LEU:HD22	1:C:755:ILE:HD11	1.99	0.44
1:C:3151:GLN:O	1:C:3155:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3285:TYR:CD1	1:C:3325:LYS:HD2	2.53	0.44
1:C:3975:GLN:O	1:C:3979:VAL:HG23	2.18	0.44
1:C:4276:VAL:O	1:C:4280:VAL:HG23	2.18	0.44
1:D:58:VAL:HG13	1:D:319:LYS:HG2	2.00	0.44
1:D:358:ASP:OD1	1:D:359:SER:N	2.50	0.44
1:D:1047:LYS:HG3	1:D:1051:ARG:NE	2.33	0.44
1:D:1689:ILE:HG23	1:D:1703:TYR:CZ	2.53	0.44
1:D:2319:VAL:O	1:D:2323:LEU:HG	2.16	0.44
1:D:2666:LEU:HB3	1:D:2667:PRO:HD3	1.99	0.44
1:D:3016:ARG:HA	1:D:3096:TYR:OH	2.18	0.44
1:D:3123:LEU:HB3	1:D:3124:GLU:H	1.72	0.44
1:D:3192:ARG:HH12	1:D:3197:LEU:HD23	1.82	0.44
1:D:3227:ARG:HE	1:D:3228:TYR:N	1.96	0.44
1:A:1649:GLU:HG2	1:A:1650:LEU:N	2.33	0.44
1:A:2440:PHE:CZ	1:A:2465:LYS:HD3	2.53	0.44
1:A:2593:VAL:HG11	1:A:2640:LEU:HG	2.00	0.44
1:A:2666:LEU:HB3	1:A:2667:PRO:HD3	1.99	0.44
1:A:2971:ILE:HG23	1:A:2975:PHE:HE2	1.83	0.44
1:A:3325:LYS:HD2	1:A:3328:LYS:HZ2	1.82	0.44
2:E:18:LYS:HE2	2:E:21:GLN:OE1	2.17	0.44
1:B:624:ALA:HB2	1:B:1667:LEU:HD12	1.99	0.44
1:B:2440:PHE:CZ	1:B:2465:LYS:HD3	2.53	0.44
1:B:2728:SER:HA	1:B:2731:LYS:HG2	1.99	0.44
1:B:3069:GLU:N	1:B:3069:GLU:OE2	2.51	0.44
1:C:58:VAL:HG13	1:C:319:LYS:HG2	2.00	0.44
1:D:2261:ASP:O	1:D:2265:VAL:HG23	2.17	0.44
1:D:2593:VAL:HG12	1:D:2644:LEU:HD13	1.99	0.44
1:D:3100:ALA:C	1:D:3103:PRO:HD2	2.43	0.44
1:A:895:MET:HA	1:A:898:ILE:HG22	1.99	0.44
1:A:1750:GLY:HA3	1:A:1839:LEU:HD21	2.00	0.44
1:A:2179:LEU:HD13	1:A:2227:VAL:HG21	1.99	0.44
1:A:3250:TRP:HE1	1:A:3256:ASN:HD21	1.66	0.44
1:A:4658:GLY:HA3	1:A:4663:ARG:HD3	1.99	0.44
1:B:1649:GLU:HG2	1:B:1650:LEU:N	2.33	0.44
1:B:2593:VAL:HG11	1:B:2640:LEU:HG	2.00	0.44
1:B:3050:LEU:HG	1:B:3052:SER:H	1.82	0.44
1:B:3131:TYR:HE1	1:B:3166:PHE:HZ	1.66	0.44
1:B:4197:ILE:HG12	1:B:4923:MET:HE3	2.00	0.44
1:C:1432:ILE:HB	1:C:1505:LEU:HB3	1.99	0.44
1:C:1689:ILE:HG23	1:C:1703:TYR:CZ	2.53	0.44
1:C:3016:ARG:HG2	1:C:3017:HIS:ND1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4159:GLN:HB3	1:C:4200:MET:HG2	1.98	0.44
1:D:240:HIS:HB2	1:D:243:GLU:OE1	2.18	0.44
1:D:853:PRO:HB3	1:D:1083:GLU:OE2	2.18	0.44
1:D:2179:LEU:HD13	1:D:2227:VAL:HG21	1.99	0.44
1:D:3250:TRP:HE1	1:D:3256:ASN:HD21	1.66	0.44
1:D:3321:PRO:O	1:D:3325:LYS:HG2	2.17	0.44
1:A:3261:ALA:C	1:A:3263:MET:H	2.26	0.44
1:A:3975:GLN:O	1:A:3979:VAL:HG23	2.18	0.44
1:A:4664:ASP:O	1:A:4668:GLU:OE1	2.36	0.44
2:H:32:GLN:HG2	1:D:1312:GLU:OE1	2.18	0.44
1:B:989:THR:HB	1:B:992:GLN:OE1	2.17	0.44
1:B:1166:VAL:HG23	1:B:1173:MET:HG2	2.00	0.44
1:B:2759:PRO:HD2	1:B:2762:LEU:HD12	2.00	0.44
1:C:1166:VAL:HG23	1:C:1173:MET:HG2	2.00	0.44
1:C:2497:ARG:NH1	1:C:2876:THR:O	2.51	0.44
1:C:4664:ASP:O	1:C:4668:GLU:OE1	2.35	0.44
1:D:749:LEU:HD22	1:D:755:ILE:HD11	1.99	0.44
1:D:3016:ARG:HG2	1:D:3017:HIS:ND1	2.33	0.44
1:A:1140:PHE:CD2	1:A:1141:LYS:HE3	2.53	0.43
1:A:1689:ILE:HG23	1:A:1703:TYR:CZ	2.53	0.43
1:A:2172:MET:O	1:A:2176:VAL:HG23	2.18	0.43
1:A:2186:GLU:HG3	1:A:2187:ILE:H	1.82	0.43
1:A:2605:MET:HB3	1:A:2606:PRO:HD3	2.00	0.43
1:A:2622:CYS:HA	1:A:2677:PRO:HG3	2.00	0.43
1:A:2642:ARG:HD2	1:A:2680:TYR:HE2	1.83	0.43
1:A:2833:LEU:HB3	1:A:2837:LEU:HB2	2.00	0.43
1:A:3320:LEU:HB2	1:A:3321:PRO:HD3	2.00	0.43
1:B:2077:ASP:O	1:B:2081:VAL:HG23	2.19	0.43
1:B:2442:MET:SD	1:B:2498:ALA:HB1	2.58	0.43
1:B:2666:LEU:HB3	1:B:2667:PRO:HD3	1.99	0.43
1:B:2833:LEU:HB3	1:B:2837:LEU:HB2	2.00	0.43
1:B:3305:PRO:O	1:B:3309:LYS:HG3	2.18	0.43
1:B:4658:GLY:HA3	1:B:4663:ARG:HD3	1.99	0.43
1:C:1047:LYS:C	1:C:1051:ARG:HE	2.25	0.43
1:C:2172:MET:O	1:C:2176:VAL:HG23	2.18	0.43
1:D:1016:TRP:CE3	1:D:1029:ASN:HB2	2.53	0.43
1:D:1039:ASP:O	1:D:1043:LYS:HB2	2.17	0.43
1:D:1047:LYS:C	1:D:1051:ARG:HE	2.25	0.43
1:D:2657:TYR:HA	1:D:2662:PHE:HE1	1.75	0.43
1:D:3305:PRO:O	1:D:3309:LYS:HG3	2.18	0.43
1:A:28:ILE:HD11	1:A:201:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3285:TYR:CD1	1:A:3325:LYS:HD2	2.53	0.43
1:B:1021:GLN:NE2	1:B:1022:GLN:O	2.51	0.43
1:B:1718:ARG:HD3	1:B:1831:MET:HA	2.00	0.43
1:B:2261:ASP:O	1:B:2265:VAL:HG23	2.17	0.43
1:B:3187:LYS:HZ1	1:B:3195:LEU:HD13	1.83	0.43
1:C:1016:TRP:CE3	1:C:1029:ASN:HB2	2.53	0.43
1:C:2884:LYS:O	1:C:2887:GLU:HG3	2.18	0.43
1:C:3101:LEU:HA	1:C:3104:MET:HE2	2.00	0.43
1:C:3325:LYS:HD2	1:C:3328:LYS:HZ2	1.83	0.43
1:C:4197:ILE:HG12	1:C:4923:MET:HE3	2.00	0.43
1:D:989:THR:HB	1:D:992:GLN:OE1	2.17	0.43
1:D:2146:LEU:HD23	1:D:2146:LEU:HA	1.83	0.43
1:D:2440:PHE:CZ	1:D:2465:LYS:HD3	2.53	0.43
1:D:2971:ILE:HG23	1:D:2975:PHE:HE2	1.83	0.43
1:D:3285:TYR:CD1	1:D:3325:LYS:HD2	2.53	0.43
1:D:4197:ILE:HG12	1:D:4923:MET:HE3	2.00	0.43
1:A:240:HIS:HB2	1:A:243:GLU:OE1	2.18	0.43
1:A:749:LEU:HD22	1:A:755:ILE:HD11	1.99	0.43
1:A:1444:GLY:HA3	1:A:1487:MET:HA	2.01	0.43
1:A:1892:GLY:H	1:A:1895:GLN:NE2	2.16	0.43
1:A:3131:TYR:HE1	1:A:3166:PHE:HZ	1.66	0.43
1:B:877:HIS:O	1:B:880:ARG:HD3	2.19	0.43
1:B:1047:LYS:HG3	1:B:1051:ARG:NE	2.33	0.43
1:B:2146:LEU:HD23	1:B:2146:LEU:HA	1.83	0.43
1:B:2723:LYS:N	1:B:2726:GLU:OE1	2.45	0.43
1:B:3320:LEU:HB2	1:B:3321:PRO:HD3	2.00	0.43
1:C:1444:GLY:HA3	1:C:1487:MET:HA	2.01	0.43
1:C:1718:ARG:HD3	1:C:1831:MET:HA	2.01	0.43
1:C:2621:TYR:OH	1:C:2637:GLU:OE2	2.17	0.43
1:C:2923:TYR:CE2	1:C:2999:LYS:HB3	2.52	0.43
1:C:3038:GLN:HA	1:C:3111:HIS:CD2	2.53	0.43
1:C:3100:ALA:C	1:C:3103:PRO:HD2	2.43	0.43
1:C:3305:PRO:O	1:C:3309:LYS:HG3	2.18	0.43
1:D:28:ILE:HD11	1:D:201:LEU:HD21	2.00	0.43
1:D:877:HIS:O	1:D:880:ARG:HD3	2.18	0.43
1:D:931:TYR:CD2	4:D:5003:ATP:C2'	3.02	0.43
1:D:2497:ARG:NH1	1:D:2876:THR:O	2.50	0.43
1:D:2593:VAL:HG11	1:D:2640:LEU:HG	2.00	0.43
1:D:2670:SER:HB2	1:D:2973:GLN:CG	2.47	0.43
1:D:3975:GLN:O	1:D:3979:VAL:HG23	2.18	0.43
1:A:12:GLN:HG3	1:A:177:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:TRP:CE3	1:A:1029:ASN:HB2	2.53	0.43
1:A:2593:VAL:HG12	1:A:2644:LEU:HD13	1.99	0.43
1:A:2670:SER:HB2	1:A:2973:GLN:CG	2.47	0.43
1:A:3793:LEU:HD23	1:A:3793:LEU:HA	1.89	0.43
1:A:4014:LEU:HD13	1:A:4122:ALA:HB2	2.00	0.43
1:B:2155:PHE:HA	1:B:2162:MET:HE3	2.01	0.43
1:B:2622:CYS:HA	1:B:2677:PRO:HG3	2.01	0.43
1:B:3948:LEU:HD23	1:B:3948:LEU:HA	1.88	0.43
1:B:4664:ASP:O	1:B:4668:GLU:OE1	2.35	0.43
1:C:433:LEU:HD23	1:C:433:LEU:HA	1.89	0.43
1:C:1021:GLN:NE2	1:C:1022:GLN:O	2.51	0.43
1:C:1047:LYS:HG3	1:C:1051:ARG:NE	2.33	0.43
1:C:1750:GLY:HA3	1:C:1839:LEU:HD21	2.00	0.43
1:C:2247:VAL:HG11	1:C:2257:LEU:HD12	2.00	0.43
1:C:2642:ARG:HD2	1:C:2680:TYR:HE2	1.83	0.43
1:C:2967:VAL:O	1:C:2971:ILE:HG13	2.19	0.43
1:C:3069:GLU:N	1:C:3069:GLU:OE2	2.51	0.43
1:C:4014:LEU:HD13	1:C:4122:ALA:HB2	2.00	0.43
1:D:1300:MET:HE3	1:D:1300:MET:HB3	1.87	0.43
1:D:2719:TYR:HD1	1:D:2723:LYS:HZ2	1.64	0.43
1:D:3101:LEU:HA	1:D:3104:MET:HE2	2.00	0.43
1:D:3237:VAL:C	1:D:3240:PRO:HD2	2.43	0.43
1:A:58:VAL:HG13	1:A:319:LYS:HG2	2.00	0.43
1:A:661:LEU:HD13	1:A:673:TRP:CD1	2.53	0.43
1:A:678:MET:HE1	1:A:812:LYS:NZ	2.32	0.43
1:A:1021:GLN:NE2	1:A:1022:GLN:O	2.51	0.43
1:A:1043:LYS:O	1:A:1047:LYS:CB	2.65	0.43
1:A:2279:MET:SD	1:A:2283:LYS:HD3	2.57	0.43
2:G:89:PRO:HB2	1:C:1671:ARG:HH22	1.83	0.43
1:B:58:VAL:HG13	1:B:319:LYS:HG2	2.00	0.43
1:B:240:HIS:HB2	1:B:243:GLU:OE1	2.18	0.43
1:B:661:LEU:HD13	1:B:673:TRP:CD1	2.53	0.43
1:B:962:LYS:NZ	1:B:982:ASP:OD1	2.36	0.43
1:B:1432:ILE:HB	1:B:1505:LEU:HB3	1.99	0.43
1:B:1689:ILE:HG23	1:B:1703:TYR:CZ	2.53	0.43
1:B:1784:LEU:HD13	1:B:1833:ILE:HD11	1.98	0.43
1:B:2607:LEU:CD1	1:B:2664:LEU:HG	2.47	0.43
1:B:2638:LEU:HB3	1:B:2680:TYR:CE1	2.54	0.43
1:B:2884:LYS:O	1:B:2887:GLU:HG3	2.18	0.43
1:B:2971:ILE:HG23	1:B:2975:PHE:HE2	1.83	0.43
1:B:3285:TYR:CD1	1:B:3325:LYS:HD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4030:ASP:OD2	1:B:4031:THR:N	2.52	0.43
1:C:661:LEU:HD13	1:C:673:TRP:CD1	2.53	0.43
1:C:829:LYS:NZ	1:C:1037:LEU:O	2.39	0.43
1:C:982:ASP:HB2	1:C:985:PHE:HD1	1.83	0.43
1:C:1649:GLU:HG2	1:C:1650:LEU:N	2.32	0.43
1:C:2155:PHE:HA	1:C:2162:MET:HE3	2.01	0.43
1:C:2222:LEU:HA	1:C:2222:LEU:HD23	1.79	0.43
1:C:2440:PHE:CZ	1:C:2465:LYS:HD3	2.53	0.43
1:C:2759:PRO:HD2	1:C:2762:LEU:HD12	2.00	0.43
1:C:2833:LEU:HB3	1:C:2837:LEU:HB2	2.00	0.43
1:C:4673:ASP:OD1	1:C:4673:ASP:N	2.51	0.43
1:D:1892:GLY:H	1:D:1895:GLN:NE2	2.16	0.43
1:D:2087:LEU:O	1:D:2091:GLN:HG2	2.19	0.43
1:A:655:MET:SD	1:A:836:HIS:HA	2.59	0.43
1:A:2146:LEU:HD23	1:A:2146:LEU:HA	1.83	0.43
1:A:4197:ILE:HG12	1:A:4923:MET:HE3	2.00	0.43
1:B:12:GLN:HG3	1:B:177:VAL:HG11	2.01	0.43
1:B:579:LEU:HD13	1:B:617:LEU:HG	2.00	0.43
1:B:931:TYR:CD2	4:B:5003:ATP:C2'	3.01	0.43
1:B:1016:TRP:CE3	1:B:1029:ASN:HB2	2.53	0.43
1:B:3101:LEU:HA	1:B:3104:MET:HE2	2.00	0.43
1:B:4014:LEU:HD13	1:B:4122:ALA:HB2	2.00	0.43
1:C:240:HIS:HB2	1:C:243:GLU:OE1	2.18	0.43
1:C:2087:LEU:O	1:C:2091:GLN:HG2	2.19	0.43
1:C:2442:MET:SD	1:C:2498:ALA:HB1	2.58	0.43
1:C:3237:VAL:C	1:C:3240:PRO:HD2	2.43	0.43
1:D:661:LEU:HD13	1:D:673:TRP:CD1	2.53	0.43
1:D:1931:ASP:OD1	1:D:1932:PHE:N	2.52	0.43
1:D:2172:MET:O	1:D:2176:VAL:HG23	2.18	0.43
1:D:2409:ILE:HD13	1:D:2420:ARG:NH1	2.34	0.43
1:D:2442:MET:SD	1:D:2498:ALA:HB1	2.58	0.43
1:D:2549:LEU:HD13	1:D:2573:LEU:HD11	2.00	0.43
1:D:4276:VAL:O	1:D:4280:VAL:HG23	2.18	0.43
1:A:877:HIS:O	1:A:880:ARG:HD3	2.19	0.43
1:A:1039:ASP:O	1:A:1043:LYS:HB2	2.17	0.43
1:A:1047:LYS:HG3	1:A:1051:ARG:NE	2.33	0.43
1:A:2187:ILE:HD11	1:A:2193:VAL:HG21	2.01	0.43
1:A:2759:PRO:HD2	1:A:2762:LEU:HD12	2.00	0.43
1:A:2884:LYS:O	1:A:2887:GLU:HG3	2.18	0.43
1:A:3305:PRO:O	1:A:3309:LYS:HG3	2.18	0.43
2:F:50:ARG:HH21	2:F:53:LYS:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:SER:HB2	1:B:190:ARG:HH11	1.84	0.43
1:B:853:PRO:HB3	1:B:1083:GLU:OE2	2.18	0.43
1:B:2549:LEU:HD13	1:B:2573:LEU:HD11	1.99	0.43
1:B:2788:ARG:NH2	1:B:2906:GLY:O	2.45	0.43
1:C:2077:ASP:O	1:C:2081:VAL:HG23	2.19	0.43
1:C:2638:LEU:HB3	1:C:2680:TYR:CE1	2.54	0.43
1:C:2682:GLU:HG3	1:C:2919:LYS:HD3	2.00	0.43
1:C:2719:TYR:CE2	1:C:2799:ALA:HB2	2.38	0.43
1:D:188:SER:HB2	1:D:190:ARG:HH11	1.84	0.43
1:D:2988:ARG:N	1:D:2989:PRO:HD3	2.34	0.43
1:A:931:TYR:CD2	4:A:5003:ATP:C2'	3.02	0.43
1:A:1166:VAL:HG23	1:A:1173:MET:HG2	2.00	0.43
1:A:2967:VAL:O	1:A:2971:ILE:HG13	2.19	0.43
1:A:4070:ALA:HB1	1:A:4078:LEU:HD13	2.01	0.43
1:A:4276:VAL:O	1:A:4280:VAL:HG23	2.18	0.43
1:A:4673:ASP:OD1	1:A:4673:ASP:N	2.51	0.43
1:B:1608:VAL:HA	1:B:1618:LEU:O	2.19	0.43
1:B:2726:GLU:OE1	1:B:2726:GLU:N	2.51	0.43
1:B:3227:ARG:NE	1:B:3228:TYR:H	1.96	0.43
1:C:1892:GLY:H	1:C:1895:GLN:NE2	2.16	0.43
1:C:1931:ASP:OD1	1:C:1932:PHE:N	2.52	0.43
1:C:3123:LEU:HB3	1:C:3124:GLU:H	1.72	0.43
1:C:4617:ILE:HD13	1:C:4666:ILE:HD12	2.01	0.43
1:C:4867:ILE:HG12	1:D:4864:GLY:HA2	2.01	0.43
1:D:1021:GLN:NE2	1:D:1022:GLN:O	2.51	0.43
1:D:2187:ILE:HD11	1:D:2193:VAL:HG21	2.01	0.43
1:D:2621:TYR:OH	1:D:2637:GLU:OE2	2.17	0.43
1:D:2638:LEU:HB3	1:D:2680:TYR:CE1	2.54	0.43
1:D:2684:ASN:ND2	1:D:2909:ASP:OD1	2.39	0.43
1:D:2833:LEU:HB3	1:D:2837:LEU:HB2	2.00	0.43
1:D:3069:GLU:N	1:D:3069:GLU:OE2	2.51	0.43
1:D:4617:ILE:HD13	1:D:4666:ILE:HD12	2.01	0.43
1:A:188:SER:HB2	1:A:190:ARG:HH11	1.84	0.43
1:A:579:LEU:HD13	1:A:617:LEU:HG	2.00	0.43
1:A:848:ARG:HD3	1:A:1599:MET:HE1	2.01	0.43
1:A:1914:CYS:O	1:A:1918:VAL:HG23	2.19	0.43
1:A:2087:LEU:O	1:A:2091:GLN:HG2	2.19	0.43
1:A:2155:PHE:HA	1:A:2162:MET:HE3	2.01	0.43
1:A:2442:MET:SD	1:A:2498:ALA:HB1	2.58	0.43
1:A:3054:LYS:O	1:A:3057:LEU:HD23	2.19	0.43
1:B:28:ILE:HD11	1:B:201:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:MET:SD	1:B:836:HIS:HA	2.59	0.43
1:B:896:ASN:O	1:B:899:GLU:HG3	2.19	0.43
1:B:1931:ASP:OD1	1:B:1932:PHE:N	2.52	0.43
1:B:2581:ARG:HB3	1:B:2584:MET:SD	2.59	0.43
1:B:3250:TRP:HE1	1:B:3256:ASN:HD21	1.66	0.43
1:C:877:HIS:HA	1:C:880:ARG:NE	2.34	0.43
1:C:877:HIS:O	1:C:880:ARG:HD3	2.19	0.43
1:D:655:MET:SD	1:D:836:HIS:HA	2.59	0.43
1:D:896:ASN:O	1:D:899:GLU:HG3	2.19	0.43
1:D:982:ASP:HB2	1:D:985:PHE:HD1	1.83	0.43
1:D:2581:ARG:HB3	1:D:2584:MET:SD	2.59	0.43
1:D:2967:VAL:O	1:D:2971:ILE:HG13	2.19	0.43
1:D:3187:LYS:HZ2	1:D:3195:LEU:HD13	1.83	0.43
1:D:3320:LEU:HB2	1:D:3321:PRO:HD3	2.00	0.43
1:A:1967:SER:O	1:A:3605:MET:HE1	2.19	0.43
1:A:2077:ASP:O	1:A:2081:VAL:HG23	2.19	0.43
1:A:2409:ILE:HD13	1:A:2420:ARG:NH1	2.34	0.43
1:A:2719:TYR:HE2	1:A:2799:ALA:CB	2.24	0.43
1:A:2768:LYS:O	1:A:2771:TYR:HB3	2.19	0.43
1:A:2999:LYS:O	1:A:3002:GLU:HG3	2.19	0.43
1:A:4040:LYS:HE3	1:A:4040:LYS:HB2	1.83	0.43
1:A:4617:ILE:HD13	1:A:4666:ILE:HD12	2.01	0.43
1:B:281:ARG:NH1	1:B:345:GLU:HB3	2.34	0.43
1:B:937:LEU:HG	1:B:941:LYS:HE2	2.01	0.43
1:B:1444:GLY:HA3	1:B:1487:MET:HA	2.01	0.43
1:B:1750:GLY:HA3	1:B:1839:LEU:HD21	2.00	0.43
1:B:1972:GLN:OE1	1:B:3608:LEU:HG	2.19	0.43
1:B:2682:GLU:HG3	1:B:2919:LYS:HD3	2.00	0.43
1:C:188:SER:HB2	1:C:190:ARG:HH11	1.84	0.43
1:C:2605:MET:HB3	1:C:2606:PRO:HD3	2.00	0.43
1:C:2607:LEU:CD1	1:C:2664:LEU:HG	2.47	0.43
1:C:2768:LYS:O	1:C:2771:TYR:HB3	2.19	0.43
1:C:3054:LYS:O	1:C:3057:LEU:HD23	2.18	0.43
1:C:3250:TRP:HE1	1:C:3256:ASN:HD21	1.66	0.43
1:D:848:ARG:HD3	1:D:1599:MET:HE1	2.01	0.43
1:D:1166:VAL:HG23	1:D:1173:MET:HG2	2.00	0.43
1:D:2622:CYS:HA	1:D:2677:PRO:HG3	2.00	0.43
1:D:2998:ASN:ND2	1:D:3048:THR:HG1	2.16	0.43
1:A:881:ILE:HG21	1:A:1062:TYR:CE2	2.54	0.42
1:A:3227:ARG:NH2	1:A:3295:TRP:HZ2	2.17	0.42
1:A:3969:LYS:HE2	1:A:3969:LYS:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:50:ARG:HE	2:F:53:LYS:HE3	1.84	0.42
1:B:877:HIS:HA	1:B:880:ARG:NE	2.34	0.42
1:B:2768:LYS:O	1:B:2771:TYR:HB3	2.19	0.42
1:B:3261:ALA:C	1:B:3263:MET:H	2.26	0.42
1:B:3823:GLU:OE1	1:B:3826:GLY:N	2.41	0.42
1:C:28:ILE:HD11	1:C:201:LEU:HD21	2.00	0.42
1:C:937:LEU:HG	1:C:941:LYS:HE2	2.01	0.42
1:C:2409:ILE:HD13	1:C:2420:ARG:NH1	2.34	0.42
1:D:12:GLN:HG3	1:D:177:VAL:HG11	2.01	0.42
1:D:877:HIS:HA	1:D:880:ARG:NE	2.34	0.42
1:D:1444:GLY:HA3	1:D:1487:MET:HA	2.01	0.42
1:D:1608:VAL:HA	1:D:1618:LEU:O	2.19	0.42
1:D:1914:CYS:O	1:D:1918:VAL:HG23	2.19	0.42
1:D:2155:PHE:HA	1:D:2162:MET:HE3	2.01	0.42
1:D:2247:VAL:HG11	1:D:2257:LEU:HD12	2.00	0.42
1:D:2768:LYS:O	1:D:2771:TYR:HB3	2.19	0.42
1:D:2884:LYS:O	1:D:2887:GLU:HG3	2.18	0.42
1:D:2999:LYS:O	1:D:3002:GLU:HG3	2.19	0.42
1:D:3183:ILE:CG1	1:D:3187:LYS:HE2	2.49	0.42
1:D:4070:ALA:HB1	1:D:4078:LEU:HD13	2.01	0.42
1:A:896:ASN:O	1:A:899:GLU:HG3	2.19	0.42
1:A:1256:PRO:HG3	1:A:1593:HIS:NE2	2.34	0.42
1:A:1608:VAL:HA	1:A:1618:LEU:O	2.19	0.42
1:A:2549:LEU:HD13	1:A:2573:LEU:HD11	1.99	0.42
1:A:2914:THR:N	1:A:2915:PRO:HD2	2.34	0.42
1:A:2988:ARG:N	1:A:2989:PRO:HD3	2.34	0.42
1:A:3183:ILE:CG1	1:A:3187:LYS:HE2	2.49	0.42
1:A:4694:LEU:HD21	1:D:4264:LEU:HB3	2.02	0.42
2:E:50:ARG:HH21	2:E:53:LYS:HG2	1.83	0.42
1:B:2409:ILE:HD13	1:B:2420:ARG:NH1	2.34	0.42
1:B:2719:TYR:CE2	1:B:2799:ALA:HB2	2.38	0.42
1:B:2999:LYS:O	1:B:3002:GLU:HG3	2.19	0.42
1:B:3134:LEU:HD12	1:B:3162:PHE:CE2	2.54	0.42
1:B:3697:LYS:HD3	1:B:3700:HIS:NE2	2.34	0.42
1:B:4617:ILE:HD13	1:B:4666:ILE:HD12	2.01	0.42
1:C:579:LEU:HD13	1:C:617:LEU:HG	2.00	0.42
1:C:722:LEU:HD23	1:C:722:LEU:HA	1.91	0.42
1:C:1942:PHE:O	1:C:1946:GLU:HG2	2.20	0.42
1:C:2622:CYS:HA	1:C:2677:PRO:HG3	2.00	0.42
1:C:2726:GLU:OE1	1:C:2726:GLU:N	2.51	0.42
1:C:2918:GLU:HG3	1:C:2923:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2988:ARG:N	1:C:2989:PRO:HD3	2.34	0.42
1:C:3320:LEU:HB2	1:C:3321:PRO:HD3	2.00	0.42
1:C:3793:LEU:HD23	1:C:3793:LEU:HA	1.89	0.42
1:D:608:HIS:HB2	1:D:1656:HIS:ND1	2.34	0.42
1:D:1283:LEU:HD11	1:D:1582:CYS:SG	2.60	0.42
1:D:1718:ARG:HD3	1:D:1831:MET:HA	2.01	0.42
1:D:2222:LEU:HA	1:D:2222:LEU:HD23	1.79	0.42
1:D:2759:PRO:HD2	1:D:2762:LEU:HD12	2.00	0.42
1:D:2944:ASP:O	1:D:2947:SER:OG	2.35	0.42
1:D:3298:ARG:O	1:D:3301:VAL:HG12	2.19	0.42
1:D:4014:LEU:HD13	1:D:4122:ALA:HB2	2.00	0.42
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.87	0.42
1:A:877:HIS:HA	1:A:880:ARG:NE	2.34	0.42
1:A:1161:VAL:HG21	1:A:1225:LYS:HE2	2.01	0.42
1:A:1718:ARG:HD3	1:A:1831:MET:HA	2.01	0.42
1:A:2268:TYR:HB3	1:A:2298:TYR:CZ	2.55	0.42
1:A:2682:GLU:HG3	1:A:2919:LYS:HD3	2.01	0.42
1:A:3069:GLU:OE2	1:A:3069:GLU:N	2.51	0.42
1:A:3697:LYS:HA	1:A:3700:HIS:NE2	2.34	0.42
1:B:2918:GLU:HG3	1:B:2923:TYR:CD1	2.54	0.42
1:B:2988:ARG:N	1:B:2989:PRO:HD3	2.34	0.42
1:C:1283:LEU:HD11	1:C:1582:CYS:SG	2.60	0.42
1:C:2971:ILE:HG23	1:C:2975:PHE:HE2	1.83	0.42
1:C:3131:TYR:HE1	1:C:3166:PHE:HZ	1.66	0.42
1:C:3699:CYS:SG	1:C:3731:LEU:HD12	2.60	0.42
1:C:4030:ASP:OD2	1:C:4031:THR:N	2.52	0.42
1:D:1256:PRO:HG3	1:D:1593:HIS:NE2	2.34	0.42
1:D:2726:GLU:OE1	1:D:2726:GLU:N	2.51	0.42
1:D:2775:ILE:H	1:D:2775:ILE:HD12	1.84	0.42
1:D:3697:LYS:HD3	1:D:3700:HIS:NE2	2.34	0.42
1:D:4266:LYS:HB2	1:D:4266:LYS:HE2	1.83	0.42
1:A:267:VAL:HG22	1:A:273:SER:HB3	2.02	0.42
1:A:281:ARG:NH1	1:A:345:GLU:HB3	2.34	0.42
1:A:608:HIS:HB2	1:A:1656:HIS:ND1	2.34	0.42
1:A:3697:LYS:HD3	1:A:3700:HIS:NE2	2.34	0.42
1:A:4030:ASP:OD2	1:A:4031:THR:N	2.52	0.42
2:G:50:ARG:HH21	2:G:53:LYS:HG2	1.83	0.42
1:B:848:ARG:HD3	1:B:1599:MET:HE1	2.01	0.42
1:B:1283:LEU:HD11	1:B:1582:CYS:SG	2.60	0.42
1:B:1892:GLY:H	1:B:1895:GLN:NE2	2.16	0.42
1:B:1967:SER:O	1:B:3605:MET:HE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2775:ILE:H	1:B:2775:ILE:HD12	1.84	0.42
1:B:3054:LYS:O	1:B:3057:LEU:HD23	2.19	0.42
1:B:3183:ILE:CG1	1:B:3187:LYS:HE2	2.49	0.42
1:B:4015:LYS:HE2	1:B:4015:LYS:HB3	1.88	0.42
1:C:12:GLN:HG3	1:C:177:VAL:HG11	2.01	0.42
1:C:281:ARG:NH1	1:C:345:GLU:HB3	2.34	0.42
1:C:848:ARG:HD3	1:C:1599:MET:HE1	2.01	0.42
1:C:871:GLN:OE1	1:C:871:GLN:N	2.50	0.42
1:C:881:ILE:HG21	1:C:1062:TYR:CE2	2.54	0.42
1:C:1608:VAL:HA	1:C:1618:LEU:O	2.19	0.42
1:C:2549:LEU:HD13	1:C:2573:LEU:HD11	2.00	0.42
1:C:2581:ARG:HB3	1:C:2584:MET:SD	2.59	0.42
1:C:2841:ALA:HA	1:C:2844:MET:HG3	2.02	0.42
1:C:3697:LYS:HD3	1:C:3700:HIS:NE2	2.34	0.42
1:C:3889:TYR:HB2	1:C:3954:MET:HE2	2.01	0.42
1:D:281:ARG:NH1	1:D:345:GLU:HB3	2.34	0.42
1:D:579:LEU:HD13	1:D:617:LEU:HG	2.00	0.42
1:D:631:LEU:O	1:D:635:ASN:ND2	2.53	0.42
1:D:1967:SER:O	1:D:3605:MET:HE1	2.19	0.42
1:D:3697:LYS:HA	1:D:3700:HIS:NE2	2.34	0.42
1:D:3699:CYS:SG	1:D:3731:LEU:HD12	2.59	0.42
1:D:4040:LYS:HE3	1:D:4040:LYS:HB2	1.83	0.42
1:A:496:ASN:O	1:A:500:GLU:OE1	2.38	0.42
1:A:937:LEU:HG	1:A:941:LYS:HE2	2.01	0.42
1:A:2929:LEU:O	1:A:2933:VAL:HG23	2.20	0.42
1:B:732:LEU:HD23	1:B:732:LEU:HA	1.87	0.42
1:B:881:ILE:HG21	1:B:1062:TYR:CE2	2.54	0.42
1:B:1256:PRO:HG3	1:B:1593:HIS:NE2	2.34	0.42
1:B:1937:GLN:HG2	1:B:3609:TYR:HA	2.02	0.42
1:B:2187:ILE:HD11	1:B:2193:VAL:HG21	2.01	0.42
1:B:3227:ARG:NH2	1:B:3295:TRP:HZ2	2.18	0.42
1:B:3298:ARG:O	1:B:3301:VAL:HG12	2.19	0.42
1:B:3699:CYS:SG	1:B:3731:LEU:HD12	2.59	0.42
1:B:4031:THR:HA	1:B:4034:GLU:HG3	2.01	0.42
1:C:896:ASN:O	1:C:899:GLU:HG3	2.19	0.42
1:C:2775:ILE:H	1:C:2775:ILE:HD12	1.84	0.42
1:C:2998:ASN:ND2	1:C:3048:THR:HG1	2.16	0.42
1:C:3697:LYS:HA	1:C:3700:HIS:NE2	2.34	0.42
1:C:4031:THR:HA	1:C:4034:GLU:HG3	2.01	0.42
1:D:1729:MET:SD	1:D:1930:ASP:HB2	2.60	0.42
1:D:1937:GLN:HG2	1:D:3609:TYR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2858:MET:O	1:D:2861:GLU:HG3	2.20	0.42
1:D:3054:LYS:O	1:D:3057:LEU:HD23	2.19	0.42
1:D:3641:ILE:HD11	1:D:3694:ILE:HG22	2.02	0.42
1:D:3783:GLU:OE2	1:D:3784:LYS:HG2	2.20	0.42
1:A:1283:LEU:HD11	1:A:1582:CYS:SG	2.60	0.42
1:A:1931:ASP:OD1	1:A:1932:PHE:N	2.52	0.42
1:A:1937:GLN:HG2	1:A:3609:TYR:HA	2.02	0.42
1:A:2581:ARG:HB3	1:A:2584:MET:SD	2.59	0.42
1:A:2638:LEU:HB3	1:A:2680:TYR:CE1	2.54	0.42
1:A:3101:LEU:HA	1:A:3104:MET:HE2	2.00	0.42
1:A:3783:GLU:OE2	1:A:3784:LYS:HG2	2.20	0.42
1:B:39:ALA:O	1:B:123:HIS:HE1	2.03	0.42
1:B:1179:GLY:HA3	1:B:1229:ILE:HD11	2.02	0.42
1:B:3293:GLY:O	1:B:3296:MET:HG2	2.20	0.42
1:B:3641:ILE:HD11	1:B:3694:ILE:HG22	2.02	0.42
1:B:3697:LYS:HA	1:B:3700:HIS:NE2	2.34	0.42
1:B:4710:LEU:HD23	1:B:4710:LEU:HA	1.90	0.42
1:B:4867:ILE:HG12	1:C:4864:GLY:HA2	2.01	0.42
1:C:608:HIS:HB2	1:C:1656:HIS:ND1	2.34	0.42
1:C:1967:SER:O	1:C:3605:MET:HE1	2.19	0.42
1:C:2146:LEU:HD23	1:C:2146:LEU:HA	1.83	0.42
1:C:2268:TYR:HB3	1:C:2298:TYR:CZ	2.55	0.42
1:C:2999:LYS:O	1:C:3002:GLU:HG3	2.19	0.42
1:C:3134:LEU:HB2	1:C:3162:PHE:HE2	1.85	0.42
1:C:3293:GLY:O	1:C:3296:MET:HG2	2.20	0.42
1:D:411:GLU:OE2	1:D:485:ARG:NE	2.35	0.42
1:D:1942:PHE:O	1:D:1946:GLU:HG2	2.19	0.42
1:D:2077:ASP:O	1:D:2081:VAL:HG23	2.19	0.42
1:D:2481:GLN:O	1:D:2485:LEU:HD23	2.19	0.42
1:D:4925:LEU:HD12	1:D:4933:HIS:CE1	2.55	0.42
1:A:2841:ALA:HA	1:A:2844:MET:HG3	2.02	0.42
1:A:3102:LEU:HD21	1:A:3154:ALA:O	2.20	0.42
1:A:3298:ARG:O	1:A:3301:VAL:HG12	2.19	0.42
1:A:4031:THR:HA	1:A:4034:GLU:HG3	2.01	0.42
1:A:4484:ILE:O	1:A:4488:GLN:HG2	2.20	0.42
1:A:4818:TYR:HA	1:B:4848:ILE:HD11	2.00	0.42
2:H:75:LEU:HD22	2:H:102:VAL:HG21	2.02	0.42
1:B:267:VAL:HG22	1:B:273:SER:HB3	2.02	0.42
1:B:496:ASN:O	1:B:500:GLU:OE1	2.38	0.42
1:B:631:LEU:O	1:B:635:ASN:ND2	2.53	0.42
1:B:1161:VAL:HG21	1:B:1225:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4484:ILE:O	1:B:4488:GLN:HG2	2.20	0.42
1:C:931:TYR:CD2	4:C:5003:ATP:C2'	3.01	0.42
1:C:2187:ILE:HD11	1:C:2193:VAL:HG21	2.01	0.42
1:C:3187:LYS:HZ1	1:C:3195:LEU:HD13	1.84	0.42
1:D:2268:TYR:HB3	1:D:2298:TYR:CZ	2.54	0.42
1:D:2605:MET:HB3	1:D:2606:PRO:HD3	2.00	0.42
1:D:2642:ARG:HD2	1:D:2680:TYR:HE2	1.83	0.42
1:D:2841:ALA:HA	1:D:2844:MET:HG3	2.02	0.42
1:A:631:LEU:O	1:A:635:ASN:ND2	2.53	0.42
1:A:1729:MET:SD	1:A:1930:ASP:HB2	2.60	0.42
1:A:2895:PHE:HA	1:A:2898:ILE:HG12	2.02	0.42
1:A:2918:GLU:HG3	1:A:2923:TYR:CD1	2.54	0.42
1:A:4512:ALA:O	1:A:4516:ILE:HG13	2.20	0.42
2:H:50:ARG:HE	2:H:53:LYS:HE3	1.84	0.42
1:B:2222:LEU:HD23	1:B:2222:LEU:HA	1.79	0.42
1:B:2605:MET:HB3	1:B:2606:PRO:HD3	2.00	0.42
1:B:2841:ALA:HA	1:B:2844:MET:HG3	2.02	0.42
1:C:732:LEU:HD23	1:C:732:LEU:HA	1.87	0.42
1:C:1729:MET:SD	1:C:1930:ASP:HB2	2.60	0.42
1:C:1937:GLN:HG2	1:C:3609:TYR:HA	2.02	0.42
1:C:1972:GLN:OE1	1:C:3608:LEU:HG	2.19	0.42
1:C:2481:GLN:O	1:C:2485:LEU:HD23	2.19	0.42
1:C:2858:MET:O	1:C:2861:GLU:HG3	2.20	0.42
1:C:3102:LEU:HD21	1:C:3154:ALA:O	2.20	0.42
1:C:3212:GLU:HG2	1:C:3213:LYS:N	2.35	0.42
1:C:3783:GLU:OE2	1:C:3784:LYS:HG2	2.20	0.42
1:D:2828:MET:HE1	1:D:2891:ASP:O	2.20	0.42
1:D:4030:ASP:OD2	1:D:4031:THR:N	2.52	0.42
1:D:4484:ILE:O	1:D:4488:GLN:HG2	2.20	0.42
1:A:881:ILE:HD11	1:A:1060:TYR:CE2	2.55	0.42
1:A:1991:GLU:HG2	1:A:1992:ILE:N	2.35	0.42
1:A:2525:LEU:HD21	1:A:2569:ILE:HA	2.02	0.42
1:A:3187:LYS:HD2	1:A:3192:ARG:HD2	2.02	0.42
1:A:3641:ILE:HD11	1:A:3694:ILE:HG22	2.02	0.42
1:A:4795:LYS:HD2	1:A:4795:LYS:HA	1.80	0.42
2:E:36:LYS:HB3	2:E:36:LYS:HE3	1.81	0.42
2:E:58:LYS:O	2:E:61:GLU:HB3	2.20	0.42
2:H:50:ARG:HH21	2:H:53:LYS:HG2	1.83	0.42
2:H:58:LYS:O	2:H:61:GLU:HB3	2.20	0.42
1:B:1914:CYS:O	1:B:1918:VAL:HG23	2.19	0.42
1:B:2858:MET:O	1:B:2861:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2967:VAL:O	1:B:2971:ILE:HG13	2.19	0.42
1:B:3212:GLU:HG2	1:B:3213:LYS:N	2.35	0.42
1:B:3783:GLU:OE2	1:B:3784:LYS:HG2	2.20	0.42
1:C:23:GLN:NE2	1:C:215:ALA:HB2	2.35	0.42
1:C:881:ILE:HD11	1:C:1060:TYR:CE2	2.55	0.42
1:C:1256:PRO:HG3	1:C:1593:HIS:NE2	2.34	0.42
1:C:1914:CYS:HB3	1:C:2090:ARG:NH2	2.35	0.42
1:C:2914:THR:N	1:C:2915:PRO:HD2	2.34	0.42
1:C:3183:ILE:CG1	1:C:3187:LYS:HE2	2.49	0.42
1:C:3298:ARG:O	1:C:3301:VAL:HG12	2.19	0.42
1:C:4925:LEU:HD12	1:C:4933:HIS:CE1	2.55	0.42
1:D:1161:VAL:HG21	1:D:1225:LYS:HE2	2.01	0.42
1:D:1179:GLY:HA3	1:D:1229:ILE:HD11	2.02	0.42
1:D:2682:GLU:HG3	1:D:2919:LYS:HD3	2.00	0.42
1:D:2914:THR:N	1:D:2915:PRO:HD2	2.34	0.42
1:D:3183:ILE:HG13	1:D:3187:LYS:HE2	2.02	0.42
1:D:3293:GLY:O	1:D:3296:MET:HG2	2.20	0.42
1:A:911:ASN:OD1	1:A:912:LYS:N	2.53	0.42
1:A:3134:LEU:HD12	1:A:3162:PHE:CE2	2.54	0.42
1:A:3699:CYS:SG	1:A:3731:LEU:HD12	2.59	0.42
1:A:3942:ASP:O	1:A:3945:VAL:HG12	2.20	0.42
2:E:26:HIS:CD2	2:E:46:PRO:HA	2.55	0.42
2:E:50:ARG:HE	2:E:53:LYS:HE3	1.85	0.42
2:F:58:LYS:O	2:F:61:GLU:HB3	2.20	0.42
1:B:608:HIS:HB2	1:B:1656:HIS:ND1	2.34	0.42
1:B:895:MET:O	1:B:898:ILE:HG22	2.20	0.42
1:B:1500:ARG:HD2	1:B:1505:LEU:HB2	2.02	0.42
1:B:2087:LEU:O	1:B:2091:GLN:HG2	2.19	0.42
1:B:2268:TYR:HB3	1:B:2298:TYR:CZ	2.54	0.42
1:C:39:ALA:O	1:C:123:HIS:HE1	2.03	0.42
1:C:655:MET:SD	1:C:836:HIS:HA	2.59	0.42
1:C:2929:LEU:O	1:C:2933:VAL:HG23	2.20	0.42
1:C:3227:ARG:NH2	1:C:3295:TRP:HZ2	2.18	0.42
1:C:3641:ILE:HD11	1:C:3694:ILE:HG22	2.02	0.42
1:C:4832:GLU:HG2	1:C:4833:ASP:H	1.85	0.42
1:D:267:VAL:HG22	1:D:273:SER:HB3	2.02	0.42
1:D:881:ILE:HD11	1:D:1060:TYR:CE2	2.55	0.42
1:D:1004:HIS:CD2	1:D:1038:LEU:HD11	2.55	0.42
1:D:3131:TYR:HE1	1:D:3166:PHE:HZ	1.66	0.42
1:D:3213:LYS:O	1:D:3216:GLU:HG3	2.20	0.42
1:A:877:HIS:HA	1:A:880:ARG:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:GLY:O	1:A:1140:PHE:HB2	2.20	0.41
1:A:1914:CYS:HB3	1:A:2090:ARG:NH2	2.35	0.41
2:E:75:LEU:HD22	2:E:102:VAL:HG21	2.02	0.41
2:H:89:PRO:HB2	1:D:1671:ARG:HH22	1.85	0.41
1:B:804:LEU:HD13	1:B:832:LEU:HD21	2.02	0.41
1:B:1240:ALA:HB2	1:B:1247:ILE:HD11	2.02	0.41
1:B:1942:PHE:O	1:B:1946:GLU:HG2	2.20	0.41
1:B:2525:LEU:HD21	1:B:2569:ILE:HA	2.02	0.41
1:C:962:LYS:NZ	1:C:982:ASP:OD1	2.36	0.41
1:C:1991:GLU:HG2	1:C:1992:ILE:N	2.35	0.41
1:C:2525:LEU:HD21	1:C:2569:ILE:HA	2.02	0.41
1:C:2828:MET:HE1	1:C:2891:ASP:O	2.20	0.41
1:C:3187:LYS:HD2	1:C:3192:ARG:HD2	2.02	0.41
1:C:3942:ASP:O	1:C:3945:VAL:HG12	2.20	0.41
1:D:263:GLU:OE1	1:D:272:ARG:NH1	2.40	0.41
1:D:881:ILE:HG21	1:D:1062:TYR:CE2	2.54	0.41
1:D:1991:GLU:HG2	1:D:1992:ILE:N	2.35	0.41
1:D:2186:GLU:HG3	1:D:2187:ILE:HG22	2.03	0.41
1:D:2200:LEU:HD23	1:D:2200:LEU:HA	1.84	0.41
1:D:2895:PHE:HA	1:D:2898:ILE:HG12	2.02	0.41
1:D:2918:GLU:HG3	1:D:2923:TYR:CD1	2.54	0.41
1:D:2959:GLU:OE1	1:D:2959:GLU:N	2.53	0.41
1:D:3227:ARG:NH2	1:D:3295:TRP:HZ2	2.17	0.41
1:A:513:HIS:O	1:A:517:VAL:HG23	2.20	0.41
1:A:890:HIS:HB3	1:A:929:ARG:HH12	1.86	0.41
1:A:904:TYR:OH	1:A:923:LYS:NZ	2.53	0.41
1:A:1004:HIS:CD2	1:A:1038:LEU:HD11	2.55	0.41
1:A:2333:PRO:HA	1:A:2336:ARG:NE	2.33	0.41
1:A:2775:ILE:HD12	1:A:2775:ILE:H	1.84	0.41
1:A:4817:MET:HE3	1:A:4817:MET:HB3	1.91	0.41
1:B:878:LEU:HD13	1:B:944:LEU:HD11	2.02	0.41
1:B:1991:GLU:HG2	1:B:1992:ILE:N	2.35	0.41
1:B:2481:GLN:O	1:B:2485:LEU:HD23	2.19	0.41
1:B:2934:ASP:HB2	1:B:3010:LYS:HZ1	1.85	0.41
1:B:3123:LEU:HB3	1:B:3124:GLU:H	1.72	0.41
1:B:3942:ASP:O	1:B:3945:VAL:HG12	2.20	0.41
1:B:4832:GLU:HG2	1:B:4833:ASP:H	1.86	0.41
1:C:411:GLU:OE2	1:C:485:ARG:NE	2.35	0.41
1:C:877:HIS:HA	1:C:880:ARG:CD	2.50	0.41
1:C:1240:ALA:HB2	1:C:1247:ILE:HD11	2.03	0.41
1:C:2333:PRO:HA	1:C:2336:ARG:NE	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2385:GLY:O	1:C:2389:MET:HG3	2.21	0.41
1:C:2480:VAL:HG12	1:C:2483:PHE:H	1.85	0.41
1:C:2645:PHE:CD2	1:C:2921:PHE:HZ	2.38	0.41
1:C:2852:TRP:CH2	1:C:2856:LYS:HG3	2.55	0.41
1:C:3001:LYS:HD2	1:C:3041:ASP:HB3	2.02	0.41
1:C:3134:LEU:HD12	1:C:3162:PHE:CE2	2.54	0.41
1:C:3172:GLU:OE2	1:C:3175:LEU:HG	2.20	0.41
1:C:3213:LYS:O	1:C:3216:GLU:HG3	2.20	0.41
1:D:804:LEU:HD13	1:D:832:LEU:HD21	2.02	0.41
1:D:937:LEU:HG	1:D:941:LYS:HE2	2.01	0.41
1:D:1972:GLN:OE1	1:D:3608:LEU:HG	2.19	0.41
1:D:2645:PHE:CD2	1:D:2921:PHE:HZ	2.38	0.41
1:D:3134:LEU:HB2	1:D:3162:PHE:HE2	1.85	0.41
1:A:248:PRO:C	1:A:272:ARG:HH21	2.28	0.41
1:A:411:GLU:OE2	1:A:485:ARG:NE	2.35	0.41
1:A:1477:HIS:CE1	1:A:1478:GLU:HG2	2.56	0.41
1:A:2481:GLN:O	1:A:2485:LEU:HD23	2.19	0.41
1:A:2607:LEU:CD1	1:A:2664:LEU:HG	2.47	0.41
1:A:2726:GLU:OE1	1:A:2726:GLU:N	2.51	0.41
1:A:2858:MET:O	1:A:2861:GLU:HG3	2.20	0.41
1:A:3035:ILE:O	1:A:3039:THR:HG23	2.21	0.41
1:B:881:ILE:HD11	1:B:1060:TYR:CE2	2.55	0.41
1:B:2895:PHE:HA	1:B:2898:ILE:HG12	2.02	0.41
1:B:3102:LEU:HD21	1:B:3154:ALA:O	2.20	0.41
1:C:878:LEU:HD13	1:C:944:LEU:HD11	2.02	0.41
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.86	0.41
1:C:3183:ILE:HG13	1:C:3187:LYS:HE2	2.02	0.41
1:C:3227:ARG:CZ	1:C:3291:ASP:HB3	2.51	0.41
1:C:4070:ALA:HB1	1:C:4078:LEU:HD13	2.01	0.41
1:D:911:ASN:OD1	1:D:912:LYS:N	2.54	0.41
1:D:1477:HIS:CE1	1:D:1478:GLU:HG2	2.55	0.41
1:D:1500:ARG:HD2	1:D:1505:LEU:HB2	2.02	0.41
1:D:2333:PRO:HA	1:D:2336:ARG:NE	2.33	0.41
1:D:4031:THR:HA	1:D:4034:GLU:HG3	2.01	0.41
1:A:23:GLN:NE2	1:A:215:ALA:HB2	2.35	0.41
1:A:39:ALA:O	1:A:123:HIS:HE1	2.03	0.41
1:A:2172:MET:HE2	1:A:2172:MET:HB2	1.97	0.41
1:A:3861:GLN:HB3	1:A:3864:ASN:HD22	1.86	0.41
1:A:3889:TYR:HB2	1:A:3954:MET:HE2	2.01	0.41
2:H:26:HIS:CD2	2:H:46:PRO:HA	2.56	0.41
2:H:51:ILE:C	2:H:53:LYS:HZ1	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:HIS:HA	1:B:880:ARG:CD	2.50	0.41
1:B:2929:LEU:O	1:B:2933:VAL:HG23	2.20	0.41
1:B:3227:ARG:CZ	1:B:3291:ASP:HB3	2.51	0.41
1:C:911:ASN:OD1	1:C:912:LYS:N	2.53	0.41
1:C:2186:GLU:HG3	1:C:2187:ILE:HG22	2.03	0.41
1:C:2868:HIS:HB3	1:C:2871:LEU:HB2	2.03	0.41
1:D:496:ASN:O	1:D:500:GLU:OE1	2.38	0.41
1:D:2525:LEU:HD21	1:D:2569:ILE:HA	2.02	0.41
1:D:2659:GLN:O	1:D:2663:LYS:HG2	2.21	0.41
1:D:2852:TRP:CH2	1:D:2856:LYS:HG3	2.55	0.41
1:D:3889:TYR:HB2	1:D:3954:MET:HE2	2.01	0.41
1:D:4512:ALA:O	1:D:4516:ILE:HG13	2.20	0.41
1:A:989:THR:HG22	1:A:991:SER:H	1.85	0.41
1:A:1942:PHE:O	1:A:1946:GLU:HG2	2.20	0.41
1:A:2243:ALA:O	1:A:2247:VAL:HG22	2.20	0.41
1:A:3293:GLY:O	1:A:3296:MET:HG2	2.20	0.41
1:A:4925:LEU:HD12	1:A:4933:HIS:CE1	2.55	0.41
2:F:26:HIS:CD2	2:F:46:PRO:HA	2.55	0.41
2:F:89:PRO:HB2	1:B:1671:ARG:HH22	1.85	0.41
1:B:248:PRO:C	1:B:272:ARG:HH21	2.28	0.41
1:B:456:LEU:O	1:B:460:ILE:HG12	2.21	0.41
1:B:1477:HIS:CE1	1:B:1478:GLU:HG2	2.56	0.41
1:B:1494:MET:HE2	1:B:1497:GLY:HA2	2.02	0.41
1:B:2186:GLU:HG3	1:B:2187:ILE:HG22	2.03	0.41
1:B:2243:ALA:O	1:B:2247:VAL:HG22	2.20	0.41
1:B:2645:PHE:CD2	1:B:2921:PHE:HZ	2.38	0.41
1:B:2752:LYS:HD3	1:B:2752:LYS:HA	1.92	0.41
1:B:3046:MET:HE1	1:B:3057:LEU:HD21	2.02	0.41
1:B:3142:THR:HA	1:B:3233:HIS:HB3	2.02	0.41
1:B:3172:GLU:OE2	1:B:3175:LEU:HG	2.20	0.41
1:B:3889:TYR:HB2	1:B:3954:MET:HE2	2.01	0.41
1:B:4070:ALA:HB1	1:B:4078:LEU:HD13	2.01	0.41
1:B:4832:GLU:N	1:B:4843:ARG:HH22	2.19	0.41
1:B:4925:LEU:HD12	1:B:4933:HIS:CE1	2.55	0.41
1:C:267:VAL:HG22	1:C:273:SER:HB3	2.02	0.41
1:C:631:LEU:O	1:C:635:ASN:ND2	2.53	0.41
1:C:670:TYR:CE2	1:C:672:LYS:HB2	2.56	0.41
1:C:804:LEU:HD13	1:C:832:LEU:HD21	2.02	0.41
1:C:1016:TRP:HZ3	1:C:1022:GLN:HE22	1.69	0.41
1:C:1748:LEU:HB2	1:C:1751:ILE:HD13	2.03	0.41
1:C:1914:CYS:O	1:C:1918:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2243:ALA:O	1:C:2247:VAL:HG22	2.20	0.41
1:C:2659:GLN:O	1:C:2663:LYS:HG2	2.21	0.41
1:C:3843:LEU:HD23	1:C:3846:LEU:HD12	2.03	0.41
1:D:513:HIS:O	1:D:517:VAL:HG23	2.20	0.41
1:D:670:TYR:CE2	1:D:672:LYS:HB2	2.56	0.41
1:D:895:MET:O	1:D:898:ILE:HG22	2.20	0.41
1:D:1016:TRP:HZ3	1:D:1022:GLN:HE22	1.69	0.41
1:D:1111:GLY:O	1:D:1140:PHE:HB2	2.20	0.41
1:D:1748:LEU:HB2	1:D:1751:ILE:HD13	2.03	0.41
1:D:2243:ALA:O	1:D:2247:VAL:HG22	2.20	0.41
1:A:670:TYR:CE2	1:A:672:LYS:HB2	2.56	0.41
1:A:4649:VAL:O	1:A:4653:VAL:HG23	2.21	0.41
2:G:75:LEU:HD22	2:G:102:VAL:HG21	2.02	0.41
1:B:1111:GLY:O	1:B:1140:PHE:HB2	2.20	0.41
1:B:2385:GLY:O	1:B:2389:MET:HG3	2.21	0.41
1:B:2659:GLN:O	1:B:2663:LYS:HG2	2.20	0.41
1:B:2845:ALA:HB1	1:B:2885:ASP:OD1	2.21	0.41
1:B:2852:TRP:CH2	1:B:2856:LYS:HG3	2.55	0.41
1:B:3213:LYS:O	1:B:3216:GLU:HG3	2.20	0.41
1:B:3292:GLU:HB3	1:B:3293:GLY:H	1.70	0.41
1:B:3843:LEU:HD23	1:B:3846:LEU:HD12	2.03	0.41
1:B:4512:ALA:O	1:B:4516:ILE:HG13	2.20	0.41
1:B:4859:LEU:O	1:B:4863:GLN:HG2	2.21	0.41
1:C:895:MET:O	1:C:898:ILE:HG22	2.20	0.41
1:C:1304:LEU:HD23	1:C:1304:LEU:HA	1.91	0.41
1:C:2895:PHE:HA	1:C:2898:ILE:HG12	2.02	0.41
1:D:39:ALA:O	1:D:123:HIS:HE1	2.03	0.41
1:D:1054:VAL:O	1:D:1057:LEU:HG	2.21	0.41
1:D:2868:HIS:HB3	1:D:2871:LEU:HB2	2.03	0.41
1:D:3840:PHE:CE1	1:D:3874:THR:HG23	2.56	0.41
1:D:4832:GLU:N	1:D:4843:ARG:HH22	2.19	0.41
1:A:804:LEU:HD13	1:A:832:LEU:HD21	2.02	0.41
1:A:1016:TRP:HZ3	1:A:1022:GLN:HE22	1.69	0.41
1:A:1179:GLY:HA3	1:A:1229:ILE:HD11	2.02	0.41
1:A:1288:LYS:H	1:A:1288:LYS:HG3	1.72	0.41
1:A:2186:GLU:HG3	1:A:2187:ILE:HG22	2.03	0.41
1:A:3142:THR:HA	1:A:3233:HIS:HB3	2.02	0.41
1:A:3840:PHE:CE1	1:A:3874:THR:HG23	2.56	0.41
1:A:4832:GLU:HG2	1:A:4833:ASP:H	1.86	0.41
2:E:51:ILE:C	2:E:53:LYS:HZ1	2.15	0.41
1:B:513:HIS:O	1:B:517:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1729:MET:SD	1:B:1930:ASP:HB2	2.60	0.41
1:B:2828:MET:HE1	1:B:2891:ASP:O	2.20	0.41
1:B:3148:VAL:O	1:B:3152:ARG:HB3	2.21	0.41
1:B:3166:PHE:CD1	1:B:3167:PRO:HD2	2.56	0.41
1:C:890:HIS:HB3	1:C:929:ARG:HH12	1.86	0.41
1:C:904:TYR:OH	1:C:923:LYS:NZ	2.53	0.41
1:C:1958:THR:O	1:C:1962:THR:HG22	2.21	0.41
1:C:2175:MET:HE2	1:C:2175:MET:HB3	1.88	0.41
1:C:3035:ILE:O	1:C:3039:THR:HG23	2.21	0.41
1:C:3166:PHE:CD1	1:C:3167:PRO:HD2	2.56	0.41
1:D:330:THR:HG23	1:D:366:VAL:HG22	2.03	0.41
1:D:871:GLN:OE1	1:D:871:GLN:N	2.50	0.41
1:D:917:CYS:HA	1:D:924:LEU:HG	2.02	0.41
1:D:1421:MET:O	1:D:1576:LYS:NZ	2.51	0.41
1:D:1494:MET:HE2	1:D:1497:GLY:HA2	2.02	0.41
1:D:1958:THR:O	1:D:1962:THR:HG22	2.21	0.41
1:D:2736:LYS:HB3	1:D:2741:TRP:CB	2.51	0.41
1:D:3046:MET:HE1	1:D:3057:LEU:HD21	2.02	0.41
1:D:3102:LEU:HD21	1:D:3154:ALA:O	2.20	0.41
1:D:4575:LEU:HD23	1:D:4575:LEU:HA	1.96	0.41
1:A:456:LEU:O	1:A:460:ILE:HG12	2.21	0.41
1:A:2852:TRP:CH2	1:A:2856:LYS:HG3	2.56	0.41
1:A:3172:GLU:OE2	1:A:3175:LEU:HG	2.20	0.41
1:A:3183:ILE:HG13	1:A:3187:LYS:HE2	2.02	0.41
1:A:3213:LYS:O	1:A:3216:GLU:HG3	2.20	0.41
1:A:3906:PHE:HB3	1:A:3967:LEU:HD11	2.03	0.41
1:A:4806:CYS:HA	1:A:4812:CYS:HB2	2.03	0.41
1:A:4832:GLU:N	1:A:4843:ARG:HH22	2.19	0.41
2:F:3:VAL:HG13	2:F:5:ILE:HD11	2.03	0.41
2:G:50:ARG:HE	2:G:53:LYS:HE3	1.84	0.41
1:B:670:TYR:CE2	1:B:672:LYS:HB2	2.56	0.41
1:B:1748:LEU:HB2	1:B:1751:ILE:HD13	2.03	0.41
1:B:2333:PRO:HA	1:B:2336:ARG:NE	2.33	0.41
1:B:4673:ASP:OD1	1:B:4673:ASP:N	2.51	0.41
1:C:137:ARG:HG3	1:C:139:SER:HB3	2.03	0.41
1:C:456:LEU:O	1:C:460:ILE:HG12	2.21	0.41
1:C:496:ASN:O	1:C:500:GLU:OE1	2.38	0.41
1:C:3148:VAL:O	1:C:3152:ARG:HB3	2.21	0.41
1:C:3901:GLN:CD	1:C:3904:ARG:HH21	2.29	0.41
1:C:3969:LYS:HB2	1:C:3969:LYS:HE2	1.76	0.41
1:D:23:GLN:NE2	1:D:215:ALA:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:PRO:C	1:D:272:ARG:HH21	2.28	0.41
1:D:2179:LEU:HD22	1:D:2227:VAL:HG11	2.03	0.41
1:D:2929:LEU:O	1:D:2933:VAL:HG23	2.20	0.41
1:D:3035:ILE:O	1:D:3039:THR:HG23	2.21	0.41
1:D:3935:LEU:HD23	1:D:3935:LEU:HA	1.88	0.41
1:A:1047:LYS:HD2	1:A:1050:LEU:HD11	2.02	0.41
1:A:1748:LEU:HB2	1:A:1751:ILE:HD13	2.03	0.41
1:A:1972:GLN:OE1	1:A:3608:LEU:HG	2.19	0.41
1:A:2645:PHE:CD2	1:A:2921:PHE:HZ	2.38	0.41
1:A:2659:GLN:O	1:A:2663:LYS:HG2	2.21	0.41
1:A:3227:ARG:CZ	1:A:3291:ASP:HB3	2.51	0.41
1:A:4569:GLU:HB3	1:A:4570:PRO:HD3	2.02	0.41
2:E:32:GLN:OE1	2:E:97:THR:HB	2.21	0.41
2:G:26:HIS:CD2	2:G:46:PRO:HA	2.56	0.41
1:B:23:GLN:NE2	1:B:215:ALA:HB2	2.35	0.41
1:B:827:LEU:HD23	1:B:827:LEU:HA	1.89	0.41
1:B:911:ASN:OD1	1:B:912:LYS:N	2.53	0.41
1:B:1046:ASN:OD1	1:B:1047:LYS:N	2.54	0.41
1:B:1502:ASN:OD1	1:B:1503:ASN:N	2.54	0.41
1:B:2071:GLN:CD	1:B:3648:GLY:HA3	2.46	0.41
1:B:2480:VAL:HG12	1:B:2483:PHE:H	1.86	0.41
1:B:2998:ASN:ND2	1:B:3048:THR:HG1	2.16	0.41
1:B:3068:LEU:HD21	1:B:3133:ILE:HG12	2.03	0.41
1:B:3208:ILE:HA	1:B:3209:PRO:HD3	1.91	0.41
1:B:4063:THR:O	1:B:4067:LEU:HD23	2.21	0.41
1:C:513:HIS:O	1:C:517:VAL:HG23	2.20	0.41
1:C:1046:ASN:OD1	1:C:1047:LYS:N	2.54	0.41
1:C:1161:VAL:HG21	1:C:1225:LYS:HE2	2.01	0.41
1:C:2071:GLN:CD	1:C:3648:GLY:HA3	2.46	0.41
1:C:2122:SER:O	1:C:2126:ILE:HG12	2.21	0.41
1:C:2619:LYS:HZ1	1:C:2627:TRP:CD1	2.37	0.41
1:C:2845:ALA:HB1	1:C:2885:ASP:OD1	2.21	0.41
1:C:2886:ARG:O	1:C:2890:GLN:OE1	2.39	0.41
1:C:2957:GLU:HB2	1:C:2961:LYS:HZ1	1.86	0.41
1:C:3046:MET:HE1	1:C:3057:LEU:HD21	2.02	0.41
1:C:3227:ARG:NH2	1:C:3287:ASN:HB2	2.36	0.41
1:C:3858:LEU:HD23	1:C:3858:LEU:HA	1.96	0.41
1:C:3920:LEU:O	1:C:3924:ILE:HG12	2.21	0.41
1:C:4063:THR:O	1:C:4067:LEU:HD23	2.21	0.41
1:C:4484:ILE:O	1:C:4488:GLN:HG2	2.20	0.41
1:C:4512:ALA:O	1:C:4516:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4832:GLU:N	1:C:4843:ARG:HH22	2.19	0.41
1:C:4859:LEU:O	1:C:4863:GLN:HG2	2.21	0.41
1:D:281:ARG:NE	1:D:283:ALA:O	2.41	0.41
1:D:467:ASP:OD1	1:D:469:HIS:ND1	2.51	0.41
1:D:877:HIS:HA	1:D:880:ARG:CD	2.50	0.41
1:D:890:HIS:HB3	1:D:929:ARG:HH12	1.86	0.41
1:D:893:TRP:CD2	4:D:5003:ATP:N6	2.89	0.41
1:D:946:LEU:HB2	1:D:998:LYS:HZ3	1.85	0.41
1:D:989:THR:HG22	1:D:991:SER:H	1.85	0.41
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.86	0.41
1:D:2071:GLN:CD	1:D:3648:GLY:HA3	2.46	0.41
1:D:2480:VAL:HG12	1:D:2483:PHE:H	1.86	0.41
1:D:2934:ASP:HB2	1:D:3010:LYS:HZ1	1.86	0.41
1:D:3001:LYS:HD2	1:D:3041:ASP:HB3	2.02	0.41
1:D:3134:LEU:HD12	1:D:3162:PHE:CE2	2.54	0.41
1:D:3187:LYS:HD2	1:D:3192:ARG:HD2	2.02	0.41
1:D:3192:ARG:NH2	1:D:3197:LEU:HD23	2.26	0.41
1:D:3227:ARG:CZ	1:D:3291:ASP:HB3	2.51	0.41
1:D:3227:ARG:NH2	1:D:3287:ASN:HB2	2.36	0.41
1:D:3906:PHE:HB3	1:D:3967:LEU:HD11	2.03	0.41
1:A:372:LEU:HA	1:A:393:MET:HG2	2.03	0.41
1:A:895:MET:O	1:A:898:ILE:HG22	2.20	0.41
1:A:1240:ALA:HB2	1:A:1247:ILE:HD11	2.02	0.41
1:A:1300:MET:HE3	1:A:1300:MET:HB3	1.87	0.41
1:A:1732:GLU:HB2	1:A:1753:LEU:HD21	2.03	0.41
1:A:2179:LEU:HD22	1:A:2227:VAL:HG11	2.03	0.41
1:A:2347:MET:O	1:A:2351:ILE:HG12	2.21	0.41
1:A:2480:VAL:HG12	1:A:2483:PHE:H	1.85	0.41
1:A:2886:ARG:O	1:A:2890:GLN:OE1	2.39	0.41
1:A:3200:ASN:O	1:A:3204:VAL:HG23	2.21	0.41
1:A:3920:LEU:O	1:A:3924:ILE:HG12	2.21	0.41
2:H:25:VAL:HG12	2:H:104:LEU:HA	2.04	0.41
1:B:1088:PHE:HB2	1:B:1205:CYS:SG	2.61	0.41
1:B:1914:CYS:HB3	1:B:2090:ARG:NH2	2.35	0.41
1:B:2796:ASP:OD1	1:B:2797:SER:N	2.54	0.41
1:B:3187:LYS:HD2	1:B:3192:ARG:HD2	2.02	0.41
1:C:248:PRO:C	1:C:272:ARG:HH21	2.28	0.41
1:C:2200:LEU:HD23	1:C:2200:LEU:HA	1.84	0.41
1:C:2489:GLU:OE1	1:C:2544:LEU:HD13	2.21	0.41
1:C:2736:LYS:HB3	1:C:2741:TRP:CB	2.51	0.41
1:C:2796:ASP:OD1	1:C:2797:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3068:LEU:HD21	1:C:3133:ILE:HG12	2.03	0.41
1:D:137:ARG:HG3	1:D:139:SER:HB3	2.03	0.41
1:D:1240:ALA:HB2	1:D:1247:ILE:HD11	2.03	0.41
1:D:1502:ASN:OD1	1:D:1503:ASN:N	2.54	0.41
1:D:2122:SER:O	1:D:2126:ILE:HG12	2.21	0.41
1:D:2347:MET:O	1:D:2351:ILE:HG12	2.21	0.41
1:D:2886:ARG:O	1:D:2890:GLN:OE1	2.39	0.41
1:A:62:LEU:O	1:A:66:THR:HG23	2.21	0.40
1:A:137:ARG:HG3	1:A:139:SER:HB3	2.03	0.40
1:A:907:VAL:HG13	1:A:909:ASP:HB2	2.04	0.40
1:A:917:CYS:HA	1:A:924:LEU:HG	2.02	0.40
1:A:1088:PHE:HB2	1:A:1205:CYS:SG	2.61	0.40
1:A:1829:LEU:HD12	1:A:1829:LEU:HA	1.95	0.40
1:A:3843:LEU:HD23	1:A:3846:LEU:HD12	2.03	0.40
1:A:4484:ILE:HG13	1:A:4485:ILE:N	2.37	0.40
1:B:871:GLN:OE1	1:B:871:GLN:N	2.50	0.40
1:B:989:THR:HG22	1:B:991:SER:H	1.85	0.40
1:B:2179:LEU:HD22	1:B:2227:VAL:HG11	2.03	0.40
1:B:2556:SER:HA	1:B:2569:ILE:HD12	2.04	0.40
1:B:2868:HIS:HB3	1:B:2871:LEU:HB2	2.03	0.40
1:B:3035:ILE:O	1:B:3039:THR:HG23	2.21	0.40
1:B:3840:PHE:CE1	1:B:3874:THR:HG23	2.56	0.40
1:B:3846:LEU:O	1:B:3854:PHE:HD2	2.04	0.40
1:C:989:THR:HG22	1:C:991:SER:H	1.85	0.40
1:C:2347:MET:O	1:C:2351:ILE:HG12	2.21	0.40
1:C:3861:GLN:HB3	1:C:3864:ASN:HD22	1.86	0.40
1:C:4079:ASP:HB3	1:C:4082:GLU:CG	2.52	0.40
1:C:4831:ILE:CG1	1:C:4843:ARG:HH21	2.34	0.40
1:D:456:LEU:O	1:D:460:ILE:HG12	2.21	0.40
1:D:816:PRO:HB2	1:D:819:TYR:CD2	2.56	0.40
1:D:3172:GLU:OE2	1:D:3175:LEU:HG	2.20	0.40
1:D:3728:GLN:HG2	1:D:3765:ILE:HA	2.03	0.40
1:D:3920:LEU:O	1:D:3924:ILE:HG12	2.21	0.40
1:D:4735:ASN:HB3	1:D:4738:PHE:HD2	1.86	0.40
1:A:241:MET:HE1	1:A:404:SER:HB2	2.04	0.40
1:A:630:HIS:CE1	1:A:1671:ARG:HD3	2.57	0.40
1:A:816:PRO:HB2	1:A:819:TYR:CD2	2.56	0.40
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.86	0.40
1:A:1929:SER:OG	1:A:3617:VAL:HG13	2.22	0.40
1:A:2489:GLU:OE1	1:A:2544:LEU:HD13	2.21	0.40
1:A:2556:SER:HA	1:A:2569:ILE:HD12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2828:MET:HE1	1:A:2891:ASP:O	2.20	0.40
1:A:3134:LEU:HB2	1:A:3162:PHE:HE2	1.85	0.40
2:F:75:LEU:HD22	2:F:102:VAL:HG21	2.02	0.40
2:H:32:GLN:OE1	2:H:97:THR:HB	2.21	0.40
1:B:630:HIS:CE1	1:B:1671:ARG:HD3	2.57	0.40
1:B:890:HIS:HB3	1:B:929:ARG:HH12	1.86	0.40
1:B:917:CYS:HA	1:B:924:LEU:HG	2.02	0.40
1:B:1960:ARG:O	1:B:1963:LYS:HG2	2.21	0.40
1:B:2200:LEU:HD23	1:B:2200:LEU:HA	1.84	0.40
1:B:2486:HIS:O	1:B:2490:VAL:HG22	2.22	0.40
1:B:2914:THR:N	1:B:2915:PRO:HD2	2.34	0.40
1:B:4828:GLY:HA2	1:B:4831:ILE:HG12	2.04	0.40
1:C:274:LEU:HD23	1:C:274:LEU:HA	1.83	0.40
1:C:282:VAL:O	1:C:285:SER:OG	2.39	0.40
1:C:1088:PHE:HB2	1:C:1205:CYS:SG	2.61	0.40
1:C:1477:HIS:CE1	1:C:1478:GLU:HG2	2.56	0.40
1:C:2431:ASP:O	1:C:2435:VAL:HG23	2.21	0.40
1:C:2486:HIS:O	1:C:2490:VAL:HG22	2.22	0.40
1:C:3026:ALA:HA	1:C:3029:ILE:HD13	2.04	0.40
1:C:4484:ILE:HG13	1:C:4485:ILE:N	2.37	0.40
1:D:62:LEU:O	1:D:66:THR:HG23	2.22	0.40
1:D:521:GLU:HG2	1:D:522:ALA:N	2.36	0.40
1:D:878:LEU:HD13	1:D:944:LEU:HD11	2.02	0.40
1:D:907:VAL:HG13	1:D:909:ASP:HB2	2.04	0.40
1:D:1108:VAL:HB	1:D:1212:VAL:HB	2.03	0.40
1:D:1283:LEU:HB2	1:D:1555:PHE:HB2	2.04	0.40
1:D:3843:LEU:HD23	1:D:3846:LEU:HD12	2.03	0.40
1:D:3861:GLN:HB3	1:D:3864:ASN:HD22	1.86	0.40
1:D:3942:ASP:O	1:D:3945:VAL:HG12	2.20	0.40
1:D:4702:ASP:O	1:D:4706:GLN:HG2	2.21	0.40
1:D:4831:ILE:CG1	1:D:4843:ARG:HH21	2.34	0.40
1:A:330:THR:HG23	1:A:366:VAL:HG22	2.03	0.40
1:A:1046:ASN:OD1	1:A:1047:LYS:N	2.54	0.40
1:A:1500:ARG:HD2	1:A:1505:LEU:HB2	2.02	0.40
1:A:2071:GLN:CD	1:A:3648:GLY:HA3	2.46	0.40
1:A:2796:ASP:OD1	1:A:2797:SER:N	2.54	0.40
1:A:2959:GLU:OE1	1:A:2959:GLU:N	2.53	0.40
1:A:3001:LYS:HD2	1:A:3041:ASP:HB3	2.02	0.40
1:A:4055:HIS:HB3	1:A:4057:HIS:CE1	2.57	0.40
2:E:104:LEU:HD21	2:E:107:LEU:HD21	2.03	0.40
1:B:137:ARG:HG3	1:B:139:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:HIS:O	1:B:241:MET:HE2	2.22	0.40
1:B:816:PRO:HB2	1:B:819:TYR:CD2	2.56	0.40
1:B:946:LEU:HB2	1:B:998:LYS:HZ3	1.85	0.40
1:B:1004:HIS:CD2	1:B:1038:LEU:HD11	2.55	0.40
1:B:1011:ARG:HB3	1:B:1016:TRP:HB2	2.04	0.40
1:B:1016:TRP:HZ3	1:B:1022:GLN:HE22	1.69	0.40
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.86	0.40
1:B:1108:VAL:HB	1:B:1212:VAL:HB	2.03	0.40
1:B:3001:LYS:HD2	1:B:3041:ASP:HB3	2.02	0.40
1:B:3183:ILE:HG13	1:B:3187:LYS:HE2	2.02	0.40
1:B:3200:ASN:O	1:B:3204:VAL:HG23	2.21	0.40
1:C:1004:HIS:CD2	1:C:1038:LEU:HD11	2.55	0.40
1:C:1011:ARG:HH21	1:C:1014:GLN:CD	2.30	0.40
1:C:1111:GLY:O	1:C:1140:PHE:HB2	2.20	0.40
1:C:4569:GLU:HB3	1:C:4570:PRO:HD3	2.02	0.40
1:C:4702:ASP:O	1:C:4706:GLN:HG2	2.22	0.40
1:D:904:TYR:OH	1:D:923:LYS:NZ	2.53	0.40
1:D:2127:ARG:O	1:D:2130:LEU:HB2	2.21	0.40
1:D:2658:GLU:O	1:D:2662:PHE:HD1	2.04	0.40
1:D:3026:ALA:HA	1:D:3029:ILE:HD13	2.04	0.40
1:D:3208:ILE:HA	1:D:3209:PRO:HD3	1.91	0.40
1:D:4063:THR:O	1:D:4067:LEU:HD23	2.21	0.40
1:D:4806:CYS:HA	1:D:4812:CYS:HB2	2.03	0.40
1:A:1011:ARG:HB3	1:A:1016:TRP:HB2	2.04	0.40
1:A:1494:MET:HE2	1:A:1497:GLY:HA2	2.02	0.40
1:A:1829:LEU:HG	1:A:1912:TYR:CE2	2.57	0.40
1:A:2658:GLU:O	1:A:2662:PHE:HD1	2.04	0.40
1:A:2736:LYS:HB3	1:A:2741:TRP:CB	2.51	0.40
1:A:3046:MET:HE1	1:A:3057:LEU:HD21	2.02	0.40
1:A:3123:LEU:HB3	1:A:3124:GLU:H	1.72	0.40
1:A:4693:SER:O	1:A:4697:VAL:HG23	2.22	0.40
2:E:25:VAL:HG12	2:E:104:LEU:HA	2.04	0.40
2:G:25:VAL:HG12	2:G:104:LEU:HA	2.03	0.40
2:G:58:LYS:O	2:G:61:GLU:HB3	2.20	0.40
1:B:2070:ALA:HA	1:B:2075:ILE:HD11	2.03	0.40
1:B:2658:GLU:O	1:B:2662:PHE:HD1	2.04	0.40
1:B:2736:LYS:HB3	1:B:2741:TRP:CB	2.51	0.40
1:B:2886:ARG:O	1:B:2890:GLN:OE1	2.39	0.40
1:B:3026:ALA:HA	1:B:3029:ILE:HD13	2.03	0.40
1:B:3728:GLN:HG2	1:B:3765:ILE:HA	2.03	0.40
1:B:4649:VAL:O	1:B:4653:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1732:GLU:HB2	1:C:1753:LEU:HD21	2.03	0.40
1:C:2179:LEU:HD22	1:C:2227:VAL:HG11	2.03	0.40
1:C:3200:ASN:O	1:C:3204:VAL:HG23	2.21	0.40
1:C:3840:PHE:CE1	1:C:3874:THR:HG23	2.56	0.40
1:C:3846:LEU:O	1:C:3854:PHE:HD2	2.05	0.40
1:C:3935:LEU:HA	1:C:3935:LEU:HD23	1.88	0.40
1:D:966:LEU:HD23	1:D:966:LEU:HA	1.98	0.40
1:D:1011:ARG:HB3	1:D:1016:TRP:HB2	2.04	0.40
1:D:1113:MET:HB2	1:D:1156:TRP:CZ2	2.57	0.40
1:D:1960:ARG:O	1:D:1963:LYS:HG2	2.22	0.40
1:D:2385:GLY:O	1:D:2389:MET:HG3	2.20	0.40
1:D:2845:ALA:HB1	1:D:2885:ASP:OD1	2.21	0.40
1:D:3142:THR:HA	1:D:3233:HIS:HB3	2.02	0.40
1:D:3200:ASN:O	1:D:3204:VAL:HG23	2.21	0.40
1:D:4194:GLU:HG2	1:D:4645:TRP:HZ3	1.86	0.40
1:A:1283:LEU:HB2	1:A:1555:PHE:HB2	2.04	0.40
1:A:1958:THR:O	1:A:1962:THR:HG22	2.21	0.40
1:A:2868:HIS:HB3	1:A:2871:LEU:HB2	2.03	0.40
1:A:3166:PHE:CD1	1:A:3167:PRO:HD2	2.56	0.40
1:A:3250:TRP:HE3	1:A:3309:LYS:HE3	1.87	0.40
1:A:4194:GLU:HG2	1:A:4645:TRP:HZ3	1.86	0.40
2:G:3:VAL:HG13	2:G:5:ILE:HD11	2.03	0.40
1:B:241:MET:HE1	1:B:404:SER:HB2	2.04	0.40
1:B:904:TYR:OH	1:B:923:LYS:NZ	2.53	0.40
1:B:2122:SER:O	1:B:2126:ILE:HG12	2.21	0.40
1:B:2489:GLU:OE1	1:B:2544:LEU:HD13	2.21	0.40
1:B:2959:GLU:OE1	1:B:2959:GLU:N	2.53	0.40
1:B:3134:LEU:HB2	1:B:3162:PHE:HE2	1.85	0.40
1:B:3250:TRP:HE3	1:B:3309:LYS:HE3	1.87	0.40
1:C:521:GLU:HG2	1:C:522:ALA:N	2.36	0.40
1:C:816:PRO:HB2	1:C:819:TYR:CD2	2.56	0.40
1:C:1500:ARG:HD2	1:C:1505:LEU:HB2	2.02	0.40
1:C:1502:ASN:OD1	1:C:1503:ASN:N	2.54	0.40
1:C:3142:THR:HA	1:C:3233:HIS:HB3	2.02	0.40
1:C:4930:GLU:HA	1:C:4933:HIS:HD2	1.84	0.40
1:D:238:HIS:O	1:D:241:MET:HE2	2.21	0.40
1:D:274:LEU:HD23	1:D:274:LEU:HA	1.83	0.40
1:D:1047:LYS:HD2	1:D:1050:LEU:HD11	2.02	0.40
1:D:1914:CYS:HB3	1:D:2090:ARG:NH2	2.35	0.40
1:D:3316:LYS:O	1:D:3317:THR:OG1	2.30	0.40
1:D:3700:HIS:HD1	1:D:3702:GLU:H	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3793:LEU:HD23	1:D:3793:LEU:HA	1.89	0.40
1:D:4767:LEU:HD23	1:D:4767:LEU:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4198/4967 (84%)	4073 (97%)	123 (3%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4075 (97%)	121 (3%)	2 (0%)	100	100
1	C	4198/4967 (84%)	4073 (97%)	123 (3%)	2 (0%)	100	100
1	D	4198/4967 (84%)	4075 (97%)	121 (3%)	2 (0%)	100	100
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17212/20300 (85%)	16700 (97%)	504 (3%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4641	PRO
1	B	4641	PRO
1	C	4641	PRO
1	D	4641	PRO
1	A	2770	ILE
1	B	2770	ILE
1	C	2770	ILE
1	D	2770	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3708/4358 (85%)	3702 (100%)	6 (0%)	87	88
1	B	3708/4358 (85%)	3702 (100%)	6 (0%)	87	88
1	C	3708/4358 (85%)	3702 (100%)	6 (0%)	87	88
1	D	3708/4358 (85%)	3702 (100%)	6 (0%)	87	88
2	E	88/89 (99%)	87 (99%)	1 (1%)	65	77
2	F	88/89 (99%)	87 (99%)	1 (1%)	65	77
2	G	88/89 (99%)	87 (99%)	1 (1%)	65	77
2	H	88/89 (99%)	87 (99%)	1 (1%)	65	77
All	All	15184/17788 (85%)	15156 (100%)	28 (0%)	85	88

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2004	MET
1	A	2192	MET
1	A	2640	LEU
1	A	3102	LEU
1	A	3140	LEU
1	A	4809	MET
2	E	53	LYS
2	F	53	LYS
2	G	53	LYS
2	H	53	LYS
1	B	2004	MET
1	B	2192	MET
1	B	2640	LEU
1	B	3102	LEU
1	B	3140	LEU
1	B	4809	MET
1	C	2004	MET
1	C	2192	MET
1	C	2640	LEU

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Mol	Chain	Res	Type
1	C	3102	LEU
1	C	3140	LEU
1	C	4809	MET
1	D	2004	MET
1	D	2192	MET
1	D	2640	LEU
1	D	3102	LEU
1	D	3140	LEU
1	D	4809	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	29	HIS
1	A	32	GLN
1	A	110	HIS
1	A	150	GLN
1	A	375	GLN
1	A	472	HIS
1	A	635	ASN
1	A	658	ASN
1	A	808	HIS
1	A	836	HIS
1	A	1021	GLN
1	A	1244	ASN
1	A	1577	ASN
1	A	1589	GLN
1	A	1656	HIS
1	A	1970	GLN
1	A	2059	GLN
1	A	2224	ASN
1	A	2250	ASN
1	A	2486	HIS
1	A	2722	ASN
1	A	2802	ASN
1	A	2998	ASN
1	A	3095	ASN
1	A	3111	HIS
1	A	3114	GLN
1	A	3115	HIS
1	A	3185	ASN

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Mol	Chain	Res	Type
1	A	3622	GLN
1	A	3722	GLN
1	A	3770	ASN
1	A	3775	GLN
1	A	3812	ASN
1	A	3831	GLN
1	A	3905	ASN
1	A	4159	GLN
1	A	4178	ASN
1	A	4638	GLN
1	A	4879	GLN
1	A	4933	HIS
1	B	23	GLN
1	B	29	HIS
1	B	32	GLN
1	B	110	HIS
1	B	150	GLN
1	B	375	GLN
1	B	472	HIS
1	B	635	ASN
1	B	650	ASN
1	B	658	ASN
1	B	808	HIS
1	B	949	HIS
1	B	1004	HIS
1	B	1021	GLN
1	B	1211	GLN
1	B	1244	ASN
1	B	1577	ASN
1	B	1589	GLN
1	B	1656	HIS
1	B	1970	GLN
1	B	2059	GLN
1	B	2250	ASN
1	B	2486	HIS
1	B	2722	ASN
1	B	2802	ASN
1	B	2998	ASN
1	B	3095	ASN
1	B	3111	HIS
1	B	3114	GLN
1	B	3115	HIS

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Mol	Chain	Res	Type
1	B	3185	ASN
1	B	3622	GLN
1	B	3722	GLN
1	B	3767	ASN
1	B	3770	ASN
1	B	3775	GLN
1	B	3812	ASN
1	B	3831	GLN
1	B	3905	ASN
1	B	4178	ASN
1	B	4251	ASN
1	B	4489	GLN
1	B	4638	GLN
1	B	4879	GLN
1	B	4933	HIS
1	C	23	GLN
1	C	29	HIS
1	C	32	GLN
1	C	110	HIS
1	C	150	GLN
1	C	375	GLN
1	C	472	HIS
1	C	635	ASN
1	C	650	ASN
1	C	658	ASN
1	C	808	HIS
1	C	836	HIS
1	C	949	HIS
1	C	1004	HIS
1	C	1244	ASN
1	C	1577	ASN
1	C	1589	GLN
1	C	1656	HIS
1	C	1970	GLN
1	C	2059	GLN
1	C	2224	ASN
1	C	2250	ASN
1	C	2486	HIS
1	C	2722	ASN
1	C	2802	ASN
1	C	2998	ASN
1	C	3095	ASN

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Mol	Chain	Res	Type
1	C	3111	HIS
1	C	3114	GLN
1	C	3115	HIS
1	C	3185	ASN
1	C	3622	GLN
1	C	3722	GLN
1	C	3767	ASN
1	C	3770	ASN
1	C	3775	GLN
1	C	3812	ASN
1	C	3831	GLN
1	C	3905	ASN
1	C	3975	GLN
1	C	4178	ASN
1	C	4251	ASN
1	C	4489	GLN
1	C	4638	GLN
1	C	4879	GLN
1	C	4933	HIS
1	D	23	GLN
1	D	29	HIS
1	D	32	GLN
1	D	110	HIS
1	D	150	GLN
1	D	375	GLN
1	D	472	HIS
1	D	650	ASN
1	D	658	ASN
1	D	808	HIS
1	D	836	HIS
1	D	949	HIS
1	D	1021	GLN
1	D	1244	ASN
1	D	1577	ASN
1	D	1589	GLN
1	D	1593	HIS
1	D	1656	HIS
1	D	1970	GLN
1	D	2059	GLN
1	D	2224	ASN
1	D	2250	ASN
1	D	2486	HIS

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Mol	Chain	Res	Type
1	D	2722	ASN
1	D	2802	ASN
1	D	2995	HIS
1	D	2998	ASN
1	D	3095	ASN
1	D	3111	HIS
1	D	3114	GLN
1	D	3115	HIS
1	D	3185	ASN
1	D	3622	GLN
1	D	3722	GLN
1	D	3767	ASN
1	D	3770	ASN
1	D	3775	GLN
1	D	3812	ASN
1	D	3831	GLN
1	D	3905	ASN
1	D	3975	GLN
1	D	4178	ASN
1	D	4489	GLN
1	D	4638	GLN
1	D	4879	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	KVR	D	5004	-	24,25,25	1.44	3 (12%)	31,34,34	1.71	3 (9%)
4	ATP	D	5003	-	32,33,33	0.26	0	48,52,52	0.32	0
5	KVR	A	5004	-	24,25,25	1.44	3 (12%)	31,34,34	1.71	4 (12%)
5	KVR	C	5004	-	24,25,25	1.44	3 (12%)	31,34,34	1.71	4 (12%)
4	ATP	B	5003	-	32,33,33	0.26	0	48,52,52	0.31	0
5	KVR	B	5004	-	24,25,25	1.43	3 (12%)	31,34,34	1.71	4 (12%)
4	ATP	C	5003	-	32,33,33	0.26	0	48,52,52	0.32	0
4	ATP	D	5002	-	32,33,33	0.28	0	48,52,52	0.32	0
4	ATP	B	5002	-	32,33,33	0.28	0	48,52,52	0.32	0
4	ATP	A	5002	-	32,33,33	0.28	0	48,52,52	0.32	0
4	ATP	C	5002	-	32,33,33	0.28	0	48,52,52	0.32	0
4	ATP	A	5003	-	32,33,33	0.26	0	48,52,52	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	KVR	D	5004	-	-	8/10/20/20	0/2/3/3
4	ATP	D	5003	-	-	9/22/38/38	0/3/3/3
5	KVR	A	5004	-	-	8/10/20/20	0/2/3/3
5	KVR	C	5004	-	-	8/10/20/20	0/2/3/3
4	ATP	B	5003	-	-	9/22/38/38	0/3/3/3
5	KVR	B	5004	-	-	8/10/20/20	0/2/3/3
4	ATP	C	5003	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	5/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	9/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5004	KVR	C06-S09	4.90	1.82	1.77
5	D	5004	KVR	C06-S09	4.90	1.82	1.77
5	A	5004	KVR	C06-S09	4.88	1.82	1.77
5	B	5004	KVR	C06-S09	4.86	1.82	1.77
5	A	5004	KVR	C13-C05	2.61	1.55	1.51
5	B	5004	KVR	C13-C05	2.59	1.55	1.51
5	C	5004	KVR	C13-C05	2.59	1.55	1.51
5	D	5004	KVR	C13-C05	2.56	1.55	1.51
5	D	5004	KVR	C13-N12	-2.31	1.45	1.47
5	A	5004	KVR	C13-N12	-2.30	1.45	1.47
5	B	5004	KVR	C13-N12	-2.30	1.45	1.47
5	C	5004	KVR	C13-N12	-2.28	1.45	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5004	KVR	C10-S09-C06	7.29	113.03	102.71
5	A	5004	KVR	C10-S09-C06	7.27	113.02	102.71
5	C	5004	KVR	C10-S09-C06	7.27	113.00	102.71
5	B	5004	KVR	C10-S09-C06	7.25	112.99	102.71
5	C	5004	KVR	C15-C14-N12	-2.91	107.20	113.15
5	D	5004	KVR	C15-C14-N12	-2.90	107.20	113.15
5	B	5004	KVR	C15-C14-N12	-2.90	107.21	113.15
5	A	5004	KVR	C15-C14-N12	-2.90	107.22	113.15
5	C	5004	KVR	C04-C05-C06	2.05	120.11	118.17
5	A	5004	KVR	C04-C05-C06	2.04	120.10	118.17
5	B	5004	KVR	O23-C21-C18	2.03	120.04	114.84
5	B	5004	KVR	C04-C05-C06	2.02	120.08	118.17
5	D	5004	KVR	O23-C21-C18	2.02	120.02	114.84
5	C	5004	KVR	O23-C21-C18	2.02	120.01	114.84
5	A	5004	KVR	O23-C21-C18	2.00	119.98	114.84

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5003	ATP	PB-O3B-PG-O2G
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	B	5003	ATP	PB-O3B-PG-O2G
4	B	5003	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	B	5003	ATP	C5'-O5'-PA-O2A
4	B	5003	ATP	C5'-O5'-PA-O3A
4	C	5003	ATP	PB-O3B-PG-O2G
4	C	5003	ATP	C5'-O5'-PA-O1A
4	C	5003	ATP	C5'-O5'-PA-O2A
4	C	5003	ATP	C5'-O5'-PA-O3A
4	D	5003	ATP	PB-O3B-PG-O2G
4	D	5003	ATP	C5'-O5'-PA-O1A
4	D	5003	ATP	C5'-O5'-PA-O2A
4	D	5003	ATP	C5'-O5'-PA-O3A
5	A	5004	KVR	C15-C14-N12-C11
5	A	5004	KVR	C15-C14-N12-C13
5	B	5004	KVR	C15-C14-N12-C11
5	B	5004	KVR	C15-C14-N12-C13
5	C	5004	KVR	C15-C14-N12-C11
5	C	5004	KVR	C15-C14-N12-C13
5	D	5004	KVR	C15-C14-N12-C11
5	D	5004	KVR	C15-C14-N12-C13
5	A	5004	KVR	C17-C18-C21-O22
5	A	5004	KVR	C19-C18-C21-O22
5	B	5004	KVR	C17-C18-C21-O22
5	B	5004	KVR	C19-C18-C21-O22
5	C	5004	KVR	C17-C18-C21-O22
5	C	5004	KVR	C19-C18-C21-O22
5	D	5004	KVR	C17-C18-C21-O22
5	D	5004	KVR	C19-C18-C21-O22
5	A	5004	KVR	C17-C18-C21-O23
5	A	5004	KVR	C19-C18-C21-O23
5	B	5004	KVR	C17-C18-C21-O23
5	B	5004	KVR	C19-C18-C21-O23
5	C	5004	KVR	C17-C18-C21-O23
5	C	5004	KVR	C19-C18-C21-O23
5	D	5004	KVR	C17-C18-C21-O23
5	D	5004	KVR	C19-C18-C21-O23
5	A	5004	KVR	C04-C03-O02-C01
5	A	5004	KVR	C08-C03-O02-C01
5	B	5004	KVR	C04-C03-O02-C01
5	B	5004	KVR	C08-C03-O02-C01
5	C	5004	KVR	C04-C03-O02-C01
5	C	5004	KVR	C08-C03-O02-C01
5	D	5004	KVR	C04-C03-O02-C01
5	D	5004	KVR	C08-C03-O02-C01

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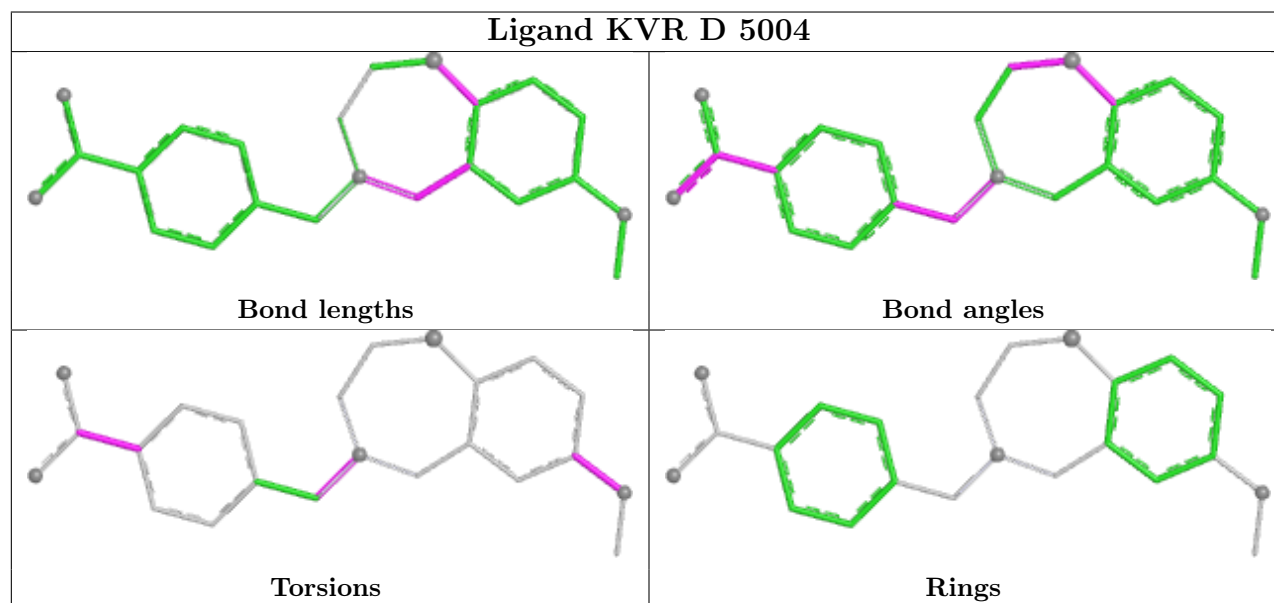
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PG-O3B-PB-O3A
4	B	5002	ATP	PG-O3B-PB-O3A
4	C	5002	ATP	PG-O3B-PB-O3A
4	D	5002	ATP	PG-O3B-PB-O3A
4	A	5002	ATP	PB-O3A-PA-O5'
4	B	5002	ATP	PB-O3A-PA-O5'
4	C	5002	ATP	PB-O3A-PA-O5'
4	D	5002	ATP	PB-O3A-PA-O5'
4	A	5003	ATP	PA-O3A-PB-O2B
4	B	5003	ATP	PA-O3A-PB-O2B
4	C	5003	ATP	PA-O3A-PB-O2B
4	D	5003	ATP	PA-O3A-PB-O2B
4	A	5002	ATP	PB-O3A-PA-O1A
4	B	5002	ATP	PB-O3A-PA-O1A
4	C	5002	ATP	PB-O3A-PA-O1A
4	D	5002	ATP	PB-O3A-PA-O1A
4	A	5002	ATP	O4'-C1'-N9-C8
4	B	5002	ATP	O4'-C1'-N9-C8
4	C	5002	ATP	O4'-C1'-N9-C8
4	D	5002	ATP	O4'-C1'-N9-C8
4	A	5003	ATP	PB-O3B-PG-O1G
4	B	5003	ATP	PB-O3B-PG-O1G
4	C	5003	ATP	PB-O3B-PG-O1G
4	D	5003	ATP	PB-O3B-PG-O1G
4	A	5002	ATP	O4'-C1'-N9-C4
4	B	5002	ATP	O4'-C1'-N9-C4
4	C	5002	ATP	O4'-C1'-N9-C4
4	D	5002	ATP	O4'-C1'-N9-C4
4	C	5003	ATP	O4'-C4'-C5'-O5'
4	A	5003	ATP	PA-O3A-PB-O1B
4	B	5003	ATP	PA-O3A-PB-O1B
4	C	5003	ATP	PA-O3A-PB-O1B
4	D	5003	ATP	PA-O3A-PB-O1B
4	A	5003	ATP	O4'-C4'-C5'-O5'
4	B	5003	ATP	O4'-C4'-C5'-O5'
4	D	5003	ATP	O4'-C4'-C5'-O5'
4	A	5003	ATP	PB-O3A-PA-O2A
4	B	5003	ATP	PB-O3A-PA-O2A
4	C	5003	ATP	PB-O3A-PA-O2A
4	D	5003	ATP	PB-O3A-PA-O2A

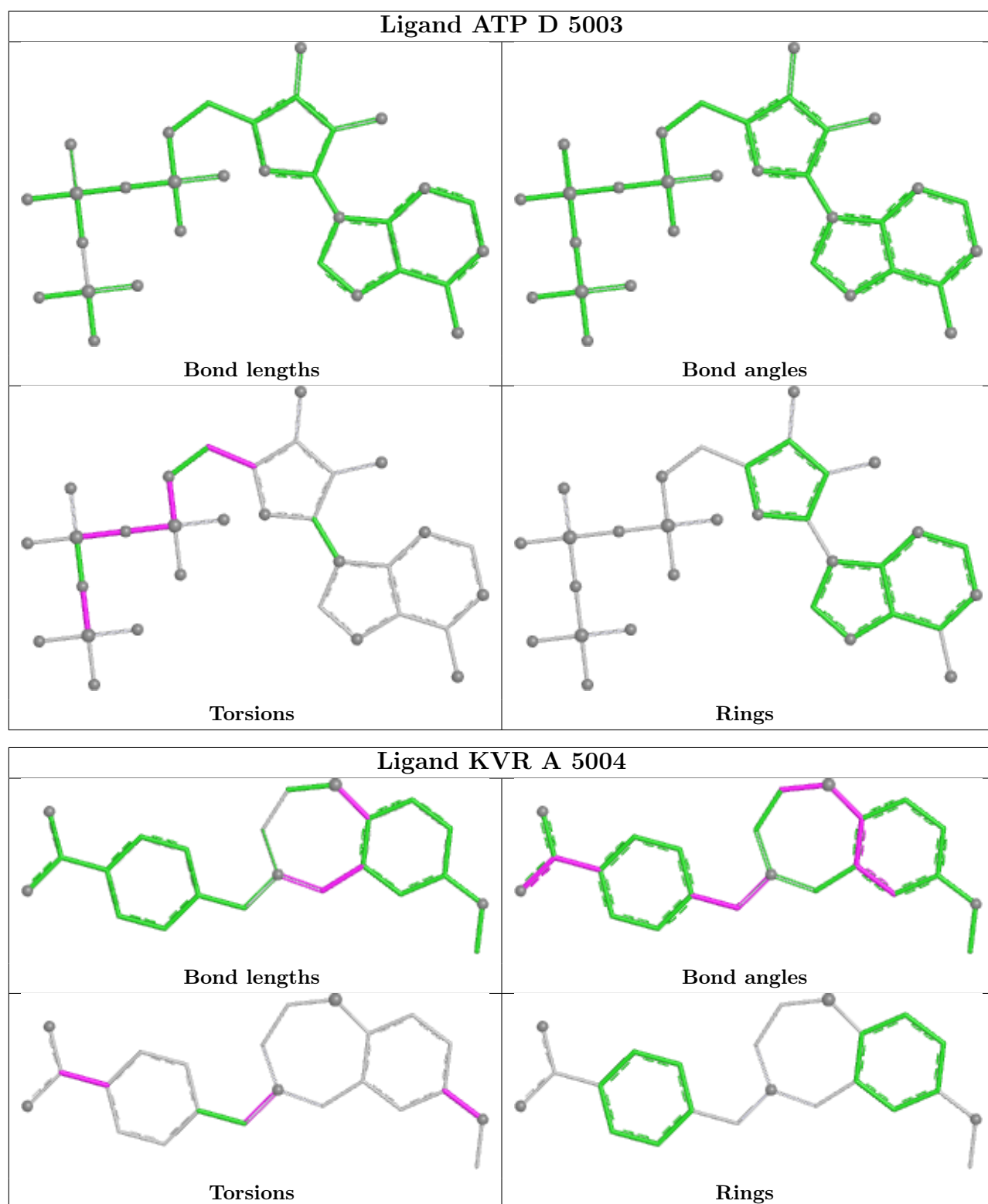
There are no ring outliers.

8 monomers are involved in 41 short contacts:

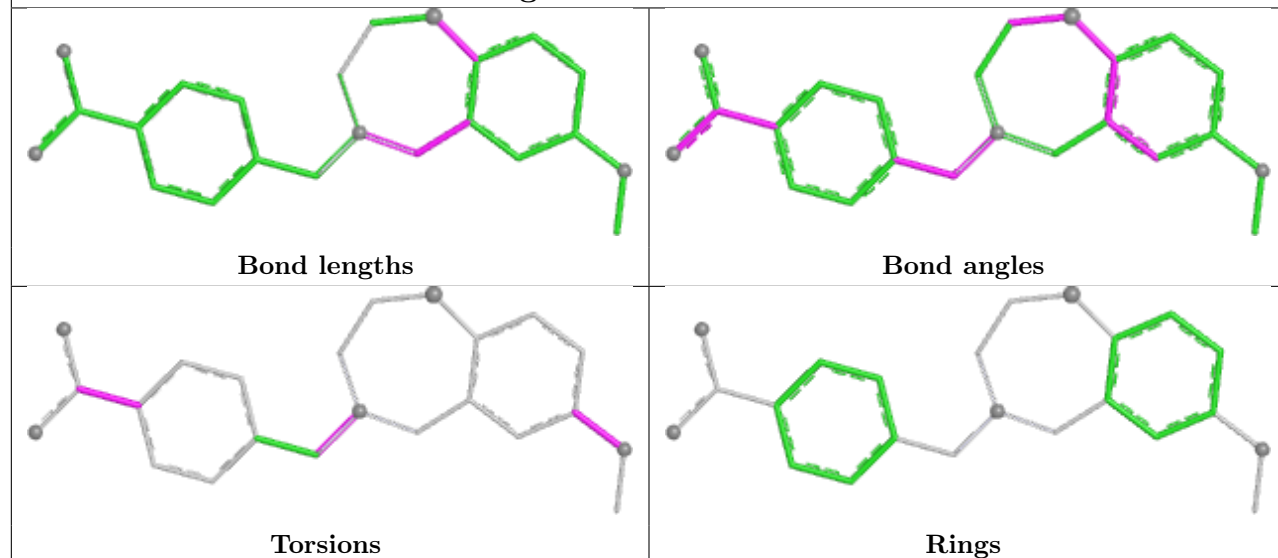
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5004	KVR	7	0
4	D	5003	ATP	10	0
5	A	5004	KVR	7	0
5	C	5004	KVR	7	0
4	B	5003	ATP	9	0
5	B	5004	KVR	7	0
4	C	5003	ATP	9	0
4	A	5003	ATP	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

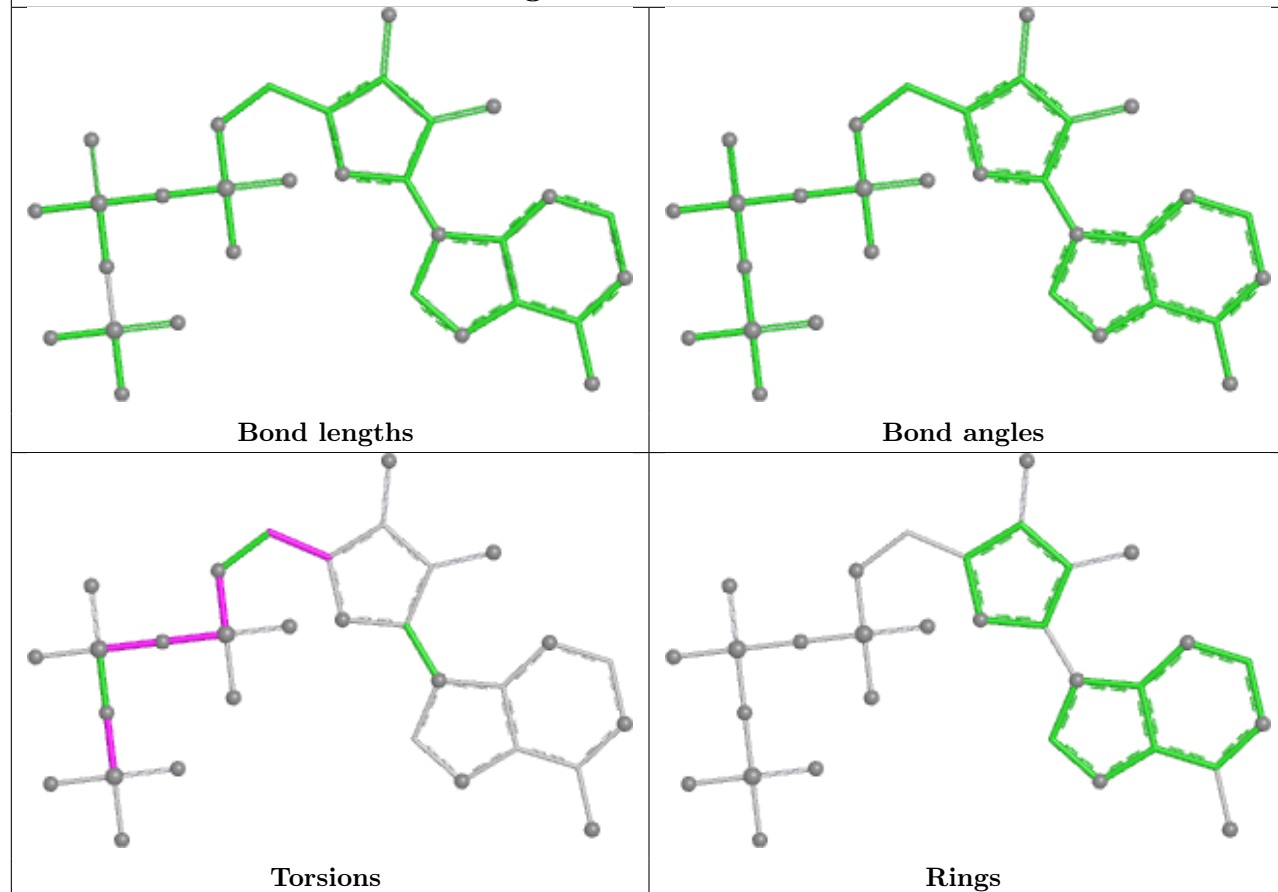




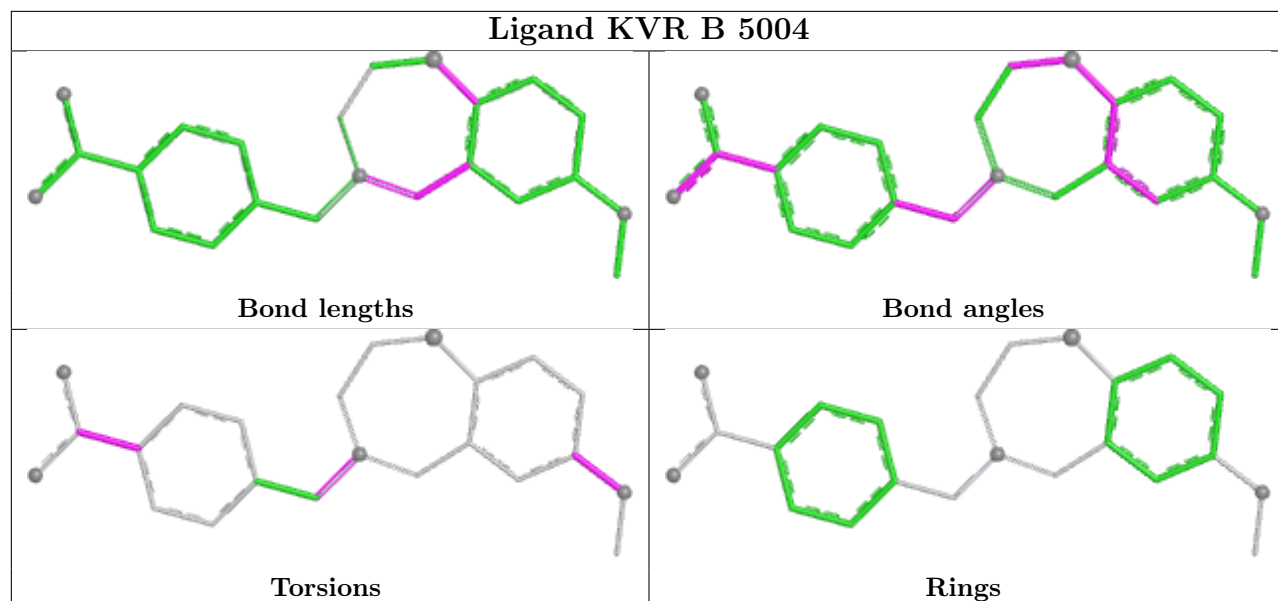
Ligand KVR C 5004



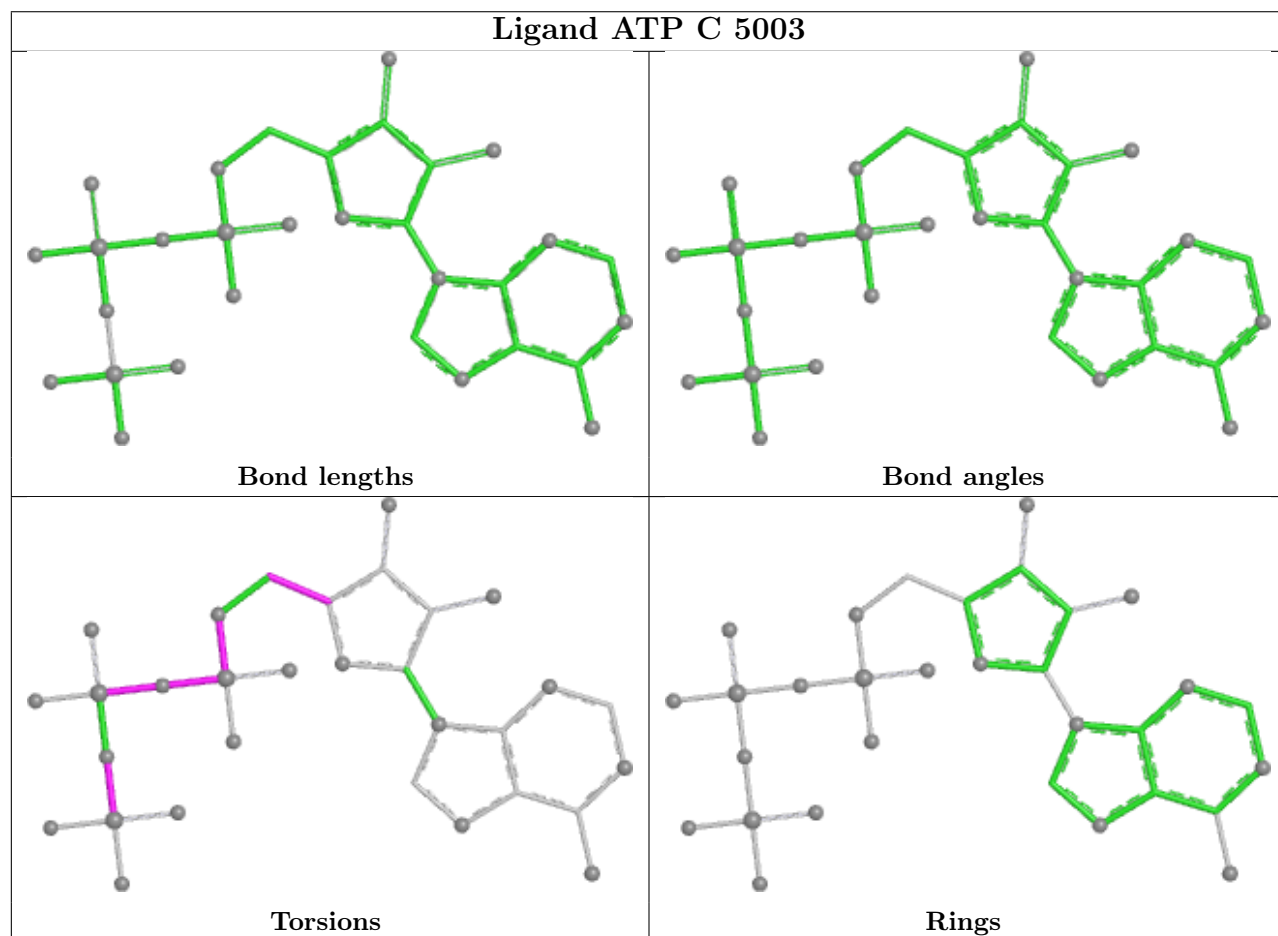
Ligand ATP B 5003

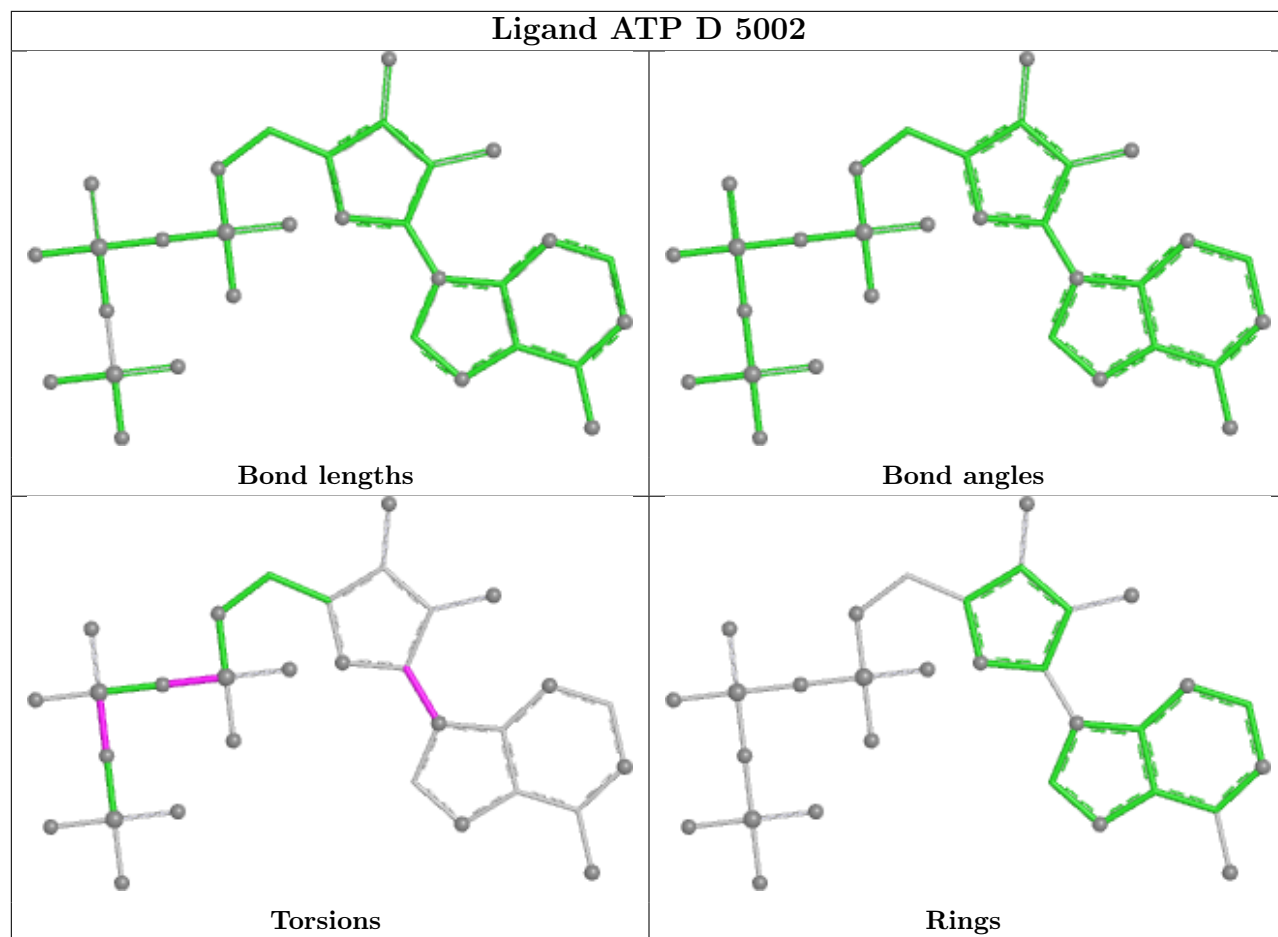


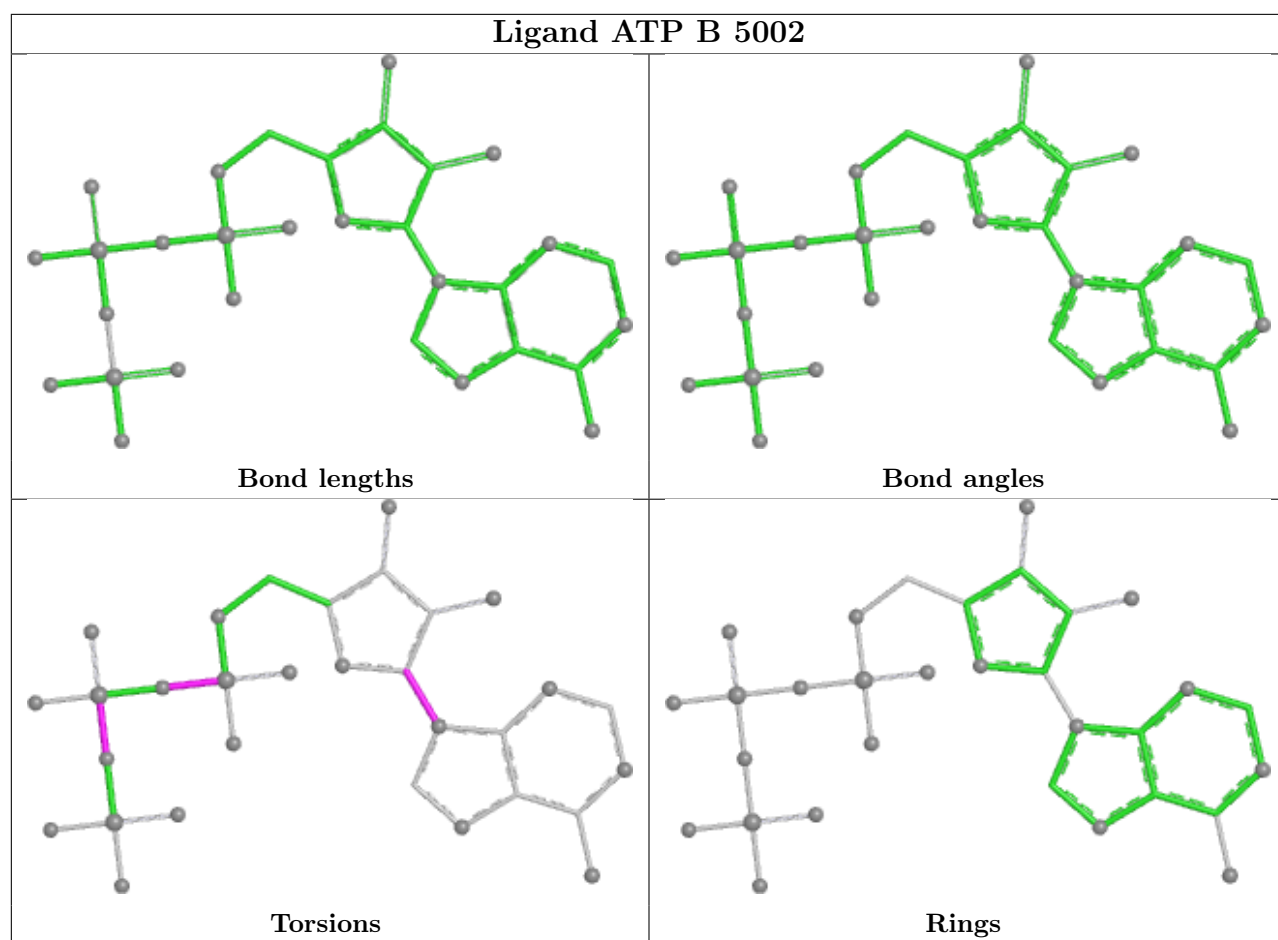
Ligand KVR B 5004

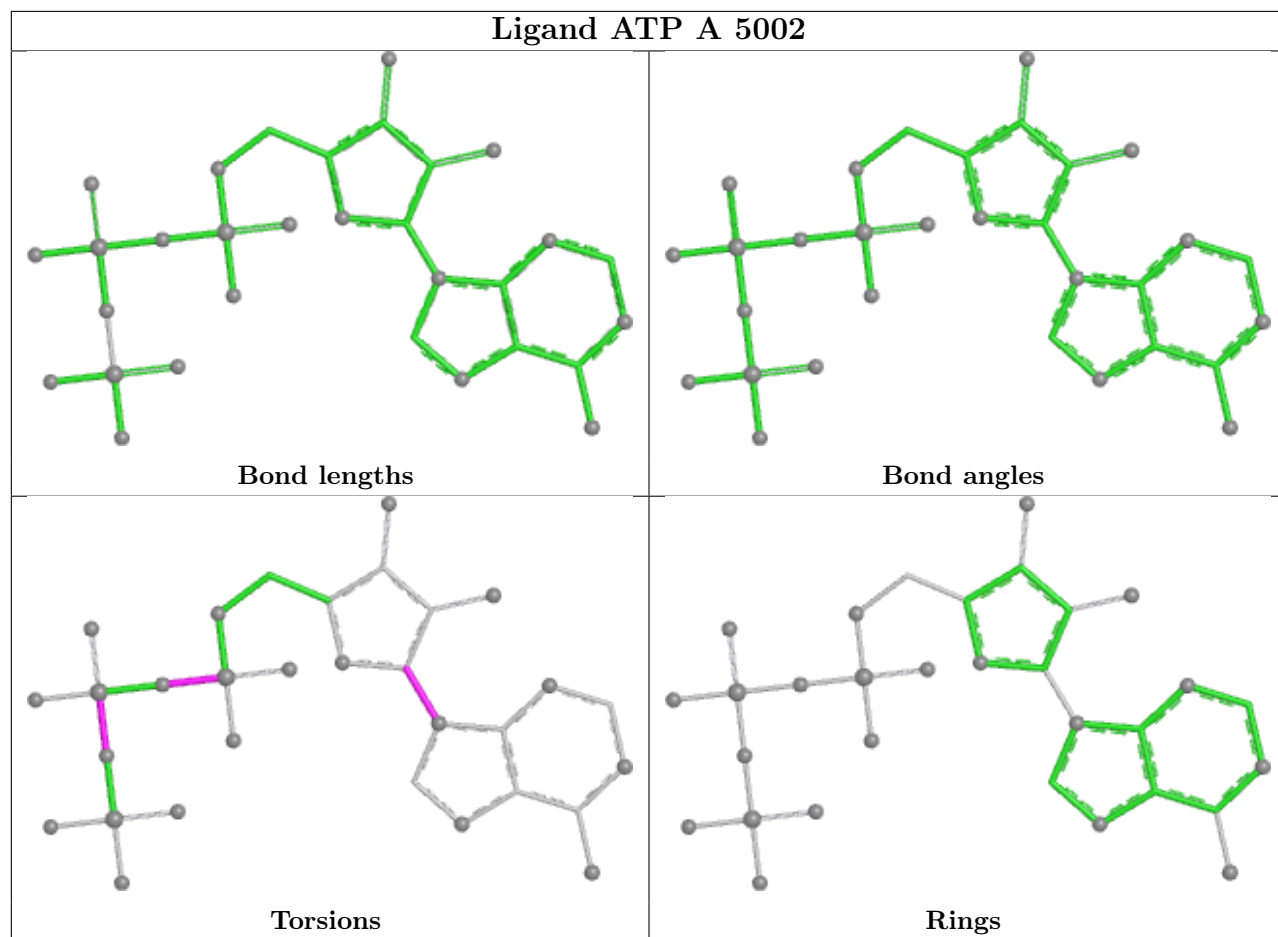


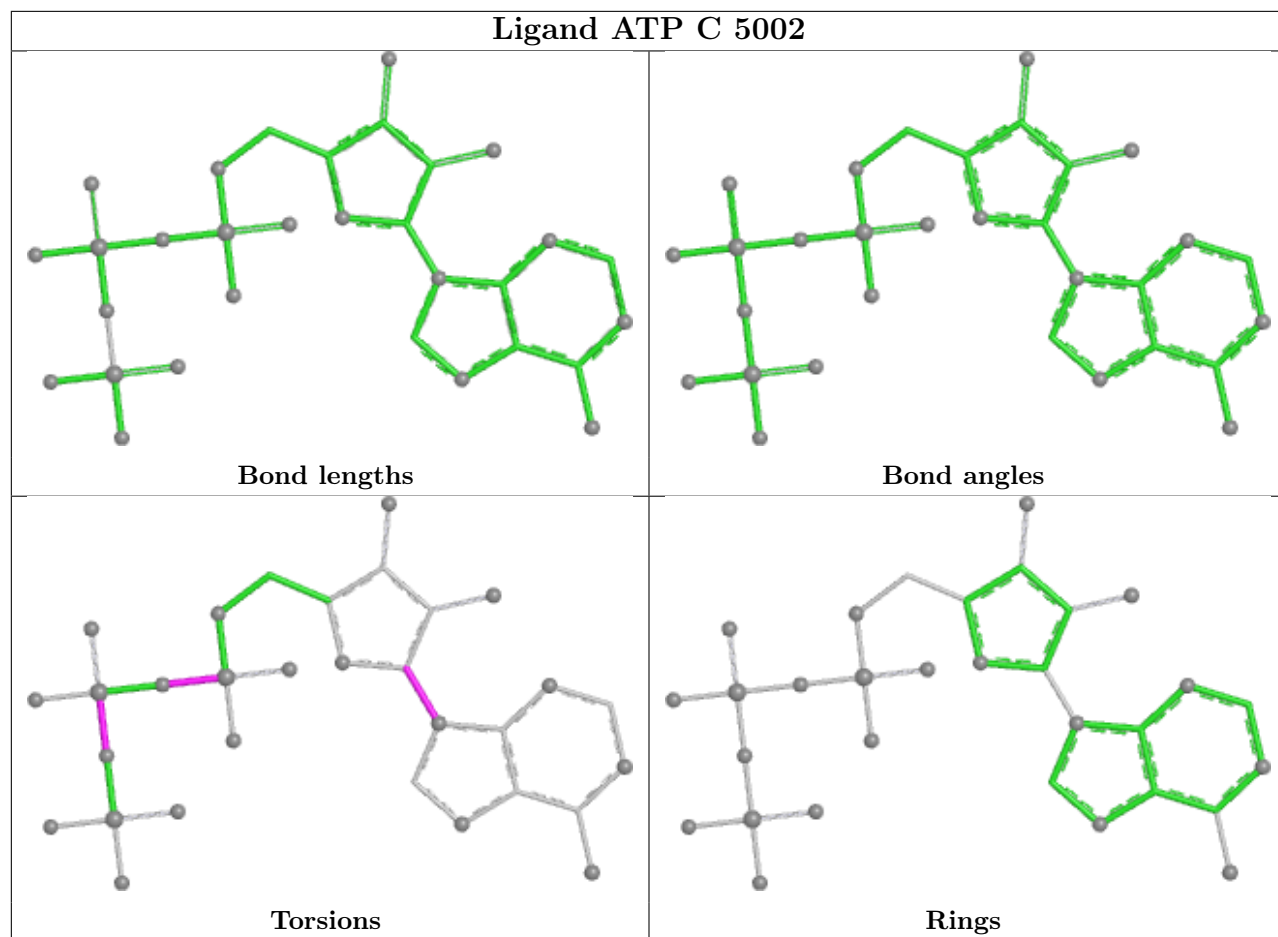
Ligand ATP C 5003

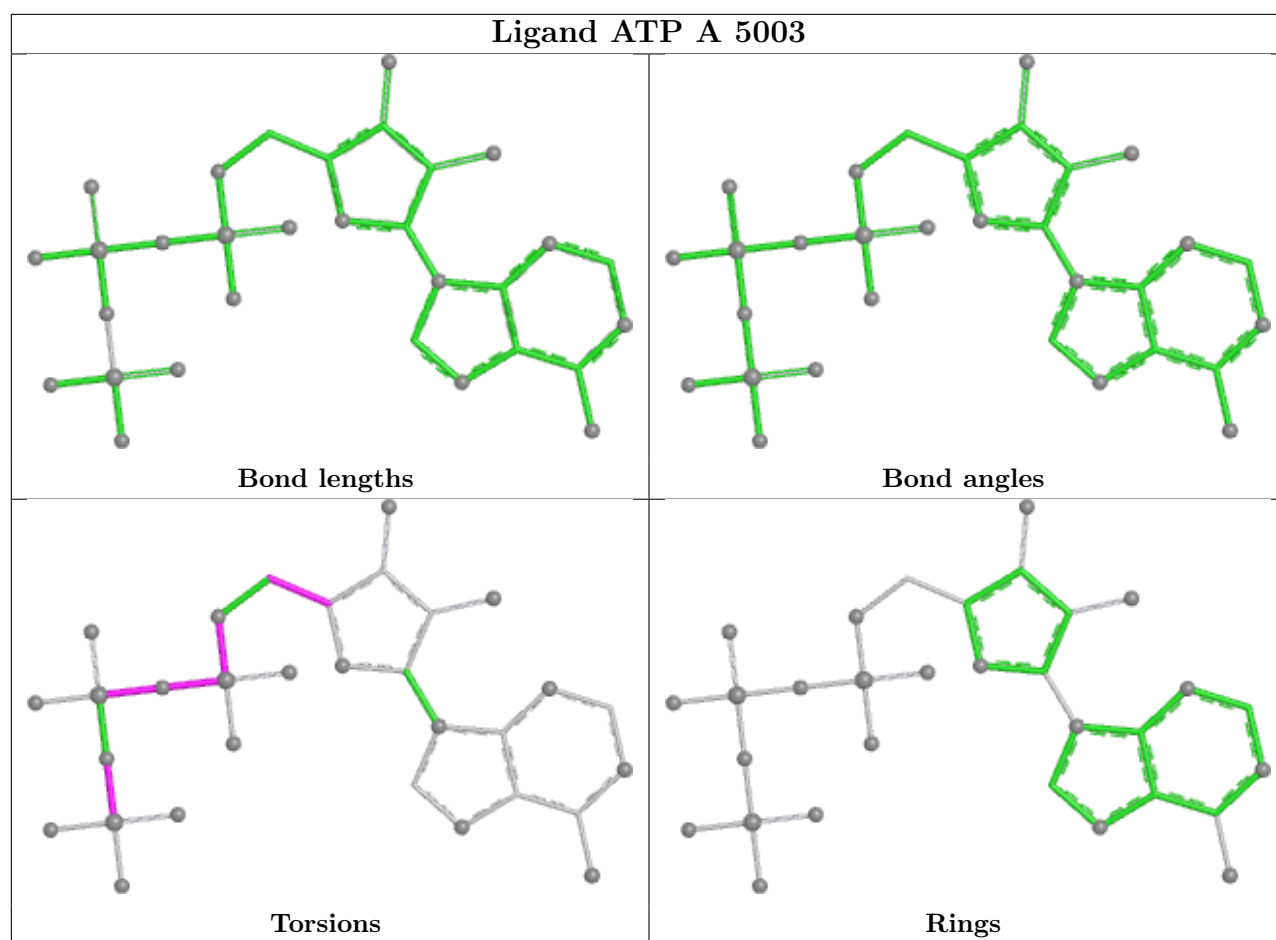












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

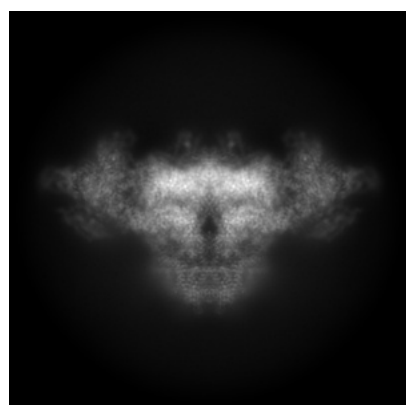
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42459. These allow visual inspection of the internal detail of the map and identification of artifacts.

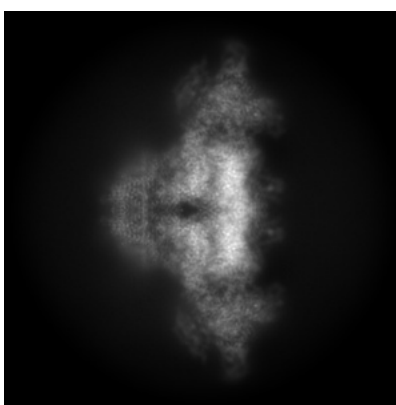
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

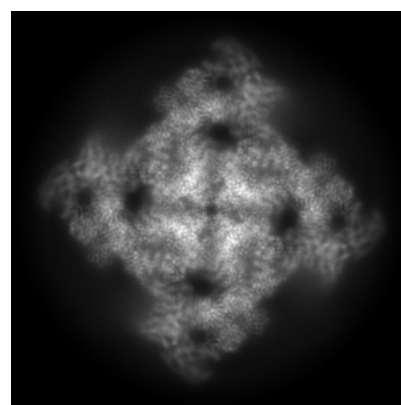
6.1.1 Primary map



X



Y

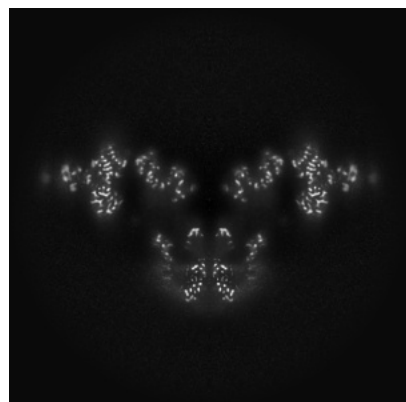


Z

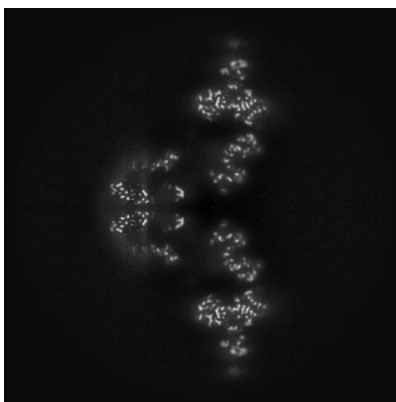
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

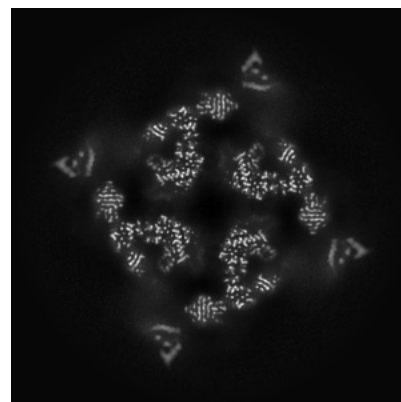
6.2.1 Primary map



X Index: 256



Y Index: 256

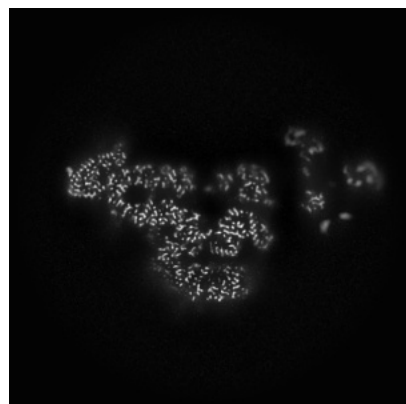


Z Index: 256

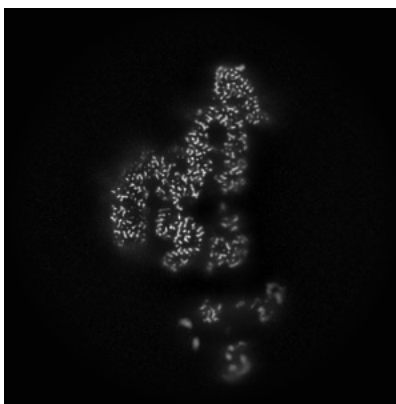
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

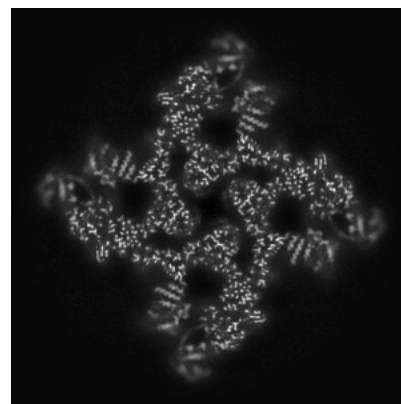
6.3.1 Primary map



X Index: 279



Y Index: 279

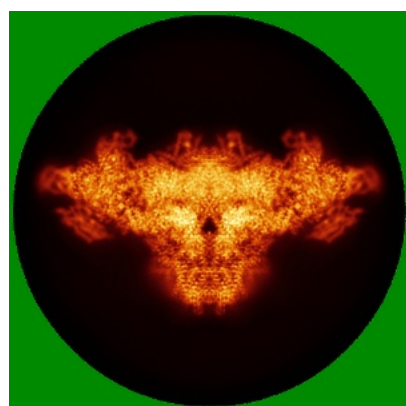


Z Index: 287

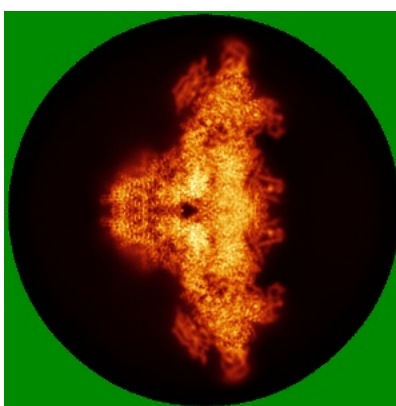
The images above show the largest variance slices of the map in three orthogonal directions.

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

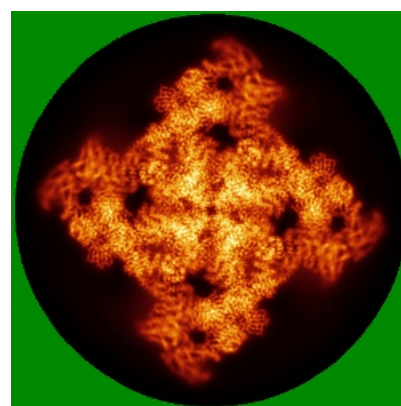
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

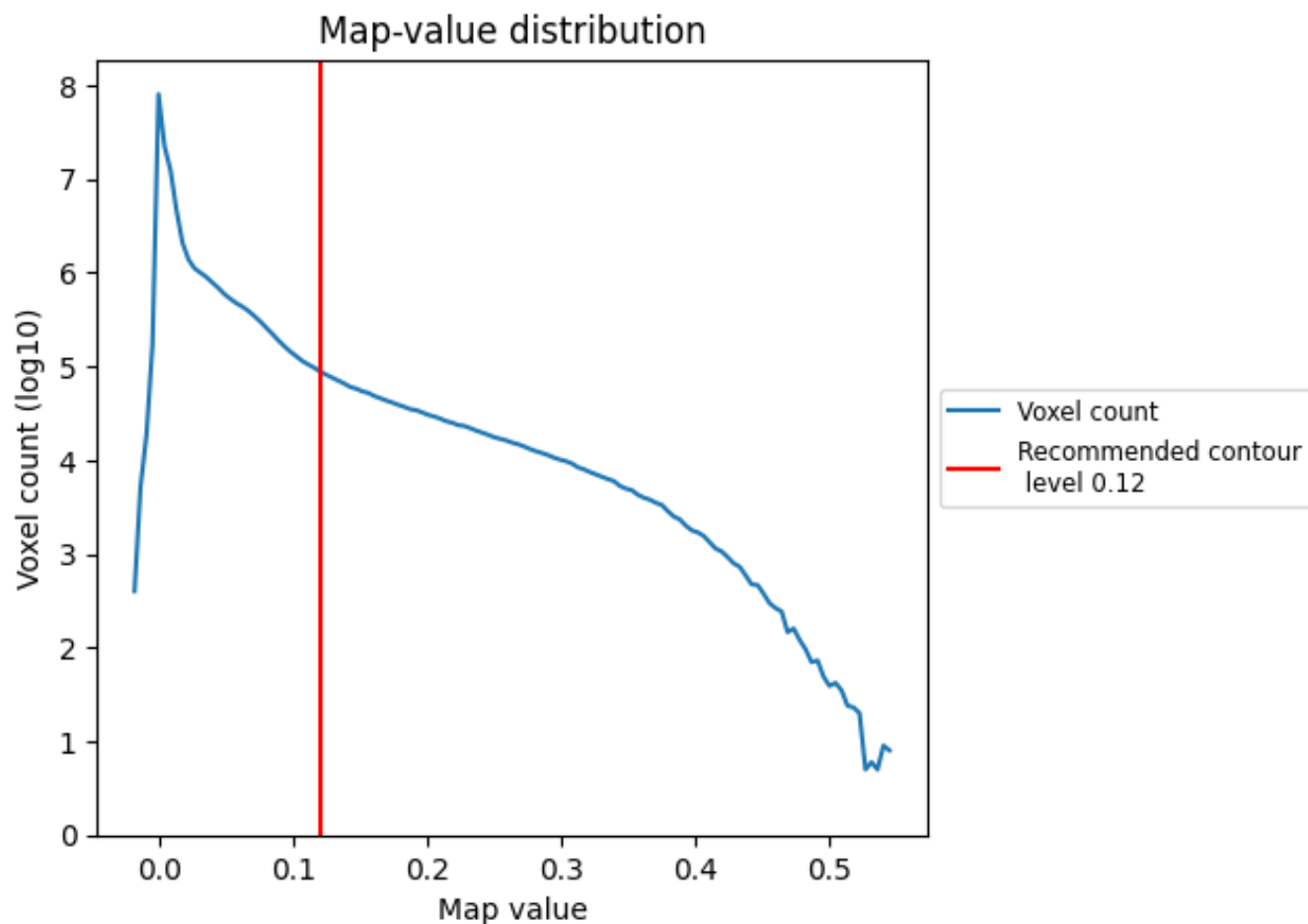
6.6 Mask visualisation

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

7 Map analysis [i](#)

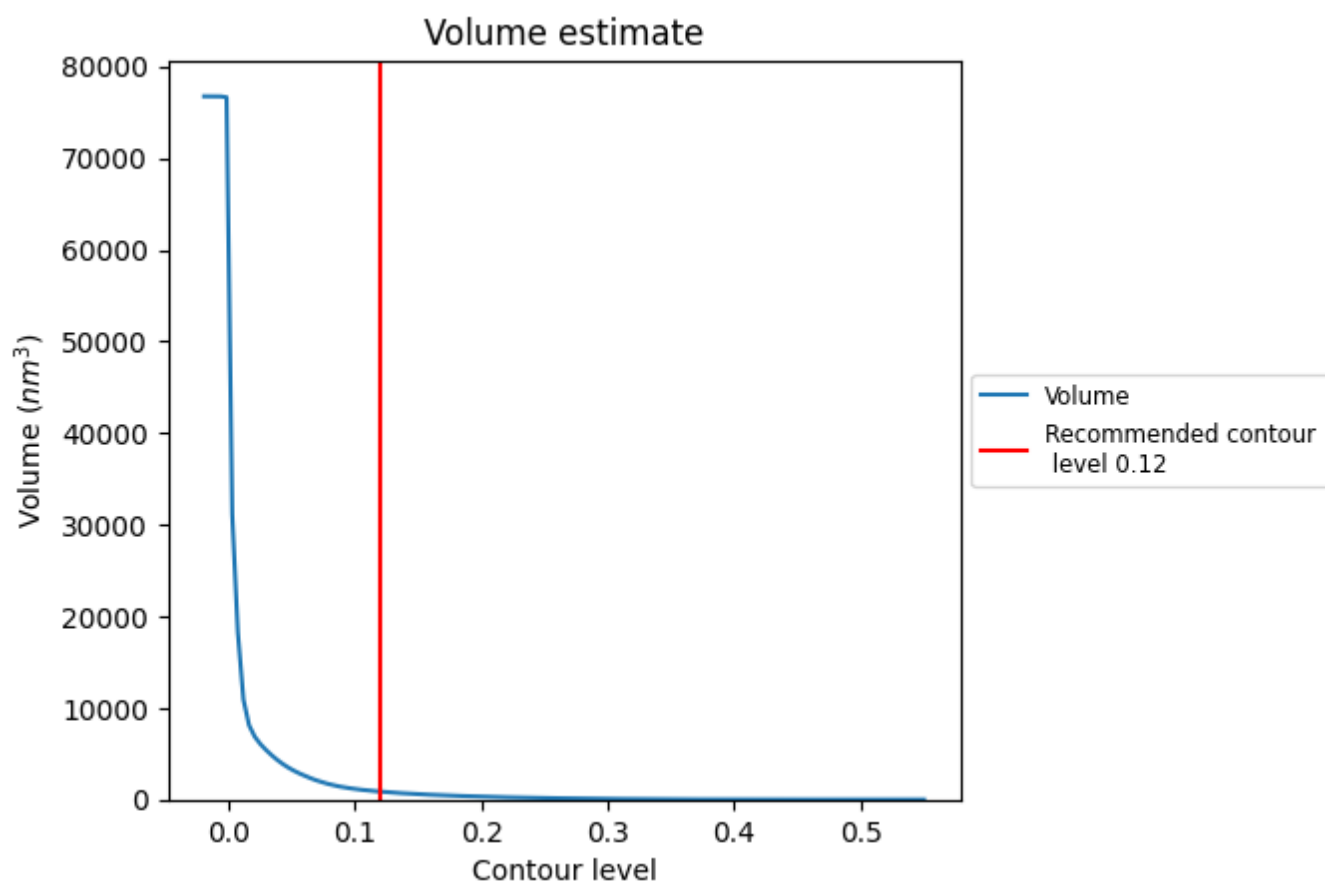
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

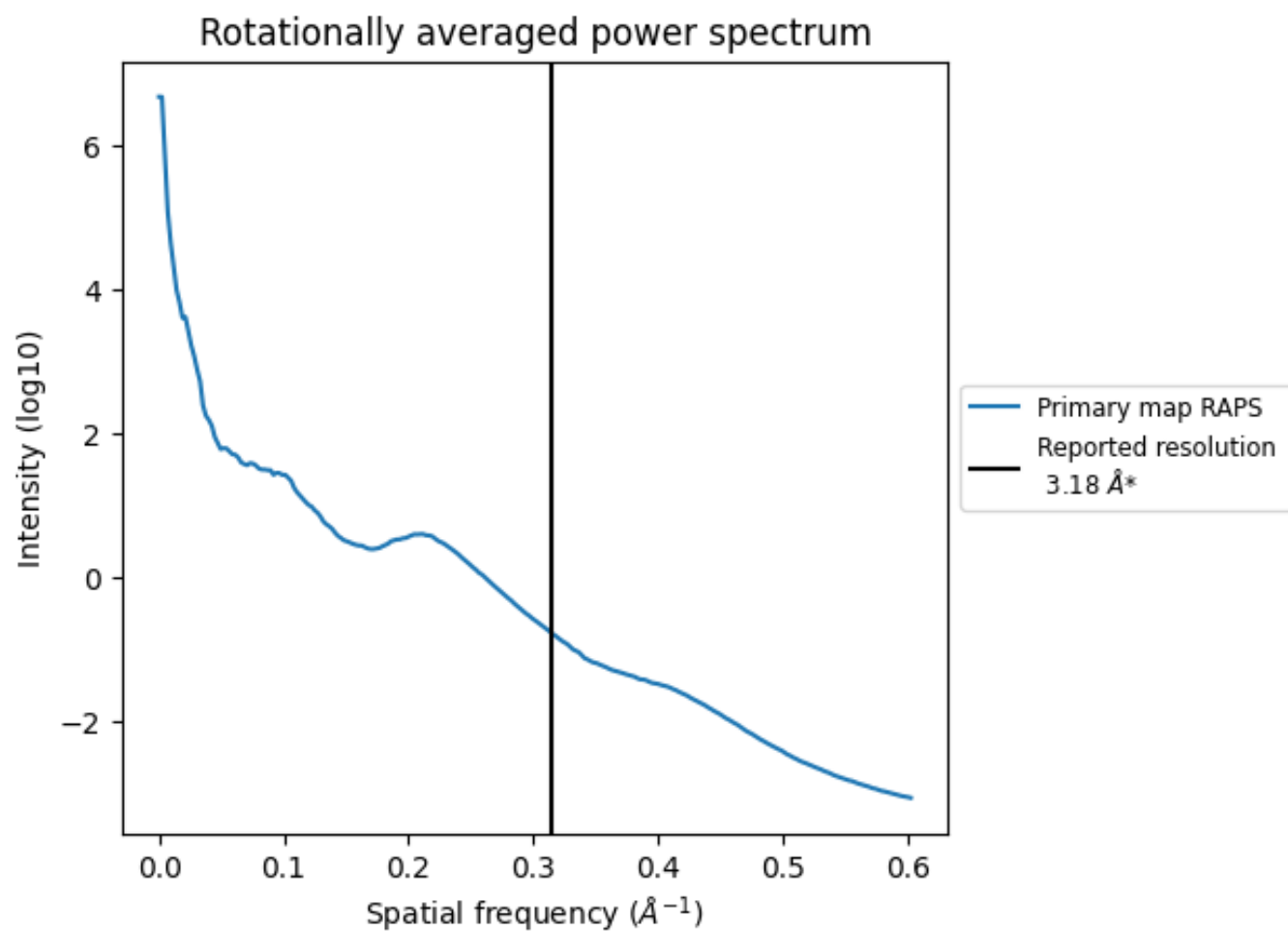
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 868 nm^3 ; this corresponds to an approximate mass of 784 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.314 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

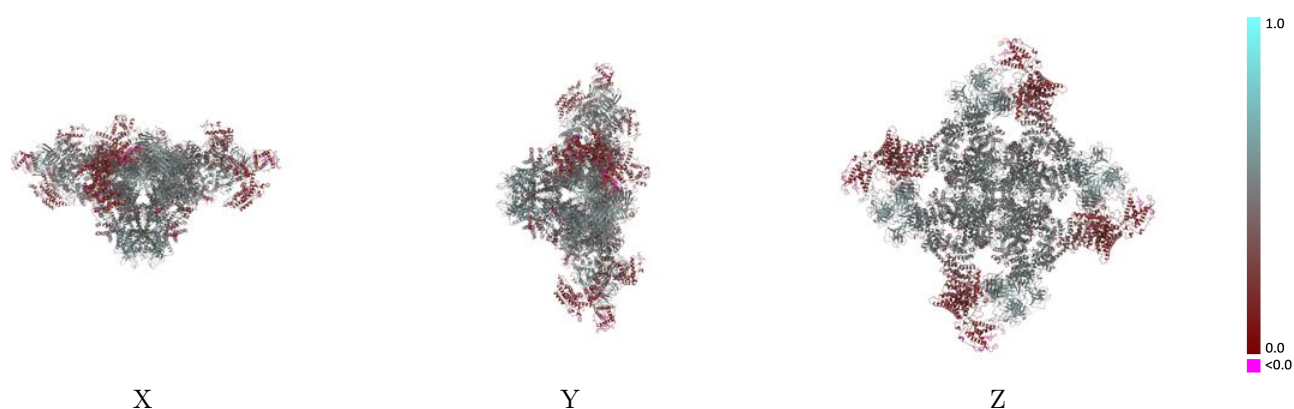
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42459 and PDB model 8UQ3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

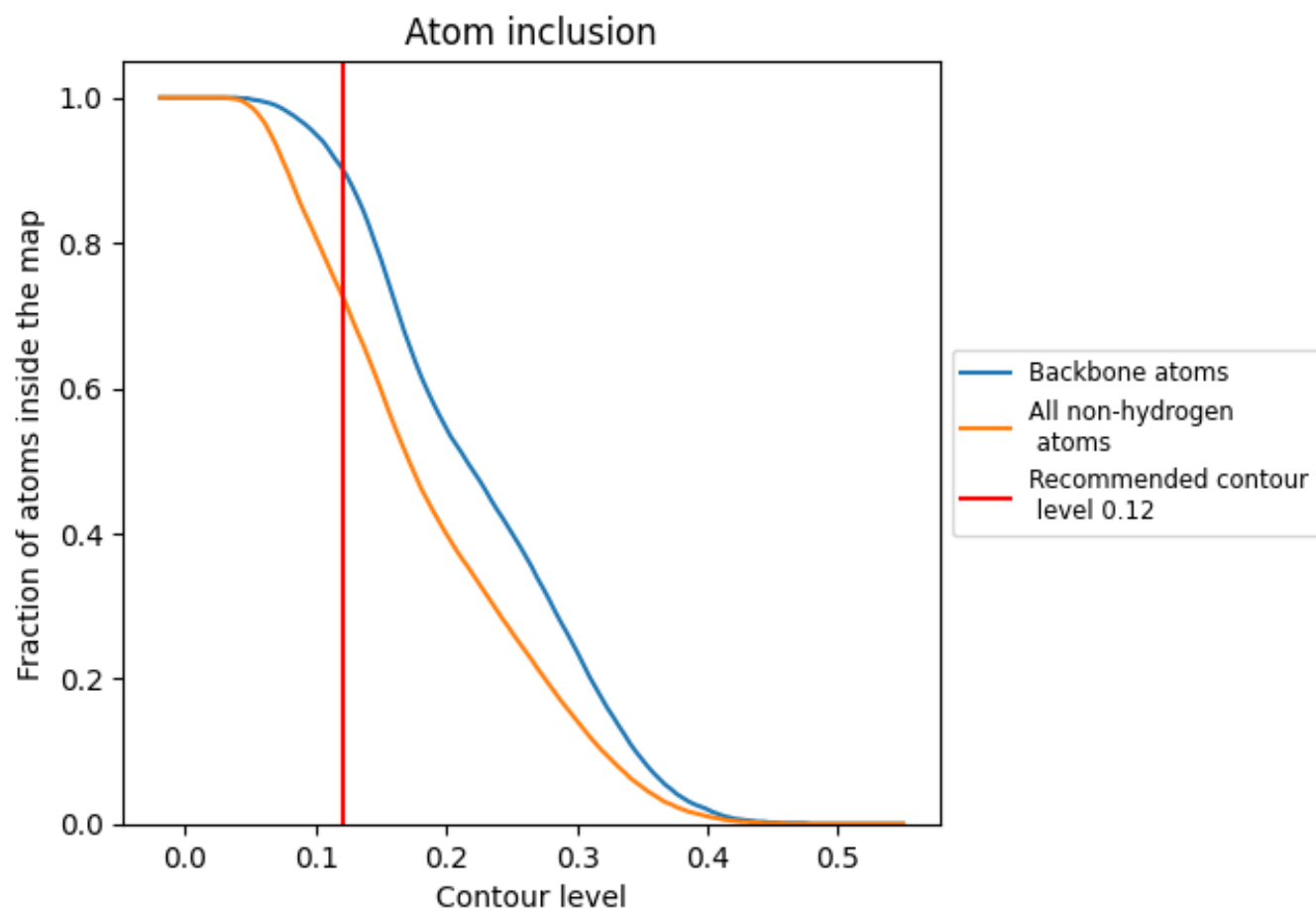


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7280	0.4180
A	0.7260	0.4160
B	0.7260	0.4160
C	0.7250	0.4150
D	0.7250	0.4160
E	0.8490	0.5070
F	0.8500	0.5100
G	0.8540	0.5100
H	0.8490	0.5110

