



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:18 AM UTC

PDB ID : 8UXH / pdb_00008uxh
EMDB ID : EMD-42764
Title : Structure of PKA phosphorylated human RyR2-R420W in the primed state
in the presence of calcium
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.52 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:

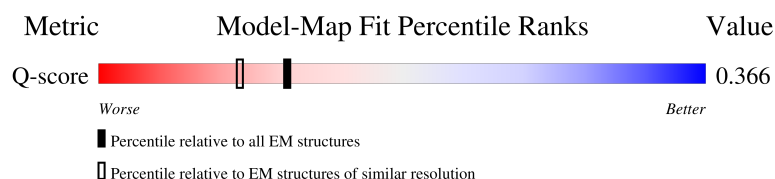
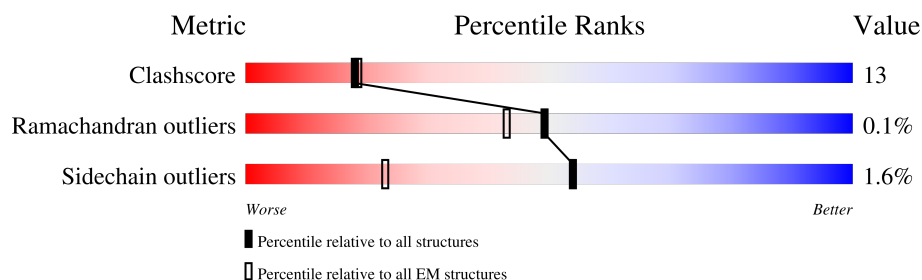
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.52 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	13017 (3.02 - 4.02)

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% 56% 23% • 19%
1	B	4967	 10% 56% 24% • 19%
1	C	4967	 10% 56% 24% • 19%
1	D	4967	 11% 57% 23% • 19%

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Mol	Chain	Length	Quality of chain
2	E	108	 78%20%..
2	F	108	 80%19%..
2	G	108	 79%19%..
2	H	108	 79%19%..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 131656 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	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	B	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	C	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	D	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

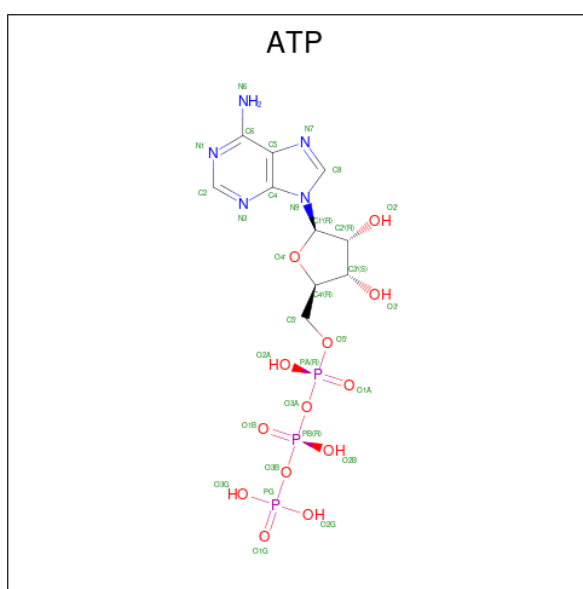
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- 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	

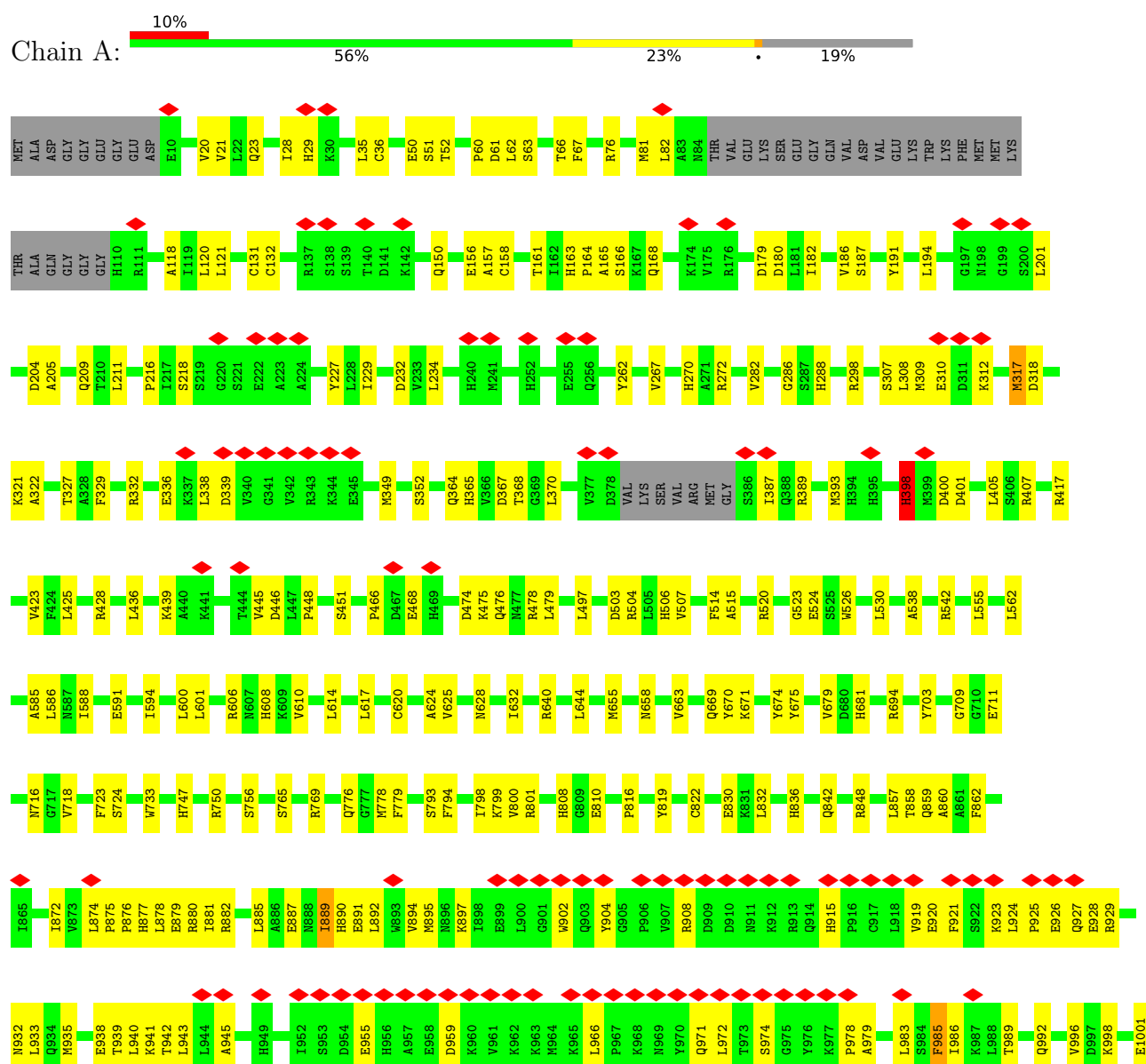
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	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.

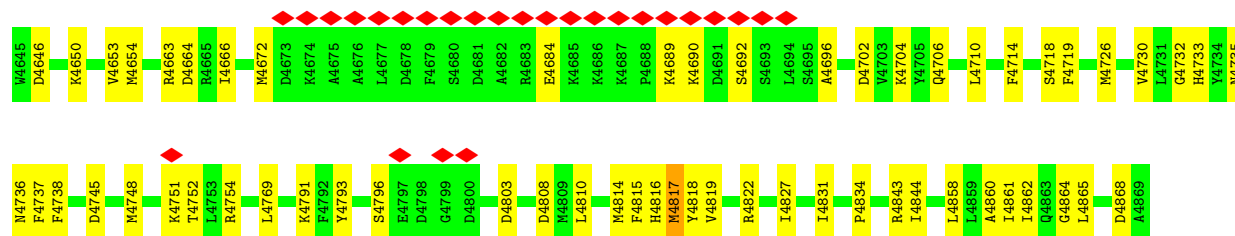
• Molecule 1: Ryanodine receptor 2



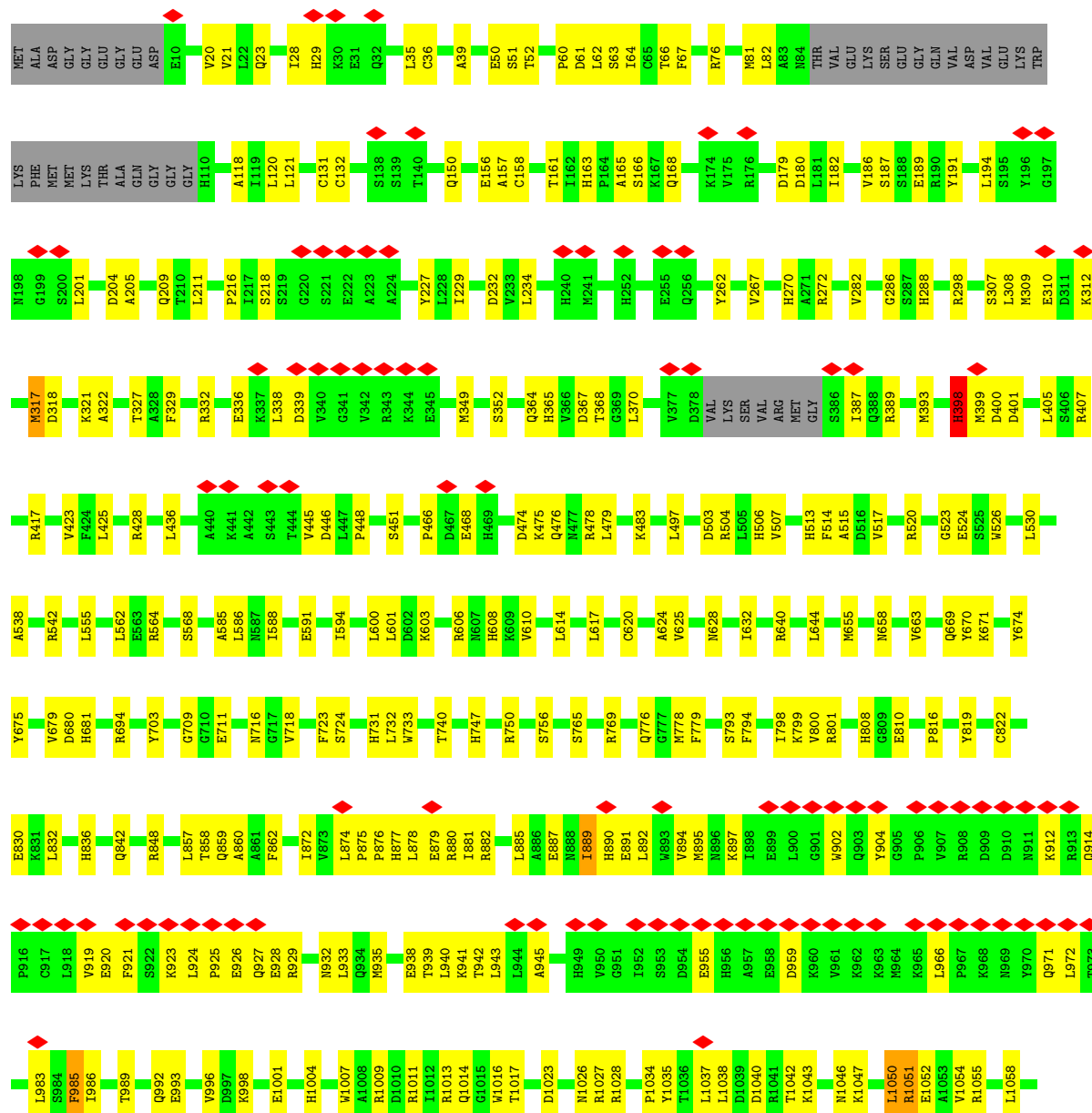


LEU	ILE	GLN	GLY	ALA	ILE	V3004	L2930	H2867	Y2801	W2741	P2678	L2569	M2442	R2336
ARG	THR	LEU	PRO	ALA	THR	T3005	V2933	H2868	W2802	L2742	D2679	E2570	D2455	G2337
GLU	SER	LEU	ASN	LEU	SER	S3006	P2869	L2870	ARG	Y2743	Y2680	C2572	M2456	R2337
THR	LEU	ASN	H2937	L2871	ARG	L3007	L2870	L2871	THR	G2744	M2681	L2573	S2457	E2348
ASP	THR	PRO	H2940	D2875	ARG	C3009	D2875	D2876	ARG	E2745	Y2684	L2576	A2458	E2349
TYR	ALA	K3010	L2943	T2877	SER	K3010	T2876	T2877	ILE	L2746	Y2685	L2580	E2350	A2350
ASN	LEU	V3013	F2943	L2878	THR	K3011	L2878	L2879	GLN	G2747	Y2686	L2581	F2460	E2351
GLY	GLY	R3016	D2944	T2879	SER	L3012	T2879	T2880	THR	S2748	S2687	P2582	K2465	E2352
THR	SER	H3017	S2947	L2880	VAL	F3013	L2880	L2881	GLN	D2749	M2688	M2584	F2471	R2359
LEU	SER	R3018	R2948	K2881	SER	K3014	K2881	K2882	VAL	S2750	M2689	M2585	V2475	D2360
PRO	ILE	L3019	G2949	L2883	THR	L3015	G2949	L2884	ASP	K2691	K2691	L2589	V2480	F2364
ASN	THR	S3020	K2950	K2885	ASP	F3016	K2950	K2886	ALA	Q2692	Q2692	R2590	Q2481	SER
GLN	THR	F3022	G2951	D2886	ALA	L3017	G2951	D2887	ALA	S2694	S2694	R2591	D2482	GLY
PRO	THR	A3026	H2953	E2887	HIS	A3027	H2953	E2888	HIS	P2755	M2695	L2592	F2483	SER
GLY	THR	T3029	Y2956	K2889	THR	T3028	Y2956	K2890	THR	L2756	D2696	V2593	L2488	LYS
LEU	THR	H3034	F2957	A2889	THR	H3035	F2957	A2890	THR	M2757	D2697	L2589	F2492	THR
LEU	THR	L3036	Q2958	Q2890	THR	L3037	Q2958	Q2891	THR	K2758	E2698	R2590	L2493	LEU
GLY	GLY	G3037	E2959	D2891	THR	G3038	E2959	D2892	THR	P2759	E2699	M2605	P2494	ASP
CYS	CYS	Q3038	F2962	L2893	THR	Q3039	F2962	L2894	THR	Y2760	G2699	P2606	D2495	THR
LEU	ALA	Q3039	F2963	L2895	THR	Q3040	F2963	L2896	THR	K2761	M2700	L2610	L2496	GLU
ALA	ALA	L3040	K2964	L2897	THR	L3041	K2964	L2898	THR	L2762	F2701	R2616	L2502	E2377
ALA	PHE	D3041	K2965	Q2897	THR	D3042	K2965	Q2898	THR	L2763	P2702	K2619	L2503	E2378
GLY	GLY	A3042	K2966	L2899	THR	A3043	K2966	L2900	THR	S2764	Q2704	L2623	L2504	D2379
ALA	ALA	Q3043	V2967	L2900	THR	Q3044	V2967	L2901	THR	E2765	P2705	L2624	T2504	D2380
PRO	THR	T3044	V2968	Q2901	THR	T3045	V2968	Q2902	THR	K2766	P2706	G2626	S2508	H2383
VAL	THR	V3045	P2969	G2903	THR	V3046	P2969	G2904	THR	E2767	T2707	W2627	A2513	H2384
GLN	THR	M3046	L2970	Y2903	THR	M3047	L2970	Y2904	THR	K2768	T2708	W2628	L2388	L2388
LEU	THR	K3047	Q2973	V2903	THR	K3048	Q2973	V2904	THR	E2769	T2709	G2629	L2395	L2395
GLY	THR	T3048	K2976	S2903	THR	T3049	K2976	S2904	THR	L2770	S2710	P2630	L2396	L2396
GLY	THR	G3049	L2979	R2905	THR	G3050	L2979	R2906	THR	L2771	L2711	E2635	L2397	L2397
LEU	HIS	L3050	L2980	Q2906	THR	L3051	L2980	Q2907	THR	L2772	L2712	E2636	R2401	R2401
ASP	ASP	E3051	Y2981	F2907	THR	E3052	Y2981	F2908	THR	L2773	L2713	E2637	E2415	E2415
LYS	LYS	S3052	F2982	K2908	THR	S3053	F2982	K2909	THR	L2774	L2714	E2644	R2418	R2418
HIS	HIS	K3054	L2983	D2909	THR	K3055	L2983	D2910	THR	L2775	L2715	L2644	L2419	L2419
ASN	ASN	V3055	L2984	L2910	THR	V3056	L2984	L2911	THR	L2776	E2716	L2645	R2420	R2420
ILE	ILE	S3056	A2985	L2911	THR	S3057	A2985	L2912	THR	L2777	L2716	P2526	S2421	S2421
SER	SER	A3058	A2986	E2911	THR	A3059	A2986	E2912	THR	L2778	L2717	P2527	L2422	L2422
ILE	ILE	L3059	S2987	T2914	THR	L3060	S2987	T2915	THR	L2779	L2718	Q2659	L2427	L2427
ASN	ASN	F3060	R2988	P2915	THR	F3061	R2988	P2916	THR	L2780	E2719	E2660	L2432	L2432
THR	THR	F3061	L2990	S2916	THR	F3062	L2990	S2917	THR	L2781	Y2719	L2652	V2435	V2435
LYS	LYS	D3062	L2993	L2917	THR	D3063	L2993	L2918	THR	L2782	F2720	K2655	I2436	I2436
SER	SER	N3063	G2993	E2918	THR	N3064	G2993	E2919	THR	L2783	Y2721	K2656	F2440	F2440
ARG	ARG	A3065	N2998	R2919	THR	A3066	N2998	R2920	THR	A2784	Y2724	Q2659	S2568	S2568
GLY	GLY	L3067	E3000	P2921	THR	L3068	E3000	P2922	THR	G2785	Y2725	E2660	K2557	K2557
ASP	ASP	F3069	K3001	S2922	THR	F3070	K3001	S2923	THR	G2786	K2663	K2663	D2567	D2567
VAL	VAL	D3070	E3002	Y2923	THR	D3071	E3002	Y2924	THR	G2787	L2666	L2666	S2568	S2568
GLN	GLN	L3070	E3003	L2926	THR	L3071	E3003	L2927	THR	A2788	L2667	L2667	F2441	F2441
SER	SER	K3070	Q2927	Q2928	THR	K3071	Q2927	Q2929	THR	R2788	L2668	L2668		
TYR	TYR	T3071	Q2929	L2929	THR	T3072	Q2929	L2930	THR	R2789	L2669	L2669		
ARG	ARG				THR	R2790	L2670	L2671	THR	S2789	L2670	L2670		
					THR	E2791	L2671	L2672	THR	D2789	L2671	L2671		
					THR	R2791	L2672	L2673	THR	S2790	L2672	L2672		
					THR	E2792	L2673	L2674	THR	D2790	L2673	L2673		
					THR	R2792	L2674	L2675	THR	S2791	L2674	L2674		
					THR	E2793	L2675	L2676	THR	D2791	L2675	L2675		
					THR	R2793	L2676	L2677	THR	S2792	L2676	L2676		
					THR	E2794	L2677	L2678	THR	D2792	L2677	L2677		
					THR	R2794	L2678	L2679	THR	S2793	L2678	L2678		
					THR	E2795	L2679	L2680	THR	D2793	L2679	L2679		
					THR	R2795	L2680	L2681	THR	S2794	L2680	L2680		
					THR	E2796	L2681	L2682	THR	D2794	L2681	L2681		
					THR	R2796	L2682	L2683	THR	S2795	L2682	L2682		
					THR	E2797	L2683	L2684	THR	D2795	L2683	L2683		
					THR	R2797	L2684	L2685	THR	S2796	L2684	L2684		
					THR	E2798	L2685	L2686	THR	D2796	L2685	L2685		
					THR	R2798	L2686	L2687	THR	S2797	L2686	L2686		
					THR	E2799	L2687	L2688	THR	D2797	L2687	L2687		
					THR	R2799	L2688	L2689	THR	S2798	L2688	L2688		
					THR	E2800	L2689	L2690	THR	D2798	L2689	L2689		
					THR				THR	S2799	L2690	L2690		





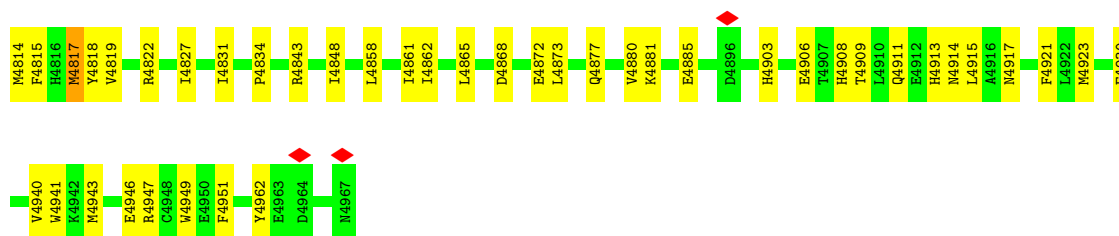
• Molecule 1: Ryanodine receptor 2



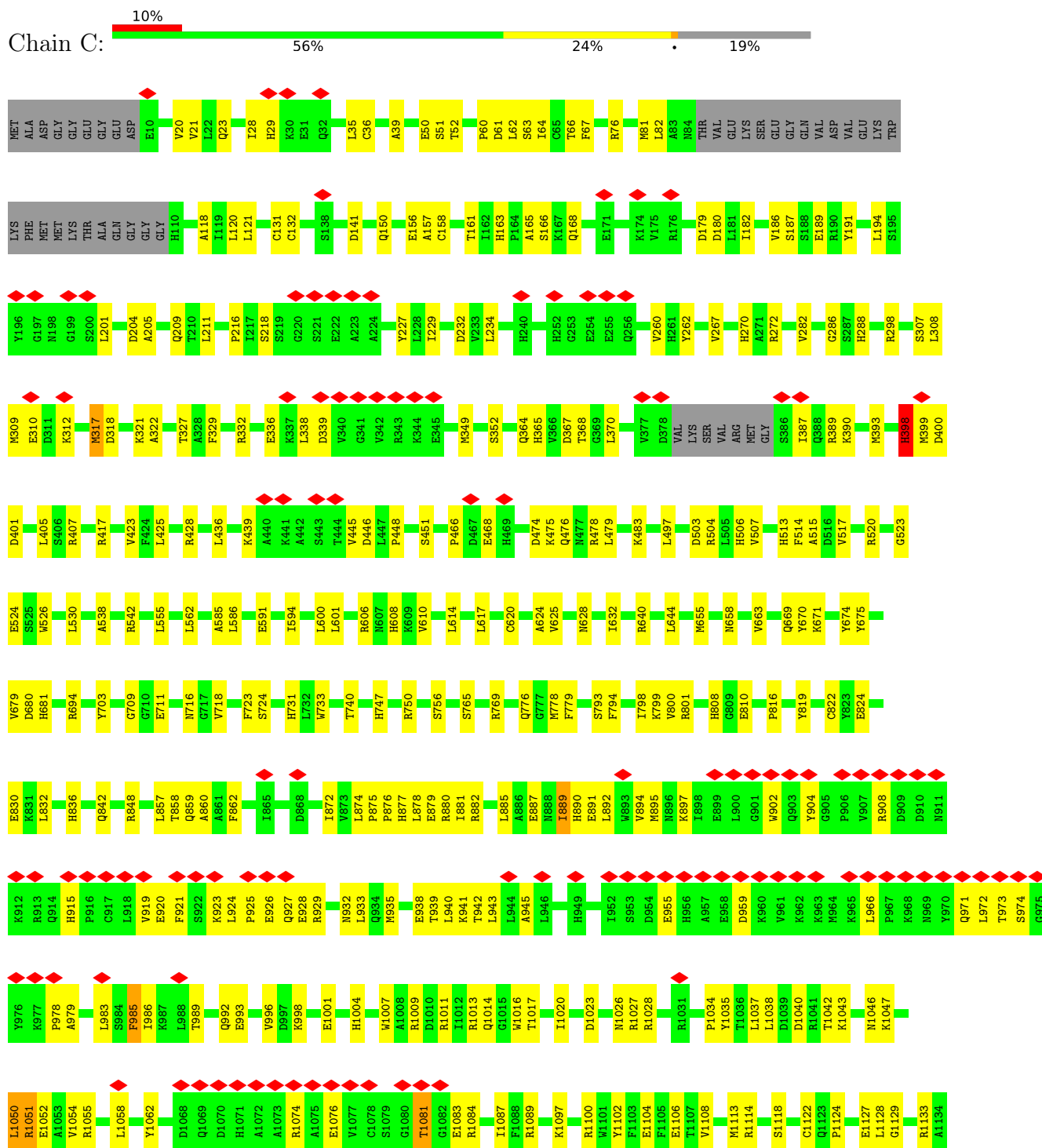
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R2401	R2307	V2178	L2058	K1983	S1788	I1641	K1525	ALA	ASP	M1165	Q1069
E2415	F2307	G2181	I2062	S1984	T1791	E1642	Y1531	ASP	H1277	V1166	H1071
R2418	N2318	G2182	M2066	P1989	I1792	I1644	E1534	R1414	L1283	M1173	A1072
I2419	V2321	E2183	V2074	E1990	Q1793	T1645	F1540	D1415	T1286	M1174	A1073
R2420	R2322	S2184	M2084	I1991	M1794	E1646	F1540	D1416	ASP	L1177	R1074
S2421	R2322	K2185	F2085	I1992	L1795	E1649	Q1546	Y1426	ARG	E1180	A1075
I2422	E2186	E2187	V2086	R1993	E1797	L1650	Q1546	Y1427	ASP	I1181	E1076
L2427	C2330	M2192	L2087	L1996	E1801	L1851	S1549	Y1428	LYS	E1184	V1077
L2432	F2331	N2195	R2090	E2010	D1808	K1852	P1550	S1429	ASP	E1189	G1078
G2433	G2332	G2434	Q2091	LEU	F1825	F1656	M1551	Y1428	LYS	A1191	S1079
G2434	P2333	R2198	Q2092	ASP	Y1826	L1667	Q1554	Y1429	ASP	L1190	T1081
V2435	A2334	F2199	G2096	GLY	T1827	H1670	F1555	Y1430	ASP	K1193	G1082
L2436	R2336	Y2202	V2099	ASP	L1828	H1674	E1556	I1432	ASP	G1198	E1083
F2440	G2337	F2203	I2126	LEU	L1829	I1830	Q1553	I1432	ASP	V1204	R1084
Q2441	L2344	C2204	R2127	ASP	M1831	H1674	Q1553	I1432	ASP	G1206	I1087
M2442	L2344	R2205	S2128	GLY	T1842	D1681	M1563	M1440	ASP	V1212	F1088
D2455	M2347	I2206	L2129	ASN	L1843	E1882	M1564	I1446	ASP	G1213	R1089
M2456	E2346	Q2209	L2130	GLY	R1918	P1683	P1565	I1446	ASP	R1214	K1092
A2457	A2350	R2209	S2131	ASP	R1919	Q1684	L1586	H1451	ASP	V1217	K1097
A2458	K2351	K2212	S2132	LEU	V1926	L1685	L1570	H1451	ASP	R1220	R1100
G2459	K2352	R2213	R2133	THR	V1850	L1686	L1570	V1467	ASP	D1220	Y1101
F2460	L2353	M2214	M2134	ILE	F1851	Y1687	C1582	T1468	ASP	V1221	Y1102
K2465	R2359	Y2220	G2135	ARG	K1852	A1888	Q1589	D1471	ASP	G1222	F1103
F2471	D2360	V2227	E2138	GLY	A1854	I1689	F1590	E1472	ASP	S1222	E1104
V2475	S2363	G2228	M2142	ARG	ALA	E1690	M1694	E1477	ASP	Y1226	F1106
V2480	P2364	L2229	I2143	LEU	THR	M1694	M1596	H1477	ASP	E1234	Y1107
Q2481	ASN	R2234	L2146	LEU	PRO	P1695	M1599	S1483	ASP	E1237	V1108
D2482	GLY	R2235	L2146	VAL	GLU	Y1703	F1603	Y1486	ASP	T1243	M1113
F2483	SER	T2238	M2150	VAL	GLU	L1706	L1605	A1490	ASP	T1244	R1114
L2488	SER	D2241	V2154	THR	ASP	L1711	K1606	A1490	ASP	M1249	S1118
F2492	THR	M2248	Q2157	LEU	THR	M1721	R1610	S1493	ASP	W1250	C1122
L2493	THR	M2248	H2158	LYS	GLU	E1724	I1611	M1494	ASP	L1251	Q1123
P2494	GLU	L2253	P2159	LYS	GLU	Y1725	Q1615	S1495	ASP	G1252	P1124
L2496	GLU	L2253	L2161	LYS	LEU	I1726	G1616	P1496	ASP	S1252	E1127
R2497	E2377	P2260	R2162	ALA	VAL	V1727	W1617	G1497	ASP	L1255	G1129
L2502	E2378	L2262	R2163	LYS	ASP	E1732	V1619	Q1498	ASP	Q1267	R1133
D2503	D2379	E2263	A2164	PRO	ALA	A1959	Q1620	G1499	ASP	F1258	A1134
T2504	D2380	E2263	L2165	VAL	LYS	I1736	L1622	R1500	ASP	L1259	F1135
S2508	H2383	V2266	T2170	GLU	GLN	L1748	D1623	N1501	ASP	Q1267	R1133
A2513	M2384	L2274	V2171	SER	GLY	P1749	D1623	N1502	ASP	P1266	Q1260
	L2388	M2279	M2172	ASP	ALA	D1785	M1628	N1503	ASP	F1258	L1259
	L2395	K2054	M2175	SER	GLY		S1629	E1506	ASP	Q1260	V1261
		S2055		THR	GLU				ASP	VAL	R1144
				LYS					ASP	THR	W1145
				LYS					ASP	THR	Y1152







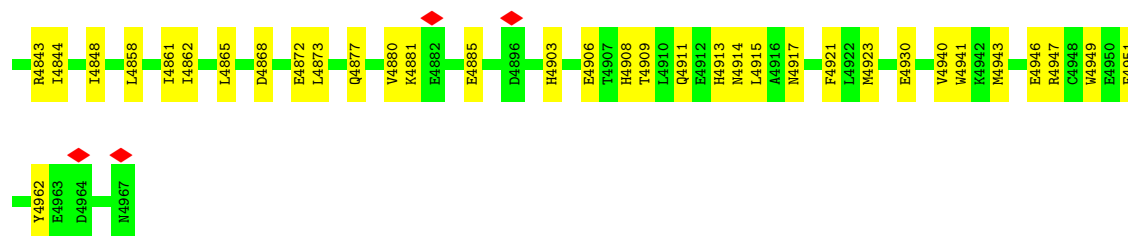
• Molecule 1: Ryanodine receptor 2



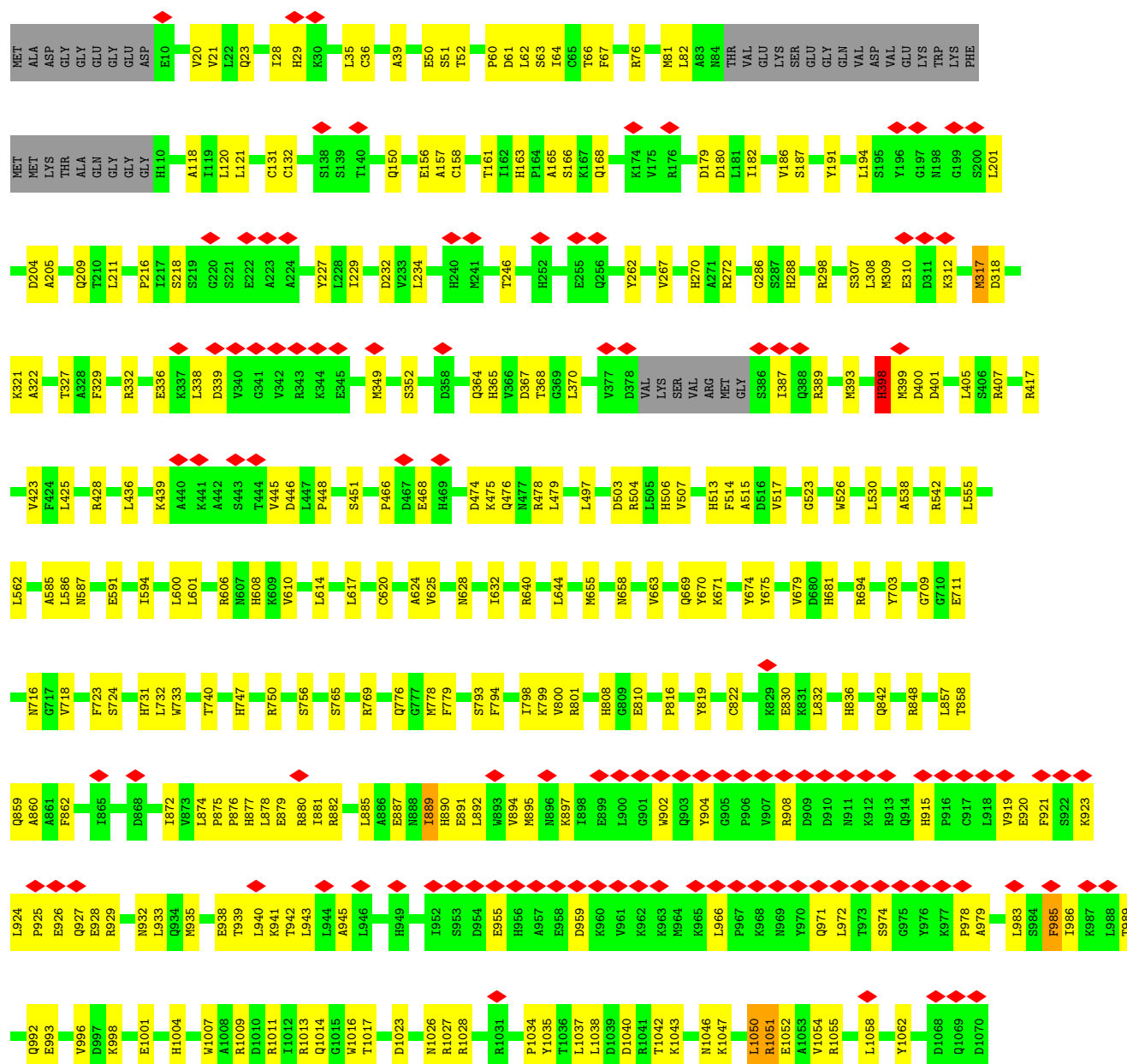








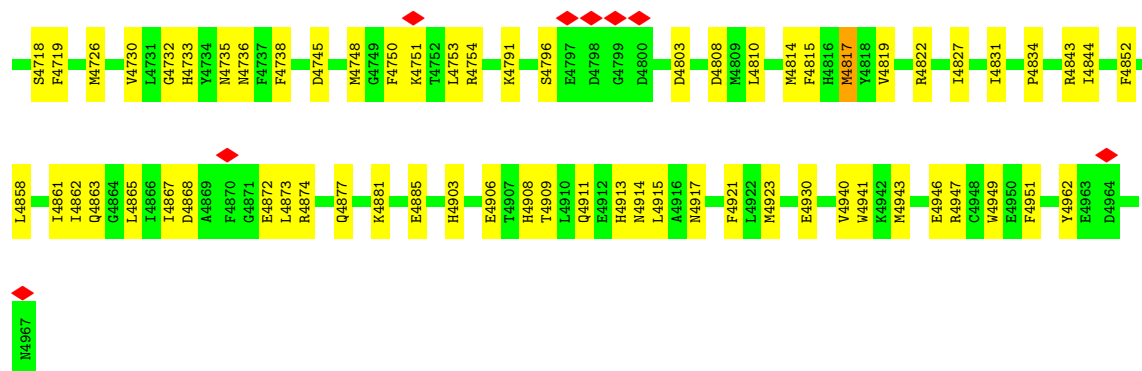
• Molecule 1: Ryanodine receptor 2





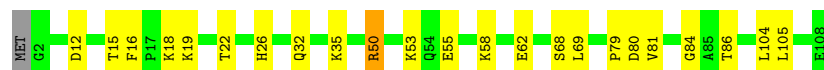
PHE	GLU	GLU	PRO	GLU	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	GLU	THR	
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- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 78% 20% ..



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

Chain F: 80% 19% ..



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

Chain G: 79% 19% ..



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

Chain H: 79% 19% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55886	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	0.564	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	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, CA

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	0.18	0/32738	0.49	18/44213 (0.0%)
1	B	0.18	0/32738	0.49	18/44213 (0.0%)
1	C	0.18	0/32738	0.49	18/44213 (0.0%)
1	D	0.18	0/32738	0.49	18/44213 (0.0%)
2	E	0.14	0/834	0.39	0/1123
2	F	0.14	0/834	0.39	0/1123
2	G	0.14	0/834	0.40	0/1123
2	H	0.14	0/834	0.39	0/1123
All	All	0.18	0/134288	0.49	72/181344 (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 (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2279	MET	CB-CG-SD	10.64	144.62	112.70
1	C	2279	MET	CB-CG-SD	10.64	144.61	112.70
1	B	2279	MET	CB-CG-SD	10.63	144.60	112.70
1	D	2279	MET	CB-CG-SD	10.63	144.58	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2788	ARG	CB-CG-CD	8.98	131.96	111.30
1	B	2788	ARG	CB-CG-CD	8.96	131.92	111.30
1	A	2788	ARG	CB-CG-CD	8.95	131.89	111.30
1	D	2788	ARG	CB-CG-CD	8.94	131.87	111.30
1	D	2279	MET	CA-CB-CG	8.46	131.03	114.10
1	B	2279	MET	CA-CB-CG	8.46	131.02	114.10
1	C	2279	MET	CA-CB-CG	8.46	131.01	114.10
1	A	2279	MET	CA-CB-CG	8.45	131.00	114.10
1	D	4208	GLU	CA-CB-CG	8.40	130.91	114.10
1	C	4208	GLU	CA-CB-CG	8.39	130.89	114.10
1	A	4208	GLU	CA-CB-CG	8.38	130.87	114.10
1	B	4208	GLU	CA-CB-CG	8.38	130.86	114.10
1	D	2530	ARG	CB-CG-CD	7.23	127.93	111.30
1	B	2530	ARG	CB-CG-CD	7.23	127.93	111.30
1	C	2530	ARG	CB-CG-CD	7.23	127.92	111.30
1	A	2530	ARG	CB-CG-CD	7.21	127.88	111.30
1	B	1051	ARG	CB-CG-CD	-6.53	96.28	111.30
1	D	1051	ARG	CB-CG-CD	-6.51	96.32	111.30
1	C	1051	ARG	CB-CG-CD	-6.51	96.33	111.30
1	A	1051	ARG	CB-CG-CD	-6.50	96.34	111.30
1	D	2788	ARG	CA-CB-CG	-6.45	101.21	114.10
1	A	2788	ARG	CA-CB-CG	-6.44	101.21	114.10
1	B	2788	ARG	CA-CB-CG	-6.43	101.24	114.10
1	C	2788	ARG	CA-CB-CG	-6.42	101.25	114.10
1	A	1960	ARG	CA-CB-CG	-6.39	101.32	114.10
1	D	1960	ARG	CA-CB-CG	-6.38	101.34	114.10
1	B	1960	ARG	CA-CB-CG	-6.37	101.36	114.10
1	C	1960	ARG	CA-CB-CG	-6.37	101.37	114.10
1	D	1050	LEU	CA-C-N	-6.26	111.79	122.56
1	D	1050	LEU	C-N-CA	-6.26	111.79	122.56
1	C	1050	LEU	CA-C-N	-6.24	111.83	122.56
1	C	1050	LEU	C-N-CA	-6.24	111.83	122.56
1	A	1050	LEU	CA-C-N	-6.23	111.84	122.56
1	A	1050	LEU	C-N-CA	-6.23	111.84	122.56
1	B	1050	LEU	CA-C-N	-6.23	111.85	122.56
1	B	1050	LEU	C-N-CA	-6.23	111.85	122.56
1	C	1948	MET	CB-CG-SD	6.22	131.36	112.70
1	B	1948	MET	CB-CG-SD	6.21	131.33	112.70
1	D	1948	MET	CB-CG-SD	6.21	131.32	112.70
1	A	1948	MET	CB-CG-SD	6.20	131.31	112.70
1	C	2689	MET	CA-CB-CG	6.05	126.21	114.10
1	B	2689	MET	CA-CB-CG	6.05	126.20	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2689	MET	CA-CB-CG	6.05	126.20	114.10
1	A	2689	MET	CA-CB-CG	6.03	126.17	114.10
1	D	4109	MET	CA-CB-CG	5.55	125.19	114.10
1	C	4109	MET	CA-CB-CG	5.52	125.15	114.10
1	B	4109	MET	CA-CB-CG	5.52	125.14	114.10
1	A	4109	MET	CA-CB-CG	5.52	125.14	114.10
1	D	2788	ARG	CG-CD-NE	5.49	124.08	112.00
1	A	2788	ARG	CG-CD-NE	5.48	124.05	112.00
1	C	2788	ARG	CG-CD-NE	5.47	124.04	112.00
1	B	2788	ARG	CG-CD-NE	5.47	124.03	112.00
1	A	4046	ARG	CB-CG-CD	5.30	123.49	111.30
1	D	4046	ARG	CB-CG-CD	5.29	123.46	111.30
1	B	4046	ARG	CB-CG-CD	5.28	123.45	111.30
1	C	4046	ARG	CB-CG-CD	5.28	123.45	111.30
1	D	1493	SER	CA-C-N	-5.20	115.62	122.85
1	D	1493	SER	C-N-CA	-5.20	115.62	122.85
1	A	1493	SER	CA-C-N	-5.18	115.65	122.85
1	A	1493	SER	C-N-CA	-5.18	115.65	122.85
1	C	1493	SER	CA-C-N	-5.17	115.66	122.85
1	C	1493	SER	C-N-CA	-5.17	115.66	122.85
1	B	1493	SER	CA-C-N	-5.17	115.66	122.85
1	B	1493	SER	C-N-CA	-5.17	115.66	122.85
1	C	1293	GLN	CA-CB-CG	5.13	124.37	114.10
1	D	1293	GLN	CA-CB-CG	5.12	124.34	114.10
1	A	1293	GLN	CA-CB-CG	5.10	124.30	114.10
1	B	1293	GLN	CA-CB-CG	5.09	124.29	114.10

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2530	ARG	Sidechain
1	A	2788	ARG	Sidechain
1	A	398	HIS	Peptide
1	B	2530	ARG	Sidechain
1	B	2788	ARG	Sidechain
1	B	398	HIS	Peptide
1	C	2530	ARG	Sidechain
1	C	2788	ARG	Sidechain
1	C	398	HIS	Peptide
1	D	2530	ARG	Sidechain
1	D	2788	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	398	HIS	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	32032	0	31689	881	0
1	B	32032	0	31689	883	0
1	C	32032	0	31689	868	0
1	D	32032	0	31689	866	0
2	E	818	0	821	14	0
2	F	818	0	821	12	0
2	G	818	0	821	13	0
2	H	818	0	821	13	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	0	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	131656	0	130136	3472	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 (3472) 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:4814:MET:HE1	1:D:4844:ILE:HD13	1.35	1.03
1:D:2857:LYS:HE3	1:D:2871:LEU:HD23	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2857:LYS:HE3	1:A:2871:LEU:HD23	1.52	0.92
1:C:2857:LYS:HE3	1:C:2871:LEU:HD23	1.52	0.91
1:B:2857:LYS:HE3	1:B:2871:LEU:HD23	1.52	0.90
1:D:1564:MET:HE3	1:D:1565:PRO:HD2	1.58	0.86
1:A:4844:ILE:HD13	1:D:4814:MET:CE	2.04	0.86
1:C:1564:MET:HE3	1:C:1565:PRO:HD2	1.58	0.86
1:A:1564:MET:HE3	1:A:1565:PRO:HD2	1.58	0.85
1:B:1564:MET:HE3	1:B:1565:PRO:HD2	1.58	0.84
1:D:4834:PRO:HB3	1:D:4843:ARG:HD3	1.59	0.84
1:A:4834:PRO:HB3	1:A:4843:ARG:HD3	1.59	0.83
1:B:2130:LEU:HD11	1:B:2170:THR:HG23	1.61	0.83
1:B:986:ILE:HD11	1:B:1055:ARG:HD3	1.59	0.83
1:D:986:ILE:HD11	1:D:1055:ARG:HD3	1.59	0.83
1:C:4834:PRO:HB3	1:C:4843:ARG:HD3	1.59	0.83
1:B:4834:PRO:HB3	1:B:4843:ARG:HD3	1.59	0.82
1:A:875:PRO:HD2	1:A:878:LEU:HD13	1.62	0.82
1:B:875:PRO:HD2	1:B:878:LEU:HD13	1.62	0.82
1:A:2130:LEU:HD11	1:A:2170:THR:HG23	1.61	0.82
1:C:2130:LEU:HD11	1:C:2170:THR:HG23	1.61	0.82
1:C:4641:PRO:HB3	1:C:4644:TYR:HB3	1.61	0.82
1:A:986:ILE:HD11	1:A:1055:ARG:HD3	1.59	0.82
1:B:4641:PRO:HB3	1:B:4644:TYR:HB3	1.61	0.82
1:C:986:ILE:HD11	1:C:1055:ARG:HD3	1.59	0.82
1:D:875:PRO:HD2	1:D:878:LEU:HD13	1.62	0.81
1:D:2130:LEU:HD11	1:D:2170:THR:HG23	1.61	0.81
1:D:4641:PRO:HB3	1:D:4644:TYR:HB3	1.61	0.81
1:B:476:GLN:NE2	1:B:3678:GLU:OE1	2.14	0.81
1:C:875:PRO:HD2	1:C:878:LEU:HD13	1.61	0.81
1:D:476:GLN:NE2	1:D:3678:GLU:OE1	2.14	0.81
1:A:476:GLN:NE2	1:A:3678:GLU:OE1	2.14	0.81
1:B:2882:LYS:O	1:B:2886:ARG:HG3	1.81	0.81
1:C:476:GLN:NE2	1:C:3678:GLU:OE1	2.14	0.81
1:A:4641:PRO:HB3	1:A:4644:TYR:HB3	1.61	0.80
1:A:2882:LYS:O	1:A:2886:ARG:HG3	1.81	0.80
1:B:3951:PHE:HB3	1:B:3975:GLN:HE21	1.46	0.80
1:C:3951:PHE:HB3	1:C:3975:GLN:HE21	1.46	0.80
1:D:2882:LYS:O	1:D:2886:ARG:HG3	1.81	0.80
1:C:2882:LYS:O	1:C:2886:ARG:HG3	1.81	0.79
1:A:4831:ILE:HG13	1:A:4843:ARG:HH21	1.47	0.79
1:B:4831:ILE:HG13	1:B:4843:ARG:HH21	1.47	0.79
1:A:3951:PHE:HB3	1:A:3975:GLN:HE21	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3951:PHE:HB3	1:D:3975:GLN:HE21	1.46	0.78
1:C:2465:LYS:NZ	1:C:2495:ASP:OD2	2.17	0.78
1:D:23:GLN:NE2	1:D:36:CYS:SG	2.57	0.78
1:A:23:GLN:NE2	1:A:36:CYS:SG	2.57	0.78
1:C:4044:SER:HA	1:C:4077:THR:HG22	1.66	0.78
1:B:23:GLN:NE2	1:B:36:CYS:SG	2.57	0.78
1:C:23:GLN:NE2	1:C:36:CYS:SG	2.57	0.78
1:D:4831:ILE:HG13	1:D:4843:ARG:HH21	1.47	0.78
1:B:4044:SER:HA	1:B:4077:THR:HG22	1.66	0.77
1:C:4831:ILE:HG13	1:C:4843:ARG:HH21	1.48	0.77
1:A:2465:LYS:NZ	1:A:2495:ASP:OD2	2.17	0.77
1:A:4844:ILE:HD13	1:D:4814:MET:HE1	1.64	0.77
1:C:2760:TYR:OH	1:C:2772:ARG:NH1	2.18	0.77
1:D:4044:SER:HA	1:D:4077:THR:HG22	1.66	0.77
1:B:2465:LYS:NZ	1:B:2495:ASP:OD2	2.17	0.77
1:D:4637:THR:HG22	1:D:4704:LYS:HG3	1.66	0.77
1:C:4637:THR:HG22	1:C:4704:LYS:HG3	1.66	0.77
1:A:4044:SER:HA	1:A:4077:THR:HG22	1.66	0.76
1:D:4640:PHE:CG	1:D:4641:PRO:HD2	2.20	0.76
1:D:996:VAL:HG21	1:D:1051:ARG:HB3	1.67	0.76
1:A:4637:THR:HG22	1:A:4704:LYS:HG3	1.66	0.76
1:A:4640:PHE:CG	1:A:4641:PRO:HD2	2.20	0.76
1:A:4737:PHE:HD2	1:B:4783:VAL:HG13	1.51	0.76
1:C:996:VAL:HG21	1:C:1051:ARG:HB3	1.68	0.76
1:A:3051:GLU:OE1	1:A:3051:GLU:N	2.14	0.76
1:D:2465:LYS:NZ	1:D:2495:ASP:OD2	2.17	0.76
1:C:4640:PHE:CG	1:C:4641:PRO:HD2	2.20	0.76
1:A:2832:THR:HG21	1:B:1290:PHE:HE2	1.50	0.75
1:B:4637:THR:HG22	1:B:4704:LYS:HG3	1.66	0.75
1:B:4640:PHE:CG	1:B:4641:PRO:HD2	2.20	0.75
1:A:4864:GLY:CA	1:D:4867:ILE:HG12	2.16	0.75
1:B:2760:TYR:OH	1:B:2772:ARG:NH1	2.18	0.75
1:C:2627:TRP:HB2	1:C:2630:PHE:HB2	1.69	0.75
1:D:2627:TRP:HB2	1:D:2630:PHE:HB2	1.69	0.75
1:D:3901:GLN:OE1	1:D:3904:ARG:NH2	2.20	0.75
1:A:2760:TYR:OH	1:A:2772:ARG:NH1	2.18	0.75
1:A:996:VAL:HG21	1:A:1051:ARG:HB3	1.67	0.74
1:D:2787:TRP:HD1	1:D:2906:GLY:H	1.34	0.74
1:A:3770:ASN:HB3	1:A:3773:VAL:HG12	1.69	0.74
1:B:996:VAL:HG21	1:B:1051:ARG:HB3	1.67	0.74
1:B:3770:ASN:HB3	1:B:3773:VAL:HG12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3770:ASN:HB3	1:C:3773:VAL:HG12	1.70	0.74
1:C:3901:GLN:OE1	1:C:3904:ARG:NH2	2.20	0.74
1:D:3770:ASN:HB3	1:D:3773:VAL:HG12	1.69	0.74
1:A:2627:TRP:HB2	1:A:2630:PHE:HB2	1.69	0.74
1:D:2760:TYR:OH	1:D:2772:ARG:NH1	2.18	0.74
1:C:2787:TRP:HD1	1:C:2906:GLY:H	1.34	0.74
1:A:1958:THR:HA	1:A:1961:LYS:HD2	1.70	0.74
1:B:2627:TRP:HB2	1:B:2630:PHE:HB2	1.69	0.74
1:A:2787:TRP:HD1	1:A:2906:GLY:H	1.34	0.73
1:D:1958:THR:HA	1:D:1961:LYS:HD2	1.70	0.73
1:A:2782:MET:HE1	1:A:2789:ILE:HB	1.70	0.73
1:A:3901:GLN:OE1	1:A:3904:ARG:NH2	2.20	0.73
1:B:2782:MET:HE1	1:B:2789:ILE:HB	1.70	0.73
1:B:3901:GLN:OE1	1:B:3904:ARG:NH2	2.20	0.73
1:A:2793:ARG:NH1	1:A:2793:ARG:HG2	2.04	0.73
1:B:3051:GLU:OE1	1:B:3051:GLU:N	2.14	0.73
1:C:586:LEU:HD11	1:C:617:LEU:HA	1.71	0.73
1:C:1711:LEU:HB3	1:C:1831:MET:HE1	1.70	0.73
1:A:2787:TRP:CD1	1:A:2906:GLY:H	2.07	0.73
1:D:2793:ARG:NH1	1:D:2793:ARG:HG2	2.04	0.73
1:D:2787:TRP:CD1	1:D:2906:GLY:H	2.07	0.72
1:C:1958:THR:HA	1:C:1961:LYS:HD2	1.70	0.72
1:D:2730:ASP:O	1:D:2734:MET:HG2	1.90	0.72
1:A:2730:ASP:O	1:A:2734:MET:HG2	1.90	0.72
1:B:1711:LEU:HB3	1:B:1831:MET:HE1	1.70	0.72
1:B:1958:THR:HA	1:B:1961:LYS:HD2	1.70	0.72
1:B:4079:ASP:HB3	1:B:4082:GLU:HG2	1.72	0.72
1:C:2787:TRP:CD1	1:C:2906:GLY:H	2.07	0.72
1:D:586:LEU:HD11	1:D:617:LEU:HA	1.70	0.72
1:A:2436:ILE:HA	1:A:2465:LYS:HE3	1.72	0.72
1:A:2824:ARG:HE	1:B:1502:ASN:HB2	1.55	0.72
1:B:2730:ASP:O	1:B:2734:MET:HG2	1.89	0.72
1:B:2787:TRP:HD1	1:B:2906:GLY:H	1.34	0.72
1:B:2436:ILE:HA	1:B:2465:LYS:HE3	1.71	0.72
1:C:2436:ILE:HA	1:C:2465:LYS:HE3	1.71	0.72
1:C:2730:ASP:O	1:C:2734:MET:HG2	1.90	0.72
1:C:2552:VAL:HG13	1:C:2569:ILE:HD11	1.72	0.72
1:D:2436:ILE:HA	1:D:2465:LYS:HE3	1.72	0.72
1:A:586:LEU:HD11	1:A:617:LEU:HA	1.71	0.72
1:A:4079:ASP:HB3	1:A:4082:GLU:HG2	1.72	0.72
1:B:2787:TRP:CD1	1:B:2906:GLY:H	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1166:VAL:HG23	1:D:1173:MET:HG2	1.72	0.72
1:D:2782:MET:HE1	1:D:2789:ILE:HB	1.70	0.72
1:C:1122:CYS:HA	1:C:1133:ARG:HD3	1.71	0.72
1:C:2782:MET:HE1	1:C:2789:ILE:HB	1.70	0.72
1:D:2552:VAL:HG13	1:D:2569:ILE:HD11	1.72	0.72
1:D:4079:ASP:HB3	1:D:4082:GLU:HG2	1.72	0.72
1:C:3051:GLU:OE1	1:C:3051:GLU:N	2.14	0.72
1:D:1711:LEU:HB3	1:D:1831:MET:HE1	1.70	0.72
1:A:1711:LEU:HB3	1:A:1831:MET:HE1	1.70	0.72
1:A:2552:VAL:HG13	1:A:2569:ILE:HD11	1.72	0.72
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.72	0.72
1:B:1122:CYS:HA	1:B:1133:ARG:HD3	1.71	0.71
1:C:1166:VAL:HG23	1:C:1173:MET:HG2	1.72	0.71
1:B:2976:LYS:O	1:B:2979:ARG:NH1	2.24	0.71
1:C:4079:ASP:HB3	1:C:4082:GLU:HG2	1.72	0.71
1:B:586:LEU:HD11	1:B:617:LEU:HA	1.71	0.71
1:D:2976:LYS:O	1:D:2979:ARG:NH1	2.24	0.71
1:A:2830:ASN:OD1	1:B:1549:SER:HB2	1.91	0.71
1:D:2736:LYS:HB3	1:D:2741:TRP:CD1	2.26	0.71
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.72	0.71
1:A:2824:ARG:NH2	1:B:1502:ASN:O	2.24	0.71
1:D:3051:GLU:OE1	1:D:3051:GLU:N	2.14	0.71
1:A:1166:VAL:HG23	1:A:1173:MET:HG2	1.72	0.71
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.72	0.71
1:B:2552:VAL:HG13	1:B:2569:ILE:HD11	1.72	0.70
1:C:2793:ARG:NH1	1:C:2793:ARG:HG2	2.04	0.70
1:A:2736:LYS:HB3	1:A:2741:TRP:CD1	2.26	0.70
1:A:4818:TYR:HD1	1:B:4848:ILE:HD11	1.56	0.70
1:D:1122:CYS:HA	1:D:1133:ARG:HD3	1.72	0.70
1:D:799:LYS:NZ	1:D:1620:GLN:OE1	2.24	0.70
1:A:799:LYS:NZ	1:A:1620:GLN:OE1	2.24	0.70
1:D:878:LEU:HG	1:D:940:LEU:HD12	1.74	0.70
1:B:1166:VAL:HG23	1:B:1173:MET:HG2	1.72	0.70
1:A:878:LEU:HG	1:A:940:LEU:HD12	1.74	0.70
1:A:1122:CYS:HA	1:A:1133:ARG:HD3	1.72	0.70
1:B:2793:ARG:HG2	1:B:2793:ARG:NH1	2.04	0.70
1:C:878:LEU:HG	1:C:940:LEU:HD12	1.74	0.70
1:C:2788:ARG:HD3	1:C:2905:ARG:O	1.92	0.70
1:C:2976:LYS:O	1:C:2979:ARG:NH1	2.24	0.70
1:D:2788:ARG:HD3	1:D:2905:ARG:O	1.92	0.70
1:B:2788:ARG:HD3	1:B:2905:ARG:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:LYS:NZ	1:B:1620:GLN:OE1	2.24	0.69
1:B:878:LEU:HG	1:B:940:LEU:HD12	1.74	0.69
1:D:2690:GLU:HB2	1:D:2692:GLN:OE1	1.92	0.69
1:B:2736:LYS:HB3	1:B:2741:TRP:CD1	2.26	0.69
1:C:2690:GLU:HB2	1:C:2692:GLN:OE1	1.92	0.69
1:C:2736:LYS:HB3	1:C:2741:TRP:CD1	2.26	0.69
1:A:2788:ARG:HD3	1:A:2905:ARG:O	1.92	0.69
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.26	0.69
1:D:4654:MET:HE3	1:D:4663:ARG:HE	1.58	0.69
1:A:2976:LYS:O	1:A:2979:ARG:NH1	2.24	0.69
1:B:2690:GLU:HB2	1:B:2692:GLN:OE1	1.92	0.69
1:B:2832:THR:OG1	1:C:1548:THR:O	2.09	0.69
1:C:799:LYS:NZ	1:C:1620:GLN:OE1	2.24	0.69
1:A:4872:GLU:HG2	1:D:4874:ARG:CD	2.22	0.69
1:C:2832:THR:OG1	1:D:1548:THR:O	2.10	0.69
1:A:1949:GLN:O	1:A:1953:MET:HE2	1.93	0.69
1:B:1949:GLN:O	1:B:1953:MET:HE2	1.93	0.69
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.72	0.69
1:D:1947:VAL:HG23	1:D:1961:LYS:HB3	1.75	0.69
1:D:2332:GLY:H	1:D:2336:ARG:HH21	1.40	0.69
1:A:2690:GLU:HB2	1:A:2692:GLN:OE1	1.92	0.69
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.26	0.69
1:C:1949:GLN:O	1:C:1953:MET:HE2	1.93	0.69
1:A:1947:VAL:HG23	1:A:1961:LYS:HB3	1.75	0.68
1:A:2332:GLY:H	1:A:2336:ARG:HH21	1.40	0.68
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.26	0.68
1:C:4654:MET:HE3	1:C:4663:ARG:HE	1.58	0.68
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.26	0.68
1:B:1898:LEU:HD23	1:B:1902:VAL:HG12	1.76	0.68
1:C:2711:ILE:HG21	1:C:2783:LEU:HB2	1.76	0.68
1:B:2332:GLY:H	1:B:2336:ARG:HH21	1.40	0.68
1:B:4654:MET:HE3	1:B:4663:ARG:HE	1.58	0.68
1:A:4521:LYS:NZ	1:B:4807:ASP:HB3	2.08	0.68
1:B:1035:TYR:HA	1:B:1038:LEU:HD12	1.76	0.68
1:B:1947:VAL:HG23	1:B:1961:LYS:HB3	1.75	0.68
1:C:1035:TYR:HA	1:C:1038:LEU:HD12	1.76	0.68
1:B:2782:MET:HG2	1:B:2783:LEU:HD12	1.76	0.67
1:C:1947:VAL:HG23	1:C:1961:LYS:HB3	1.75	0.67
1:A:3043:ARG:HA	1:A:3046:MET:HE2	1.76	0.67
1:D:1265:HIS:O	1:D:1288:LYS:NZ	2.27	0.67
1:D:1949:GLN:O	1:D:1953:MET:HE2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2882:LYS:HB3	1:A:2886:ARG:HD3	1.76	0.67
1:B:2882:LYS:HB3	1:B:2886:ARG:HD3	1.76	0.67
1:C:2332:GLY:H	1:C:2336:ARG:HH21	1.40	0.67
1:A:4860:ALA:HB2	1:D:4863:GLN:HG2	1.76	0.67
1:B:3001:LYS:HD3	1:B:3044:THR:HG21	1.76	0.67
1:D:2782:MET:HG2	1:D:2783:LEU:HD12	1.76	0.67
1:A:4654:MET:HE3	1:A:4663:ARG:HE	1.58	0.67
1:D:1035:TYR:HA	1:D:1038:LEU:HD12	1.76	0.67
1:B:2576:ILE:O	1:B:2580:LEU:HB2	1.95	0.67
1:C:655:MET:HE1	1:C:836:HIS:CD2	2.30	0.67
1:C:2782:MET:HG2	1:C:2783:LEU:HD12	1.76	0.67
1:A:1035:TYR:HA	1:A:1038:LEU:HD12	1.76	0.67
1:D:2711:ILE:HG21	1:D:2783:LEU:HB2	1.76	0.67
1:B:476:GLN:NE2	1:B:3677:THR:HA	2.10	0.67
1:B:2711:ILE:HG21	1:B:2783:LEU:HB2	1.76	0.67
1:C:2502:LEU:HD21	1:C:2516:LEU:HD23	1.77	0.67
1:A:166:SER:OG	1:A:168:GLN:OE1	2.13	0.67
1:A:4011:GLU:HG2	1:A:4121:LEU:HD21	1.77	0.67
1:D:476:GLN:NE2	1:D:3677:THR:HA	2.10	0.67
1:D:1898:LEU:HD23	1:D:1902:VAL:HG12	1.76	0.67
1:A:476:GLN:NE2	1:A:3677:THR:HA	2.10	0.66
1:A:1265:HIS:O	1:A:1288:LYS:NZ	2.27	0.66
1:D:2576:ILE:O	1:D:2580:LEU:HB2	1.95	0.66
1:A:2576:ILE:O	1:A:2580:LEU:HB2	1.95	0.66
1:A:4810:LEU:HD13	1:D:4518:LEU:HD21	1.75	0.66
1:B:1844:GLN:NE2	1:B:1853:GLU:OE1	2.26	0.66
1:D:3001:LYS:HD3	1:D:3044:THR:HG21	1.76	0.66
1:A:2711:ILE:HG21	1:A:2783:LEU:HB2	1.76	0.66
1:B:1265:HIS:O	1:B:1288:LYS:NZ	2.27	0.66
1:C:2693:SER:OG	1:C:2704:GLN:NE2	2.28	0.66
1:D:2693:SER:OG	1:D:2704:GLN:NE2	2.28	0.66
1:D:4011:GLU:HG2	1:D:4121:LEU:HD21	1.77	0.66
1:B:4011:GLU:HG2	1:B:4121:LEU:HD21	1.77	0.66
1:D:3043:ARG:HA	1:D:3046:MET:HE2	1.76	0.66
1:A:2260:PRO:HA	1:A:2263:GLU:HG2	1.77	0.66
1:B:2756:LEU:HD13	1:B:2766:LYS:HE2	1.78	0.66
1:C:2576:ILE:O	1:C:2580:LEU:HB2	1.95	0.66
1:C:4011:GLU:HG2	1:C:4121:LEU:HD21	1.77	0.66
1:A:2693:SER:OG	1:A:2704:GLN:NE2	2.28	0.66
1:B:655:MET:HE1	1:B:836:HIS:CD2	2.30	0.66
1:B:2693:SER:OG	1:B:2704:GLN:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2756:LEU:HD13	1:C:2766:LYS:HE2	1.78	0.66
1:D:166:SER:OG	1:D:168:GLN:OE1	2.13	0.66
1:D:234:LEU:HD13	1:D:405:LEU:HD22	1.78	0.66
1:A:1898:LEU:HD23	1:A:1902:VAL:HG12	1.76	0.66
1:B:3900:GLU:OE2	1:B:3904:ARG:NH1	2.29	0.66
1:C:234:LEU:HD13	1:C:405:LEU:HD22	1.78	0.66
1:C:3900:GLU:OE2	1:C:3904:ARG:NH1	2.29	0.66
1:A:3001:LYS:HD3	1:A:3044:THR:HG21	1.76	0.66
1:A:3900:GLU:OE2	1:A:3904:ARG:NH1	2.29	0.66
1:B:3043:ARG:HA	1:B:3046:MET:HE2	1.76	0.66
1:C:2882:LYS:HB3	1:C:2886:ARG:HD3	1.76	0.66
1:D:655:MET:HE1	1:D:836:HIS:CD2	2.30	0.66
1:D:2717:LEU:HD12	1:D:2779:LEU:HD13	1.77	0.66
1:C:166:SER:OG	1:C:168:GLN:OE1	2.13	0.66
1:C:1898:LEU:HD23	1:C:1902:VAL:HG12	1.76	0.66
1:C:2717:LEU:HD12	1:C:2779:LEU:HD13	1.77	0.66
1:C:2958:GLN:HA	1:C:2961:LYS:HE2	1.78	0.66
1:C:3001:LYS:HD3	1:C:3044:THR:HG21	1.76	0.66
1:D:887:GLU:HA	1:D:890:HIS:CD2	2.31	0.66
1:A:267:VAL:HA	1:A:270:HIS:HD2	1.61	0.66
2:E:22:THR:HG22	2:E:50:ARG:HG2	1.79	0.66
1:A:2782:MET:HG2	1:A:2783:LEU:HD12	1.76	0.65
1:D:3900:GLU:OE2	1:D:3904:ARG:NH1	2.29	0.65
1:A:2648:ILE:O	1:A:2652:LEU:HB2	1.97	0.65
1:B:669:GLN:HE22	1:B:862:PHE:H	1.44	0.65
1:B:2648:ILE:O	1:B:2652:LEU:HB2	1.97	0.65
1:C:476:GLN:NE2	1:C:3677:THR:HA	2.10	0.65
1:C:669:GLN:HE22	1:C:862:PHE:H	1.44	0.65
1:C:1052:GLU:HA	1:C:1055:ARG:HG2	1.79	0.65
1:D:2582:PRO:HA	1:D:2585:MET:HG3	1.79	0.65
1:B:267:VAL:HA	1:B:270:HIS:HD2	1.61	0.65
1:C:2648:ILE:O	1:C:2652:LEU:HB2	1.97	0.65
1:A:655:MET:HE1	1:A:836:HIS:CD2	2.30	0.65
1:A:996:VAL:HG11	1:A:1051:ARG:HD2	1.78	0.65
1:A:1052:GLU:HA	1:A:1055:ARG:HG2	1.79	0.65
1:A:2502:LEU:HD21	1:A:2516:LEU:HD23	1.77	0.65
1:B:166:SER:OG	1:B:168:GLN:OE1	2.13	0.65
1:B:2717:LEU:HD12	1:B:2779:LEU:HD13	1.77	0.65
1:A:4521:LYS:HZ2	1:B:4807:ASP:HB3	1.61	0.65
1:C:887:GLU:HA	1:C:890:HIS:CD2	2.31	0.65
1:C:2582:PRO:HA	1:C:2585:MET:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:996:VAL:HG11	1:B:1051:ARG:HD2	1.79	0.65
1:B:2154:VAL:HG13	1:B:2158:HIS:HD2	1.62	0.65
1:C:1265:HIS:O	1:C:1288:LYS:NZ	2.27	0.65
1:C:2933:VAL:HA	1:C:2963:PHE:HZ	1.62	0.65
1:D:1052:GLU:HA	1:D:1055:ARG:HG2	1.78	0.65
1:D:2648:ILE:O	1:D:2652:LEU:HB2	1.97	0.65
1:A:2958:GLN:HA	1:A:2961:LYS:HE2	1.78	0.65
2:F:22:THR:HG22	2:F:50:ARG:HG2	1.79	0.65
2:H:22:THR:HG22	2:H:50:ARG:HG2	1.79	0.65
1:B:1052:GLU:HA	1:B:1055:ARG:HG2	1.79	0.65
1:B:2502:LEU:HD21	1:B:2516:LEU:HD23	1.77	0.65
1:D:2882:LYS:HB3	1:D:2886:ARG:HD3	1.76	0.65
1:A:2756:LEU:HD13	1:A:2766:LYS:HE2	1.78	0.65
1:B:2958:GLN:HA	1:B:2961:LYS:HE2	1.78	0.65
1:B:4255:LEU:HB2	1:B:4293:THR:HG21	1.78	0.65
1:C:2154:VAL:HG13	1:C:2158:HIS:HD2	1.62	0.65
1:A:2717:LEU:HD12	1:A:2779:LEU:HD13	1.77	0.65
1:B:298:ARG:HH12	1:B:417:ARG:HH12	1.45	0.65
1:B:2582:PRO:HA	1:B:2585:MET:HG3	1.79	0.65
1:C:2260:PRO:HA	1:C:2263:GLU:HG2	1.77	0.65
1:D:2502:LEU:HD21	1:D:2516:LEU:HD23	1.77	0.65
1:A:298:ARG:HH12	1:A:417:ARG:HH12	1.45	0.65
1:A:2154:VAL:HG13	1:A:2158:HIS:HD2	1.62	0.65
1:C:3043:ARG:HA	1:C:3046:MET:HE2	1.76	0.65
1:D:298:ARG:HH12	1:D:417:ARG:HH12	1.45	0.65
1:D:2933:VAL:HA	1:D:2963:PHE:HZ	1.62	0.65
1:D:2958:GLN:HA	1:D:2961:LYS:HE2	1.78	0.65
1:D:4255:LEU:HB2	1:D:4293:THR:HG21	1.78	0.65
1:A:234:LEU:HD13	1:A:405:LEU:HD22	1.78	0.64
1:A:887:GLU:HA	1:A:890:HIS:CD2	2.31	0.64
1:B:234:LEU:HD13	1:B:405:LEU:HD22	1.78	0.64
1:D:2756:LEU:HD13	1:D:2766:LYS:HE2	1.78	0.64
1:A:669:GLN:HE22	1:A:862:PHE:H	1.44	0.64
1:C:1502:ASN:OD1	1:C:1503:ASN:N	2.30	0.64
1:D:1502:ASN:OD1	1:D:1503:ASN:N	2.30	0.64
1:A:1502:ASN:OD1	1:A:1503:ASN:N	2.30	0.64
1:A:4031:THR:HA	1:A:4034:GLU:HG2	1.80	0.64
1:B:2593:VAL:HA	1:B:2644:LEU:HD13	1.78	0.64
1:C:4031:THR:HA	1:C:4034:GLU:HG2	1.80	0.64
1:D:2260:PRO:HA	1:D:2263:GLU:HG2	1.77	0.64
1:A:2933:VAL:HA	1:A:2963:PHE:HZ	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:22:THR:HG22	2:G:50:ARG:HG2	1.79	0.64
1:C:298:ARG:HH12	1:C:417:ARG:HH12	1.45	0.64
1:D:2593:VAL:HA	1:D:2644:LEU:HD13	1.78	0.64
1:A:4255:LEU:HB2	1:A:4293:THR:HG21	1.78	0.64
1:B:2260:PRO:HA	1:B:2263:GLU:HG2	1.77	0.64
1:B:2927:GLN:HE21	1:B:3003:MET:HE3	1.63	0.64
1:D:669:GLN:HE22	1:D:862:PHE:H	1.44	0.64
1:C:4049:HIS:HD2	1:C:4067:LEU:HD11	1.63	0.64
1:D:996:VAL:HG11	1:D:1051:ARG:HD2	1.78	0.64
1:B:887:GLU:HA	1:B:890:HIS:CD2	2.31	0.64
1:B:1502:ASN:OD1	1:B:1503:ASN:N	2.30	0.64
1:C:4255:LEU:HB2	1:C:4293:THR:HG21	1.78	0.64
1:D:267:VAL:HA	1:D:270:HIS:HD2	1.62	0.64
1:A:2582:PRO:HA	1:A:2585:MET:HG3	1.79	0.64
1:A:2927:GLN:HE21	1:A:3003:MET:HE3	1.63	0.64
1:A:4618:THR:OG1	1:A:4619:GLU:OE1	2.15	0.64
1:D:4031:THR:HA	1:D:4034:GLU:HG2	1.80	0.64
1:B:4031:THR:HA	1:B:4034:GLU:HG2	1.80	0.64
1:C:2688:MET:HG2	1:C:2689:MET:HG3	1.80	0.64
1:D:1844:GLN:NE2	1:D:1853:GLU:OE1	2.26	0.64
1:D:2154:VAL:HG13	1:D:2158:HIS:HD2	1.62	0.64
1:A:2688:MET:HG2	1:A:2689:MET:HG3	1.80	0.64
1:B:2933:VAL:HA	1:B:2963:PHE:HZ	1.62	0.64
1:C:267:VAL:HA	1:C:270:HIS:HD2	1.61	0.64
1:D:2927:GLN:HE21	1:D:3003:MET:HE3	1.63	0.64
1:A:2593:VAL:HA	1:A:2644:LEU:HD13	1.78	0.63
1:B:4049:HIS:HD2	1:B:4067:LEU:HD11	1.63	0.63
1:C:425:LEU:HD12	1:C:428:ARG:HD3	1.80	0.63
1:C:694:ARG:NH1	1:C:718:VAL:O	2.31	0.63
1:C:996:VAL:HG11	1:C:1051:ARG:HD2	1.78	0.63
1:C:2593:VAL:HA	1:C:2644:LEU:HD13	1.78	0.63
1:D:312:LYS:HG3	1:D:370:LEU:HD13	1.80	0.63
1:B:601:LEU:HB2	1:B:610:VAL:HG11	1.80	0.63
1:B:2793:ARG:HG2	1:B:2793:ARG:HH11	1.63	0.63
1:C:1989:PRO:HD2	1:C:1992:ILE:HD12	1.80	0.63
1:C:2927:GLN:HE21	1:C:3003:MET:HE3	1.63	0.63
1:A:601:LEU:HB2	1:A:610:VAL:HG11	1.81	0.63
1:B:694:ARG:NH1	1:B:718:VAL:O	2.32	0.63
1:B:2688:MET:HG2	1:B:2689:MET:HG3	1.80	0.63
1:C:1844:GLN:NE2	1:C:1853:GLU:OE1	2.26	0.63
1:D:601:LEU:HB2	1:D:610:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1989:PRO:HD2	1:A:1992:ILE:HD12	1.80	0.63
1:D:2688:MET:HG2	1:D:2689:MET:HG3	1.80	0.63
1:B:194:LEU:HD11	1:B:201:LEU:HB3	1.81	0.63
1:B:425:LEU:HD12	1:B:428:ARG:HD3	1.80	0.63
1:A:2129:LEU:HA	1:A:2132:VAL:HG22	1.81	0.63
1:B:466:PRO:HG2	1:B:479:LEU:HD12	1.81	0.63
1:D:3604:ARG:O	1:D:3605:MET:HE2	1.99	0.63
1:B:218:SER:HB3	1:B:286:GLY:HA3	1.80	0.63
1:B:776:GLN:OE1	1:B:776:GLN:N	2.32	0.63
1:A:694:ARG:NH1	1:A:718:VAL:O	2.32	0.62
1:A:3604:ARG:O	1:A:3605:MET:HE2	1.99	0.62
1:A:4049:HIS:HD2	1:A:4067:LEU:HD11	1.63	0.62
1:D:776:GLN:N	1:D:776:GLN:OE1	2.32	0.62
1:A:1844:GLN:NE2	1:A:1853:GLU:OE1	2.26	0.62
1:A:4864:GLY:HA3	1:D:4867:ILE:HG12	1.79	0.62
1:D:218:SER:HB3	1:D:286:GLY:HA3	1.80	0.62
1:A:312:LYS:HG3	1:A:370:LEU:HD13	1.80	0.62
1:B:1482:ARG:NH1	1:B:1534:GLU:OE2	2.33	0.62
1:B:3604:ARG:O	1:B:3605:MET:HE2	1.99	0.62
1:D:425:LEU:HD12	1:D:428:ARG:HD3	1.80	0.62
1:A:218:SER:HB3	1:A:286:GLY:HA3	1.80	0.62
1:A:466:PRO:HG2	1:A:479:LEU:HD12	1.81	0.62
1:A:4245:LEU:HD11	1:B:4626:ILE:HG13	1.82	0.62
1:C:194:LEU:HD11	1:C:201:LEU:HB3	1.81	0.62
1:D:998:LYS:HA	1:D:1001:GLU:HG2	1.81	0.62
1:D:2711:ILE:HG23	1:D:2783:LEU:HD22	1.81	0.62
1:D:4049:HIS:HD2	1:D:4067:LEU:HD11	1.63	0.62
1:A:882:ARG:NH1	1:A:933:LEU:HD22	2.15	0.62
1:B:2126:ILE:HA	1:B:2142:MET:HE1	1.81	0.62
1:C:218:SER:HB3	1:C:286:GLY:HA3	1.80	0.62
1:A:1026:ASN:HB3	1:A:1028:ARG:HG2	1.82	0.62
1:C:1113:MET:HB2	1:C:1156:TRP:CZ2	2.35	0.62
1:C:2126:ILE:HA	1:C:2142:MET:HE1	1.81	0.62
1:C:2129:LEU:HA	1:C:2132:VAL:HG22	1.81	0.62
1:C:2711:ILE:HG23	1:C:2783:LEU:HD22	1.81	0.62
1:C:4618:THR:OG1	1:C:4619:GLU:OE1	2.15	0.62
1:D:882:ARG:NH1	1:D:933:LEU:HD22	2.15	0.62
1:D:4046:ARG:NE	1:D:4046:ARG:HA	2.15	0.62
1:A:1113:MET:HB2	1:A:1156:TRP:CZ2	2.35	0.62
1:B:1989:PRO:HD2	1:B:1992:ILE:HD12	1.80	0.62
1:B:2322:ARG:HH12	1:C:189:GLU:HG3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4618:THR:OG1	1:B:4619:GLU:OE1	2.15	0.62
1:C:466:PRO:HG2	1:C:479:LEU:HD12	1.81	0.62
1:D:4617:ILE:HG12	1:D:4666:ILE:HD11	1.82	0.62
1:A:972:LEU:HD23	1:A:974:SER:H	1.65	0.62
1:C:882:ARG:NH1	1:C:933:LEU:HD22	2.15	0.62
1:C:2793:ARG:HG2	1:C:2793:ARG:HH11	1.64	0.62
1:D:1113:MET:HB2	1:D:1156:TRP:CZ2	2.35	0.62
1:D:1989:PRO:HD2	1:D:1992:ILE:HD12	1.80	0.62
1:A:1482:ARG:NH1	1:A:1534:GLU:OE2	2.33	0.62
1:A:4872:GLU:HG2	1:D:4874:ARG:HD2	1.80	0.62
1:B:882:ARG:NH1	1:B:933:LEU:HD22	2.15	0.62
1:B:1303:ARG:NH1	1:B:1589:GLN:OE1	2.32	0.62
1:C:312:LYS:HG3	1:C:370:LEU:HD13	1.80	0.62
1:C:601:LEU:HB2	1:C:610:VAL:HG11	1.81	0.62
1:C:1303:ARG:NH1	1:C:1589:GLN:OE1	2.32	0.62
1:D:194:LEU:HD11	1:D:201:LEU:HB3	1.81	0.62
1:D:1026:ASN:HB3	1:D:1028:ARG:HG2	1.82	0.62
1:A:2793:ARG:HG2	1:A:2793:ARG:HH11	1.64	0.62
1:A:4617:ILE:HG12	1:A:4666:ILE:HD11	1.82	0.62
1:B:312:LYS:HG3	1:B:370:LEU:HD13	1.80	0.62
1:B:940:LEU:HA	1:B:943:LEU:HD12	1.82	0.62
1:B:1249:MET:HB2	1:B:1599:MET:HE2	1.82	0.62
1:B:2898:ILE:HG23	1:C:1500:ARG:HH22	1.64	0.62
1:B:4046:ARG:NE	1:B:4046:ARG:HA	2.15	0.62
1:B:4617:ILE:HG12	1:B:4666:ILE:HD11	1.82	0.62
1:C:972:LEU:HD23	1:C:974:SER:H	1.65	0.62
1:C:1249:MET:HB2	1:C:1599:MET:HE2	1.82	0.62
1:C:3604:ARG:O	1:C:3605:MET:HE2	1.99	0.62
1:D:1303:ARG:NH1	1:D:1589:GLN:OE1	2.32	0.62
1:D:4819:VAL:HG12	1:D:4822:ARG:HH21	1.65	0.62
1:A:1434:PRO:O	1:D:2830:ASN:ND2	2.33	0.61
1:D:2129:LEU:HA	1:D:2132:VAL:HG22	1.81	0.61
1:A:2797:SER:HB3	1:A:2801:TYR:CE2	2.35	0.61
1:A:4279:MET:HE2	1:B:4487:TYR:HD1	1.64	0.61
1:B:2797:SER:HB3	1:B:2801:TYR:CE2	2.35	0.61
1:B:2956:TYR:O	1:B:2960:ILE:HG22	2.00	0.61
1:C:4046:ARG:HA	1:C:4046:ARG:NE	2.15	0.61
1:D:4004:VAL:HG11	1:D:4114:ARG:HD2	1.82	0.61
1:A:902:TRP:HZ2	1:A:915:HIS:HB3	1.65	0.61
1:A:998:LYS:HA	1:A:1001:GLU:HG2	1.82	0.61
1:A:4004:VAL:HG11	1:A:4114:ARG:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4046:ARG:NE	1:A:4046:ARG:HA	2.15	0.61
1:B:2711:ILE:HG23	1:B:2783:LEU:HD22	1.81	0.61
1:C:940:LEU:HA	1:C:943:LEU:HD12	1.82	0.61
1:D:1482:ARG:NH1	1:D:1534:GLU:OE2	2.33	0.61
1:D:2126:ILE:HA	1:D:2142:MET:HE1	1.81	0.61
1:D:3729:ALA:HA	1:D:3732:HIS:CE1	2.36	0.61
1:A:1303:ARG:NH1	1:A:1589:GLN:OE1	2.33	0.61
1:B:2129:LEU:HA	1:B:2132:VAL:HG22	1.81	0.61
1:C:2797:SER:HB3	1:C:2801:TYR:CE2	2.35	0.61
1:D:694:ARG:NH1	1:D:718:VAL:O	2.31	0.61
1:A:425:LEU:HD12	1:A:428:ARG:HD3	1.80	0.61
1:A:2926:LEU:HB3	1:A:3003:MET:HE1	1.83	0.61
1:B:4819:VAL:HG12	1:B:4822:ARG:HH21	1.65	0.61
1:C:776:GLN:OE1	1:C:776:GLN:N	2.32	0.61
1:C:902:TRP:HZ2	1:C:915:HIS:HB3	1.64	0.61
1:C:998:LYS:HA	1:C:1001:GLU:HG2	1.82	0.61
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.34	0.61
1:A:4814:MET:HA	1:A:4817:MET:HB2	1.83	0.61
1:B:3729:ALA:HA	1:B:3732:HIS:CE1	2.36	0.61
1:C:4819:VAL:HG12	1:C:4822:ARG:HH21	1.65	0.61
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.34	0.61
1:D:466:PRO:HG2	1:D:479:LEU:HD12	1.81	0.61
1:D:2926:LEU:HB3	1:D:3003:MET:HE1	1.83	0.61
1:D:3034:HIS:O	1:D:3038:GLN:NE2	2.34	0.61
1:D:4618:THR:OG1	1:D:4619:GLU:OE1	2.15	0.61
1:A:194:LEU:HD11	1:A:201:LEU:HB3	1.81	0.61
1:A:4819:VAL:HG12	1:A:4822:ARG:HH21	1.65	0.61
1:B:972:LEU:HD23	1:B:974:SER:H	1.65	0.61
1:B:1113:MET:HB2	1:B:1156:TRP:CZ2	2.35	0.61
1:D:2779:LEU:O	1:D:2782:MET:HG2	2.01	0.61
1:B:4814:MET:HA	1:B:4817:MET:HB2	1.83	0.61
1:C:3034:HIS:O	1:C:3038:GLN:NE2	2.34	0.61
1:D:972:LEU:HD23	1:D:974:SER:H	1.65	0.61
1:D:1249:MET:HB2	1:D:1599:MET:HE2	1.82	0.61
1:A:2787:TRP:HD1	1:A:2906:GLY:N	1.99	0.61
1:B:902:TRP:HZ2	1:B:915:HIS:HB3	1.64	0.61
1:B:2779:LEU:O	1:B:2782:MET:HG2	2.01	0.61
1:A:776:GLN:N	1:A:776:GLN:OE1	2.32	0.61
1:A:842:GLN:HB2	1:A:1603:PHE:HB2	1.83	0.61
1:A:3034:HIS:O	1:A:3038:GLN:NE2	2.34	0.61
1:A:4864:GLY:HA2	1:D:4867:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.34	0.61
1:B:4004:VAL:HG11	1:B:4114:ARG:HD2	1.82	0.61
1:C:1026:ASN:HB3	1:C:1028:ARG:HG2	1.82	0.61
1:C:3729:ALA:HA	1:C:3732:HIS:CE1	2.36	0.61
1:C:4617:ILE:HG12	1:C:4666:ILE:HD11	1.82	0.61
1:D:2797:SER:HB3	1:D:2801:TYR:CE2	2.35	0.61
1:A:2779:LEU:O	1:A:2782:MET:HG2	2.01	0.60
1:B:3034:HIS:O	1:B:3038:GLN:NE2	2.34	0.60
1:C:1482:ARG:NH1	1:C:1534:GLU:OE2	2.33	0.60
1:D:2956:TYR:O	1:D:2960:ILE:HG22	2.00	0.60
1:A:2711:ILE:HG23	1:A:2783:LEU:HD22	1.81	0.60
1:B:1606:VAL:HG12	1:B:1621:CYS:HB2	1.83	0.60
1:C:2956:TYR:O	1:C:2960:ILE:HG22	2.00	0.60
1:D:2793:ARG:HG2	1:D:2793:ARG:HH11	1.64	0.60
1:A:2956:TYR:O	1:A:2960:ILE:HG22	2.00	0.60
1:A:940:LEU:HA	1:A:943:LEU:HD12	1.82	0.60
1:A:1249:MET:HB2	1:A:1599:MET:HE2	1.82	0.60
1:A:2187:ILE:HG13	1:A:2227:VAL:HG13	1.83	0.60
1:A:3729:ALA:HA	1:A:3732:HIS:CE1	2.36	0.60
1:C:2187:ILE:HG13	1:C:2227:VAL:HG13	1.83	0.60
1:C:2926:LEU:HB3	1:C:3003:MET:HE1	1.83	0.60
1:C:3890:TRP:O	1:D:76:ARG:NH2	2.34	0.60
1:C:4004:VAL:HG11	1:C:4114:ARG:HD2	1.82	0.60
1:D:902:TRP:HZ2	1:D:915:HIS:HB3	1.65	0.60
1:D:2187:ILE:HG13	1:D:2227:VAL:HG13	1.83	0.60
1:A:1606:VAL:HG12	1:A:1621:CYS:HB2	1.83	0.60
1:B:998:LYS:HA	1:B:1001:GLU:HG2	1.82	0.60
1:D:2787:TRP:HD1	1:D:2906:GLY:N	1.99	0.60
1:A:4737:PHE:CD2	1:B:4783:VAL:HG13	2.36	0.60
1:B:1026:ASN:HB3	1:B:1028:ARG:HG2	1.82	0.60
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.34	0.60
1:D:2318:ASN:O	1:D:2322:ARG:HG3	2.01	0.60
1:A:2126:ILE:HA	1:A:2142:MET:HE1	1.81	0.60
1:D:940:LEU:HA	1:D:943:LEU:HD12	1.82	0.60
1:D:4814:MET:HA	1:D:4817:MET:HB2	1.83	0.60
1:A:2318:ASN:O	1:A:2322:ARG:HG3	2.01	0.60
1:C:1606:VAL:HG12	1:C:1621:CYS:HB2	1.83	0.60
1:B:2857:LYS:CE	1:B:2871:LEU:HD23	2.30	0.60
1:D:842:GLN:HB2	1:D:1603:PHE:HB2	1.83	0.60
1:A:1685:LEU:O	1:A:1689:ILE:HG12	2.02	0.59
2:H:69:LEU:HA	2:H:104:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1113:MET:HB2	1:B:1156:TRP:HZ2	1.67	0.59
1:B:1685:LEU:O	1:B:1689:ILE:HG12	2.02	0.59
1:B:2926:LEU:HB3	1:B:3003:MET:HE1	1.82	0.59
1:C:1113:MET:HB2	1:C:1156:TRP:HZ2	1.67	0.59
1:C:2779:LEU:O	1:C:2782:MET:HG2	2.01	0.59
1:C:810:GLU:OE1	1:C:810:GLU:N	2.35	0.59
1:C:2787:TRP:HD1	1:C:2906:GLY:N	1.99	0.59
1:C:4814:MET:HA	1:C:4817:MET:HB2	1.83	0.59
1:D:2765:GLU:HA	1:D:2768:LYS:HZ1	1.67	0.59
2:F:69:LEU:HA	2:F:104:LEU:HD23	1.85	0.59
1:B:842:GLN:HB2	1:B:1603:PHE:HB2	1.83	0.59
1:D:1785:ASP:OD1	1:D:1786:ILE:N	2.36	0.59
1:C:2318:ASN:O	1:C:2322:ARG:HG3	2.01	0.59
1:A:1113:MET:HB2	1:A:1156:TRP:HZ2	1.67	0.59
1:B:2318:ASN:O	1:B:2322:ARG:HG3	2.01	0.59
1:D:1606:VAL:HG12	1:D:1621:CYS:HB2	1.83	0.59
1:C:2146:LEU:O	1:C:2150:MET:HG2	2.03	0.59
1:A:4844:ILE:HG21	1:D:4814:MET:CE	2.33	0.59
1:B:2773:TRP:HB3	1:B:2774:PRO:HD3	1.85	0.59
1:A:2202:TYR:O	1:A:2206:ILE:HG12	2.03	0.59
1:A:2441:GLN:NE2	1:A:2442:MET:O	2.36	0.59
2:G:69:LEU:HA	2:G:104:LEU:HD23	1.85	0.59
1:B:810:GLU:N	1:B:810:GLU:OE1	2.35	0.59
1:C:1685:LEU:O	1:C:1689:ILE:HG12	2.02	0.59
1:C:2773:TRP:HB3	1:C:2774:PRO:HD3	1.85	0.59
1:C:3999:MET:HG3	1:C:4002:MET:HE3	1.84	0.59
1:D:810:GLU:OE1	1:D:810:GLU:N	2.35	0.59
1:D:1113:MET:HB2	1:D:1156:TRP:HZ2	1.67	0.59
1:D:2146:LEU:O	1:D:2150:MET:HG2	2.03	0.59
1:D:2441:GLN:NE2	1:D:2442:MET:O	2.36	0.59
2:E:69:LEU:HA	2:E:104:LEU:HD23	1.84	0.59
1:C:310:GLU:OE2	1:C:310:GLU:N	2.34	0.59
1:D:1950:ALA:HB1	1:D:1961:LYS:NZ	2.18	0.59
1:A:1785:ASP:OD1	1:A:1786:ILE:N	2.36	0.59
1:B:2187:ILE:HG13	1:B:2227:VAL:HG13	1.83	0.59
1:C:842:GLN:HB2	1:C:1603:PHE:HB2	1.83	0.59
1:C:4187:GLU:OE1	1:C:4949:TRP:NE1	2.35	0.59
1:A:191:TYR:CD1	1:A:209:GLN:HG3	2.38	0.58
1:B:3999:MET:HG3	1:B:4002:MET:HE3	1.84	0.58
1:C:2441:GLN:NE2	1:C:2442:MET:O	2.36	0.58
1:D:1685:LEU:O	1:D:1689:ILE:HG12	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:GLU:OE1	1:A:810:GLU:N	2.35	0.58
1:B:885:LEU:O	1:B:889:ILE:HG12	2.03	0.58
1:B:1043:LYS:HA	1:B:1046:ASN:HD21	1.68	0.58
1:C:1785:ASP:OD1	1:C:1786:ILE:N	2.36	0.58
1:D:191:TYR:CD1	1:D:209:GLN:HG3	2.38	0.58
1:A:2146:LEU:O	1:A:2150:MET:HG2	2.03	0.58
1:C:562:LEU:HG	1:C:600:LEU:HD13	1.85	0.58
1:C:1043:LYS:HA	1:C:1046:ASN:HD21	1.68	0.58
1:D:2773:TRP:HB3	1:D:2774:PRO:HD3	1.85	0.58
1:A:1950:ALA:HB1	1:A:1961:LYS:NZ	2.18	0.58
1:D:2202:TYR:O	1:D:2206:ILE:HG12	2.03	0.58
1:D:2905:ARG:HH11	1:D:2906:GLY:H	1.52	0.58
1:B:1670:HIS:O	1:B:1674:HIS:ND1	2.32	0.58
1:B:1950:ALA:HB1	1:B:1961:LYS:NZ	2.18	0.58
1:B:2441:GLN:NE2	1:B:2442:MET:O	2.36	0.58
1:D:4517:LEU:HD21	1:D:4736:ASN:HB3	1.86	0.58
1:A:2834:SER:OG	1:A:2836:ASP:OD1	2.20	0.58
1:C:4517:LEU:HD21	1:C:4736:ASN:HB3	1.86	0.58
1:A:4818:TYR:CD1	1:B:4848:ILE:HD11	2.37	0.58
1:B:2146:LEU:O	1:B:2150:MET:HG2	2.03	0.58
1:C:2905:ARG:HH11	1:C:2906:GLY:H	1.52	0.58
1:D:1102:TYR:N	1:D:1237:GLU:O	2.37	0.58
1:A:76:ARG:NH2	1:D:3890:TRP:O	2.36	0.58
1:A:885:LEU:O	1:A:889:ILE:HG12	2.03	0.58
1:A:1255:LEU:HD11	1:A:1451:HIS:HB3	1.86	0.58
1:A:3999:MET:HG3	1:A:4002:MET:HE3	1.84	0.58
1:D:2834:SER:OG	1:D:2836:ASP:OD1	2.19	0.58
1:A:3845:LEU:HD23	1:A:3848:GLU:HG3	1.86	0.58
1:B:4517:LEU:HD21	1:B:4736:ASN:HB3	1.86	0.58
1:C:2307:PHE:HB2	1:C:2401:ARG:HB3	1.86	0.58
1:D:881:ILE:HG13	1:D:885:LEU:HG	1.86	0.58
1:A:4870:PHE:HD2	1:B:4868:ASP:OD2	1.87	0.58
1:B:191:TYR:CD1	1:B:209:GLN:HG3	2.38	0.58
1:B:310:GLU:OE2	1:B:310:GLU:N	2.34	0.58
1:C:191:TYR:CD1	1:C:209:GLN:HG3	2.38	0.58
1:C:1102:TYR:N	1:C:1237:GLU:O	2.37	0.58
1:C:2202:TYR:O	1:C:2206:ILE:HG12	2.03	0.58
1:C:2877:LEU:O	1:C:2882:LYS:NZ	2.37	0.58
1:C:4116:GLN:HA	1:C:4119:LEU:HD12	1.85	0.58
1:D:562:LEU:HG	1:D:600:LEU:HD13	1.85	0.58
1:D:3999:MET:HG3	1:D:4002:MET:HE3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:LYS:HA	1:A:1046:ASN:HD21	1.68	0.57
1:A:2773:TRP:HB3	1:A:2774:PRO:HD3	1.85	0.57
1:B:1255:LEU:HD11	1:B:1451:HIS:HB3	1.86	0.57
1:B:1785:ASP:OD1	1:B:1786:ILE:N	2.36	0.57
1:B:2787:TRP:HD1	1:B:2906:GLY:N	1.99	0.57
1:B:2832:THR:HG21	1:C:1550:PRO:HD3	1.86	0.57
1:B:2877:LEU:O	1:B:2882:LYS:NZ	2.36	0.57
1:B:2905:ARG:HH11	1:B:2906:GLY:H	1.52	0.57
1:C:1950:ALA:HB1	1:C:1961:LYS:NZ	2.18	0.57
1:D:885:LEU:O	1:D:889:ILE:HG12	2.03	0.57
1:A:2877:LEU:O	1:A:2882:LYS:NZ	2.36	0.57
1:B:2202:TYR:O	1:B:2206:ILE:HG12	2.03	0.57
1:C:885:LEU:O	1:C:889:ILE:HG12	2.03	0.57
1:D:4116:GLN:HA	1:D:4119:LEU:HD12	1.85	0.57
1:A:1217:PHE:HE2	1:A:1249:MET:HE1	1.70	0.57
1:A:2905:ARG:HH11	1:A:2906:GLY:H	1.52	0.57
1:A:4914:ASN:HB3	1:A:4917:ASN:HB2	1.87	0.57
1:B:562:LEU:HG	1:B:600:LEU:HD13	1.85	0.57
1:C:2894:LYS:O	1:C:2898:ILE:HG12	2.05	0.57
1:C:4144:ARG:NH2	1:C:4962:TYR:OH	2.34	0.57
1:D:1689:ILE:HA	1:D:1703:TYR:HE1	1.69	0.57
1:D:2790:GLU:N	1:D:2902:ALA:O	2.33	0.57
1:A:562:LEU:HG	1:A:600:LEU:HD13	1.85	0.57
1:A:4517:LEU:HD21	1:A:4736:ASN:HB3	1.86	0.57
1:C:3845:LEU:HD23	1:C:3848:GLU:HG3	1.86	0.57
1:D:4245:LEU:O	1:D:4249:ARG:HG3	2.04	0.57
1:A:881:ILE:HG13	1:A:885:LEU:HG	1.86	0.57
1:A:1689:ILE:HA	1:A:1703:TYR:HE1	1.69	0.57
1:B:891:GLU:O	1:B:895:MET:HG3	2.05	0.57
1:C:874:LEU:HD23	1:C:941:LYS:HD3	1.86	0.57
1:C:1255:LEU:HD11	1:C:1451:HIS:HB3	1.86	0.57
1:D:670:TYR:HD1	1:D:1017:THR:HG21	1.70	0.57
1:D:874:LEU:HD23	1:D:941:LYS:HD3	1.86	0.57
1:D:1043:LYS:HA	1:D:1046:ASN:HD21	1.68	0.57
1:D:4187:GLU:OE1	1:D:4949:TRP:NE1	2.35	0.57
1:A:4116:GLN:HA	1:A:4119:LEU:HD12	1.85	0.57
1:B:3778:LEU:HD13	1:B:3854:PHE:HD1	1.70	0.57
1:B:4116:GLN:HA	1:B:4119:LEU:HD12	1.85	0.57
1:B:4245:LEU:O	1:B:4249:ARG:HG3	2.04	0.57
1:C:881:ILE:HG13	1:C:885:LEU:HG	1.86	0.57
1:D:2877:LEU:O	1:D:2882:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2307:PHE:HB2	1:B:2401:ARG:HB3	1.86	0.57
1:C:3778:LEU:HD13	1:C:3854:PHE:HD1	1.70	0.57
1:D:317:MET:HE2	1:D:321:LYS:HG3	1.86	0.57
1:D:3845:LEU:HD23	1:D:3848:GLU:HG3	1.86	0.57
1:A:989:THR:OG1	1:A:992:GLN:HG3	2.05	0.57
1:A:2790:GLU:N	1:A:2902:ALA:O	2.33	0.57
1:B:262:TYR:HB2	1:B:389:ARG:HG3	1.86	0.57
1:B:874:LEU:HD23	1:B:941:LYS:HD3	1.86	0.57
1:B:4914:ASN:HB3	1:B:4917:ASN:HB2	1.87	0.57
1:C:670:TYR:HD1	1:C:1017:THR:HG21	1.69	0.57
1:C:4245:LEU:O	1:C:4249:ARG:HG3	2.04	0.57
1:D:1217:PHE:HE2	1:D:1249:MET:HE1	1.70	0.57
1:D:4914:ASN:HB3	1:D:4917:ASN:HB2	1.87	0.57
1:A:2857:LYS:CE	1:A:2871:LEU:HD23	2.30	0.57
1:B:4481:TRP:CD1	1:B:4692:SER:HA	2.40	0.57
1:C:317:MET:HE2	1:C:321:LYS:HG3	1.86	0.57
1:C:1217:PHE:HE2	1:C:1249:MET:HE1	1.70	0.57
1:C:2765:GLU:HA	1:C:2768:LYS:HZ1	1.69	0.57
1:D:2757:MET:O	1:D:2820:GLY:N	2.38	0.57
1:A:874:LEU:HD23	1:A:941:LYS:HD3	1.86	0.57
1:A:891:GLU:O	1:A:895:MET:HG3	2.05	0.57
1:A:2757:MET:O	1:A:2820:GLY:N	2.38	0.57
1:B:989:THR:OG1	1:B:992:GLN:HG3	2.05	0.57
1:C:891:GLU:O	1:C:895:MET:HG3	2.05	0.57
1:C:2757:MET:O	1:C:2820:GLY:N	2.38	0.57
1:C:4481:TRP:CD1	1:C:4692:SER:HA	2.40	0.57
1:D:891:GLU:HA	1:D:894:VAL:HG22	1.87	0.57
1:B:1217:PHE:HE2	1:B:1249:MET:HE1	1.70	0.56
1:D:2307:PHE:HB2	1:D:2401:ARG:HB3	1.86	0.56
1:A:891:GLU:HA	1:A:894:VAL:HG22	1.87	0.56
1:B:1689:ILE:HA	1:B:1703:TYR:HE1	1.69	0.56
1:B:4026:LEU:HD13	1:B:4055:HIS:CG	2.40	0.56
1:C:204:ASP:OD1	1:C:205:ALA:N	2.38	0.56
1:C:1250:TRP:HE3	1:C:1596:TRP:HB3	1.70	0.56
1:D:989:THR:OG1	1:D:992:GLN:HG3	2.05	0.56
1:D:3022:PHE:HB2	1:D:3026:ALA:HB2	1.86	0.56
1:A:1250:TRP:HE3	1:A:1596:TRP:HB3	1.70	0.56
1:A:4026:LEU:HD13	1:A:4055:HIS:CG	2.40	0.56
1:A:4481:TRP:CD1	1:A:4692:SER:HA	2.40	0.56
1:A:4868:ASP:O	1:A:4872:GLU:HG3	2.05	0.56
1:B:204:ASP:OD1	1:B:205:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2757:MET:O	1:B:2820:GLY:N	2.38	0.56
1:B:2855:LYS:HA	1:B:2858:MET:HG2	1.87	0.56
1:B:2894:LYS:O	1:B:2898:ILE:HG12	2.05	0.56
1:B:3022:PHE:HB2	1:B:3026:ALA:HB2	1.86	0.56
1:C:4814:MET:CE	1:D:4844:ILE:HD13	2.22	0.56
1:D:891:GLU:O	1:D:895:MET:HG3	2.05	0.56
1:D:1670:HIS:O	1:D:1674:HIS:ND1	2.32	0.56
1:D:2708:THR:O	1:D:2780:LYS:HD2	2.06	0.56
1:D:4026:LEU:HD13	1:D:4055:HIS:CG	2.40	0.56
1:D:4481:TRP:CD1	1:D:4692:SER:HA	2.40	0.56
1:A:204:ASP:OD1	1:A:205:ALA:N	2.38	0.56
1:A:262:TYR:HB2	1:A:389:ARG:HG3	1.86	0.56
1:A:4245:LEU:O	1:A:4249:ARG:HG3	2.04	0.56
1:B:881:ILE:HG13	1:B:885:LEU:HG	1.86	0.56
1:B:2440:PHE:HB3	1:B:2460:PHE:HD2	1.71	0.56
1:B:4868:ASP:O	1:B:4872:GLU:HG3	2.05	0.56
1:C:989:THR:OG1	1:C:992:GLN:HG3	2.05	0.56
1:C:1689:ILE:HA	1:C:1703:TYR:HE1	1.69	0.56
1:C:2440:PHE:HB3	1:C:2460:PHE:HD2	1.71	0.56
1:C:4279:MET:HE3	1:D:4488:GLN:HG3	1.88	0.56
1:D:2894:LYS:O	1:D:2898:ILE:HG12	2.05	0.56
1:A:317:MET:HE2	1:A:321:LYS:HG3	1.86	0.56
1:A:2307:PHE:HB2	1:A:2401:ARG:HB3	1.86	0.56
1:A:2440:PHE:HB3	1:A:2460:PHE:HD2	1.71	0.56
1:A:2855:LYS:HA	1:A:2858:MET:HG2	1.87	0.56
1:B:436:LEU:HG	1:B:445:VAL:HG11	1.88	0.56
1:B:670:TYR:HD1	1:B:1017:THR:HG21	1.69	0.56
1:B:3845:LEU:HD23	1:B:3848:GLU:HG3	1.86	0.56
1:C:985:PHE:H	1:C:985:PHE:HD2	1.53	0.56
1:C:3022:PHE:HB2	1:C:3026:ALA:HB2	1.86	0.56
1:C:4868:ASP:O	1:C:4872:GLU:HG3	2.05	0.56
1:D:1255:LEU:HD11	1:D:1451:HIS:HB3	1.86	0.56
1:D:2212:LYS:NZ	1:D:3822:GLU:OE1	2.32	0.56
2:H:88:HIS:NE2	1:D:1776:TYR:OH	2.30	0.56
1:B:1549:SER:OG	1:B:1551:ASN:O	2.24	0.56
1:C:4644:TYR:CE2	1:C:4646:ASP:HB3	2.41	0.56
1:D:4868:ASP:O	1:D:4872:GLU:HG3	2.05	0.56
1:B:1467:VAL:HG21	1:B:1482:ARG:HH21	1.71	0.56
1:C:398:HIS:HB3	1:C:400:ASP:H	1.70	0.56
1:C:436:LEU:HG	1:C:445:VAL:HG11	1.88	0.56
1:C:1549:SER:OG	1:C:1551:ASN:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2708:THR:O	1:C:2780:LYS:HD2	2.06	0.56
1:C:2855:LYS:HA	1:C:2858:MET:HG2	1.86	0.56
1:C:4914:ASN:HB3	1:C:4917:ASN:HB2	1.87	0.56
1:D:204:ASP:OD1	1:D:205:ALA:N	2.38	0.56
1:A:398:HIS:HB3	1:A:400:ASP:H	1.70	0.56
1:A:670:TYR:HD1	1:A:1017:THR:HG21	1.70	0.56
1:A:1258:PHE:CG	1:A:1303:ARG:HD3	2.41	0.56
1:A:2480:VAL:HB	1:A:2483:PHE:HB3	1.88	0.56
1:A:3778:LEU:HD13	1:A:3854:PHE:HD1	1.69	0.56
1:B:317:MET:HE2	1:B:321:LYS:HG3	1.86	0.56
1:B:4644:TYR:CE2	1:B:4646:ASP:HB3	2.41	0.56
1:C:262:TYR:HB2	1:C:389:ARG:HG3	1.86	0.56
1:D:1250:TRP:HE3	1:D:1596:TRP:HB3	1.71	0.56
1:D:2440:PHE:HB3	1:D:2460:PHE:HD2	1.71	0.56
1:A:3022:PHE:HB2	1:A:3026:ALA:HB2	1.86	0.56
1:B:1102:TYR:N	1:B:1237:GLU:O	2.37	0.56
1:B:2708:THR:O	1:B:2780:LYS:HD2	2.06	0.56
1:B:4016:PHE:HA	1:B:4019:MET:HE2	1.88	0.56
1:D:398:HIS:HB3	1:D:400:ASP:H	1.70	0.56
1:D:2855:LYS:HA	1:D:2858:MET:HG2	1.86	0.56
1:A:2195:ASN:HD22	1:A:2198:ARG:HH12	1.54	0.56
1:A:2894:LYS:O	1:A:2898:ILE:HG12	2.05	0.56
1:C:2195:ASN:HD22	1:C:2198:ARG:HH12	1.54	0.56
1:B:398:HIS:HB3	1:B:400:ASP:H	1.70	0.55
1:B:1258:PHE:CG	1:B:1303:ARG:HD3	2.41	0.55
1:C:1467:VAL:HG21	1:C:1482:ARG:HH21	1.71	0.55
1:C:2635:GLU:HG2	1:C:2680:TYR:HE1	1.71	0.55
1:C:2777:GLU:O	1:C:2781:THR:OG1	2.19	0.55
1:C:4026:LEU:HD13	1:C:4055:HIS:CG	2.40	0.55
1:D:436:LEU:HG	1:D:445:VAL:HG11	1.88	0.55
1:D:1467:VAL:HG21	1:D:1482:ARG:HH21	1.71	0.55
1:A:3962:SER:HB3	1:A:4071:GLU:HG2	1.88	0.55
1:C:2659:GLN:OE1	1:C:2659:GLN:N	2.37	0.55
1:D:262:TYR:HB2	1:D:389:ARG:HG3	1.86	0.55
1:D:3778:LEU:HD13	1:D:3854:PHE:HD1	1.69	0.55
1:C:2480:VAL:HB	1:C:2483:PHE:HB3	1.88	0.55
1:A:2504:THR:O	1:A:2508:SER:N	2.40	0.55
1:A:4144:ARG:NH2	1:A:4962:TYR:OH	2.34	0.55
1:B:3962:SER:HB3	1:B:4071:GLU:HG2	1.88	0.55
1:C:1724:GLU:HG2	1:C:2165:LEU:HD23	1.89	0.55
1:D:756:SER:OG	1:D:769:ARG:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3962:SER:HB3	1:D:4071:GLU:HG2	1.88	0.55
1:A:436:LEU:HG	1:A:445:VAL:HG11	1.88	0.55
1:A:985:PHE:H	1:A:985:PHE:HD2	1.53	0.55
1:A:1108:VAL:HB	1:A:1212:VAL:HG23	1.89	0.55
1:A:1724:GLU:HG2	1:A:2165:LEU:HD23	1.89	0.55
1:A:2635:GLU:HG2	1:A:2680:TYR:HE1	1.71	0.55
1:A:2708:THR:O	1:A:2780:LYS:HD2	2.06	0.55
1:A:4014:LEU:HD13	1:A:4122:ALA:HB2	1.88	0.55
1:A:4016:PHE:HA	1:A:4019:MET:HE2	1.88	0.55
1:B:857:LEU:HG	1:B:860:ALA:HB2	1.88	0.55
1:B:2195:ASN:HD22	1:B:2198:ARG:HH12	1.54	0.55
1:B:3622:GLN:O	1:B:3626:LYS:NZ	2.39	0.55
1:C:2619:LYS:HB2	1:C:2627:TRP:CH2	2.41	0.55
1:D:889:ILE:HA	1:D:892:LEU:HB2	1.88	0.55
1:D:1549:SER:OG	1:D:1551:ASN:O	2.24	0.55
1:D:4114:ARG:O	1:D:4117:THR:OG1	2.22	0.55
1:B:2062:ILE:O	1:B:2066:MET:HG2	2.07	0.55
1:C:1258:PHE:CG	1:C:1303:ARG:HD3	2.41	0.55
1:C:3622:GLN:O	1:C:3626:LYS:NZ	2.39	0.55
1:D:894:VAL:HA	1:D:897:LYS:HG2	1.89	0.55
1:D:985:PHE:H	1:D:985:PHE:HD2	1.53	0.55
1:D:2195:ASN:HD22	1:D:2198:ARG:HH12	1.54	0.55
1:A:889:ILE:HA	1:A:892:LEU:HB2	1.88	0.55
1:A:1467:VAL:HG21	1:A:1482:ARG:HH21	1.71	0.55
1:C:2212:LYS:NZ	1:C:3822:GLU:OE1	2.32	0.55
1:C:2521:CYS:HA	1:C:2525:LEU:HD12	1.89	0.55
1:D:1945:ASN:O	1:D:1949:GLN:HG2	2.07	0.55
1:D:2521:CYS:HA	1:D:2525:LEU:HD12	1.89	0.55
1:D:4093:ASP:OD1	1:D:4094:ILE:HD12	2.07	0.55
1:A:857:LEU:HG	1:A:860:ALA:HB2	1.88	0.55
1:B:1945:ASN:O	1:B:1949:GLN:HG2	2.07	0.55
1:B:4831:ILE:HG13	1:B:4843:ARG:NH2	2.21	0.55
1:C:1628:MET:HG3	1:C:1687:TYR:CD2	2.42	0.55
1:C:2062:ILE:O	1:C:2066:MET:HG2	2.07	0.55
1:C:2834:SER:OG	1:C:2836:ASP:OD1	2.20	0.55
1:D:625:VAL:HG12	1:D:628:ASN:H	1.72	0.55
1:D:919:VAL:HB	1:D:923:LYS:HG3	1.89	0.55
1:D:1258:PHE:CG	1:D:1303:ARG:HD3	2.41	0.55
1:D:2758:LYS:NZ	1:D:2762:LEU:O	2.40	0.55
1:D:4144:ARG:NH2	1:D:4962:TYR:OH	2.34	0.55
1:A:919:VAL:HB	1:A:923:LYS:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1628:MET:HG3	1:A:1687:TYR:CD2	2.42	0.55
1:A:3622:GLN:O	1:A:3626:LYS:NZ	2.39	0.55
1:B:4827:ILE:O	1:B:4831:ILE:HG12	2.07	0.55
1:C:1610:ARG:HA	1:C:1617:TRP:HA	1.89	0.55
1:C:4016:PHE:HA	1:C:4019:MET:HE2	1.88	0.55
1:D:857:LEU:HG	1:D:860:ALA:HB2	1.88	0.55
1:D:1108:VAL:HB	1:D:1212:VAL:HG23	1.89	0.55
1:A:625:VAL:HG12	1:A:628:ASN:H	1.72	0.55
1:A:1102:TYR:N	1:A:1237:GLU:O	2.37	0.55
1:B:891:GLU:HA	1:B:894:VAL:HG22	1.87	0.55
1:B:1250:TRP:HE3	1:B:1596:TRP:HB3	1.70	0.55
1:B:1628:MET:HG3	1:B:1687:TYR:CD2	2.42	0.55
1:C:891:GLU:HA	1:C:894:VAL:HG22	1.87	0.55
1:D:2480:VAL:HB	1:D:2483:PHE:HB3	1.88	0.55
1:D:2619:LYS:HB2	1:D:2627:TRP:CH2	2.41	0.55
1:D:4014:LEU:HD13	1:D:4122:ALA:HB2	1.88	0.55
1:D:4016:PHE:HA	1:D:4019:MET:HE2	1.88	0.55
1:A:2605:MET:HB3	1:A:2606:PRO:HD3	1.89	0.54
1:A:4644:TYR:CE2	1:A:4646:ASP:HB3	2.41	0.54
1:B:2619:LYS:HB2	1:B:2627:TRP:CH2	2.41	0.54
1:B:2635:GLU:HG2	1:B:2680:TYR:HE1	1.71	0.54
1:B:2659:GLN:OE1	1:B:2659:GLN:N	2.37	0.54
1:B:2777:GLU:O	1:B:2781:THR:OG1	2.19	0.54
1:B:2998:ASN:OD1	1:B:2999:LYS:N	2.40	0.54
1:C:1670:HIS:O	1:C:1674:HIS:ND1	2.32	0.54
1:C:2234:MET:HE2	1:C:2238:THR:HG22	1.88	0.54
1:C:2790:GLU:N	1:C:2902:ALA:O	2.33	0.54
1:D:2160:ASN:OD1	1:D:2163:ARG:NH2	2.40	0.54
1:D:2605:MET:HB3	1:D:2606:PRO:HD3	1.89	0.54
1:D:2635:GLU:HG2	1:D:2680:TYR:HE1	1.71	0.54
1:D:2998:ASN:OD1	1:D:2999:LYS:N	2.40	0.54
1:D:3846:LEU:HB3	1:D:3854:PHE:CE2	2.42	0.54
1:A:894:VAL:HA	1:A:897:LYS:HG2	1.89	0.54
1:A:2619:LYS:HB2	1:A:2627:TRP:CH2	2.41	0.54
1:A:2998:ASN:OD1	1:A:2999:LYS:N	2.40	0.54
1:A:4183:LYS:HE2	1:D:4906:GLU:OE2	2.08	0.54
1:B:2480:VAL:HB	1:B:2483:PHE:HB3	1.88	0.54
1:C:857:LEU:HG	1:C:860:ALA:HB2	1.88	0.54
1:D:2062:ILE:O	1:D:2066:MET:HG2	2.07	0.54
1:D:2719:TYR:OH	1:D:2799:ALA:HB2	2.07	0.54
1:D:2768:LYS:O	1:D:2772:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3013:VAL:O	1:D:3018:ARG:NH2	2.40	0.54
1:D:4644:TYR:CE2	1:D:4646:ASP:HB3	2.41	0.54
1:A:756:SER:OG	1:A:769:ARG:O	2.25	0.54
1:A:1945:ASN:O	1:A:1949:GLN:HG2	2.07	0.54
1:A:2719:TYR:OH	1:A:2799:ALA:HB2	2.07	0.54
1:A:4279:MET:CE	1:B:4487:TYR:HD1	2.20	0.54
1:B:756:SER:OG	1:B:769:ARG:O	2.25	0.54
1:B:2504:THR:O	1:B:2508:SER:N	2.40	0.54
1:B:2758:LYS:NZ	1:B:2762:LEU:O	2.40	0.54
1:D:1628:MET:HG3	1:D:1687:TYR:CD2	2.42	0.54
1:D:2767:GLU:O	1:D:2771:TYR:N	2.40	0.54
1:A:310:GLU:OE2	1:A:310:GLU:N	2.34	0.54
1:A:801:ARG:NH1	1:A:1615:GLN:O	2.40	0.54
1:A:1670:HIS:O	1:A:1674:HIS:ND1	2.32	0.54
1:A:2521:CYS:HA	1:A:2525:LEU:HD12	1.89	0.54
1:B:625:VAL:HG12	1:B:628:ASN:H	1.72	0.54
1:B:2855:LYS:HA	1:B:2858:MET:HE3	1.90	0.54
1:B:3013:VAL:O	1:B:3018:ARG:NH2	2.40	0.54
1:C:889:ILE:HA	1:C:892:LEU:HB2	1.88	0.54
1:C:1471:ASP:OD2	1:C:1473:LYS:NZ	2.40	0.54
1:C:2998:ASN:OD1	1:C:2999:LYS:N	2.40	0.54
1:C:4186:MET:HE2	1:C:4186:MET:HA	1.90	0.54
1:D:1610:ARG:HA	1:D:1617:TRP:HA	1.89	0.54
1:A:4827:ILE:O	1:A:4831:ILE:HG12	2.07	0.54
2:H:80:ASP:OD1	2:H:81:VAL:N	2.41	0.54
1:B:2234:MET:HE2	1:B:2238:THR:HG22	1.88	0.54
1:B:2834:SER:OG	1:B:2836:ASP:OD1	2.20	0.54
1:C:801:ARG:NH1	1:C:1615:GLN:O	2.40	0.54
1:C:877:HIS:HA	1:C:880:ARG:CD	2.38	0.54
1:C:919:VAL:HB	1:C:923:LYS:HG3	1.89	0.54
1:C:2797:SER:HB3	1:C:2801:TYR:HE2	1.72	0.54
1:D:28:ILE:HG22	1:D:29:HIS:CD2	2.43	0.54
1:A:2927:GLN:NE2	1:A:3003:MET:HE3	2.22	0.54
1:A:4197:ILE:HG23	1:A:4923:MET:HE2	1.90	0.54
1:A:4844:ILE:HG21	1:D:4814:MET:HE2	1.90	0.54
2:F:80:ASP:OD1	2:F:81:VAL:N	2.41	0.54
1:B:985:PHE:H	1:B:985:PHE:HD2	1.53	0.54
1:B:3846:LEU:HB3	1:B:3854:PHE:CE2	2.42	0.54
1:B:4014:LEU:HD13	1:B:4122:ALA:HB2	1.88	0.54
1:C:625:VAL:HG12	1:C:628:ASN:H	1.72	0.54
1:C:1440:ASN:HB3	1:C:1546:GLN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1896:MET:HB3	1:C:1898:LEU:HD11	1.90	0.54
1:C:2605:MET:HB3	1:C:2606:PRO:HD3	1.90	0.54
1:C:4093:ASP:OD1	1:C:4094:ILE:HD12	2.07	0.54
1:A:2234:MET:HE2	1:A:2238:THR:HG22	1.88	0.54
1:A:3846:LEU:HB3	1:A:3854:PHE:CE2	2.42	0.54
1:A:4093:ASP:OD1	1:A:4094:ILE:HD12	2.07	0.54
1:A:4520:TYR:CD1	1:A:4561:LEU:HD13	2.43	0.54
1:B:2160:ASN:OD1	1:B:2163:ARG:NH2	2.40	0.54
1:B:2719:TYR:OH	1:B:2799:ALA:HB2	2.07	0.54
1:C:28:ILE:HG22	1:C:29:HIS:CD2	2.43	0.54
1:C:28:ILE:HG22	1:C:29:HIS:HD2	1.73	0.54
1:C:1989:PRO:O	1:C:1993:ARG:HG3	2.08	0.54
1:C:3846:LEU:HB3	1:C:3854:PHE:CE2	2.42	0.54
1:C:3962:SER:HB3	1:C:4071:GLU:HG2	1.88	0.54
1:D:679:VAL:HA	1:D:800:VAL:HG12	1.90	0.54
1:D:1896:MET:HB3	1:D:1898:LEU:HD11	1.90	0.54
1:D:2234:MET:HE2	1:D:2238:THR:HG22	1.88	0.54
1:D:4502:MET:HE1	1:D:4585:PHE:HD2	1.73	0.54
2:F:16:PHE:O	2:F:18:LYS:NZ	2.37	0.54
1:B:1471:ASP:OD2	1:B:1473:LYS:NZ	2.40	0.54
1:B:1610:ARG:HA	1:B:1617:TRP:HA	1.89	0.54
1:B:1989:PRO:O	1:B:1993:ARG:HG3	2.08	0.54
1:B:2521:CYS:HA	1:B:2525:LEU:HD12	1.89	0.54
1:B:2832:THR:HG21	1:C:1290:PHE:HE2	1.73	0.54
1:B:2927:GLN:NE2	1:B:3003:MET:HE3	2.23	0.54
1:C:20:VAL:HG12	1:C:216:PRO:HA	1.90	0.54
1:C:2768:LYS:O	1:C:2772:ARG:HD3	2.07	0.54
1:C:2855:LYS:HA	1:C:2858:MET:HE3	1.90	0.54
1:D:877:HIS:HA	1:D:880:ARG:CD	2.38	0.54
1:D:1440:ASN:HB3	1:D:1546:GLN:HB3	1.90	0.54
1:D:2092:TYR:CD2	1:D:3640:LEU:HD13	2.43	0.54
1:D:4827:ILE:O	1:D:4831:ILE:HG12	2.07	0.54
1:A:1303:ARG:HD2	1:A:1446:ILE:HD11	1.90	0.54
1:B:887:GLU:HB2	1:B:921:PHE:HZ	1.73	0.54
1:B:919:VAL:HB	1:B:923:LYS:HG3	1.89	0.54
1:C:3921:THR:O	1:C:3925:GLN:HG2	2.08	0.54
1:C:4520:TYR:CD1	1:C:4561:LEU:HD13	2.43	0.54
1:D:2927:GLN:NE2	1:D:3003:MET:HE3	2.22	0.54
1:A:28:ILE:HG22	1:A:29:HIS:CD2	2.43	0.54
1:B:28:ILE:HG22	1:B:29:HIS:CD2	2.43	0.54
1:B:227:TYR:CG	1:B:352:SER:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:ARG:NH1	1:B:1615:GLN:O	2.40	0.54
1:B:1011:ARG:HH21	1:B:1014:GLN:NE2	2.06	0.54
1:B:1645:THR:HG22	1:B:1695:PRO:HG3	1.90	0.54
1:B:1896:MET:HB3	1:B:1898:LEU:HD11	1.90	0.54
1:B:2605:MET:HB3	1:B:2606:PRO:HD3	1.90	0.54
1:B:4197:ILE:HG23	1:B:4923:MET:HE2	1.90	0.54
1:C:227:TYR:CG	1:C:352:SER:HB2	2.43	0.54
1:C:2526:PRO:HB3	1:C:2530:ARG:NH1	2.23	0.54
1:C:2585:MET:HE1	1:C:2589:LEU:HD21	1.90	0.54
1:C:4827:ILE:O	1:C:4831:ILE:HG12	2.07	0.54
1:D:1724:GLU:HG2	1:D:2165:LEU:HD23	1.89	0.54
1:D:1989:PRO:O	1:D:1993:ARG:HG3	2.08	0.54
1:D:3622:GLN:O	1:D:3626:LYS:NZ	2.39	0.54
1:D:4186:MET:HE2	1:D:4186:MET:HA	1.90	0.54
1:A:28:ILE:HG22	1:A:29:HIS:HD2	1.73	0.53
1:A:1429:SER:HB2	1:A:1556:GLU:HB2	1.90	0.53
1:A:3879:LEU:O	1:A:3882:GLN:HG3	2.08	0.53
1:B:966:LEU:HD12	1:B:979:ALA:HB2	1.90	0.53
1:B:1724:GLU:HG2	1:B:2165:LEU:HD23	1.89	0.53
1:B:2337:GLY:O	1:C:141:ASP:HA	2.08	0.53
1:B:2797:SER:HB3	1:B:2801:TYR:HE2	1.72	0.53
1:B:3879:LEU:O	1:B:3882:GLN:HG3	2.08	0.53
1:B:4881:LYS:O	1:B:4885:GLU:HG2	2.08	0.53
1:C:1023:ASP:HB2	1:C:1028:ARG:HB2	1.90	0.53
1:C:2092:TYR:CD2	1:C:3640:LEU:HD13	2.43	0.53
1:C:2719:TYR:OH	1:C:2799:ALA:HB2	2.08	0.53
1:C:2855:LYS:HE3	1:C:2856:LYS:HZ2	1.73	0.53
1:C:4502:MET:HE1	1:C:4585:PHE:HD2	1.73	0.53
1:D:2782:MET:CG	1:D:2783:LEU:HD12	2.38	0.53
1:A:679:VAL:HA	1:A:800:VAL:HG12	1.90	0.53
1:A:1014:GLN:O	1:A:1027:ARG:NH1	2.42	0.53
1:A:1896:MET:HB3	1:A:1898:LEU:HD11	1.90	0.53
1:A:2062:ILE:O	1:A:2066:MET:HG2	2.07	0.53
1:A:3013:VAL:O	1:A:3018:ARG:NH2	2.40	0.53
2:G:58:LYS:O	2:G:62:GLU:HG3	2.08	0.53
2:G:80:ASP:OD1	2:G:81:VAL:N	2.41	0.53
1:B:679:VAL:HA	1:B:800:VAL:HG12	1.90	0.53
1:B:894:VAL:HA	1:B:897:LYS:HG2	1.89	0.53
1:B:1303:ARG:HD2	1:B:1446:ILE:HD11	1.90	0.53
1:B:2729:HIS:NE2	1:B:2763:LEU:HD22	2.24	0.53
1:C:1097:LYS:NZ	1:C:1198:GLY:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1907:CYS:SG	1:C:2066:MET:HE1	2.49	0.53
1:C:2782:MET:CG	1:C:2783:LEU:HD12	2.38	0.53
1:C:2857:LYS:CE	1:C:2871:LEU:HD23	2.30	0.53
1:C:2927:GLN:NE2	1:C:3003:MET:HE3	2.22	0.53
1:C:4014:LEU:HD13	1:C:4122:ALA:HB2	1.88	0.53
1:D:1689:ILE:HA	1:D:1703:TYR:CE1	2.44	0.53
1:A:877:HIS:HA	1:A:880:ARG:CD	2.38	0.53
1:A:1477:HIS:CE1	1:A:1478:GLU:HG3	2.43	0.53
1:A:2782:MET:CG	1:A:2783:LEU:HD12	2.38	0.53
1:B:1023:ASP:HB2	1:B:1028:ARG:HB2	1.90	0.53
1:B:1108:VAL:HB	1:B:1212:VAL:HG23	1.89	0.53
1:B:1477:HIS:CE1	1:B:1478:GLU:HG3	2.43	0.53
1:B:1907:CYS:SG	1:B:2066:MET:HE1	2.48	0.53
1:B:2585:MET:HE1	1:B:2589:LEU:HD21	1.90	0.53
1:B:4502:MET:HE1	1:B:4585:PHE:HD2	1.73	0.53
1:C:1011:ARG:HH21	1:C:1014:GLN:NE2	2.06	0.53
1:C:1108:VAL:HB	1:C:1212:VAL:HG23	1.89	0.53
1:C:1945:ASN:O	1:C:1949:GLN:HG2	2.07	0.53
1:C:2832:THR:HG21	1:D:1550:PRO:HD3	1.90	0.53
1:C:4197:ILE:HG23	1:C:4923:MET:HE2	1.90	0.53
1:D:310:GLU:OE2	1:D:310:GLU:N	2.34	0.53
1:D:2397:ASP:O	1:D:2401:ARG:HG2	2.09	0.53
1:D:2659:GLN:O	1:D:2965:LYS:NZ	2.41	0.53
1:D:2797:SER:HB3	1:D:2801:TYR:HE2	1.72	0.53
1:D:2855:LYS:HA	1:D:2858:MET:HE3	1.89	0.53
1:D:2857:LYS:CE	1:D:2871:LEU:HD23	2.30	0.53
1:D:4520:TYR:CD1	1:D:4561:LEU:HD13	2.43	0.53
1:A:1023:ASP:HB2	1:A:1028:ARG:HB2	1.90	0.53
1:A:2659:GLN:O	1:A:2965:LYS:NZ	2.41	0.53
1:A:2768:LYS:O	1:A:2772:ARG:HD3	2.07	0.53
2:G:16:PHE:O	2:G:18:LYS:NZ	2.37	0.53
1:B:1429:SER:HB2	1:B:1556:GLU:HB2	1.90	0.53
1:C:966:LEU:HD12	1:C:979:ALA:HB2	1.91	0.53
1:C:2127:ARG:NH2	1:C:2165:LEU:O	2.42	0.53
1:D:227:TYR:CG	1:D:352:SER:HB2	2.43	0.53
1:D:887:GLU:HB2	1:D:921:PHE:HZ	1.73	0.53
1:D:1014:GLN:O	1:D:1027:ARG:NH1	2.42	0.53
1:D:1711:LEU:CB	1:D:1831:MET:HE1	2.38	0.53
1:D:2729:HIS:NE2	1:D:2763:LEU:HD22	2.24	0.53
1:D:4018:ASP:OD2	1:D:4022:LYS:NZ	2.38	0.53
1:A:20:VAL:HG12	1:A:216:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:LEU:HD12	1:A:979:ALA:HB2	1.90	0.53
1:A:1097:LYS:NZ	1:A:1198:GLY:O	2.42	0.53
1:A:2526:PRO:HB3	1:A:2530:ARG:NH1	2.23	0.53
1:B:877:HIS:HA	1:B:880:ARG:CD	2.38	0.53
1:B:889:ILE:HA	1:B:892:LEU:HB2	1.88	0.53
1:B:4520:TYR:CD1	1:B:4561:LEU:HD13	2.43	0.53
1:C:1477:HIS:CE1	1:C:1478:GLU:HG3	2.43	0.53
1:C:2729:HIS:NE2	1:C:2763:LEU:HD22	2.24	0.53
1:C:4265:LYS:O	1:C:4269:LYS:HG2	2.09	0.53
1:C:4831:ILE:HG13	1:C:4843:ARG:NH2	2.21	0.53
1:C:4881:LYS:O	1:C:4885:GLU:HG2	2.08	0.53
1:D:966:LEU:HD12	1:D:979:ALA:HB2	1.90	0.53
1:D:1011:ARG:HH21	1:D:1014:GLN:NE2	2.06	0.53
1:D:1023:ASP:HB2	1:D:1028:ARG:HB2	1.90	0.53
1:D:1429:SER:HB2	1:D:1556:GLU:HB2	1.90	0.53
1:D:2127:ARG:NH2	1:D:2165:LEU:O	2.42	0.53
1:D:2868:HIS:CD2	1:D:2870:LEU:HB2	2.44	0.53
1:D:3668:ILE:HD12	1:D:3734:ARG:HB2	1.91	0.53
1:A:2729:HIS:NE2	1:A:2763:LEU:HD22	2.24	0.53
1:A:4502:MET:HE1	1:A:4585:PHE:HD2	1.73	0.53
2:E:80:ASP:OD1	2:E:81:VAL:N	2.41	0.53
2:H:16:PHE:O	2:H:18:LYS:NZ	2.37	0.53
2:H:58:LYS:O	2:H:62:GLU:HG3	2.08	0.53
1:C:874:LEU:HB2	1:C:878:LEU:HD22	1.91	0.53
1:D:20:VAL:HG12	1:D:216:PRO:HA	1.90	0.53
1:D:28:ILE:HG22	1:D:29:HIS:HD2	1.73	0.53
1:D:1097:LYS:NZ	1:D:1198:GLY:O	2.42	0.53
1:A:1610:ARG:HA	1:A:1617:TRP:HA	1.89	0.53
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.90	0.53
1:A:2832:THR:HG21	1:B:1290:PHE:CE2	2.39	0.53
1:A:2855:LYS:HA	1:A:2858:MET:HE3	1.89	0.53
2:E:58:LYS:O	2:E:62:GLU:HG3	2.08	0.53
1:B:874:LEU:HB2	1:B:878:LEU:HD22	1.91	0.53
1:B:2066:MET:HE3	1:B:2084:MET:HG2	1.91	0.53
1:B:2526:PRO:HB3	1:B:2530:ARG:NH1	2.23	0.53
1:B:2765:GLU:HA	1:B:2768:LYS:HZ1	1.74	0.53
1:C:679:VAL:HA	1:C:800:VAL:HG12	1.90	0.53
1:C:1711:LEU:CB	1:C:1831:MET:HE1	2.38	0.53
1:D:229:ILE:HG22	1:D:288:HIS:HD2	1.74	0.53
1:D:3921:THR:O	1:D:3925:GLN:HG2	2.08	0.53
1:D:4881:LYS:O	1:D:4885:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:GLU:HB2	1:A:921:PHE:HZ	1.73	0.53
1:A:2659:GLN:OE1	1:A:2659:GLN:N	2.37	0.53
1:A:2765:GLU:HA	1:A:2768:LYS:HZ1	1.74	0.53
1:A:4654:MET:HB2	1:A:4672:MET:HE1	1.91	0.53
2:F:58:LYS:O	2:F:62:GLU:HG3	2.08	0.53
1:B:20:VAL:HG12	1:B:216:PRO:HA	1.90	0.53
1:B:1440:ASN:HB3	1:B:1546:GLN:HB3	1.90	0.53
1:B:2767:GLU:O	1:B:2771:TYR:N	2.40	0.53
1:B:2790:GLU:N	1:B:2902:ALA:O	2.33	0.53
1:C:894:VAL:HA	1:C:897:LYS:HG2	1.89	0.53
1:C:4287:TYR:HA	1:C:4290:ILE:HD12	1.91	0.53
1:D:4197:ILE:HG23	1:D:4923:MET:HE2	1.90	0.53
1:D:4265:LYS:O	1:D:4269:LYS:HG2	2.09	0.53
1:D:4654:MET:HB2	1:D:4672:MET:HE1	1.91	0.53
1:A:1011:ARG:HH21	1:A:1014:GLN:NE2	2.06	0.53
1:A:3668:ILE:HD12	1:A:3734:ARG:HB2	1.91	0.53
1:B:1004:HIS:CE1	1:B:1038:LEU:HD21	2.44	0.53
1:B:2768:LYS:O	1:B:2772:ARG:HD3	2.07	0.53
1:B:4093:ASP:OD1	1:B:4094:ILE:HD12	2.07	0.53
1:B:4186:MET:HE2	1:B:4186:MET:HA	1.90	0.53
1:B:4187:GLU:OE1	1:B:4949:TRP:NE1	2.35	0.53
1:B:4287:TYR:HA	1:B:4290:ILE:HD12	1.91	0.53
1:C:1303:ARG:HD2	1:C:1446:ILE:HD11	1.90	0.53
1:C:1689:ILE:HA	1:C:1703:TYR:CE1	2.44	0.53
1:D:1907:CYS:SG	1:D:2066:MET:HE1	2.48	0.53
1:A:663:VAL:HG23	1:A:671:LYS:HE3	1.91	0.53
1:A:1689:ILE:HA	1:A:1703:TYR:CE1	2.44	0.53
1:A:1989:PRO:O	1:A:1993:ARG:HG3	2.08	0.53
1:A:2066:MET:HE3	1:A:2084:MET:HG2	1.91	0.53
1:A:2092:TYR:CD2	1:A:3640:LEU:HD13	2.43	0.53
1:A:2212:LYS:NZ	1:A:3822:GLU:OE1	2.32	0.53
1:A:2585:MET:HE1	1:A:2589:LEU:HD21	1.90	0.53
1:A:4872:GLU:HG2	1:D:4874:ARG:HD3	1.91	0.53
2:G:12:ASP:OD1	2:G:68:SER:OG	2.27	0.53
1:B:1690:GLU:OE1	1:B:1790:LYS:NZ	2.42	0.53
1:B:2092:TYR:CD2	1:B:3640:LEU:HD13	2.43	0.53
1:B:2127:ARG:NH2	1:B:2165:LEU:O	2.42	0.53
1:B:2397:ASP:O	1:B:2401:ARG:HG2	2.09	0.53
1:B:3803:LEU:HB2	1:B:3884:SER:HB2	1.92	0.53
1:B:3921:THR:O	1:B:3925:GLN:HG2	2.08	0.53
1:B:4114:ARG:O	1:B:4117:THR:OG1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1014:GLN:O	1:C:1027:ARG:NH1	2.42	0.53
1:C:2066:MET:HE3	1:C:2084:MET:HG2	1.91	0.53
1:C:2504:THR:O	1:C:2508:SER:N	2.40	0.53
1:D:1181:ILE:HG22	1:D:1189:GLU:OE2	2.09	0.53
1:D:1477:HIS:CE1	1:D:1478:GLU:HG3	2.43	0.53
1:D:2526:PRO:HB3	1:D:2530:ARG:NH1	2.23	0.53
1:A:2724:TYR:HD1	1:A:2895:PHE:CD2	2.27	0.52
2:E:16:PHE:O	2:E:18:LYS:NZ	2.37	0.52
1:B:229:ILE:HG22	1:B:288:HIS:HD2	1.74	0.52
1:B:663:VAL:HG23	1:B:671:LYS:HE3	1.91	0.52
1:B:1087:ILE:HD11	1:B:1204:VAL:HG22	1.91	0.52
1:B:1689:ILE:HA	1:B:1703:TYR:CE1	2.44	0.52
1:B:2333:PRO:HA	1:B:2336:ARG:HG2	1.92	0.52
1:C:1181:ILE:HG22	1:C:1189:GLU:OE2	2.09	0.52
1:C:1429:SER:HB2	1:C:1556:GLU:HB2	1.90	0.52
1:C:2703:PRO:HB2	1:C:2854:LYS:HB2	1.91	0.52
1:D:3669:LEU:HB3	1:D:3673:ARG:HH21	1.74	0.52
1:A:229:ILE:HG22	1:A:288:HIS:HD2	1.74	0.52
1:A:1181:ILE:HG22	1:A:1189:GLU:OE2	2.09	0.52
1:A:1471:ASP:OD2	1:A:1473:LYS:NZ	2.40	0.52
1:A:1711:LEU:CB	1:A:1831:MET:HE1	2.38	0.52
1:A:1907:CYS:SG	1:A:2066:MET:HE1	2.49	0.52
1:A:2127:ARG:NH2	1:A:2165:LEU:O	2.42	0.52
1:A:2703:PRO:HB2	1:A:2854:LYS:HB2	1.91	0.52
1:B:1014:GLN:O	1:B:1027:ARG:NH1	2.42	0.52
1:B:2930:ILE:HA	1:B:3010:LYS:HZ1	1.74	0.52
1:B:4265:LYS:O	1:B:4269:LYS:HG2	2.09	0.52
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	1.90	0.52
1:C:2791:ARG:HH21	1:C:2795:GLY:C	2.17	0.52
1:C:3803:LEU:HB2	1:C:3884:SER:HB2	1.92	0.52
1:C:4654:MET:HB2	1:C:4672:MET:HE1	1.91	0.52
1:D:663:VAL:HG23	1:D:671:LYS:HE3	1.91	0.52
1:D:1004:HIS:CE1	1:D:1038:LEU:HD21	2.44	0.52
1:D:1431:ARG:NE	1:D:1506:GLU:OE1	2.30	0.52
1:D:2333:PRO:HA	1:D:2336:ARG:HG2	1.92	0.52
1:A:1440:ASN:HB3	1:A:1546:GLN:HB3	1.90	0.52
1:A:2333:PRO:HA	1:A:2336:ARG:HG2	1.92	0.52
1:A:2729:HIS:CD2	1:A:2763:LEU:HD22	2.44	0.52
1:A:2868:HIS:CD2	1:A:2870:LEU:HB2	2.44	0.52
2:F:12:ASP:OD1	2:F:68:SER:OG	2.27	0.52
1:B:28:ILE:HG22	1:B:29:HIS:HD2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2729:HIS:CD2	1:B:2763:LEU:HD22	2.44	0.52
1:B:2791:ARG:HH21	1:B:2795:GLY:C	2.17	0.52
1:B:4144:ARG:NH2	1:B:4962:TYR:OH	2.34	0.52
1:C:663:VAL:HG23	1:C:671:LYS:HE3	1.91	0.52
1:C:887:GLU:HB2	1:C:921:PHE:HZ	1.73	0.52
1:D:1303:ARG:HD2	1:D:1446:ILE:HD11	1.90	0.52
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.90	0.52
1:D:4831:ILE:HG13	1:D:4843:ARG:NH2	2.21	0.52
1:A:1549:SER:OG	1:A:1551:ASN:O	2.24	0.52
1:A:4186:MET:HA	1:A:4186:MET:HE2	1.90	0.52
1:A:4640:PHE:HB3	1:A:4650:LYS:HE2	1.92	0.52
1:A:4881:LYS:O	1:A:4885:GLU:HG2	2.08	0.52
1:B:1097:LYS:NZ	1:B:1198:GLY:O	2.42	0.52
1:B:4654:MET:HB2	1:B:4672:MET:HE1	1.91	0.52
1:C:1690:GLU:OE1	1:C:1790:LYS:NZ	2.42	0.52
1:C:2397:ASP:O	1:C:2401:ARG:HG2	2.09	0.52
1:C:2729:HIS:CD2	1:C:2763:LEU:HD22	2.44	0.52
1:C:2868:HIS:CD2	1:C:2870:LEU:HB2	2.44	0.52
1:D:2066:MET:HE3	1:D:2084:MET:HG2	1.91	0.52
1:D:2791:ARG:HH21	1:D:2795:GLY:C	2.17	0.52
1:A:227:TYR:CG	1:A:352:SER:HB2	2.43	0.52
1:A:428:ARG:NH2	1:A:446:ASP:OD2	2.42	0.52
1:A:3921:THR:O	1:A:3925:GLN:HG2	2.08	0.52
1:B:428:ARG:NH2	1:B:446:ASP:OD2	2.43	0.52
1:B:2659:GLN:O	1:B:2965:LYS:NZ	2.41	0.52
1:C:367:ASP:OD1	1:C:368:THR:N	2.43	0.52
1:C:756:SER:OG	1:C:769:ARG:O	2.25	0.52
1:C:2333:PRO:HA	1:C:2336:ARG:HG2	1.92	0.52
1:C:3669:LEU:HB3	1:C:3673:ARG:HH21	1.74	0.52
1:D:332:ARG:NH1	1:D:339:ASP:OD1	2.43	0.52
1:A:2054:LYS:HE2	1:A:2056:SER:HA	1.92	0.52
1:B:332:ARG:NH1	1:B:339:ASP:OD1	2.43	0.52
1:B:1711:LEU:CB	1:B:1831:MET:HE1	2.38	0.52
1:C:4106:SER:HA	1:C:4115:LEU:HD21	1.92	0.52
1:C:4943:MET:HA	1:C:4946:GLU:HG2	1.91	0.52
1:D:2585:MET:HE1	1:D:2589:LEU:HD21	1.90	0.52
1:A:2142:MET:HA	1:A:2142:MET:HE2	1.91	0.52
1:A:4287:TYR:HA	1:A:4290:ILE:HD12	1.91	0.52
1:B:2054:LYS:HE2	1:B:2056:SER:HA	1.92	0.52
1:B:2868:HIS:CD2	1:B:2870:LEU:HB2	2.44	0.52
1:B:4702:ASP:O	1:B:4706:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1087:ILE:HD11	1:C:1204:VAL:HG22	1.91	0.52
1:C:2659:GLN:O	1:C:2965:LYS:NZ	2.41	0.52
1:C:2724:TYR:HD1	1:C:2895:PHE:CD2	2.27	0.52
1:D:986:ILE:CD1	1:D:1055:ARG:HA	2.40	0.52
1:D:1471:ASP:OD2	1:D:1473:LYS:NZ	2.40	0.52
1:D:2724:TYR:HD1	1:D:2895:PHE:CD2	2.27	0.52
1:D:3803:LEU:HB2	1:D:3884:SER:HB2	1.92	0.52
1:D:4287:TYR:HA	1:D:4290:ILE:HD12	1.91	0.52
1:D:4664:ASP:OD1	1:D:4664:ASP:N	2.42	0.52
1:D:4702:ASP:O	1:D:4706:GLN:HG2	2.10	0.52
1:A:927:GLN:NE2	1:A:928:GLU:HG3	2.25	0.52
1:A:2397:ASP:O	1:A:2401:ARG:HG2	2.09	0.52
1:B:927:GLN:NE2	1:B:928:GLU:HG3	2.25	0.52
1:B:1827:THR:HG22	1:B:1831:MET:HE3	1.92	0.52
1:B:2142:MET:HE2	1:B:2142:MET:HA	1.91	0.52
1:B:2150:MET:HE1	1:B:2199:PHE:HA	1.92	0.52
1:B:2782:MET:CG	1:B:2783:LEU:HD12	2.38	0.52
1:B:4664:ASP:OD1	1:B:4664:ASP:N	2.42	0.52
1:C:229:ILE:HG22	1:C:288:HIS:HD2	1.74	0.52
1:C:428:ARG:NH2	1:C:446:ASP:OD2	2.43	0.52
1:C:1004:HIS:CE1	1:C:1038:LEU:HD21	2.44	0.52
1:C:3823:GLU:HG3	1:C:3826:GLY:HA2	1.92	0.52
1:D:1087:ILE:HD11	1:D:1204:VAL:HG22	1.91	0.52
1:D:2142:MET:HE2	1:D:2142:MET:HA	1.91	0.52
1:D:2930:ILE:HA	1:D:3010:LYS:HZ1	1.75	0.52
1:D:3879:LEU:O	1:D:3882:GLN:HG3	2.08	0.52
1:A:1087:ILE:HD11	1:A:1204:VAL:HG22	1.91	0.52
1:A:1950:ALA:HB1	1:A:1961:LYS:HZ2	1.75	0.52
1:A:2160:ASN:OD1	1:A:2163:ARG:NH2	2.40	0.52
1:A:2767:GLU:O	1:A:2771:TYR:N	2.40	0.52
1:A:4943:MET:HA	1:A:4946:GLU:HG2	1.91	0.52
1:B:986:ILE:CD1	1:B:1055:ARG:HA	2.40	0.52
1:B:4640:PHE:HB3	1:B:4650:LYS:HE2	1.92	0.52
1:C:996:VAL:HG13	1:C:1047:LYS:HE2	1.91	0.52
1:C:1827:THR:HG22	1:C:1831:MET:HE3	1.92	0.52
1:C:3879:LEU:O	1:C:3882:GLN:HG3	2.08	0.52
1:D:428:ARG:NH2	1:D:446:ASP:OD2	2.42	0.52
1:D:2054:LYS:HE2	1:D:2056:SER:HA	1.92	0.52
1:D:2150:MET:HE1	1:D:2199:PHE:HA	1.92	0.52
1:D:4943:MET:HA	1:D:4946:GLU:HG2	1.91	0.52
1:A:902:TRP:HZ2	1:A:915:HIS:CB	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1501:ASN:OD1	1:A:1502:ASN:N	2.43	0.52
1:A:2581:ARG:HB3	1:A:2584:MET:HG2	1.92	0.52
2:E:12:ASP:OD1	2:E:68:SER:OG	2.27	0.52
1:B:902:TRP:HZ2	1:B:915:HIS:CB	2.23	0.52
1:B:2703:PRO:HB2	1:B:2854:LYS:HB2	1.91	0.52
1:B:4107:GLU:OE1	1:B:4149:TYR:OH	2.22	0.52
1:B:4520:TYR:HD1	1:B:4561:LEU:HD13	1.75	0.52
1:C:986:ILE:CD1	1:C:1055:ARG:HA	2.40	0.52
1:C:3668:ILE:HD12	1:C:3734:ARG:HB2	1.91	0.52
1:A:1827:THR:HG22	1:A:1831:MET:HE3	1.92	0.51
1:A:4265:LYS:O	1:A:4269:LYS:HG2	2.09	0.51
1:A:4520:TYR:HD1	1:A:4561:LEU:HD13	1.75	0.51
1:B:848:ARG:NH1	1:B:1599:MET:SD	2.84	0.51
1:B:1181:ILE:HG22	1:B:1189:GLU:OE2	2.09	0.51
1:B:2581:ARG:HB3	1:B:2584:MET:HG2	1.92	0.51
1:C:1688:ALA:HA	1:C:1694:MET:HE3	1.92	0.51
1:D:801:ARG:NH1	1:D:1615:GLN:O	2.40	0.51
1:A:1004:HIS:CE1	1:A:1038:LEU:HD21	2.44	0.51
1:A:1688:ALA:HA	1:A:1694:MET:HE3	1.92	0.51
1:A:2758:LYS:NZ	1:A:2762:LEU:O	2.40	0.51
1:A:3823:GLU:HG3	1:A:3826:GLY:HA2	1.92	0.51
1:B:996:VAL:HG13	1:B:1047:LYS:HE2	1.91	0.51
1:B:1688:ALA:HA	1:B:1694:MET:HE3	1.92	0.51
1:B:2724:TYR:HD1	1:B:2895:PHE:CD2	2.27	0.51
1:B:2833:LEU:HB3	1:B:2838[A]:HIS:NE2	2.25	0.51
1:B:4943:MET:HA	1:B:4946:GLU:HG2	1.91	0.51
1:C:332:ARG:NH1	1:C:339:ASP:OD1	2.43	0.51
1:C:848:ARG:NH1	1:C:1599:MET:SD	2.83	0.51
1:C:2160:ASN:OD1	1:C:2163:ARG:NH2	2.40	0.51
1:C:2420:ARG:NH2	1:C:2475:VAL:O	2.44	0.51
1:D:874:LEU:HB2	1:D:878:LEU:HD22	1.91	0.51
1:D:2729:HIS:CD2	1:D:2763:LEU:HD22	2.44	0.51
1:A:2349:GLU:OE2	1:A:2359:ARG:NH2	2.42	0.51
1:A:2791:ARG:HH21	1:A:2795:GLY:C	2.18	0.51
1:A:3954:MET:HE3	1:A:3954:MET:HA	1.93	0.51
1:A:4702:ASP:O	1:A:4706:GLN:HG2	2.10	0.51
1:C:2150:MET:HE1	1:C:2199:PHE:HA	1.92	0.51
1:C:2758:LYS:NZ	1:C:2762:LEU:O	2.40	0.51
1:C:2767:GLU:O	1:C:2771:TYR:N	2.40	0.51
1:C:2930:ILE:HG23	1:C:3010:LYS:HZ3	1.75	0.51
1:C:3013:VAL:O	1:C:3018:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4702:ASP:O	1:C:4706:GLN:HG2	2.10	0.51
1:D:927:GLN:NE2	1:D:928:GLU:HG3	2.25	0.51
1:D:2420:ARG:NH2	1:D:2475:VAL:O	2.44	0.51
1:D:4640:PHE:HB3	1:D:4650:LYS:HE2	1.92	0.51
1:A:2290:TRP:CZ2	1:A:2388:ILE:HG12	2.46	0.51
1:A:3803:LEU:HB2	1:A:3884:SER:HB2	1.92	0.51
1:B:367:ASP:OD1	1:B:368:THR:N	2.43	0.51
1:B:1501:ASN:OD1	1:B:1502:ASN:N	2.43	0.51
1:B:2349:GLU:OE2	1:B:2359:ARG:NH2	2.42	0.51
1:B:3823:GLU:HG3	1:B:3826:GLY:HA2	1.92	0.51
1:C:2054:LYS:HE2	1:C:2056:SER:HA	1.92	0.51
1:D:848:ARG:NH1	1:D:1599:MET:SD	2.84	0.51
1:D:1688:ALA:HA	1:D:1694:MET:HE3	1.92	0.51
1:D:2503:ASP:HB3	1:D:2554:ARG:NH2	2.25	0.51
1:A:118:ALA:HA	1:A:161:THR:HA	1.93	0.51
1:A:874:LEU:HB2	1:A:878:LEU:HD22	1.91	0.51
1:A:996:VAL:HG13	1:A:1047:LYS:HE2	1.91	0.51
1:B:1286:THR:OG1	1:B:1550:PRO:O	2.27	0.51
1:B:3668:ILE:HD12	1:B:3734:ARG:HB2	1.91	0.51
1:D:2290:TRP:CZ2	1:D:2388:ILE:HG12	2.46	0.51
1:A:332:ARG:NH1	1:A:339:ASP:OD1	2.43	0.51
1:A:848:ARG:NH1	1:A:1599:MET:SD	2.83	0.51
1:A:939:THR:O	1:A:943:LEU:HG	2.11	0.51
1:A:2420:ARG:NH2	1:A:2475:VAL:O	2.44	0.51
1:A:2930:ILE:HA	1:A:3010:LYS:HZ1	1.75	0.51
1:B:3669:LEU:HB3	1:B:3673:ARG:HH21	1.74	0.51
1:B:4106:SER:HA	1:B:4115:LEU:HD21	1.92	0.51
1:C:118:ALA:HA	1:C:161:THR:HA	1.93	0.51
1:C:902:TRP:HZ2	1:C:915:HIS:CB	2.23	0.51
1:C:2142:MET:HE2	1:C:2142:MET:HA	1.91	0.51
1:C:2349:GLU:OE2	1:C:2359:ARG:NH2	2.42	0.51
1:C:2503:ASP:HB3	1:C:2554:ARG:NH2	2.25	0.51
1:D:538:ALA:O	1:D:542:ARG:HG3	2.11	0.51
1:D:2777:GLU:O	1:D:2781:THR:OG1	2.19	0.51
1:D:3823:GLU:HG3	1:D:3826:GLY:HA2	1.92	0.51
1:D:3954:MET:HA	1:D:3954:MET:HE3	1.93	0.51
1:D:4106:SER:HA	1:D:4115:LEU:HD21	1.92	0.51
1:A:2150:MET:HE1	1:A:2199:PHE:HA	1.92	0.51
1:A:2503:ASP:HB3	1:A:2554:ARG:NH2	2.25	0.51
1:A:3669:LEU:HB3	1:A:3673:ARG:HH21	1.74	0.51
1:B:2833:LEU:HB3	1:B:2838[B]:HIS:NE2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:890:HIS:CE1	1:C:891:GLU:HG2	2.46	0.51
1:C:4569:GLU:HB3	1:C:4570:PRO:HD3	1.92	0.51
1:C:4943:MET:SD	1:C:4951:PHE:HB3	2.51	0.51
1:D:35:LEU:HD23	1:D:51:SER:HA	1.93	0.51
1:D:902:TRP:HZ2	1:D:915:HIS:CB	2.23	0.51
1:D:2504:THR:O	1:D:2508:SER:N	2.40	0.51
1:D:4520:TYR:HD1	1:D:4561:LEU:HD13	1.76	0.51
1:D:4569:GLU:HB3	1:D:4570:PRO:HD3	1.92	0.51
1:C:939:THR:O	1:C:943:LEU:HG	2.11	0.51
1:C:1431:ARG:NE	1:C:1506:GLU:OE1	2.30	0.51
1:C:2798:MET:SD	1:C:2799:ALA:N	2.84	0.51
1:C:4520:TYR:HD1	1:C:4561:LEU:HD13	1.76	0.51
1:C:4862:ILE:HD13	1:D:4852:PHE:HE1	1.75	0.51
1:D:890:HIS:CE1	1:D:891:GLU:HG2	2.46	0.51
1:D:1501:ASN:OD1	1:D:1502:ASN:N	2.43	0.51
1:D:1827:THR:HG22	1:D:1831:MET:HE3	1.92	0.51
1:D:2703:PRO:HB2	1:D:2854:LYS:HB2	1.91	0.51
1:D:2798:MET:SD	1:D:2799:ALA:N	2.84	0.51
1:D:4943:MET:SD	1:D:4951:PHE:HB3	2.51	0.51
1:B:1016:TRP:HA	1:B:1027:ARG:HB3	1.93	0.51
1:C:927:GLN:NE2	1:C:928:GLU:HG3	2.25	0.51
1:C:1501:ASN:OD1	1:C:1502:ASN:N	2.43	0.51
1:C:4631:ASP:O	1:C:4634:VAL:HG12	2.11	0.51
1:C:4640:PHE:CD2	1:C:4641:PRO:HD2	2.46	0.51
1:D:2982:PHE:O	1:D:3001:LYS:NZ	2.44	0.51
1:D:4631:ASP:O	1:D:4634:VAL:HG12	2.11	0.51
1:A:538:ALA:O	1:A:542:ARG:HG3	2.11	0.51
1:A:986:ILE:CD1	1:A:1055:ARG:HA	2.40	0.51
1:A:2797:SER:HB3	1:A:2801:TYR:HE2	1.72	0.51
1:A:4114:ARG:O	1:A:4117:THR:OG1	2.22	0.51
1:A:4187:GLU:OE1	1:A:4949:TRP:NE1	2.35	0.51
2:H:12:ASP:OD1	2:H:68:SER:OG	2.27	0.51
1:B:1432:ILE:HB	1:B:1505:LEU:HB3	1.94	0.51
1:B:1851:PHE:HZ	1:B:2058:LEU:HD13	1.76	0.51
1:C:35:LEU:HD23	1:C:51:SER:HA	1.93	0.51
1:C:1016:TRP:HA	1:C:1027:ARG:HB3	1.93	0.51
1:C:1432:ILE:HB	1:C:1505:LEU:HB3	1.94	0.51
1:C:2290:TRP:CZ2	1:C:2388:ILE:HG12	2.46	0.51
1:C:2794:GLU:O	1:C:2797:SER:HB2	2.11	0.51
1:C:2930:ILE:HA	1:C:3010:LYS:HZ1	1.76	0.51
1:C:4018:ASP:OD2	1:C:4022:LYS:NZ	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1851:PHE:HZ	1:D:2058:LEU:HD13	1.76	0.51
1:D:2732:TRP:CD1	1:D:2736:LYS:HZ3	2.29	0.51
1:D:2794:GLU:O	1:D:2797:SER:HB2	2.11	0.51
1:A:367:ASP:OD1	1:A:368:THR:N	2.43	0.50
1:A:890:HIS:CE1	1:A:891:GLU:HG2	2.46	0.50
1:A:1851:PHE:HZ	1:A:2058:LEU:HD13	1.76	0.50
1:A:4943:MET:SD	1:A:4951:PHE:HB3	2.51	0.50
1:B:538:ALA:O	1:B:542:ARG:HG3	2.11	0.50
1:B:2212:LYS:NZ	1:B:3822:GLU:OE1	2.32	0.50
1:C:2782:MET:HE2	1:C:2787:TRP:O	2.12	0.50
1:C:4640:PHE:HB3	1:C:4650:LYS:HE2	1.92	0.50
1:D:1007:TRP:CD1	1:D:1011:ARG:HH11	2.30	0.50
1:A:2488:LEU:HD12	1:A:2492:PHE:HB2	1.93	0.50
1:A:2794:GLU:O	1:A:2797:SER:HB2	2.11	0.50
1:A:4569:GLU:HB3	1:A:4570:PRO:HD3	1.92	0.50
1:A:4631:ASP:O	1:A:4634:VAL:HG12	2.11	0.50
1:B:890:HIS:CE1	1:B:891:GLU:HG2	2.46	0.50
1:B:1243:THR:HG22	1:B:1808:ASP:HB2	1.93	0.50
1:B:2290:TRP:CZ2	1:B:2388:ILE:HG12	2.46	0.50
1:B:2488:LEU:HD12	1:B:2492:PHE:HB2	1.93	0.50
1:B:2794:GLU:O	1:B:2797:SER:HB2	2.11	0.50
1:B:3097:THR:HA	1:B:3101:LEU:HD23	1.94	0.50
1:C:1007:TRP:CD1	1:C:1011:ARG:HH11	2.30	0.50
1:C:1685:LEU:HD22	1:C:1706:LEU:HB2	1.93	0.50
1:C:3996:GLY:O	1:C:4000:VAL:HG23	2.12	0.50
1:D:996:VAL:HG13	1:D:1047:LYS:HE2	1.91	0.50
1:D:2659:GLN:OE1	1:D:2659:GLN:N	2.37	0.50
1:A:842:GLN:OE1	1:A:1603:PHE:N	2.43	0.50
1:A:1220:ASP:OD2	1:A:1222:SER:OG	2.30	0.50
1:A:1286:THR:OG1	1:A:1550:PRO:O	2.27	0.50
1:A:1826:TYR:O	1:A:1830:ILE:HG12	2.12	0.50
1:A:2418:ARG:O	1:A:2422:ILE:HG12	2.12	0.50
1:A:4769:LEU:HB3	1:D:4753:LEU:CD2	2.41	0.50
1:B:67:PHE:HB3	1:B:121:LEU:HD22	1.93	0.50
1:B:1559:ARG:HD3	1:B:1565:PRO:HD3	1.93	0.50
1:B:1685:LEU:HD22	1:B:1706:LEU:HB2	1.93	0.50
1:B:4631:ASP:O	1:B:4634:VAL:HG12	2.11	0.50
1:C:929:ARG:HH22	1:C:933:LEU:HD21	1.75	0.50
1:C:2172:MET:O	1:C:2176:VAL:HG23	2.11	0.50
1:D:4634:VAL:O	1:D:4637:THR:OG1	2.26	0.50
1:A:35:LEU:HD23	1:A:51:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2782:MET:HE2	1:A:2787:TRP:O	2.11	0.50
1:A:2933:VAL:HA	1:A:2963:PHE:CZ	2.46	0.50
1:A:4106:SER:HA	1:A:4115:LEU:HD21	1.92	0.50
1:B:2856:LYS:O	1:B:2860:LEU:HD23	2.12	0.50
1:C:538:ALA:O	1:C:542:ARG:HG3	2.11	0.50
1:C:1559:ARG:HD3	1:C:1565:PRO:HD3	1.93	0.50
1:A:1947:VAL:HG11	1:A:1965:PHE:CE2	2.46	0.50
1:A:2129:LEU:HD23	1:A:2132:VAL:HG21	1.94	0.50
1:A:2172:MET:O	1:A:2176:VAL:HG23	2.11	0.50
1:B:1220:ASP:OD2	1:B:1222:SER:OG	2.30	0.50
1:B:2420:ARG:NH2	1:B:2475:VAL:O	2.44	0.50
1:B:4903:HIS:HB3	1:B:4906:GLU:OE2	2.12	0.50
1:C:1152:TYR:HD1	1:C:1184:ASP:HB3	1.76	0.50
1:C:1851:PHE:HZ	1:C:2058:LEU:HD13	1.76	0.50
1:C:1947:VAL:CG2	1:C:1961:LYS:HB3	2.42	0.50
1:C:2856:LYS:O	1:C:2860:LEU:HD23	2.12	0.50
1:D:398:HIS:HB3	1:D:400:ASP:N	2.26	0.50
1:D:939:THR:O	1:D:943:LEU:HG	2.11	0.50
1:D:1947:VAL:HG11	1:D:1965:PHE:CE2	2.46	0.50
1:D:2172:MET:O	1:D:2176:VAL:HG23	2.11	0.50
1:A:1007:TRP:CD1	1:A:1011:ARG:HH11	2.30	0.50
1:A:2798:MET:SD	1:A:2799:ALA:N	2.84	0.50
1:A:2982:PHE:O	1:A:3001:LYS:NZ	2.44	0.50
1:A:4245:LEU:CD1	1:B:4626:ILE:HG13	2.40	0.50
1:B:118:ALA:HA	1:B:161:THR:HA	1.93	0.50
1:B:2798:MET:SD	1:B:2799:ALA:N	2.84	0.50
1:B:2933:VAL:HA	1:B:2963:PHE:CZ	2.46	0.50
1:B:3891:TYR:HA	1:C:76:ARG:NH2	2.25	0.50
1:C:1711:LEU:HB3	1:C:1831:MET:CE	2.40	0.50
1:C:2488:LEU:HD12	1:C:2492:PHE:HB2	1.93	0.50
1:C:2982:PHE:O	1:C:3001:LYS:NZ	2.44	0.50
1:D:1685:LEU:HD22	1:D:1706:LEU:HB2	1.93	0.50
1:D:2129:LEU:HD23	1:D:2132:VAL:HG21	1.94	0.50
1:A:4640:PHE:CD2	1:A:4641:PRO:HD2	2.46	0.50
1:B:132:CYS:H	1:B:157:ALA:HB1	1.77	0.50
1:B:939:THR:O	1:B:943:LEU:HG	2.11	0.50
1:B:1947:VAL:HG11	1:B:1965:PHE:CE2	2.46	0.50
1:B:2331:PHE:HB3	1:B:2335:LEU:HB2	1.94	0.50
1:B:2503:ASP:HB3	1:B:2554:ARG:NH2	2.25	0.50
1:B:3954:MET:HA	1:B:3954:MET:HE3	1.93	0.50
1:B:4569:GLU:HB3	1:B:4570:PRO:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1293:GLN:OE1	1:C:1294:ASN:N	2.45	0.50
1:C:2418:ARG:O	1:C:2422:ILE:HG12	2.12	0.50
1:C:2852:TRP:CZ2	1:C:2856:LYS:HE2	2.47	0.50
1:D:118:ALA:HA	1:D:161:THR:HA	1.93	0.50
1:D:929:ARG:HH22	1:D:933:LEU:HD21	1.75	0.50
1:D:1826:TYR:O	1:D:1830:ILE:HG12	2.12	0.50
1:D:3912:VAL:O	1:D:3916:VAL:HG23	2.12	0.50
1:D:3940:LEU:HD11	1:D:3981:MET:HE1	1.93	0.50
1:D:4903:HIS:HB3	1:D:4906:GLU:OE2	2.12	0.50
1:A:1293:GLN:OE1	1:A:1294:ASN:N	2.45	0.50
1:A:2732:TRP:CD1	1:A:2736:LYS:HZ3	2.30	0.50
1:A:2777:GLU:O	1:A:2781:THR:OG1	2.19	0.50
1:B:929:ARG:HH22	1:B:933:LEU:HD21	1.75	0.50
1:B:2988:ARG:HB2	1:B:2989:PRO:HD3	1.94	0.50
1:C:398:HIS:HB3	1:C:400:ASP:N	2.26	0.50
1:C:625:VAL:HG22	1:C:2133:ARG:HD2	1.94	0.50
1:C:2129:LEU:HD23	1:C:2132:VAL:HG21	1.94	0.50
1:C:3097:THR:HA	1:C:3101:LEU:HD23	1.94	0.50
1:D:1559:ARG:HD3	1:D:1565:PRO:HD3	1.93	0.50
1:D:2782:MET:HE2	1:D:2787:TRP:O	2.11	0.50
1:D:2856:LYS:O	1:D:2860:LEU:HD23	2.12	0.50
1:A:398:HIS:HB3	1:A:400:ASP:N	2.27	0.50
1:A:1432:ILE:HB	1:A:1505:LEU:HB3	1.93	0.50
1:A:1559:ARG:HD3	1:A:1565:PRO:HD3	1.93	0.50
1:A:1685:LEU:HD22	1:A:1706:LEU:HB2	1.93	0.50
1:A:2331:PHE:HB3	1:A:2335:LEU:HB2	1.94	0.50
1:A:2526:PRO:O	1:A:2529:THR:N	2.45	0.50
1:A:2833:LEU:HB3	1:A:2838[A]:HIS:CE1	2.47	0.50
1:A:3811:GLN:NE2	1:A:3823:GLU:OE2	2.45	0.50
1:B:1007:TRP:CD1	1:B:1011:ARG:HH11	2.30	0.50
1:B:1947:VAL:CG2	1:B:1961:LYS:HB3	2.42	0.50
1:B:2990:LEU:HB3	1:B:2993:GLY:O	2.12	0.50
1:B:4943:MET:SD	1:B:4951:PHE:HB3	2.51	0.50
1:C:2581:ARG:HB3	1:C:2584:MET:HG2	1.92	0.50
1:C:3043:ARG:HB3	1:C:3047:LYS:NZ	2.27	0.50
1:C:3954:MET:HA	1:C:3954:MET:HE3	1.93	0.50
1:D:1293:GLN:OE1	1:D:1294:ASN:N	2.45	0.50
1:D:1432:ILE:HB	1:D:1505:LEU:HB3	1.93	0.50
1:D:2888:LYS:HA	1:D:2891:ASP:OD2	2.12	0.50
1:D:3043:ARG:HB3	1:D:3047:LYS:NZ	2.27	0.50
1:A:929:ARG:HH22	1:A:933:LEU:HD21	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2593:VAL:HG12	1:A:2644:LEU:HD22	1.94	0.49
1:A:3890:TRP:O	1:B:76:ARG:NH2	2.45	0.49
1:A:4831:ILE:HG13	1:A:4843:ARG:NH2	2.21	0.49
1:B:514:PHE:HD2	1:B:526:TRP:HB2	1.77	0.49
1:B:3996:GLY:O	1:B:4000:VAL:HG23	2.12	0.49
1:B:4930:GLU:OE2	1:B:4941:TRP:NE1	2.45	0.49
1:C:4903:HIS:HB3	1:C:4906:GLU:OE2	2.12	0.49
1:D:132:CYS:H	1:D:157:ALA:HB1	1.77	0.49
1:D:503:ASP:O	1:D:507:VAL:HG13	2.12	0.49
1:D:625:VAL:HG22	1:D:2133:ARG:HD2	1.94	0.49
1:D:1016:TRP:HA	1:D:1027:ARG:HB3	1.93	0.49
1:D:1711:LEU:HB3	1:D:1831:MET:CE	2.40	0.49
1:D:2581:ARG:HB3	1:D:2584:MET:HG2	1.92	0.49
1:D:2852:TRP:CZ2	1:D:2856:LYS:HE2	2.47	0.49
1:D:3996:GLY:O	1:D:4000:VAL:HG23	2.12	0.49
1:D:4267:GLN:O	1:D:4271:VAL:HG12	2.12	0.49
1:A:1016:TRP:HA	1:A:1027:ARG:HB3	1.93	0.49
1:A:2856:LYS:O	1:A:2860:LEU:HD23	2.12	0.49
1:A:2988:ARG:HB2	1:A:2989:PRO:HD3	1.94	0.49
1:A:3912:VAL:O	1:A:3916:VAL:HG23	2.12	0.49
1:A:4047:ASP:HA	1:A:4050:LYS:HG2	1.93	0.49
1:B:3940:LEU:HD11	1:B:3981:MET:HE1	1.93	0.49
1:B:4267:GLN:O	1:B:4271:VAL:HG12	2.12	0.49
1:C:1243:THR:HG22	1:C:1808:ASP:HB2	1.93	0.49
1:C:4114:ARG:O	1:C:4117:THR:OG1	2.22	0.49
1:C:4664:ASP:OD1	1:C:4664:ASP:N	2.42	0.49
1:D:161:THR:HG23	1:D:186:VAL:HG22	1.94	0.49
1:D:2933:VAL:HA	1:D:2963:PHE:CZ	2.46	0.49
1:D:4047:ASP:HA	1:D:4050:LYS:HG2	1.93	0.49
1:D:4640:PHE:CD2	1:D:4641:PRO:HD2	2.46	0.49
1:A:161:THR:HG23	1:A:186:VAL:HG22	1.94	0.49
1:A:503:ASP:O	1:A:507:VAL:HG13	2.13	0.49
1:A:1152:TYR:HD1	1:A:1184:ASP:HB3	1.76	0.49
1:A:4903:HIS:HB3	1:A:4906:GLU:OE2	2.12	0.49
1:B:1293:GLN:OE1	1:B:1294:ASN:N	2.45	0.49
1:B:1298:ASP:OD1	1:B:1299:ILE:N	2.46	0.49
1:B:2782:MET:HE2	1:B:2787:TRP:O	2.11	0.49
1:B:2885:ASP:O	1:B:2888:LYS:HG3	2.13	0.49
1:B:2982:PHE:O	1:B:3001:LYS:NZ	2.44	0.49
1:C:132:CYS:H	1:C:157:ALA:HB1	1.77	0.49
1:C:1042:THR:O	1:C:1046:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3912:VAL:O	1:C:3916:VAL:HG23	2.12	0.49
1:C:4267:GLN:O	1:C:4271:VAL:HG12	2.12	0.49
1:D:67:PHE:HB3	1:D:121:LEU:HD22	1.93	0.49
1:D:1152:TYR:HD1	1:D:1184:ASP:HB3	1.76	0.49
1:D:1690:GLU:OE1	1:D:1790:LYS:NZ	2.42	0.49
1:D:4633:LEU:O	1:D:4637:THR:HG23	2.13	0.49
1:A:67:PHE:HB3	1:A:121:LEU:HD22	1.93	0.49
1:A:1042:THR:O	1:A:1046:ASN:ND2	2.46	0.49
1:A:1283:LEU:HB2	1:A:1555:PHE:HB2	1.94	0.49
1:A:1468:THR:HG22	1:A:1479:SER:HB2	1.95	0.49
1:A:3043:ARG:HB3	1:A:3047:LYS:NZ	2.27	0.49
1:A:3996:GLY:O	1:A:4000:VAL:HG23	2.12	0.49
1:A:4267:GLN:O	1:A:4271:VAL:HG12	2.12	0.49
1:B:35:LEU:HD23	1:B:51:SER:HA	1.93	0.49
1:B:971:GLN:HG3	1:B:978:PRO:HG2	1.94	0.49
1:B:2172:MET:O	1:B:2176:VAL:HG23	2.11	0.49
1:B:2418:ARG:O	1:B:2422:ILE:HG12	2.12	0.49
1:B:3042:ALA:HB3	1:B:3117:PHE:CE2	2.48	0.49
1:B:3074:ASN:OD1	1:B:3075:LEU:N	2.46	0.49
1:B:4633:LEU:HD22	1:B:4704:LYS:HE3	1.95	0.49
1:C:971:GLN:HG3	1:C:978:PRO:HG2	1.94	0.49
1:C:1102:TYR:HD2	1:C:1165:MET:HG2	1.77	0.49
1:C:2593:VAL:HG12	1:C:2644:LEU:HD22	1.94	0.49
1:C:2732:TRP:CD1	1:C:2736:LYS:HZ3	2.30	0.49
1:C:4640:PHE:CD1	1:C:4641:PRO:HD2	2.47	0.49
1:D:1243:THR:HG22	1:D:1808:ASP:HB2	1.93	0.49
1:A:1243:THR:HG22	1:A:1808:ASP:HB2	1.93	0.49
1:A:2885:ASP:O	1:A:2888:LYS:HG3	2.13	0.49
1:A:4633:LEU:HD22	1:A:4704:LYS:HE3	1.95	0.49
1:B:842:GLN:OE1	1:B:1603:PHE:N	2.43	0.49
1:B:1102:TYR:HD2	1:B:1165:MET:HG2	1.77	0.49
1:B:2129:LEU:HD23	1:B:2132:VAL:HG21	1.94	0.49
1:B:3811:GLN:NE2	1:B:3823:GLU:OE2	2.45	0.49
1:B:4640:PHE:CD1	1:B:4641:PRO:HD2	2.47	0.49
1:B:4640:PHE:CD2	1:B:4641:PRO:HD2	2.46	0.49
1:C:67:PHE:HB3	1:C:121:LEU:HD22	1.93	0.49
1:C:1826:TYR:O	1:C:1830:ILE:HG12	2.12	0.49
1:C:3940:LEU:HD11	1:C:3981:MET:HE1	1.93	0.49
1:D:367:ASP:OD1	1:D:368:THR:N	2.43	0.49
1:D:1468:THR:HG22	1:D:1479:SER:HB2	1.95	0.49
1:D:2418:ARG:O	1:D:2422:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2526:PRO:O	1:D:2529:THR:N	2.45	0.49
1:D:2990:LEU:HB3	1:D:2993:GLY:O	2.12	0.49
1:A:625:VAL:HG22	1:A:2133:ARG:HD2	1.94	0.49
1:A:1102:TYR:HD2	1:A:1165:MET:HG2	1.77	0.49
1:A:1298:ASP:OD1	1:A:1299:ILE:N	2.46	0.49
1:A:2852:TRP:CZ2	1:A:2856:LYS:HE2	2.47	0.49
1:A:3074:ASN:OD1	1:A:3075:LEU:N	2.46	0.49
1:A:3097:THR:HA	1:A:3101:LEU:HD23	1.94	0.49
1:B:161:THR:HG23	1:B:186:VAL:HG22	1.94	0.49
1:B:398:HIS:HB3	1:B:400:ASP:N	2.26	0.49
1:B:625:VAL:HG22	1:B:2133:ARG:HD2	1.94	0.49
1:B:1711:LEU:HB3	1:B:1831:MET:CE	2.40	0.49
1:B:2888:LYS:HA	1:B:2891:ASP:OD2	2.12	0.49
1:C:1947:VAL:HG11	1:C:1965:PHE:CE2	2.46	0.49
1:C:2933:VAL:HA	1:C:2963:PHE:CZ	2.46	0.49
1:C:3074:ASN:OD1	1:C:3075:LEU:N	2.46	0.49
1:C:3920:LEU:O	1:C:3924:ILE:HG12	2.13	0.49
1:C:4633:LEU:HD22	1:C:4704:LYS:HE3	1.95	0.49
1:D:926:GLU:O	1:D:929:ARG:HB3	2.13	0.49
1:D:1298:ASP:OD1	1:D:1299:ILE:N	2.46	0.49
1:D:3074:ASN:OD1	1:D:3075:LEU:N	2.46	0.49
1:D:4633:LEU:HD22	1:D:4704:LYS:HE3	1.95	0.49
1:D:4930:GLU:OE2	1:D:4941:TRP:NE1	2.45	0.49
1:A:2681:MET:HE1	1:A:2920:ARG:HG2	1.95	0.49
1:A:4279:MET:HE3	1:B:4488:GLN:HG3	1.94	0.49
2:H:35:LYS:NZ	1:D:640:ARG:O	2.46	0.49
1:B:503:ASP:O	1:B:507:VAL:HG13	2.12	0.49
1:B:1042:THR:O	1:B:1046:ASN:ND2	2.46	0.49
1:B:2593:VAL:HG12	1:B:2644:LEU:HD22	1.94	0.49
1:B:2929:LEU:O	1:B:2933:VAL:HG23	2.13	0.49
1:B:3912:VAL:O	1:B:3916:VAL:HG23	2.12	0.49
1:D:971:GLN:HG3	1:D:978:PRO:HG2	1.94	0.49
1:D:2229:LEU:O	1:D:2235:ARG:NH1	2.46	0.49
1:D:2711:ILE:CG2	1:D:2783:LEU:HD22	2.43	0.49
1:D:2930:ILE:HG23	1:D:3010:LYS:HZ3	1.78	0.49
1:D:2988:ARG:HB2	1:D:2989:PRO:HD3	1.94	0.49
1:D:3811:GLN:NE2	1:D:3823:GLU:OE2	2.45	0.49
1:A:1788:LYS:O	1:A:1792:ILE:HG13	2.13	0.49
1:A:2868:HIS:CD2	1:A:2870:LEU:H	2.31	0.49
1:A:2888:LYS:HA	1:A:2891:ASP:OD2	2.12	0.49
1:B:2229:LEU:O	1:B:2235:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2990:LEU:HB3	1:C:2993:GLY:O	2.12	0.49
1:C:3042:ALA:HB3	1:C:3117:PHE:CE2	2.48	0.49
1:D:2331:PHE:HB3	1:D:2335:LEU:HB2	1.94	0.49
1:D:2681:MET:HE1	1:D:2920:ARG:HG2	1.95	0.49
1:A:2711:ILE:CG2	1:A:2783:LEU:HD22	2.43	0.49
1:A:3763:ILE:HD11	1:A:3838:ASP:O	2.13	0.49
1:A:3940:LEU:HD11	1:A:3981:MET:HE1	1.93	0.49
1:A:4633:LEU:O	1:A:4637:THR:HG23	2.13	0.49
1:B:681:HIS:O	1:B:799:LYS:N	2.46	0.49
1:B:1089:ARG:HB3	1:B:1204:VAL:HG23	1.94	0.49
1:B:3043:ARG:HB3	1:B:3047:LYS:NZ	2.27	0.49
1:C:555:LEU:HD11	1:C:585:ALA:HB1	1.95	0.49
1:C:2526:PRO:O	1:C:2529:THR:N	2.45	0.49
1:C:3001:LYS:O	1:C:3005:THR:HG23	2.13	0.49
1:C:4047:ASP:HA	1:C:4050:LYS:HG2	1.93	0.49
1:D:2593:VAL:HG12	1:D:2644:LEU:HD22	1.94	0.49
1:D:3042:ALA:HB3	1:D:3117:PHE:CE2	2.48	0.49
1:D:4640:PHE:CD1	1:D:4641:PRO:HD2	2.47	0.49
1:A:681:HIS:O	1:A:799:LYS:N	2.46	0.49
1:A:1051:ARG:O	1:A:1055:ARG:HG2	2.13	0.49
1:A:3042:ALA:HB3	1:A:3117:PHE:CE2	2.48	0.49
1:A:3920:LEU:O	1:A:3924:ILE:HG12	2.13	0.49
1:A:4268:MET:HE1	1:B:4480:PHE:HZ	1.77	0.49
1:A:4714:PHE:CD1	1:D:4294:LEU:HD12	2.48	0.49
1:B:1468:THR:HG22	1:B:1479:SER:HB2	1.95	0.49
1:B:2526:PRO:O	1:B:2529:THR:N	2.45	0.49
1:B:2553:TYR:HD2	1:B:2591:ARG:HH21	1.61	0.49
1:B:2826:ILE:HG22	1:C:1502:ASN:HA	1.94	0.49
1:B:3920:LEU:O	1:B:3924:ILE:HG12	2.13	0.49
1:C:681:HIS:O	1:C:799:LYS:N	2.46	0.49
1:C:926:GLU:O	1:C:929:ARG:HB3	2.13	0.49
1:C:1298:ASP:OD1	1:C:1299:ILE:N	2.46	0.49
1:C:2331:PHE:HB3	1:C:2335:LEU:HB2	1.94	0.49
1:C:2347:MET:O	1:C:2351:ILE:HG12	2.13	0.49
1:C:2868:HIS:CD2	1:C:2870:LEU:H	2.31	0.49
1:D:2349:GLU:OE2	1:D:2359:ARG:NH2	2.42	0.49
1:D:3920:LEU:O	1:D:3924:ILE:HG12	2.13	0.49
1:A:2840:MET:HA	1:A:2843:MET:HE3	1.95	0.48
1:A:3001:LYS:O	1:A:3005:THR:HG23	2.13	0.48
1:A:4587:ILE:HG23	1:A:4719:PHE:HE1	1.78	0.48
1:A:4860:ALA:CB	1:D:4863:GLN:HG2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1152:TYR:HD1	1:B:1184:ASP:HB3	1.76	0.48
1:B:1826:TYR:O	1:B:1830:ILE:HG12	2.12	0.48
1:B:2852:TRP:CZ2	1:B:2856:LYS:HE2	2.47	0.48
1:B:3001:LYS:O	1:B:3005:THR:HG23	2.13	0.48
1:C:2681:MET:HE1	1:C:2920:ARG:HG2	1.95	0.48
1:C:2885:ASP:O	1:C:2888:LYS:HG3	2.13	0.48
1:C:2888:LYS:HA	1:C:2891:ASP:OD2	2.12	0.48
1:C:3763:ILE:HD11	1:C:3838:ASP:O	2.13	0.48
1:C:4633:LEU:O	1:C:4637:THR:HG23	2.13	0.48
1:D:1089:ARG:HB3	1:D:1204:VAL:HG23	1.94	0.48
1:D:2488:LEU:HD12	1:D:2492:PHE:HB2	1.93	0.48
1:D:2840:MET:HA	1:D:2843:MET:HE3	1.95	0.48
1:D:3097:THR:HA	1:D:3101:LEU:HD23	1.94	0.48
1:A:336:GLU:OE2	1:A:338:LEU:HB3	2.14	0.48
1:A:514:PHE:HD2	1:A:526:TRP:HB2	1.77	0.48
1:A:926:GLU:O	1:A:929:ARG:HB3	2.13	0.48
1:A:4640:PHE:CD1	1:A:4641:PRO:HD2	2.47	0.48
1:B:1051:ARG:O	1:B:1055:ARG:HG2	2.13	0.48
1:C:514:PHE:HD2	1:C:526:TRP:HB2	1.77	0.48
1:C:2840:MET:HA	1:C:2843:MET:HE3	1.95	0.48
1:C:3811:GLN:NE2	1:C:3823:GLU:OE2	2.45	0.48
1:D:1042:THR:O	1:D:1046:ASN:ND2	2.46	0.48
1:D:1283:LEU:HB2	1:D:1555:PHE:HB2	1.94	0.48
1:D:2553:TYR:HD2	1:D:2591:ARG:HH21	1.61	0.48
1:D:2732:TRP:NE1	1:D:2736:LYS:HZ3	2.12	0.48
1:A:132:CYS:H	1:A:157:ALA:HB1	1.77	0.48
1:A:555:LEU:HD11	1:A:585:ALA:HB1	1.95	0.48
1:A:1089:ARG:HB3	1:A:1204:VAL:HG23	1.94	0.48
1:B:1244:ASN:HD22	1:B:1801:GLU:HG2	1.78	0.48
1:B:2681:MET:HE1	1:B:2920:ARG:HG2	1.95	0.48
1:B:2868:HIS:CD2	1:B:2870:LEU:H	2.31	0.48
1:B:2917:ILE:HD12	1:B:2920:ARG:HD2	1.95	0.48
1:B:3890:TRP:O	1:C:76:ARG:NH2	2.46	0.48
1:B:4587:ILE:HG23	1:B:4719:PHE:HE1	1.78	0.48
1:C:1051:ARG:O	1:C:1055:ARG:HG2	2.13	0.48
1:C:4930:GLU:OE2	1:C:4941:TRP:NE1	2.45	0.48
1:D:1051:ARG:O	1:D:1055:ARG:HG2	2.13	0.48
1:D:1102:TYR:HD2	1:D:1165:MET:HG2	1.77	0.48
1:D:1244:ASN:HD22	1:D:1801:GLU:HG2	1.78	0.48
1:D:1788:LYS:O	1:D:1792:ILE:HG13	2.13	0.48
1:D:2885:ASP:O	1:D:2888:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:GLU:HA	1:A:1055:ARG:CG	2.44	0.48
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.39	0.48
1:A:1260:GLN:NE2	1:A:1261:VAL:O	2.47	0.48
1:B:555:LEU:HD11	1:B:585:ALA:HB1	1.95	0.48
1:B:1260:GLN:NE2	1:B:1261:VAL:O	2.47	0.48
1:B:1283:LEU:HB2	1:B:1555:PHE:HB2	1.94	0.48
1:B:2157:GLN:O	1:B:3615:ARG:NH2	2.44	0.48
1:B:2455:ASP:HB3	1:B:2458:ALA:HB3	1.95	0.48
1:B:3763:ILE:HD11	1:B:3838:ASP:O	2.13	0.48
1:B:4047:ASP:HA	1:B:4050:LYS:HG2	1.93	0.48
1:C:2455:ASP:HB3	1:C:2458:ALA:HB3	1.95	0.48
1:D:336:GLU:OE2	1:D:338:LEU:HB3	2.14	0.48
1:D:681:HIS:O	1:D:799:LYS:N	2.46	0.48
1:D:1052:GLU:HA	1:D:1055:ARG:CG	2.44	0.48
1:D:1518:LEU:HB2	1:D:1531:TYR:HB2	1.96	0.48
1:D:1947:VAL:CG2	1:D:1961:LYS:HB3	2.42	0.48
1:D:4109:MET:HB2	1:D:4115:LEU:HD22	1.96	0.48
1:B:3944:VAL:HG13	1:B:3978:MET:HE3	1.95	0.48
1:C:1260:GLN:NE2	1:C:1261:VAL:O	2.47	0.48
1:C:1518:LEU:HB2	1:C:1531:TYR:HB2	1.96	0.48
1:C:2092:TYR:HD2	1:C:3640:LEU:HD13	1.78	0.48
1:C:2229:LEU:O	1:C:2235:ARG:NH1	2.46	0.48
1:C:2918:GLU:HA	1:C:2923:TYR:CD2	2.49	0.48
1:C:2929:LEU:O	1:C:2933:VAL:HG23	2.13	0.48
1:D:555:LEU:HD11	1:D:585:ALA:HB1	1.95	0.48
1:D:3763:ILE:HD11	1:D:3838:ASP:O	2.13	0.48
1:A:983:LEU:HD12	1:A:1055:ARG:HG3	1.96	0.48
1:A:2229:LEU:O	1:A:2235:ARG:NH1	2.46	0.48
1:A:2990:LEU:HB3	1:A:2993:GLY:O	2.12	0.48
1:A:3730:ARG:O	1:A:3734:ARG:NH1	2.47	0.48
1:A:3944:VAL:HG13	1:A:3978:MET:HE3	1.95	0.48
2:F:12:ASP:OD2	2:F:15:THR:HG22	2.13	0.48
1:B:1788:LYS:O	1:B:1792:ILE:HG13	2.13	0.48
1:B:2711:ILE:CG2	1:B:2783:LEU:HD22	2.43	0.48
1:B:3889:TYR:CD1	1:B:3954:MET:SD	3.07	0.48
1:C:2553:TYR:HD2	1:C:2591:ARG:HH21	1.61	0.48
1:C:2841:ALA:HB2	1:C:2893:LEU:HD21	1.96	0.48
1:C:2988:ARG:HB2	1:C:2989:PRO:HD3	1.94	0.48
1:C:2998:ASN:O	1:C:3002:GLU:HG2	2.13	0.48
1:A:1690:GLU:OE1	1:A:1790:LYS:NZ	2.42	0.48
1:A:2918:GLU:HA	1:A:2923:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3944:VAL:HG11	1:A:4002:MET:HE2	1.96	0.48
1:A:4930:GLU:OE2	1:A:4941:TRP:NE1	2.45	0.48
1:B:2238:THR:OG1	1:B:2241:ASP:OD2	2.24	0.48
1:C:161:THR:HG23	1:C:186:VAL:HG22	1.94	0.48
1:C:1089:ARG:HB3	1:C:1204:VAL:HG23	1.94	0.48
1:C:2917:ILE:HD12	1:C:2920:ARG:HD2	1.95	0.48
1:C:3770:ASN:HB3	1:C:3773:VAL:CG1	2.42	0.48
1:C:4267:GLN:HA	1:C:4270:LYS:HE2	1.96	0.48
1:C:4587:ILE:HG23	1:C:4719:PHE:HE1	1.78	0.48
1:D:1220:ASP:OD2	1:D:1222:SER:OG	2.30	0.48
1:D:2868:HIS:CD2	1:D:2870:LEU:H	2.31	0.48
1:A:1711:LEU:HB3	1:A:1831:MET:CE	2.40	0.48
1:A:1947:VAL:CG2	1:A:1961:LYS:HB3	2.42	0.48
1:A:2497:ARG:HH22	1:A:2878:THR:N	2.12	0.48
1:A:4048:PHE:O	1:A:4052:MET:HG2	2.14	0.48
2:E:12:ASP:OD2	2:E:15:THR:HG22	2.13	0.48
1:B:614:LEU:HA	1:B:617:LEU:HD12	1.96	0.48
1:B:926:GLU:O	1:B:929:ARG:HB3	2.13	0.48
1:B:1518:LEU:HB2	1:B:1531:TYR:HB2	1.96	0.48
1:B:2347:MET:O	1:B:2351:ILE:HG12	2.13	0.48
1:C:336:GLU:OE2	1:C:338:LEU:HB3	2.13	0.48
1:C:718:VAL:HG23	1:C:793:SER:HB3	1.96	0.48
1:C:1468:THR:HG22	1:C:1479:SER:HB2	1.95	0.48
1:C:2432:LEU:O	1:C:2436:ILE:HG13	2.14	0.48
1:C:2930:ILE:HD12	1:C:3003:MET:HE2	1.96	0.48
1:C:4109:MET:HB2	1:C:4115:LEU:HD22	1.96	0.48
1:D:50:GLU:CD	1:D:61:ASP:H	2.21	0.48
1:D:932:ASN:HA	1:D:935:MET:HG3	1.96	0.48
1:D:2855:LYS:HE3	1:D:2856:LYS:HZ2	1.79	0.48
1:D:4048:PHE:O	1:D:4052:MET:HG2	2.14	0.48
1:A:971:GLN:HG3	1:A:978:PRO:HG2	1.94	0.48
1:A:1518:LEU:HB2	1:A:1531:TYR:HB2	1.96	0.48
1:A:2763:LEU:HG	1:A:2764:SER:N	2.29	0.48
1:A:2930:ILE:HG23	1:A:3010:LYS:HZ3	1.79	0.48
1:A:4107:GLU:OE1	1:A:4149:TYR:OH	2.22	0.48
1:A:4109:MET:HB2	1:A:4115:LEU:HD22	1.96	0.48
2:G:50:ARG:N	2:G:55:GLU:OE2	2.37	0.48
1:B:932:ASN:HA	1:B:935:MET:HG3	1.96	0.48
1:B:2497:ARG:HH22	1:B:2878:THR:N	2.12	0.48
1:B:4048:PHE:O	1:B:4052:MET:HG2	2.14	0.48
1:B:4633:LEU:O	1:B:4637:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1787:LEU:HD23	1:C:1828:LEU:HD21	1.96	0.48
1:C:2763:LEU:HG	1:C:2764:SER:N	2.29	0.48
1:D:514:PHE:HD2	1:D:526:TRP:HB2	1.77	0.48
1:D:2763:LEU:HD23	1:D:2767:GLU:CD	2.39	0.48
1:D:2929:LEU:O	1:D:2933:VAL:HG23	2.13	0.48
1:D:4587:ILE:HG23	1:D:4719:PHE:HE1	1.78	0.48
1:D:4873:LEU:O	1:D:4877:GLN:HG2	2.14	0.48
1:A:2157:GLN:O	1:A:3615:ARG:NH2	2.44	0.48
1:A:2929:LEU:O	1:A:2933:VAL:HG23	2.13	0.48
1:A:4518:LEU:HD21	1:B:4810:LEU:HD13	1.96	0.48
1:A:4664:ASP:N	1:A:4664:ASP:OD1	2.42	0.48
2:G:12:ASP:OD2	2:G:15:THR:HG22	2.13	0.48
2:H:12:ASP:OD2	2:H:15:THR:HG22	2.13	0.48
1:B:2432:LEU:O	1:B:2436:ILE:HG13	2.14	0.48
1:B:4267:GLN:HA	1:B:4270:LYS:HE2	1.96	0.48
1:C:503:ASP:O	1:C:507:VAL:HG13	2.12	0.48
1:C:1911:GLN:OE1	1:C:2090:ARG:NH1	2.47	0.48
1:C:3889:TYR:CD1	1:C:3954:MET:SD	3.07	0.48
1:C:4008:ASN:OD1	1:C:4009:ASN:N	2.47	0.48
1:C:4730:VAL:HA	1:C:4733:HIS:HD2	1.78	0.48
1:C:4873:LEU:O	1:C:4877:GLN:HG2	2.14	0.48
1:D:448:PRO:HB2	1:D:451:SER:OG	2.14	0.48
1:D:614:LEU:HA	1:D:617:LEU:HD12	1.96	0.48
1:D:3944:VAL:HG11	1:D:4002:MET:HE2	1.96	0.48
1:A:50:GLU:CD	1:A:61:ASP:H	2.21	0.47
1:A:2841:ALA:HB2	1:A:2893:LEU:HD21	1.96	0.47
1:A:4008:ASN:OD1	1:A:4009:ASN:N	2.47	0.47
1:B:336:GLU:OE2	1:B:338:LEU:HB3	2.13	0.47
1:B:2685:TYR:CE1	1:B:2909:ASP:HB2	2.49	0.47
1:B:2732:TRP:CD1	1:B:2736:LYS:HZ3	2.31	0.47
1:B:2763:LEU:HG	1:B:2764:SER:N	2.28	0.47
1:B:2840:MET:HA	1:B:2843:MET:HE3	1.95	0.47
1:B:2905:ARG:HH11	1:B:2906:GLY:N	2.12	0.47
1:B:2998:ASN:O	1:B:3002:GLU:HG2	2.13	0.47
1:C:718:VAL:HG13	1:C:724:SER:HB2	1.96	0.47
1:C:932:ASN:HA	1:C:935:MET:HG3	1.96	0.47
1:C:1052:GLU:HA	1:C:1055:ARG:CG	2.44	0.47
1:C:1283:LEU:HB2	1:C:1555:PHE:HB2	1.94	0.47
1:C:2763:LEU:HD23	1:C:2767:GLU:CD	2.39	0.47
1:D:718:VAL:HG23	1:D:793:SER:HB3	1.96	0.47
1:D:2998:ASN:O	1:D:3002:GLU:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3662:ASP:O	1:D:3666:GLN:HG3	2.14	0.47
1:D:3944:VAL:HG13	1:D:3978:MET:HE3	1.95	0.47
1:D:4026:LEU:O	1:D:4029:SER:OG	2.29	0.47
1:A:908:ARG:NH1	1:A:928:GLU:OE2	2.35	0.47
1:A:2526:PRO:HB3	1:A:2530:ARG:HH11	1.80	0.47
1:A:3004:VAL:O	1:A:3007:LEU:HG	2.15	0.47
1:A:4730:VAL:HA	1:A:4733:HIS:HD2	1.79	0.47
1:B:718:VAL:HG13	1:B:724:SER:HB2	1.96	0.47
1:B:1009:ARG:O	1:B:1013:ARG:HG2	2.15	0.47
1:B:1911:GLN:OE1	1:B:2090:ARG:NH1	2.47	0.47
1:B:2791:ARG:HH21	1:B:2796:ASP:N	2.12	0.47
1:C:1244:ASN:HD22	1:C:1801:GLU:HG2	1.78	0.47
1:C:2497:ARG:HH22	1:C:2878:THR:N	2.12	0.47
1:D:1950:ALA:HB1	1:D:1961:LYS:HZ3	1.78	0.47
1:D:2497:ARG:HH22	1:D:2878:THR:N	2.12	0.47
1:D:2917:ILE:HD12	1:D:2920:ARG:HD2	1.95	0.47
1:A:2553:TYR:HD2	1:A:2591:ARG:HH21	1.61	0.47
1:B:983:LEU:HD12	1:B:1055:ARG:HG3	1.96	0.47
1:B:1007:TRP:O	1:B:1011:ARG:HG2	2.14	0.47
1:B:2092:TYR:HD2	1:B:3640:LEU:HD13	1.79	0.47
1:C:889:ILE:HA	1:C:892:LEU:HD12	1.97	0.47
1:C:1788:LYS:O	1:C:1792:ILE:HG13	2.13	0.47
1:C:4048:PHE:O	1:C:4052:MET:HG2	2.14	0.47
1:C:4120:GLU:HA	1:C:4123:GLU:HG2	1.97	0.47
1:D:983:LEU:HD12	1:D:1055:ARG:HG3	1.96	0.47
1:D:1260:GLN:NE2	1:D:1261:VAL:O	2.47	0.47
1:D:2775:ILE:O	1:D:2779:LEU:HG	2.14	0.47
1:D:3770:ASN:HB3	1:D:3773:VAL:CG1	2.42	0.47
1:A:718:VAL:HG13	1:A:724:SER:HB2	1.96	0.47
1:A:1007:TRP:O	1:A:1011:ARG:HG2	2.14	0.47
1:A:1009:ARG:O	1:A:1013:ARG:HG2	2.14	0.47
1:A:2943:PHE:CE2	1:A:2947:SER:HB3	2.50	0.47
1:B:1954:SER:O	1:B:1958:THR:OG1	2.33	0.47
1:B:2763:LEU:HD23	1:B:2767:GLU:CD	2.39	0.47
1:B:2775:ILE:O	1:B:2779:LEU:HG	2.14	0.47
1:B:4730:VAL:HA	1:B:4733:HIS:HD2	1.78	0.47
1:C:2791:ARG:HH21	1:C:2796:ASP:N	2.12	0.47
1:C:3701:ASP:OD2	1:C:3727:GLN:NE2	2.48	0.47
1:D:1911:GLN:OE1	1:D:2090:ARG:NH1	2.47	0.47
1:D:2526:PRO:HB3	1:D:2530:ARG:HH11	1.79	0.47
1:D:2918:GLU:HA	1:D:2923:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3001:LYS:O	1:D:3005:THR:HG23	2.13	0.47
1:D:3016:ARG:O	1:D:3018:ARG:NH1	2.48	0.47
1:A:131:CYS:SG	1:A:150:GLN:HB2	2.55	0.47
1:A:920:GLU:O	1:A:924:LEU:N	2.48	0.47
1:A:1087:ILE:HG22	1:A:1252:SER:OG	2.15	0.47
1:A:1244:ASN:HD22	1:A:1801:GLU:HG2	1.78	0.47
1:A:3889:TYR:CD1	1:A:3954:MET:SD	3.07	0.47
1:B:232:ASP:OD2	1:B:407:ARG:NH1	2.48	0.47
1:B:1787:LEU:HD23	1:B:1828:LEU:HD21	1.95	0.47
1:B:2918:GLU:HA	1:B:2923:TYR:CD2	2.49	0.47
1:B:3016:ARG:O	1:B:3018:ARG:NH1	2.48	0.47
1:B:3730:ARG:O	1:B:3734:ARG:NH1	2.47	0.47
1:C:448:PRO:HB2	1:C:451:SER:OG	2.14	0.47
1:C:1954:SER:O	1:C:1958:THR:OG1	2.33	0.47
1:C:2711:ILE:CG2	1:C:2783:LEU:HD22	2.43	0.47
1:C:2886:ARG:O	1:C:2890:GLN:OE1	2.33	0.47
1:C:3004:VAL:O	1:C:3007:LEU:HG	2.15	0.47
1:C:3016:ARG:O	1:C:3018:ARG:NH1	2.48	0.47
1:D:718:VAL:HG13	1:D:724:SER:HB2	1.97	0.47
1:D:1787:LEU:HD23	1:D:1828:LEU:HD21	1.95	0.47
1:D:2347:MET:O	1:D:2351:ILE:HG12	2.13	0.47
1:D:2930:ILE:HD12	1:D:3003:MET:HE2	1.96	0.47
1:D:2943:PHE:CE2	1:D:2947:SER:HB3	2.50	0.47
1:D:4730:VAL:HA	1:D:4733:HIS:HD2	1.78	0.47
1:A:889:ILE:HA	1:A:892:LEU:HD12	1.97	0.47
1:A:2763:LEU:HD23	1:A:2767:GLU:CD	2.39	0.47
1:A:2791:ARG:HH21	1:A:2796:ASP:N	2.12	0.47
1:A:4873:LEU:O	1:A:4877:GLN:HG2	2.14	0.47
1:B:50:GLU:CD	1:B:61:ASP:H	2.21	0.47
1:B:889:ILE:HA	1:B:892:LEU:HD12	1.97	0.47
1:B:1092:LYS:NZ	1:B:1646:GLU:OE1	2.39	0.47
1:B:2526:PRO:HB3	1:B:2530:ARG:HH11	1.80	0.47
1:B:2898:ILE:HG23	1:C:1500:ARG:NH2	2.27	0.47
1:B:2930:ILE:HD12	1:B:3003:MET:HE2	1.96	0.47
1:B:3108:LEU:O	1:B:3112:ILE:HG12	2.15	0.47
1:C:4049:HIS:CD2	1:C:4067:LEU:HD11	2.47	0.47
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.39	0.47
1:D:1177:LEU:O	1:D:1180:GLU:HG3	2.15	0.47
1:D:2685:TYR:CE1	1:D:2909:ASP:HB2	2.49	0.47
1:D:2791:ARG:HH21	1:D:2796:ASP:N	2.12	0.47
1:D:2886:ARG:O	1:D:2890:GLN:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3730:ARG:O	1:D:3734:ARG:NH1	2.47	0.47
1:A:232:ASP:OD2	1:A:407:ARG:NH1	2.48	0.47
1:A:932:ASN:HA	1:A:935:MET:HG3	1.96	0.47
1:A:1954:SER:O	1:A:1958:THR:OG1	2.33	0.47
1:A:2775:ILE:O	1:A:2779:LEU:HG	2.14	0.47
1:A:2917:ILE:HD12	1:A:2920:ARG:HD2	1.95	0.47
1:A:2930:ILE:HD12	1:A:3003:MET:HE2	1.96	0.47
1:A:2998:ASN:O	1:A:3002:GLU:HG2	2.13	0.47
1:A:3077:GLN:HG2	1:A:3078:GLY:N	2.30	0.47
1:A:4684:GLU:N	1:A:4684:GLU:OE2	2.48	0.47
1:B:2841:ALA:HB2	1:B:2893:LEU:HD21	1.96	0.47
1:B:2943:PHE:CE2	1:B:2947:SER:HB3	2.50	0.47
1:B:3701:ASP:OD2	1:B:3727:GLN:NE2	2.48	0.47
1:B:4109:MET:HB2	1:B:4115:LEU:HD22	1.96	0.47
1:B:4120:GLU:HA	1:B:4123:GLU:HG2	1.97	0.47
1:B:4873:LEU:O	1:B:4877:GLN:HG2	2.14	0.47
1:C:131:CYS:SG	1:C:150:GLN:HB2	2.55	0.47
1:C:1007:TRP:O	1:C:1011:ARG:HG2	2.14	0.47
1:C:1009:ARG:O	1:C:1013:ARG:HG2	2.14	0.47
1:C:1087:ILE:HG22	1:C:1252:SER:OG	2.15	0.47
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.39	0.47
1:C:3730:ARG:O	1:C:3734:ARG:NH1	2.47	0.47
1:C:3944:VAL:HG11	1:C:4002:MET:HE2	1.96	0.47
1:C:3944:VAL:HG13	1:C:3978:MET:HE3	1.95	0.47
1:D:474:ASP:O	1:D:478:ARG:HG2	2.15	0.47
1:D:1007:TRP:O	1:D:1011:ARG:HG2	2.14	0.47
1:D:2432:LEU:O	1:D:2436:ILE:HG13	2.14	0.47
1:D:2841:ALA:HB2	1:D:2893:LEU:HD21	1.96	0.47
1:D:3889:TYR:CD1	1:D:3954:MET:SD	3.07	0.47
1:D:4120:GLU:HA	1:D:4123:GLU:HG2	1.97	0.47
1:A:1177:LEU:O	1:A:1180:GLU:HG3	2.15	0.47
1:A:1787:LEU:HD23	1:A:1828:LEU:HD21	1.96	0.47
1:B:3077:GLN:HG2	1:B:3078:GLY:N	2.30	0.47
1:C:423:VAL:HG23	1:C:497:LEU:HD22	1.97	0.47
1:C:874:LEU:HD13	1:C:878:LEU:HB3	1.96	0.47
1:C:1220:ASP:OD2	1:C:1222:SER:OG	2.30	0.47
1:C:2526:PRO:HB3	1:C:2530:ARG:HH11	1.79	0.47
1:C:2775:ILE:O	1:C:2779:LEU:HG	2.14	0.47
1:C:2789:ILE:HD12	1:C:2903:VAL:HA	1.96	0.47
1:D:889:ILE:HA	1:D:892:LEU:HD12	1.97	0.47
1:D:2092:TYR:HD2	1:D:3640:LEU:HD13	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2629:ASN:OD1	1:D:2630:PHE:N	2.48	0.47
1:A:448:PRO:HB2	1:A:451:SER:OG	2.14	0.47
1:A:614:LEU:HA	1:A:617:LEU:HD12	1.96	0.47
1:A:1911:GLN:OE1	1:A:2090:ARG:NH1	2.47	0.47
1:A:2979:ARG:H	1:A:2979:ARG:HD3	1.80	0.47
1:A:3662:ASP:O	1:A:3666:GLN:HG3	2.14	0.47
1:A:3770:ASN:HB3	1:A:3773:VAL:CG1	2.42	0.47
1:A:4049:HIS:CD2	1:A:4067:LEU:HD11	2.47	0.47
1:A:4187:GLU:OE2	1:A:4947:ARG:NH2	2.41	0.47
1:B:448:PRO:HB2	1:B:451:SER:OG	2.14	0.47
1:B:874:LEU:HD13	1:B:878:LEU:HB3	1.96	0.47
1:B:1611:ILE:HB	1:B:1615:GLN:HB2	1.97	0.47
1:B:2886:ARG:O	1:B:2890:GLN:OE1	2.33	0.47
1:B:3662:ASP:O	1:B:3666:GLN:HG3	2.14	0.47
1:B:3944:VAL:HG11	1:B:4002:MET:HE2	1.96	0.47
1:C:983:LEU:HD12	1:C:1055:ARG:HG3	1.96	0.47
1:C:1611:ILE:HB	1:C:1615:GLN:HB2	1.97	0.47
1:D:874:LEU:HD13	1:D:878:LEU:HB3	1.96	0.47
1:D:4269:LYS:HA	1:D:4272:LYS:HE3	1.96	0.47
1:A:2204:CYS:SG	1:A:2214:MET:HG2	2.55	0.47
1:A:2455:ASP:HB3	1:A:2458:ALA:HB3	1.95	0.47
1:A:4267:GLN:HA	1:A:4270:LYS:HE2	1.96	0.47
1:B:1431:ARG:NE	1:B:1506:GLU:OE1	2.30	0.47
1:B:2782:MET:O	1:B:2786:GLY:N	2.48	0.47
1:B:3728:GLN:O	1:B:3732:HIS:ND1	2.46	0.47
1:C:1177:LEU:O	1:C:1180:GLU:HG3	2.15	0.47
1:C:1940:GLN:OE1	1:C:3608:LEU:HB2	2.15	0.47
1:C:2943:PHE:CE2	1:C:2947:SER:HB3	2.50	0.47
1:C:4269:LYS:HA	1:C:4272:LYS:HE3	1.96	0.47
1:C:4639:SER:OG	1:C:4642:ASN:HB2	2.15	0.47
1:D:232:ASP:OD2	1:D:407:ARG:NH1	2.48	0.47
1:D:920:GLU:O	1:D:924:LEU:N	2.48	0.47
1:D:1009:ARG:O	1:D:1013:ARG:HG2	2.15	0.47
1:D:2204:CYS:SG	1:D:2214:MET:HG2	2.55	0.47
1:D:2526:PRO:O	1:D:2530:ARG:HG3	2.15	0.47
1:D:2610:LEU:HD13	1:D:2644:LEU:HD21	1.97	0.47
1:A:2629:ASN:OD1	1:A:2630:PHE:N	2.48	0.46
1:A:2855:LYS:HE3	1:A:2856:LYS:HZ2	1.80	0.46
1:B:131:CYS:SG	1:B:150:GLN:HB2	2.55	0.46
1:B:1523:ASN:HB2	1:B:1525:LYS:NZ	2.30	0.46
1:B:2694:SER:O	1:B:2701:PHE:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:920:GLU:O	1:C:924:LEU:N	2.48	0.46
1:C:2685:TYR:CE1	1:C:2909:ASP:HB2	2.49	0.46
1:C:3662:ASP:O	1:C:3666:GLN:HG3	2.14	0.46
1:C:3892:TYR:OH	1:C:3899:ASP:OD1	2.32	0.46
1:D:131:CYS:SG	1:D:150:GLN:HB2	2.55	0.46
1:D:4584:PHE:HD1	1:D:4726:MET:HE2	1.81	0.46
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.97	0.46
1:A:1523:ASN:HB2	1:A:1525:LYS:NZ	2.30	0.46
1:A:1940:GLN:OE1	1:A:3608:LEU:HB2	2.15	0.46
1:A:2347:MET:O	1:A:2351:ILE:HG12	2.13	0.46
1:A:4584:PHE:HD1	1:A:4726:MET:HE2	1.81	0.46
1:B:920:GLU:O	1:B:924:LEU:N	2.48	0.46
1:B:2629:ASN:OD1	1:B:2630:PHE:N	2.48	0.46
1:D:61:ASP:OD1	1:D:63:SER:OG	2.32	0.46
1:D:842:GLN:OE1	1:D:1603:PHE:N	2.43	0.46
1:D:1940:GLN:OE1	1:D:3608:LEU:HB2	2.15	0.46
1:D:1954:SER:O	1:D:1958:THR:OG1	2.33	0.46
1:D:3701:ASP:OD2	1:D:3727:GLN:NE2	2.48	0.46
1:D:4267:GLN:HA	1:D:4270:LYS:HE2	1.96	0.46
1:D:4796:SER:HB3	1:D:4803:ASP:HB3	1.97	0.46
1:A:2732:TRP:NE1	1:A:2736:LYS:HZ3	2.14	0.46
1:B:61:ASP:OD1	1:B:63:SER:OG	2.32	0.46
1:B:718:VAL:HG23	1:B:793:SER:HB3	1.96	0.46
1:B:1052:GLU:HA	1:B:1055:ARG:CG	2.44	0.46
1:B:4008:ASN:OD1	1:B:4009:ASN:N	2.47	0.46
1:B:4684:GLU:N	1:B:4684:GLU:OE2	2.48	0.46
1:B:4796:SER:HB3	1:B:4803:ASP:HB3	1.98	0.46
1:C:50:GLU:CD	1:C:61:ASP:H	2.21	0.46
1:C:2659:GLN:C	1:C:2663:LYS:HZ2	2.24	0.46
1:C:2905:ARG:HH11	1:C:2906:GLY:N	2.12	0.46
1:C:3077:GLN:HG2	1:C:3078:GLY:N	2.30	0.46
1:D:1490:ALA:HA	1:D:1493:SER:HB2	1.98	0.46
1:D:2455:ASP:HB3	1:D:2458:ALA:HB3	1.95	0.46
1:D:2763:LEU:HG	1:D:2764:SER:N	2.29	0.46
1:D:2782:MET:O	1:D:2786:GLY:N	2.48	0.46
1:D:2905:ARG:HH11	1:D:2906:GLY:N	2.12	0.46
1:A:2303:ARG:NH1	1:A:2307:PHE:HB3	2.31	0.46
1:A:2526:PRO:O	1:A:2530:ARG:HG3	2.15	0.46
1:A:2666:LEU:HD13	1:A:2966:VAL:HA	1.97	0.46
1:A:2685:TYR:CE1	1:A:2909:ASP:HB2	2.49	0.46
1:A:4017:PHE:O	1:A:4021:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.97	0.46
1:B:1262:PRO:HD3	1:B:1590:PHE:HE1	1.81	0.46
1:B:3004:VAL:O	1:B:3007:LEU:HG	2.15	0.46
1:B:4017:PHE:O	1:B:4021:LEU:HG	2.16	0.46
1:B:4639:SER:OG	1:B:4642:ASN:HB2	2.15	0.46
1:C:1262:PRO:HD3	1:C:1590:PHE:HE1	1.81	0.46
1:C:2629:ASN:OD1	1:C:2630:PHE:N	2.48	0.46
1:C:2789:ILE:HD12	1:C:2903:VAL:CA	2.46	0.46
1:C:4796:SER:HB3	1:C:4803:ASP:HB3	1.97	0.46
1:D:1087:ILE:HG22	1:D:1252:SER:OG	2.15	0.46
1:D:2789:ILE:HD12	1:D:2903:VAL:HA	1.96	0.46
1:D:3004:VAL:O	1:D:3007:LEU:HG	2.14	0.46
1:D:3108:LEU:O	1:D:3112:ILE:HG12	2.15	0.46
1:D:4008:ASN:OD1	1:D:4009:ASN:N	2.47	0.46
1:A:2092:TYR:HD2	1:A:3640:LEU:HD13	1.78	0.46
1:A:2905:ARG:HH11	1:A:2906:GLY:N	2.12	0.46
1:B:1494:MET:CE	1:B:1505:LEU:HD22	2.46	0.46
1:B:2303:ARG:NH1	1:B:2307:PHE:HB3	2.31	0.46
1:B:2980:LEU:HD23	1:B:2990:LEU:HG	1.98	0.46
1:B:4815:PHE:O	1:B:4819:VAL:HG22	2.16	0.46
1:C:474:ASP:O	1:C:478:ARG:HG2	2.15	0.46
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.97	0.46
1:C:2855:LYS:HE3	1:C:2856:LYS:NZ	2.31	0.46
1:C:4187:GLU:OE2	1:C:4947:ARG:NH2	2.41	0.46
1:D:317:MET:HB2	1:D:321:LYS:HZ2	1.81	0.46
1:D:1262:PRO:HD3	1:D:1590:PHE:HE1	1.81	0.46
1:D:2303:ARG:NH1	1:D:2307:PHE:HB3	2.31	0.46
1:D:2660:GLU:HA	1:D:2663:LYS:HZ2	1.80	0.46
1:D:3077:GLN:HG2	1:D:3078:GLY:N	2.30	0.46
1:D:4049:HIS:CD2	1:D:4067:LEU:HD11	2.47	0.46
1:D:4815:PHE:O	1:D:4819:VAL:HG22	2.16	0.46
1:A:474:ASP:O	1:A:478:ARG:HG2	2.15	0.46
1:A:1431:ARG:NE	1:A:1506:GLU:OE1	2.30	0.46
1:A:1490:ALA:HA	1:A:1493:SER:HB2	1.98	0.46
1:A:2432:LEU:O	1:A:2436:ILE:HG13	2.14	0.46
1:A:2610:LEU:HD13	1:A:2644:LEU:HD21	1.97	0.46
1:A:2782:MET:O	1:A:2786:GLY:N	2.48	0.46
1:A:2980:LEU:HD23	1:A:2990:LEU:HG	1.98	0.46
1:A:3016:ARG:O	1:A:3018:ARG:NH1	2.48	0.46
1:A:3108:LEU:O	1:A:3112:ILE:HG12	2.15	0.46
1:B:423:VAL:HG23	1:B:497:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ASP:O	1:B:478:ARG:HG2	2.15	0.46
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.39	0.46
1:B:1234:GLU:H	1:B:1234:GLU:CD	2.23	0.46
1:B:1953:MET:N	1:B:1953:MET:SD	2.89	0.46
1:B:2610:LEU:HD13	1:B:2644:LEU:HD21	1.97	0.46
1:B:2666:LEU:HD13	1:B:2966:VAL:HA	1.97	0.46
1:B:2979:ARG:HD3	1:B:2979:ARG:H	1.80	0.46
1:C:232:ASP:OD2	1:C:407:ARG:NH1	2.48	0.46
1:C:2526:PRO:O	1:C:2530:ARG:HG3	2.15	0.46
1:C:2666:LEU:HD13	1:C:2966:VAL:HA	1.97	0.46
1:C:2782:MET:O	1:C:2786:GLY:N	2.48	0.46
1:C:3749:GLY:HA2	1:C:3796:LEU:HG	1.97	0.46
1:C:3961:ASP:OD2	1:C:3963:SER:OG	2.34	0.46
1:D:4017:PHE:O	1:D:4021:LEU:HG	2.16	0.46
1:A:1427:TYR:HB2	1:A:1563:VAL:HG11	1.98	0.46
1:A:2886:ARG:O	1:A:2890:GLN:OE1	2.33	0.46
1:A:4269:LYS:HA	1:A:4272:LYS:HE3	1.96	0.46
1:A:4796:SER:HB3	1:A:4803:ASP:HB3	1.98	0.46
1:B:317:MET:HB2	1:B:321:LYS:HZ2	1.80	0.46
1:B:624:ALA:HB2	1:B:1667:LEU:HD12	1.97	0.46
1:B:2789:ILE:HD12	1:B:2903:VAL:HA	1.96	0.46
1:B:4049:HIS:CD2	1:B:4067:LEU:HD11	2.47	0.46
1:B:4269:LYS:HA	1:B:4272:LYS:HE3	1.96	0.46
1:B:4751:LYS:HG3	1:B:4754:ARG:NH1	2.31	0.46
1:C:317:MET:HB2	1:C:321:LYS:HZ2	1.81	0.46
1:C:2732:TRP:NE1	1:C:2736:LYS:HZ3	2.14	0.46
1:C:2979:ARG:H	1:C:2979:ARG:HD3	1.80	0.46
1:C:4684:GLU:N	1:C:4684:GLU:OE2	2.48	0.46
1:C:4815:PHE:O	1:C:4819:VAL:HG22	2.16	0.46
1:A:2772:ARG:O	1:A:2776:LYS:HG2	2.16	0.46
1:A:4120:GLU:HA	1:A:4123:GLU:HG2	1.97	0.46
1:B:504:ARG:O	1:B:507:VAL:HG22	2.16	0.46
1:B:1087:ILE:HG22	1:B:1252:SER:OG	2.15	0.46
1:B:1177:LEU:O	1:B:1180:GLU:HG3	2.15	0.46
1:B:1523:ASN:HB2	1:B:1525:LYS:HZ1	1.81	0.46
1:B:3613:ARG:O	1:B:3617:VAL:HG23	2.16	0.46
1:B:4584:PHE:HD1	1:B:4726:MET:HE2	1.81	0.46
1:C:61:ASP:OD1	1:C:63:SER:OG	2.32	0.46
1:C:614:LEU:HA	1:C:617:LEU:HD12	1.96	0.46
1:C:2204:CYS:SG	1:C:2214:MET:HG2	2.55	0.46
1:C:3108:LEU:O	1:C:3112:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4584:PHE:HD1	1:C:4726:MET:HE2	1.81	0.46
1:D:1523:ASN:HB2	1:D:1525:LYS:NZ	2.31	0.46
1:D:2979:ARG:H	1:D:2979:ARG:HD3	1.80	0.46
1:D:3693:ASP:O	1:D:3697:LYS:HG2	2.16	0.46
1:D:4684:GLU:N	1:D:4684:GLU:OE2	2.48	0.46
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.97	0.46
1:A:2589:LEU:O	1:A:2593:VAL:HG13	2.16	0.46
1:A:2855:LYS:HE3	1:A:2856:LYS:NZ	2.31	0.46
1:A:3994:THR:HA	1:A:3997:LYS:HD2	1.98	0.46
1:B:2589:LEU:O	1:B:2593:VAL:HG13	2.16	0.46
1:B:2659:GLN:C	1:B:2663:LYS:HZ2	2.23	0.46
1:B:2772:ARG:O	1:B:2776:LYS:HG2	2.16	0.46
1:B:2930:ILE:HG23	1:B:3010:LYS:HZ3	1.80	0.46
1:C:1234:GLU:H	1:C:1234:GLU:CD	2.23	0.46
1:C:1427:TYR:HB2	1:C:1563:VAL:HG11	1.98	0.46
1:C:2303:ARG:NH1	1:C:2307:PHE:HB3	2.31	0.46
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.97	0.46
1:D:1689:ILE:HG22	1:D:1794:MET:HE1	1.98	0.46
1:D:4639:SER:OG	1:D:4642:ASN:HB2	2.15	0.46
1:A:423:VAL:HG23	1:A:497:LEU:HD22	1.97	0.46
1:A:718:VAL:HG23	1:A:793:SER:HB3	1.96	0.46
1:A:2789:ILE:HD12	1:A:2903:VAL:HA	1.97	0.46
1:A:3728:GLN:O	1:A:3732:HIS:ND1	2.46	0.46
1:A:3891:TYR:HA	1:B:76:ARG:NH2	2.31	0.46
1:A:4018:ASP:OD2	1:A:4022:LYS:NZ	2.38	0.46
1:B:1429:SER:HB3	1:B:1506:GLU:OE2	2.16	0.46
1:B:4814:MET:HE1	1:C:4844:ILE:HD13	1.98	0.46
1:C:2157:GLN:O	1:C:3615:ARG:NH2	2.44	0.46
1:C:3613:ARG:O	1:C:3617:VAL:HG23	2.16	0.46
1:C:3693:ASP:O	1:C:3697:LYS:HG2	2.16	0.46
1:C:4862:ILE:HA	1:C:4865:LEU:HD12	1.98	0.46
1:D:423:VAL:HG23	1:D:497:LEU:HD22	1.97	0.46
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	1.97	0.46
1:D:1611:ILE:HB	1:D:1615:GLN:HB2	1.97	0.46
1:D:2694:SER:O	1:D:2701:PHE:HA	2.15	0.46
1:D:3961:ASP:OD2	1:D:3963:SER:OG	2.34	0.46
1:D:4819:VAL:HG12	1:D:4822:ARG:NH2	2.31	0.46
1:D:4862:ILE:HA	1:D:4865:LEU:HD12	1.98	0.46
1:A:874:LEU:HD13	1:A:878:LEU:HB3	1.96	0.45
1:A:1960:ARG:H	1:A:1960:ARG:HG3	0.96	0.45
1:A:2789:ILE:HD12	1:A:2903:VAL:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3693:ASP:O	1:A:3697:LYS:HG2	2.16	0.45
1:A:4815:PHE:O	1:A:4819:VAL:HG22	2.16	0.45
1:B:1040:ASP:HA	1:B:1043:LYS:HG2	1.98	0.45
1:B:2526:PRO:O	1:B:2530:ARG:HG3	2.15	0.45
1:B:2789:ILE:HD12	1:B:2903:VAL:CA	2.46	0.45
1:C:942:THR:HA	1:C:945:ALA:HB3	1.98	0.45
1:C:2980:LEU:HD23	1:C:2990:LEU:HG	1.98	0.45
1:D:1106:GLU:HB3	1:D:1214:ARG:HB2	1.98	0.45
1:D:1953:MET:N	1:D:1953:MET:SD	2.89	0.45
1:D:2666:LEU:HD13	1:D:2966:VAL:HA	1.97	0.45
1:D:2980:LEU:HD23	1:D:2990:LEU:HG	1.98	0.45
1:D:3009:CYS:O	1:D:3013:VAL:HG23	2.17	0.45
1:D:3749:GLY:HA2	1:D:3796:LEU:HG	1.97	0.45
1:A:3613:ARG:O	1:A:3617:VAL:HG23	2.16	0.45
1:A:3701:ASP:OD2	1:A:3727:GLN:NE2	2.48	0.45
1:A:4862:ILE:HA	1:A:4865:LEU:HD12	1.98	0.45
1:B:1940:GLN:OE1	1:B:3608:LEU:HB2	2.15	0.45
1:B:2855:LYS:HE3	1:B:2856:LYS:NZ	2.31	0.45
1:B:2968:LEU:HD22	1:B:3029:ILE:HG23	1.98	0.45
1:B:3009:CYS:O	1:B:3013:VAL:HG23	2.17	0.45
1:B:3994:THR:HA	1:B:3997:LYS:HD2	1.98	0.45
1:B:4018:ASP:OD2	1:B:4022:LYS:NZ	2.38	0.45
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.97	0.45
1:C:2973:GLN:O	1:C:2976:LYS:HG3	2.17	0.45
1:D:942:THR:HA	1:D:945:ALA:HB3	1.98	0.45
1:D:1427:TYR:HB2	1:D:1563:VAL:HG11	1.98	0.45
1:D:2973:GLN:O	1:D:2976:LYS:HG3	2.17	0.45
1:A:1052:GLU:O	1:A:1055:ARG:HB2	2.16	0.45
1:A:1262:PRO:HD3	1:A:1590:PHE:HE1	1.81	0.45
1:A:2660:GLU:HA	1:A:2663:LYS:HZ2	1.81	0.45
1:B:322:ALA:HB1	1:B:327:THR:HG21	1.99	0.45
1:B:942:THR:HA	1:B:945:ALA:HB3	1.98	0.45
1:B:4026:LEU:O	1:B:4029:SER:OG	2.30	0.45
1:B:4189:PHE:CE1	1:B:4915:LEU:HG	2.52	0.45
1:B:4249:ARG:O	1:B:4253:LEU:HD23	2.17	0.45
1:C:1523:ASN:HB2	1:C:1525:LYS:NZ	2.30	0.45
1:C:3019:ILE:HD12	1:C:3026:ALA:HB1	1.99	0.45
1:C:4751:LYS:HG3	1:C:4754:ARG:NH1	2.31	0.45
1:D:2154:VAL:HG13	1:D:2158:HIS:CD2	2.48	0.45
1:D:3019:ILE:HD12	1:D:3026:ALA:HB1	1.99	0.45
1:D:3797:MET:HG3	1:D:3839:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:GLU:H	1:A:1234:GLU:CD	2.23	0.45
1:A:1429:SER:HB3	1:A:1506:GLU:OE2	2.16	0.45
1:A:1494:MET:CE	1:A:1505:LEU:HD22	2.46	0.45
1:A:3009:CYS:O	1:A:3013:VAL:HG23	2.16	0.45
1:A:3878:LEU:HA	1:A:3881:VAL:HG12	1.99	0.45
1:A:4639:SER:OG	1:A:4642:ASN:HB2	2.15	0.45
1:B:468:GLU:HA	1:B:475:LYS:NZ	2.32	0.45
1:B:1490:ALA:HA	1:B:1493:SER:HB2	1.98	0.45
1:B:4862:ILE:HA	1:B:4865:LEU:HD12	1.98	0.45
1:C:1523:ASN:HB2	1:C:1525:LYS:HZ1	1.81	0.45
1:C:1689:ILE:HG22	1:C:1794:MET:HE1	1.98	0.45
1:C:1953:MET:SD	1:C:1953:MET:N	2.89	0.45
1:C:2694:SER:O	1:C:2701:PHE:HA	2.15	0.45
1:D:504:ARG:O	1:D:507:VAL:HG22	2.16	0.45
1:D:1307:PRO:HB3	1:D:1540:PHE:CE2	2.52	0.45
1:D:1415:ASP:OD2	1:D:1559:ARG:NH2	2.49	0.45
1:D:2157:GLN:O	1:D:3615:ARG:NH2	2.44	0.45
1:D:2789:ILE:HD12	1:D:2903:VAL:CA	2.46	0.45
1:D:2855:LYS:HE3	1:D:2856:LYS:NZ	2.31	0.45
1:A:322:ALA:HB1	1:A:327:THR:HG21	1.99	0.45
1:A:504:ARG:O	1:A:507:VAL:HG22	2.16	0.45
1:A:1611:ILE:HB	1:A:1615:GLN:HB2	1.97	0.45
1:A:1953:MET:N	1:A:1953:MET:SD	2.89	0.45
1:A:4249:ARG:O	1:A:4253:LEU:HD23	2.17	0.45
1:A:4751:LYS:HG3	1:A:4754:ARG:NH1	2.31	0.45
1:B:1052:GLU:O	1:B:1055:ARG:HB2	2.16	0.45
1:B:2204:CYS:SG	1:B:2214:MET:HG2	2.55	0.45
1:B:3749:GLY:HA2	1:B:3796:LEU:HG	1.97	0.45
1:B:3878:LEU:HA	1:B:3881:VAL:HG12	1.99	0.45
1:C:908:ARG:NH1	1:C:928:GLU:OE2	2.35	0.45
1:C:1052:GLU:O	1:C:1055:ARG:HB2	2.16	0.45
1:C:2589:LEU:O	1:C:2593:VAL:HG13	2.16	0.45
1:C:2610:LEU:HD13	1:C:2644:LEU:HD21	1.97	0.45
1:C:2772:ARG:O	1:C:2776:LYS:HG2	2.16	0.45
1:C:3889:TYR:OH	1:C:3953:HIS:HB3	2.17	0.45
1:C:4921:PHE:HE2	1:C:4940:VAL:HG11	1.82	0.45
1:D:1040:ASP:HA	1:D:1043:LYS:HG2	1.98	0.45
1:D:3878:LEU:HA	1:D:3881:VAL:HG12	1.99	0.45
1:D:4751:LYS:HG3	1:D:4754:ARG:NH1	2.31	0.45
1:A:468:GLU:HA	1:A:475:LYS:NZ	2.32	0.45
1:A:2933:VAL:HB	1:A:3010:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3961:ASP:OD2	1:A:3963:SER:OG	2.34	0.45
1:A:4819:VAL:HG12	1:A:4822:ARG:NH2	2.31	0.45
1:B:1727:VAL:HG11	1:B:1926:VAL:HG21	1.99	0.45
1:B:2973:GLN:O	1:B:2976:LYS:HG3	2.17	0.45
1:C:504:ARG:O	1:C:507:VAL:HG22	2.16	0.45
1:C:1494:MET:CE	1:C:1505:LEU:HD22	2.46	0.45
1:C:3009:CYS:O	1:C:3013:VAL:HG23	2.17	0.45
1:C:3878:LEU:HA	1:C:3881:VAL:HG12	1.99	0.45
1:C:3994:THR:HA	1:C:3997:LYS:HD2	1.98	0.45
1:C:4017:PHE:O	1:C:4021:LEU:HG	2.16	0.45
1:C:4249:ARG:O	1:C:4253:LEU:HD23	2.17	0.45
1:C:4819:VAL:HG12	1:C:4822:ARG:NH2	2.31	0.45
1:D:322:ALA:HB1	1:D:327:THR:HG21	1.99	0.45
1:D:2933:VAL:HB	1:D:3010:LYS:NZ	2.32	0.45
1:D:4249:ARG:O	1:D:4253:LEU:HD23	2.17	0.45
1:A:765:SER:HA	1:A:779:PHE:O	2.16	0.45
1:A:2694:SER:O	1:A:2701:PHE:HA	2.15	0.45
1:A:3892:TYR:OH	1:A:3899:ASP:OD1	2.32	0.45
1:A:4262:LYS:HD2	1:A:4265:LYS:HD3	1.99	0.45
2:F:58:LYS:HB3	2:F:81:VAL:O	2.17	0.45
1:B:765:SER:HA	1:B:779:PHE:O	2.16	0.45
1:B:902:TRP:CZ2	1:B:915:HIS:HB3	2.50	0.45
1:B:3693:ASP:O	1:B:3697:LYS:HG2	2.16	0.45
1:C:1307:PRO:HB3	1:C:1540:PHE:CE2	2.52	0.45
1:C:1490:ALA:HA	1:C:1493:SER:HB2	1.98	0.45
1:C:2968:LEU:HD22	1:C:3029:ILE:HG23	1.98	0.45
1:D:1234:GLU:H	1:D:1234:GLU:CD	2.23	0.45
1:D:1523:ASN:HB2	1:D:1525:LYS:HZ1	1.81	0.45
1:D:2248:MET:HE3	1:D:2248:MET:HB2	1.86	0.45
1:D:3994:THR:HA	1:D:3997:LYS:HD2	1.98	0.45
1:D:4262:LYS:HD2	1:D:4265:LYS:HD3	1.99	0.45
1:A:317:MET:HB2	1:A:321:LYS:HZ2	1.81	0.45
1:A:1106:GLU:HB3	1:A:1214:ARG:HB2	1.98	0.45
1:A:1523:ASN:HB2	1:A:1525:LYS:HZ1	1.81	0.45
1:A:1825:PHE:CE1	1:A:1842:ILE:HD13	2.52	0.45
1:A:2332:GLY:N	1:A:2336:ARG:HH21	2.12	0.45
1:A:2973:GLN:O	1:A:2976:LYS:HG3	2.17	0.45
1:B:1307:PRO:HB3	1:B:1540:PHE:CE2	2.52	0.45
1:B:1427:TYR:HB2	1:B:1563:VAL:HG11	1.98	0.45
1:C:468:GLU:HA	1:C:475:LYS:NZ	2.32	0.45
1:D:468:GLU:HA	1:D:475:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1052:GLU:O	1:D:1055:ARG:HB2	2.16	0.45
1:D:2176:VAL:HG22	1:D:2220:TYR:CE2	2.52	0.45
1:D:2589:LEU:O	1:D:2593:VAL:HG13	2.16	0.45
1:D:2772:ARG:O	1:D:2776:LYS:HG2	2.16	0.45
1:D:2968:LEU:HD22	1:D:3029:ILE:HG23	1.98	0.45
1:D:4189:PHE:CE1	1:D:4915:LEU:HG	2.52	0.45
1:D:4906:GLU:HA	1:D:4909:THR:OG1	2.16	0.45
1:A:2886:ARG:O	1:A:2889:ALA:HB3	2.17	0.45
1:A:3019:ILE:HD12	1:A:3026:ALA:HB1	1.99	0.45
1:A:4689:LYS:HD2	1:A:4696:ALA:HB2	1.99	0.45
1:A:4710:LEU:HD23	1:A:4710:LEU:HA	1.86	0.45
2:H:58:LYS:HB3	2:H:81:VAL:O	2.16	0.45
1:B:318:ASP:O	1:B:322:ALA:HB2	2.17	0.45
1:B:2248:MET:HE3	1:B:2248:MET:HB2	1.86	0.45
1:B:2843:MET:HE2	1:B:2843:MET:HB3	1.85	0.45
1:B:3961:ASP:OD2	1:B:3963:SER:OG	2.34	0.45
1:C:1106:GLU:HB3	1:C:1214:ARG:HB2	1.98	0.45
1:C:1429:SER:HB3	1:C:1506:GLU:OE2	2.16	0.45
1:C:2332:GLY:N	1:C:2336:ARG:HH21	2.13	0.45
1:D:2855:LYS:O	1:D:2858:MET:HG2	2.17	0.45
1:D:3889:TYR:OH	1:D:3953:HIS:HB3	2.17	0.45
1:A:942:THR:HA	1:A:945:ALA:HB3	1.98	0.45
1:A:1114:ARG:HB2	1:A:1206:SER:OG	2.18	0.45
1:A:1689:ILE:HG22	1:A:1794:MET:HE1	1.98	0.45
1:A:2322:ARG:HH12	1:B:189:GLU:HG3	1.82	0.45
1:A:2581:ARG:HG3	1:A:2583:SER:H	1.82	0.45
1:A:3602:CYS:O	1:A:3605:MET:HE3	2.17	0.45
1:A:3797:MET:HG3	1:A:3839:LEU:HD21	1.98	0.45
1:A:4071:GLU:HB2	1:A:4086:ARG:HH12	1.82	0.45
1:A:4189:PHE:CE1	1:A:4915:LEU:HG	2.52	0.45
1:B:816:PRO:HB2	1:B:819:TYR:CD1	2.52	0.45
1:B:2427:ILE:HD13	1:B:2471:PHE:CZ	2.52	0.45
1:B:3019:ILE:HD12	1:B:3026:ALA:HB1	1.99	0.45
1:B:3797:MET:HG3	1:B:3839:LEU:HD21	1.98	0.45
1:B:3889:TYR:OH	1:B:3953:HIS:HB3	2.17	0.45
1:B:4906:GLU:HA	1:B:4909:THR:OG1	2.16	0.45
1:B:4921:PHE:HE2	1:B:4940:VAL:HG11	1.82	0.45
1:C:765:SER:HA	1:C:779:PHE:O	2.16	0.45
1:C:1040:ASP:HA	1:C:1043:LYS:HG2	1.98	0.45
1:C:1100:ARG:NH2	1:C:1234:GLU:O	2.50	0.45
1:C:1415:ASP:OD2	1:C:1559:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1724:GLU:O	1:C:1919:ARG:NH2	2.50	0.45
1:C:1825:PHE:CE1	1:C:1842:ILE:HD13	2.52	0.45
1:C:2222:LEU:HD23	1:C:2222:LEU:HA	1.80	0.45
1:C:2855:LYS:O	1:C:2858:MET:HG2	2.17	0.45
1:C:2898:ILE:HG23	1:D:1500:ARG:HH22	1.81	0.45
1:C:3797:MET:HG3	1:C:3839:LEU:HD21	1.98	0.45
1:C:4071:GLU:OE1	1:C:4086:ARG:NH1	2.50	0.45
1:D:874:LEU:HA	1:D:875:PRO:HD3	1.82	0.45
1:D:1429:SER:HB3	1:D:1506:GLU:OE2	2.16	0.45
1:D:1494:MET:CE	1:D:1505:LEU:HD22	2.46	0.45
1:D:1727:VAL:HG11	1:D:1926:VAL:HG21	1.99	0.45
1:D:4921:PHE:HE2	1:D:4940:VAL:HG11	1.82	0.45
1:A:179:ASP:OD1	1:A:180:ASP:N	2.51	0.44
1:A:1040:ASP:HA	1:A:1043:LYS:HG2	1.98	0.44
1:A:1727:VAL:HG11	1:A:1926:VAL:HG21	1.99	0.44
1:A:2176:VAL:HG22	1:A:2220:TYR:CE2	2.52	0.44
1:A:3749:GLY:HA2	1:A:3796:LEU:HG	1.97	0.44
1:A:4071:GLU:OE1	1:A:4086:ARG:NH1	2.50	0.44
1:A:4906:GLU:HA	1:A:4909:THR:OG1	2.16	0.44
1:B:801:ARG:HG3	1:B:1618:LEU:HD13	2.00	0.44
1:B:4071:GLU:HB2	1:B:4086:ARG:HH12	1.82	0.44
1:B:4262:LYS:HD2	1:B:4265:LYS:HD3	1.99	0.44
1:B:4710:LEU:HD23	1:B:4710:LEU:HA	1.86	0.44
1:C:318:ASP:O	1:C:322:ALA:HB2	2.17	0.44
1:C:322:ALA:HB1	1:C:327:THR:HG21	1.99	0.44
1:C:816:PRO:HB2	1:C:819:TYR:CD1	2.52	0.44
1:C:2192:MET:HE2	1:C:2192:MET:HB3	1.80	0.44
1:C:4262:LYS:HD2	1:C:4265:LYS:HD3	1.99	0.44
1:D:904:TYR:HB3	1:D:972:LEU:CD1	2.47	0.44
1:D:1724:GLU:O	1:D:1919:ARG:NH2	2.51	0.44
1:D:1825:PHE:CE1	1:D:1842:ILE:HD13	2.52	0.44
1:D:2581:ARG:HG3	1:D:2583:SER:H	1.82	0.44
1:D:2651:ALA:O	1:D:2655:LYS:HG2	2.17	0.44
1:D:3613:ARG:O	1:D:3617:VAL:HG23	2.16	0.44
1:B:1106:GLU:HB3	1:B:1214:ARG:HB2	1.98	0.44
1:B:1114:ARG:HB2	1:B:1206:SER:OG	2.18	0.44
1:B:1255:LEU:HD12	1:B:1256:PRO:HD2	1.99	0.44
1:B:1724:GLU:O	1:B:1919:ARG:NH2	2.50	0.44
1:B:2855:LYS:HE3	1:B:2856:LYS:HZ2	1.83	0.44
1:B:3968:LEU:O	1:B:3972:MET:HG2	2.18	0.44
1:C:904:TYR:HB3	1:C:972:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1255:LEU:HD12	1:C:1256:PRO:HD2	1.99	0.44
1:C:3968:LEU:O	1:C:3972:MET:HG2	2.17	0.44
1:C:4189:PHE:CE1	1:C:4915:LEU:HG	2.52	0.44
1:D:318:ASP:O	1:D:322:ALA:HB2	2.17	0.44
1:D:765:SER:HA	1:D:779:PHE:O	2.16	0.44
1:D:875:PRO:HB2	1:D:877:HIS:CE1	2.53	0.44
1:D:2383:HIS:CG	1:D:2458:ALA:HB2	2.53	0.44
1:D:3968:LEU:O	1:D:3972:MET:HG2	2.17	0.44
1:D:4187:GLU:OE2	1:D:4947:ARG:NH2	2.41	0.44
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.87	0.44
1:A:2238:THR:OG1	1:A:2241:ASP:OD2	2.24	0.44
1:A:2248:MET:HE3	1:A:2248:MET:HB2	1.86	0.44
1:A:2415:GLU:O	1:A:2419:ILE:HG12	2.18	0.44
1:A:2855:LYS:O	1:A:2858:MET:HG2	2.17	0.44
1:A:2968:LEU:HD22	1:A:3029:ILE:HG23	1.98	0.44
1:A:2985:ALA:HB2	1:A:3001:LYS:HE2	2.00	0.44
1:A:3889:TYR:OH	1:A:3953:HIS:HB3	2.17	0.44
1:A:4252:ILE:O	1:A:4256:MET:HG2	2.18	0.44
1:B:120:LEU:HD12	1:B:120:LEU:HA	1.87	0.44
1:B:1689:ILE:HG22	1:B:1794:MET:HE1	1.98	0.44
1:B:1853:GLU:OE1	1:B:1853:GLU:N	2.49	0.44
1:B:3077:GLN:HG2	1:B:3078:GLY:H	1.82	0.44
1:C:842:GLN:OE1	1:C:1603:PHE:N	2.43	0.44
1:C:1087:ILE:HG21	1:C:1124:PRO:HA	2.00	0.44
1:C:2581:ARG:HG3	1:C:2583:SER:H	1.82	0.44
1:C:3077:GLN:HG2	1:C:3078:GLY:H	1.83	0.44
1:C:4071:GLU:HB2	1:C:4086:ARG:HH12	1.82	0.44
1:C:4732:GLY:HA2	1:C:4738:PHE:HB2	1.98	0.44
1:D:801:ARG:HG3	1:D:1618:LEU:HD13	2.00	0.44
1:D:1087:ILE:HG21	1:D:1124:PRO:HA	2.00	0.44
1:D:2440:PHE:HB3	1:D:2460:PHE:CD2	2.51	0.44
1:D:3602:CYS:O	1:D:3605:MET:HE3	2.17	0.44
1:A:703:TYR:HD2	1:A:858:THR:HG23	1.83	0.44
1:A:2440:PHE:HB3	1:A:2460:PHE:CD2	2.51	0.44
1:A:4047:ASP:HA	1:A:4050:LYS:HE3	2.00	0.44
1:A:4732:GLY:HA2	1:A:4738:PHE:HB2	1.98	0.44
1:A:4921:PHE:HE2	1:A:4940:VAL:HG11	1.82	0.44
1:B:921:PHE:HD1	1:B:929:ARG:NE	2.16	0.44
1:B:2195:ASN:ND2	1:B:2198:ARG:HH12	2.15	0.44
1:B:2554:ARG:HA	1:B:2554:ARG:HD2	1.85	0.44
1:B:2855:LYS:O	1:B:2858:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2886:ARG:O	1:B:2889:ALA:HB3	2.17	0.44
1:C:935:MET:HA	1:C:938:GLU:HG3	2.00	0.44
1:C:2176:VAL:HG22	1:C:2220:TYR:CE2	2.52	0.44
1:C:2383:HIS:CG	1:C:2458:ALA:HB2	2.53	0.44
1:C:2415:GLU:O	1:C:2419:ILE:HG12	2.18	0.44
1:C:2789:ILE:HD11	1:C:2896:LEU:HD21	2.00	0.44
1:D:2222:LEU:HD23	1:D:2222:LEU:HA	1.80	0.44
1:D:2332:GLY:N	1:D:2336:ARG:HH21	2.13	0.44
1:D:3008:PHE:CD1	1:D:3040:LEU:HD11	2.53	0.44
1:D:4071:GLU:HB2	1:D:4086:ARG:HH12	1.82	0.44
1:A:904:TYR:HB3	1:A:972:LEU:CD1	2.48	0.44
1:A:2096:GLY:HA2	1:A:2099:VAL:HG22	1.99	0.44
1:A:2321:VAL:HG11	1:A:2419:ILE:HD12	2.00	0.44
1:A:4769:LEU:HB3	1:D:4753:LEU:HD23	1.99	0.44
2:E:58:LYS:HB3	2:E:81:VAL:O	2.17	0.44
2:G:58:LYS:HB3	2:G:81:VAL:O	2.16	0.44
1:B:703:TYR:HD2	1:B:858:THR:HG23	1.83	0.44
1:B:875:PRO:HB2	1:B:877:HIS:CE1	2.53	0.44
1:B:1087:ILE:HG21	1:B:1124:PRO:HA	2.00	0.44
1:B:1100:ARG:NH2	1:B:1234:GLU:O	2.51	0.44
1:B:2581:ARG:HG3	1:B:2583:SER:H	1.82	0.44
1:B:2789:ILE:HD11	1:B:2896:LEU:HD21	2.00	0.44
1:B:3050:LEU:HD12	1:B:3051:GLU:OE1	2.18	0.44
1:B:3770:ASN:HB3	1:B:3773:VAL:CG1	2.42	0.44
1:B:4047:ASP:HA	1:B:4050:LYS:HE3	1.99	0.44
1:B:4071:GLU:OE1	1:B:4086:ARG:NH1	2.50	0.44
1:B:4689:LYS:HD2	1:B:4696:ALA:HB2	1.99	0.44
1:C:267:VAL:HG23	1:C:272:ARG:NH1	2.33	0.44
1:C:594:ILE:HD11	1:C:632:ILE:HG13	2.00	0.44
1:C:2933:VAL:HB	1:C:3010:LYS:NZ	2.32	0.44
1:C:3008:PHE:CD1	1:C:3040:LEU:HD11	2.53	0.44
1:C:3602:CYS:O	1:C:3605:MET:HE3	2.17	0.44
1:C:4906:GLU:HA	1:C:4909:THR:OG1	2.16	0.44
1:D:1853:GLU:OE1	1:D:1853:GLU:N	2.49	0.44
1:D:2321:VAL:HG11	1:D:2419:ILE:HD12	2.00	0.44
1:D:4732:GLY:HA2	1:D:4738:PHE:HB2	1.98	0.44
1:A:61:ASP:OD1	1:A:63:SER:OG	2.32	0.44
1:A:640:ARG:O	2:E:35:LYS:NZ	2.49	0.44
1:A:711:GLU:OE1	1:A:716:ASN:HB2	2.18	0.44
1:A:4481:TRP:HA	1:A:4484:ILE:HG12	2.00	0.44
1:B:2176:VAL:HG22	1:B:2220:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2933:VAL:HB	1:B:3010:LYS:NZ	2.32	0.44
1:B:4252:ILE:O	1:B:4256:MET:HG2	2.18	0.44
1:C:120:LEU:HD12	1:C:120:LEU:HA	1.87	0.44
1:C:515:ALA:HB2	1:C:523:GLY:HA3	2.00	0.44
1:C:703:TYR:HD2	1:C:858:THR:HG23	1.83	0.44
1:C:2427:ILE:HD13	1:C:2471:PHE:CZ	2.53	0.44
1:C:4689:LYS:HD2	1:C:4696:ALA:HB2	1.99	0.44
1:A:387:ILE:HD11	1:A:389:ARG:HH21	1.83	0.44
1:A:1307:PRO:HB3	1:A:1540:PHE:CE2	2.52	0.44
1:A:4752:THR:OG1	1:B:4766:GLN:OE1	2.36	0.44
1:B:1825:PHE:CE1	1:B:1842:ILE:HD13	2.52	0.44
1:B:2321:VAL:HG11	1:B:2419:ILE:HD12	2.00	0.44
1:B:3008:PHE:CD1	1:B:3040:LEU:HD11	2.53	0.44
1:B:4481:TRP:HA	1:B:4484:ILE:HG12	2.00	0.44
1:B:4819:VAL:HG12	1:B:4822:ARG:NH2	2.31	0.44
1:C:2248:MET:HE3	1:C:2248:MET:HB2	1.86	0.44
1:C:2886:ARG:O	1:C:2889:ALA:HB3	2.17	0.44
1:D:703:TYR:HD2	1:D:858:THR:HG23	1.83	0.44
1:D:4071:GLU:OE1	1:D:4086:ARG:NH1	2.50	0.44
1:D:4481:TRP:HA	1:D:4484:ILE:HG12	2.00	0.44
1:A:21:VAL:HG12	1:A:66:THR:HA	2.00	0.44
1:A:2518:ARG:O	1:A:2522:THR:OG1	2.23	0.44
1:A:2651:ALA:O	1:A:2655:LYS:HG2	2.17	0.44
1:A:2877:LEU:HG	1:A:2882:LYS:HG3	2.00	0.44
1:A:3008:PHE:CD1	1:A:3040:LEU:HD11	2.53	0.44
1:B:308:LEU:HD13	1:B:393:MET:HG3	2.00	0.44
1:B:694:ARG:HD3	1:B:733:TRP:CD1	2.53	0.44
1:B:935:MET:HA	1:B:938:GLU:HG3	1.99	0.44
1:B:1642:LEU:HD21	1:B:1691:ASN:ND2	2.33	0.44
1:B:1910:LEU:HD13	1:B:2062:ILE:HG12	1.99	0.44
1:B:2096:GLY:HA2	1:B:2099:VAL:HG22	1.99	0.44
1:B:2440:PHE:HB3	1:B:2460:PHE:CD2	2.51	0.44
1:B:2688:MET:O	1:B:2689:MET:C	2.61	0.44
1:B:2789:ILE:CD1	1:B:2903:VAL:HB	2.48	0.44
1:B:2887:GLU:HA	1:B:2890:GLN:OE1	2.18	0.44
1:B:2985:ALA:HB2	1:B:3001:LYS:HE2	2.00	0.44
1:B:3602:CYS:O	1:B:3605:MET:HE3	2.17	0.44
1:B:4052:MET:HG3	1:B:4063:THR:HG23	2.00	0.44
1:B:4732:GLY:HA2	1:B:4738:PHE:HB2	1.98	0.44
1:C:921:PHE:HD1	1:C:929:ARG:NE	2.16	0.44
1:C:1114:ARG:HB2	1:C:1206:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3050:LEU:HD12	1:C:3051:GLU:OE1	2.18	0.44
1:D:1427:TYR:CE2	1:D:1560:ILE:HG23	2.53	0.44
1:D:1932:PHE:CE2	1:D:1996:LEU:HD22	2.53	0.44
1:D:2415:GLU:O	1:D:2419:ILE:HG12	2.18	0.44
1:A:308:LEU:HD13	1:A:393:MET:HG3	2.00	0.44
1:A:1415:ASP:OD2	1:A:1559:ARG:NH2	2.49	0.44
1:A:1566:LEU:O	1:A:1570:LEU:HG	2.18	0.44
1:A:3642:GLU:O	1:A:3646:LYS:HG3	2.18	0.44
1:A:4052:MET:HG3	1:A:4063:THR:HG23	2.00	0.44
1:A:4094:ILE:O	1:A:4098:VAL:HG23	2.18	0.44
2:E:50:ARG:N	2:E:55:GLU:OE2	2.37	0.44
2:H:26:HIS:CD2	2:H:105:LEU:HD11	2.53	0.44
1:B:794:PHE:CG	1:B:798:ILE:HD13	2.53	0.44
1:B:2877:LEU:HG	1:B:2882:LYS:HG3	2.00	0.44
1:B:2917:ILE:HG12	1:B:2999:LYS:HD3	2.00	0.44
1:C:1727:VAL:HG11	1:C:1926:VAL:HG21	1.99	0.44
1:C:2154:VAL:HG13	1:C:2158:HIS:CD2	2.48	0.44
1:C:4481:TRP:HA	1:C:4484:ILE:HG12	2.00	0.44
1:D:179:ASP:OD1	1:D:180:ASP:N	2.51	0.44
1:D:711:GLU:OE1	1:D:716:ASN:HB2	2.18	0.44
1:D:1566:LEU:O	1:D:1570:LEU:HG	2.18	0.44
1:D:2427:ILE:HD13	1:D:2471:PHE:CZ	2.52	0.44
1:D:4247:ALA:HA	1:D:4250:TYR:CE1	2.53	0.44
1:A:1724:GLU:O	1:A:1919:ARG:NH2	2.50	0.43
1:A:1932:PHE:CE2	1:A:1996:LEU:HD22	2.53	0.43
1:A:2383:HIS:CG	1:A:2458:ALA:HB2	2.53	0.43
1:A:2427:ILE:HD13	1:A:2471:PHE:CZ	2.52	0.43
1:A:3948:LEU:HG	1:A:3978:MET:HE1	2.00	0.43
1:A:3968:LEU:O	1:A:3972:MET:HG2	2.17	0.43
1:A:4016:PHE:HA	1:A:4019:MET:CE	2.48	0.43
1:A:4611:GLU:HA	1:A:4653:VAL:HG22	2.00	0.43
2:E:26:HIS:CD2	2:E:105:LEU:HD11	2.53	0.43
1:B:594:ILE:HD11	1:B:632:ILE:HG13	2.00	0.43
1:B:1050:LEU:HD12	1:B:1050:LEU:HA	1.81	0.43
1:B:1721:MET:HA	1:B:1721:MET:HE3	2.00	0.43
1:B:1947:VAL:HG11	1:B:1965:PHE:HE2	1.83	0.43
1:B:4634:VAL:O	1:B:4637:THR:OG1	2.26	0.43
1:C:308:LEU:HD13	1:C:393:MET:HG3	2.00	0.43
1:C:875:PRO:HB2	1:C:877:HIS:CE1	2.53	0.43
1:C:1642:LEU:HD21	1:C:1691:ASN:ND2	2.33	0.43
1:C:1749:PRO:HB2	1:C:1913:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2887:GLU:HA	1:C:2890:GLN:OE1	2.18	0.43
1:C:4252:ILE:O	1:C:4256:MET:HG2	2.18	0.43
1:D:794:PHE:CG	1:D:798:ILE:HD13	2.53	0.43
1:D:816:PRO:HB2	1:D:819:TYR:CD1	2.52	0.43
1:D:1100:ARG:NH2	1:D:1234:GLU:O	2.51	0.43
1:D:1642:LEU:HD21	1:D:1691:ASN:ND2	2.33	0.43
1:D:1749:PRO:HB2	1:D:1913:LEU:HD22	2.00	0.43
1:D:2758:LYS:HE3	1:D:2763:LEU:HA	2.00	0.43
1:D:3077:GLN:HG2	1:D:3078:GLY:H	1.83	0.43
1:D:4052:MET:HG3	1:D:4063:THR:HG23	2.00	0.43
1:D:4689:LYS:HD2	1:D:4696:ALA:HB2	1.99	0.43
1:A:307:SER:OG	1:A:317:MET:HG2	2.19	0.43
1:A:935:MET:HA	1:A:938:GLU:HG3	1.99	0.43
1:A:1038:LEU:HB2	1:A:1043:LYS:HE2	2.00	0.43
1:A:4748:MET:N	1:A:4748:MET:SD	2.92	0.43
1:A:4815:PHE:CZ	1:A:4819:VAL:HG21	2.53	0.43
1:B:387:ILE:HD11	1:B:389:ARG:HH21	1.83	0.43
1:B:658:ASN:HB2	1:B:832:LEU:HD12	2.00	0.43
1:B:1084:ARG:NH1	1:B:1127:GLU:OE1	2.50	0.43
1:B:4016:PHE:HA	1:B:4019:MET:CE	2.48	0.43
1:B:4748:MET:N	1:B:4748:MET:SD	2.92	0.43
1:C:658:ASN:HB2	1:C:832:LEU:HD12	2.00	0.43
1:C:1286:THR:OG1	1:C:1550:PRO:O	2.27	0.43
1:C:1427:TYR:CE2	1:C:1560:ILE:HG23	2.53	0.43
1:C:2688:MET:O	1:C:2689:MET:C	2.61	0.43
1:C:4052:MET:HG3	1:C:4063:THR:HG23	2.00	0.43
1:D:515:ALA:HB2	1:D:523:GLY:HA3	2.00	0.43
1:D:594:ILE:HD11	1:D:632:ILE:HG13	2.00	0.43
1:D:1038:LEU:HB2	1:D:1043:LYS:HE2	2.00	0.43
1:D:1114:ARG:HB2	1:D:1206:SER:OG	2.18	0.43
1:D:1910:LEU:HD13	1:D:2062:ILE:HG12	1.99	0.43
1:D:2074:VAL:HG23	1:D:3660:ARG:HB2	2.01	0.43
1:D:4561:LEU:HD11	1:D:4563:GLU:OE2	2.19	0.43
1:D:4815:PHE:CZ	1:D:4819:VAL:HG21	2.53	0.43
1:A:658:ASN:HB2	1:A:832:LEU:HD12	2.00	0.43
1:A:794:PHE:CG	1:A:798:ILE:HD13	2.53	0.43
1:A:875:PRO:HB2	1:A:877:HIS:CE1	2.52	0.43
1:A:1034:PRO:HD2	1:A:1037:LEU:HD12	2.00	0.43
1:A:1087:ILE:HG21	1:A:1124:PRO:HA	2.00	0.43
1:A:1749:PRO:HB2	1:A:1913:LEU:HD22	2.00	0.43
1:A:2143:ILE:HG12	1:A:2195:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2758:LYS:HE3	1:A:2763:LEU:HA	2.00	0.43
2:F:35:LYS:NZ	1:B:640:ARG:O	2.51	0.43
2:G:26:HIS:CD2	2:G:105:LEU:HD11	2.53	0.43
1:B:2383:HIS:CG	1:B:2458:ALA:HB2	2.53	0.43
1:B:3642:GLU:O	1:B:3646:LYS:HG3	2.18	0.43
1:B:3948:LEU:HG	1:B:3978:MET:HE1	2.00	0.43
1:C:179:ASP:OD1	1:C:180:ASP:N	2.51	0.43
1:C:711:GLU:OE1	1:C:716:ASN:HB2	2.18	0.43
1:C:1034:PRO:HD2	1:C:1037:LEU:HD12	2.00	0.43
1:C:1947:VAL:HG11	1:C:1965:PHE:HE2	1.83	0.43
1:C:2074:VAL:HG23	1:C:3660:ARG:HB2	2.00	0.43
1:C:2321:VAL:HG11	1:C:2419:ILE:HD12	2.00	0.43
1:C:4016:PHE:HA	1:C:4019:MET:CE	2.48	0.43
1:C:4561:LEU:HD11	1:C:4563:GLU:OE2	2.19	0.43
1:D:267:VAL:HG23	1:D:272:ARG:NH1	2.33	0.43
1:D:1641:ILE:HA	1:D:1644:LEU:HD13	2.00	0.43
1:D:2886:ARG:O	1:D:2889:ALA:HB3	2.17	0.43
1:D:3892:TYR:OH	1:D:3899:ASP:OD1	2.32	0.43
1:D:4047:ASP:HA	1:D:4050:LYS:HE3	2.00	0.43
1:D:4611:GLU:HA	1:D:4653:VAL:HG22	2.00	0.43
1:A:52:THR:HG22	1:A:60:PRO:HB3	2.00	0.43
1:A:267:VAL:HG23	1:A:272:ARG:NH1	2.33	0.43
1:A:902:TRP:CZ2	1:A:915:HIS:HB3	2.50	0.43
1:A:1642:LEU:HD21	1:A:1691:ASN:ND2	2.33	0.43
1:A:1795:LEU:HD23	1:A:1842:ILE:HD11	2.01	0.43
1:A:2074:VAL:HG23	1:A:3660:ARG:HB2	2.00	0.43
1:A:4070:ALA:HB1	1:A:4078:LEU:HD22	2.01	0.43
1:B:307:SER:OG	1:B:317:MET:HG2	2.19	0.43
1:B:1749:PRO:HB2	1:B:1913:LEU:HD22	2.00	0.43
1:B:1795:LEU:HD23	1:B:1842:ILE:HD11	2.01	0.43
1:B:4070:ALA:HB1	1:B:4078:LEU:HD22	2.01	0.43
1:B:4094:ILE:O	1:B:4098:VAL:HG23	2.18	0.43
1:C:794:PHE:CG	1:C:798:ILE:HD13	2.53	0.43
1:C:1038:LEU:HB2	1:C:1043:LYS:HE2	2.00	0.43
1:C:1795:LEU:HD23	1:C:1842:ILE:HD11	2.01	0.43
1:C:3649:ALA:C	1:C:3652:PRO:HD2	2.44	0.43
1:D:880:ARG:NH1	1:D:1062:TYR:OH	2.52	0.43
1:D:921:PHE:HD1	1:D:929:ARG:NE	2.16	0.43
1:D:2789:ILE:HD11	1:D:2896:LEU:HD21	2.00	0.43
1:D:4020:PHE:HA	1:D:4023:LEU:HB3	2.00	0.43
1:D:4252:ILE:O	1:D:4256:MET:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4294:LEU:O	1:D:4298:VAL:HG23	2.19	0.43
1:A:816:PRO:HB2	1:A:819:TYR:CD1	2.52	0.43
1:A:1100:ARG:NH2	1:A:1234:GLU:O	2.51	0.43
1:A:1427:TYR:CE2	1:A:1560:ILE:HG23	2.53	0.43
1:A:1641:ILE:HA	1:A:1644:LEU:HD13	2.00	0.43
1:A:1947:VAL:HG11	1:A:1965:PHE:HE2	1.83	0.43
1:A:2789:ILE:HD11	1:A:2896:LEU:HD21	2.00	0.43
1:A:2833:LEU:HB3	1:A:2838[B]:HIS:CE1	2.53	0.43
1:A:4247:ALA:HA	1:A:4250:TYR:CE1	2.53	0.43
1:B:179:ASP:OD1	1:B:180:ASP:N	2.51	0.43
1:B:1415:ASP:OD2	1:B:1559:ARG:NH2	2.49	0.43
1:B:3060:PHE:HE2	1:B:3108:LEU:HD13	1.84	0.43
1:B:3649:ALA:C	1:B:3652:PRO:HD2	2.43	0.43
1:B:4247:ALA:HA	1:B:4250:TYR:CE1	2.53	0.43
1:C:21:VAL:HG12	1:C:66:THR:HA	2.00	0.43
1:C:747:HIS:HD2	1:C:750:ARG:HG3	1.84	0.43
1:C:880:ARG:NH1	1:C:1062:TYR:OH	2.52	0.43
1:C:2651:ALA:O	1:C:2655:LYS:HG2	2.17	0.43
1:C:2966:VAL:O	1:C:2970:LEU:N	2.46	0.43
1:C:4294:LEU:O	1:C:4298:VAL:HG23	2.19	0.43
1:C:4748:MET:N	1:C:4748:MET:SD	2.92	0.43
1:C:4815:PHE:CZ	1:C:4819:VAL:HG21	2.53	0.43
1:D:2688:MET:O	1:D:2689:MET:C	2.61	0.43
1:D:2887:GLU:HA	1:D:2890:GLN:OE1	2.18	0.43
1:D:3050:LEU:HD12	1:D:3051:GLU:OE1	2.18	0.43
1:D:3642:GLU:O	1:D:3646:LYS:HG3	2.18	0.43
1:D:4748:MET:N	1:D:4748:MET:SD	2.92	0.43
1:A:808:HIS:HA	1:A:1610:ARG:HH21	1.84	0.43
1:A:921:PHE:HD1	1:A:929:ARG:NE	2.16	0.43
1:A:1910:LEU:HD13	1:A:2062:ILE:HG12	1.99	0.43
1:A:3077:GLN:HG2	1:A:3078:GLY:H	1.83	0.43
2:H:79:PRO:O	2:H:84:GLY:HA2	2.19	0.43
1:B:877:HIS:HA	1:B:880:ARG:NE	2.34	0.43
1:B:2074:VAL:HG23	1:B:3660:ARG:HB2	2.01	0.43
1:B:2192:MET:O	1:B:2192:MET:HG2	2.17	0.43
1:B:2651:ALA:O	1:B:2655:LYS:HG2	2.17	0.43
1:C:307:SER:OG	1:C:317:MET:HG2	2.18	0.43
1:C:694:ARG:HD3	1:C:733:TRP:CD1	2.53	0.43
1:C:877:HIS:HA	1:C:880:ARG:NE	2.34	0.43
1:C:1028:ARG:HA	1:C:1028:ARG:HD2	1.83	0.43
1:C:1050:LEU:HD12	1:C:1050:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1853:GLU:OE1	1:C:1853:GLU:N	2.49	0.43
1:C:1932:PHE:CE2	1:C:1996:LEU:HD22	2.53	0.43
1:C:2917:ILE:HG12	1:C:2999:LYS:HD3	2.00	0.43
1:C:3102:LEU:HA	1:C:3105:LEU:HG	2.00	0.43
1:C:3948:LEU:HG	1:C:3978:MET:HE1	2.00	0.43
1:D:387:ILE:HD11	1:D:389:ARG:HH21	1.83	0.43
1:D:747:HIS:HD2	1:D:750:ARG:HG3	1.84	0.43
1:D:1255:LEU:HD12	1:D:1256:PRO:HD2	1.99	0.43
1:D:1721:MET:HA	1:D:1721:MET:HE3	2.00	0.43
1:D:2096:GLY:HA2	1:D:2099:VAL:HG22	1.99	0.43
1:D:2554:ARG:HA	1:D:2554:ARG:HD2	1.85	0.43
1:D:2789:ILE:CD1	1:D:2903:VAL:HB	2.48	0.43
1:D:2877:LEU:HG	1:D:2882:LYS:HG3	2.00	0.43
1:D:2985:ALA:HB2	1:D:3001:LYS:HE2	2.00	0.43
1:D:4016:PHE:HA	1:D:4019:MET:CE	2.48	0.43
1:D:4254:THR:HA	1:D:4257:ARG:HE	1.84	0.43
1:A:318:ASP:O	1:A:322:ALA:HB2	2.17	0.43
1:A:2192:MET:HE2	1:A:2192:MET:HB3	1.80	0.43
1:A:4561:LEU:HD11	1:A:4563:GLU:OE2	2.19	0.43
1:A:4690:LYS:HD3	1:A:4692:SER:OG	2.19	0.43
2:G:35:LYS:NZ	1:C:640:ARG:O	2.51	0.43
1:B:711:GLU:OE1	1:B:716:ASN:HB2	2.18	0.43
1:B:747:HIS:HD2	1:B:750:ARG:HG3	1.84	0.43
1:B:2691:LYS:O	1:B:2695:MET:HG3	2.19	0.43
1:B:4245:LEU:HD11	1:C:4626:ILE:HG13	2.00	0.43
1:B:4815:PHE:CZ	1:B:4819:VAL:HG21	2.53	0.43
1:C:52:THR:HG22	1:C:60:PRO:HB3	2.00	0.43
1:C:674:TYR:HE1	1:C:756:SER:HB2	1.84	0.43
1:C:986:ILE:HD11	1:C:1055:ARG:HA	2.01	0.43
1:C:2096:GLY:HA2	1:C:2099:VAL:HG22	1.99	0.43
1:D:52:THR:HG22	1:D:60:PRO:HB3	1.99	0.43
1:D:308:LEU:HD13	1:D:393:MET:HG3	2.00	0.43
1:D:608:HIS:HB2	1:D:1656:HIS:ND1	2.34	0.43
1:D:694:ARG:HD3	1:D:733:TRP:CD1	2.53	0.43
1:D:2691:LYS:O	1:D:2695:MET:HG3	2.19	0.43
1:D:2836:ASP:OD1	1:D:2836:ASP:N	2.52	0.43
1:D:3948:LEU:HG	1:D:3978:MET:HE1	2.00	0.43
1:A:1190:LEU:HD11	1:A:1193:LYS:HA	2.01	0.43
1:A:1255:LEU:HD12	1:A:1256:PRO:HD2	1.99	0.43
1:A:2135:GLY:H	1:A:2138:GLU:HB2	1.84	0.43
1:A:2603:ALA:C	1:A:2606:PRO:HD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2688:MET:O	1:A:2689:MET:C	2.61	0.43
1:A:2789:ILE:CD1	1:A:2903:VAL:HB	2.48	0.43
1:A:2917:ILE:HG12	1:A:2999:LYS:HD3	2.00	0.43
1:A:3050:LEU:HD12	1:A:3051:GLU:OE1	2.18	0.43
2:F:26:HIS:CD2	2:F:105:LEU:HD11	2.53	0.43
1:B:515:ALA:HB2	1:B:523:GLY:HA3	2.00	0.43
1:B:904:TYR:HB3	1:B:972:LEU:CD1	2.48	0.43
1:C:120:LEU:HD11	1:C:158:CYS:HB3	2.01	0.43
1:C:1494:MET:HE3	1:C:1505:LEU:HD22	2.01	0.43
1:C:1566:LEU:O	1:C:1570:LEU:HG	2.18	0.43
1:C:1726:ILE:HD11	1:C:2161:LEU:HD11	2.01	0.43
1:C:2691:LYS:O	1:C:2695:MET:HG3	2.19	0.43
1:C:3642:GLU:O	1:C:3646:LYS:HG3	2.18	0.43
1:C:4663:ARG:CB	1:C:4674:LYS:HZ3	2.32	0.43
1:D:21:VAL:HG12	1:D:66:THR:HA	2.00	0.43
1:D:658:ASN:HB2	1:D:832:LEU:HD12	2.00	0.43
1:D:674:TYR:HE1	1:D:756:SER:HB2	1.84	0.43
1:D:908:ARG:NH1	1:D:928:GLU:OE2	2.35	0.43
1:D:4094:ILE:O	1:D:4098:VAL:HG23	2.18	0.43
1:A:515:ALA:HB2	1:A:523:GLY:HA3	2.00	0.43
1:A:801:ARG:HG3	1:A:1618:LEU:HD13	2.00	0.43
1:A:1605:LYS:HE2	1:A:1623:ASP:OD2	2.19	0.43
1:A:2154:VAL:HG13	1:A:2158:HIS:CD2	2.48	0.43
1:A:3906:PHE:HB3	1:A:3967:LEU:HD11	2.01	0.43
1:A:4245:LEU:HD21	1:B:4629:GLN:HB3	2.01	0.43
1:B:267:VAL:HG23	1:B:272:ARG:NH1	2.33	0.43
1:B:591:GLU:O	1:B:594:ILE:HG22	2.19	0.43
1:B:732:LEU:HD23	1:B:732:LEU:HA	1.89	0.43
1:B:1427:TYR:CE2	1:B:1560:ILE:HG23	2.53	0.43
1:B:2415:GLU:O	1:B:2419:ILE:HG12	2.18	0.43
1:C:439:LYS:HD3	1:C:439:LYS:HA	1.73	0.43
1:C:801:ARG:HG3	1:C:1618:LEU:HD13	2.00	0.43
1:C:2758:LYS:HE3	1:C:2763:LEU:HA	2.00	0.43
1:C:4247:ALA:HA	1:C:4250:TYR:CE1	2.53	0.43
1:D:307:SER:OG	1:D:317:MET:HG2	2.18	0.43
1:D:732:LEU:HD23	1:D:732:LEU:HA	1.89	0.43
1:D:1034:PRO:HD2	1:D:1037:LEU:HD12	2.00	0.43
1:D:1726:ILE:HD11	1:D:2161:LEU:HD11	2.01	0.43
1:A:2887:GLU:HA	1:A:2890:GLN:OE1	2.18	0.43
1:B:156:GLU:HB2	1:B:187:SER:HB3	2.01	0.43
1:B:675:TYR:HB3	1:B:822:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:808:HIS:HA	1:B:1610:ARG:HH21	1.84	0.43
1:B:1566:LEU:O	1:B:1570:LEU:HG	2.18	0.43
1:B:1932:PHE:CE2	1:B:1996:LEU:HD22	2.53	0.43
1:B:2135:GLY:H	1:B:2138:GLU:HB2	1.84	0.43
1:B:4690:LYS:HD3	1:B:4692:SER:OG	2.19	0.43
1:C:675:TYR:HB3	1:C:822:CYS:SG	2.59	0.43
1:C:830:GLU:OE1	1:C:830:GLU:N	2.52	0.43
1:C:1426:TYR:HA	1:C:1564:MET:O	2.19	0.43
1:C:1960:ARG:H	1:C:1960:ARG:HG3	0.96	0.43
1:C:2440:PHE:HB3	1:C:2460:PHE:CD2	2.51	0.43
1:C:2937:HIS:O	1:C:2940:ILE:HG22	2.19	0.43
1:C:4047:ASP:HA	1:C:4050:LYS:HE3	2.00	0.43
1:D:156:GLU:HB2	1:D:187:SER:HB3	2.01	0.43
1:D:935:MET:HA	1:D:938:GLU:HG3	2.00	0.43
1:D:1284:LYS:HZ1	1:D:1552:VAL:N	2.16	0.43
1:D:3960:GLN:HA	1:D:4069:CYS:HA	2.00	0.43
1:A:439:LYS:HA	1:A:439:LYS:HD3	1.73	0.42
1:A:694:ARG:HD3	1:A:733:TRP:CD1	2.53	0.42
1:A:830:GLU:OE1	1:A:830:GLU:N	2.52	0.42
1:A:874:LEU:HA	1:A:875:PRO:HD3	1.82	0.42
1:A:880:ARG:NH1	1:A:1062:TYR:OH	2.52	0.42
1:A:2066:MET:CE	1:A:2084:MET:HA	2.49	0.42
1:A:2704:GLN:O	1:A:2704:GLN:HG2	2.19	0.42
1:A:3926:GLY:O	1:A:3927:PRO:C	2.62	0.42
1:A:4480:PHE:N	1:A:4482:LYS:HZ3	2.17	0.42
2:G:19:LYS:HB2	2:G:19:LYS:HE3	1.83	0.42
1:B:399:MET:HE3	1:B:399:MET:HB3	1.94	0.42
1:B:564:ARG:O	1:B:568:SER:OG	2.31	0.42
1:B:1038:LEU:HB2	1:B:1043:LYS:HE2	2.01	0.42
1:B:1051:ARG:HA	1:B:1054:VAL:HG23	2.01	0.42
1:B:1605:LYS:HE2	1:B:1623:ASP:OD2	2.19	0.42
1:B:1732:GLU:O	1:B:1736:ILE:HG12	2.19	0.42
1:B:3102:LEU:HA	1:B:3105:LEU:HG	2.00	0.42
1:B:4561:LEU:HD11	1:B:4563:GLU:OE2	2.19	0.42
1:C:165:ALA:HB2	1:C:182:ILE:HG23	2.01	0.42
1:C:1605:LYS:HE2	1:C:1623:ASP:OD2	2.19	0.42
1:C:2143:ILE:HG12	1:C:2195:ASN:OD1	2.18	0.42
1:C:2877:LEU:HG	1:C:2882:LYS:HG3	2.00	0.42
1:C:2985:ALA:HB2	1:C:3001:LYS:HE2	2.00	0.42
1:C:3036:LEU:O	1:C:3040:LEU:HG	2.19	0.42
1:C:4094:ILE:O	1:C:4098:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:HD13	1:D:156:GLU:HG2	2.01	0.42
1:D:120:LEU:HD11	1:D:158:CYS:HB3	2.01	0.42
1:D:308:LEU:HG	1:D:309:MET:O	2.19	0.42
1:D:2195:ASN:ND2	1:D:2198:ARG:HH12	2.15	0.42
1:D:2603:ALA:C	1:D:2606:PRO:HD2	2.44	0.42
1:D:2636:GLU:HG2	1:D:2637:GLU:N	2.34	0.42
1:D:2704:GLN:O	1:D:2704:GLN:HG2	2.19	0.42
1:D:2843:MET:HE2	1:D:2843:MET:HB3	1.85	0.42
1:D:3060:PHE:HE2	1:D:3108:LEU:HD13	1.84	0.42
1:D:3649:ALA:C	1:D:3652:PRO:HD2	2.43	0.42
1:A:608:HIS:HB2	1:A:1656:HIS:ND1	2.34	0.42
1:A:872:ILE:HG13	1:A:941:LYS:HE3	2.01	0.42
1:A:877:HIS:HA	1:A:880:ARG:NE	2.34	0.42
1:A:1426:TYR:HA	1:A:1564:MET:O	2.19	0.42
1:A:1721:MET:HE3	1:A:1721:MET:HA	2.00	0.42
1:A:3649:ALA:C	1:A:3652:PRO:HD2	2.44	0.42
1:A:4055:HIS:O	1:B:4660:PHE:HE1	2.02	0.42
2:F:79:PRO:O	2:F:84:GLY:HA2	2.19	0.42
2:G:79:PRO:O	2:G:84:GLY:HA2	2.19	0.42
1:B:165:ALA:HB2	1:B:182:ILE:HG23	2.01	0.42
1:B:468:GLU:HA	1:B:475:LYS:HZ3	1.84	0.42
1:B:996:VAL:HG11	1:B:1051:ARG:CD	2.46	0.42
1:B:1034:PRO:HD2	1:B:1037:LEU:HD12	2.00	0.42
1:B:2143:ILE:HG12	1:B:2195:ASN:OD1	2.18	0.42
1:B:2937:HIS:O	1:B:2940:ILE:HG22	2.19	0.42
1:B:3926:GLY:O	1:B:3927:PRO:C	2.62	0.42
1:C:606:ARG:HB2	1:C:1653:PHE:CE1	2.55	0.42
1:C:1051:ARG:HA	1:C:1054:VAL:HG23	2.01	0.42
1:C:1721:MET:HA	1:C:1721:MET:HE3	2.00	0.42
1:C:1732:GLU:O	1:C:1736:ILE:HG12	2.19	0.42
1:C:2636:GLU:HG2	1:C:2637:GLU:N	2.34	0.42
1:C:4611:GLU:HA	1:C:4653:VAL:HG22	2.00	0.42
1:D:872:ILE:HG13	1:D:941:LYS:HE3	2.01	0.42
1:D:877:HIS:HA	1:D:880:ARG:NE	2.34	0.42
1:D:1426:TYR:HA	1:D:1564:MET:O	2.19	0.42
1:D:2143:ILE:HG12	1:D:2195:ASN:OD1	2.18	0.42
1:D:3102:LEU:HA	1:D:3105:LEU:HG	2.00	0.42
1:D:3728:GLN:O	1:D:3732:HIS:ND1	2.46	0.42
1:D:4208:GLU:OE1	1:D:4208:GLU:O	2.37	0.42
1:A:329:PHE:CE1	1:A:365:HIS:HD2	2.37	0.42
1:A:675:TYR:HB3	1:A:822:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2347:MET:HE3	1:A:2435:VAL:HG13	2.02	0.42
1:A:3036:LEU:O	1:A:3040:LEU:HG	2.19	0.42
1:A:4020:PHE:HA	1:A:4023:LEU:HB3	2.00	0.42
1:A:4030:ASP:HA	1:A:4033:LYS:HE2	2.01	0.42
1:A:4732:GLY:HA2	1:A:4735:ASN:O	2.19	0.42
1:B:880:ARG:NH1	1:B:1062:TYR:OH	2.52	0.42
1:B:1011:ARG:HB3	1:B:1016:TRP:HB2	2.00	0.42
1:B:1652:LYS:NZ	1:B:1656:HIS:HE1	2.17	0.42
1:B:2347:MET:HE3	1:B:2435:VAL:HG13	2.02	0.42
1:B:2732:TRP:NE1	1:B:2736:LYS:HZ3	2.17	0.42
1:C:308:LEU:HG	1:C:309:MET:O	2.19	0.42
1:C:3960:GLN:HA	1:C:4069:CYS:HA	2.00	0.42
1:C:4208:GLU:OE1	1:C:4208:GLU:O	2.37	0.42
1:C:4862:ILE:HD13	1:D:4852:PHE:CE1	2.54	0.42
1:D:165:ALA:HB2	1:D:182:ILE:HG23	2.01	0.42
1:D:830:GLU:N	1:D:830:GLU:OE1	2.52	0.42
1:D:985:PHE:CD2	1:D:985:PHE:N	2.88	0.42
1:D:4480:PHE:N	1:D:4482:LYS:HZ3	2.17	0.42
1:D:4663:ARG:CB	1:D:4674:LYS:HZ3	2.32	0.42
1:A:594:ILE:HD11	1:A:632:ILE:HG13	2.00	0.42
1:A:747:HIS:CD2	1:A:750:ARG:HG3	2.54	0.42
1:A:747:HIS:HD2	1:A:750:ARG:HG3	1.84	0.42
1:A:986:ILE:HD11	1:A:1055:ARG:HA	2.01	0.42
1:A:1011:ARG:HB3	1:A:1016:TRP:HB2	2.00	0.42
1:A:1652:LYS:NZ	1:A:1656:HIS:HE1	2.18	0.42
1:A:2678:PRO:HA	1:A:2921:PHE:HD2	1.84	0.42
1:A:2714:PRO:O	1:A:2718:GLU:HG2	2.20	0.42
1:A:2937:HIS:O	1:A:2940:ILE:HG22	2.19	0.42
1:A:3060:PHE:HE2	1:A:3108:LEU:HD13	1.84	0.42
1:A:4254:THR:HA	1:A:4257:ARG:HE	1.84	0.42
1:B:747:HIS:CD2	1:B:750:ARG:HG3	2.54	0.42
1:B:830:GLU:N	1:B:830:GLU:OE1	2.52	0.42
1:B:872:ILE:HG13	1:B:941:LYS:HE3	2.01	0.42
1:B:889:ILE:HG12	1:B:889:ILE:H	1.75	0.42
1:B:2678:PRO:HA	1:B:2921:PHE:HD2	1.84	0.42
1:B:3637:GLU:HG2	1:B:3697:LYS:HB2	2.02	0.42
1:B:4208:GLU:OE1	1:B:4208:GLU:O	2.37	0.42
1:C:387:ILE:HD11	1:C:389:ARG:HH21	1.83	0.42
1:C:398:HIS:HB2	1:C:401:ASP:OD1	2.19	0.42
1:C:808:HIS:HA	1:C:1610:ARG:HH21	1.84	0.42
1:C:872:ILE:HG13	1:C:941:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:996:VAL:HG11	1:C:1051:ARG:CD	2.46	0.42
1:C:1011:ARG:HB3	1:C:1016:TRP:HB2	2.00	0.42
1:C:2347:MET:HE3	1:C:2435:VAL:HG13	2.02	0.42
1:C:4254:THR:HA	1:C:4257:ARG:HE	1.84	0.42
1:D:808:HIS:HA	1:D:1610:ARG:HH21	1.84	0.42
1:D:1166:VAL:HG23	1:D:1173:MET:CG	2.46	0.42
1:D:2347:MET:HE3	1:D:2435:VAL:HG13	2.02	0.42
1:D:2714:PRO:O	1:D:2718:GLU:HG2	2.20	0.42
1:D:4030:ASP:HA	1:D:4033:LYS:HE2	2.02	0.42
1:D:4732:GLY:HA2	1:D:4735:ASN:O	2.20	0.42
1:A:120:LEU:HD11	1:A:158:CYS:HB3	2.01	0.42
1:A:165:ALA:HB2	1:A:182:ILE:HG23	2.01	0.42
1:A:674:TYR:HE1	1:A:756:SER:HB2	1.84	0.42
1:A:2691:LYS:O	1:A:2695:MET:HG3	2.19	0.42
1:A:3960:GLN:HA	1:A:4069:CYS:HA	2.00	0.42
1:A:4503:ARG:NH2	1:A:4745:ASP:OD2	2.53	0.42
2:E:79:PRO:O	2:E:84:GLY:HA2	2.19	0.42
1:B:52:THR:HG22	1:B:60:PRO:HB3	2.00	0.42
1:B:163:HIS:HB2	1:B:182:ILE:HG13	2.02	0.42
1:B:882:ARG:HH11	1:B:933:LEU:HD22	1.85	0.42
1:B:2567:ASP:O	1:B:2571:VAL:HG23	2.20	0.42
1:B:3827:GLU:O	1:B:3831:GLN:HA	2.19	0.42
1:B:4030:ASP:HA	1:B:4033:LYS:HE2	2.02	0.42
1:B:4187:GLU:OE2	1:B:4947:ARG:NH2	2.41	0.42
1:B:4279:MET:HE3	1:C:4488:GLN:HG3	2.01	0.42
1:B:4503:ARG:NH2	1:B:4745:ASP:OD2	2.53	0.42
1:C:591:GLU:O	1:C:594:ILE:HG22	2.19	0.42
1:C:1652:LYS:NZ	1:C:1656:HIS:HE1	2.18	0.42
1:C:1910:LEU:HD13	1:C:2062:ILE:HG12	1.99	0.42
1:C:2195:ASN:ND2	1:C:2198:ARG:HH12	2.15	0.42
1:C:2274:LEU:HD21	1:C:2329:GLU:HB2	2.01	0.42
1:C:2898:ILE:HD12	1:D:1500:ARG:HH22	1.84	0.42
1:C:4070:ALA:HB1	1:C:4078:LEU:HD22	2.01	0.42
1:C:4690:LYS:HD3	1:C:4692:SER:OG	2.19	0.42
1:D:606:ARG:HB2	1:D:1653:PHE:CE1	2.55	0.42
1:D:1050:LEU:HD12	1:D:1050:LEU:HA	1.81	0.42
1:D:1795:LEU:HD23	1:D:1842:ILE:HD11	2.01	0.42
1:D:2917:ILE:HG12	1:D:2999:LYS:HD3	2.00	0.42
1:D:3637:GLU:HG2	1:D:3697:LYS:HB2	2.02	0.42
1:D:4070:ALA:HB1	1:D:4078:LEU:HD22	2.01	0.42
1:D:4135:ARG:HD2	1:D:4911:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:ILE:HD12	1:A:1058:LEU:HD12	2.01	0.42
1:A:1084:ARG:NH1	1:A:1127:GLU:OE1	2.50	0.42
1:A:1595:LEU:HD23	1:A:1595:LEU:HA	1.89	0.42
1:A:1611:ILE:HD11	1:A:1618:LEU:HD23	2.02	0.42
1:A:1649:GLU:HG2	1:A:1650:LEU:N	2.35	0.42
1:B:21:VAL:HG12	1:B:66:THR:HA	2.00	0.42
1:B:1190:LEU:HD11	1:B:1193:LYS:HA	2.01	0.42
1:B:1641:ILE:HA	1:B:1644:LEU:HD13	2.00	0.42
1:B:2636:GLU:HG2	1:B:2637:GLU:N	2.34	0.42
1:B:2701:PHE:CE2	1:B:2703:PRO:HG3	2.55	0.42
1:B:3698:SER:O	1:B:3727:GLN:NE2	2.49	0.42
1:B:4294:LEU:O	1:B:4298:VAL:HG23	2.18	0.42
1:C:329:PHE:CE1	1:C:365:HIS:HD2	2.37	0.42
1:C:2066:MET:CE	1:C:2084:MET:HA	2.49	0.42
1:C:2135:GLY:H	1:C:2138:GLU:HB2	1.84	0.42
1:C:2789:ILE:CD1	1:C:2903:VAL:HB	2.48	0.42
1:C:3637:GLU:HG2	1:C:3697:LYS:HB2	2.02	0.42
1:C:4480:PHE:N	1:C:4482:LYS:HZ3	2.17	0.42
1:D:877:HIS:ND1	1:D:878:LEU:HD12	2.35	0.42
1:D:902:TRP:CZ2	1:D:915:HIS:HB3	2.50	0.42
1:D:1190:LEU:HD11	1:D:1193:LYS:HA	2.01	0.42
1:D:1286:THR:OG1	1:D:1550:PRO:O	2.27	0.42
1:D:1552:VAL:HG12	1:D:1553:PHE:HD1	1.85	0.42
1:D:1649:GLU:HG2	1:D:1650:LEU:N	2.35	0.42
1:D:2937:HIS:O	1:D:2940:ILE:HG22	2.19	0.42
1:A:1284:LYS:HZ1	1:A:1552:VAL:N	2.16	0.42
1:A:3102:LEU:HA	1:A:3105:LEU:HG	2.00	0.42
1:A:4135:ARG:HD2	1:A:4911:GLN:HB3	2.02	0.42
1:A:4208:GLU:OE1	1:A:4208:GLU:O	2.37	0.42
1:B:506:HIS:CE1	1:B:530:LEU:HD21	2.55	0.42
1:B:1494:MET:HE3	1:B:1505:LEU:HD22	2.00	0.42
1:B:2066:MET:CE	1:B:2084:MET:HA	2.49	0.42
1:B:2603:ALA:C	1:B:2606:PRO:HD2	2.44	0.42
1:B:2758:LYS:HE3	1:B:2763:LEU:HA	2.00	0.42
1:B:3821:THR:HG22	1:B:3823:GLU:H	1.85	0.42
1:B:4020:PHE:HA	1:B:4023:LEU:HB3	2.00	0.42
1:B:4611:GLU:HA	1:B:4653:VAL:HG22	2.00	0.42
1:B:4663:ARG:CB	1:B:4674:LYS:HZ3	2.33	0.42
1:C:874:LEU:HA	1:C:875:PRO:HD3	1.82	0.42
1:C:986:ILE:HD12	1:C:1058:LEU:HD12	2.01	0.42
1:C:1944:TYR:HA	1:C:1947:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2701:PHE:CE2	1:C:2703:PRO:HG3	2.55	0.42
1:C:2714:PRO:O	1:C:2718:GLU:HG2	2.20	0.42
1:C:2836:ASP:OD1	1:C:2836:ASP:N	2.52	0.42
1:C:3060:PHE:HE2	1:C:3108:LEU:HD13	1.84	0.42
1:C:3821:THR:HG22	1:C:3823:GLU:H	1.85	0.42
1:C:4634:VAL:O	1:C:4637:THR:OG1	2.26	0.42
1:C:4732:GLY:HA2	1:C:4735:ASN:O	2.20	0.42
1:D:398:HIS:HB2	1:D:401:ASP:OD1	2.19	0.42
1:D:1732:GLU:O	1:D:1736:ILE:HG12	2.19	0.42
1:D:2274:LEU:HD21	1:D:2329:GLU:HB2	2.01	0.42
1:D:2567:ASP:O	1:D:2571:VAL:HG23	2.20	0.42
1:D:2857:LYS:O	1:D:2861:GLU:OE1	2.38	0.42
1:D:3926:GLY:O	1:D:3927:PRO:C	2.62	0.42
1:A:591:GLU:O	1:A:594:ILE:HG22	2.19	0.42
1:A:882:ARG:HH11	1:A:933:LEU:HD22	1.85	0.42
1:A:996:VAL:HG11	1:A:1051:ARG:CD	2.46	0.42
1:A:3642:GLU:HB3	1:A:3646:LYS:NZ	2.35	0.42
1:A:3827:GLU:O	1:A:3831:GLN:HA	2.20	0.42
1:B:120:LEU:HD11	1:B:158:CYS:HB3	2.01	0.42
1:B:398:HIS:HB2	1:B:401:ASP:OD1	2.19	0.42
1:B:608:HIS:HB2	1:B:1656:HIS:ND1	2.34	0.42
1:B:674:TYR:HE1	1:B:756:SER:HB2	1.84	0.42
1:B:955:GLU:HG3	1:B:959:ASP:OD2	2.20	0.42
1:B:1081:THR:HG23	1:B:1083:GLU:H	1.85	0.42
1:B:1426:TYR:HA	1:B:1564:MET:O	2.19	0.42
1:B:1726:ILE:HD11	1:B:2161:LEU:HD11	2.01	0.42
1:B:2154:VAL:HG13	1:B:2158:HIS:CD2	2.48	0.42
1:B:2714:PRO:O	1:B:2718:GLU:HG2	2.20	0.42
1:B:2857:LYS:O	1:B:2861:GLU:OE1	2.38	0.42
1:B:3906:PHE:HB3	1:B:3967:LEU:HD11	2.01	0.42
1:C:747:HIS:CD2	1:C:750:ARG:HG3	2.54	0.42
1:C:1552:VAL:HG12	1:C:1553:PHE:HD1	1.85	0.42
1:C:2603:ALA:C	1:C:2606:PRO:HD2	2.44	0.42
1:D:675:TYR:HB3	1:D:822:CYS:SG	2.59	0.42
1:D:1944:TYR:HA	1:D:1947:VAL:HG12	2.02	0.42
1:D:2163:ARG:NH1	1:D:2209:GLN:HB3	2.35	0.42
1:D:2678:PRO:HA	1:D:2921:PHE:HD2	1.84	0.42
1:A:191:TYR:CE1	1:A:209:GLN:HG3	2.55	0.42
1:A:985:PHE:CD2	1:A:985:PHE:N	2.88	0.42
1:A:1494:MET:HE3	1:A:1505:LEU:HD22	2.01	0.42
1:A:1726:ILE:HD11	1:A:2161:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1914:CYS:O	1:A:1918:VAL:HG23	2.20	0.42
1:A:1931:ASP:OD1	1:A:1932:PHE:N	2.53	0.42
1:B:874:LEU:HA	1:B:875:PRO:HD3	1.82	0.42
1:B:986:ILE:HD11	1:B:1055:ARG:HA	2.01	0.42
1:B:986:ILE:HD13	1:B:1055:ARG:HA	2.02	0.42
1:B:1004:HIS:HE1	1:B:1038:LEU:HD21	1.84	0.42
1:B:1931:ASP:OD1	1:B:1932:PHE:N	2.53	0.42
1:B:1944:TYR:HA	1:B:1947:VAL:HG12	2.02	0.42
1:B:2163:ARG:NH1	1:B:2209:GLN:HB3	2.35	0.42
1:B:2704:GLN:O	1:B:2704:GLN:HG2	2.19	0.42
1:B:3960:GLN:HA	1:B:4069:CYS:HA	2.00	0.42
1:B:4254:THR:HA	1:B:4257:ARG:HE	1.84	0.42
1:C:483:LYS:HB2	1:C:483:LYS:HE3	1.84	0.42
1:C:506:HIS:CE1	1:C:530:LEU:HD21	2.55	0.42
1:C:955:GLU:HG3	1:C:959:ASP:OD2	2.20	0.42
1:C:2299:LEU:HD22	1:C:2395:LEU:HA	2.01	0.42
1:C:2552:VAL:HG11	1:C:2573:LEU:HD13	2.01	0.42
1:C:2678:PRO:HA	1:C:2921:PHE:HD2	1.84	0.42
1:C:2737:LEU:HD23	1:C:2737:LEU:HA	1.93	0.42
1:C:2857:LYS:O	1:C:2861:GLU:OE1	2.38	0.42
1:C:3827:GLU:O	1:C:3831:GLN:HA	2.19	0.42
1:C:4020:PHE:HA	1:C:4023:LEU:HB3	2.01	0.42
1:D:747:HIS:CD2	1:D:750:ARG:HG3	2.54	0.42
1:D:1475:LYS:HE3	1:D:1475:LYS:HB3	1.90	0.42
1:D:1605:LYS:HE2	1:D:1623:ASP:OD2	2.19	0.42
1:D:2066:MET:CE	1:D:2084:MET:HA	2.49	0.42
1:D:2238:THR:OG1	1:D:2241:ASP:OD2	2.24	0.42
1:D:3827:GLU:O	1:D:3831:GLN:HA	2.19	0.42
1:A:606:ARG:HB2	1:A:1653:PHE:CE1	2.55	0.42
1:A:644:LEU:HD22	1:A:1630:LEU:HD21	2.02	0.42
1:A:1028:ARG:HA	1:A:1028:ARG:HD2	1.83	0.42
1:A:1502:ASN:O	1:D:2824:ARG:NH2	2.53	0.42
1:A:1944:TYR:HA	1:A:1947:VAL:HG12	2.02	0.42
1:B:82:LEU:HD13	1:B:156:GLU:HG2	2.01	0.42
1:B:1174:MET:HG3	1:B:1190:LEU:HA	2.02	0.42
1:B:1611:ILE:HD11	1:B:1618:LEU:HD23	2.02	0.42
1:B:2836:ASP:OD1	1:B:2836:ASP:N	2.52	0.42
1:B:3036:LEU:O	1:B:3040:LEU:HG	2.19	0.42
1:B:4135:ARG:HD2	1:B:4911:GLN:HB3	2.02	0.42
1:C:163:HIS:HB2	1:C:182:ILE:HG13	2.02	0.42
1:C:608:HIS:HB2	1:C:1656:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:985:PHE:CD2	1:C:985:PHE:N	2.88	0.42
1:C:986:ILE:HD13	1:C:1055:ARG:HA	2.02	0.42
1:C:1190:LEU:HD11	1:C:1193:LYS:HA	2.01	0.42
1:C:1641:ILE:HA	1:C:1644:LEU:HD13	2.00	0.42
1:C:1649:GLU:HG2	1:C:1650:LEU:N	2.35	0.42
1:C:2353:ILE:O	1:C:2360:ASP:HB2	2.20	0.42
1:C:2567:ASP:O	1:C:2571:VAL:HG23	2.20	0.42
1:C:4030:ASP:HA	1:C:4033:LYS:HE2	2.02	0.42
1:D:191:TYR:CE1	1:D:209:GLN:HG3	2.55	0.42
1:D:591:GLU:O	1:D:594:ILE:HG22	2.19	0.42
1:D:644:LEU:HD22	1:D:1630:LEU:HD21	2.02	0.42
1:D:986:ILE:HD11	1:D:1055:ARG:HA	2.01	0.42
1:D:1494:MET:HE3	1:D:1505:LEU:HD22	2.01	0.42
1:D:2353:ILE:O	1:D:2360:ASP:HB2	2.20	0.42
1:D:2552:VAL:HG11	1:D:2573:LEU:HD13	2.01	0.42
1:D:2702:ASN:HA	1:D:2703:PRO:HD3	1.84	0.42
1:D:2841:ALA:HA	1:D:2844:MET:HG3	2.02	0.42
1:D:4690:LYS:HD3	1:D:4692:SER:OG	2.19	0.42
1:A:398:HIS:HB2	1:A:401:ASP:OD1	2.19	0.41
1:A:2636:GLU:HG2	1:A:2637:GLU:N	2.34	0.41
1:B:308:LEU:HG	1:B:309:MET:O	2.19	0.41
1:B:606:ARG:HB2	1:B:1653:PHE:CE1	2.55	0.41
1:B:2623:LEU:HB3	1:B:2626:GLY:HA2	2.02	0.41
1:B:4947:ARG:HA	1:B:4947:ARG:HD2	1.92	0.41
1:C:156:GLU:HB2	1:C:187:SER:HB3	2.01	0.41
1:C:1135:PHE:HB3	1:C:1173:MET:HE1	2.02	0.41
1:C:2175:MET:HA	1:C:2178:VAL:HG12	2.02	0.41
1:C:2704:GLN:O	1:C:2704:GLN:HG2	2.19	0.41
1:C:3018:ARG:HG3	1:C:3021:LEU:HD22	2.02	0.41
1:C:3723:LYS:NZ	1:C:3727:GLN:OE1	2.52	0.41
1:C:4135:ARG:HD2	1:C:4911:GLN:HB3	2.02	0.41
1:D:399:MET:HE3	1:D:399:MET:HB3	1.94	0.41
1:D:1483:SER:HB3	1:D:1486:TYR:CE1	2.55	0.41
1:D:2262:LEU:O	1:D:2266:VAL:HG23	2.20	0.41
1:D:3018:ARG:HG3	1:D:3021:LEU:HD22	2.02	0.41
1:D:3723:LYS:NZ	1:D:3727:GLN:OE1	2.52	0.41
1:A:506:HIS:CE1	1:A:530:LEU:HD21	2.55	0.41
1:A:586:LEU:HD22	1:A:620:CYS:HB2	2.02	0.41
1:A:921:PHE:HD1	1:A:929:ARG:CZ	2.34	0.41
1:A:1732:GLU:O	1:A:1736:ILE:HG12	2.19	0.41
1:A:2274:LEU:HD21	1:A:2329:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2857:LYS:O	1:A:2861:GLU:OE1	2.38	0.41
1:A:3637:GLU:HG2	1:A:3697:LYS:HB2	2.02	0.41
1:A:4294:LEU:O	1:A:4298:VAL:HG23	2.18	0.41
1:B:165:ALA:HB1	1:B:211:LEU:HD22	2.03	0.41
1:B:329:PHE:CE1	1:B:365:HIS:HD2	2.37	0.41
1:B:2175:MET:HA	1:B:2178:VAL:HG12	2.02	0.41
1:B:2353:ILE:O	1:B:2360:ASP:HB2	2.20	0.41
1:B:3065:ALA:O	1:B:3069:GLU:HG2	2.20	0.41
1:B:3677:THR:HB	1:B:3679:LYS:NZ	2.35	0.41
1:B:4038:ASP:OD2	1:B:4040:LYS:NZ	2.36	0.41
1:C:1081:THR:HG23	1:C:1083:GLU:H	1.85	0.41
1:C:2163:ARG:NH1	1:C:2209:GLN:HB3	2.35	0.41
1:C:2623:LEU:HB3	1:C:2626:GLY:HA2	2.02	0.41
1:C:3926:GLY:O	1:C:3927:PRO:C	2.62	0.41
1:C:4710:LEU:HD23	1:C:4710:LEU:HA	1.86	0.41
1:D:1914:CYS:O	1:D:1918:VAL:HG23	2.20	0.41
1:D:1947:VAL:HG11	1:D:1965:PHE:HE2	1.83	0.41
1:D:2833:LEU:HB3	1:D:2838[B]:HIS:NE2	2.35	0.41
1:D:3036:LEU:O	1:D:3040:LEU:HG	2.19	0.41
1:D:3906:PHE:HB3	1:D:3967:LEU:HD11	2.01	0.41
1:D:4306:PHE:HA	1:D:4309:ILE:HG12	2.01	0.41
1:A:308:LEU:HG	1:A:309:MET:O	2.19	0.41
1:A:955:GLU:HG3	1:A:959:ASP:OD2	2.19	0.41
1:A:1161:VAL:HB	1:A:1226:TYR:HE2	1.85	0.41
1:A:1552:VAL:HG12	1:A:1553:PHE:HD1	1.85	0.41
1:A:2134:MET:HE2	1:A:2192:MET:CE	2.50	0.41
1:A:2175:MET:HA	1:A:2178:VAL:HG12	2.02	0.41
1:A:2737:LEU:HD23	1:A:2737:LEU:HA	1.93	0.41
1:A:2843:MET:HE2	1:A:2843:MET:HB3	1.85	0.41
1:B:2552:VAL:HG11	1:B:2573:LEU:HD13	2.01	0.41
1:B:4818:TYR:HD1	1:C:4848:ILE:HD11	1.85	0.41
1:C:260:VAL:O	1:C:390:LYS:NZ	2.37	0.41
1:C:399:MET:HE3	1:C:399:MET:HB3	1.94	0.41
1:C:1931:ASP:OD1	1:C:1932:PHE:N	2.53	0.41
1:C:2134:MET:HE2	1:C:2192:MET:CE	2.50	0.41
1:C:2837:LEU:HA	1:C:2840:MET:HB2	2.02	0.41
1:C:2943:PHE:CE1	1:C:2952:GLU:HG2	2.55	0.41
1:C:2953:HIS:O	1:C:2953:HIS:CG	2.73	0.41
1:C:4568:MET:HA	1:C:4571:THR:HB	2.02	0.41
1:D:996:VAL:HG11	1:D:1051:ARG:CD	2.46	0.41
1:D:1011:ARG:HB3	1:D:1016:TRP:HB2	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1135:PHE:HB3	1:D:1173:MET:HE1	2.02	0.41
1:D:2135:GLY:H	1:D:2138:GLU:HB2	1.84	0.41
1:D:2943:PHE:CE2	1:D:3021:LEU:HD23	2.55	0.41
1:D:3642:GLU:HB3	1:D:3646:LYS:NZ	2.35	0.41
1:D:3992:ASN:O	1:D:3997:LYS:NZ	2.51	0.41
1:D:4107:GLU:OE1	1:D:4149:TYR:OH	2.22	0.41
1:D:4503:ARG:NH2	1:D:4745:ASP:OD2	2.53	0.41
1:A:82:LEU:HD13	1:A:156:GLU:HG2	2.01	0.41
1:A:163:HIS:HB2	1:A:182:ILE:HG13	2.02	0.41
1:A:1051:ARG:HA	1:A:1054:VAL:HG23	2.02	0.41
1:A:1312:GLU:OE1	2:E:32:GLN:HG2	2.20	0.41
1:A:2567:ASP:O	1:A:2571:VAL:HG23	2.20	0.41
1:A:2841:ALA:HA	1:A:2844:MET:HG3	2.02	0.41
1:A:4793:TYR:HH	1:A:4816:HIS:CE1	2.32	0.41
2:E:19:LYS:HE3	2:E:19:LYS:HB2	1.83	0.41
1:B:483:LYS:HB2	1:B:483:LYS:HE3	1.84	0.41
1:B:877:HIS:ND1	1:B:878:LEU:HD12	2.35	0.41
1:B:924:LEU:HD12	1:B:925:PRO:O	2.21	0.41
1:B:993:GLU:OE2	1:B:1047:LYS:NZ	2.52	0.41
1:B:1190:LEU:HD11	1:B:1193:LYS:HD3	2.03	0.41
1:B:1483:SER:HB3	1:B:1486:TYR:CE1	2.55	0.41
1:B:2943:PHE:CE2	1:B:3021:LEU:HD23	2.55	0.41
1:C:1084:ARG:NH1	1:C:1127:GLU:OE1	2.50	0.41
1:C:2238:THR:OG1	1:C:2241:ASP:OD2	2.24	0.41
1:C:3677:THR:HB	1:C:3679:LYS:HZ3	1.86	0.41
1:C:3728:GLN:O	1:C:3732:HIS:ND1	2.46	0.41
1:D:955:GLU:HG3	1:D:959:ASP:OD2	2.20	0.41
1:D:993:GLU:OE2	1:D:1047:LYS:NZ	2.52	0.41
1:D:2701:PHE:CE2	1:D:2703:PRO:HG3	2.55	0.41
1:D:2953:HIS:CG	1:D:2953:HIS:O	2.73	0.41
1:D:3821:THR:HG22	1:D:3823:GLU:H	1.85	0.41
1:A:156:GLU:HB2	1:A:187:SER:HB3	2.01	0.41
1:A:877:HIS:ND1	1:A:878:LEU:HD12	2.35	0.41
1:A:1004:HIS:HE1	1:A:1038:LEU:HD21	1.84	0.41
1:A:2195:ASN:ND2	1:A:2198:ARG:HH12	2.15	0.41
1:A:2460:PHE:CE2	1:A:2465:LYS:HD2	2.56	0.41
1:A:2701:PHE:CE2	1:A:2703:PRO:HG3	2.55	0.41
1:A:2857:LYS:HE3	1:A:2871:LEU:CD2	2.37	0.41
1:A:4306:PHE:HA	1:A:4309:ILE:HG12	2.02	0.41
1:A:4858:LEU:HD23	1:A:4861:ILE:HD12	2.03	0.41
1:B:62:LEU:HD11	1:B:282:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:921:PHE:HD1	1:B:929:ARG:CZ	2.33	0.41
1:B:985:PHE:N	1:B:985:PHE:CD2	2.88	0.41
1:B:986:ILE:HD12	1:B:1058:LEU:HD12	2.01	0.41
1:B:1028:ARG:HA	1:B:1028:ARG:HD2	1.83	0.41
1:B:1304:LEU:HD23	1:B:1304:LEU:HA	1.95	0.41
1:B:2134:MET:HE2	1:B:2192:MET:CE	2.50	0.41
1:B:2274:LEU:HD21	1:B:2329:GLU:HB2	2.01	0.41
1:B:2841:ALA:HA	1:B:2844:MET:HG3	2.02	0.41
1:B:2943:PHE:CE1	1:B:2952:GLU:HG2	2.56	0.41
1:B:4045:LYS:HE3	1:B:4067:LEU:HD22	2.03	0.41
1:B:4805:LYS:HA	1:B:4805:LYS:HD2	1.82	0.41
1:C:62:LEU:HD11	1:C:282:VAL:HG13	2.03	0.41
1:C:165:ALA:HB1	1:C:211:LEU:HD22	2.03	0.41
1:C:586:LEU:HD22	1:C:620:CYS:HB2	2.02	0.41
1:C:1074:ARG:NH1	1:C:1076:GLU:HA	2.36	0.41
1:C:1475:LYS:HE3	1:C:1475:LYS:HB3	1.90	0.41
1:C:2943:PHE:CE2	1:C:3021:LEU:HD23	2.56	0.41
1:C:3891:TYR:HA	1:D:76:ARG:NH2	2.36	0.41
1:D:329:PHE:CE1	1:D:365:HIS:HD2	2.37	0.41
1:D:506:HIS:CE1	1:D:530:LEU:HD21	2.55	0.41
1:D:1051:ARG:HA	1:D:1054:VAL:HG23	2.01	0.41
1:D:1174:MET:HG3	1:D:1190:LEU:HA	2.02	0.41
1:D:2966:VAL:O	1:D:2970:LEU:N	2.46	0.41
1:D:4045:LYS:HE3	1:D:4067:LEU:HD22	2.03	0.41
1:D:4908:HIS:CE1	1:D:4913:HIS:ND1	2.89	0.41
1:A:2192:MET:O	1:A:2192:MET:HG2	2.16	0.41
1:A:2262:LEU:O	1:A:2266:VAL:HG23	2.20	0.41
1:A:2552:VAL:HG11	1:A:2573:LEU:HD13	2.01	0.41
1:A:3065:ALA:O	1:A:3069:GLU:HG2	2.20	0.41
1:B:201:LEU:H	1:B:201:LEU:HD12	1.85	0.41
1:B:1074:ARG:NH1	1:B:1076:GLU:HA	2.36	0.41
1:B:1468:THR:HG22	1:B:1479:SER:CB	2.51	0.41
1:B:1950:ALA:HB1	1:B:1961:LYS:HZ3	1.85	0.41
1:B:2262:LEU:O	1:B:2266:VAL:HG23	2.20	0.41
1:B:2299:LEU:HD22	1:B:2395:LEU:HA	2.01	0.41
1:B:2460:PHE:CE2	1:B:2465:LYS:HD2	2.56	0.41
1:B:4306:PHE:HA	1:B:4309:ILE:HG12	2.01	0.41
1:B:4480:PHE:N	1:B:4482:LYS:HZ3	2.18	0.41
1:B:4908:HIS:CE1	1:B:4913:HIS:ND1	2.89	0.41
1:C:39:ALA:O	1:C:64:ILE:HB	2.21	0.41
1:C:82:LEU:HD13	1:C:156:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LEU:H	1:C:201:LEU:HD12	1.85	0.41
1:C:857:LEU:HD12	1:C:859:GLN:NE2	2.36	0.41
1:C:876:PRO:HA	1:C:879:GLU:OE1	2.21	0.41
1:C:1004:HIS:HE1	1:C:1038:LEU:HD21	1.84	0.41
1:C:1161:VAL:HB	1:C:1226:TYR:HE2	1.85	0.41
1:C:1174:MET:HG3	1:C:1190:LEU:HA	2.02	0.41
1:C:1483:SER:HB3	1:C:1486:TYR:CE1	2.55	0.41
1:C:1681:ASP:HB3	1:C:1683:PRO:HD2	2.03	0.41
1:C:2460:PHE:CE2	1:C:2465:LYS:HD2	2.56	0.41
1:C:2841:ALA:HA	1:C:2844:MET:HG3	2.02	0.41
1:C:3025:ASP:O	1:C:3028:SER:OG	2.25	0.41
1:C:3642:GLU:HB3	1:C:3646:LYS:NZ	2.35	0.41
1:C:3833:ASP:OD2	1:C:3908:LYS:HD2	2.21	0.41
1:D:439:LYS:HA	1:D:439:LYS:HD3	1.73	0.41
1:D:857:LEU:HD12	1:D:859:GLN:NE2	2.36	0.41
1:D:924:LEU:HD12	1:D:925:PRO:O	2.21	0.41
1:D:1004:HIS:HE1	1:D:1038:LEU:HD21	1.85	0.41
1:D:1652:LYS:NZ	1:D:1656:HIS:HE1	2.18	0.41
1:D:1948:MET:HA	1:D:1948:MET:CE	2.51	0.41
1:D:1979:PHE:CD1	1:D:1993:ARG:HG2	2.56	0.41
1:D:2299:LEU:HD22	1:D:2395:LEU:HA	2.01	0.41
1:D:2837:LEU:HA	1:D:2840:MET:HB2	2.02	0.41
1:D:4503:ARG:HD2	1:D:4503:ARG:HA	1.93	0.41
1:A:1640:ASP:OD2	1:A:1641:ILE:N	2.54	0.41
1:A:1853:GLU:OE1	1:A:1853:GLU:N	2.49	0.41
1:A:1979:PHE:CD1	1:A:1993:ARG:HG2	2.56	0.41
1:A:2554:ARG:HH11	1:A:2557:LYS:HB2	1.86	0.41
1:A:2836:ASP:OD1	1:A:2836:ASP:N	2.52	0.41
1:A:2837:LEU:HA	1:A:2840:MET:HB2	2.02	0.41
1:A:2943:PHE:CE1	1:A:2952:GLU:HG2	2.56	0.41
1:A:2953:HIS:O	1:A:2953:HIS:CG	2.73	0.41
1:B:191:TYR:CE1	1:B:209:GLN:HG3	2.55	0.41
1:B:876:PRO:HA	1:B:879:GLU:OE1	2.21	0.41
1:B:1135:PHE:HB3	1:B:1173:MET:HE1	2.02	0.41
1:B:1649:GLU:HG2	1:B:1650:LEU:N	2.35	0.41
1:B:1948:MET:CE	1:B:1948:MET:HA	2.51	0.41
1:B:2502:LEU:HD13	1:B:2513:ALA:HB1	2.03	0.41
1:B:2953:HIS:CG	1:B:2953:HIS:O	2.73	0.41
1:B:4061:SER:O	1:B:4064:GLU:HG3	2.21	0.41
1:B:4502:MET:HE1	1:B:4585:PHE:CD2	2.55	0.41
1:B:4732:GLY:HA2	1:B:4735:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4858:LEU:HD23	1:B:4861:ILE:HD12	2.03	0.41
1:C:709:GLY:HA3	1:C:723:PHE:CD2	2.55	0.41
1:C:1152:TYR:CD1	1:C:1184:ASP:HB3	2.56	0.41
1:C:2843:MET:HE2	1:C:2843:MET:HB3	1.85	0.41
1:C:4908:HIS:CE1	1:C:4913:HIS:ND1	2.89	0.41
1:D:3861:GLN:H	1:D:3867:THR:HG23	1.86	0.41
1:A:876:PRO:HA	1:A:879:GLU:OE1	2.21	0.41
1:A:986:ILE:HD13	1:A:1055:ARG:HA	2.02	0.41
1:A:1081:THR:HG23	1:A:1083:GLU:H	1.85	0.41
1:A:2279:MET:HE3	1:A:2283:LYS:HD3	2.03	0.41
1:A:2943:PHE:CE2	1:A:3021:LEU:HD23	2.55	0.41
1:A:3833:ASP:OD2	1:A:3908:LYS:HD2	2.21	0.41
1:A:4177:VAL:HG11	1:A:4880:VAL:HA	2.03	0.41
1:B:585:ALA:O	1:B:588:ILE:HG22	2.21	0.41
1:B:603:LYS:HE3	1:B:603:LYS:HB3	1.94	0.41
1:C:62:LEU:O	1:C:66:THR:HG23	2.21	0.41
1:C:520:ARG:O	1:C:524:GLU:HG2	2.21	0.41
1:C:993:GLU:OE2	1:C:1047:LYS:NZ	2.52	0.41
1:C:3065:ALA:O	1:C:3069:GLU:HG2	2.20	0.41
1:C:3861:GLN:H	1:C:3867:THR:HG23	1.86	0.41
1:D:1124:PRO:HD2	1:D:1594:VAL:HG23	2.03	0.41
1:D:1611:ILE:HD11	1:D:1618:LEU:HD23	2.02	0.41
1:A:165:ALA:HB1	1:A:211:LEU:HD22	2.02	0.41
1:A:201:LEU:HD12	1:A:201:LEU:H	1.85	0.41
1:A:1043:LYS:HA	1:A:1046:ASN:ND2	2.35	0.41
1:A:1050:LEU:HD12	1:A:1050:LEU:HA	1.81	0.41
1:A:1092:LYS:NZ	1:A:1646:GLU:OE1	2.39	0.41
1:A:1489:CYS:O	1:A:1493:SER:OG	2.27	0.41
1:A:1793:GLN:NE2	1:A:1797:GLU:OE2	2.54	0.41
1:A:2353:ILE:O	1:A:2360:ASP:HB2	2.20	0.41
1:A:2502:LEU:HD13	1:A:2513:ALA:HB1	2.03	0.41
1:A:2678:PRO:HB2	1:A:2981:TYR:CE1	2.56	0.41
1:A:2733:SER:HB3	1:A:2821:TYR:CZ	2.56	0.41
1:A:3107:SER:O	1:A:3110:GLU:HG3	2.21	0.41
1:A:3739:MET:HE2	1:A:3739:MET:HB3	1.92	0.41
1:A:3821:THR:HG22	1:A:3823:GLU:H	1.85	0.41
1:A:3861:GLN:H	1:A:3867:THR:HG23	1.86	0.41
1:A:4568:MET:HA	1:A:4571:THR:HB	2.02	0.41
1:A:4908:HIS:CE1	1:A:4913:HIS:ND1	2.89	0.41
1:B:513:HIS:O	1:B:517:VAL:HG23	2.21	0.41
1:B:680:ASP:N	1:B:799:LYS:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1552:VAL:HG12	1:B:1553:PHE:HD1	1.85	0.41
1:B:1914:CYS:O	1:B:1918:VAL:HG23	2.20	0.41
1:B:1978:ASN:HB3	1:B:1983:LYS:HE2	2.03	0.41
1:B:1979:PHE:CD1	1:B:1993:ARG:HG2	2.56	0.41
1:B:2550:HIS:HE1	1:B:2875:ASP:CG	2.29	0.41
1:B:2554:ARG:HH11	1:B:2557:LYS:HB2	1.86	0.41
1:B:2801:TYR:CE2	1:C:1496:PRO:O	2.74	0.41
1:B:3833:ASP:OD2	1:B:3908:LYS:HD2	2.21	0.41
1:B:4177:VAL:HG11	1:B:4880:VAL:HA	2.03	0.41
1:C:191:TYR:CE1	1:C:209:GLN:HG3	2.55	0.41
1:C:298:ARG:NH1	1:C:417:ARG:HH12	2.15	0.41
1:C:877:HIS:ND1	1:C:878:LEU:HD12	2.35	0.41
1:C:1166:VAL:HG23	1:C:1173:MET:CG	2.46	0.41
1:C:1630:LEU:HD13	1:C:1644:LEU:HD21	2.03	0.41
1:C:1793:GLN:NE2	1:C:1797:GLU:OE2	2.54	0.41
1:C:1914:CYS:O	1:C:1918:VAL:HG23	2.20	0.41
1:C:1979:PHE:CD1	1:C:1993:ARG:HG2	2.55	0.41
1:C:2087:LEU:O	1:C:2091:GLN:HG2	2.21	0.41
1:C:2555:LEU:HD12	1:C:2555:LEU:HA	1.97	0.41
1:C:2678:PRO:HB2	1:C:2981:TYR:CE1	2.56	0.41
1:C:3639:LYS:NZ	1:C:3643:ASP:OD2	2.54	0.41
1:C:3906:PHE:HB3	1:C:3967:LEU:HD11	2.01	0.41
1:C:4503:ARG:HD2	1:C:4503:ARG:HA	1.93	0.41
1:C:4503:ARG:NH2	1:C:4745:ASP:OD2	2.53	0.41
1:D:39:ALA:O	1:D:64:ILE:HB	2.21	0.41
1:D:163:HIS:HB2	1:D:182:ILE:HG13	2.02	0.41
1:D:513:HIS:O	1:D:517:VAL:HG23	2.21	0.41
1:D:709:GLY:HA3	1:D:723:PHE:CD2	2.55	0.41
1:D:986:ILE:HD12	1:D:1058:LEU:HD12	2.01	0.41
1:D:1102:TYR:CE1	1:D:1104:GLU:HG3	2.56	0.41
1:D:1161:VAL:HB	1:D:1226:TYR:HE2	1.85	0.41
1:D:1468:THR:HG22	1:D:1479:SER:CB	2.51	0.41
1:D:1564:MET:HE3	1:D:1565:PRO:CD	2.42	0.41
1:D:1681:ASP:HB3	1:D:1683:PRO:HD2	2.03	0.41
1:D:1793:GLN:NE2	1:D:1797:GLU:OE2	2.54	0.41
1:D:1931:ASP:OD1	1:D:1932:PHE:N	2.53	0.41
1:D:2175:MET:HA	1:D:2178:VAL:HG12	2.02	0.41
1:D:2678:PRO:HB2	1:D:2981:TYR:CE1	2.56	0.41
1:D:2721:ILE:HG21	1:D:2772:ARG:HG3	2.03	0.41
1:D:3065:ALA:O	1:D:3069:GLU:HG2	2.20	0.41
1:D:3698:SER:O	1:D:3727:GLN:NE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3833:ASP:OD2	1:D:3908:LYS:HD2	2.21	0.41
1:D:4750:PHE:HD2	1:D:4753:LEU:HD12	1.86	0.41
1:A:924:LEU:HD12	1:A:925:PRO:O	2.21	0.41
1:A:1190:LEU:HD11	1:A:1193:LYS:HD3	2.03	0.41
1:A:2163:ARG:NH1	1:A:2209:GLN:HB3	2.35	0.41
1:A:3018:ARG:HG3	1:A:3021:LEU:HD22	2.02	0.41
1:A:3639:LYS:NZ	1:A:3643:ASP:OD2	2.54	0.41
1:A:3677:THR:HB	1:A:3679:LYS:NZ	2.36	0.41
2:F:50:ARG:N	2:F:55:GLU:OE2	2.37	0.41
2:H:50:ARG:N	2:H:55:GLU:OE2	2.37	0.41
1:B:39:ALA:O	1:B:64:ILE:HB	2.21	0.41
1:B:709:GLY:HA3	1:B:723:PHE:CD2	2.56	0.41
1:B:1475:LYS:HB3	1:B:1475:LYS:HE3	1.90	0.41
1:B:2253:LEU:HD23	1:B:2253:LEU:HA	1.93	0.41
1:B:2344:LEU:HD22	1:B:2434:GLY:HA3	2.03	0.41
1:B:2733:SER:HB3	1:B:2821:TYR:CZ	2.56	0.41
1:B:3642:GLU:HB3	1:B:3646:LYS:NZ	2.35	0.41
1:B:3687:LEU:HD12	1:B:3687:LEU:HA	1.94	0.41
1:C:680:ASP:N	1:C:799:LYS:O	2.54	0.41
1:C:1640:ASP:OD2	1:C:1641:ILE:N	2.54	0.41
1:C:2262:LEU:O	1:C:2266:VAL:HG23	2.20	0.41
1:C:3972:MET:HE1	1:C:4016:PHE:CE2	2.56	0.41
1:C:4045:LYS:HE3	1:C:4067:LEU:HD22	2.03	0.41
1:C:4061:SER:O	1:C:4064:GLU:HG3	2.21	0.41
1:C:4306:PHE:HA	1:C:4309:ILE:HG12	2.02	0.41
1:D:876:PRO:HA	1:D:879:GLU:OE1	2.21	0.41
1:D:921:PHE:HD1	1:D:929:ARG:CZ	2.34	0.41
1:D:929:ARG:NH2	1:D:933:LEU:HD21	2.36	0.41
1:D:1152:TYR:CD1	1:D:1184:ASP:HB3	2.56	0.41
1:D:2134:MET:HE2	1:D:2192:MET:CE	2.50	0.41
1:D:2192:MET:HE2	1:D:2192:MET:HB3	1.80	0.41
1:D:2550:HIS:HE1	1:D:2875:ASP:CG	2.29	0.41
1:D:2943:PHE:CE1	1:D:2952:GLU:HG2	2.56	0.41
1:A:62:LEU:O	1:A:66:THR:HG23	2.21	0.40
1:A:520:ARG:O	1:A:524:GLU:HG2	2.21	0.40
1:A:585:ALA:O	1:A:588:ILE:HG22	2.21	0.40
1:A:709:GLY:HA3	1:A:723:PHE:CD2	2.55	0.40
1:A:1174:MET:HG3	1:A:1190:LEU:HA	2.02	0.40
1:A:1483:SER:HB3	1:A:1486:TYR:CE1	2.55	0.40
1:A:2299:LEU:HD22	1:A:2395:LEU:HA	2.01	0.40
1:A:2966:VAL:O	1:A:2970:LEU:N	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4609:LYS:HD3	1:A:4615:LEU:HD13	2.03	0.40
1:A:4844:ILE:HD13	1:D:4814:MET:HE2	1.95	0.40
1:B:644:LEU:HD22	1:B:1630:LEU:HD21	2.02	0.40
1:B:1161:VAL:HB	1:B:1226:TYR:HE2	1.85	0.40
1:B:1630:LEU:HD13	1:B:1644:LEU:HD21	2.03	0.40
1:B:1977:LEU:HD23	1:B:1977:LEU:HA	1.88	0.40
1:B:2087:LEU:O	1:B:2091:GLN:HG2	2.21	0.40
1:B:2837:LEU:HA	1:B:2840:MET:HB2	2.02	0.40
1:B:3882:GLN:HB3	1:B:3947:PHE:CE2	2.56	0.40
1:B:4609:LYS:HD3	1:B:4615:LEU:HD13	2.03	0.40
1:C:731:HIS:CE1	1:C:740:THR:HG22	2.57	0.40
1:C:892:LEU:HD13	1:C:1052:GLU:OE1	2.21	0.40
1:C:1102:TYR:CE1	1:C:1104:GLU:HG3	2.56	0.40
1:C:1611:ILE:HD11	1:C:1618:LEU:HD23	2.02	0.40
1:C:1948:MET:HA	1:C:1948:MET:CE	2.51	0.40
1:C:2502:LEU:HD13	1:C:2513:ALA:HB1	2.03	0.40
1:C:2721:ILE:HG21	1:C:2772:ARG:HG3	2.03	0.40
1:C:2733:SER:HB3	1:C:2821:TYR:CZ	2.56	0.40
1:C:4750:PHE:HD2	1:C:4753:LEU:HD12	1.86	0.40
1:D:165:ALA:HB1	1:D:211:LEU:HD22	2.02	0.40
1:D:586:LEU:HD22	1:D:620:CYS:HB2	2.02	0.40
1:D:674:TYR:CE1	1:D:756:SER:HB2	2.56	0.40
1:D:2146:LEU:HD23	1:D:2146:LEU:HA	1.94	0.40
1:D:2554:ARG:HH11	1:D:2557:LYS:HB2	1.86	0.40
1:D:2635:GLU:HG2	1:D:2680:TYR:CE1	2.55	0.40
1:D:4609:LYS:HD3	1:D:4615:LEU:HD13	2.03	0.40
1:A:2721:ILE:HG21	1:A:2772:ARG:HG3	2.03	0.40
1:A:3651:PRO:HB2	1:A:3652:PRO:HD3	2.04	0.40
1:A:4061:SER:O	1:A:4064:GLU:HG3	2.21	0.40
1:A:4172:PHE:CZ	1:A:4189:PHE:HA	2.57	0.40
1:A:4808:ASP:OD2	1:A:4810:LEU:HB3	2.22	0.40
1:B:731:HIS:CE1	1:B:740:THR:HG22	2.56	0.40
1:B:912:LYS:NZ	1:B:914:GLN:HG3	2.37	0.40
1:B:1640:ASP:OD2	1:B:1641:ILE:N	2.54	0.40
1:B:1681:ASP:HB3	1:B:1683:PRO:HD2	2.03	0.40
1:B:1793:GLN:NE2	1:B:1797:GLU:OE2	2.54	0.40
1:B:4113:THR:O	1:B:4117:THR:HG23	2.21	0.40
1:C:370:LEU:HB2	1:C:393:MET:HE2	2.03	0.40
1:C:824:GLU:OE2	1:C:1020:ILE:N	2.55	0.40
1:C:972:LEU:HG	1:C:973:THR:H	1.86	0.40
1:C:3651:PRO:HB2	1:C:3652:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3872:ILE:O	1:C:3875:VAL:HG12	2.22	0.40
1:C:4502:MET:HE1	1:C:4585:PHE:CD2	2.55	0.40
1:D:246:THR:HG21	1:D:267:VAL:HG21	2.03	0.40
1:D:288:HIS:CE1	1:D:352:SER:HB3	2.57	0.40
1:D:298:ARG:NH1	1:D:417:ARG:HH12	2.15	0.40
1:D:1084:ARG:NH1	1:D:1127:GLU:OE1	2.50	0.40
1:D:1978:ASN:HB3	1:D:1983:LYS:HE2	2.03	0.40
1:D:2502:LEU:HD13	1:D:2513:ALA:HB1	2.03	0.40
1:D:2733:SER:HB3	1:D:2821:TYR:CZ	2.56	0.40
1:D:2793:ARG:HH11	1:D:2793:ARG:CG	2.31	0.40
1:D:3107:SER:O	1:D:3110:GLU:HG3	2.21	0.40
1:D:3639:LYS:NZ	1:D:3643:ASP:OD2	2.54	0.40
1:D:4858:LEU:HD23	1:D:4861:ILE:HD12	2.03	0.40
1:A:163:HIS:HA	1:A:164:PRO:HD3	1.95	0.40
1:A:929:ARG:NH2	1:A:933:LEU:HD21	2.36	0.40
1:A:1135:PHE:HB3	1:A:1173:MET:HE1	2.02	0.40
1:A:1166:VAL:HG23	1:A:1173:MET:CG	2.46	0.40
1:A:1948:MET:HA	1:A:1948:MET:CE	2.51	0.40
1:A:2623:LEU:HB3	1:A:2626:GLY:HA2	2.02	0.40
1:A:3882:GLN:HB3	1:A:3947:PHE:CE2	2.57	0.40
1:A:4045:LYS:HE3	1:A:4067:LEU:HD22	2.03	0.40
1:A:4622:SER:C	1:A:4624:ASP:H	2.29	0.40
1:B:62:LEU:O	1:B:66:THR:HG23	2.21	0.40
1:B:857:LEU:HD12	1:B:859:GLN:NE2	2.36	0.40
1:B:880:ARG:NH1	1:B:881:ILE:HB	2.37	0.40
1:B:929:ARG:NH2	1:B:933:LEU:HD21	2.36	0.40
1:B:1786:ILE:O	1:B:1790:LYS:HG2	2.22	0.40
1:B:2678:PRO:HB2	1:B:2981:TYR:CE1	2.56	0.40
1:B:2966:VAL:O	1:B:2970:LEU:N	2.46	0.40
1:B:3018:ARG:HG3	1:B:3021:LEU:HD22	2.02	0.40
1:B:4568:MET:HA	1:B:4571:THR:HB	2.02	0.40
1:C:514:PHE:CD2	1:C:526:TRP:HB2	2.56	0.40
1:C:902:TRP:CZ2	1:C:915:HIS:HB3	2.50	0.40
1:C:921:PHE:HD1	1:C:929:ARG:CZ	2.34	0.40
1:C:1978:ASN:HB3	1:C:1983:LYS:HE2	2.03	0.40
1:C:2508:SER:HB3	1:C:2560:SER:OG	2.22	0.40
1:C:3107:SER:O	1:C:3110:GLU:HG3	2.21	0.40
1:C:3677:THR:HB	1:C:3679:LYS:NZ	2.35	0.40
1:C:3882:GLN:HB3	1:C:3947:PHE:CE2	2.57	0.40
1:C:4858:LEU:HD23	1:C:4861:ILE:HD12	2.03	0.40
1:D:731:HIS:CE1	1:D:740:THR:HG22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1190:LEU:HD11	1:D:1193:LYS:HD3	2.03	0.40
1:D:1304:LEU:HD23	1:D:1304:LEU:HA	1.95	0.40
1:D:3651:PRO:HB2	1:D:3652:PRO:HD3	2.04	0.40
1:D:4042:VAL:HG12	1:D:4077:THR:HB	2.04	0.40
1:D:4808:ASP:OD2	1:D:4810:LEU:HB3	2.21	0.40
1:A:880:ARG:NH1	1:A:881:ILE:HB	2.37	0.40
1:A:1468:THR:HG22	1:A:1479:SER:CB	2.51	0.40
1:A:1757:LEU:HD23	1:A:1757:LEU:HA	1.87	0.40
1:A:3043:ARG:HB3	1:A:3047:LYS:HZ1	1.86	0.40
1:A:3073:GLU:O	1:A:3077:GLN:OE1	2.40	0.40
1:A:3723:LYS:NZ	1:A:3727:GLN:OE1	2.52	0.40
1:A:4585:PHE:HA	1:A:4588:ILE:HD12	2.04	0.40
1:B:520:ARG:O	1:B:524:GLU:HG2	2.21	0.40
1:B:1102:TYR:CE1	1:B:1104:GLU:HG3	2.56	0.40
1:B:2086:VAL:HG22	1:B:3687:LEU:HD13	2.04	0.40
1:B:2721:ILE:HG21	1:B:2772:ARG:HG3	2.03	0.40
1:B:3639:LYS:NZ	1:B:3643:ASP:OD2	2.54	0.40
1:B:3972:MET:HE1	1:B:4016:PHE:CE2	2.56	0.40
1:C:644:LEU:HD22	1:C:1630:LEU:HD21	2.02	0.40
1:C:924:LEU:HD12	1:C:925:PRO:O	2.21	0.40
1:C:2554:ARG:HH11	1:C:2557:LYS:HB2	1.86	0.40
1:C:2843:MET:O	1:C:2846:GLU:HG2	2.22	0.40
1:C:2844:MET:CE	1:C:2848:TYR:HE2	2.35	0.40
1:C:4177:VAL:HG11	1:C:4880:VAL:HA	2.03	0.40
1:C:4609:LYS:HD3	1:C:4615:LEU:HD13	2.03	0.40
1:D:587:ASN:OD1	1:D:2133:ARG:NH1	2.53	0.40
1:D:986:ILE:HD13	1:D:1055:ARG:HA	2.02	0.40
1:D:1640:ASP:OD2	1:D:1641:ILE:N	2.54	0.40
1:D:1960:ARG:H	1:D:1960:ARG:HG3	0.96	0.40
1:D:2460:PHE:CE2	1:D:2465:LYS:HD2	2.56	0.40
1:D:2844:MET:CE	1:D:2848:TYR:HE2	2.35	0.40
1:D:3972:MET:HE1	1:D:4016:PHE:CE2	2.56	0.40
1:A:62:LEU:HD11	1:A:282:VAL:HG13	2.03	0.40
1:A:857:LEU:HD12	1:A:859:GLN:NE2	2.36	0.40
1:A:1786:ILE:O	1:A:1790:LYS:HG2	2.22	0.40
1:A:1977:LEU:HD23	1:A:1977:LEU:HA	1.88	0.40
1:A:2701:PHE:HD2	1:A:2857:LYS:HZ3	1.68	0.40
1:A:2721:ILE:HG12	1:A:2775:ILE:CG2	2.52	0.40
1:A:3043:ARG:O	1:A:3047:LYS:HE2	2.22	0.40
1:A:3642:GLU:OE2	1:A:3730:ARG:NH1	2.55	0.40
1:A:3972:MET:HE1	1:A:4016:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LEU:HD22	1:B:620:CYS:HB2	2.02	0.40
1:B:1283:LEU:HD11	1:B:1582:CYS:SG	2.62	0.40
1:B:1850:VAL:HA	1:B:2054:LYS:HE3	2.03	0.40
1:B:2721:ILE:HG12	1:B:2775:ILE:CG2	2.52	0.40
1:B:3642:GLU:OE2	1:B:3730:ARG:NH1	2.55	0.40
1:B:4622:SER:C	1:B:4624:ASP:H	2.29	0.40
1:B:4808:ASP:OD2	1:B:4810:LEU:HB3	2.21	0.40
1:C:513:HIS:O	1:C:517:VAL:HG23	2.21	0.40
1:C:929:ARG:NH2	1:C:933:LEU:HD21	2.36	0.40
1:C:1433:PHE:HE1	1:C:1554:GLN:HB2	1.87	0.40
1:C:1642:LEU:HD21	1:C:1691:ASN:HD21	1.87	0.40
1:C:1786:ILE:O	1:C:1790:LYS:HG2	2.22	0.40
1:C:2192:MET:O	1:C:2192:MET:HG2	2.17	0.40
1:C:2279:MET:HE3	1:C:2283:LYS:HD3	2.03	0.40
1:C:2554:ARG:HA	1:C:2554:ARG:HD2	1.85	0.40
1:C:4026:LEU:O	1:C:4029:SER:OG	2.30	0.40
1:D:62:LEU:O	1:D:66:THR:HG23	2.21	0.40
1:D:201:LEU:HD12	1:D:201:LEU:H	1.85	0.40
1:D:1081:THR:HG23	1:D:1083:GLU:H	1.85	0.40
1:D:2279:MET:HE3	1:D:2283:LYS:HD3	2.03	0.40
1:D:2623:LEU:HB3	1:D:2626:GLY:HA2	2.02	0.40
1:D:2635:GLU:HA	1:D:2638:LEU:HD12	2.03	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	3978/4967 (80%)	3861 (97%)	113 (3%)	4 (0%)	48	79
1	B	3978/4967 (80%)	3862 (97%)	112 (3%)	4 (0%)	48	79
1	C	3978/4967 (80%)	3861 (97%)	113 (3%)	4 (0%)	48	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	3978/4967 (80%)	3862 (97%)	112 (3%)	4 (0%)	48	79
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	16332/20300 (80%)	15850 (97%)	466 (3%)	16 (0%)	49	79

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2988	ARG
1	A	3927	PRO
1	A	4641	PRO
1	B	2988	ARG
1	B	3927	PRO
1	B	4641	PRO
1	C	2988	ARG
1	C	3927	PRO
1	C	4641	PRO
1	D	2988	ARG
1	D	3927	PRO
1	D	4641	PRO
1	A	1081	THR
1	B	1081	THR
1	C	1081	THR
1	D	1081	THR

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	3513/4358 (81%)	3459 (98%)	54 (2%)	57	71
1	B	3513/4358 (81%)	3459 (98%)	54 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	3513/4358 (81%)	3459 (98%)	54 (2%)	57	71
1	D	3513/4358 (81%)	3459 (98%)	54 (2%)	57	71
2	E	88/89 (99%)	85 (97%)	3 (3%)	32	58
2	F	88/89 (99%)	85 (97%)	3 (3%)	32	58
2	G	88/89 (99%)	85 (97%)	3 (3%)	32	58
2	H	88/89 (99%)	85 (97%)	3 (3%)	32	58
All	All	14404/17788 (81%)	14176 (98%)	228 (2%)	54	70

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	MET
1	A	317	MET
1	A	349	MET
1	A	398	HIS
1	A	778	MET
1	A	889	ILE
1	A	985	PHE
1	A	1181	ILE
1	A	1249	MET
1	A	1293	GLN
1	A	1300	MET
1	A	1748	LEU
1	A	1948	MET
1	A	1953	MET
1	A	1957	LEU
1	A	1960	ARG
1	A	2192	MET
1	A	2279	MET
1	A	2347	MET
1	A	2384	MET
1	A	2456	MET
1	A	2482	ASP
1	A	2493	LEU
1	A	2530	ARG
1	A	2580	LEU
1	A	2652	LEU
1	A	2689	MET
1	A	2695	MET
1	A	2730	ASP

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Mol	Chain	Res	Type
1	A	2734	MET
1	A	2788	ARG
1	A	2793	ARG
1	A	2828	MET
1	A	2843	MET
1	A	2870	LEU
1	A	2880	LYS
1	A	2897	GLN
1	A	2960	ILE
1	A	2968	LEU
1	A	3051	GLU
1	A	3061	LEU
1	A	3105	LEU
1	A	3611	LEU
1	A	3739	MET
1	A	3999	MET
1	A	4046	ARG
1	A	4109	MET
1	A	4208	GLU
1	A	4292	MET
1	A	4504	MET
1	A	4555	ILE
1	A	4718	SER
1	A	4791	LYS
1	A	4817	MET
2	E	50	ARG
2	E	53	LYS
2	E	86	THR
2	F	50	ARG
2	F	53	LYS
2	F	86	THR
2	G	50	ARG
2	G	53	LYS
2	G	86	THR
2	H	50	ARG
2	H	53	LYS
2	H	86	THR
1	B	81	MET
1	B	317	MET
1	B	349	MET
1	B	398	HIS
1	B	778	MET

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Mol	Chain	Res	Type
1	B	889	ILE
1	B	985	PHE
1	B	1181	ILE
1	B	1249	MET
1	B	1293	GLN
1	B	1300	MET
1	B	1748	LEU
1	B	1948	MET
1	B	1953	MET
1	B	1957	LEU
1	B	1960	ARG
1	B	2192	MET
1	B	2279	MET
1	B	2347	MET
1	B	2384	MET
1	B	2456	MET
1	B	2482	ASP
1	B	2493	LEU
1	B	2530	ARG
1	B	2580	LEU
1	B	2652	LEU
1	B	2689	MET
1	B	2695	MET
1	B	2730	ASP
1	B	2734	MET
1	B	2788	ARG
1	B	2793	ARG
1	B	2828	MET
1	B	2843	MET
1	B	2870	LEU
1	B	2880	LYS
1	B	2897	GLN
1	B	2960	ILE
1	B	2968	LEU
1	B	3051	GLU
1	B	3061	LEU
1	B	3105	LEU
1	B	3611	LEU
1	B	3739	MET
1	B	3999	MET
1	B	4046	ARG
1	B	4109	MET

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Mol	Chain	Res	Type
1	B	4208	GLU
1	B	4292	MET
1	B	4504	MET
1	B	4555	ILE
1	B	4718	SER
1	B	4791	LYS
1	B	4817	MET
1	C	81	MET
1	C	317	MET
1	C	349	MET
1	C	398	HIS
1	C	778	MET
1	C	889	ILE
1	C	985	PHE
1	C	1181	ILE
1	C	1249	MET
1	C	1293	GLN
1	C	1300	MET
1	C	1748	LEU
1	C	1948	MET
1	C	1953	MET
1	C	1957	LEU
1	C	1960	ARG
1	C	2192	MET
1	C	2279	MET
1	C	2347	MET
1	C	2384	MET
1	C	2456	MET
1	C	2482	ASP
1	C	2493	LEU
1	C	2530	ARG
1	C	2580	LEU
1	C	2652	LEU
1	C	2689	MET
1	C	2695	MET
1	C	2730	ASP
1	C	2734	MET
1	C	2788	ARG
1	C	2793	ARG
1	C	2828	MET
1	C	2843	MET
1	C	2870	LEU

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Mol	Chain	Res	Type
1	C	2880	LYS
1	C	2897	GLN
1	C	2960	ILE
1	C	2968	LEU
1	C	3051	GLU
1	C	3061	LEU
1	C	3105	LEU
1	C	3611	LEU
1	C	3739	MET
1	C	3999	MET
1	C	4046	ARG
1	C	4109	MET
1	C	4208	GLU
1	C	4292	MET
1	C	4504	MET
1	C	4555	ILE
1	C	4718	SER
1	C	4791	LYS
1	C	4817	MET
1	D	81	MET
1	D	317	MET
1	D	349	MET
1	D	398	HIS
1	D	778	MET
1	D	889	ILE
1	D	985	PHE
1	D	1181	ILE
1	D	1249	MET
1	D	1293	GLN
1	D	1300	MET
1	D	1748	LEU
1	D	1948	MET
1	D	1953	MET
1	D	1957	LEU
1	D	1960	ARG
1	D	2192	MET
1	D	2279	MET
1	D	2347	MET
1	D	2384	MET
1	D	2456	MET
1	D	2482	ASP
1	D	2493	LEU

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Mol	Chain	Res	Type
1	D	2530	ARG
1	D	2580	LEU
1	D	2652	LEU
1	D	2689	MET
1	D	2695	MET
1	D	2730	ASP
1	D	2734	MET
1	D	2788	ARG
1	D	2793	ARG
1	D	2828	MET
1	D	2843	MET
1	D	2870	LEU
1	D	2880	LYS
1	D	2897	GLN
1	D	2960	ILE
1	D	2968	LEU
1	D	3051	GLU
1	D	3061	LEU
1	D	3105	LEU
1	D	3611	LEU
1	D	3739	MET
1	D	3999	MET
1	D	4046	ARG
1	D	4109	MET
1	D	4208	GLU
1	D	4292	MET
1	D	4504	MET
1	D	4555	ILE
1	D	4718	SER
1	D	4791	LYS
1	D	4817	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (230) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	270	HIS
1	A	288	HIS
1	A	476	GLN
1	A	692	HIS
1	A	746	GLN
1	A	781	ASN

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Mol	Chain	Res	Type
1	A	836	HIS
1	A	890	HIS
1	A	932	ASN
1	A	992	GLN
1	A	1004	HIS
1	A	1046	ASN
1	A	1063	ASN
1	A	1126	GLN
1	A	1265	HIS
1	A	1551	ASN
1	A	1577	ASN
1	A	1602	GLN
1	A	1626	GLN
1	A	1631	HIS
1	A	1656	HIS
1	A	1670	HIS
1	A	1835	HIS
1	A	1920	HIS
1	A	1970	GLN
1	A	2118	ASN
1	A	2177	ASN
1	A	2224	ASN
1	A	2250	ASN
1	A	2579	GLN
1	A	2702	ASN
1	A	2704	GLN
1	A	2722	ASN
1	A	2868	HIS
1	A	2977	ASN
1	A	3038	GLN
1	A	3614	HIS
1	A	3770	ASN
1	A	3775	GLN
1	A	3844	GLN
1	A	3850	HIS
1	A	3856	ASN
1	A	3869	ASN
1	A	3915	GLN
1	A	3931	ASN
1	A	3933	GLN
1	A	3937	HIS
1	A	3975	GLN

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Mol	Chain	Res	Type
1	A	4009	ASN
1	A	4049	HIS
1	A	4075	ASN
1	A	4296	HIS
1	A	4620	GLN
1	A	4706	GLN
1	A	4735	ASN
1	A	4742	HIS
1	A	4762	HIS
1	A	4927	ASN
1	B	23	GLN
1	B	163	HIS
1	B	270	HIS
1	B	288	HIS
1	B	476	GLN
1	B	692	HIS
1	B	746	GLN
1	B	781	ASN
1	B	836	HIS
1	B	932	ASN
1	B	992	GLN
1	B	1004	HIS
1	B	1046	ASN
1	B	1126	GLN
1	B	1551	ASN
1	B	1577	ASN
1	B	1602	GLN
1	B	1626	GLN
1	B	1631	HIS
1	B	1656	HIS
1	B	1670	HIS
1	B	1762	GLN
1	B	1835	HIS
1	B	1920	HIS
1	B	1970	GLN
1	B	2118	ASN
1	B	2224	ASN
1	B	2579	GLN
1	B	2702	ASN
1	B	2704	GLN
1	B	2830	ASN
1	B	2868	HIS

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Mol	Chain	Res	Type
1	B	2927	GLN
1	B	2977	ASN
1	B	3038	GLN
1	B	3614	HIS
1	B	3770	ASN
1	B	3775	GLN
1	B	3844	GLN
1	B	3850	HIS
1	B	3856	ASN
1	B	3869	ASN
1	B	3915	GLN
1	B	3931	ASN
1	B	3933	GLN
1	B	3937	HIS
1	B	3975	GLN
1	B	4049	HIS
1	B	4075	ASN
1	B	4514	ASN
1	B	4620	GLN
1	B	4706	GLN
1	B	4735	ASN
1	B	4967	ASN
1	C	23	GLN
1	C	270	HIS
1	C	288	HIS
1	C	476	GLN
1	C	607	ASN
1	C	692	HIS
1	C	746	GLN
1	C	781	ASN
1	C	836	HIS
1	C	932	ASN
1	C	992	GLN
1	C	1004	HIS
1	C	1046	ASN
1	C	1063	ASN
1	C	1126	GLN
1	C	1551	ASN
1	C	1577	ASN
1	C	1602	GLN
1	C	1626	GLN
1	C	1631	HIS

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Mol	Chain	Res	Type
1	C	1656	HIS
1	C	1670	HIS
1	C	1920	HIS
1	C	1970	GLN
1	C	2118	ASN
1	C	2177	ASN
1	C	2224	ASN
1	C	2579	GLN
1	C	2702	ASN
1	C	2704	GLN
1	C	2722	ASN
1	C	2868	HIS
1	C	3038	GLN
1	C	3614	HIS
1	C	3770	ASN
1	C	3775	GLN
1	C	3844	GLN
1	C	3850	HIS
1	C	3856	ASN
1	C	3869	ASN
1	C	3915	GLN
1	C	3931	ASN
1	C	3933	GLN
1	C	3937	HIS
1	C	3975	GLN
1	C	4009	ASN
1	C	4049	HIS
1	C	4075	ASN
1	C	4108	HIS
1	C	4296	HIS
1	C	4514	ASN
1	C	4620	GLN
1	C	4706	GLN
1	C	4735	ASN
1	C	4742	HIS
1	C	4967	ASN
1	D	23	GLN
1	D	270	HIS
1	D	288	HIS
1	D	476	GLN
1	D	692	HIS
1	D	731	HIS

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Mol	Chain	Res	Type
1	D	746	GLN
1	D	781	ASN
1	D	836	HIS
1	D	890	HIS
1	D	932	ASN
1	D	956	HIS
1	D	992	GLN
1	D	1004	HIS
1	D	1021	GLN
1	D	1046	ASN
1	D	1063	ASN
1	D	1126	GLN
1	D	1244	ASN
1	D	1265	HIS
1	D	1551	ASN
1	D	1577	ASN
1	D	1602	GLN
1	D	1631	HIS
1	D	1656	HIS
1	D	1670	HIS
1	D	1762	GLN
1	D	1920	HIS
1	D	1970	GLN
1	D	2118	ASN
1	D	2158	HIS
1	D	2177	ASN
1	D	2224	ASN
1	D	2541	HIS
1	D	2579	GLN
1	D	2702	ASN
1	D	2704	GLN
1	D	2868	HIS
1	D	2977	ASN
1	D	3038	GLN
1	D	3614	HIS
1	D	3770	ASN
1	D	3775	GLN
1	D	3850	HIS
1	D	3856	ASN
1	D	3869	ASN
1	D	3931	ASN
1	D	3933	GLN

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Mol	Chain	Res	Type
1	D	3937	HIS
1	D	3975	GLN
1	D	4009	ASN
1	D	4049	HIS
1	D	4075	ASN
1	D	4296	HIS
1	D	4514	ASN
1	D	4620	GLN
1	D	4706	GLN
1	D	4735	ASN
1	D	4742	HIS
1	D	4762	HIS
1	D	4967	ASN

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, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	D	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	A	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	B	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	A	5004	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	D	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	C	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	C	5004	-	32,33,33	0.26	0	48,52,52	0.27	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
4	ATP	B	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5004	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	B	5004	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5004	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	C	5004	-	-	9/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O3G
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5004	ATP	C5'-O5'-PA-O2A
4	A	5004	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	PB-O3B-PG-O3G
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	B	5002	ATP	C4'-C5'-O5'-PA
4	B	5004	ATP	C5'-O5'-PA-O2A
4	B	5004	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	PB-O3B-PG-O3G
4	C	5002	ATP	C5'-O5'-PA-O1A
4	C	5002	ATP	C5'-O5'-PA-O2A
4	C	5002	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	C4'-C5'-O5'-PA
4	C	5004	ATP	C5'-O5'-PA-O2A
4	C	5004	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	PB-O3B-PG-O3G
4	D	5002	ATP	C5'-O5'-PA-O1A
4	D	5002	ATP	C5'-O5'-PA-O2A
4	D	5002	ATP	C5'-O5'-PA-O3A
4	D	5004	ATP	C5'-O5'-PA-O2A
4	D	5004	ATP	C5'-O5'-PA-O3A
4	A	5002	ATP	C4'-C5'-O5'-PA
4	D	5002	ATP	C4'-C5'-O5'-PA
4	A	5004	ATP	O4'-C4'-C5'-O5'
4	B	5004	ATP	O4'-C4'-C5'-O5'
4	C	5004	ATP	O4'-C4'-C5'-O5'
4	D	5004	ATP	O4'-C4'-C5'-O5'
4	A	5004	ATP	PB-O3A-PA-O5'
4	B	5004	ATP	PB-O3A-PA-O5'
4	C	5004	ATP	PB-O3A-PA-O5'
4	D	5004	ATP	PB-O3A-PA-O5'
4	A	5002	ATP	PA-O3A-PB-O3B
4	B	5002	ATP	PA-O3A-PB-O3B
4	C	5002	ATP	PA-O3A-PB-O3B
4	D	5002	ATP	PA-O3A-PB-O3B
4	A	5004	ATP	PG-O3B-PB-O2B
4	B	5004	ATP	PG-O3B-PB-O2B
4	C	5004	ATP	PG-O3B-PB-O2B
4	D	5004	ATP	PG-O3B-PB-O2B
4	A	5004	ATP	C5'-O5'-PA-O1A
4	B	5004	ATP	C5'-O5'-PA-O1A
4	C	5004	ATP	C5'-O5'-PA-O1A
4	D	5004	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	PB-O3B-PG-O1G
4	B	5002	ATP	PB-O3B-PG-O1G
4	C	5002	ATP	PB-O3B-PG-O1G
4	D	5002	ATP	PB-O3B-PG-O1G

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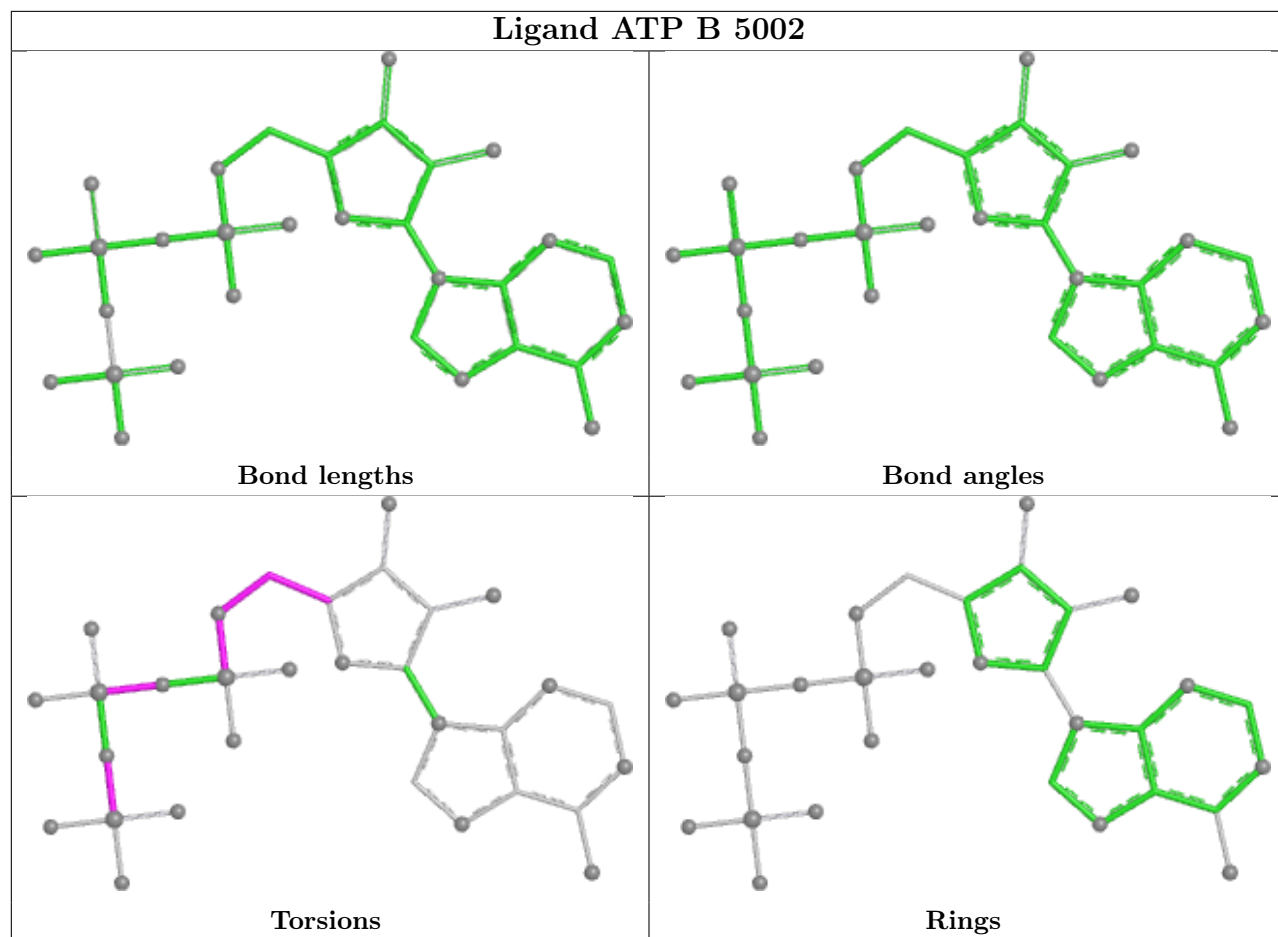
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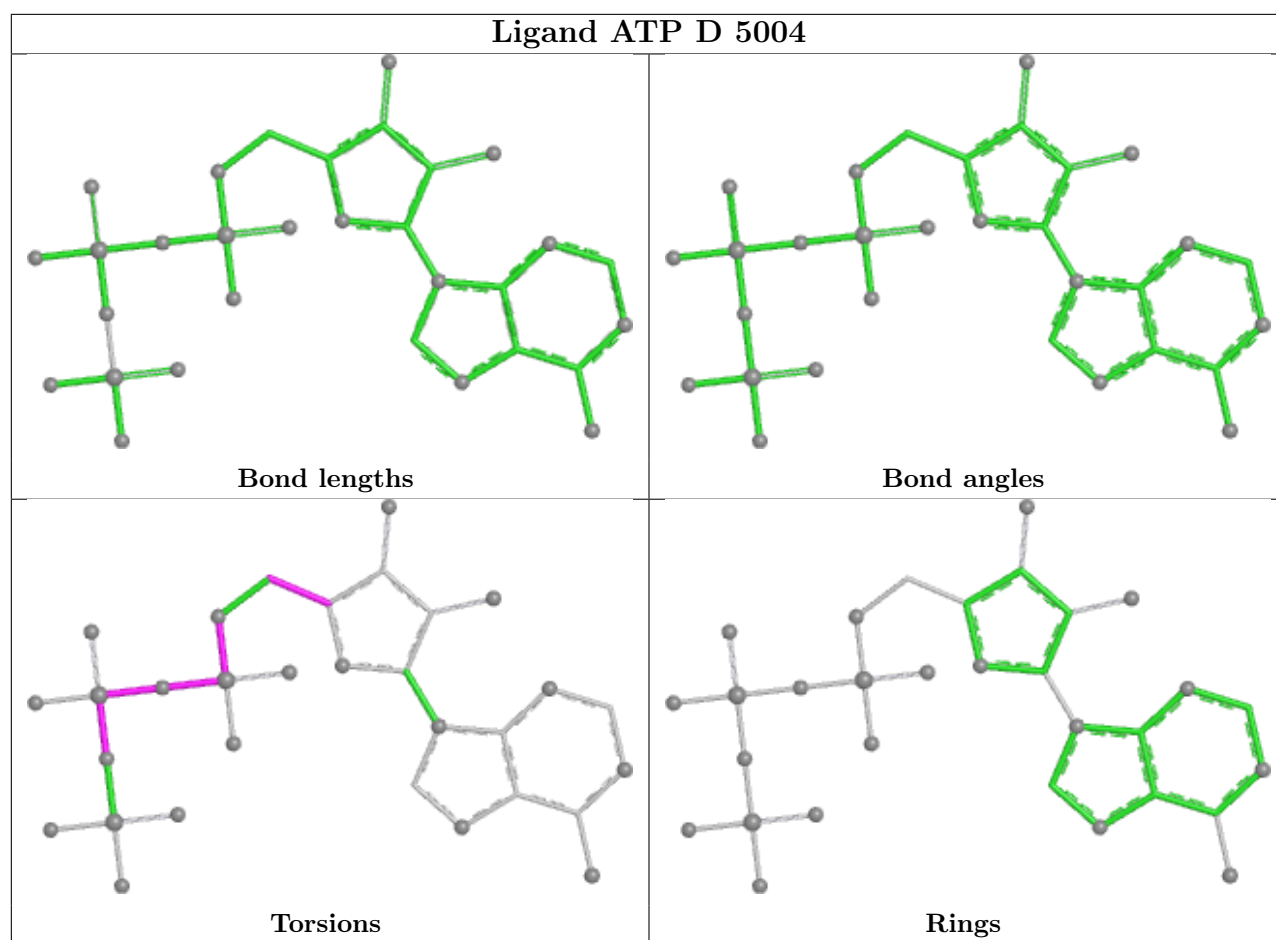
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PA-O3A-PB-O1B
4	A	5004	ATP	PG-O3B-PB-O1B
4	A	5004	ATP	PB-O3A-PA-O1A
4	B	5002	ATP	PA-O3A-PB-O1B
4	B	5004	ATP	PG-O3B-PB-O1B
4	B	5004	ATP	PB-O3A-PA-O1A
4	C	5002	ATP	PA-O3A-PB-O1B
4	C	5004	ATP	PG-O3B-PB-O1B
4	C	5004	ATP	PB-O3A-PA-O1A
4	D	5002	ATP	PA-O3A-PB-O1B
4	D	5004	ATP	PG-O3B-PB-O1B
4	D	5004	ATP	PB-O3A-PA-O1A
4	A	5004	ATP	PA-O3A-PB-O2B
4	B	5004	ATP	PA-O3A-PB-O2B
4	C	5004	ATP	PA-O3A-PB-O2B
4	D	5004	ATP	PA-O3A-PB-O2B
4	A	5002	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	O4'-C4'-C5'-O5'
4	C	5002	ATP	O4'-C4'-C5'-O5'
4	D	5002	ATP	O4'-C4'-C5'-O5'

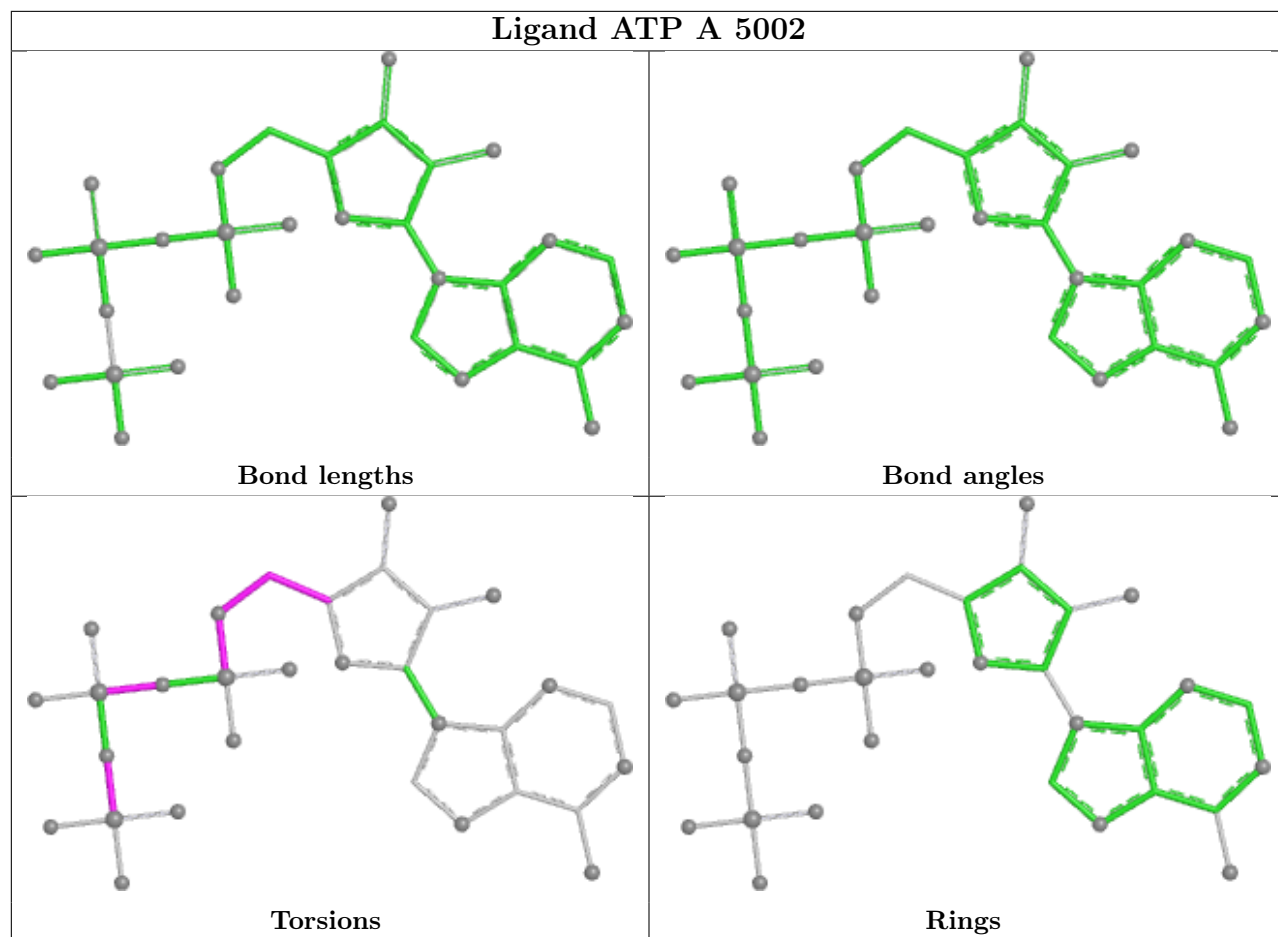
There are no ring outliers.

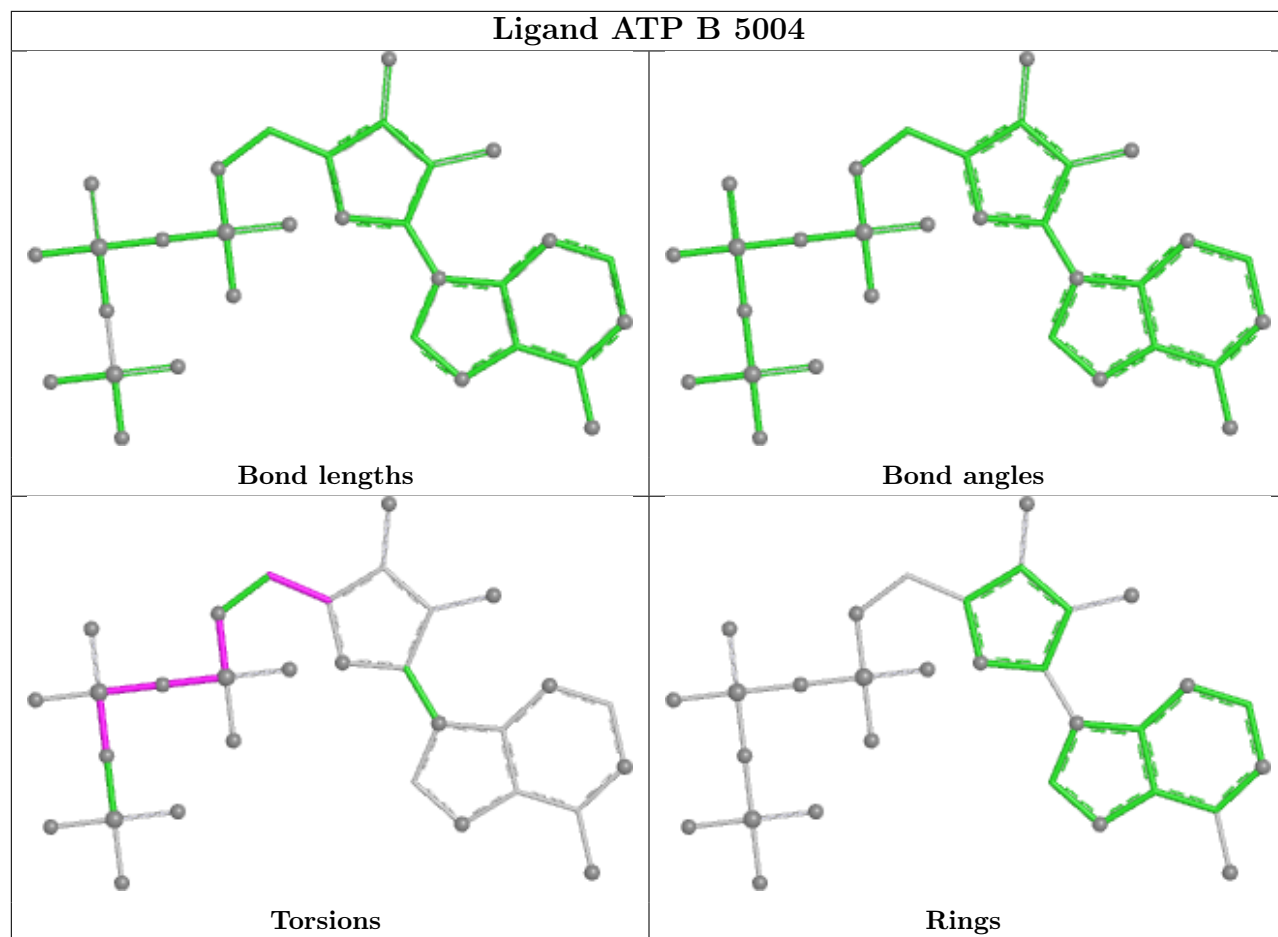
No monomer is involved in short contacts.

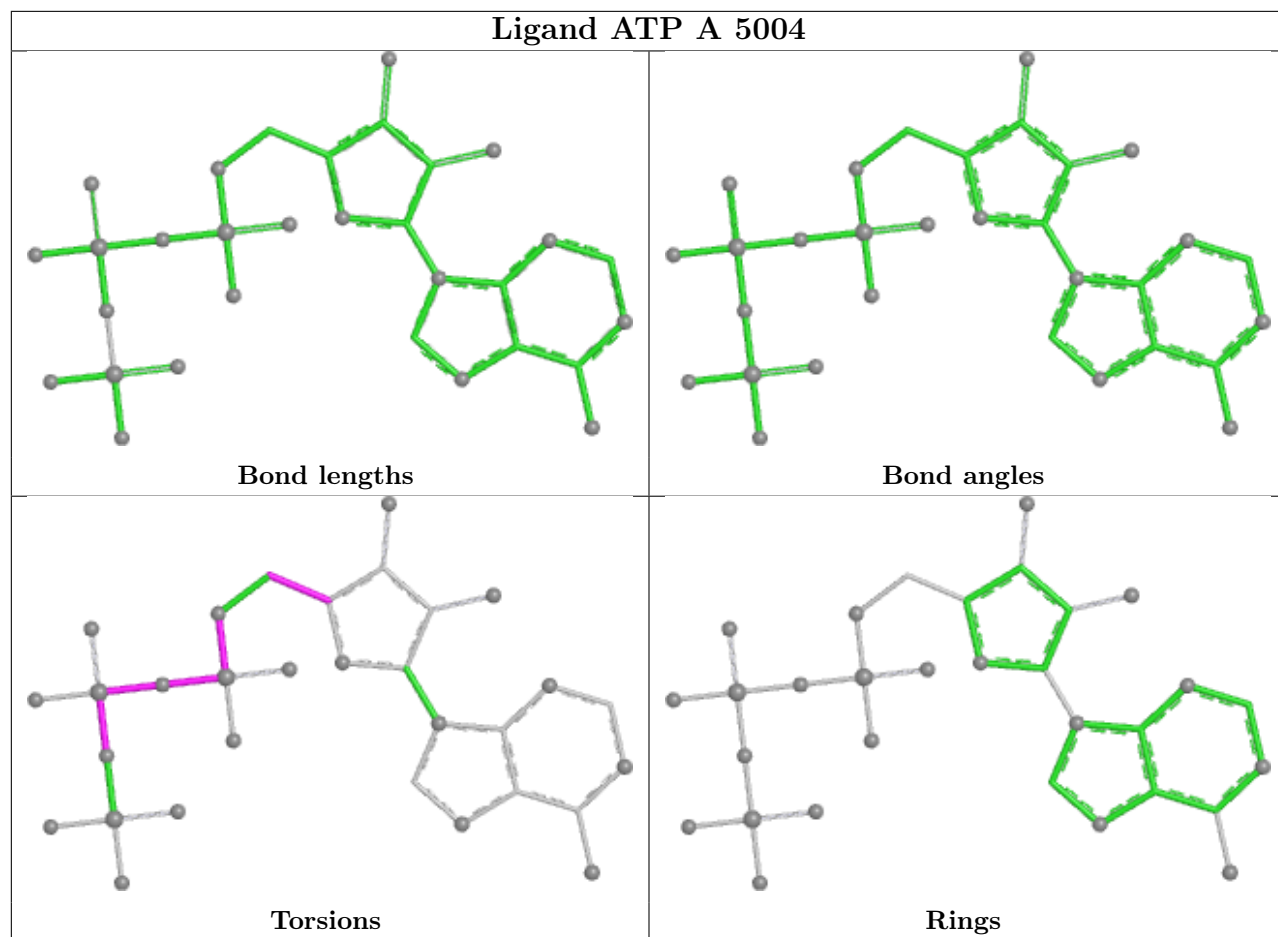
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

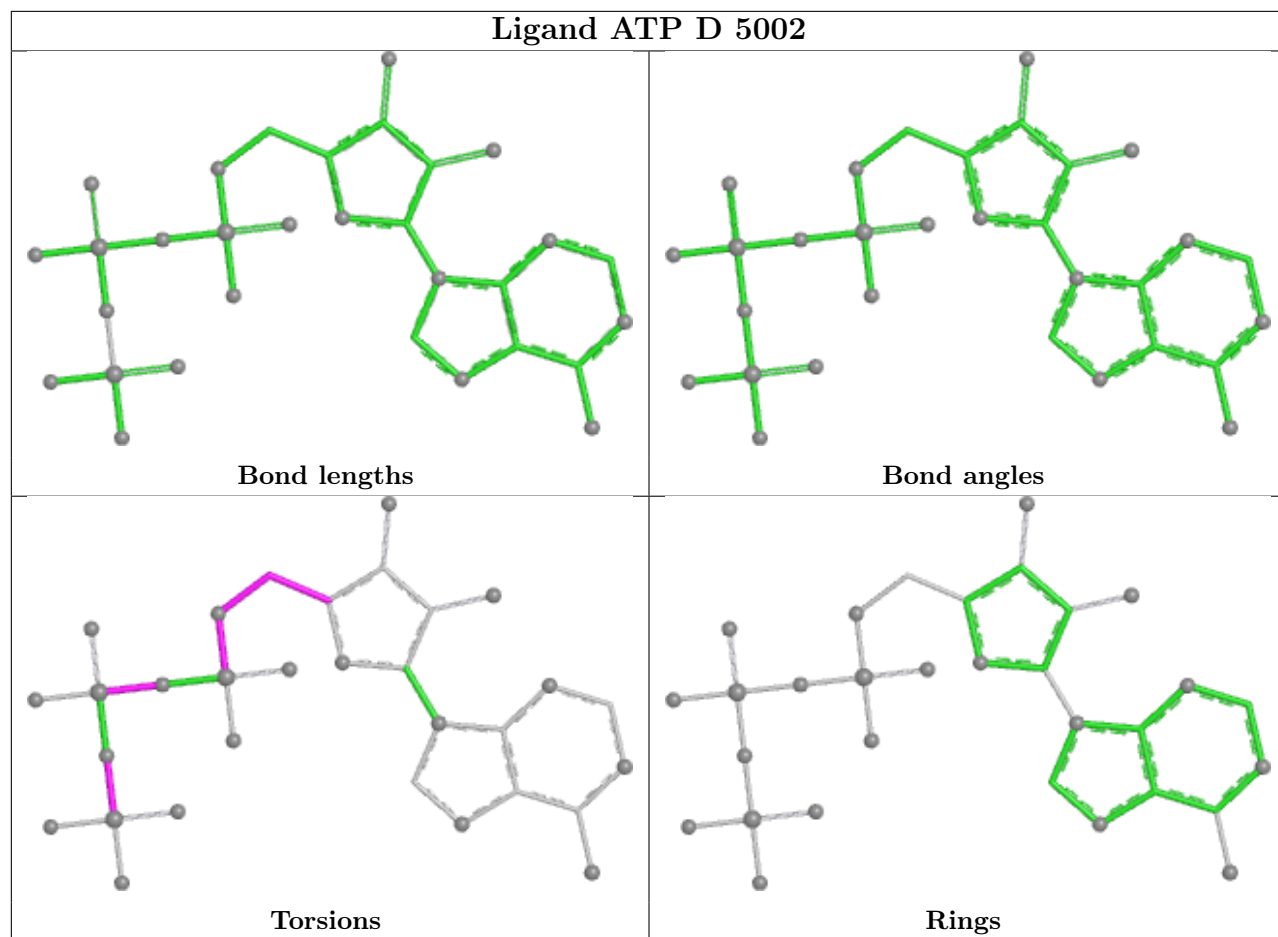


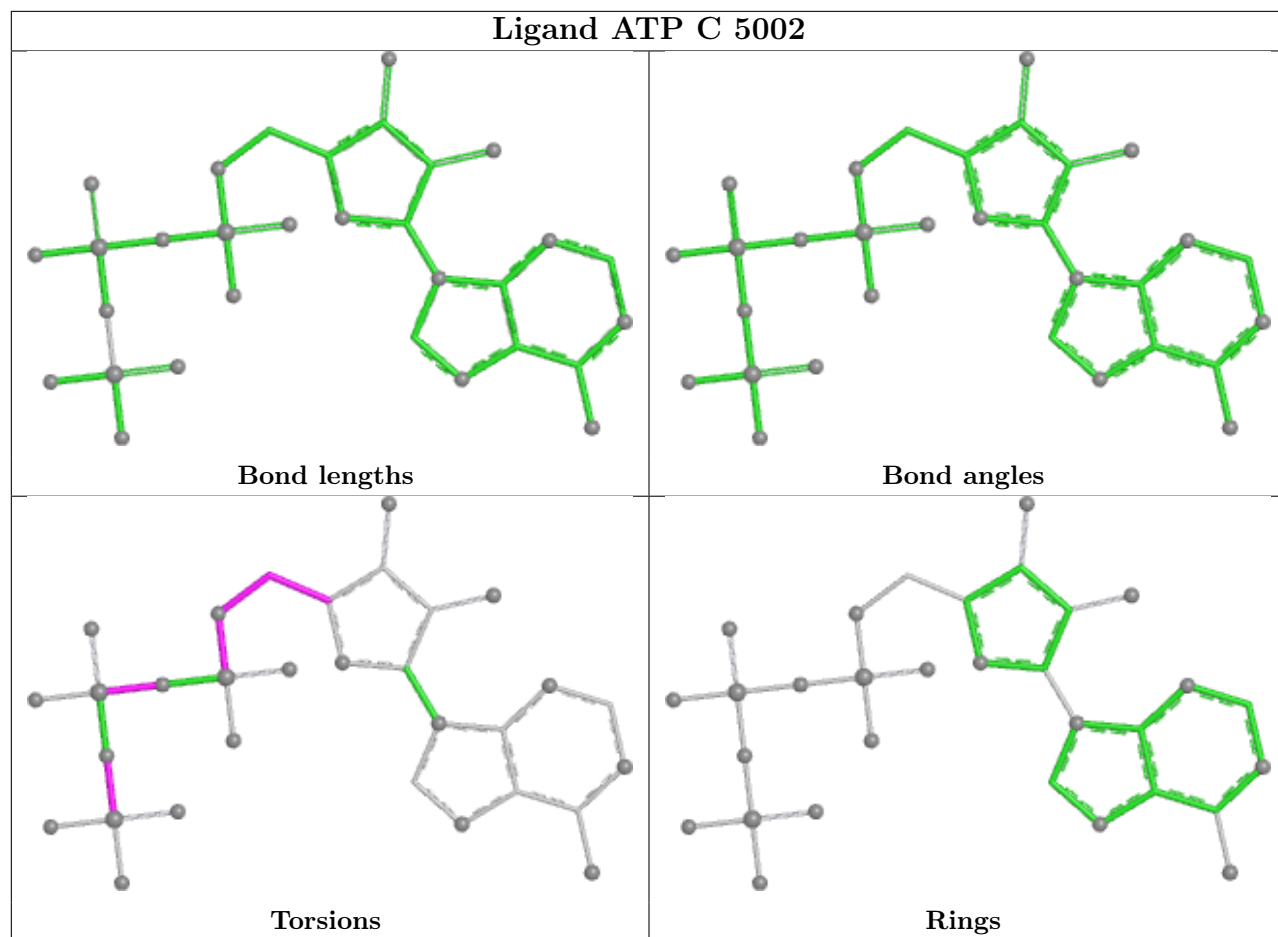


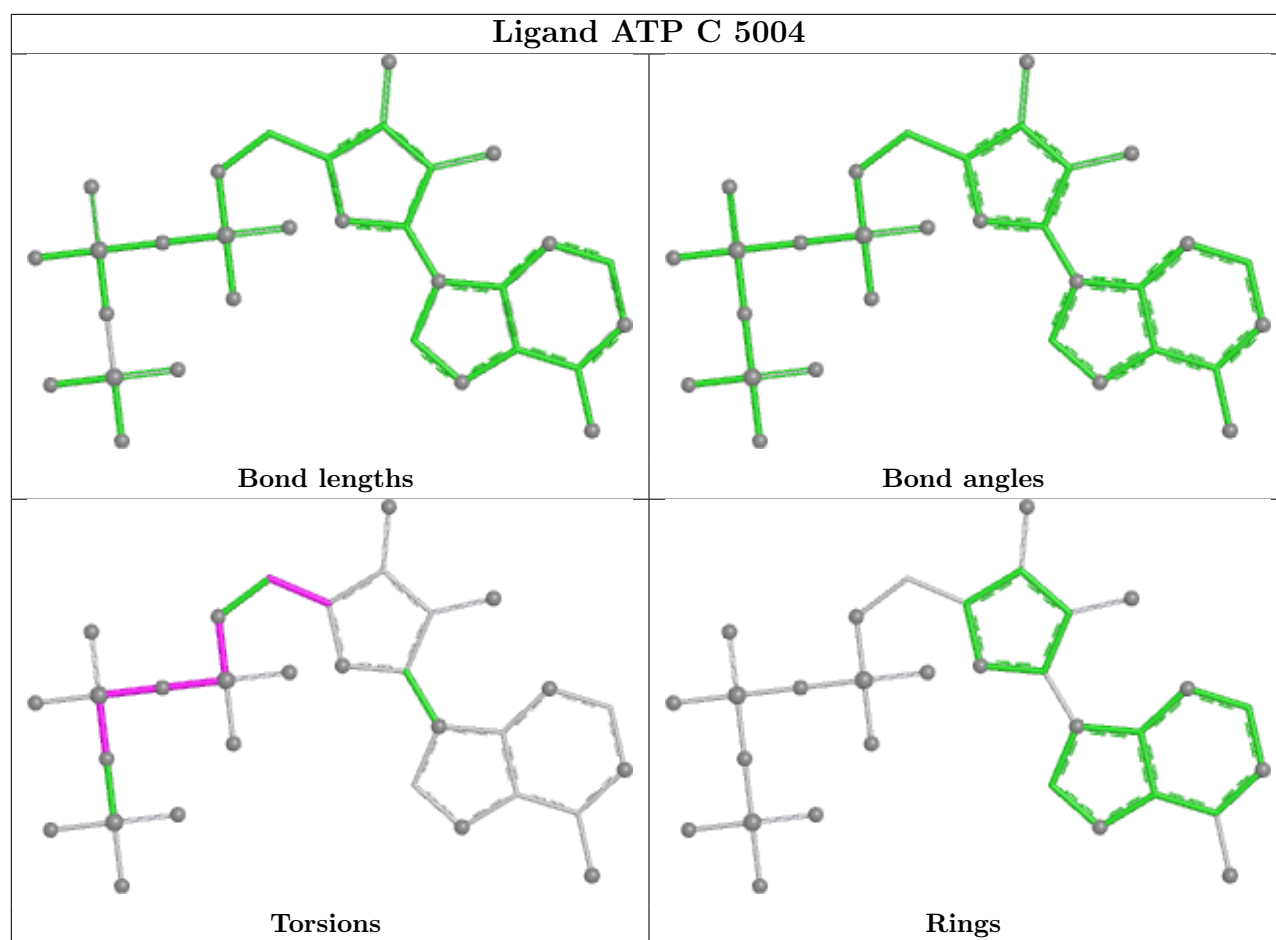












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42764. These allow visual inspection of the internal detail of the map and identification of artifacts.

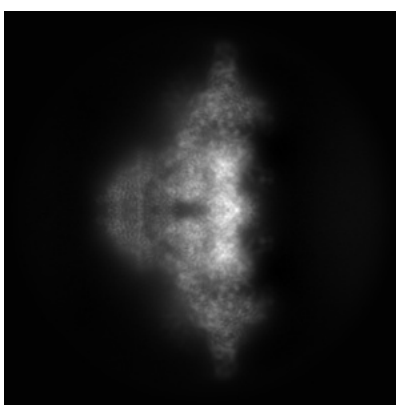
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

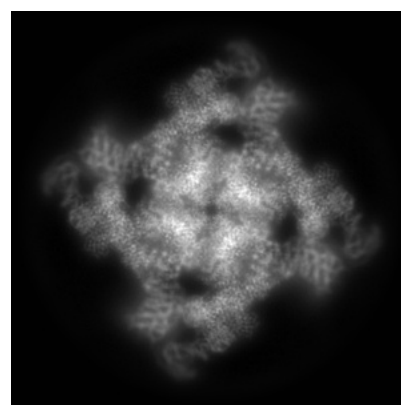
6.1.1 Primary map



X



Y

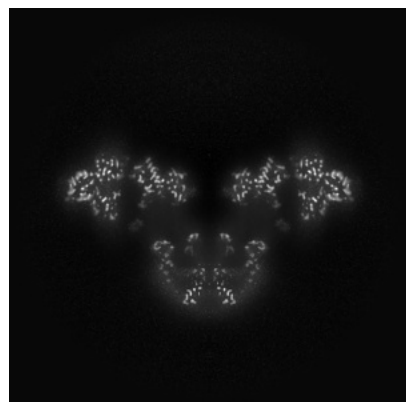


Z

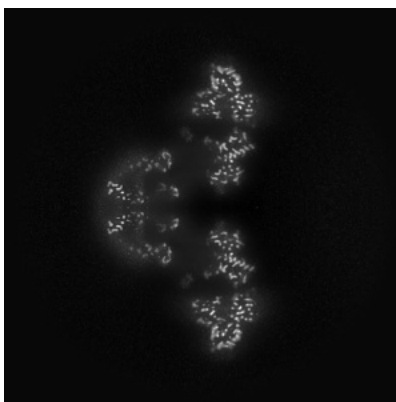
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

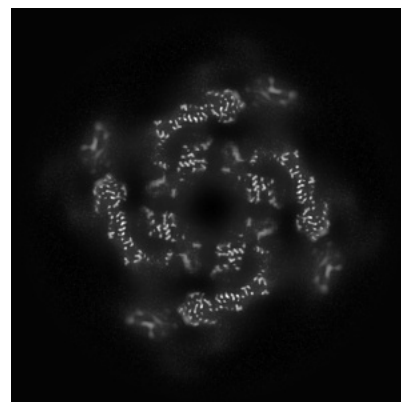
6.2.1 Primary map



X Index: 256



Y Index: 256

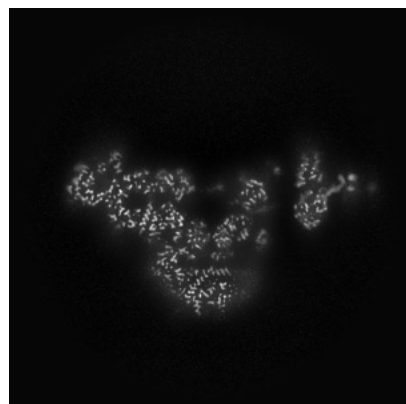


Z Index: 256

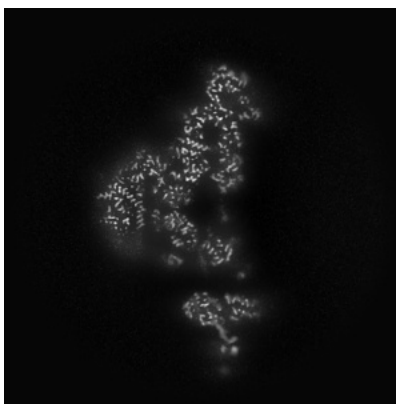
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

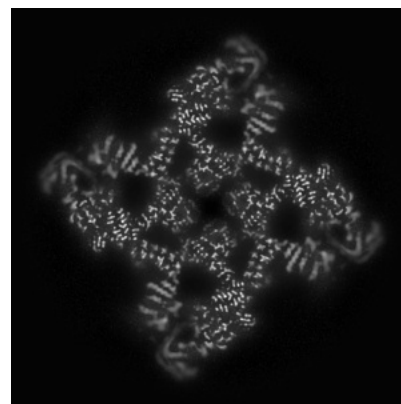
6.3.1 Primary map



X Index: 274



Y Index: 274



Z Index: 277

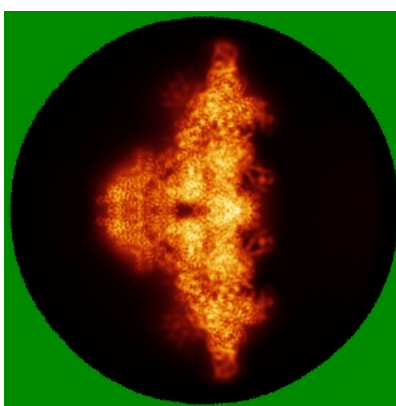
The images above show the largest variance slices of the map in three orthogonal directions.

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

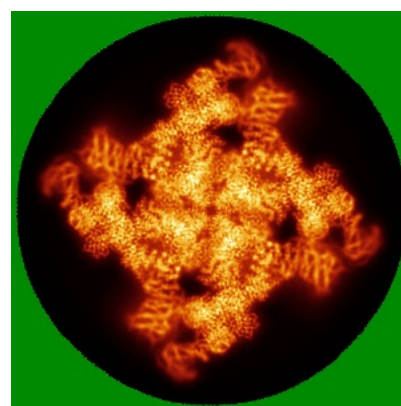
6.4.1 Primary map



X



Y

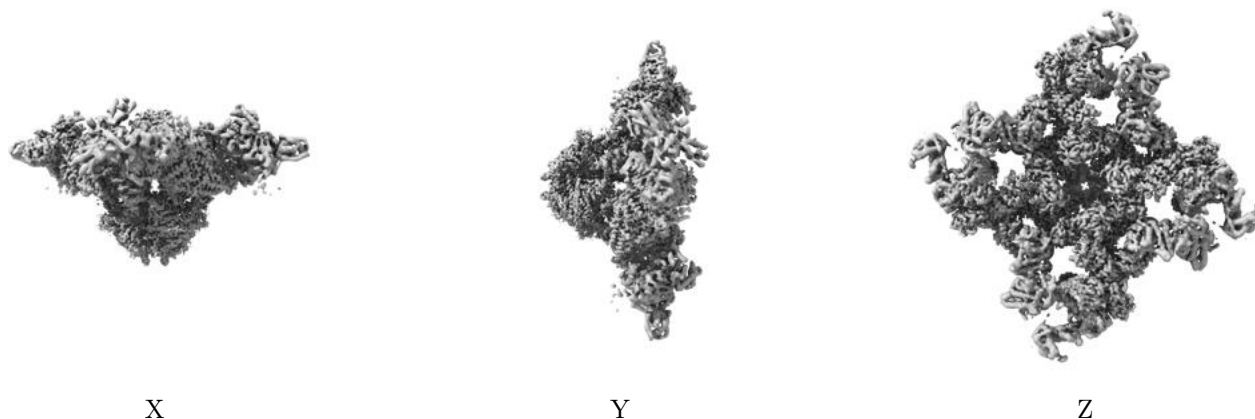


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

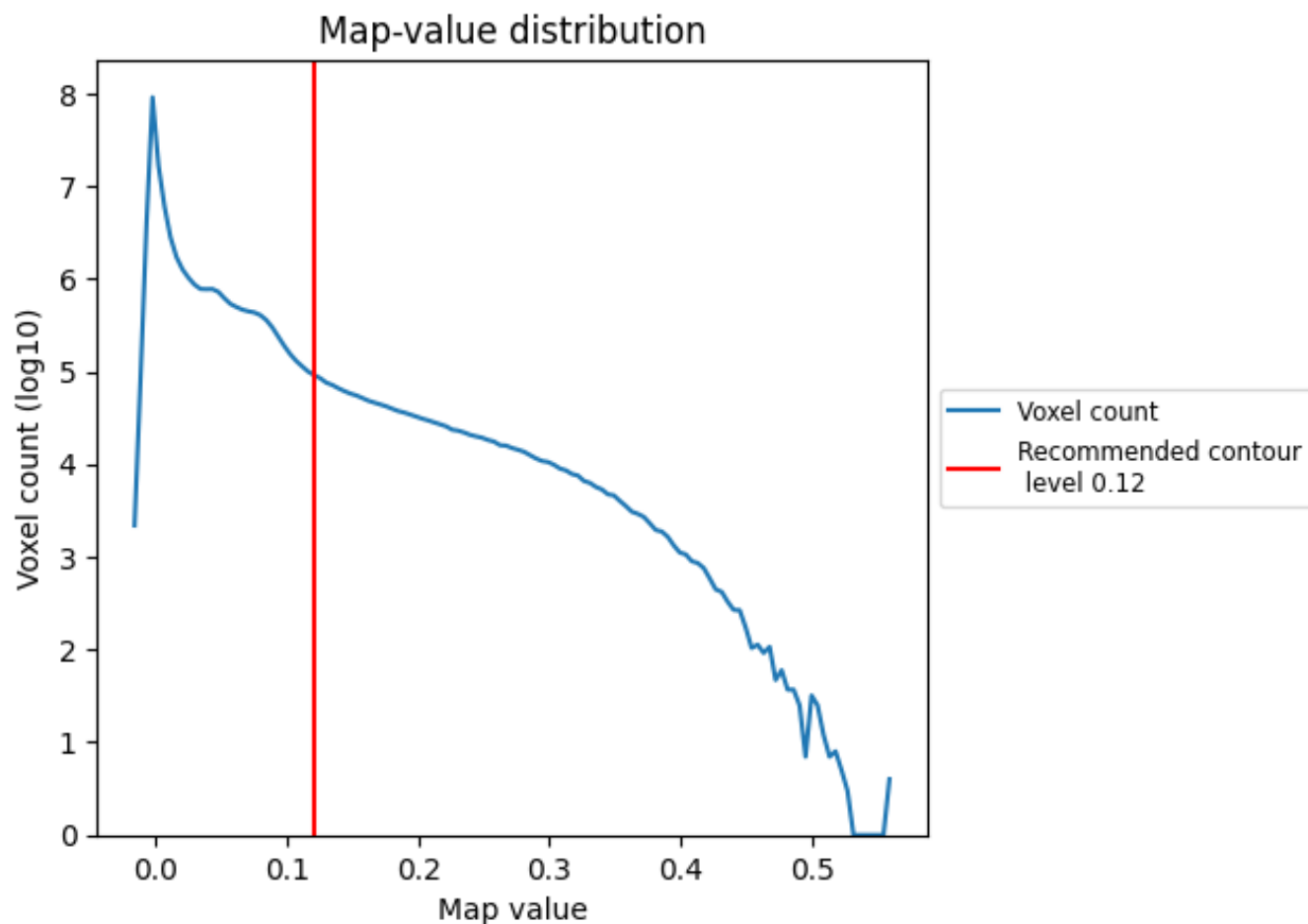
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

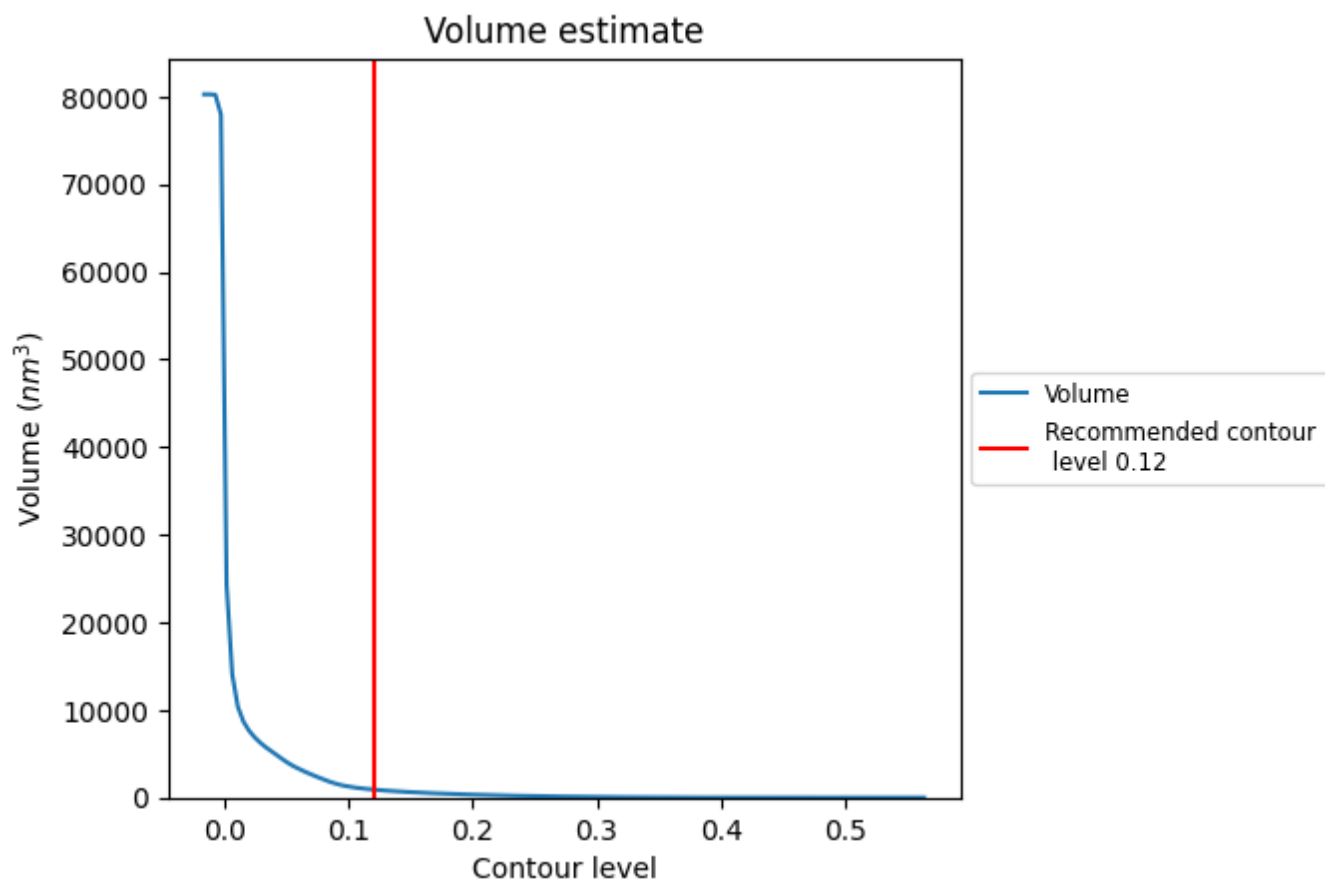
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

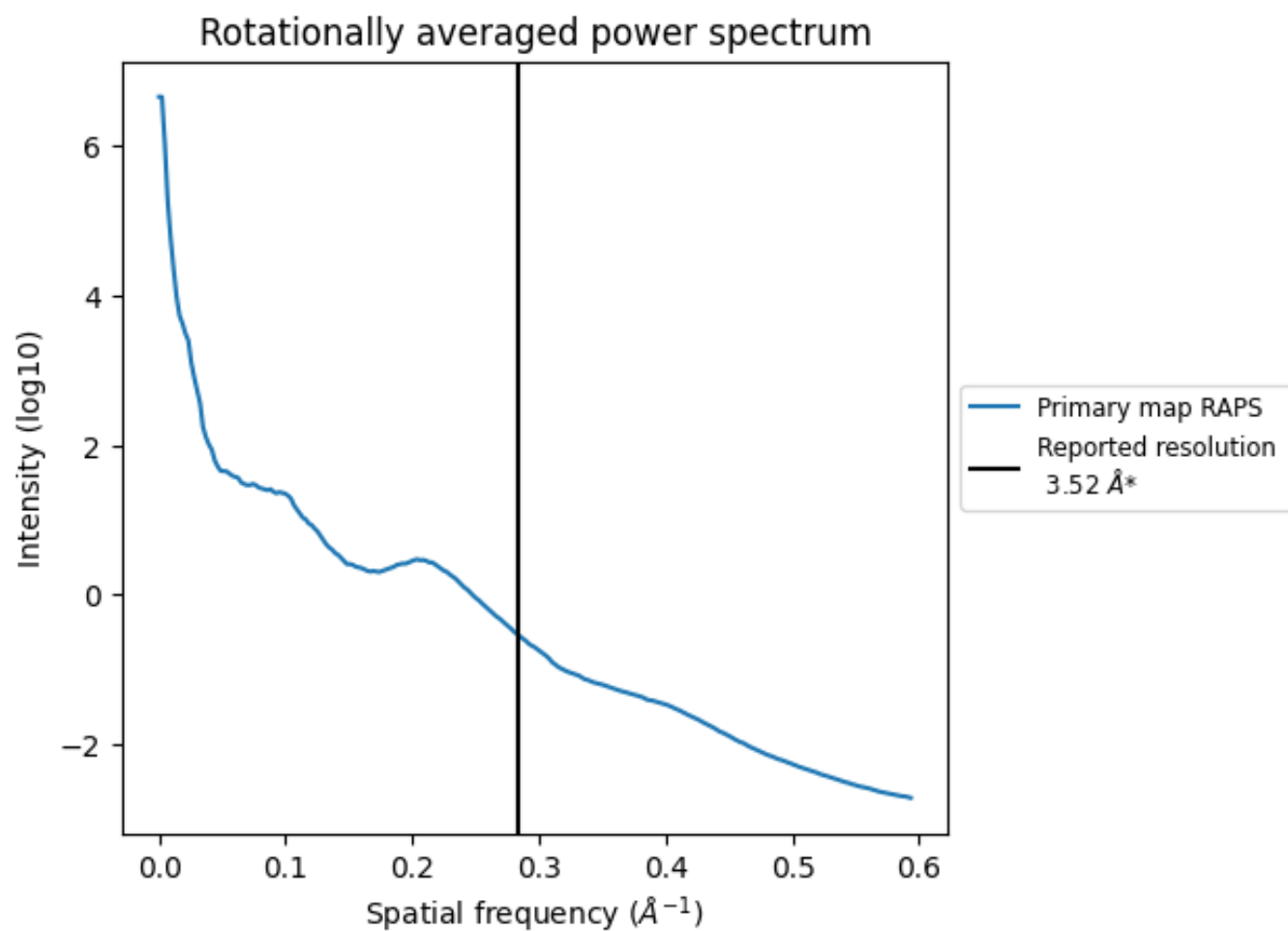
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 911 nm³; this corresponds to an approximate mass of 823 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 0.284 Å⁻¹

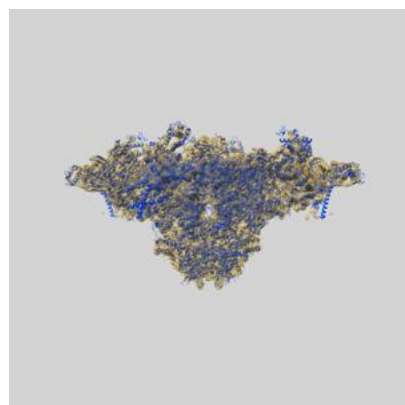
8 Fourier-Shell correlation

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

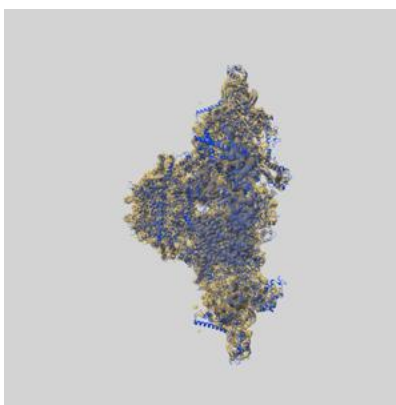
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42764 and PDB model 8UXH. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

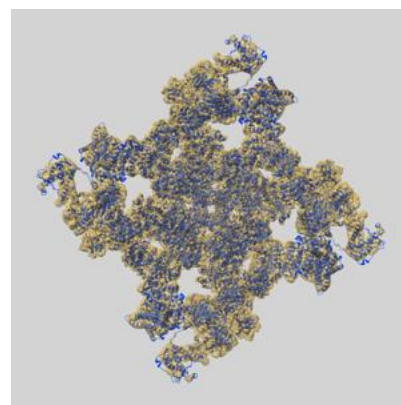
9.1 Map-model overlay [i](#)



X



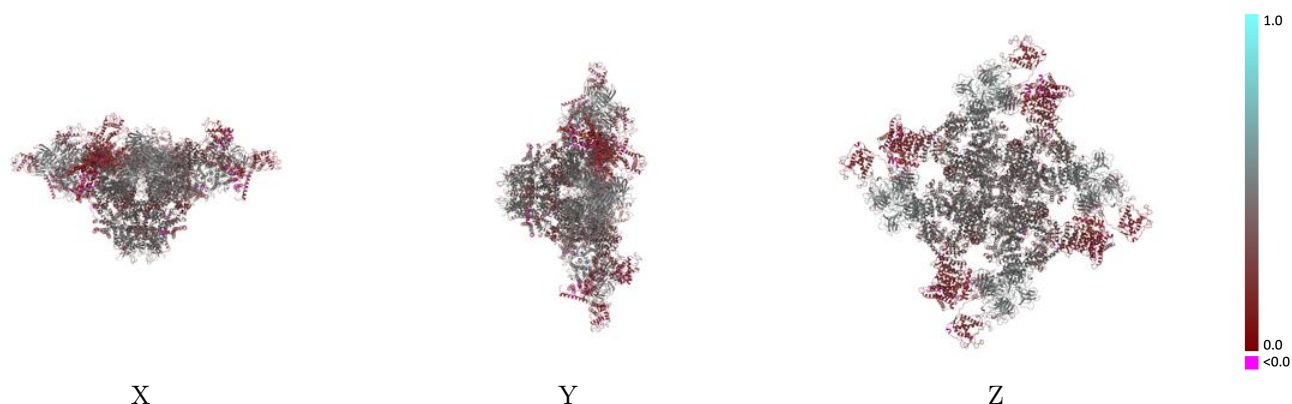
Y



Z

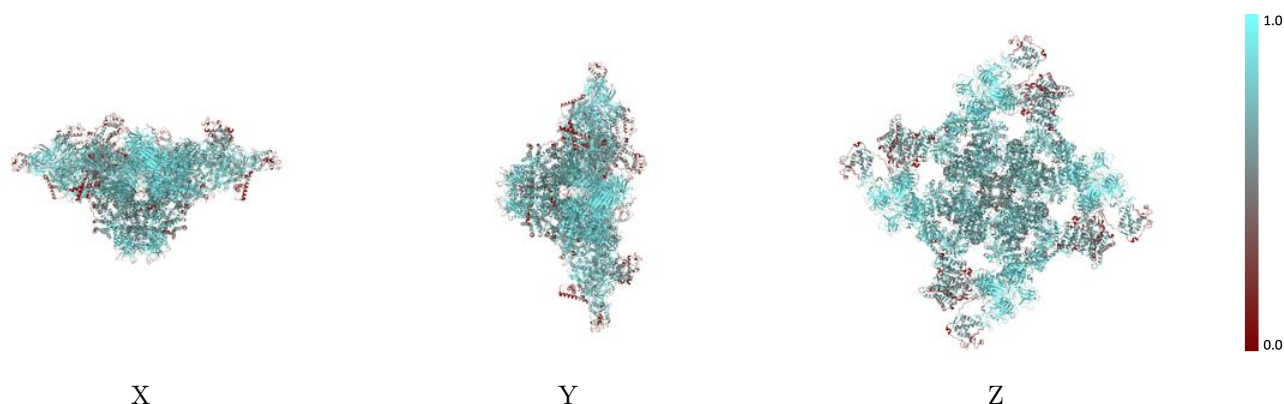
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



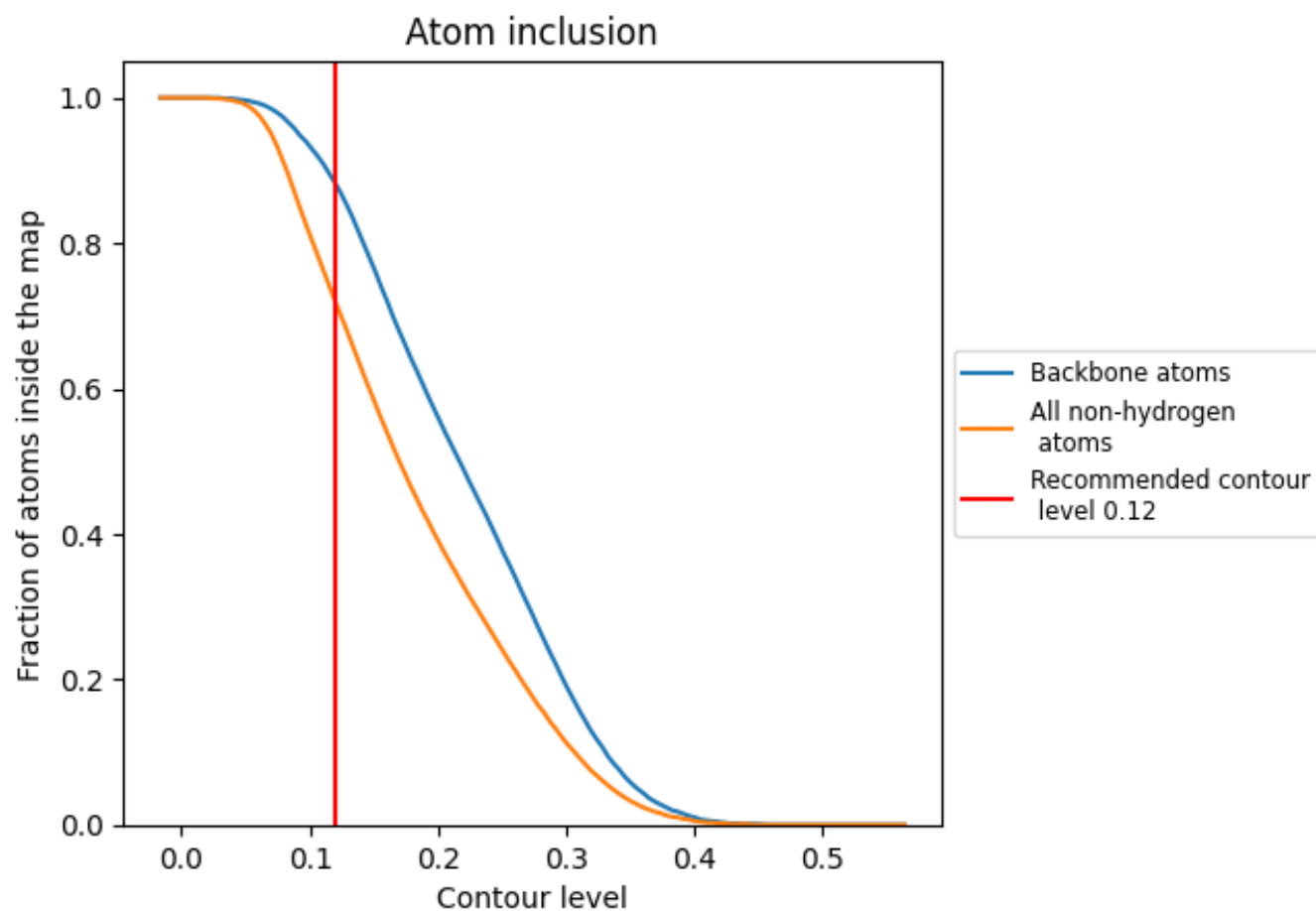
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 72% 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	0.7190	0.3660
A	0.7170	0.3650
B	0.7160	0.3640
C	0.7180	0.3660
D	0.7120	0.3560
E	0.8560	0.5050
F	0.8510	0.5030
G	0.8590	0.5060
H	0.8570	0.5040

1.0

0.0

<0.0