



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 01:53 AM UTC

PDB ID : 9E18 / pdb_00009e18
EMDB ID : EMD-47385
Title : Structure of RyR1 in the primed state in the presence of pentoxifylline
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 2.68 Å(reported)
Based on initial model : 7TZC

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:

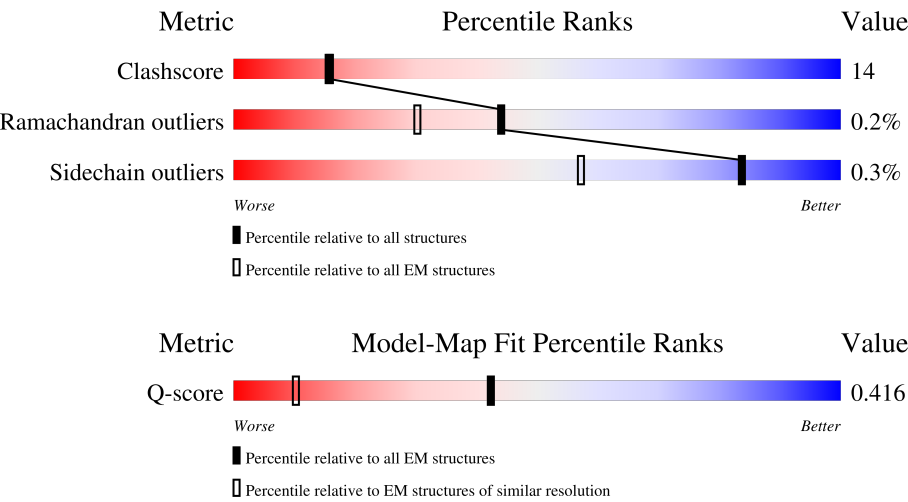
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	5037	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	108	5% 72% 20%
2	F	108	6% 72% 20%
2	G	108	5% 71% 21%
2	H	108	71% 21%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144144 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.

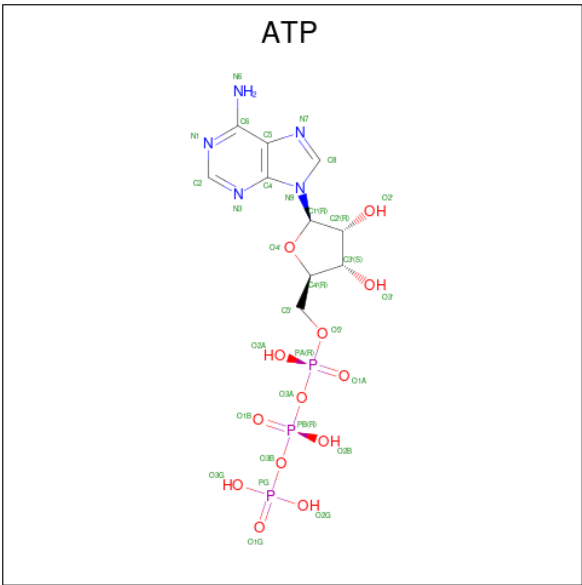
- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	G	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

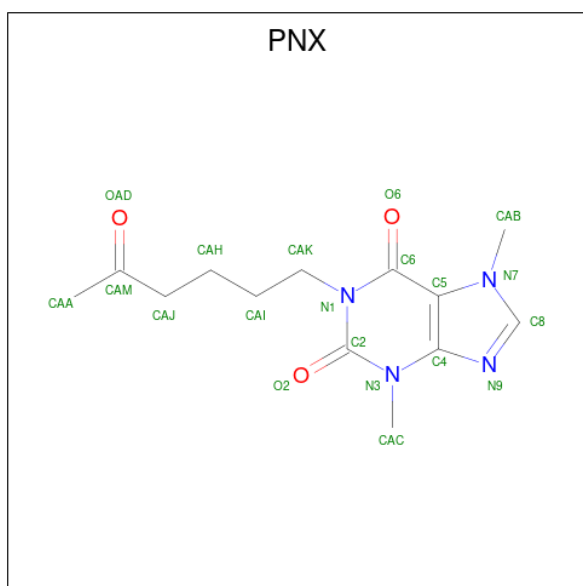
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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

- Molecule 6 is 3,7-DIMETHYL-1-(5-OXOHEXYL)-3,7-DIHYDRO-1H-PURINE-2,6-DIONE (CCD ID: PNK) (formula: C₁₃H₁₈N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			20	13	4	3	
6	B	1	Total	C	N	O	0
			20	13	4	3	
6	D	1	Total	C	N	O	0
			20	13	4	3	
6	C	1	Total	C	N	O	0
			20	13	4	3	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	O	0
			2	2	
7	B	2	Total	O	0
			2	2	

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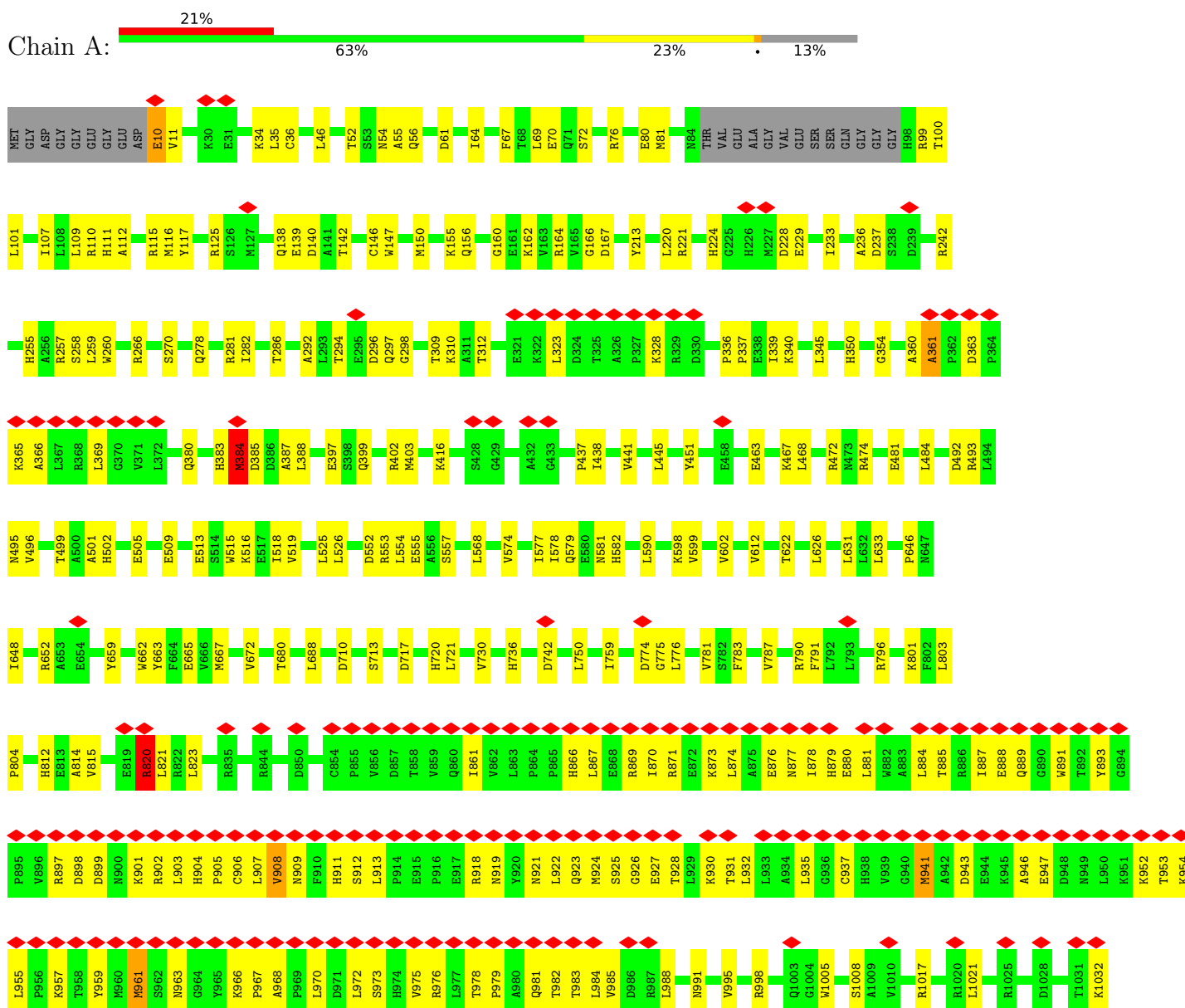
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Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	O	0
			2	2	
7	C	2	Total	O	0
			2	2	

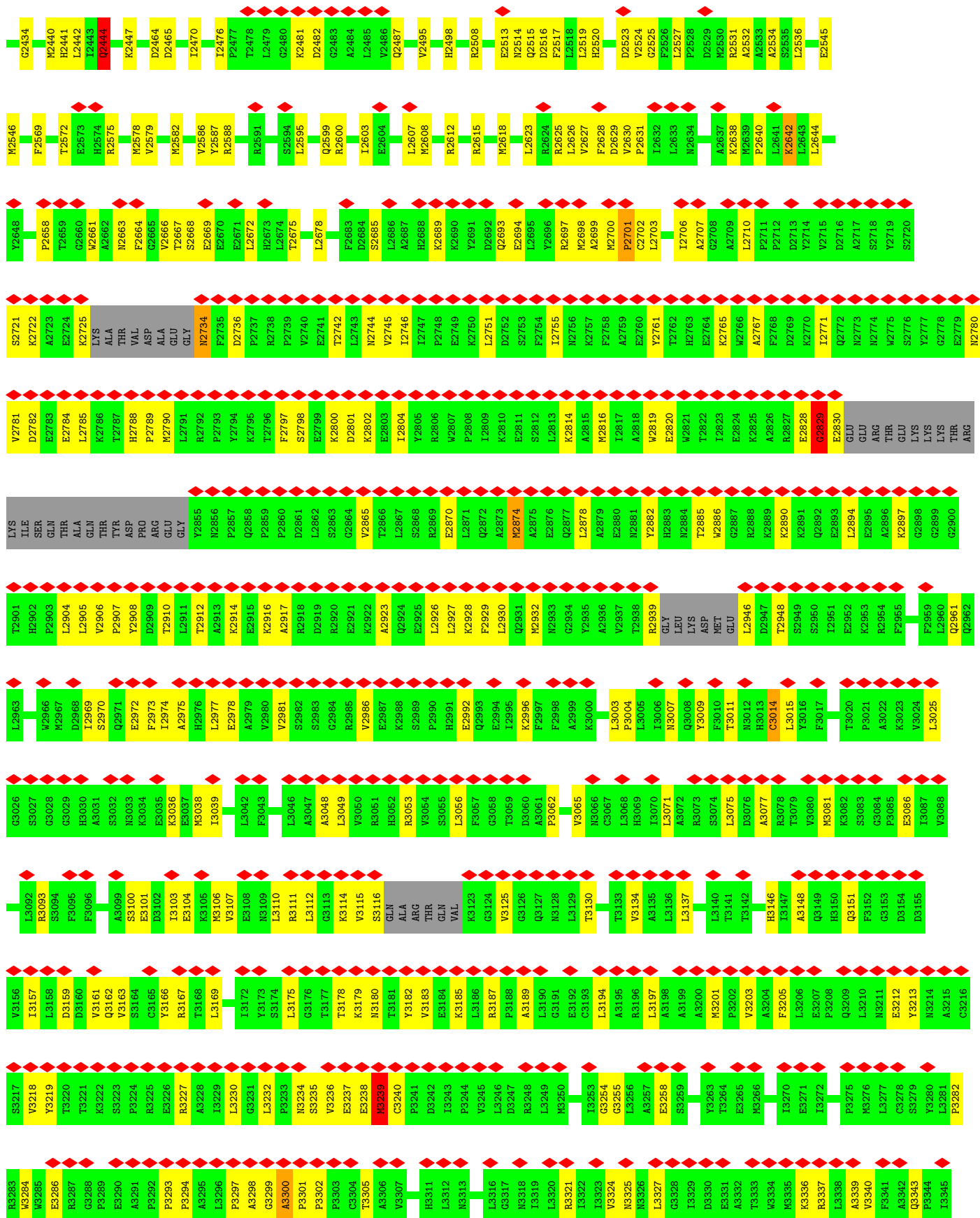
3 Residue-property plots

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.

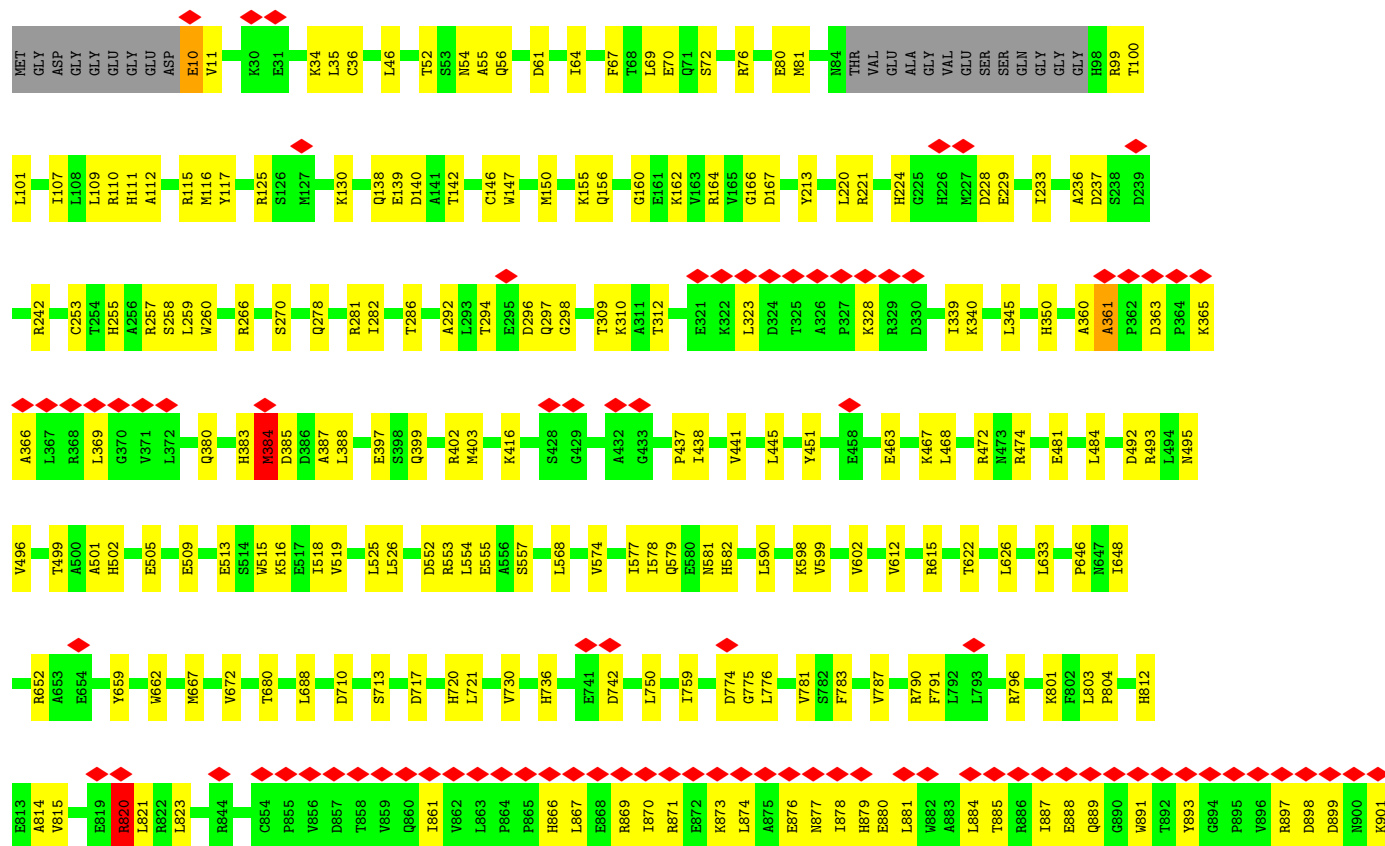
• Molecule 1: Ryanodine receptor 1



Q2308	G2217	M2101	D2017	L1926	G1855	R1727	D1513	ASP	LYS	M1286	H1127	M1035
M2312	G2218	Q2107	E2018	L1927	D1858	R1728	L1514	VAL	GLU	R1128	R1127	M1036
L2313	E2219	Q2107	E2019	Q1928	V1859	M1729	V1515	VAL	THR	W1132	W1132	D1037
Y2318	T2220	V2117	D2020	M1929	I1866	L1731	A1531	ALA	PRO	P1142	P1142	S1038
P2319	K2221	M2120	C2021	L1931	E1873	S1732	E1535	D1419	GLY	W1143	W1143	L1039
D2320	E2222	F2121	R2028	V1935	E1874	E1733	S1536	M1420	THR	D1147	D1147	C1040
E2329	R2223	S2122	A2040	M1939	GLU	T1742	M1537	R1421	GLN	M1152	M1152	Q1041
R2330	P2226	L2123	Q2045	L1943	GLU	R1743	V1552	D1422	PRO	Q1299	Q1299	A1042
D2333	K2227	L2135	L2046	E1944	GLU	F1748	F1553	D1423	GLY	ALA	ALA	V1043
A2350	M2228	P2146	GLU	A1960	GLU	F1749	V1554	P1424	VAL	GLY	GLY	V1044
R2351	C2283	Q2149	GLU	F1961	GLU	P1750	Q1559	T1427	GLU	L1153	L1153	R1044
V2352	R2234	V2149	GLU	A1962	GLU	G1751	M1560	L1428	ALA	L1154	L1154	T1045
V2353	F2235	E2157	GLU	A1965	GLU	R1752	V1561	M1429	GLN	T1156	T1156	L1046
V2354	L2236	E2157	PRO	V1966	GLU	K1753	Q1562	T1430	VAL	E1157	E1157	L1047
R2355	C2237	Q2161	GLU	D1967	GLU	G1754	Q1563	Y1434	LEU	M1158	M1158	G1048
R2369	C2240	L2165	GLU	K1968	GLU	F1755	F1564	Y1435	ALA	PRO	PRO	Y1049
G2373	R2244	L2167	THR	L1969	GLU	M1756	E1565	S1436	GLY	GLY	GLY	G1050
S2374	M2250	I2167	GLU	Q1973	GLU	A1757	K1568	F1440	ASN	S1171	S1171	Y1051
G2375	G2375	R1974	GLU	R1974	GLU	R1758	Q1569	A1441	GLN	D1172	D1172	N1052
L2376	H2253	S1975	GLU	S1975	GLU	P1787	K1570	T1454	LYS	S1173	S1173	I1053
L2377	L2254	L2177	GLU	L1979	ASP	A1788	N1571	T1456	ASP	G1174	G1174	E1054
A2378	S2255	L2182	GLU	L1980	GLU	A1789	I1572	D1456	THR	S1176	S1176	P1055
E2382	Y2256	I2182	GLU	M1981	LYS	A1790	A1577	D1461	GLU	E1181	E1181	P1056
R2385	S2261	I2185	LEU	R1982	GLU	V1791	R1584	F1464	LYS	I1182	I1182	D1057
R2392	G2262	M2186	LEU	A1983	ASP	A1792	P1593	K1468	LYS	D1186	D1186	Q1058
D2393	G2263	V2190	THR	F1984	GLU	E1793	M1599	R1470	ALA	E1059	E1059	P1060
G2396	G2264	F2191	VAL	T1985	GLU	A1794	P1603	M1476	GLY	L1189	L1189	S1061
V2397	L2265	Y2192	ARG	M1986	GLU	L1804	V1603	G1477	PRO	P1190	P1190	Q1062
ARG	G2266	Q2193	LEU	S1987	GLU	A1806	V1603	D1478	ASP	L1194	L1194	V1063
ASP	M2267	P2195	VAL	A1988	LYS	L1807	R1619	E1479	ASP	Q1198	Q1198	E1064
ARG	T2271	N2196	LYS	A1989	ASP	R1808	V1626	E1479	TYR	E1221	E1221	N1065
ASP	V2275	L2197	LYS	E1990	ALA	D1809	K1639	G1480	GLU	S1241	S1241	Q1066
ARG	A2276	R2198	GLU	T1991	GLU	A1810	L1639	G1481	LEU	H1252	H1252	S1067
ARG	V2280	G2202	LYS	A1992	GLU	L1812	L1676	M1482	ARG	Y1255	Y1255	W1069
GLU	M2283	H2204	GLU	R1993	GLU	R1813	R1680	H1484	SER	M1280	M1280	D1070
HIS	L2288	E2205	ALA	R1994	GLU	M1814	A1684	G1497	ALA	Q1077	Q1077	R1071
PHE	E2292	M2208	PRO	R1995	ALA	R1819	L1694	V1501	TRP	T1263	T1263	V1072
GLY	G2293	M2211	GLU	R1996	GLU	D1820	L1694	S1502	ALA	D1265	D1265	Q1084
GLU	D2294	V2212	ALA	F1998	GLU	G1822	L1698	P1503	GLY	T1286	T1286	S1085
F2410	E2296	N2213	GLU	S2000	LYS	D1828	G1705	G1504	LEU	L1272	L1272	G1086
P2411	K2297	V2214	ASP	P2001	ASP	S1833	Y1712	Q1505	LYS	R1276	R1276	R1087
E2412	V2298	G2216	L1922	Q2005	L1922	F1836	Q1837	Q1506	ARG	Q1280	Q1280	W1088
E2413	L2418	L2418	E1923	I2006	E1923	Q1837	P1840	G1507	LEU	N1281	N1281	R1101
N2414	A2303	L2418	E1924	H2011	E1924	P1840	I1853	R1508	THR	A1105	A1105	D1112
L2418	L2307	Y2426	G1925	D2014	G1925	I1853	F1854	I1509	ALA	D1113	D1113	V1113
Y2426				E2015		F1854		S1510	THR	E1114	E1114	L1115
				A2016				T1512	ALA	V1123	V1123	G1126



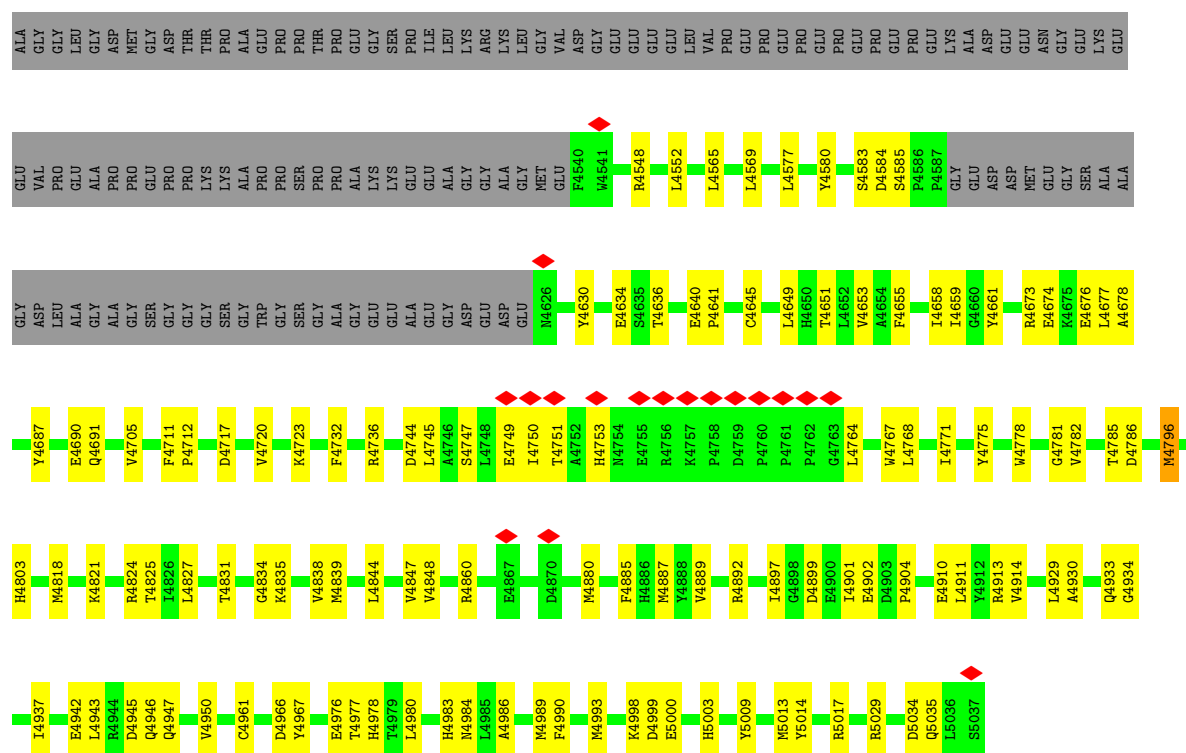




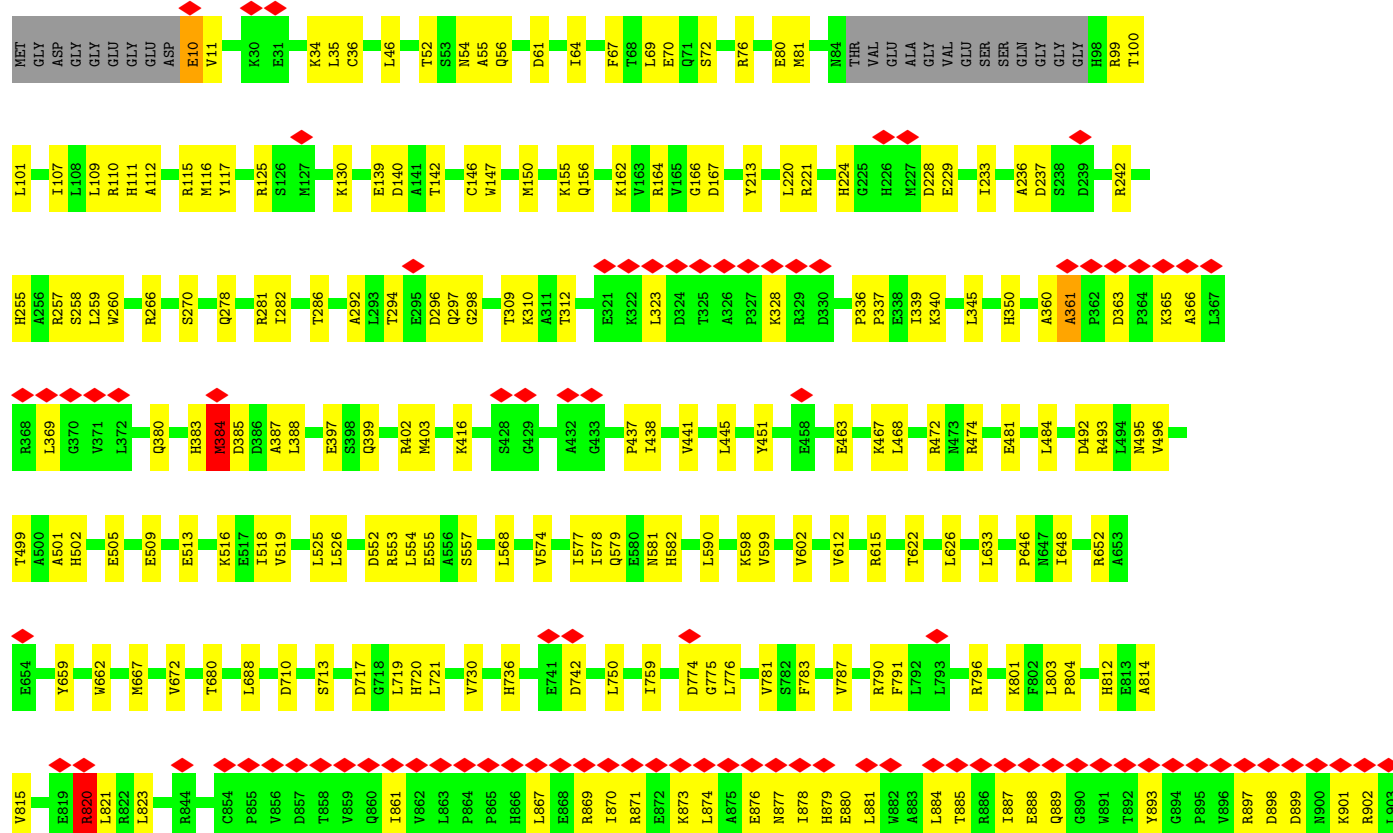








• Molecule 1: Ryanodine receptor 1



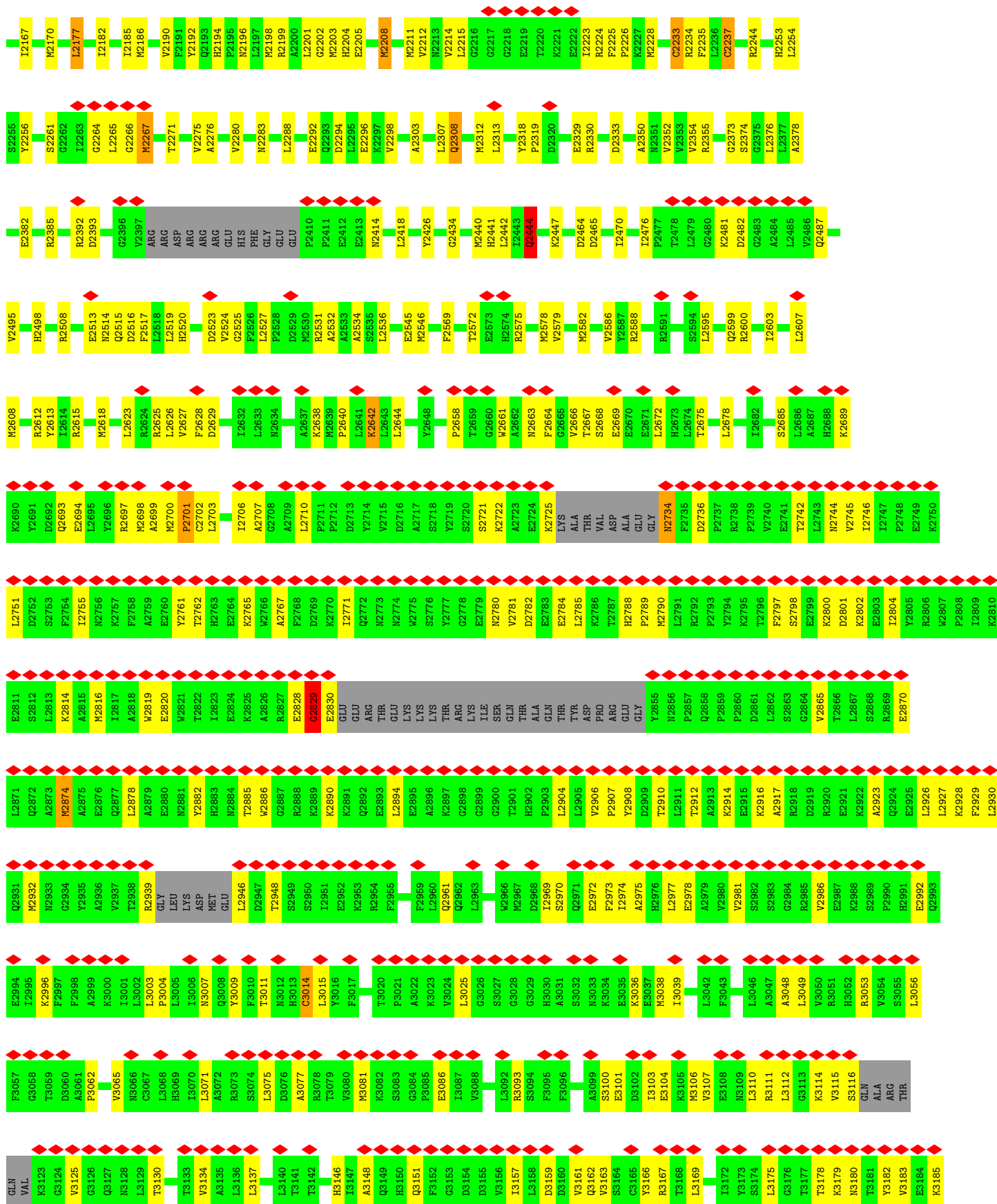


L3175	G3176	T3177	T3178	T3179	N3180	T3181	Y3182	Y3183	Y3184	Y3185	Y3186	L3187	L3188	P3188	A3189	L3190	G3191	E3192	C3193	L3194	A3195	L3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	N3211	E3212	Y3213	N3214	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	P3233	N3234	
L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	Q3126	N3128	L3129	T3130	T3133	V3134	A3135	L3136	L3137	L3140	T3141	T3142	H3146	I3147	A3148	K3149	H3150	Q3151	F3152	G3153	E3086	I3087	V3088	L3092	R3093	S3094	D3160	V3161	Q3162	V3163	S3164	G3165	P3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	P3233	N3234	
L3046	A3047	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3061	P3062	V3065	N3066	C3067	L3068	H3069	L3070	L3071	A3072	R3073	S3074	L3075	D3076	A3077	R3078	Y3079	V3080	M3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	L3092	R3093	S3094	F3095	F3096	A3099	S3100	E3101	D3102	I3103	E3104	K3105	N3106	V3107	E3108	N3109		
S2983	Q2984	E2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	Q2993	E2994	I2995	K2996	F2997	P2998	A2999	K3000	I3001	L3002	P3003	L3005	I3006	N3007	Q3008	Y3009	F3010	T3011	N3012	H3013	C3014	L3015	Y3016	F3017	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	N3033	K3034	E3035	K3036	E3037	M3038	I3039	L3042	F3043			
R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	GLY	LEU	LYS	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	I2951	E2952	K2953	R2954	F2955	F2959	L2960	Q2961	Q2962	L2963	V2966	K2967	D2968	L2969	S2970	Q2971	E2972	F2973	I2974	A2975	H2976	L2977	E2978	A2979	V2980	Y2981	S2982		
P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	E2877	L2878	A2879	E2880	N2881	Y2882	H2883	T2884	T2885	W2886	G2887	K2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	K2914	E2915	K2916	A2917	R2918	D2919
K2800	D2801	K2802	E2803	L2804	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	A2818	W2819	E2820	Y2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	Q2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859		
V2740	E2741	T2742	L2743	V2745	L2746	L2747	L2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	W2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	D2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	W2790	L2791	P2792	Y2794	K2795	T2796	T2797	S2798	E2799	
L2674	T2675	L2678	L2682	S2685	H2686	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	Y2696	R2697	M2698	A2699	M2700	P2701	C2702	L2703	I2706	A2707	G2708	A2709	L2710	P2711	K2712	D2713	Y2714	V2715	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	D2735	F2736	P2737	R2738	P2739				
E2591	S2594	L2595	Q2599	R2600	I2603	L2607	M2608	R2612	Y2613	L2614	R2615	M2618	L2623	R2624	R2625	L2626	V2627	F2628	D2629	I2632	L2633	N2634	A2637	K2638	M2639	P2640	L2641	L2642	L2643	L2644	Y2648	P2658	T2659	G2660	W2661	A2662	N2663	F2664	G2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673											
T2478	L2479	G2480	K2481	D2482	Q2483	A2484	L2485	V2486	Q2487	V2495	H2498	R2508	E2513	N2514	Q2515	D2516	F2517	L2518	L2519	H2520	D2523	V2524	G2525	F2526	L2527	P2528	D2529	M2530	D2531	A2532	A2533	A2534	S2535	L2536	E2545	M2546	F2569	T2572	E2573	H2574	R2575	A2576	I2577	M2578	V2579	M2582	V2586	Y2587	R2588									
N2351	V2352	V2353	V2354	R2355	S2374	G2375	L2376	L2377	A2378	E2382	R2385	R2386	R2389	D2393	G2396	V2397	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	P2410	P2411	K2412	E2413	L2414	L2418	Y2426	G2434	N2440	H2441	L2442	I2443	Q2444	K2447	D2464	D2465	I2470	L2476	P2477													
F2235	L2236	C2237	C2240	R2244	M2250	H2253	L2254	S2255	Y2256	S2261	G2262	T2263	G2264	L2265	G2266	H2267	T2271	V2275	A2276	V2280	N2283	L2288	E2292	K2293	D2294	L2295	E2296	V2297	V2298	A2303	L2307	Q2308	M2312	L2313	Y2318	P2319	D2320	E2329	R2330	D2333	A2350																	

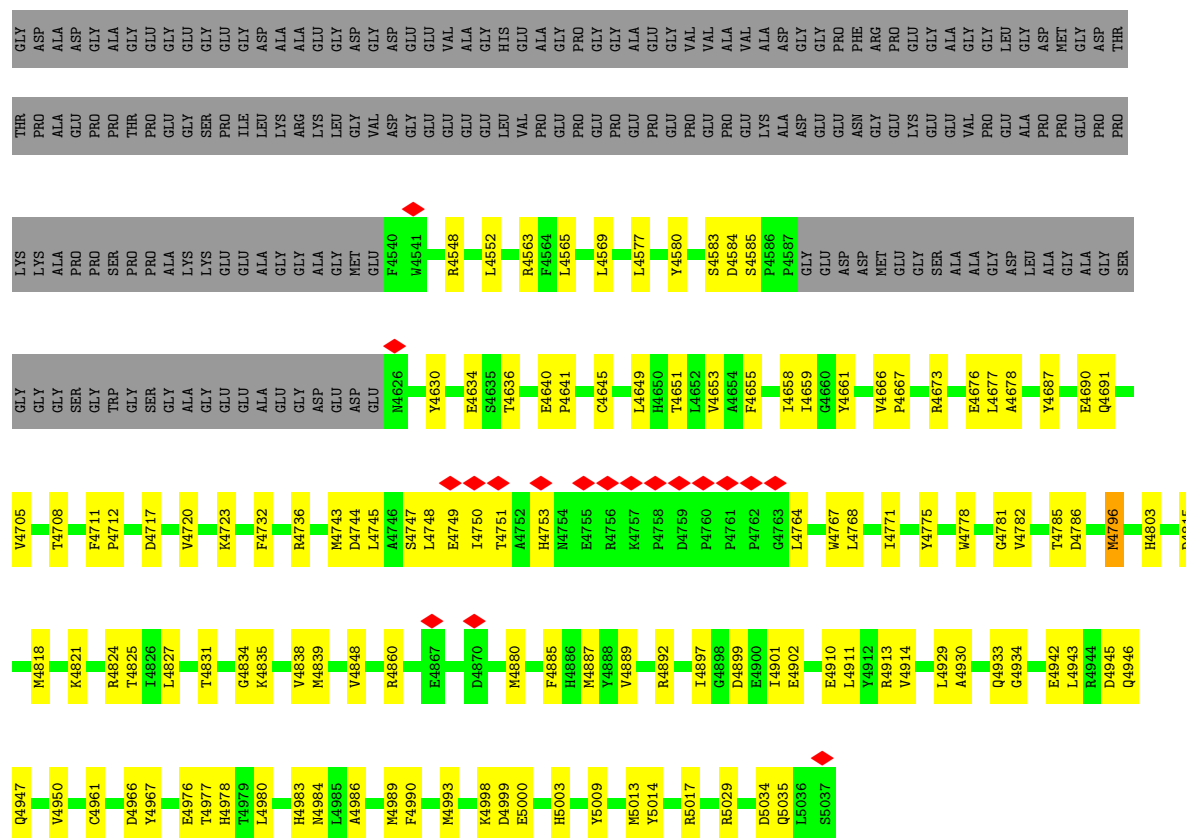




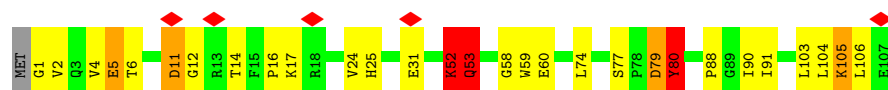




ALA	ARG	GLY	L3186	L3246	L3316	A3385	E3463	P3527	E3590	L3663	C3786	Y3902	E4032	G4179	GLY
ARG	ALA	GLU	R3187	D3247	L3316	E3386	I3464	T3528	K3591	T3664	E3789	L3903	E4032	R4180	GLU
ALA	GLY	GLY	F3188	R3248	N3318	A3387	N3465	I3529	I3592	D3671	E3789	R3904	M4039	E4181	GLY
ALA	ALA	ALA	A3189	L3249	I3319	E3388	N3466	Q3530	V3593	M3793	M3793	T3910	A4041	E4182	ALA
GLY	GLY	GLY	L3190	M3250	L3320	E3389	M3467	D3531	R3594	M3672	T3802	T3911	R4042	S4187	ALA
ALA	ALA	THR	G3191		L3321	E3390	S3468	L3532	Q3597	M3673	T3803	I3916	V4045	R4188	ALA
GLY	VAL	VAL	I3192		I3322	E3391	F3469	T3534	E3598	E3682	S3803	D3941	V4045	R4188	THR
ALA	ALA	ALA	G3193		L3323	E3392	L3470	M3534	V3602	Q3683	E3825	D3942	V4049	R4192	ALA
GLY	ALA	ALA	L3194		G3255	L3393	T3471	L3535	L3603	E3684	E3825	V3942	V4049	R4192	ALA
ALA	GLY	ALA	A3195		L3256	L3394	T3472	A3536	L3604	E3685	S3831	I3943	M4057	I4197	ALA
ALA	THR	ALA	R3196		A3257	R3395	A3472	H3605	L3605	E3686	A3834	Q3946	M4057	I4197	ALA
GLY	ALA	ALA	L3197		E3258	R3396	D3473	L3606	H3606	E3687	L3835	G3947	K4060	R4202	ALA
ALA	ALA	ALA	A3198		G3260	D3397	S3474	T3538	L3607	E3688	L3835	K3947	F4061	W4205	ALA
ALA	ALA	ALA	A3199			I3329	K3475	I3539	E3607	E3689	L3836	R3949	F4062	W4205	ALA
ALA	ALA	ALA	A3200			I3330	S3476		T3608	E3690	T3838	A3954	D4063	Q4209	ALA
GLY	ALA	ALA	F3202		Y3263	E3331	K3477	L3542	T3609	V3690	C3839	A3954	M4064	Q4209	ALA
ALA	ALA	ALA	V3203		T3264	A3332	M3478	K3543	E3610	E3692	S3840		M4064	W4222	ALA
ALA	ALA	ALA	A3204		E3265	T3333	A3479	T3545	H3611	K3693	V3841				ALA
ALA	ALA	ALA	F3205		M3266	T3334	L3401	D3546	T3612	K3694	R3849				ALA
ALA	ALA	ALA	L3206			W3334	L3402	E3547	P3613	K3694	K3852				ALA
ALA	ALA	ALA	E3207			M3335	C3402	E3548	K3614	L3721					ALA
ALA	ALA	ALA	P3208			K3336	D3405	V3549	S3615	Y3722					ALA
ALA	ALA	ALA	Q3209			R3337	L3406	R3550	S3616	M3723					ALA
ALA	ALA	ALA	L3210			L3338	L3408	E3551	K3617	A3724					ALA
ALA	ALA	ALA	N3211			A3339	Y3409	F3552	K3618	Y3725					ALA
ALA	ALA	ALA	E3212			V3340	G3410	G3553	V3619	A3726					ALA
ALA	ALA	ALA	Y3213			F3341	L3411	Q3554	W3620	D3727					ALA
ALA	ALA	ALA	N3214			A3342	L3412	N3555	H3621	I3728					ALA
ALA	ALA	ALA	A3215			Q3343	L3413	N3556	H3622	K3731					ALA
ALA	ALA	ALA	C3216			F3344	L3414	L3557	L3623	S3732					ALA
ALA	ALA	ALA	S3217			V3345	D3417	H3558	S3625	C3733					ALA
ALA	ALA	ALA	R3218			R3347	A3429	Q3560	K3626	E3736					ALA
ALA	ALA	ALA	Y3219			K3348	E3432	G3561	Q3627	GLU					ALA
ALA	ALA	ALA	T3220			H3357	E3433	K3562	R3628	GLY					ALA
ALA	ALA	ALA	T3221			F3358	L3434	V3563	R3629	GLY					ALA
ALA	ALA	ALA	K3222			R3358	F3435	E3564	R3630	GLU					ALA
ALA	ALA	ALA	S3223			T3361	R3436	G3565	A3631	ASN					ALA
ALA	ALA	ALA	P3224			I3362	M3437	S3566	V3632	GLU					ALA
ALA	ALA	ALA	K3225			R3363	Y3442	F3567	A3633	ALA					ALA
ALA	ALA	ALA	E3226			R3364	F3443	S3568	A3634	GLU					ALA
ALA	ALA	ALA	R3227			L3365	I3443	L3569	C3635	GLU					ALA
ALA	ALA	ALA	A3228			R3366	Y3444	R3570	F3636	GLU					ALA
ALA	ALA	ALA	I3229			K3367	K3447	K3573	R3637	V3749					ALA
ALA	ALA	ALA	L3230			R3368	E3447	A3574	M3638	E3750					ALA
ALA	ALA	ALA	G3231			V3372	N3450	K3577	T3639	E3755					ALA
ALA	ALA	ALA	L3232			V3373	F3451	G3578	P3640	E3759					ALA
ALA	ALA	ALA	F3233			A3374	K3452	L3579	L3641						ALA
ALA	ALA	ALA	N3234			E3375	R3453	P3580	Y3642						ALA
ALA	ALA	ALA	V3236			E3376	E3454	Q3581	N3651	Q3766					ALA
ALA	ALA	ALA	E3237			E3377	E3455	R3582	E3655	L3770					ALA
ALA	ALA	ALA	E3238			Q3378	F3458	E3583	K3658						ALA
ALA	ALA	ALA	R3239			L3379	V3459	E3584	A3659						ALA
ALA	ALA	ALA	C3240			R3380	V3460	D3585	A3660						ALA
ALA	ALA	ALA	P3241			L3381	Q3461	A3586	W3661						ALA
ALA	ALA	ALA	I3242			E3382	N3462	D3587	I3662						ALA
ALA	ALA	ALA	I3243			A3383		D3588							ALA
ALA	ALA	ALA	P3244			K3384		P3589							ALA
ALA	ALA	ALA	V3245												ALA



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



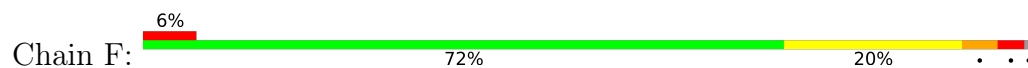
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	64353	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.555	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.48	61/35977 (0.2%)	0.57	65/48726 (0.1%)
1	B	0.48	61/35977 (0.2%)	0.57	65/48726 (0.1%)
1	C	0.48	61/35977 (0.2%)	0.57	66/48726 (0.1%)
1	D	0.48	61/35977 (0.2%)	0.57	65/48726 (0.1%)
2	E	1.69	18/850 (2.1%)	2.45	24/1146 (2.1%)
2	F	1.69	18/850 (2.1%)	2.45	24/1146 (2.1%)
2	G	1.69	18/850 (2.1%)	2.45	24/1146 (2.1%)
2	H	1.69	18/850 (2.1%)	2.45	24/1146 (2.1%)
All	All	0.54	316/147308 (0.2%)	0.67	357/199488 (0.2%)

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	14
1	B	0	14
1	C	0	14
1	D	0	14
2	E	0	5
2	F	0	5
2	G	0	5
2	H	0	5
All	All	0	76

All (316) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	80	TYR	CD1-CE1	23.90	2.10	1.38
2	F	80	TYR	CD1-CE1	23.89	2.10	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	80	TYR	CD1-CE1	23.88	2.10	1.38
2	G	80	TYR	CD1-CE1	23.86	2.10	1.38
1	D	1036	ARG	CZ-NH1	-20.77	1.03	1.32
1	A	1036	ARG	CZ-NH1	-20.75	1.03	1.32
1	B	1036	ARG	CZ-NH1	-20.75	1.03	1.32
1	C	1036	ARG	CZ-NH1	-20.75	1.03	1.32
2	F	52	LYS	CE-NZ	-19.62	0.90	1.49
2	G	52	LYS	CE-NZ	-19.60	0.90	1.49
2	H	52	LYS	CE-NZ	-19.59	0.90	1.49
2	E	52	LYS	CE-NZ	-19.58	0.90	1.49
1	A	3239	MET	CB-CG	19.32	2.10	1.52
1	D	3239	MET	CB-CG	19.32	2.10	1.52
1	B	3239	MET	CB-CG	19.31	2.10	1.52
1	C	3239	MET	CB-CG	19.31	2.10	1.52
2	G	80	TYR	CD2-CE2	18.42	1.94	1.38
2	H	80	TYR	CD2-CE2	18.40	1.93	1.38
2	F	80	TYR	CD2-CE2	18.40	1.93	1.38
2	E	80	TYR	CD2-CE2	18.39	1.93	1.38
1	B	2444	GLN	CG-CD	-17.91	1.07	1.52
1	D	2444	GLN	CG-CD	-17.91	1.07	1.52
1	A	2444	GLN	CG-CD	-17.89	1.07	1.52
1	C	2444	GLN	CG-CD	-17.89	1.07	1.52
1	B	2642	LYS	CG-CD	17.69	2.05	1.52
1	C	2642	LYS	CG-CD	17.68	2.05	1.52
1	A	2642	LYS	CG-CD	17.68	2.05	1.52
1	D	2642	LYS	CG-CD	17.66	2.05	1.52
1	A	2237	CYS	CB-SG	16.41	2.35	1.81
1	D	2237	CYS	CB-SG	16.41	2.35	1.81
1	B	2237	CYS	CB-SG	16.40	2.35	1.81
1	C	2237	CYS	CB-SG	16.40	2.35	1.81
1	A	2233	CYS	CB-SG	-15.44	1.30	1.81
1	D	2233	CYS	CB-SG	-15.44	1.30	1.81
1	C	2233	CYS	CB-SG	-15.44	1.30	1.81
1	B	2233	CYS	CB-SG	-15.42	1.30	1.81
1	B	1036	ARG	CB-CG	-14.40	1.09	1.52
1	D	1036	ARG	CB-CG	-14.38	1.09	1.52
1	A	1036	ARG	CB-CG	-14.38	1.09	1.52
1	C	1036	ARG	CB-CG	-14.38	1.09	1.52
1	B	2177	LEU	CB-CG	-11.78	1.29	1.53
1	D	2177	LEU	CB-CG	-11.78	1.29	1.53
1	A	2177	LEU	CB-CG	-11.76	1.29	1.53
1	C	2177	LEU	CB-CG	-11.74	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3239	MET	CG-SD	11.64	2.09	1.80
1	A	3239	MET	CG-SD	11.61	2.09	1.80
1	B	3239	MET	CG-SD	11.59	2.09	1.80
1	D	3239	MET	CG-SD	11.59	2.09	1.80
1	D	820	ARG	CZ-NH1	11.55	1.49	1.32
1	A	820	ARG	CZ-NH1	11.54	1.48	1.32
1	B	820	ARG	CZ-NH1	11.54	1.48	1.32
1	C	820	ARG	CZ-NH1	11.54	1.48	1.32
1	A	1036	ARG	NE-CZ	-11.38	1.20	1.33
1	C	1036	ARG	NE-CZ	-11.38	1.20	1.33
1	B	1036	ARG	NE-CZ	-11.33	1.20	1.33
1	D	1036	ARG	NE-CZ	-11.33	1.20	1.33
1	D	1036	ARG	CD-NE	-11.16	1.30	1.46
1	B	1036	ARG	CD-NE	-11.15	1.30	1.46
1	A	1036	ARG	CD-NE	-11.14	1.30	1.46
1	C	1036	ARG	CD-NE	-11.14	1.30	1.46
1	B	3557	LEU	CG-CD1	-11.12	1.15	1.52
1	A	3557	LEU	CG-CD1	-11.10	1.16	1.52
1	C	3557	LEU	CG-CD1	-11.10	1.16	1.52
1	D	3557	LEU	CG-CD1	-11.08	1.16	1.52
1	A	1559	GLN	CD-NE2	-10.74	1.10	1.33
1	B	1559	GLN	CD-NE2	-10.74	1.10	1.33
1	D	1559	GLN	CD-NE2	-10.74	1.10	1.33
1	C	1559	GLN	CD-NE2	-10.74	1.10	1.33
1	C	416	LYS	CD-CE	-10.68	1.20	1.52
1	A	416	LYS	CD-CE	-10.67	1.20	1.52
1	B	416	LYS	CD-CE	-10.67	1.20	1.52
1	D	416	LYS	CD-CE	-10.64	1.20	1.52
1	B	3478	MET	SD-CE	-10.62	1.52	1.79
1	D	3478	MET	SD-CE	-10.62	1.52	1.79
1	C	3478	MET	SD-CE	-10.62	1.52	1.79
1	C	384	MET	SD-CE	-10.60	1.53	1.79
1	A	3478	MET	SD-CE	-10.60	1.53	1.79
1	A	384	MET	SD-CE	-10.59	1.53	1.79
1	D	384	MET	SD-CE	-10.59	1.53	1.79
1	B	384	MET	SD-CE	-10.58	1.53	1.79
1	A	1036	ARG	CG-CD	-10.57	1.20	1.52
1	B	1036	ARG	CG-CD	-10.57	1.20	1.52
1	C	1036	ARG	CG-CD	-10.57	1.20	1.52
1	D	1036	ARG	CG-CD	-10.56	1.20	1.52
1	D	2308	GLN	CD-OE1	-10.51	1.03	1.23
1	A	2308	GLN	CD-OE1	-10.48	1.03	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2308	GLN	CD-OE1	-10.48	1.03	1.23
1	C	2308	GLN	CD-OE1	-10.48	1.03	1.23
1	B	2308	GLN	CD-NE2	-10.42	1.11	1.33
1	A	2308	GLN	CD-NE2	-10.41	1.11	1.33
1	D	2308	GLN	CD-NE2	-10.39	1.11	1.33
2	H	80	TYR	CA-CB	-10.39	1.37	1.53
1	C	2308	GLN	CD-NE2	-10.39	1.11	1.33
2	G	80	TYR	CA-CB	-10.35	1.37	1.53
2	F	80	TYR	CA-CB	-10.35	1.37	1.53
2	E	80	TYR	CA-CB	-10.35	1.37	1.53
1	C	4880	MET	SD-CE	-9.85	1.54	1.79
1	A	4880	MET	SD-CE	-9.82	1.54	1.79
1	B	4880	MET	SD-CE	-9.81	1.55	1.79
1	D	4880	MET	SD-CE	-9.81	1.55	1.79
1	D	2308	GLN	CB-CG	-9.31	1.24	1.52
1	C	2308	GLN	CB-CG	-9.30	1.24	1.52
1	A	2308	GLN	CB-CG	-9.30	1.24	1.52
1	B	2308	GLN	CB-CG	-9.27	1.24	1.52
1	B	1036	ARG	C-N	-9.26	1.22	1.33
1	D	1036	ARG	C-N	-9.26	1.22	1.33
1	C	1036	ARG	C-N	-9.26	1.22	1.33
1	A	1036	ARG	C-N	-9.23	1.22	1.33
1	B	941	MET	CG-SD	-9.09	1.58	1.80
1	A	941	MET	CG-SD	-9.08	1.58	1.80
1	D	941	MET	CG-SD	-9.07	1.58	1.80
1	C	941	MET	CG-SD	-9.07	1.58	1.80
2	H	80	TYR	CE1-CZ	-8.95	1.16	1.38
2	E	80	TYR	CE1-CZ	-8.94	1.16	1.38
2	G	80	TYR	CE1-CZ	-8.92	1.16	1.38
2	F	80	TYR	CE1-CZ	-8.92	1.16	1.38
2	G	53	GLN	CG-CD	8.80	1.74	1.52
2	H	53	GLN	CG-CD	8.78	1.74	1.52
2	F	53	GLN	CG-CD	8.77	1.74	1.52
2	E	53	GLN	CG-CD	8.74	1.74	1.52
2	H	80	TYR	CB-CG	-8.69	1.32	1.51
2	E	80	TYR	CB-CG	-8.67	1.32	1.51
2	F	80	TYR	CB-CG	-8.66	1.32	1.51
2	G	80	TYR	CB-CG	-8.66	1.32	1.51
1	C	3478	MET	CB-CG	-8.28	1.27	1.52
2	F	79	ASP	C-O	-8.28	1.14	1.24
2	G	79	ASP	C-O	-8.27	1.14	1.24
2	E	79	ASP	C-O	-8.25	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3478	MET	CB-CG	-8.25	1.27	1.52
1	D	3478	MET	CB-CG	-8.25	1.27	1.52
1	B	3478	MET	CB-CG	-8.24	1.27	1.52
2	H	79	ASP	C-O	-8.22	1.14	1.24
2	F	53	GLN	CB-CG	-8.20	1.27	1.52
2	H	53	GLN	CB-CG	-8.20	1.27	1.52
2	G	53	GLN	CB-CG	-8.19	1.27	1.52
2	E	53	GLN	CB-CG	-8.17	1.27	1.52
1	B	820	ARG	CD-NE	7.78	1.57	1.46
1	B	3239	MET	CA-C	-7.75	1.42	1.52
1	C	3239	MET	CA-C	-7.75	1.42	1.52
1	A	820	ARG	CD-NE	7.75	1.57	1.46
1	D	820	ARG	CD-NE	7.75	1.57	1.46
1	C	820	ARG	CD-NE	7.72	1.57	1.46
1	A	3239	MET	CA-C	-7.71	1.42	1.52
1	B	2267	MET	SD-CE	-7.67	1.60	1.79
1	D	3239	MET	CA-C	-7.67	1.42	1.52
1	C	2267	MET	SD-CE	-7.67	1.60	1.79
1	A	2267	MET	SD-CE	-7.65	1.60	1.79
1	D	2267	MET	CA-CB	-7.65	1.41	1.53
1	C	2267	MET	CA-CB	-7.65	1.41	1.53
1	D	2267	MET	SD-CE	-7.65	1.60	1.79
1	A	2267	MET	CA-CB	-7.63	1.41	1.53
1	B	2267	MET	CA-CB	-7.63	1.41	1.53
1	A	2874	MET	CB-CG	-7.51	1.29	1.52
1	B	2874	MET	CB-CG	-7.51	1.29	1.52
1	D	2874	MET	CB-CG	-7.50	1.29	1.52
1	C	2874	MET	CB-CG	-7.50	1.29	1.52
2	H	105	LYS	CE-NZ	-7.28	1.27	1.49
1	B	2312	MET	CB-CG	-7.28	1.30	1.52
2	G	105	LYS	CE-NZ	-7.26	1.27	1.49
2	E	105	LYS	CE-NZ	-7.25	1.27	1.49
1	A	2312	MET	CB-CG	-7.25	1.30	1.52
2	F	105	LYS	CE-NZ	-7.25	1.27	1.49
1	D	2312	MET	CB-CG	-7.25	1.30	1.52
1	C	2312	MET	CB-CG	-7.25	1.30	1.52
1	C	2444	GLN	CB-CG	-7.22	1.30	1.52
1	A	2444	GLN	CB-CG	-7.21	1.30	1.52
1	B	2444	GLN	CB-CG	-7.20	1.30	1.52
1	D	2444	GLN	CB-CG	-7.20	1.30	1.52
1	B	2734	ASN	CB-CG	-7.13	1.34	1.52
1	A	2734	ASN	CB-CG	-7.12	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2734	ASN	CB-CG	-7.12	1.34	1.52
1	A	1260	MET	CG-SD	-7.08	1.63	1.80
1	B	1260	MET	CG-SD	-7.08	1.63	1.80
1	D	1260	MET	CG-SD	-7.08	1.63	1.80
1	C	1260	MET	CG-SD	-7.08	1.63	1.80
1	D	2734	ASN	CB-CG	-7.07	1.34	1.52
1	A	1559	GLN	CD-OE1	-7.00	1.10	1.23
1	B	1559	GLN	CD-OE1	-7.00	1.10	1.23
1	D	1559	GLN	CD-OE1	-7.00	1.10	1.23
1	C	1559	GLN	CD-OE1	-7.00	1.10	1.23
2	H	52	LYS	CA-C	-6.87	1.43	1.52
2	G	52	LYS	CA-C	-6.83	1.43	1.52
2	F	52	LYS	CA-C	-6.82	1.43	1.52
2	E	52	LYS	CA-C	-6.80	1.43	1.52
1	B	3467	MET	CB-CG	6.80	1.72	1.52
1	D	3467	MET	CB-CG	6.80	1.72	1.52
1	C	3467	MET	CB-CG	6.80	1.72	1.52
1	A	3467	MET	CB-CG	6.80	1.72	1.52
1	B	1559	GLN	CB-CG	-6.77	1.32	1.52
1	D	1559	GLN	CB-CG	-6.77	1.32	1.52
1	C	1559	GLN	CB-CG	-6.77	1.32	1.52
1	A	1559	GLN	CB-CG	-6.76	1.32	1.52
1	D	4161	ARG	NE-CZ	-6.69	1.25	1.33
1	A	4161	ARG	NE-CZ	-6.68	1.25	1.33
1	C	2444	GLN	CD-OE1	-6.65	1.10	1.23
1	A	2444	GLN	CD-OE1	-6.64	1.10	1.23
1	B	2444	GLN	CD-OE1	-6.64	1.10	1.23
1	D	2444	GLN	CD-OE1	-6.63	1.10	1.23
1	B	4161	ARG	NE-CZ	-6.63	1.25	1.33
1	C	4161	ARG	NE-CZ	-6.63	1.25	1.33
2	F	80	TYR	C-N	-6.62	1.22	1.33
1	A	3239	MET	N-CA	6.61	1.54	1.46
1	D	3239	MET	N-CA	6.61	1.54	1.46
2	E	80	TYR	C-N	-6.60	1.22	1.33
2	G	80	TYR	C-N	-6.59	1.22	1.33
1	B	3239	MET	N-CA	6.58	1.54	1.46
1	C	3239	MET	N-CA	6.58	1.54	1.46
2	H	80	TYR	C-N	-6.57	1.22	1.33
1	B	3239	MET	CA-CB	6.57	1.64	1.53
1	C	3239	MET	CA-CB	6.57	1.64	1.53
1	D	3239	MET	CA-CB	6.56	1.64	1.53
1	A	3239	MET	CA-CB	6.56	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	80	TYR	CZ-OH	-6.52	1.24	1.38
2	E	80	TYR	CZ-OH	-6.51	1.24	1.38
2	G	80	TYR	CZ-OH	-6.50	1.24	1.38
2	F	80	TYR	CZ-OH	-6.49	1.24	1.38
1	C	3238	GLU	C-N	6.40	1.42	1.33
1	B	2722	LYS	N-CA	-6.37	1.38	1.46
1	B	3238	GLU	C-N	6.36	1.42	1.33
1	A	3238	GLU	C-N	6.33	1.42	1.33
1	A	2722	LYS	N-CA	-6.31	1.38	1.46
1	C	2722	LYS	N-CA	-6.31	1.38	1.46
1	D	3238	GLU	C-N	6.28	1.42	1.33
1	D	2722	LYS	N-CA	-6.25	1.38	1.46
1	B	2444	GLN	N-CA	-6.23	1.38	1.46
1	B	2237	CYS	CA-CB	6.22	1.63	1.53
1	C	2237	CYS	CA-CB	6.22	1.63	1.53
1	C	820	ARG	CA-C	-6.21	1.45	1.52
1	A	2237	CYS	CA-CB	6.20	1.63	1.53
1	D	2237	CYS	CA-CB	6.20	1.63	1.53
1	A	2444	GLN	N-CA	-6.20	1.38	1.46
1	D	2444	GLN	N-CA	-6.20	1.38	1.46
1	D	820	ARG	CA-C	-6.19	1.45	1.52
1	A	820	ARG	CA-C	-6.19	1.45	1.52
1	C	2444	GLN	N-CA	-6.15	1.38	1.46
1	B	820	ARG	CA-CB	6.15	1.68	1.53
1	B	820	ARG	CA-C	-6.14	1.45	1.52
1	D	820	ARG	CA-CB	6.14	1.68	1.53
1	C	820	ARG	CA-CB	6.14	1.68	1.53
1	A	820	ARG	CA-CB	6.14	1.68	1.53
1	B	1128	ARG	CB-CG	-5.97	1.34	1.52
1	A	1128	ARG	CB-CG	-5.96	1.34	1.52
1	D	1128	ARG	CB-CG	-5.94	1.34	1.52
1	C	1128	ARG	CB-CG	-5.94	1.34	1.52
1	D	2722	LYS	CE-NZ	-5.92	1.31	1.49
1	D	961	MET	CG-SD	-5.92	1.66	1.80
1	A	2722	LYS	CE-NZ	-5.91	1.31	1.49
1	B	2722	LYS	CE-NZ	-5.91	1.31	1.49
1	A	961	MET	CG-SD	-5.91	1.66	1.80
1	B	961	MET	CG-SD	-5.91	1.66	1.80
1	C	961	MET	CG-SD	-5.90	1.66	1.80
1	C	2722	LYS	CE-NZ	-5.89	1.31	1.49
1	A	1036	ARG	CA-CB	-5.88	1.43	1.53
1	C	1036	ARG	CA-CB	-5.88	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1036	ARG	CA-CB	-5.84	1.43	1.53
1	D	1036	ARG	CA-CB	-5.84	1.43	1.53
1	A	383	HIS	C-N	5.82	1.41	1.33
1	D	383	HIS	C-N	5.82	1.41	1.33
1	B	383	HIS	C-N	5.80	1.41	1.33
1	C	383	HIS	C-N	5.75	1.41	1.33
1	A	3014	CYS	CB-SG	-5.74	1.62	1.81
1	D	3014	CYS	CB-SG	-5.74	1.62	1.81
1	B	3014	CYS	CB-SG	-5.72	1.62	1.81
1	C	3014	CYS	CB-SG	-5.72	1.62	1.81
1	A	4796	MET	CG-SD	-5.66	1.66	1.80
2	E	5	GLU	CD-OE1	-5.66	1.14	1.25
2	H	5	GLU	CD-OE1	-5.66	1.14	1.25
1	B	4796	MET	CG-SD	-5.65	1.66	1.80
1	D	4796	MET	CG-SD	-5.65	1.66	1.80
1	C	4796	MET	CG-SD	-5.65	1.66	1.80
2	G	5	GLU	CD-OE1	-5.65	1.14	1.25
2	F	5	GLU	CD-OE1	-5.63	1.14	1.25
1	D	3240	CYS	N-CA	5.61	1.54	1.46
1	A	2267	MET	CG-SD	-5.58	1.66	1.80
1	D	2267	MET	CG-SD	-5.58	1.66	1.80
1	B	2267	MET	CG-SD	-5.57	1.66	1.80
1	C	2267	MET	CG-SD	-5.57	1.66	1.80
1	A	3240	CYS	N-CA	5.57	1.53	1.46
1	B	3240	CYS	N-CA	5.56	1.53	1.46
1	C	3240	CYS	N-CA	5.56	1.53	1.46
2	F	53	GLN	CD-OE1	-5.56	1.12	1.23
2	F	53	GLN	CA-CB	-5.55	1.45	1.53
2	H	53	GLN	CD-OE1	-5.54	1.13	1.23
2	G	53	GLN	CD-OE1	-5.54	1.13	1.23
2	E	53	GLN	CA-CB	-5.51	1.45	1.53
2	H	53	GLN	CA-CB	-5.50	1.45	1.53
2	G	53	GLN	CA-CB	-5.50	1.45	1.53
2	E	53	GLN	CD-OE1	-5.49	1.13	1.23
1	D	820	ARG	CG-CD	-5.46	1.36	1.52
1	A	820	ARG	CG-CD	-5.43	1.36	1.52
1	B	820	ARG	CG-CD	-5.41	1.36	1.52
1	C	820	ARG	CG-CD	-5.41	1.36	1.52
1	D	1260	MET	SD-CE	-5.38	1.66	1.79
1	C	1260	MET	SD-CE	-5.38	1.66	1.79
1	A	1260	MET	SD-CE	-5.35	1.66	1.79
1	B	1260	MET	SD-CE	-5.35	1.66	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	416	LYS	CE-NZ	5.31	1.65	1.49
1	D	416	LYS	CE-NZ	5.31	1.65	1.49
1	C	416	LYS	CE-NZ	5.30	1.65	1.49
1	A	416	LYS	CE-NZ	5.30	1.65	1.49
1	D	820	ARG	CB-CG	5.13	1.67	1.52
2	E	53	GLN	N-CA	5.13	1.53	1.46
1	A	820	ARG	CB-CG	5.12	1.67	1.52
1	B	820	ARG	CB-CG	5.12	1.67	1.52
1	C	820	ARG	CB-CG	5.12	1.67	1.52
2	G	53	GLN	N-CA	5.12	1.53	1.46
2	H	53	GLN	N-CA	5.10	1.53	1.46
2	F	11	ASP	CG-OD1	-5.10	1.15	1.25
2	F	53	GLN	N-CA	5.08	1.53	1.46
2	G	11	ASP	CG-OD1	-5.08	1.15	1.25
2	E	11	ASP	CG-OD1	-5.08	1.15	1.25
1	B	4161	ARG	CZ-NH1	-5.08	1.25	1.32
1	D	4161	ARG	CZ-NH1	-5.08	1.25	1.32
1	C	4161	ARG	CZ-NH1	-5.06	1.25	1.32
2	H	11	ASP	CG-OD1	-5.06	1.15	1.25
1	A	4161	ARG	CZ-NH1	-5.05	1.25	1.32

All (357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	TYR	CE1-CZ-CE2	-44.72	30.86	120.30
2	F	80	TYR	CE1-CZ-CE2	-44.71	30.88	120.30
2	G	80	TYR	CE1-CZ-CE2	-44.71	30.89	120.30
2	E	80	TYR	CE1-CZ-CE2	-44.70	30.90	120.30
2	H	80	TYR	CD1-CG-CD2	-32.83	68.86	118.10
2	E	80	TYR	CD1-CG-CD2	-32.81	68.89	118.10
2	G	80	TYR	CD1-CG-CD2	-32.80	68.89	118.10
2	F	80	TYR	CD1-CG-CD2	-32.79	68.91	118.10
2	H	53	GLN	OE1-CD-NE2	-29.22	93.38	122.60
2	E	53	GLN	OE1-CD-NE2	-29.20	93.40	122.60
2	G	53	GLN	OE1-CD-NE2	-29.18	93.42	122.60
2	F	53	GLN	OE1-CD-NE2	-29.18	93.42	122.60
1	A	3239	MET	CB-CG-SD	22.43	179.99	112.70
1	B	3239	MET	CB-CG-SD	22.43	179.99	112.70
1	C	3239	MET	CB-CG-SD	22.42	179.97	112.70
1	D	3239	MET	CB-CG-SD	22.42	179.97	112.70
2	F	80	TYR	CG-CD1-CE1	-21.01	89.69	121.20
2	G	80	TYR	CG-CD1-CE1	-21.00	89.70	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	80	TYR	CG-CD1-CE1	-20.99	89.71	121.20
2	H	80	TYR	CG-CD1-CE1	-20.98	89.73	121.20
2	F	80	TYR	CB-CG-CD2	18.36	148.33	120.80
2	G	80	TYR	CB-CG-CD2	18.32	148.28	120.80
2	H	80	TYR	CB-CG-CD2	18.31	148.27	120.80
2	E	80	TYR	CB-CG-CD2	18.29	148.24	120.80
1	D	384	MET	CB-CG-SD	18.15	167.14	112.70
1	A	384	MET	CB-CG-SD	18.13	167.10	112.70
1	C	384	MET	CB-CG-SD	18.12	167.07	112.70
1	B	384	MET	CB-CG-SD	18.12	167.06	112.70
1	B	2642	LYS	CD-CE-NZ	-16.62	58.72	111.90
1	D	2642	LYS	CD-CE-NZ	-16.61	58.73	111.90
1	A	2642	LYS	CD-CE-NZ	-16.61	58.75	111.90
1	C	2642	LYS	CD-CE-NZ	-16.61	58.76	111.90
1	C	1036	ARG	CG-CD-NE	16.11	147.43	112.00
1	A	1036	ARG	CG-CD-NE	16.09	147.41	112.00
1	B	1036	ARG	CG-CD-NE	16.09	147.39	112.00
1	D	1036	ARG	CG-CD-NE	16.07	147.35	112.00
1	D	3239	MET	CA-CB-CG	-15.38	83.35	114.10
1	A	3239	MET	CA-CB-CG	-15.37	83.37	114.10
1	B	3239	MET	CA-CB-CG	-15.35	83.39	114.10
1	C	3239	MET	CA-CB-CG	-15.35	83.39	114.10
1	D	1036	ARG	CD-NE-CZ	-15.11	103.24	124.40
1	A	1036	ARG	CD-NE-CZ	-15.10	103.26	124.40
1	B	1036	ARG	CD-NE-CZ	-15.09	103.28	124.40
1	C	1036	ARG	CD-NE-CZ	-15.07	103.30	124.40
2	H	53	GLN	CG-CD-NE2	-14.95	93.98	116.40
2	G	53	GLN	CG-CD-NE2	-14.94	93.99	116.40
2	F	53	GLN	CG-CD-NE2	-14.94	94.00	116.40
2	E	53	GLN	CG-CD-NE2	-14.93	94.00	116.40
2	G	53	GLN	CG-CD-OE1	14.82	150.45	120.80
2	H	53	GLN	CG-CD-OE1	14.82	150.43	120.80
2	F	53	GLN	CG-CD-OE1	14.81	150.43	120.80
2	E	53	GLN	CG-CD-OE1	14.79	150.38	120.80
1	B	384	MET	CA-CB-CG	14.13	142.36	114.10
1	D	384	MET	CA-CB-CG	14.12	142.34	114.10
1	A	384	MET	CA-CB-CG	14.11	142.33	114.10
1	C	384	MET	CA-CB-CG	14.10	142.29	114.10
1	B	820	ARG	CD-NE-CZ	-14.09	104.67	124.40
1	A	820	ARG	CD-NE-CZ	-14.07	104.70	124.40
1	D	820	ARG	CD-NE-CZ	-14.07	104.71	124.40
1	C	820	ARG	CD-NE-CZ	-14.06	104.71	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	MET	CG-SD-CE	-13.70	70.77	100.90
1	A	384	MET	CG-SD-CE	-13.69	70.79	100.90
1	C	384	MET	CG-SD-CE	-13.69	70.79	100.90
1	D	384	MET	CG-SD-CE	-13.68	70.81	100.90
1	C	2312	MET	CG-SD-CE	12.70	128.85	100.90
1	A	2312	MET	CG-SD-CE	12.70	128.83	100.90
1	B	2312	MET	CG-SD-CE	12.70	128.83	100.90
1	D	2312	MET	CG-SD-CE	12.69	128.82	100.90
1	C	820	ARG	CA-CB-CG	-12.16	89.78	114.10
1	B	820	ARG	CA-CB-CG	-12.16	89.79	114.10
1	D	820	ARG	CA-CB-CG	-12.16	89.78	114.10
1	A	820	ARG	CA-CB-CG	-12.15	89.80	114.10
1	B	820	ARG	CG-CD-NE	-11.35	87.02	112.00
1	A	820	ARG	CG-CD-NE	-11.35	87.03	112.00
1	D	820	ARG	CG-CD-NE	-11.35	87.04	112.00
1	C	820	ARG	CG-CD-NE	-11.34	87.06	112.00
2	H	80	TYR	O-C-N	11.19	133.98	122.12
2	G	80	TYR	O-C-N	11.14	133.93	122.12
2	E	80	TYR	O-C-N	11.14	133.93	122.12
2	F	80	TYR	O-C-N	11.14	133.93	122.12
1	B	1559	GLN	CA-CB-CG	10.99	136.08	114.10
1	C	1559	GLN	CA-CB-CG	10.99	136.08	114.10
1	D	1559	GLN	CA-CB-CG	10.99	136.08	114.10
1	A	1559	GLN	CA-CB-CG	10.99	136.07	114.10
1	C	3239	MET	CA-C-O	10.88	136.06	120.51
1	A	3239	MET	CA-C-O	10.87	136.05	120.51
1	B	3239	MET	CA-C-O	10.86	136.04	120.51
1	D	3239	MET	CA-C-O	10.85	136.03	120.51
2	G	80	TYR	CZ-CE2-CD2	-10.81	100.14	119.60
2	F	80	TYR	CZ-CE2-CD2	-10.80	100.17	119.60
2	E	80	TYR	CZ-CE2-CD2	-10.79	100.17	119.60
2	H	80	TYR	CZ-CE2-CD2	-10.79	100.19	119.60
2	H	80	TYR	CA-C-O	-10.65	109.26	120.55
1	C	2444	GLN	CB-CG-CD	10.65	130.70	112.60
2	E	80	TYR	CA-C-O	-10.65	109.27	120.55
2	G	80	TYR	CA-C-O	-10.65	109.27	120.55
1	B	2444	GLN	CB-CG-CD	10.64	130.69	112.60
1	D	2444	GLN	CB-CG-CD	10.64	130.69	112.60
1	A	2444	GLN	CB-CG-CD	10.63	130.67	112.60
2	F	80	TYR	CA-C-O	-10.63	109.28	120.55
2	E	52	LYS	CD-CE-NZ	10.19	144.51	111.90
2	H	52	LYS	CD-CE-NZ	10.18	144.48	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	52	LYS	CD-CE-NZ	10.18	144.46	111.90
2	F	52	LYS	CD-CE-NZ	10.17	144.45	111.90
2	E	80	TYR	CB-CG-CD1	-9.82	106.07	120.80
2	F	80	TYR	CB-CG-CD1	-9.80	106.09	120.80
2	G	80	TYR	CB-CG-CD1	-9.80	106.10	120.80
2	H	80	TYR	CB-CG-CD1	-9.80	106.10	120.80
1	D	3478	MET	CB-CG-SD	9.66	141.70	112.70
1	C	3478	MET	CB-CG-SD	9.66	141.67	112.70
1	A	3478	MET	CB-CG-SD	9.65	141.66	112.70
1	B	3478	MET	CB-CG-SD	9.64	141.62	112.70
1	B	2829	GLY	CA-C-N	9.57	138.92	121.70
1	B	2829	GLY	C-N-CA	9.57	138.92	121.70
1	A	2829	GLY	CA-C-N	9.56	138.91	121.70
1	A	2829	GLY	C-N-CA	9.56	138.91	121.70
1	D	2829	GLY	CA-C-N	9.55	138.88	121.70
1	D	2829	GLY	C-N-CA	9.55	138.88	121.70
1	C	2829	GLY	CA-C-N	9.55	138.88	121.70
1	C	2829	GLY	C-N-CA	9.55	138.88	121.70
2	G	80	TYR	N-CA-CB	-9.30	96.45	110.12
2	F	80	TYR	N-CA-CB	-9.30	96.45	110.12
2	H	80	TYR	N-CA-CB	-9.29	96.47	110.12
2	E	80	TYR	N-CA-CB	-9.28	96.47	110.12
2	G	52	LYS	CA-C-N	-9.10	109.54	123.47
2	G	52	LYS	C-N-CA	-9.10	109.54	123.47
2	F	52	LYS	CA-C-N	-9.10	109.55	123.47
2	F	52	LYS	C-N-CA	-9.10	109.55	123.47
2	H	52	LYS	CA-C-N	-9.09	109.57	123.47
2	H	52	LYS	C-N-CA	-9.09	109.57	123.47
2	E	52	LYS	CA-C-N	-9.08	109.58	123.47
2	E	52	LYS	C-N-CA	-9.08	109.58	123.47
1	C	2308	GLN	CA-CB-CG	8.73	131.56	114.10
1	D	2308	GLN	CA-CB-CG	8.73	131.56	114.10
1	A	2308	GLN	CA-CB-CG	8.73	131.55	114.10
1	B	2308	GLN	CA-CB-CG	8.70	131.51	114.10
1	A	2267	MET	CG-SD-CE	-8.66	81.85	100.90
1	B	2267	MET	CG-SD-CE	-8.66	81.85	100.90
1	D	2267	MET	CG-SD-CE	-8.66	81.85	100.90
1	C	2267	MET	CG-SD-CE	-8.66	81.86	100.90
1	D	3858	MET	CB-CG-SD	8.48	138.15	112.70
1	C	3858	MET	CB-CG-SD	8.48	138.13	112.70
1	A	3858	MET	CB-CG-SD	8.48	138.13	112.70
1	B	3858	MET	CB-CG-SD	8.47	138.12	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2444	GLN	CA-CB-CG	8.46	131.02	114.10
1	C	2444	GLN	CA-CB-CG	8.46	131.01	114.10
1	B	2444	GLN	CA-CB-CG	8.45	131.01	114.10
1	D	2444	GLN	CA-CB-CG	8.45	131.01	114.10
2	F	53	GLN	CA-CB-CG	8.24	130.58	114.10
2	H	53	GLN	CA-CB-CG	8.23	130.57	114.10
1	D	2312	MET	CB-CG-SD	8.23	137.38	112.70
1	B	2312	MET	CB-CG-SD	8.22	137.37	112.70
1	A	2312	MET	CB-CG-SD	8.22	137.35	112.70
2	E	53	GLN	CA-CB-CG	8.21	130.53	114.10
1	C	2312	MET	CB-CG-SD	8.21	137.32	112.70
2	G	53	GLN	CA-CB-CG	8.20	130.50	114.10
1	C	2308	GLN	OE1-CD-NE2	-8.16	114.44	122.60
1	A	2308	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	D	2308	GLN	OE1-CD-NE2	-8.13	114.47	122.60
1	B	2308	GLN	OE1-CD-NE2	-8.13	114.47	122.60
2	E	80	TYR	CD1-CE1-CZ	8.02	134.03	119.60
2	G	80	TYR	CD1-CE1-CZ	8.01	134.02	119.60
2	F	80	TYR	CD1-CE1-CZ	8.01	134.01	119.60
2	H	80	TYR	CD1-CE1-CZ	7.99	133.99	119.60
2	G	80	TYR	CB-CA-C	7.92	123.94	110.79
2	E	80	TYR	CB-CA-C	7.92	123.93	110.79
2	H	80	TYR	CB-CA-C	7.92	123.93	110.79
2	F	80	TYR	CB-CA-C	7.90	123.91	110.79
1	D	3239	MET	CB-CA-C	-7.87	94.75	110.42
1	A	3239	MET	CB-CA-C	-7.87	94.77	110.42
1	B	3239	MET	CB-CA-C	-7.86	94.78	110.42
1	C	3239	MET	CB-CA-C	-7.86	94.78	110.42
1	D	1036	ARG	CB-CG-CD	7.58	128.74	111.30
1	A	1036	ARG	CB-CG-CD	7.58	128.72	111.30
1	B	1036	ARG	CB-CG-CD	7.56	128.69	111.30
1	C	1036	ARG	CB-CG-CD	7.55	128.67	111.30
1	A	1559	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	B	1559	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	D	1559	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	C	1559	GLN	OE1-CD-NE2	-7.46	115.14	122.60
1	B	3467	MET	CB-CG-SD	7.45	135.04	112.70
1	D	3467	MET	CB-CG-SD	7.45	135.04	112.70
1	A	3467	MET	CB-CG-SD	7.44	135.03	112.70
1	C	3467	MET	CB-CG-SD	7.43	134.99	112.70
1	C	2444	GLN	CG-CD-OE1	-7.42	105.97	120.80
1	B	2444	GLN	CG-CD-OE1	-7.41	105.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2444	GLN	CG-CD-OE1	-7.39	106.01	120.80
1	D	2444	GLN	CG-CD-OE1	-7.39	106.03	120.80
2	F	5	GLU	OE1-CD-OE2	-7.36	105.23	122.90
2	H	5	GLU	OE1-CD-OE2	-7.36	105.24	122.90
2	G	5	GLU	OE1-CD-OE2	-7.36	105.23	122.90
2	E	5	GLU	OE1-CD-OE2	-7.35	105.25	122.90
1	B	4796	MET	CG-SD-CE	-7.06	85.36	100.90
1	D	4796	MET	CG-SD-CE	-7.06	85.36	100.90
1	C	4796	MET	CG-SD-CE	-7.06	85.36	100.90
1	A	4796	MET	CG-SD-CE	-7.06	85.37	100.90
1	D	3014	CYS	CA-CB-SG	7.00	130.51	114.40
1	A	3014	CYS	CA-CB-SG	7.00	130.49	114.40
1	B	3014	CYS	CA-CB-SG	6.99	130.48	114.40
1	C	3014	CYS	CA-CB-SG	6.98	130.45	114.40
1	D	4880	MET	CB-CG-SD	6.96	133.58	112.70
1	A	4880	MET	CB-CG-SD	6.95	133.54	112.70
1	B	4880	MET	CB-CG-SD	6.95	133.54	112.70
1	C	4880	MET	CB-CG-SD	6.94	133.53	112.70
1	B	2722	LYS	CG-CD-CE	-6.90	95.42	111.30
1	A	2722	LYS	CG-CD-CE	-6.89	95.46	111.30
1	C	2722	LYS	CG-CD-CE	-6.88	95.47	111.30
1	D	2722	LYS	CG-CD-CE	-6.88	95.48	111.30
2	H	105	LYS	CD-CE-NZ	6.82	133.72	111.90
2	F	105	LYS	CD-CE-NZ	6.82	133.71	111.90
2	E	105	LYS	CD-CE-NZ	6.80	133.67	111.90
2	G	105	LYS	CD-CE-NZ	6.80	133.66	111.90
2	H	52	LYS	CG-CD-CE	-6.79	95.68	111.30
2	G	52	LYS	CG-CD-CE	-6.78	95.70	111.30
2	F	52	LYS	CG-CD-CE	-6.77	95.72	111.30
2	E	52	LYS	CG-CD-CE	-6.76	95.74	111.30
1	D	3478	MET	CA-CB-CG	-6.71	100.69	114.10
1	A	3478	MET	CA-CB-CG	-6.70	100.70	114.10
1	D	1071	ARG	CG-CD-NE	6.69	126.72	112.00
1	C	1071	ARG	CG-CD-NE	6.69	126.71	112.00
1	A	1071	ARG	CG-CD-NE	6.68	126.71	112.00
1	B	3478	MET	CA-CB-CG	-6.68	100.73	114.10
1	B	1071	ARG	CG-CD-NE	6.68	126.69	112.00
1	C	3478	MET	CA-CB-CG	-6.67	100.75	114.10
1	A	4880	MET	CA-CB-CG	-6.66	100.77	114.10
1	B	4880	MET	CA-CB-CG	-6.66	100.78	114.10
1	C	4880	MET	CA-CB-CG	-6.66	100.78	114.10
1	D	4880	MET	CA-CB-CG	-6.65	100.80	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2734	ASN	CB-CG-ND2	6.35	125.92	116.40
1	B	2734	ASN	CB-CG-ND2	6.34	125.91	116.40
1	C	2734	ASN	CB-CG-ND2	6.34	125.90	116.40
1	D	2734	ASN	CB-CG-OD1	-6.33	108.14	120.80
1	D	2734	ASN	CB-CG-ND2	6.32	125.88	116.40
1	A	2734	ASN	CB-CG-OD1	-6.32	108.17	120.80
1	B	2734	ASN	CB-CG-OD1	-6.31	108.18	120.80
1	C	2734	ASN	CB-CG-OD1	-6.31	108.19	120.80
1	D	3731	LYS	CD-CE-NZ	6.28	132.01	111.90
1	A	3731	LYS	CD-CE-NZ	6.28	131.99	111.90
1	C	3731	LYS	CD-CE-NZ	6.27	131.98	111.90
1	B	3731	LYS	CD-CE-NZ	6.27	131.97	111.90
1	A	1559	GLN	CG-CD-OE1	6.17	133.14	120.80
1	B	1559	GLN	CG-CD-OE1	6.17	133.14	120.80
1	C	1559	GLN	CG-CD-OE1	6.17	133.14	120.80
1	D	1559	GLN	CG-CD-OE1	6.16	133.12	120.80
1	A	2237	CYS	CB-CA-C	6.15	121.31	110.85
1	B	2237	CYS	CB-CA-C	6.15	121.31	110.85
1	C	2237	CYS	CB-CA-C	6.15	121.30	110.85
1	D	2237	CYS	CB-CA-C	6.14	121.29	110.85
1	C	3557	LEU	CB-CG-CD1	6.09	128.98	110.70
1	B	3557	LEU	CB-CG-CD1	6.09	128.96	110.70
1	D	3557	LEU	CB-CG-CD1	6.09	128.96	110.70
1	A	3557	LEU	CB-CG-CD1	6.08	128.96	110.70
1	B	1260	MET	CG-SD-CE	-6.00	87.71	100.90
1	C	2642	LYS	CG-CD-CE	-6.00	97.51	111.30
1	A	1260	MET	CG-SD-CE	-5.99	87.72	100.90
1	C	2721	SER	CA-C-N	5.99	128.80	120.29
1	C	2721	SER	C-N-CA	5.99	128.80	120.29
1	A	2642	LYS	CG-CD-CE	-5.99	97.53	111.30
1	D	1260	MET	CG-SD-CE	-5.99	87.73	100.90
1	C	1260	MET	CG-SD-CE	-5.99	87.73	100.90
1	B	2642	LYS	CG-CD-CE	-5.99	97.53	111.30
1	B	1128	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	A	2721	SER	CA-C-N	5.98	128.78	120.29
1	A	2721	SER	C-N-CA	5.98	128.78	120.29
1	D	2208	MET	CG-SD-CE	-5.98	87.75	100.90
1	D	2642	LYS	CG-CD-CE	-5.98	97.55	111.30
1	B	2208	MET	CG-SD-CE	-5.97	87.76	100.90
1	B	2721	SER	CA-C-N	5.97	128.77	120.29
1	B	2721	SER	C-N-CA	5.97	128.77	120.29
1	D	2721	SER	CA-C-N	5.97	128.77	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2721	SER	C-N-CA	5.97	128.77	120.29
1	C	1128	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	A	2208	MET	CG-SD-CE	-5.97	87.77	100.90
1	A	1128	ARG	NE-CZ-NH1	5.96	127.47	121.50
1	D	1128	ARG	NE-CZ-NH1	5.96	127.47	121.50
1	C	2208	MET	CG-SD-CE	-5.96	87.80	100.90
1	D	1128	ARG	N-CA-CB	-5.93	102.69	110.88
1	A	1128	ARG	N-CA-CB	-5.92	102.70	110.88
1	C	1128	ARG	N-CA-CB	-5.92	102.71	110.88
1	B	1128	ARG	N-CA-CB	-5.91	102.73	110.88
1	D	1036	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	D	2267	MET	O-C-N	-5.88	116.00	123.06
1	A	2267	MET	O-C-N	-5.87	116.02	123.06
1	C	2267	MET	O-C-N	-5.86	116.03	123.06
1	A	1036	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	B	1036	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	C	1036	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	B	2267	MET	O-C-N	-5.85	116.04	123.06
1	D	2308	GLN	CB-CG-CD	5.82	122.49	112.60
1	B	2308	GLN	CB-CG-CD	5.81	122.47	112.60
1	A	2308	GLN	CB-CG-CD	5.81	122.47	112.60
1	C	2308	GLN	CB-CG-CD	5.78	122.43	112.60
1	C	1128	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	A	1128	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	B	1128	ARG	NE-CZ-NH2	-5.67	114.10	119.20
1	D	1128	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	D	4161	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	4161	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	B	4161	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	C	4161	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	D	1036	ARG	N-CA-C	5.52	122.56	110.80
1	B	1036	ARG	N-CA-C	5.51	122.54	110.80
1	C	1036	ARG	N-CA-C	5.50	122.52	110.80
1	A	1036	ARG	N-CA-C	5.50	122.51	110.80
1	D	3478	MET	CG-SD-CE	5.46	112.91	100.90
1	A	3478	MET	CG-SD-CE	5.45	112.88	100.90
1	C	3478	MET	CG-SD-CE	5.45	112.88	100.90
1	B	3478	MET	CG-SD-CE	5.44	112.88	100.90
1	C	1036	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	B	2642	LYS	CB-CG-CD	5.41	123.74	111.30
1	B	1036	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	D	1036	ARG	NE-CZ-NH2	-5.41	114.33	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2642	LYS	CB-CG-CD	5.40	123.72	111.30
1	A	2642	LYS	CB-CG-CD	5.40	123.72	111.30
1	D	2642	LYS	CB-CG-CD	5.40	123.72	111.30
2	F	80	TYR	OH-CZ-CE2	-5.40	103.71	119.90
1	A	1036	ARG	NE-CZ-NH2	-5.39	114.34	119.20
2	G	80	TYR	OH-CZ-CE2	-5.38	103.77	119.90
2	E	80	TYR	OH-CZ-CE2	-5.37	103.78	119.90
2	H	80	TYR	OH-CZ-CE2	-5.36	103.81	119.90
1	B	2308	GLN	N-CA-CB	5.29	118.99	111.05
1	A	2308	GLN	N-CA-CB	5.28	118.98	111.05
1	D	2308	GLN	N-CA-CB	5.27	118.96	111.05
1	A	10	GLU	N-CA-C	5.27	125.74	111.00
1	B	10	GLU	N-CA-C	5.26	125.74	111.00
1	C	2308	GLN	N-CA-CB	5.26	118.94	111.05
1	C	10	GLU	N-CA-C	5.26	125.72	111.00
1	B	2208	MET	CB-CG-SD	5.26	128.47	112.70
1	D	10	GLU	N-CA-C	5.25	125.71	111.00
1	D	2208	MET	CB-CG-SD	5.25	128.46	112.70
1	C	2208	MET	CB-CG-SD	5.25	128.44	112.70
1	A	2208	MET	CB-CG-SD	5.25	128.43	112.70
1	B	1128	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
1	A	1128	ARG	NH1-CZ-NH2	-5.18	112.56	119.30
1	B	1260	MET	CB-CG-SD	5.18	128.25	112.70
1	D	1128	ARG	NH1-CZ-NH2	-5.18	112.56	119.30
1	D	1260	MET	CB-CG-SD	5.17	128.22	112.70
1	C	1260	MET	CB-CG-SD	5.17	128.22	112.70
1	A	1260	MET	CB-CG-SD	5.17	128.22	112.70
1	C	1128	ARG	NH1-CZ-NH2	-5.16	112.60	119.30
1	B	10	GLU	CB-CG-CD	5.11	121.29	112.60
1	C	10	GLU	CB-CG-CD	5.11	121.29	112.60
2	E	53	GLN	N-CA-C	5.10	119.45	113.23
1	D	10	GLU	CB-CG-CD	5.10	121.26	112.60
1	A	10	GLU	CB-CG-CD	5.09	121.26	112.60
1	C	2177	LEU	CB-CA-C	-5.09	102.89	110.88
2	F	52	LYS	CB-CG-CD	5.08	123.00	111.30
1	B	2177	LEU	CB-CA-C	-5.08	102.91	110.88
1	D	2177	LEU	CB-CA-C	-5.08	102.91	110.88
1	A	2177	LEU	CB-CA-C	-5.08	102.91	110.88
2	E	52	LYS	CB-CG-CD	5.08	122.97	111.30
2	G	52	LYS	CB-CG-CD	5.07	122.97	111.30
2	G	53	GLN	N-CA-C	5.06	119.41	113.23
2	H	53	GLN	N-CA-C	5.06	119.41	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	52	LYS	CB-CG-CD	5.06	122.94	111.30
2	F	53	GLN	N-CA-C	5.04	119.38	113.23
1	C	156	GLN	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	ASN	Peptide
1	A	1036	ARG	Sidechain,Mainchain
1	A	1051	TYR	Sidechain
1	A	1128	ARG	Sidechain
1	A	1749	PRO	Mainchain
1	A	1758	ARG	Sidechain
1	A	1944	GLU	Sidechain
1	A	1982	ARG	Sidechain
1	A	2444	GLN	Sidechain
1	A	2701	PRO	Peptide
1	A	3453	ARG	Sidechain
1	A	4161	ARG	Sidechain
1	A	820	ARG	Sidechain
1	B	1035	ASN	Peptide
1	B	1036	ARG	Sidechain,Mainchain
1	B	1051	TYR	Sidechain
1	B	1128	ARG	Sidechain
1	B	1749	PRO	Mainchain
1	B	1758	ARG	Sidechain
1	B	1944	GLU	Sidechain
1	B	1982	ARG	Sidechain
1	B	2444	GLN	Sidechain
1	B	2701	PRO	Peptide
1	B	3453	ARG	Sidechain
1	B	4161	ARG	Sidechain
1	B	820	ARG	Sidechain
1	C	1035	ASN	Peptide
1	C	1036	ARG	Sidechain,Mainchain
1	C	1051	TYR	Sidechain
1	C	1128	ARG	Sidechain
1	C	1749	PRO	Mainchain
1	C	1758	ARG	Sidechain
1	C	1944	GLU	Sidechain
1	C	1982	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	2444	GLN	Sidechain
1	C	2701	PRO	Peptide
1	C	3453	ARG	Sidechain
1	C	4161	ARG	Sidechain
1	C	820	ARG	Sidechain
1	D	1035	ASN	Peptide
1	D	1036	ARG	Sidechain,Mainchain
1	D	1051	TYR	Sidechain
1	D	1128	ARG	Sidechain
1	D	1749	PRO	Mainchain
1	D	1758	ARG	Sidechain
1	D	1944	GLU	Sidechain
1	D	1982	ARG	Sidechain
1	D	2444	GLN	Sidechain
1	D	2701	PRO	Peptide
1	D	3453	ARG	Sidechain
1	D	4161	ARG	Sidechain
1	D	820	ARG	Sidechain
2	E	5	GLU	Sidechain
2	E	52	LYS	Mainchain
2	E	53	GLN	Sidechain
2	E	60	GLU	Sidechain
2	E	80	TYR	Sidechain
2	F	5	GLU	Sidechain
2	F	52	LYS	Mainchain
2	F	53	GLN	Sidechain
2	F	60	GLU	Sidechain
2	F	80	TYR	Sidechain
2	G	5	GLU	Sidechain
2	G	52	LYS	Mainchain
2	G	53	GLN	Sidechain
2	G	60	GLU	Sidechain
2	G	80	TYR	Sidechain
2	H	5	GLU	Sidechain
2	H	52	LYS	Mainchain
2	H	53	GLN	Sidechain
2	H	60	GLU	Sidechain
2	H	80	TYR	Sidechain

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	35150	0	34792	1042	0
1	B	35150	0	34792	1033	0
1	C	35150	0	34792	1024	0
1	D	35150	0	34792	1035	0
2	E	831	0	831	24	0
2	F	831	0	831	25	0
2	G	831	0	831	25	0
2	H	831	0	831	24	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	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
6	A	20	0	18	3	0
6	B	20	0	18	3	0
6	C	20	0	18	3	0
6	D	20	0	18	3	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	144144	0	142612	4151	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 14.

All (4151) 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:D:941:MET:HE1	1:D:1051:TYR:CD1	1.45	1.52
1:B:941:MET:HE1	1:B:1051:TYR:CD1	1.45	1.50
1:C:941:MET:HE1	1:C:1051:TYR:CD1	1.45	1.50
1:A:941:MET:HE1	1:A:1051:TYR:CD1	1.45	1.49
1:D:3239:MET:CG	1:D:3239:MET:SD	2.09	1.41
1:A:3239:MET:CG	1:A:3239:MET:SD	2.09	1.41
1:B:3239:MET:SD	1:B:3239:MET:CG	2.09	1.39
1:C:3239:MET:SD	1:C:3239:MET:CG	2.09	1.39
1:A:2642:LYS:CD	1:A:2642:LYS:CG	2.05	1.34
1:B:2642:LYS:CG	1:B:2642:LYS:CD	2.05	1.34
1:D:2642:LYS:CG	1:D:2642:LYS:CD	2.05	1.33
1:A:1749:PRO:O	1:A:1758:ARG:NH2	1.62	1.32
1:C:2642:LYS:CG	1:C:2642:LYS:CD	2.05	1.32
1:C:1749:PRO:O	1:C:1758:ARG:NH2	1.62	1.31
1:D:3239:MET:CG	1:D:3239:MET:CB	2.10	1.30
1:A:3239:MET:CG	1:A:3239:MET:CB	2.10	1.30
1:B:1749:PRO:O	1:B:1758:ARG:NH2	1.62	1.30
1:D:1749:PRO:O	1:D:1758:ARG:NH2	1.62	1.28
1:B:3239:MET:CG	1:B:3239:MET:CB	2.10	1.28
1:C:3239:MET:CG	1:C:3239:MET:CB	2.10	1.28
1:C:961:MET:CE	1:C:963:ASN:HB3	1.66	1.26
1:A:961:MET:CE	1:A:963:ASN:HB3	1.66	1.25
1:D:961:MET:CE	1:D:963:ASN:HB3	1.66	1.24
1:B:961:MET:CE	1:B:963:ASN:HB3	1.66	1.23
1:A:2523:ASP:HB3	1:A:2578:MET:HE1	1.21	1.19
1:B:972:LEU:HG	1:B:1041:GLN:NE2	1.59	1.18
1:C:972:LEU:HG	1:C:1041:GLN:NE2	1.59	1.18
1:A:941:MET:CE	1:A:1051:TYR:CD1	2.27	1.17
1:C:941:MET:CE	1:C:1051:TYR:CD1	2.27	1.17
1:B:941:MET:CE	1:B:1051:TYR:CD1	2.27	1.17
1:B:2523:ASP:HB3	1:B:2578:MET:HE1	1.21	1.17
1:D:2226:PRO:HB3	1:D:2267:MET:HE1	1.26	1.16
1:D:2523:ASP:HB3	1:D:2578:MET:HE1	1.21	1.16
1:D:972:LEU:HG	1:D:1041:GLN:NE2	1.59	1.16
1:A:972:LEU:HG	1:A:1041:GLN:NE2	1.59	1.16
1:C:2226:PRO:HB3	1:C:2267:MET:HE1	1.26	1.15
1:A:2226:PRO:HB3	1:A:2267:MET:HE1	1.26	1.15
1:B:2237:CYS:SG	1:B:2237:CYS:CB	2.35	1.15
1:D:941:MET:CE	1:D:1051:TYR:CD1	2.27	1.15
1:A:2237:CYS:CB	1:A:2237:CYS:SG	2.35	1.15
1:C:2237:CYS:SG	1:C:2237:CYS:CB	2.35	1.14
1:D:2237:CYS:SG	1:D:2275:VAL:HG22	1.88	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2237:CYS:SG	1:D:2237:CYS:CB	2.35	1.13
1:D:2642:LYS:HG3	1:D:2698:MET:HE1	1.29	1.13
1:C:2237:CYS:SG	1:C:2275:VAL:HG22	1.88	1.13
1:B:2226:PRO:HB3	1:B:2267:MET:HE1	1.26	1.13
1:A:2237:CYS:SG	1:A:2275:VAL:HG22	1.88	1.12
1:B:2237:CYS:SG	1:B:2275:VAL:HG22	1.88	1.12
1:C:2523:ASP:HB3	1:C:2578:MET:HE1	1.21	1.12
1:B:3450:ASN:OD1	1:B:3453:ARG:NH2	1.82	1.12
1:D:3450:ASN:OD1	1:D:3453:ARG:NH2	1.82	1.12
1:A:3450:ASN:OD1	1:A:3453:ARG:NH2	1.82	1.12
1:C:3450:ASN:OD1	1:C:3453:ARG:NH2	1.82	1.12
1:D:941:MET:HE1	1:D:1051:TYR:CG	1.84	1.11
1:A:2642:LYS:HG3	1:A:2698:MET:HE1	1.29	1.11
1:C:941:MET:HE1	1:C:1051:TYR:CG	1.84	1.11
1:C:2642:LYS:HG3	1:C:2698:MET:HE1	1.29	1.11
1:A:941:MET:HE1	1:A:1051:TYR:CG	1.84	1.10
1:B:941:MET:HE1	1:B:1051:TYR:CG	1.84	1.10
1:B:2642:LYS:HG3	1:B:2698:MET:HE1	1.29	1.07
1:B:2233:CYS:CB	1:B:2237:CYS:SG	2.43	1.07
1:A:2233:CYS:CB	1:A:2237:CYS:SG	2.43	1.06
1:C:2233:CYS:CB	1:C:2237:CYS:SG	2.43	1.06
1:D:2233:CYS:CB	1:D:2237:CYS:SG	2.43	1.05
1:D:2642:LYS:CG	1:D:2642:LYS:NZ	2.21	1.04
1:B:2874:MET:HE2	1:B:2939:ARG:CB	1.88	1.03
1:A:961:MET:HE1	1:A:963:ASN:HB3	1.03	1.03
1:B:961:MET:HE1	1:B:963:ASN:HB3	1.03	1.03
1:D:2874:MET:HE2	1:D:2939:ARG:HB2	1.05	1.03
1:C:961:MET:HE1	1:C:963:ASN:HB3	1.03	1.03
1:C:2874:MET:HE2	1:C:2939:ARG:CB	1.88	1.03
1:A:2874:MET:HE2	1:A:2939:ARG:HB2	1.05	1.03
1:D:961:MET:HE1	1:D:963:ASN:HB3	1.03	1.03
1:A:2642:LYS:CG	1:A:2642:LYS:NZ	2.21	1.03
1:A:2874:MET:HE2	1:A:2939:ARG:CB	1.88	1.03
1:D:941:MET:SD	1:D:1051:TYR:CE1	2.52	1.02
1:C:972:LEU:HG	1:C:1041:GLN:HE22	0.87	1.02
1:A:941:MET:SD	1:A:1051:TYR:CE1	2.52	1.02
1:B:941:MET:SD	1:B:1051:TYR:CE1	2.52	1.02
1:B:961:MET:HE1	1:B:963:ASN:CB	1.89	1.02
1:B:2874:MET:HE2	1:B:2939:ARG:HB2	1.05	1.02
1:C:941:MET:SD	1:C:1051:TYR:CE1	2.52	1.02
1:D:961:MET:HE1	1:D:963:ASN:CB	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2874:MET:HE2	1:D:2939:ARG:CB	1.88	1.02
1:C:2642:LYS:CG	1:C:2642:LYS:NZ	2.21	1.02
1:C:961:MET:HE1	1:C:963:ASN:CB	1.89	1.02
1:D:2929:PHE:HA	1:D:2932:MET:HE1	1.41	1.01
1:C:2874:MET:HE2	1:C:2939:ARG:HB2	1.05	1.01
1:A:2929:PHE:HA	1:A:2932:MET:HE1	1.41	1.01
1:A:961:MET:HE1	1:A:963:ASN:CB	1.89	1.01
1:B:2642:LYS:CG	1:B:2642:LYS:NZ	2.21	1.01
1:D:972:LEU:HG	1:D:1041:GLN:HE22	0.87	1.01
1:C:1749:PRO:C	1:C:1758:ARG:HH22	1.69	1.01
1:C:2929:PHE:HA	1:C:2932:MET:HE1	1.41	1.00
1:B:1749:PRO:C	1:B:1758:ARG:HH22	1.69	1.00
1:D:1749:PRO:C	1:D:1758:ARG:HH22	1.69	1.00
1:A:972:LEU:HG	1:A:1041:GLN:HE22	0.87	1.00
1:B:972:LEU:HG	1:B:1041:GLN:HE22	0.87	1.00
1:B:2226:PRO:CB	1:B:2267:MET:HE1	1.92	0.99
1:C:2226:PRO:CB	1:C:2267:MET:HE1	1.92	0.99
1:A:2226:PRO:CB	1:A:2267:MET:HE1	1.92	0.99
1:B:3219:TYR:HE2	1:B:3239:MET:SD	1.86	0.99
1:C:3219:TYR:HE2	1:C:3239:MET:SD	1.86	0.99
1:A:1749:PRO:C	1:A:1758:ARG:HH22	1.69	0.98
1:D:972:LEU:CG	1:D:1041:GLN:HE22	1.77	0.98
1:D:2226:PRO:CB	1:D:2267:MET:HE1	1.92	0.98
1:A:972:LEU:CG	1:A:1041:GLN:HE22	1.77	0.98
1:A:3219:TYR:HE2	1:A:3239:MET:SD	1.86	0.98
1:A:3521:GLY:HA2	1:A:3524:MET:HE2	1.46	0.97
1:B:1808:ARG:NH2	1:B:1858:ASP:OD2	1.97	0.97
1:D:3219:TYR:HE2	1:D:3239:MET:SD	1.86	0.97
1:C:972:LEU:CG	1:C:1041:GLN:HE22	1.77	0.97
1:C:2929:PHE:HA	1:C:2932:MET:CE	1.95	0.97
1:B:2929:PHE:HA	1:B:2932:MET:HE1	1.41	0.97
1:D:1808:ARG:NH2	1:D:1858:ASP:OD2	1.97	0.96
1:D:2929:PHE:HA	1:D:2932:MET:CE	1.95	0.96
1:A:1808:ARG:NH2	1:A:1858:ASP:OD2	1.97	0.96
1:A:2929:PHE:HA	1:A:2932:MET:CE	1.95	0.96
1:B:2233:CYS:HB3	1:B:2237:CYS:SG	2.05	0.96
1:D:2233:CYS:HB3	1:D:2237:CYS:SG	2.04	0.96
1:C:1808:ARG:NH2	1:C:1858:ASP:OD2	1.97	0.96
1:C:2233:CYS:HB3	1:C:2237:CYS:SG	2.04	0.96
1:A:2771:ILE:HG22	1:B:1506:GLN:OE1	1.66	0.96
1:A:2233:CYS:HB3	1:A:2237:CYS:SG	2.04	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:972:LEU:CG	1:B:1041:GLN:HE22	1.77	0.95
1:B:2929:PHE:HA	1:B:2932:MET:CE	1.95	0.95
1:B:3521:GLY:HA2	1:B:3524:MET:HE2	1.46	0.95
1:B:3521:GLY:HA2	1:B:3524:MET:CE	1.97	0.95
1:D:3521:GLY:HA2	1:D:3524:MET:CE	1.96	0.94
1:C:3521:GLY:HA2	1:C:3524:MET:HE2	1.46	0.94
1:D:3521:GLY:HA2	1:D:3524:MET:HE2	1.46	0.94
1:A:3521:GLY:HA2	1:A:3524:MET:CE	1.96	0.94
1:C:3521:GLY:HA2	1:C:3524:MET:CE	1.96	0.94
1:A:221:ARG:NH2	1:A:397:GLU:OE2	2.03	0.92
2:E:52:LYS:O	2:E:53:GLN:HB2	1.68	0.92
1:B:2771:ILE:HG22	1:C:1506:GLN:OE1	1.69	0.92
1:D:1506:GLN:OE1	1:C:2771:ILE:HG22	1.70	0.92
1:D:221:ARG:NH2	1:D:397:GLU:OE2	2.03	0.91
1:B:2572:THR:HG21	1:B:2579:VAL:CG2	2.00	0.91
1:C:2572:THR:HG21	1:C:2579:VAL:CG2	2.00	0.91
1:A:221:ARG:NH1	1:A:258:SER:OG	2.04	0.91
2:F:52:LYS:O	2:F:53:GLN:HB2	1.68	0.91
1:B:221:ARG:NH1	1:B:258:SER:OG	2.04	0.91
1:C:221:ARG:NH1	1:C:258:SER:OG	2.04	0.91
1:A:495:ASN:OD1	1:A:553:ARG:NH1	2.03	0.91
1:B:221:ARG:NH2	1:B:397:GLU:OE2	2.03	0.91
1:B:495:ASN:OD1	1:B:553:ARG:NH1	2.03	0.91
1:D:2011:HIS:HE1	1:D:2017:ASP:OD2	1.54	0.91
1:C:495:ASN:OD1	1:C:553:ARG:NH1	2.03	0.91
1:D:221:ARG:NH1	1:D:258:SER:OG	2.04	0.90
1:A:2011:HIS:HE1	1:A:2017:ASP:OD2	1.54	0.90
2:G:52:LYS:O	2:G:53:GLN:HB2	1.68	0.90
1:D:2628:PHE:CZ	1:D:2734:ASN:OD1	2.25	0.90
1:C:221:ARG:NH2	1:C:397:GLU:OE2	2.03	0.90
1:A:2572:THR:HG21	1:A:2579:VAL:CG2	2.00	0.90
1:D:2572:THR:HG21	1:D:2579:VAL:CG2	2.00	0.90
1:A:2628:PHE:CZ	1:A:2734:ASN:OD1	2.25	0.90
1:B:2628:PHE:CZ	1:B:2734:ASN:OD1	2.24	0.90
2:H:52:LYS:O	2:H:53:GLN:HB2	1.68	0.90
1:A:2874:MET:CE	1:A:2939:ARG:HB2	1.99	0.90
1:B:2011:HIS:HE1	1:B:2017:ASP:OD2	1.54	0.90
1:D:495:ASN:OD1	1:D:553:ARG:NH1	2.03	0.89
1:D:2874:MET:CE	1:D:2939:ARG:HB2	1.99	0.89
1:C:2628:PHE:CZ	1:C:2734:ASN:OD1	2.25	0.89
1:A:941:MET:HE1	1:A:1051:TYR:CE1	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2011:HIS:HE1	1:C:2017:ASP:OD2	1.54	0.89
1:C:941:MET:HE1	1:C:1051:TYR:CE1	2.08	0.89
1:D:941:MET:HE1	1:D:1051:TYR:CE1	2.08	0.89
1:D:4039:MET:SD	1:D:4042:ARG:NH2	2.46	0.89
1:B:3239:MET:CG	1:B:3239:MET:CA	2.51	0.89
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	1.91	0.88
1:B:2874:MET:CE	1:B:2939:ARG:HB2	1.99	0.88
1:B:2292:GLU:OE1	1:B:2352:VAL:HG11	1.74	0.88
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	1.91	0.88
1:C:3239:MET:CG	1:C:3239:MET:CA	2.51	0.88
1:A:952:LYS:NZ	1:A:968:ALA:O	2.06	0.88
1:A:2292:GLU:OE1	1:A:2352:VAL:HG11	1.73	0.88
1:B:941:MET:HE1	1:B:1051:TYR:CE1	2.07	0.88
1:D:3239:MET:CG	1:D:3239:MET:CA	2.51	0.88
1:A:961:MET:SD	1:A:963:ASN:HB3	2.14	0.88
1:A:2599:GLN:O	1:A:2603:ILE:HD12	1.74	0.88
1:A:4039:MET:SD	1:A:4042:ARG:NH2	2.46	0.88
1:B:952:LYS:NZ	1:B:968:ALA:O	2.06	0.88
1:B:4039:MET:SD	1:B:4042:ARG:NH2	2.46	0.88
1:C:2874:MET:CE	1:C:2939:ARG:HB2	1.99	0.88
1:A:3239:MET:CG	1:A:3239:MET:CA	2.51	0.87
1:D:4006:ASP:OD2	1:D:4008:SER:OG	1.91	0.87
1:D:952:LYS:NZ	1:D:968:ALA:O	2.06	0.87
1:C:952:LYS:NZ	1:C:968:ALA:O	2.06	0.87
1:C:2292:GLU:OE1	1:C:2352:VAL:HG11	1.74	0.87
1:C:961:MET:SD	1:C:963:ASN:HB3	2.14	0.87
1:D:961:MET:SD	1:D:963:ASN:HB3	2.14	0.87
1:C:4006:ASP:OD2	1:C:4008:SER:OG	1.91	0.87
1:C:4039:MET:SD	1:C:4042:ARG:NH2	2.46	0.87
1:A:1506:GLN:OE1	1:D:2771:ILE:HG22	1.73	0.87
1:D:3466:ASN:ND2	1:D:3507:THR:O	2.08	0.87
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	1.91	0.87
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.08	0.87
1:B:961:MET:SD	1:B:963:ASN:HB3	2.14	0.87
1:D:2292:GLU:OE1	1:D:2352:VAL:HG11	1.74	0.87
1:B:2196:ASN:OD1	1:B:2199:ARG:NH2	2.08	0.86
1:C:2271:THR:OG1	1:C:2330:ARG:NH2	2.08	0.86
1:C:2599:GLN:O	1:C:2603:ILE:HD12	1.74	0.86
1:B:2599:GLN:O	1:B:2603:ILE:HD12	1.74	0.86
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	1.91	0.86
1:C:3466:ASN:ND2	1:C:3507:THR:O	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3573:MET:HB3	1:D:3577:ARG:NH1	1.91	0.86
1:C:2196:ASN:OD1	1:C:2199:ARG:NH2	2.08	0.86
1:A:3573:MET:HB3	1:A:3577:ARG:NH1	1.91	0.86
1:A:4006:ASP:OD2	1:A:4008:SER:OG	1.91	0.86
1:B:2271:THR:OG1	1:B:2330:ARG:NH2	2.08	0.86
1:B:4006:ASP:OD2	1:B:4008:SER:OG	1.91	0.86
1:D:2599:GLN:O	1:D:2603:ILE:HD12	1.74	0.86
1:B:3466:ASN:ND2	1:B:3507:THR:O	2.08	0.86
1:C:3573:MET:HB3	1:C:3577:ARG:NH1	1.91	0.86
1:B:3573:MET:HB3	1:B:3577:ARG:NH1	1.91	0.86
1:B:3943:ILE:O	1:B:3948:LYS:NZ	2.09	0.86
1:A:972:LEU:CG	1:A:1041:GLN:NE2	2.38	0.85
1:A:3466:ASN:ND2	1:A:3507:THR:O	2.08	0.85
1:B:941:MET:CE	1:B:1051:TYR:CE1	2.59	0.85
1:D:3943:ILE:O	1:D:3948:LYS:NZ	2.09	0.85
1:C:3943:ILE:O	1:C:3948:LYS:NZ	2.09	0.85
1:A:941:MET:CE	1:A:1051:TYR:CE1	2.60	0.85
1:D:2196:ASN:OD1	1:D:2199:ARG:NH2	2.08	0.85
1:D:2271:THR:OG1	1:D:2330:ARG:NH2	2.08	0.85
1:A:2271:THR:OG1	1:A:2330:ARG:NH2	2.08	0.85
1:A:3943:ILE:O	1:A:3948:LYS:NZ	2.09	0.85
1:C:3573:MET:HB3	1:C:3577:ARG:HH12	1.42	0.85
1:B:70:GLU:OE2	1:B:110:ARG:NE	2.09	0.85
1:A:70:GLU:OE2	1:A:110:ARG:NE	2.09	0.84
1:D:70:GLU:OE2	1:D:110:ARG:NE	2.09	0.84
1:C:3219:TYR:CE2	1:C:3239:MET:SD	2.70	0.84
1:C:70:GLU:OE2	1:C:110:ARG:NE	2.09	0.84
1:D:3219:TYR:CE2	1:D:3239:MET:SD	2.70	0.84
1:D:3239:MET:CA	1:D:3239:MET:HG2	2.08	0.84
1:D:3573:MET:HB3	1:D:3577:ARG:HH12	1.42	0.84
1:A:3219:TYR:CE2	1:A:3239:MET:SD	2.70	0.84
1:A:2929:PHE:HA	1:A:2932:MET:SD	2.18	0.84
1:B:2929:PHE:HA	1:B:2932:MET:SD	2.18	0.84
1:D:941:MET:CE	1:D:1051:TYR:CE1	2.60	0.84
1:B:3219:TYR:CE2	1:B:3239:MET:SD	2.70	0.83
1:C:941:MET:CE	1:C:1051:TYR:CE1	2.60	0.83
1:A:384:MET:SD	1:B:166:GLY:C	2.61	0.83
1:A:3573:MET:HB3	1:A:3577:ARG:HH12	1.42	0.83
1:C:2929:PHE:HA	1:C:2932:MET:SD	2.18	0.83
1:B:1999:ARG:HH12	1:B:3636:PHE:HA	1.44	0.83
1:B:3573:MET:HB3	1:B:3577:ARG:HH12	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1999:ARG:HH12	1:D:3636:PHE:HA	1.44	0.83
1:D:2929:PHE:HA	1:D:2932:MET:SD	2.18	0.83
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	1.97	0.82
1:A:1999:ARG:HH12	1:A:3636:PHE:HA	1.44	0.82
1:A:4749:GLU:O	1:A:4753:HIS:ND1	2.13	0.82
1:C:3282:PRO:O	1:C:3286:GLU:OE1	1.97	0.82
1:B:871:ARG:HD2	1:B:926:GLY:CA	2.09	0.82
1:C:1999:ARG:HH12	1:C:3636:PHE:HA	1.44	0.82
1:A:871:ARG:HD2	1:A:926:GLY:CA	2.09	0.82
1:C:871:ARG:HD2	1:C:926:GLY:CA	2.09	0.82
1:D:871:ARG:HD2	1:D:926:GLY:CA	2.09	0.82
1:D:2237:CYS:SG	1:D:2275:VAL:CG2	2.68	0.82
1:C:4749:GLU:O	1:C:4753:HIS:ND1	2.12	0.82
1:D:1252:HIS:O	1:D:1275:ARG:NH1	2.13	0.81
1:A:3282:PRO:O	1:A:3286:GLU:OE1	1.97	0.81
1:B:3175:LEU:HD21	1:B:3183:VAL:HG13	1.63	0.81
1:D:871:ARG:HD2	1:D:926:GLY:HA2	1.62	0.81
1:D:3282:PRO:O	1:D:3286:GLU:OE1	1.97	0.81
1:D:4749:GLU:O	1:D:4753:HIS:ND1	2.13	0.81
1:C:2237:CYS:SG	1:C:2275:VAL:CG2	2.68	0.81
1:B:4961:CYS:SG	1:B:4983:HIS:ND1	2.54	0.81
1:C:972:LEU:CG	1:C:1041:GLN:NE2	2.38	0.81
1:B:2237:CYS:SG	1:B:2275:VAL:CG2	2.68	0.81
1:B:4749:GLU:O	1:B:4753:HIS:ND1	2.13	0.81
1:C:1252:HIS:O	1:C:1275:ARG:NH1	2.13	0.81
1:A:2237:CYS:SG	1:A:2275:VAL:CG2	2.68	0.81
1:C:4961:CYS:SG	1:C:4983:HIS:ND1	2.54	0.81
1:A:4961:CYS:SG	1:A:4983:HIS:ND1	2.54	0.81
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	1.97	0.81
1:B:1252:HIS:O	1:B:1275:ARG:NH1	2.13	0.81
1:D:3175:LEU:HD21	1:D:3183:VAL:HG13	1.62	0.81
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	1.97	0.81
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	1.97	0.81
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.13	0.80
1:B:3465:ASN:OD1	1:B:3467:MET:HG2	1.81	0.80
1:C:885:THR:O	1:C:889:GLN:NE2	2.14	0.80
1:B:871:ARG:HD2	1:B:926:GLY:HA2	1.62	0.80
1:D:885:THR:O	1:D:889:GLN:NE2	2.14	0.80
1:B:3282:PRO:O	1:B:3286:GLU:OE1	1.97	0.80
1:C:3175:LEU:HD21	1:C:3183:VAL:HG13	1.62	0.80
1:A:871:ARG:HD2	1:A:926:GLY:HA2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:THR:O	1:A:889:GLN:NE2	2.14	0.80
1:B:885:THR:O	1:B:889:GLN:NE2	2.14	0.80
1:A:3175:LEU:HD21	1:A:3183:VAL:HG13	1.62	0.80
1:A:3197:LEU:HD21	1:A:3201:MET:HE3	1.64	0.80
1:D:4961:CYS:SG	1:D:4983:HIS:ND1	2.53	0.80
1:B:972:LEU:CG	1:B:1041:GLN:NE2	2.38	0.80
1:B:3946:GLN:OE1	1:B:3949:ARG:NH1	2.15	0.80
1:A:4075:GLU:OE1	1:B:4736:ARG:NH1	2.14	0.80
1:D:3197:LEU:HD21	1:D:3201:MET:HE3	1.64	0.80
1:B:3197:LEU:HD21	1:B:3201:MET:HE3	1.64	0.79
1:A:4744:ASP:OD2	1:A:4747:SER:OG	1.99	0.79
1:D:3465:ASN:OD1	1:D:3467:MET:HG2	1.82	0.79
1:C:3465:ASN:OD1	1:C:3467:MET:HG2	1.81	0.79
1:A:3465:ASN:OD1	1:A:3467:MET:HG2	1.82	0.79
1:C:4744:ASP:OD2	1:C:4747:SER:OG	1.99	0.79
1:A:3946:GLN:OE1	1:A:3949:ARG:NH1	2.15	0.79
1:B:981:GLN:O	1:B:985:VAL:HG23	1.83	0.79
1:B:1263:THR:OG1	1:B:1265:ASP:OD1	2.01	0.79
1:B:4744:ASP:OD2	1:B:4747:SER:OG	1.99	0.79
1:A:3458:PHE:HE2	1:A:3464:ILE:CD1	1.96	0.79
1:D:3946:GLN:OE1	1:D:3949:ARG:NH1	2.15	0.79
1:C:871:ARG:HD2	1:C:926:GLY:HA2	1.62	0.79
1:C:3946:GLN:OE1	1:C:3949:ARG:NH1	2.15	0.79
1:C:3458:PHE:HE2	1:C:3464:ILE:CD1	1.96	0.79
1:C:3197:LEU:HD21	1:C:3201:MET:HE3	1.64	0.78
1:B:384:MET:SD	1:C:166:GLY:C	2.66	0.78
1:B:4885:PHE:O	1:B:4889:VAL:HG22	1.84	0.78
1:C:4885:PHE:O	1:C:4889:VAL:HG22	1.83	0.78
1:A:3236:VAL:HA	1:A:3239:MET:SD	2.24	0.78
1:A:4736:ARG:NH1	1:D:4075:GLU:OE1	2.16	0.78
1:B:3236:VAL:HA	1:B:3239:MET:SD	2.24	0.78
1:D:3236:VAL:HA	1:D:3239:MET:SD	2.24	0.78
1:D:1263:THR:OG1	1:D:1265:ASP:OD1	2.01	0.78
1:A:981:GLN:O	1:A:985:VAL:HG23	1.83	0.78
1:B:3458:PHE:HE2	1:B:3464:ILE:CD1	1.95	0.78
1:B:4075:GLU:OE1	1:C:4736:ARG:NH1	2.17	0.78
1:A:166:GLY:C	1:D:384:MET:SD	2.67	0.78
1:C:981:GLN:O	1:C:985:VAL:HG23	1.83	0.78
1:A:4885:PHE:O	1:A:4889:VAL:HG22	1.84	0.78
1:D:3458:PHE:HE2	1:D:3464:ILE:CD1	1.95	0.78
1:D:4885:PHE:O	1:D:4889:VAL:HG22	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3236:VAL:HG23	1:A:3239:MET:SD	2.25	0.77
1:A:4892:ARG:NH1	1:B:4899:ASP:OD1	2.17	0.77
1:B:110:ARG:NH2	1:B:117:TYR:OH	2.17	0.77
1:D:4736:ARG:NH1	1:C:4075:GLU:OE1	2.18	0.77
1:C:3236:VAL:HA	1:C:3239:MET:SD	2.24	0.77
1:D:961:MET:SD	1:D:963:ASN:CB	2.72	0.77
1:D:4744:ASP:OD2	1:D:4747:SER:OG	1.99	0.77
1:A:110:ARG:NH2	1:A:117:TYR:OH	2.17	0.77
1:A:961:MET:SD	1:A:963:ASN:CB	2.72	0.77
1:D:2224:ARG:HG3	1:D:2225:PHE:CD2	2.20	0.77
1:C:110:ARG:NH2	1:C:117:TYR:OH	2.17	0.77
1:C:3236:VAL:HG23	1:C:3239:MET:SD	2.24	0.77
1:B:3733:CYS:O	1:B:3766:GLN:NE2	2.18	0.77
1:C:961:MET:SD	1:C:963:ASN:CB	2.72	0.77
1:C:2742:THR:HG23	1:C:2814:LYS:HE3	1.67	0.77
1:B:961:MET:SD	1:B:963:ASN:CB	2.72	0.77
1:C:4687:TYR:O	1:C:4691:GLN:NE2	2.18	0.77
1:C:3300:ALA:HB3	1:C:3301:PRO:HD3	1.67	0.77
1:A:2742:THR:HG23	1:A:2814:LYS:HE3	1.67	0.77
1:D:166:GLY:C	1:C:384:MET:SD	2.67	0.77
1:D:1753:LYS:O	1:D:1758:ARG:HD2	1.85	0.77
1:D:2742:THR:HG23	1:D:2814:LYS:HE3	1.67	0.77
1:D:3236:VAL:HG23	1:D:3239:MET:SD	2.25	0.77
1:D:972:LEU:CG	1:D:1041:GLN:NE2	2.38	0.77
1:B:4687:TYR:O	1:B:4691:GLN:NE2	2.18	0.77
1:D:2233:CYS:CB	1:D:2237:CYS:HG	1.89	0.77
1:D:4687:TYR:O	1:D:4691:GLN:NE2	2.18	0.77
1:C:3733:CYS:O	1:C:3766:GLN:NE2	2.18	0.77
1:A:4687:TYR:O	1:A:4691:GLN:NE2	2.18	0.77
1:D:110:ARG:NH2	1:D:117:TYR:OH	2.17	0.77
1:B:2628:PHE:CE2	1:B:2734:ASN:OD1	2.38	0.76
1:D:981:GLN:O	1:D:985:VAL:HG23	1.83	0.76
1:A:2224:ARG:HG3	1:A:2225:PHE:CD2	2.20	0.76
1:A:2233:CYS:CB	1:A:2237:CYS:HG	1.91	0.76
1:B:3236:VAL:HG23	1:B:3239:MET:SD	2.25	0.76
1:A:3733:CYS:O	1:A:3766:GLN:NE2	2.18	0.76
1:B:721:LEU:HD12	1:B:1476:MET:HE1	1.68	0.76
1:C:721:LEU:HD12	1:C:1476:MET:HE1	1.68	0.76
1:C:2628:PHE:CE2	1:C:2734:ASN:OD1	2.38	0.76
1:C:1753:LYS:O	1:C:1758:ARG:HD2	1.85	0.76
1:B:2742:THR:HG23	1:B:2814:LYS:HE3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:721:LEU:HD12	1:D:1476:MET:HE1	1.68	0.76
1:D:2523:ASP:HB3	1:D:2578:MET:CE	2.11	0.76
1:A:2638:LYS:HE3	1:A:2694:GLU:OE1	1.86	0.76
1:B:3300:ALA:HB3	1:B:3301:PRO:HD3	1.67	0.76
1:A:710:ASP:OD1	1:A:713:SER:OG	2.03	0.76
1:B:710:ASP:OD1	1:B:713:SER:OG	2.03	0.76
1:B:1255:TYR:O	1:B:1275:ARG:NH1	2.19	0.76
1:D:3733:CYS:O	1:D:3766:GLN:NE2	2.18	0.76
1:B:1753:LYS:O	1:B:1758:ARG:HD2	1.85	0.76
1:C:1263:THR:OG1	1:C:1265:ASP:OD1	2.01	0.76
1:C:2224:ARG:HG3	1:C:2225:PHE:CD2	2.20	0.76
1:A:1255:TYR:O	1:A:1275:ARG:NH1	2.19	0.76
1:A:1263:THR:OG1	1:A:1265:ASP:OD1	2.01	0.76
1:C:2638:LYS:HE3	1:C:2694:GLU:OE1	1.86	0.76
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.67	0.75
1:D:1255:TYR:O	1:D:1275:ARG:NH1	2.19	0.75
1:D:3300:ALA:HB3	1:D:3301:PRO:HD3	1.67	0.75
1:A:721:LEU:HD12	1:A:1476:MET:HE1	1.68	0.75
1:A:1753:LYS:O	1:A:1758:ARG:HD2	1.85	0.75
1:A:2212:VAL:HG21	1:A:2256:TYR:OH	1.86	0.75
1:B:2224:ARG:HG3	1:B:2225:PHE:CD2	2.20	0.75
1:B:4902:GLU:O	1:B:4913:ARG:NH1	2.20	0.75
1:D:2628:PHE:CE2	1:D:2734:ASN:OD1	2.38	0.75
1:D:2638:LYS:HE3	1:D:2694:GLU:OE1	1.86	0.75
1:D:4902:GLU:O	1:D:4913:ARG:NH1	2.20	0.75
1:C:4902:GLU:O	1:C:4913:ARG:NH1	2.20	0.75
1:D:2212:VAL:HG21	1:D:2256:TYR:OH	1.86	0.75
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.67	0.75
1:A:2628:PHE:CE2	1:A:2734:ASN:OD1	2.38	0.75
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.67	0.75
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.67	0.75
1:C:1255:TYR:O	1:C:1275:ARG:NH1	2.19	0.75
1:A:870:ILE:O	1:A:874:LEU:HD12	1.87	0.74
1:A:4902:GLU:O	1:A:4913:ARG:NH1	2.20	0.74
1:B:2638:LYS:HE3	1:B:2694:GLU:OE1	1.86	0.74
1:B:2212:VAL:HG21	1:B:2256:TYR:OH	1.86	0.74
1:A:3300:ALA:HB3	1:A:3301:PRO:HD3	1.67	0.74
1:B:1999:ARG:NH1	1:B:3636:PHE:HD1	1.86	0.74
1:D:2233:CYS:HB3	1:D:2237:CYS:HG	1.47	0.74
1:C:2212:VAL:HG21	1:C:2256:TYR:OH	1.86	0.74
1:A:3159:ASP:HA	1:A:3218:VAL:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:941:MET:SD	1:B:1051:TYR:CD1	2.81	0.74
1:D:941:MET:SD	1:D:1051:TYR:CD1	2.81	0.74
1:A:2011:HIS:HE1	1:A:2017:ASP:CG	1.95	0.74
1:A:2638:LYS:CE	1:A:2694:GLU:OE1	2.36	0.74
1:B:2638:LYS:CE	1:B:2694:GLU:OE1	2.36	0.74
1:D:870:ILE:O	1:D:874:LEU:HD12	1.87	0.73
1:A:3458:PHE:HE2	1:A:3464:ILE:HD12	1.53	0.73
1:C:2011:HIS:HE1	1:C:2017:ASP:CG	1.95	0.73
1:A:2523:ASP:HB3	1:A:2578:MET:CE	2.11	0.73
1:B:2642:LYS:HG3	1:B:2698:MET:CE	2.15	0.73
1:B:2974:ILE:HD13	1:B:3049:LEU:HD12	1.71	0.73
1:D:774:ASP:OD2	1:D:1470:ARG:NH2	2.21	0.73
1:A:2186:MET:O	1:A:2192:TYR:OH	2.05	0.73
1:D:3159:ASP:HA	1:D:3218:VAL:HG22	1.69	0.73
1:A:774:ASP:OD2	1:A:1470:ARG:NH2	2.21	0.73
1:B:870:ILE:O	1:B:874:LEU:HD12	1.87	0.73
1:C:2186:MET:O	1:C:2192:TYR:OH	2.05	0.73
1:A:2974:ILE:HD13	1:A:3049:LEU:HD12	1.71	0.73
1:D:911:HIS:O	1:D:918:ARG:NH2	2.22	0.73
1:D:2011:HIS:HE1	1:D:2017:ASP:CG	1.96	0.73
1:D:1999:ARG:NH1	1:D:3636:PHE:HD1	1.86	0.73
1:C:870:ILE:O	1:C:874:LEU:HD12	1.87	0.73
1:C:1999:ARG:NH1	1:C:3636:PHE:HD1	1.86	0.73
1:C:2974:ILE:HD13	1:C:3049:LEU:HD12	1.71	0.73
1:A:2642:LYS:HG3	1:A:2698:MET:CE	2.15	0.73
1:C:2929:PHE:O	1:C:2932:MET:SD	2.47	0.73
1:A:911:HIS:O	1:A:918:ARG:NH2	2.22	0.72
1:B:911:HIS:O	1:B:918:ARG:NH2	2.22	0.72
1:B:3159:ASP:HA	1:B:3218:VAL:HG22	1.69	0.72
1:C:911:HIS:O	1:C:918:ARG:NH2	2.22	0.72
1:C:2642:LYS:HG3	1:C:2642:LYS:NZ	2.04	0.72
1:A:2929:PHE:O	1:A:2932:MET:SD	2.47	0.72
2:G:77:SER:OG	2:G:79:ASP:OD1	2.08	0.72
1:B:2011:HIS:HE1	1:B:2017:ASP:CG	1.96	0.72
1:B:3458:PHE:HE2	1:B:3464:ILE:HD12	1.53	0.72
1:D:2638:LYS:CE	1:D:2694:GLU:OE1	2.36	0.72
1:D:710:ASP:OD1	1:D:713:SER:OG	2.03	0.72
1:D:2186:MET:O	1:D:2192:TYR:OH	2.05	0.72
1:D:3458:PHE:HE2	1:D:3464:ILE:HD12	1.53	0.72
1:C:3343:GLN:OE1	1:C:3414:ARG:NE	2.23	0.72
1:A:1999:ARG:NH1	1:A:3636:PHE:HD1	1.86	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:774:ASP:OD2	1:B:1470:ARG:NH2	2.21	0.72
1:A:941:MET:SD	1:A:1051:TYR:CD1	2.81	0.72
1:B:213:TYR:CD1	1:B:340:LYS:HG2	2.25	0.72
1:B:3690:VAL:O	1:B:3693:LYS:HE3	1.90	0.72
1:C:774:ASP:OD2	1:C:1470:ARG:NH2	2.21	0.72
1:C:2638:LYS:CE	1:C:2694:GLU:OE1	2.36	0.72
1:B:4063:ASP:OD1	1:B:4064:MET:N	2.23	0.72
1:D:2628:PHE:HZ	1:D:2734:ASN:OD1	1.73	0.72
1:D:2929:PHE:O	1:D:2932:MET:SD	2.47	0.72
1:D:213:TYR:CD1	1:D:340:LYS:HG2	2.25	0.72
1:D:4093:PHE:CE1	1:D:4097:MET:HE3	2.25	0.72
1:D:4899:ASP:OD1	1:C:4892:ARG:NH1	2.23	0.72
1:C:3458:PHE:HE2	1:C:3464:ILE:HD12	1.53	0.72
1:A:213:TYR:CD1	1:A:340:LYS:HG2	2.25	0.72
1:A:4093:PHE:CE1	1:A:4097:MET:HE3	2.25	0.72
1:B:2642:LYS:HG3	1:B:2642:LYS:NZ	2.04	0.72
1:D:2572:THR:HG21	1:D:2579:VAL:HG21	1.71	0.72
1:D:2974:ILE:HD13	1:D:3049:LEU:HD12	1.71	0.72
1:D:3690:VAL:O	1:D:3693:LYS:HE3	1.90	0.72
1:B:2628:PHE:HZ	1:B:2734:ASN:OD1	1.73	0.71
1:B:2929:PHE:O	1:B:2932:MET:SD	2.47	0.71
1:D:4063:ASP:OD1	1:D:4064:MET:N	2.23	0.71
1:C:3891:LEU:HD13	1:C:3899:PHE:CZ	2.25	0.71
1:C:4063:ASP:OD1	1:C:4064:MET:N	2.23	0.71
1:A:4063:ASP:OD1	1:A:4064:MET:N	2.23	0.71
1:D:2642:LYS:HG3	1:D:2642:LYS:NZ	2.04	0.71
1:A:2572:THR:HG21	1:A:2579:VAL:HG21	1.71	0.71
1:A:3690:VAL:O	1:A:3693:LYS:HE3	1.90	0.71
2:F:77:SER:OG	2:F:79:ASP:OD1	2.08	0.71
1:B:672:VAL:O	1:B:680:THR:OG1	2.08	0.71
1:C:213:TYR:CD1	1:C:340:LYS:HG2	2.25	0.71
1:C:2572:THR:HG21	1:C:2579:VAL:HG21	1.71	0.71
1:C:3690:VAL:O	1:C:3693:LYS:HE3	1.90	0.71
1:C:4093:PHE:CE1	1:C:4097:MET:HE3	2.25	0.71
1:B:1087:ARG:NH1	1:B:1221:GLU:O	2.23	0.71
1:D:2642:LYS:HG3	1:D:2698:MET:CE	2.15	0.71
1:C:941:MET:SD	1:C:1051:TYR:CD1	2.81	0.71
1:A:384:MET:SD	1:B:166:GLY:O	2.48	0.71
1:B:3891:LEU:HD13	1:B:3899:PHE:CZ	2.25	0.71
1:D:3891:LEU:HD13	1:D:3899:PHE:CZ	2.25	0.71
1:C:3159:ASP:HA	1:C:3218:VAL:HG22	1.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3321:ARG:NH1	1:A:3325:ASN:OD1	2.23	0.71
1:B:3343:GLN:OE1	1:B:3414:ARG:NE	2.23	0.71
1:D:2761:TYR:HB3	1:D:2765:LYS:NZ	2.06	0.71
1:A:2233:CYS:O	1:A:2234:ARG:C	2.34	0.71
2:E:77:SER:OG	2:E:79:ASP:OD1	2.08	0.71
1:C:2761:TYR:HB3	1:C:2765:LYS:NZ	2.06	0.71
1:A:3891:LEU:HD13	1:A:3899:PHE:CZ	2.25	0.71
1:D:3321:ARG:NH1	1:D:3325:ASN:OD1	2.23	0.71
1:A:4899:ASP:OD1	1:D:4892:ARG:NH1	2.23	0.71
1:B:3321:ARG:NH1	1:B:3325:ASN:OD1	2.23	0.71
1:B:4093:PHE:CE1	1:B:4097:MET:HE3	2.25	0.71
1:A:3534:MET:O	1:A:3538:THR:HG23	1.91	0.70
2:E:80:TYR:CE2	2:E:80:TYR:CD1	2.38	0.70
1:B:2572:THR:HG21	1:B:2579:VAL:HG21	1.71	0.70
1:B:2761:TYR:HB3	1:B:2765:LYS:NZ	2.06	0.70
1:D:4961:CYS:SG	1:D:4978:HIS:CE1	2.84	0.70
1:A:2628:PHE:HZ	1:A:2734:ASN:OD1	1.73	0.70
1:A:2642:LYS:HG3	1:A:2642:LYS:NZ	2.04	0.70
1:A:672:VAL:O	1:A:680:THR:OG1	2.08	0.70
1:A:2011:HIS:CE1	1:A:2017:ASP:OD2	2.43	0.70
1:B:4205:TRP:CE3	1:B:4989:MET:HE2	2.27	0.70
1:B:4961:CYS:SG	1:B:4978:HIS:CE1	2.84	0.70
1:D:1821:ASP:OD1	1:D:1822:GLY:N	2.25	0.70
1:C:3321:ARG:NH1	1:C:3325:ASN:OD1	2.23	0.70
1:A:4961:CYS:SG	1:A:4978:HIS:CE1	2.84	0.70
2:H:77:SER:OG	2:H:79:ASP:OD1	2.08	0.70
2:G:1:GLY:HA2	2:G:80:TYR:CE2	2.27	0.70
1:C:2642:LYS:HG3	1:C:2698:MET:CE	2.15	0.70
1:D:1087:ARG:NH1	1:D:1221:GLU:O	2.24	0.70
1:C:672:VAL:O	1:C:680:THR:OG1	2.08	0.70
1:C:871:ARG:NH1	1:C:922:LEU:O	2.24	0.70
1:B:871:ARG:NH1	1:B:922:LEU:O	2.24	0.70
1:B:2523:ASP:HB3	1:B:2578:MET:CE	2.11	0.70
1:B:4892:ARG:NH1	1:C:4899:ASP:OD1	2.24	0.70
1:D:4205:TRP:CE3	1:D:4989:MET:HE2	2.27	0.70
1:A:871:ARG:NH1	1:A:922:LEU:O	2.24	0.70
1:D:887:ILE:HD11	1:D:907:LEU:HD22	1.73	0.70
1:C:1087:ARG:NH1	1:C:1221:GLU:O	2.23	0.70
1:C:2523:ASP:HB3	1:C:2578:MET:CE	2.11	0.70
1:A:1087:ARG:NH1	1:A:1221:GLU:O	2.24	0.70
2:H:1:GLY:HA2	2:H:80:TYR:CE2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:887:ILE:HD11	1:B:907:LEU:CD2	2.22	0.70
1:A:2761:TYR:HB3	1:A:2765:LYS:NZ	2.06	0.70
1:D:887:ILE:HD11	1:D:907:LEU:CD2	2.22	0.70
1:A:1821:ASP:OD1	1:A:1822:GLY:N	2.24	0.69
1:B:3550:ARG:NH1	1:B:3597:GLN:OE1	2.25	0.69
1:C:710:ASP:OD1	1:C:713:SER:OG	2.03	0.69
1:C:3550:ARG:NH1	1:C:3597:GLN:OE1	2.25	0.69
1:A:1733:GLU:HG2	1:A:2201:LEU:HD23	1.74	0.69
1:A:2244:ARG:NH2	1:A:3858:MET:SD	2.65	0.69
1:B:887:ILE:HD11	1:B:907:LEU:HD22	1.73	0.69
1:D:3550:ARG:NH1	1:D:3597:GLN:OE1	2.25	0.69
1:C:69:LEU:HD13	1:C:101:LEU:HD11	1.74	0.69
1:A:3343:GLN:OE1	1:A:3414:ARG:NE	2.23	0.69
1:D:871:ARG:NH1	1:D:922:LEU:O	2.24	0.69
1:D:2244:ARG:NH2	1:D:3858:MET:SD	2.65	0.69
1:A:887:ILE:HD11	1:A:907:LEU:CD2	2.22	0.69
1:A:3550:ARG:NH1	1:A:3597:GLN:OE1	2.25	0.69
1:A:4767:TRP:CE3	1:A:4768:LEU:HD23	2.28	0.69
1:B:3534:MET:O	1:B:3538:THR:HG23	1.91	0.69
1:D:925:SER:O	1:D:928:THR:OG1	2.10	0.69
1:C:887:ILE:HD11	1:C:907:LEU:CD2	2.22	0.69
1:A:69:LEU:HD13	1:A:101:LEU:HD11	1.75	0.69
1:A:4205:TRP:CE3	1:A:4989:MET:HE2	2.27	0.69
1:D:1808:ARG:HD2	1:D:1853:ILE:HG22	1.75	0.69
1:D:3534:MET:O	1:D:3538:THR:HG23	1.91	0.69
1:C:4961:CYS:SG	1:C:4978:HIS:CE1	2.84	0.69
1:B:4767:TRP:CE3	1:B:4768:LEU:HD23	2.28	0.69
1:D:2970:SER:HA	1:D:2973:PHE:CE1	2.28	0.69
1:C:2244:ARG:NH2	1:C:3858:MET:SD	2.66	0.69
1:C:2628:PHE:HZ	1:C:2734:ASN:OD1	1.73	0.69
2:F:1:GLY:HA2	2:F:80:TYR:CE2	2.27	0.69
1:B:2244:ARG:NH2	1:B:3858:MET:SD	2.65	0.69
1:B:3343:GLN:O	1:B:3346:VAL:HG12	1.93	0.69
1:D:4767:TRP:CE3	1:D:4768:LEU:HD23	2.27	0.69
1:C:925:SER:O	1:C:928:THR:OG1	2.10	0.69
1:C:1821:ASP:OD1	1:C:1822:GLY:N	2.25	0.69
1:C:3343:GLN:O	1:C:3346:VAL:HG12	1.93	0.69
1:A:581:ASN:OD1	1:A:582:HIS:N	2.26	0.69
1:A:918:ARG:O	1:A:922:LEU:HD23	1.93	0.69
1:A:1808:ARG:HD2	1:A:1853:ILE:HG22	1.75	0.69
1:A:2516:ASP:OD1	1:A:2517:PHE:N	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:GLY:HA2	2:E:80:TYR:CE2	2.27	0.69
1:B:69:LEU:HD13	1:B:101:LEU:HD11	1.75	0.69
1:B:384:MET:SD	1:C:166:GLY:O	2.51	0.69
1:B:1821:ASP:OD1	1:B:1822:GLY:N	2.25	0.69
1:D:69:LEU:HD13	1:D:101:LEU:HD11	1.75	0.69
1:D:451:TYR:O	1:D:474:ARG:NH2	2.26	0.69
1:D:581:ASN:OD1	1:D:582:HIS:N	2.26	0.69
1:D:2233:CYS:O	1:D:2234:ARG:C	2.34	0.69
1:D:2516:ASP:OD1	1:D:2517:PHE:N	2.26	0.69
1:D:3293:PRO:HB2	1:D:3298:ALA:HB2	1.75	0.69
1:C:887:ILE:HD11	1:C:907:LEU:HD22	1.73	0.69
1:C:4205:TRP:CE3	1:C:4989:MET:HE2	2.27	0.69
1:C:4767:TRP:CE3	1:C:4768:LEU:HD23	2.28	0.69
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.26	0.69
1:B:1733:GLU:HG2	1:B:2201:LEU:HD23	1.74	0.69
1:D:1733:GLU:HG2	1:D:2201:LEU:HD23	1.74	0.69
1:D:2350:ALA:O	1:D:2354:VAL:HG23	1.93	0.69
1:D:3458:PHE:CE2	1:D:3464:ILE:HD12	2.28	0.69
1:C:3284:TRP:O	1:C:3305:THR:HG21	1.93	0.69
1:C:3293:PRO:HB2	1:C:3298:ALA:HB2	1.75	0.69
1:C:3534:MET:O	1:C:3538:THR:HG23	1.91	0.69
2:F:80:TYR:CE2	2:F:80:TYR:CD1	2.38	0.69
1:A:2970:SER:HA	1:A:2973:PHE:CE1	2.28	0.68
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.26	0.68
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.26	0.68
1:B:5014:TYR:CD1	6:B:5304:PNX:HAA3	2.29	0.68
1:D:820:ARG:NH1	1:D:821:LEU:H	1.92	0.68
1:D:3343:GLN:OE1	1:D:3414:ARG:NE	2.23	0.68
1:C:918:ARG:O	1:C:922:LEU:HD23	1.93	0.68
1:C:1808:ARG:HD2	1:C:1853:ILE:HG22	1.74	0.68
1:C:2970:SER:HA	1:C:2973:PHE:CE1	2.28	0.68
1:A:820:ARG:NH1	1:A:821:LEU:H	1.92	0.68
1:A:3343:GLN:O	1:A:3346:VAL:HG12	1.93	0.68
1:D:2211:MET:O	1:D:2214:VAL:HG12	1.93	0.68
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.26	0.68
1:A:887:ILE:HD11	1:A:907:LEU:HD22	1.73	0.68
2:H:11:ASP:OD2	2:H:12:GLY:N	2.27	0.68
1:D:918:ARG:O	1:D:922:LEU:HD23	1.93	0.68
1:D:3284:TRP:O	1:D:3305:THR:HG21	1.93	0.68
1:C:2011:HIS:CE1	1:C:2017:ASP:OD2	2.43	0.68
1:A:3458:PHE:CE2	1:A:3464:ILE:HD12	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5014:TYR:CD1	6:D:5304:PNX:HAA3	2.29	0.68
1:C:581:ASN:OD1	1:C:582:HIS:N	2.26	0.68
1:C:1987:SER:O	1:C:1991:THR:OG1	2.08	0.68
1:C:2211:MET:O	1:C:2214:VAL:HG12	1.93	0.68
1:C:5014:TYR:CD1	6:C:5304:PNX:HAA3	2.28	0.68
1:A:54:ASN:O	1:A:56:GLN:N	2.27	0.68
1:B:581:ASN:OD1	1:B:582:HIS:N	2.26	0.68
1:B:3458:PHE:CE2	1:B:3464:ILE:HD12	2.28	0.68
1:D:1821:ASP:OD2	1:D:1837:GLN:NE2	2.26	0.68
1:C:820:ARG:NH1	1:C:821:LEU:H	1.92	0.68
1:A:1980:LEU:HD11	1:A:1991:THR:HG23	1.75	0.68
1:A:2350:ALA:O	1:A:2354:VAL:HG23	1.93	0.68
2:E:11:ASP:OD2	2:E:12:GLY:N	2.27	0.68
1:B:1808:ARG:HD2	1:B:1853:ILE:HG22	1.74	0.68
1:B:2970:SER:HA	1:B:2973:PHE:CE1	2.28	0.68
1:B:3293:PRO:HB2	1:B:3298:ALA:HB2	1.75	0.68
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.26	0.68
1:D:3343:GLN:O	1:D:3346:VAL:HG12	1.93	0.68
1:D:4929:LEU:O	1:D:4933:GLN:OE1	2.12	0.68
1:C:1980:LEU:HD11	1:C:1991:THR:HG23	1.75	0.68
1:A:3293:PRO:HB2	1:A:3298:ALA:HB2	1.75	0.68
1:C:2233:CYS:O	1:C:2234:ARG:C	2.34	0.68
2:F:11:ASP:OD2	2:F:12:GLY:N	2.27	0.68
1:A:4929:LEU:O	1:A:4933:GLN:OE1	2.12	0.68
1:B:451:TYR:O	1:B:474:ARG:NH2	2.26	0.68
1:B:820:ARG:NH1	1:B:821:LEU:H	1.92	0.68
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.26	0.68
1:B:2211:MET:O	1:B:2214:VAL:HG12	1.93	0.68
1:B:2350:ALA:O	1:B:2354:VAL:HG23	1.93	0.68
1:D:4749:GLU:HB3	1:D:4753:HIS:HE1	1.59	0.68
1:C:54:ASN:O	1:C:56:GLN:N	2.27	0.68
1:C:1821:ASP:OD2	1:C:1837:GLN:NE2	2.26	0.68
1:C:2350:ALA:O	1:C:2354:VAL:HG23	1.93	0.68
1:C:2516:ASP:OD1	1:C:2517:PHE:N	2.26	0.68
1:A:2211:MET:O	1:A:2214:VAL:HG12	1.93	0.67
1:B:1980:LEU:HD11	1:B:1991:THR:HG23	1.75	0.67
1:C:2288:LEU:O	1:C:3849:ARG:NH1	2.26	0.67
1:A:5014:TYR:CD1	6:A:5304:PNX:HAA3	2.28	0.67
2:G:11:ASP:OD2	2:G:12:GLY:N	2.27	0.67
1:B:54:ASN:O	1:B:56:GLN:N	2.27	0.67
1:B:918:ARG:O	1:B:922:LEU:HD23	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2186:MET:O	1:B:2192:TYR:OH	2.05	0.67
1:B:2233:CYS:O	1:B:2234:ARG:C	2.34	0.67
1:A:4749:GLU:HB3	1:A:4753:HIS:HE1	1.59	0.67
1:B:1821:ASP:OD2	1:B:1837:GLN:NE2	2.26	0.67
1:B:2516:ASP:OD1	1:B:2517:PHE:N	2.26	0.67
1:A:1821:ASP:OD2	1:A:1837:GLN:NE2	2.26	0.67
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.26	0.67
1:B:3284:TRP:O	1:B:3305:THR:HG21	1.93	0.67
1:D:3324:VAL:HG11	1:D:3361:THR:HG22	1.76	0.67
1:A:166:GLY:O	1:D:384:MET:SD	2.52	0.67
1:B:3239:MET:SD	1:B:3239:MET:HG2	2.31	0.67
1:B:3324:VAL:HG11	1:B:3361:THR:HG22	1.76	0.67
1:C:908:VAL:O	1:C:963:ASN:ND2	2.28	0.67
1:C:3458:PHE:CE2	1:C:3464:ILE:HD12	2.28	0.67
1:C:493:ARG:O	1:C:496:VAL:HG22	1.94	0.67
1:C:4749:GLU:HB3	1:C:4753:HIS:HE1	1.59	0.67
1:A:3521:GLY:HA2	1:A:3524:MET:HE3	1.77	0.67
1:A:3825:GLU:OE1	1:A:3825:GLU:N	2.28	0.67
1:D:166:GLY:O	1:C:384:MET:SD	2.53	0.67
1:C:3239:MET:SD	1:C:3239:MET:HG2	2.31	0.67
1:A:493:ARG:O	1:A:496:VAL:HG22	1.94	0.67
1:A:4070:ASP:OD1	1:A:4071:ILE:N	2.28	0.67
1:B:961:MET:SD	1:B:963:ASN:N	2.68	0.67
1:B:4749:GLU:HB3	1:B:4753:HIS:HE1	1.59	0.67
1:C:1733:GLU:HG2	1:C:2201:LEU:HD23	1.74	0.67
1:D:54:ASN:O	1:D:56:GLN:N	2.27	0.67
1:D:908:VAL:O	1:D:963:ASN:ND2	2.28	0.67
1:D:3239:MET:HG2	1:D:3239:MET:HA	1.76	0.67
1:A:2233:CYS:CA	1:A:2237:CYS:SG	2.83	0.67
1:A:3324:VAL:HG11	1:A:3361:THR:HG22	1.76	0.67
1:B:4929:LEU:O	1:B:4933:GLN:OE1	2.12	0.67
1:D:1980:LEU:HD11	1:D:1991:THR:HG23	1.75	0.67
1:C:3324:VAL:HG11	1:C:3361:THR:HG22	1.76	0.67
1:B:493:ARG:O	1:B:496:VAL:HG22	1.94	0.66
1:B:3825:GLU:OE1	1:B:3825:GLU:N	2.28	0.66
1:D:672:VAL:O	1:D:680:THR:OG1	2.08	0.66
1:C:4929:LEU:O	1:C:4933:GLN:OE1	2.12	0.66
1:A:2572:THR:O	1:A:2572:THR:HG22	1.95	0.66
1:D:493:ARG:O	1:D:496:VAL:HG22	1.94	0.66
1:C:4070:ASP:OD1	1:C:4071:ILE:N	2.28	0.66
1:A:451:TYR:O	1:A:474:ARG:NH2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1980:LEU:HD21	1:D:1995:THR:HG22	1.78	0.66
1:C:2625:ARG:NH1	1:C:2629:ASP:OD1	2.25	0.66
1:A:908:VAL:O	1:A:963:ASN:ND2	2.28	0.66
1:A:925:SER:O	1:A:928:THR:OG1	2.10	0.66
1:A:3284:TRP:O	1:A:3305:THR:HG21	1.93	0.66
2:H:80:TYR:CE2	2:H:80:TYR:CD1	2.38	0.66
1:B:2011:HIS:CE1	1:B:2017:ASP:OD2	2.43	0.66
1:C:961:MET:SD	1:C:963:ASN:N	2.68	0.66
1:A:1068:ARG:O	1:A:1072:VAL:HG12	1.96	0.66
1:A:4910:GLU:O	1:A:4914:VAL:HG13	1.96	0.66
2:F:1:GLY:HA2	2:F:80:TYR:HE2	1.60	0.66
1:D:2642:LYS:CG	1:D:2642:LYS:CE	2.74	0.66
1:C:1980:LEU:HD21	1:C:1995:THR:HG22	1.78	0.66
1:B:4070:ASP:OD1	1:B:4071:ILE:N	2.28	0.66
1:D:4070:ASP:OD1	1:D:4071:ILE:N	2.28	0.66
1:B:908:VAL:O	1:B:963:ASN:ND2	2.28	0.66
1:D:1424:PRO:O	1:D:1428:LEU:HD23	1.96	0.66
1:D:61:ASP:OD2	1:D:402:ARG:NH2	2.28	0.66
1:D:2233:CYS:CA	1:D:2237:CYS:SG	2.84	0.66
1:D:4910:GLU:O	1:D:4914:VAL:HG13	1.96	0.66
1:C:2233:CYS:CB	1:C:2237:CYS:HG	2.02	0.66
1:A:61:ASP:OD2	1:A:402:ARG:NH2	2.28	0.66
1:D:2572:THR:HG21	1:D:2579:VAL:HG23	1.78	0.66
1:C:796:ARG:HH12	1:C:1619:ARG:HH12	1.44	0.66
1:C:3825:GLU:N	1:C:3825:GLU:OE1	2.28	0.66
1:A:2572:THR:HG21	1:A:2579:VAL:HG23	1.78	0.66
1:D:1980:LEU:HD21	1:D:1995:THR:CG2	2.26	0.66
1:D:3235:SER:OG	1:D:3237:GLU:OE1	2.14	0.66
1:C:2642:LYS:CG	1:C:2642:LYS:CE	2.74	0.66
1:A:1980:LEU:HD21	1:A:1995:THR:HG22	1.78	0.65
1:D:796:ARG:HH12	1:D:1619:ARG:HH12	1.44	0.65
1:D:4148:THR:HG21	1:D:4180:ARG:HH21	1.62	0.65
1:A:146:CYS:HG	1:A:147:TRP:CD1	2.14	0.65
1:A:796:ARG:HH12	1:A:1619:ARG:HH12	1.44	0.65
2:E:1:GLY:HA2	2:E:80:TYR:HE2	1.60	0.65
1:B:796:ARG:HH12	1:B:1619:ARG:HH12	1.44	0.65
1:D:1068:ARG:O	1:D:1072:VAL:HG12	1.96	0.65
1:D:3897:ASN:OD1	1:D:3901:ASN:ND2	2.29	0.65
1:C:1975:SER:O	1:C:1979:LEU:HD23	1.96	0.65
1:C:2233:CYS:CA	1:C:2237:CYS:SG	2.84	0.65
1:C:3897:ASN:OD1	1:C:3901:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1424:PRO:O	1:A:1428:LEU:HD23	1.96	0.65
1:A:1980:LEU:HD21	1:A:1995:THR:CG2	2.26	0.65
1:A:2642:LYS:CG	1:A:2642:LYS:CE	2.74	0.65
1:A:3897:ASN:OD1	1:A:3901:ASN:ND2	2.29	0.65
1:B:2233:CYS:CA	1:B:2237:CYS:SG	2.83	0.65
1:B:3235:SER:OG	1:B:3237:GLU:OE1	2.14	0.65
1:B:3897:ASN:OD1	1:B:3901:ASN:ND2	2.29	0.65
1:C:1424:PRO:O	1:C:1428:LEU:HD23	1.96	0.65
1:B:2642:LYS:CG	1:B:2642:LYS:CE	2.74	0.65
1:C:2572:THR:HG21	1:C:2579:VAL:HG23	1.78	0.65
1:B:2625:ARG:NH1	1:B:2629:ASP:OD1	2.25	0.65
1:B:3239:MET:SD	1:B:3239:MET:HG3	2.31	0.65
1:D:1032:LYS:O	1:D:1036:ARG:HG3	1.97	0.65
1:D:2625:ARG:NH1	1:D:2629:ASP:OD1	2.25	0.65
1:C:451:TYR:O	1:C:474:ARG:NH2	2.26	0.65
1:C:4148:THR:HG21	1:C:4180:ARG:HH21	1.62	0.65
1:B:1980:LEU:HD21	1:B:1995:THR:HG22	1.78	0.65
1:C:1980:LEU:HD21	1:C:1995:THR:CG2	2.26	0.65
1:C:2440:MET:O	1:C:2444:GLN:OE1	2.15	0.65
1:A:1032:LYS:O	1:A:1036:ARG:HG3	1.97	0.65
1:B:1980:LEU:HD21	1:B:1995:THR:CG2	2.26	0.65
1:B:2224:ARG:HE	1:B:2225:PHE:H	1.44	0.65
1:B:2523:ASP:OD1	1:B:2524:VAL:HG13	1.97	0.65
1:D:2751:LEU:O	1:D:2755:ILE:HD12	1.97	0.65
1:C:61:ASP:OD2	1:C:402:ARG:NH2	2.28	0.65
2:G:1:GLY:HA2	2:G:80:TYR:HE2	1.60	0.65
1:B:296:ASP:CG	1:B:297:GLN:OE1	2.40	0.65
1:B:2440:MET:O	1:B:2444:GLN:OE1	2.15	0.65
1:B:4148:THR:HG21	1:B:4180:ARG:HH21	1.62	0.65
1:D:2523:ASP:OD1	1:D:2524:VAL:HG13	1.97	0.65
1:C:2572:THR:HG22	1:C:2572:THR:O	1.95	0.65
1:C:2751:LEU:O	1:C:2755:ILE:HD12	1.97	0.65
1:C:3235:SER:OG	1:C:3237:GLU:OE1	2.14	0.65
1:A:924:MET:O	1:A:928:THR:HG23	1.97	0.65
1:A:1975:SER:O	1:A:1979:LEU:HD23	1.96	0.65
1:A:4148:THR:HG21	1:A:4180:ARG:HH21	1.62	0.65
1:B:61:ASP:OD2	1:B:402:ARG:NH2	2.28	0.65
1:B:1424:PRO:O	1:B:1428:LEU:HD23	1.96	0.65
1:B:4910:GLU:O	1:B:4914:VAL:HG13	1.96	0.65
1:C:568:LEU:HD12	1:C:602:VAL:HG13	1.80	0.65
1:C:1068:ARG:O	1:C:1072:VAL:HG12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2440:MET:O	1:A:2444:GLN:OE1	2.14	0.64
1:A:2751:LEU:O	1:A:2755:ILE:HD12	1.97	0.64
1:A:3235:SER:OG	1:A:3237:GLU:OE1	2.14	0.64
1:B:568:LEU:HD12	1:B:602:VAL:HG13	1.79	0.64
1:D:3239:MET:SD	1:D:3239:MET:HG3	2.31	0.64
1:C:146:CYS:HG	1:C:147:TRP:CD1	2.16	0.64
1:B:1032:LYS:O	1:B:1036:ARG:HG3	1.97	0.64
1:B:1068:ARG:O	1:B:1072:VAL:HG12	1.96	0.64
1:D:2572:THR:O	1:D:2572:THR:HG22	1.95	0.64
1:A:296:ASP:CG	1:A:297:GLN:OE1	2.40	0.64
1:B:2572:THR:O	1:B:2572:THR:HG22	1.95	0.64
1:D:1975:SER:O	1:D:1979:LEU:HD23	1.96	0.64
1:D:924:MET:O	1:D:928:THR:HG23	1.97	0.64
1:D:959:TYR:HD2	1:D:966:LYS:HE2	1.63	0.64
1:A:568:LEU:HD12	1:A:602:VAL:HG13	1.79	0.64
1:A:2625:ARG:NH1	1:A:2629:ASP:OD1	2.25	0.64
1:A:4818:MET:O	1:A:4824:ARG:NH2	2.29	0.64
2:H:1:GLY:HA2	2:H:80:TYR:HE2	1.60	0.64
1:B:4634:GLU:OE1	1:B:4636:THR:OG1	2.16	0.64
1:C:4910:GLU:O	1:C:4914:VAL:HG13	1.96	0.64
1:A:2224:ARG:HE	1:A:2225:PHE:H	1.44	0.64
1:A:2523:ASP:OD1	1:A:2524:VAL:HG13	1.97	0.64
1:C:296:ASP:CG	1:C:297:GLN:OE1	2.40	0.64
1:C:924:MET:O	1:C:928:THR:HG23	1.97	0.64
1:C:2523:ASP:OD1	1:C:2524:VAL:HG13	1.97	0.64
1:A:2829:GLY:O	1:A:2830:GLU:OE1	2.16	0.64
1:B:1975:SER:O	1:B:1979:LEU:HD23	1.96	0.64
1:D:2440:MET:O	1:D:2444:GLN:OE1	2.15	0.64
1:D:2615:ARG:NH1	1:D:2663:ASN:O	2.31	0.64
1:D:3825:GLU:OE1	1:D:3825:GLU:N	2.28	0.64
1:C:1032:LYS:O	1:C:1036:ARG:HG3	1.97	0.64
1:C:2224:ARG:HE	1:C:2225:PHE:H	1.45	0.64
1:B:959:TYR:HD2	1:B:966:LYS:HE2	1.63	0.64
1:D:2011:HIS:CE1	1:D:2017:ASP:OD2	2.43	0.64
1:B:2829:GLY:O	1:B:2830:GLU:OE1	2.16	0.64
1:D:2224:ARG:HE	1:D:2225:PHE:H	1.44	0.64
1:A:959:TYR:HD2	1:A:966:LYS:HE2	1.63	0.64
1:D:568:LEU:HD12	1:D:602:VAL:HG13	1.80	0.64
1:D:880:GLU:OE1	1:D:967:PRO:HB2	1.98	0.64
1:C:880:GLU:OE1	1:C:967:PRO:HB2	1.98	0.64
1:C:4658:ILE:HD12	1:C:4796:MET:SD	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4747:SER:O	1:C:4751:THR:HG23	1.98	0.64
1:B:1987:SER:O	1:B:1991:THR:OG1	2.08	0.63
1:D:961:MET:SD	1:D:963:ASN:N	2.68	0.63
1:D:3458:PHE:CE2	1:D:3464:ILE:CD1	2.80	0.63
1:C:2829:GLY:O	1:C:2830:GLU:OE1	2.16	0.63
1:C:3521:GLY:HA2	1:C:3524:MET:HE3	1.77	0.63
1:C:4093:PHE:CZ	1:C:4097:MET:HE3	2.34	0.63
1:A:961:MET:SD	1:A:963:ASN:N	2.68	0.63
1:B:925:SER:O	1:B:928:THR:OG1	2.10	0.63
1:B:2751:LEU:O	1:B:2755:ILE:HD12	1.97	0.63
1:D:2829:GLY:O	1:D:2830:GLU:OE1	2.16	0.63
1:D:3521:GLY:HA2	1:D:3524:MET:HE3	1.77	0.63
1:C:961:MET:CE	1:C:963:ASN:CB	2.59	0.63
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.15	0.63
1:C:4711:PHE:HB3	1:C:4712:PRO:HD3	1.80	0.63
1:A:3239:MET:SD	1:A:3239:MET:HG2	2.31	0.63
1:B:880:GLU:OE1	1:B:967:PRO:HB2	1.98	0.63
1:B:2615:ARG:NH1	1:B:2663:ASN:O	2.31	0.63
1:B:4749:GLU:C	1:B:4753:HIS:HD1	2.07	0.63
1:D:2214:VAL:HG11	1:D:2228:MET:HE1	1.81	0.63
1:C:2644:LEU:HD13	1:C:2678:LEU:HD21	1.80	0.63
1:A:4093:PHE:CZ	1:A:4097:MET:HE3	2.34	0.63
1:B:924:MET:O	1:B:928:THR:HG23	1.97	0.63
1:B:3239:MET:CG	1:B:3239:MET:CE	2.77	0.63
1:C:959:TYR:HD2	1:C:966:LYS:HE2	1.63	0.63
1:C:2214:VAL:HG11	1:C:2228:MET:HE1	1.81	0.63
1:A:4711:PHE:HB3	1:A:4712:PRO:HD3	1.80	0.63
1:D:296:ASP:CG	1:D:297:GLN:OE1	2.40	0.63
1:C:870:ILE:HD11	1:C:1049:TYR:CD2	2.34	0.63
1:C:2615:ARG:NH1	1:C:2663:ASN:O	2.31	0.63
1:C:2623:LEU:O	1:C:2627:VAL:HG23	1.99	0.63
1:A:2615:ARG:NH1	1:A:2663:ASN:O	2.31	0.63
1:A:3368:ARG:O	1:A:3372:VAL:HG23	1.99	0.63
1:B:870:ILE:HD11	1:B:1049:TYR:CD2	2.34	0.63
1:D:881:LEU:O	1:D:885:THR:HG23	1.99	0.63
1:D:2623:LEU:O	1:D:2627:VAL:HG23	1.99	0.63
1:A:2157:GLU:O	1:A:2161:GLN:NE2	2.32	0.63
1:A:2644:LEU:HD13	1:A:2678:LEU:HD21	1.80	0.63
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.15	0.63
1:B:871:ARG:CD	1:B:926:GLY:HA2	2.29	0.63
1:B:881:LEU:O	1:B:885:THR:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:881:LEU:O	1:C:885:THR:HG23	1.99	0.63
1:C:4749:GLU:C	1:C:4753:HIS:HD1	2.07	0.63
1:A:3239:MET:SD	1:A:3239:MET:HG3	2.31	0.62
1:A:4658:ILE:HD12	1:A:4796:MET:SD	2.38	0.62
1:B:2233:CYS:CB	1:B:2237:CYS:HG	2.04	0.62
1:B:2572:THR:HG21	1:B:2579:VAL:HG23	1.78	0.62
1:B:2644:LEU:HD13	1:B:2678:LEU:HD21	1.80	0.62
1:B:4711:PHE:HB3	1:B:4712:PRO:HD3	1.80	0.62
1:D:4093:PHE:CZ	1:D:4097:MET:HE3	2.34	0.62
1:D:4658:ILE:HD12	1:D:4796:MET:SD	2.38	0.62
1:C:3368:ARG:O	1:C:3372:VAL:HG23	1.99	0.62
1:A:880:GLU:OE1	1:A:967:PRO:HB2	1.98	0.62
1:A:881:LEU:O	1:A:885:THR:HG23	1.99	0.62
1:A:2214:VAL:HG11	1:A:2228:MET:HE1	1.81	0.62
1:B:2623:LEU:O	1:B:2627:VAL:HG23	1.99	0.62
1:C:871:ARG:CD	1:C:926:GLY:HA2	2.29	0.62
1:C:3834:ALA:O	1:C:3838:THR:HG23	1.99	0.62
1:A:1987:SER:O	1:A:1991:THR:OG1	2.08	0.62
1:A:3239:MET:CG	1:A:3239:MET:CE	2.77	0.62
1:A:4630:TYR:OH	1:B:4860:ARG:NH1	2.30	0.62
1:B:2157:GLU:O	1:B:2161:GLN:NE2	2.32	0.62
1:B:3834:ALA:O	1:B:3838:THR:HG23	1.99	0.62
1:D:3368:ARG:O	1:D:3372:VAL:HG23	1.99	0.62
1:D:4747:SER:O	1:D:4751:THR:HG23	1.98	0.62
1:A:1577:ALA:O	1:A:1584:ARG:NH1	2.32	0.62
1:A:3458:PHE:CE2	1:A:3464:ILE:CD1	2.81	0.62
1:A:4747:SER:O	1:A:4751:THR:HG23	1.98	0.62
1:D:988:LEU:HB3	1:D:1039:LEU:HD11	1.81	0.62
1:D:1987:SER:O	1:D:1991:THR:OG1	2.08	0.62
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.15	0.62
1:A:972:LEU:CD1	1:A:1041:GLN:NE2	2.62	0.62
1:A:3834:ALA:O	1:A:3838:THR:HG23	1.99	0.62
1:B:4658:ILE:HD12	1:B:4796:MET:SD	2.38	0.62
1:D:4749:GLU:C	1:D:4753:HIS:HD1	2.07	0.62
1:A:2623:LEU:O	1:A:2627:VAL:HG23	1.99	0.62
1:A:4749:GLU:C	1:A:4753:HIS:HD1	2.07	0.62
1:B:4747:SER:O	1:B:4751:THR:HG23	1.98	0.62
1:D:3834:ALA:O	1:D:3838:THR:HG23	1.99	0.62
1:C:2203:MET:HE2	1:C:2235:PHE:CZ	2.35	0.62
1:C:3239:MET:CG	1:C:3239:MET:CE	2.77	0.62
1:A:3969:ILE:HG21	1:A:3980:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3368:ARG:O	1:B:3372:VAL:HG23	1.99	0.62
1:B:4818:MET:O	1:B:4824:ARG:NH2	2.29	0.62
1:D:870:ILE:HD11	1:D:1049:TYR:CD2	2.34	0.62
1:D:2782:ASP:OD2	1:D:2785:LEU:HD22	1.99	0.62
1:D:3213:TYR:CE1	1:D:3302:PRO:HG2	2.34	0.62
1:C:2157:GLU:O	1:C:2161:GLN:NE2	2.32	0.62
1:B:146:CYS:HG	1:B:147:TRP:CD1	2.18	0.62
1:B:988:LEU:HB3	1:B:1039:LEU:HD11	1.81	0.62
1:B:3671:ASP:OD1	1:B:3672:ARG:N	2.33	0.62
1:B:4093:PHE:CZ	1:B:4097:MET:HE3	2.34	0.62
1:D:972:LEU:CD1	1:D:1041:GLN:NE2	2.62	0.62
1:D:2157:GLU:O	1:D:2161:GLN:NE2	2.32	0.62
1:D:2644:LEU:HD13	1:D:2678:LEU:HD21	1.80	0.62
1:A:870:ILE:HD11	1:A:1049:TYR:CD2	2.34	0.62
1:A:1280:GLN:O	1:A:1281:ASN:OD1	2.18	0.62
1:A:4745:LEU:O	1:A:4749:GLU:OE1	2.18	0.62
1:B:972:LEU:CD1	1:B:1041:GLN:NE2	2.62	0.62
1:D:4711:PHE:HB3	1:D:4712:PRO:HD3	1.80	0.62
1:A:3213:TYR:CE1	1:A:3302:PRO:HG2	2.34	0.62
1:B:2203:MET:HE2	1:B:2235:PHE:CZ	2.35	0.62
1:B:2214:VAL:HG11	1:B:2228:MET:HE1	1.81	0.62
1:D:3239:MET:CG	1:D:3239:MET:CE	2.77	0.62
1:A:2744:ASN:OD1	1:A:2745:VAL:N	2.33	0.61
1:A:3671:ASP:OD1	1:A:3672:ARG:N	2.33	0.61
2:F:16:PRO:O	2:F:17:LYS:HE2	2.00	0.61
1:B:3213:TYR:CE1	1:B:3302:PRO:HG2	2.34	0.61
1:D:2203:MET:HE2	1:D:2235:PHE:CZ	2.35	0.61
1:C:3213:TYR:CE1	1:C:3302:PRO:HG2	2.34	0.61
1:C:3239:MET:SD	1:C:3239:MET:HG3	2.31	0.61
1:C:3573:MET:CB	1:C:3577:ARG:HH12	2.12	0.61
1:A:2782:ASP:OD2	1:A:2785:LEU:HD22	1.99	0.61
2:E:79:ASP:OD1	2:E:80:TYR:N	2.33	0.61
1:B:281:ARG:NH2	1:B:309:THR:OG1	2.33	0.61
1:B:2744:ASN:OD1	1:B:2745:VAL:N	2.33	0.61
1:D:2265:LEU:HD12	1:D:2266:GLY:N	2.15	0.61
1:D:3969:ILE:HG21	1:D:3980:LEU:HD12	1.82	0.61
1:A:281:ARG:NH2	1:A:309:THR:OG1	2.33	0.61
2:G:16:PRO:O	2:G:17:LYS:HE2	2.00	0.61
1:B:1577:ALA:O	1:B:1584:ARG:NH1	2.32	0.61
1:B:2782:ASP:OD2	1:B:2785:LEU:HD22	1.99	0.61
1:B:3969:ILE:HG21	1:B:3980:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4584:ASP:OD1	1:B:4585:SER:N	2.33	0.61
1:C:1280:GLN:O	1:C:1281:ASN:OD1	2.18	0.61
1:C:3671:ASP:OD1	1:C:3672:ARG:N	2.33	0.61
1:C:4634:GLU:OE1	1:C:4636:THR:OG1	2.16	0.61
1:B:906:CYS:HB2	1:B:913:LEU:HB2	1.83	0.61
1:B:1929:MET:O	1:B:1930:LYS:CB	2.49	0.61
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.35	0.61
1:C:988:LEU:HB3	1:C:1039:LEU:HD11	1.81	0.61
1:A:988:LEU:HB3	1:A:1039:LEU:HD11	1.81	0.61
1:A:2203:MET:HE2	1:A:2235:PHE:CZ	2.35	0.61
1:B:1965:TYR:O	1:B:1969:LEU:HD13	2.00	0.61
1:D:871:ARG:CD	1:D:926:GLY:HA2	2.29	0.61
1:D:906:CYS:HB2	1:D:913:LEU:HB2	1.83	0.61
1:D:978:THR:HG1	1:D:981:GLN:CD	2.07	0.61
1:C:281:ARG:NH2	1:C:309:THR:OG1	2.33	0.61
1:C:1287:LEU:HD11	1:C:1599:MET:HE3	1.83	0.61
1:C:2782:ASP:OD2	1:C:2785:LEU:HD22	1.99	0.61
1:C:3458:PHE:CE2	1:C:3464:ILE:CD1	2.81	0.61
1:C:3891:LEU:HB3	1:C:3899:PHE:CE2	2.35	0.61
1:A:906:CYS:HB2	1:A:913:LEU:HB2	1.83	0.61
1:B:1280:GLN:O	1:B:1281:ASN:OD1	2.18	0.61
1:B:1287:LEU:HD11	1:B:1599:MET:HE3	1.83	0.61
1:B:2265:LEU:HD12	1:B:2266:GLY:N	2.15	0.61
1:B:4745:LEU:O	1:B:4749:GLU:OE1	2.18	0.61
1:D:1929:MET:O	1:D:1930:LYS:CB	2.49	0.61
1:D:2744:ASN:OD1	1:D:2745:VAL:N	2.33	0.61
1:D:4745:LEU:O	1:D:4749:GLU:OE1	2.18	0.61
1:C:972:LEU:CD1	1:C:1041:GLN:NE2	2.62	0.61
1:C:2744:ASN:OD1	1:C:2745:VAL:N	2.33	0.61
1:C:3969:ILE:HG21	1:C:3980:LEU:HD12	1.82	0.61
1:C:4584:ASP:OD1	1:C:4585:SER:N	2.34	0.61
1:A:721:LEU:HD12	1:A:1476:MET:CE	2.31	0.61
1:A:1965:TYR:O	1:A:1969:LEU:HD13	2.01	0.61
1:A:4584:ASP:OD1	1:A:4585:SER:N	2.34	0.61
1:A:4634:GLU:OE1	1:A:4636:THR:OG1	2.16	0.61
1:A:4705:VAL:HG13	1:A:4711:PHE:CE1	2.36	0.61
2:H:16:PRO:O	2:H:17:LYS:HE2	2.00	0.61
1:B:2658:PRO:O	1:B:2666:VAL:HG11	2.01	0.61
1:D:1965:TYR:O	1:D:1969:LEU:HD13	2.01	0.61
1:C:4705:VAL:HG13	1:C:4711:PHE:CE1	2.36	0.61
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3521:GLY:HA2	1:B:3524:MET:HE3	1.77	0.61
1:B:3573:MET:CB	1:B:3577:ARG:HH12	2.12	0.61
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.15	0.61
1:B:4705:VAL:HG13	1:B:4711:PHE:CE1	2.36	0.61
1:D:140:ASP:OD2	1:D:142:THR:OG1	2.19	0.61
1:D:1280:GLN:O	1:D:1281:ASN:OD1	2.18	0.61
1:C:1577:ALA:O	1:C:1584:ARG:NH1	2.32	0.61
1:C:2265:LEU:HD12	1:C:2266:GLY:N	2.15	0.61
1:C:2658:PRO:O	1:C:2666:VAL:HG11	2.01	0.61
1:C:2977:LEU:O	1:C:2981:VAL:HG23	2.01	0.61
2:E:16:PRO:O	2:E:17:LYS:HE2	2.00	0.61
1:D:2382:GLU:OE1	1:D:2385:ARG:NH1	2.34	0.61
1:D:3634:ALA:O	1:D:3638:MET:HG3	2.01	0.61
1:D:3671:ASP:OD1	1:D:3672:ARG:N	2.33	0.61
1:C:4745:LEU:O	1:C:4749:GLU:OE1	2.18	0.61
1:A:1929:MET:O	1:A:1930:LYS:CB	2.49	0.60
1:A:2265:LEU:HD12	1:A:2266:GLY:N	2.15	0.60
1:B:2977:LEU:O	1:B:2981:VAL:HG23	2.01	0.60
1:D:904:HIS:ND1	1:D:906:CYS:SG	2.73	0.60
1:D:4818:MET:O	1:D:4824:ARG:NH2	2.29	0.60
1:A:2977:LEU:O	1:A:2981:VAL:HG23	2.01	0.60
1:B:140:ASP:OD2	1:B:142:THR:OG1	2.19	0.60
1:D:3692:GLU:OE1	1:D:3694:LYS:N	2.35	0.60
1:D:3891:LEU:HB3	1:D:3899:PHE:CE2	2.35	0.60
1:C:1929:MET:O	1:C:1930:LYS:CB	2.49	0.60
1:A:2890:LYS:O	1:A:2894:LEU:HD13	2.02	0.60
1:B:2890:LYS:O	1:B:2894:LEU:HD13	2.02	0.60
1:D:294:THR:O	1:D:298:GLY:N	2.35	0.60
1:D:2977:LEU:O	1:D:2981:VAL:HG23	2.01	0.60
1:C:906:CYS:HB2	1:C:913:LEU:HB2	1.83	0.60
1:C:970:LEU:HD11	1:C:1049:TYR:CE1	2.37	0.60
1:C:1965:TYR:O	1:C:1969:LEU:HD13	2.00	0.60
1:C:4677:LEU:HD23	1:C:4711:PHE:CE1	2.37	0.60
1:A:871:ARG:HD2	1:A:926:GLY:N	2.17	0.60
2:H:79:ASP:OD1	2:H:80:TYR:N	2.33	0.60
1:D:146:CYS:HG	1:D:147:TRP:CD1	2.18	0.60
1:D:281:ARG:NH2	1:D:309:THR:OG1	2.33	0.60
1:D:1287:LEU:HD11	1:D:1599:MET:HE3	1.83	0.60
1:D:1577:ALA:O	1:D:1584:ARG:NH1	2.32	0.60
1:A:3573:MET:CB	1:A:3577:ARG:HH12	2.12	0.60
1:A:4976:GLU:O	1:A:4980:LEU:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:871:ARG:HD2	1:B:926:GLY:N	2.16	0.60
1:B:4885:PHE:CE2	1:B:4897:ILE:HD11	2.36	0.60
1:D:2464:ASP:OD1	1:D:2465:ASP:N	2.35	0.60
1:D:3573:MET:CB	1:D:3577:ARG:HH12	2.12	0.60
1:D:4677:LEU:HD23	1:D:4711:PHE:CE1	2.37	0.60
1:C:1943:LEU:CD1	1:C:2101:MET:HE1	2.31	0.60
1:A:1943:LEU:CD1	1:A:2101:MET:HE1	2.31	0.60
1:A:2382:GLU:OE1	1:A:2385:ARG:NH1	2.34	0.60
1:A:2638:LYS:O	1:A:2698:MET:HE2	2.02	0.60
1:B:1441:ALA:N	1:B:1513:ASP:OD1	2.34	0.60
1:B:2382:GLU:OE1	1:B:2385:ARG:NH1	2.34	0.60
1:D:871:ARG:HD2	1:D:926:GLY:N	2.17	0.60
1:D:4584:ASP:OD1	1:D:4585:SER:N	2.33	0.60
1:A:1287:LEU:HD11	1:A:1599:MET:HE3	1.83	0.60
1:B:3458:PHE:CE2	1:B:3464:ILE:CD1	2.81	0.60
1:B:3634:ALA:O	1:B:3638:MET:HG3	2.01	0.60
1:D:970:LEU:HD11	1:D:1049:TYR:CE1	2.37	0.60
1:D:2523:ASP:CB	1:D:2578:MET:HE1	2.15	0.60
1:D:4885:PHE:CE2	1:D:4897:ILE:HD11	2.36	0.60
1:C:294:THR:O	1:C:298:GLY:N	2.35	0.60
1:C:984:LEU:O	1:C:988:LEU:HD23	2.01	0.60
1:C:2464:ASP:OD1	1:C:2465:ASP:N	2.35	0.60
1:C:4976:GLU:O	1:C:4980:LEU:HD13	2.02	0.60
1:A:932:LEU:HD12	1:A:937:CYS:SG	2.42	0.60
1:A:3227:ARG:HB3	1:A:3232:LEU:HD12	1.83	0.60
1:B:1943:LEU:CD1	1:B:2101:MET:HE1	2.31	0.60
1:B:2638:LYS:O	1:B:2698:MET:HE2	2.02	0.60
1:D:985:VAL:HG13	1:D:1039:LEU:CD2	2.32	0.60
1:C:1441:ALA:N	1:C:1513:ASP:OD1	2.34	0.60
1:C:4966:ASP:OD1	1:C:4967:TYR:N	2.35	0.60
1:A:871:ARG:CD	1:A:926:GLY:HA2	2.29	0.60
1:A:3634:ALA:O	1:A:3638:MET:HG3	2.02	0.60
1:D:4705:VAL:HG13	1:D:4711:PHE:CE1	2.36	0.60
1:C:140:ASP:OD2	1:C:142:THR:OG1	2.19	0.60
1:C:2382:GLU:OE1	1:C:2385:ARG:NH1	2.34	0.60
1:C:4827:LEU:O	1:C:4831:THR:HG23	2.02	0.60
1:A:2233:CYS:HB3	1:A:2237:CYS:HG	1.49	0.60
1:A:2658:PRO:O	1:A:2666:VAL:HG11	2.01	0.60
1:A:4677:LEU:HD23	1:A:4711:PHE:CE1	2.37	0.60
1:B:3692:GLU:OE1	1:B:3694:LYS:N	2.35	0.60
1:B:4976:GLU:O	1:B:4980:LEU:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:932:LEU:HD12	1:D:937:CYS:SG	2.42	0.60
1:D:984:LEU:O	1:D:988:LEU:HD23	2.01	0.60
1:D:1943:LEU:CD1	1:D:2101:MET:HE1	2.31	0.60
1:D:2658:PRO:O	1:D:2666:VAL:HG11	2.01	0.60
1:D:4976:GLU:O	1:D:4980:LEU:HD13	2.02	0.60
1:A:908:VAL:O	1:A:963:ASN:CG	2.45	0.59
1:A:985:VAL:HG13	1:A:1039:LEU:CD2	2.32	0.59
1:B:721:LEU:HD12	1:B:1476:MET:CE	2.31	0.59
1:B:884:LEU:O	1:B:888:GLU:OE1	2.20	0.59
1:B:932:LEU:HD12	1:B:937:CYS:SG	2.42	0.59
1:C:3692:GLU:OE1	1:C:3694:LYS:N	2.35	0.59
1:A:140:ASP:OD2	1:A:142:THR:OG1	2.19	0.59
1:A:984:LEU:O	1:A:988:LEU:HD23	2.01	0.59
1:B:970:LEU:HD11	1:B:1049:TYR:CE1	2.37	0.59
1:B:3433:GLU:HG3	1:B:3437:MET:HE3	1.84	0.59
1:B:4677:LEU:HD23	1:B:4711:PHE:CE1	2.37	0.59
1:B:4827:LEU:O	1:B:4831:THR:HG23	2.02	0.59
1:D:2638:LYS:O	1:D:2698:MET:HE2	2.02	0.59
1:D:4634:GLU:OE1	1:D:4636:THR:OG1	2.16	0.59
1:C:721:LEU:HD12	1:C:1476:MET:CE	2.31	0.59
1:C:871:ARG:HD2	1:C:926:GLY:N	2.17	0.59
1:C:932:LEU:HD12	1:C:937:CYS:SG	2.42	0.59
1:C:2890:LYS:O	1:C:2894:LEU:HD13	2.02	0.59
1:C:4885:PHE:CE2	1:C:4897:ILE:HD11	2.36	0.59
1:A:11:VAL:HG11	1:A:164:ARG:HD3	1.85	0.59
1:B:985:VAL:HG13	1:B:1039:LEU:CD2	2.32	0.59
1:D:721:LEU:HD12	1:D:1476:MET:CE	2.31	0.59
1:D:2890:LYS:O	1:D:2894:LEU:HD13	2.02	0.59
1:A:970:LEU:HD11	1:A:1049:TYR:CE1	2.37	0.59
1:A:3327:LEU:HD12	1:A:3364:ARG:NH1	2.18	0.59
1:A:3692:GLU:OE1	1:A:3694:LYS:N	2.35	0.59
1:A:4827:LEU:O	1:A:4831:THR:HG23	2.02	0.59
1:B:233:ILE:O	1:B:257:ARG:NH1	2.35	0.59
1:B:984:LEU:O	1:B:988:LEU:HD23	2.01	0.59
1:B:3327:LEU:HD12	1:B:3364:ARG:NH1	2.18	0.59
1:D:4966:ASP:OD1	1:D:4967:TYR:N	2.35	0.59
1:C:3157:ILE:HG23	1:C:3161:VAL:HG12	1.85	0.59
1:C:3634:ALA:O	1:C:3638:MET:HG3	2.02	0.59
1:A:884:LEU:O	1:A:888:GLU:OE1	2.20	0.59
1:A:2523:ASP:CB	1:A:2578:MET:HE1	2.15	0.59
1:A:4885:PHE:CE2	1:A:4897:ILE:HD11	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:79:ASP:OD1	2:G:80:TYR:N	2.33	0.59
1:C:3433:GLU:HG3	1:C:3437:MET:HE3	1.84	0.59
1:A:3433:GLU:HG3	1:A:3437:MET:HE3	1.84	0.59
2:F:79:ASP:OD1	2:F:80:TYR:N	2.33	0.59
1:B:2625:ARG:NH1	1:B:2629:ASP:CG	2.61	0.59
1:D:11:VAL:HG11	1:D:164:ARG:HD3	1.85	0.59
1:A:64:ILE:O	1:A:111:HIS:NE2	2.36	0.59
1:A:1427:ILE:HG23	1:A:1428:LEU:HD22	1.84	0.59
1:B:908:VAL:O	1:B:963:ASN:CG	2.45	0.59
1:C:908:VAL:O	1:C:963:ASN:CG	2.45	0.59
1:C:985:VAL:HG13	1:C:1039:LEU:CD2	2.32	0.59
1:C:2376:LEU:HD11	1:C:2426:TYR:HB3	1.85	0.59
1:A:294:THR:O	1:A:298:GLY:N	2.35	0.59
2:F:17:LYS:HE2	2:F:17:LYS:HA	1.85	0.59
1:B:2376:LEU:HD11	1:B:2426:TYR:HB3	1.85	0.59
1:B:2464:ASP:OD1	1:B:2465:ASP:N	2.35	0.59
1:D:908:VAL:O	1:D:963:ASN:CG	2.45	0.59
1:D:1427:ILE:HG23	1:D:1428:LEU:HD22	1.84	0.59
1:D:3327:LEU:HD12	1:D:3364:ARG:NH1	2.18	0.59
1:C:2625:ARG:NH1	1:C:2629:ASP:CG	2.61	0.59
1:C:3236:VAL:O	1:C:3239:MET:HG2	2.02	0.59
1:C:3327:LEU:HD12	1:C:3364:ARG:NH1	2.18	0.59
1:C:3357:HIS:O	1:C:3361:THR:HG23	2.03	0.59
1:A:4930:ALA:HA	1:A:4933:GLN:OE1	2.03	0.59
1:B:3157:ILE:HG23	1:B:3161:VAL:HG12	1.85	0.59
1:D:3985:LEU:O	1:D:3989:VAL:HG23	2.03	0.59
1:C:2638:LYS:O	1:C:2698:MET:HE2	2.02	0.59
1:A:2376:LEU:HD11	1:A:2426:TYR:HB3	1.85	0.59
1:A:3985:LEU:O	1:A:3989:VAL:HG23	2.03	0.59
2:E:17:LYS:HE2	2:E:17:LYS:HA	1.85	0.59
1:B:11:VAL:HG11	1:B:164:ARG:HD3	1.85	0.59
1:B:107:ILE:HG23	1:B:150:MET:HE2	1.85	0.59
1:B:2761:TYR:HB3	1:B:2765:LYS:HZ3	1.68	0.59
1:B:3227:ARG:HB3	1:B:3232:LEU:HD12	1.83	0.59
1:D:228:ASP:OD1	1:D:229:GLU:N	2.36	0.59
1:C:3227:ARG:HB3	1:C:3232:LEU:HD12	1.83	0.59
1:A:3157:ILE:HG23	1:A:3161:VAL:HG12	1.85	0.58
2:G:17:LYS:HE2	2:G:17:LYS:HA	1.85	0.58
1:B:3985:LEU:O	1:B:3989:VAL:HG23	2.03	0.58
1:B:4930:ALA:HA	1:B:4933:GLN:OE1	2.03	0.58
1:D:2974:ILE:HD13	1:D:3049:LEU:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:VAL:HG11	1:C:164:ARG:HD3	1.85	0.58
1:A:107:ILE:HG23	1:A:150:MET:HE2	1.85	0.58
1:A:228:ASP:OD1	1:A:229:GLU:N	2.36	0.58
1:A:2464:ASP:OD1	1:A:2465:ASP:N	2.35	0.58
1:A:3197:LEU:C	1:A:3197:LEU:HD23	2.29	0.58
1:A:3324:VAL:CG1	1:A:3361:THR:HG22	2.33	0.58
1:A:4998:LYS:HB3	1:A:5003:HIS:HE1	1.68	0.58
1:B:64:ILE:O	1:B:111:HIS:NE2	2.36	0.58
1:B:3324:VAL:CG1	1:B:3361:THR:HG22	2.33	0.58
1:B:3357:HIS:O	1:B:3361:THR:HG23	2.03	0.58
1:D:3433:GLU:HG3	1:D:3437:MET:HE3	1.84	0.58
1:C:2523:ASP:CB	1:C:2578:MET:HE1	2.15	0.58
1:A:4966:ASP:OD1	1:A:4967:TYR:N	2.35	0.58
1:D:3239:MET:SD	1:D:3239:MET:HG2	2.31	0.58
1:C:64:ILE:O	1:C:111:HIS:NE2	2.36	0.58
1:C:4930:ALA:HA	1:C:4933:GLN:OE1	2.03	0.58
1:A:1112:ASP:OD1	1:A:1113:VAL:HG23	2.03	0.58
1:A:3559:LEU:HD23	1:A:3559:LEU:O	2.03	0.58
2:H:17:LYS:HE2	2:H:17:LYS:HA	1.85	0.58
1:D:2376:LEU:HD11	1:D:2426:TYR:HB3	1.85	0.58
1:D:3559:LEU:HD23	1:D:3559:LEU:O	2.03	0.58
1:D:4827:LEU:O	1:D:4831:THR:HG23	2.02	0.58
1:C:1427:ILE:HG23	1:C:1428:LEU:HD22	1.84	0.58
1:C:1925:GLY:O	1:C:1929:MET:HG3	2.04	0.58
1:C:2974:ILE:HD13	1:C:3049:LEU:CD1	2.33	0.58
1:C:4818:MET:O	1:C:4824:ARG:NH2	2.29	0.58
1:A:2625:ARG:NH1	1:A:2629:ASP:CG	2.61	0.58
1:A:3357:HIS:O	1:A:3361:THR:HG23	2.03	0.58
1:B:228:ASP:OD1	1:B:229:GLU:N	2.36	0.58
1:B:294:THR:O	1:B:298:GLY:N	2.35	0.58
1:B:2572:THR:CG2	1:B:2579:VAL:HG21	2.33	0.58
1:B:2781:VAL:HG23	1:B:2789:PRO:HG3	1.85	0.58
1:D:69:LEU:CD1	1:D:101:LEU:HD11	2.34	0.58
1:C:1112:ASP:OD1	1:C:1113:VAL:HG23	2.03	0.58
1:D:64:ILE:O	1:D:111:HIS:NE2	2.36	0.58
1:D:3157:ILE:HG23	1:D:3161:VAL:HG12	1.85	0.58
1:D:3324:VAL:CG1	1:D:3361:THR:HG22	2.33	0.58
1:D:4930:ALA:HA	1:D:4933:GLN:OE1	2.03	0.58
1:A:3236:VAL:HA	1:A:3239:MET:HG2	1.85	0.58
1:A:3398:PHE:CE2	1:A:3450:ASN:HB2	2.38	0.58
1:B:1112:ASP:OD1	1:B:1113:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3197:LEU:HD23	1:B:3197:LEU:C	2.29	0.58
1:B:4966:ASP:OD1	1:B:4967:TYR:N	2.35	0.58
1:D:2572:THR:CG2	1:D:2579:VAL:HG21	2.33	0.58
1:C:69:LEU:CD1	1:C:101:LEU:HD11	2.34	0.58
1:A:1925:GLY:O	1:A:1929:MET:HG3	2.04	0.58
1:D:961:MET:CE	1:D:963:ASN:CB	2.59	0.58
1:C:228:ASP:OD1	1:C:229:GLU:N	2.36	0.58
1:C:884:LEU:O	1:C:888:GLU:OE1	2.20	0.58
1:C:3985:LEU:O	1:C:3989:VAL:HG23	2.03	0.58
1:A:904:HIS:ND1	1:A:906:CYS:SG	2.73	0.58
1:A:2572:THR:CG2	1:A:2579:VAL:HG21	2.33	0.58
1:B:3398:PHE:CE2	1:B:3450:ASN:HB2	2.38	0.58
1:B:3442:PHE:CG	1:B:3514:LEU:HD22	2.39	0.58
1:B:4998:LYS:HB3	1:B:5003:HIS:HE1	1.68	0.58
1:D:884:LEU:O	1:D:888:GLU:OE1	2.20	0.58
1:D:3227:ARG:HB3	1:D:3232:LEU:HD12	1.83	0.58
1:C:2625:ARG:HH12	1:C:2629:ASP:CG	2.12	0.58
1:A:2974:ILE:HD13	1:A:3049:LEU:CD1	2.33	0.58
1:A:3372:VAL:CG1	1:A:3398:PHE:CE1	2.87	0.58
1:B:1925:GLY:O	1:B:1929:MET:HG3	2.04	0.58
1:B:3559:LEU:O	1:B:3559:LEU:HD23	2.03	0.58
1:C:3398:PHE:CE2	1:C:3450:ASN:HB2	2.38	0.58
1:C:3442:PHE:CG	1:C:3514:LEU:HD22	2.39	0.58
1:A:2781:VAL:HG23	1:A:2789:PRO:HG3	1.86	0.57
1:B:110:ARG:HD3	1:B:115:ARG:HE	1.70	0.57
1:D:2625:ARG:NH1	1:D:2629:ASP:CG	2.61	0.57
1:D:3398:PHE:CE2	1:D:3450:ASN:HB2	2.39	0.57
1:B:1427:ILE:HG23	1:B:1428:LEU:HD22	1.84	0.57
1:D:110:ARG:HD3	1:D:115:ARG:HE	1.70	0.57
1:D:233:ILE:O	1:D:257:ARG:NH1	2.35	0.57
1:D:3197:LEU:C	1:D:3197:LEU:HD23	2.29	0.57
1:C:233:ILE:O	1:C:257:ARG:NH1	2.35	0.57
1:C:3559:LEU:O	1:C:3559:LEU:HD23	2.03	0.57
1:A:69:LEU:CD1	1:A:101:LEU:HD11	2.34	0.57
1:B:3566:SER:HB3	1:B:3569:LEU:HD12	1.86	0.57
1:D:1112:ASP:OD1	1:D:1113:VAL:HG23	2.03	0.57
1:D:3357:HIS:O	1:D:3361:THR:HG23	2.03	0.57
1:C:107:ILE:HG23	1:C:150:MET:HE2	1.85	0.57
1:C:2586:VAL:HG13	1:C:2607:LEU:HD13	1.87	0.57
1:C:3566:SER:HB3	1:C:3569:LEU:HD12	1.86	0.57
1:A:1441:ALA:N	1:A:1513:ASP:OD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2929:PHE:CA	1:A:2932:MET:HE1	2.26	0.57
1:B:69:LEU:CD1	1:B:101:LEU:HD11	2.34	0.57
1:B:1748:PHE:HB3	1:B:1758:ARG:NH1	2.20	0.57
1:D:554:LEU:HD11	1:D:1593:PRO:CG	2.35	0.57
1:D:3442:PHE:CG	1:D:3514:LEU:HD22	2.39	0.57
1:C:904:HIS:ND1	1:C:906:CYS:SG	2.73	0.57
1:C:1749:PRO:C	1:C:1758:ARG:NH2	2.45	0.57
1:C:2572:THR:CG2	1:C:2579:VAL:HG21	2.33	0.57
1:A:1748:PHE:HB3	1:A:1758:ARG:NH1	2.20	0.57
1:B:3372:VAL:CG1	1:B:3398:PHE:CE1	2.87	0.57
1:B:4630:TYR:OH	1:C:4860:ARG:NH1	2.37	0.57
1:D:4998:LYS:HB3	1:D:5003:HIS:HE1	1.68	0.57
1:C:2382:GLU:OE2	1:C:2392:ARG:NH2	2.38	0.57
1:C:3372:VAL:CG1	1:C:3398:PHE:CE1	2.87	0.57
1:C:4998:LYS:HB3	1:C:5003:HIS:HE1	1.68	0.57
1:A:3254:GLY:O	1:A:3258:GLU:OE1	2.23	0.57
1:D:107:ILE:HG23	1:D:150:MET:HE2	1.85	0.57
1:D:1441:ALA:N	1:D:1513:ASP:OD1	2.34	0.57
1:D:3498:ARG:O	1:D:3501:ASP:N	2.38	0.57
1:C:1748:PHE:HB3	1:C:1758:ARG:NH1	2.20	0.57
1:C:3254:GLY:O	1:C:3258:GLU:OE1	2.23	0.57
1:C:3324:VAL:CG1	1:C:3361:THR:HG22	2.33	0.57
1:A:110:ARG:HD3	1:A:115:ARG:HE	1.70	0.57
1:A:554:LEU:HD11	1:A:1593:PRO:CG	2.35	0.57
1:A:2382:GLU:OE2	1:A:2392:ARG:NH2	2.38	0.57
1:A:3442:PHE:CG	1:A:3514:LEU:HD22	2.39	0.57
1:D:1748:PHE:HB3	1:D:1758:ARG:NH1	2.19	0.57
1:D:1925:GLY:O	1:D:1929:MET:HG3	2.04	0.57
1:D:3179:LYS:O	1:D:3180:ASN:ND2	2.38	0.57
1:C:1497:GLY:O	1:C:1501:VAL:HG13	2.05	0.57
1:A:3498:ARG:O	1:A:3501:ASP:N	2.38	0.57
1:B:3179:LYS:O	1:B:3180:ASN:ND2	2.38	0.57
1:B:3236:VAL:HA	1:B:3239:MET:HG2	1.86	0.57
1:D:1497:GLY:O	1:D:1501:VAL:HG13	2.05	0.57
1:A:2625:ARG:HH12	1:A:2629:ASP:CG	2.12	0.57
1:B:554:LEU:HD11	1:B:1593:PRO:CG	2.35	0.57
1:B:2974:ILE:HD13	1:B:3049:LEU:CD1	2.33	0.57
1:D:3372:VAL:CG1	1:D:3398:PHE:CE1	2.87	0.57
1:C:554:LEU:HD11	1:C:1593:PRO:CG	2.35	0.57
1:C:3179:LYS:O	1:C:3180:ASN:ND2	2.38	0.57
1:A:2782:ASP:N	1:A:2782:ASP:OD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2382:GLU:OE2	1:B:2392:ARG:NH2	2.38	0.57
1:B:2586:VAL:HG13	1:B:2607:LEU:HD13	1.87	0.57
1:B:3498:ARG:O	1:B:3501:ASP:N	2.38	0.57
1:A:3179:LYS:O	1:A:3180:ASN:ND2	2.38	0.56
1:B:3137:LEU:HD23	1:B:3189:ALA:HB1	1.86	0.56
1:B:3254:GLY:O	1:B:3258:GLU:OE1	2.23	0.56
1:D:2780:ASN:OD1	1:D:2781:VAL:N	2.38	0.56
1:C:3137:LEU:HD23	1:C:3189:ALA:HB1	1.86	0.56
1:C:3197:LEU:HD23	1:C:3197:LEU:C	2.29	0.56
1:A:907:LEU:O	1:A:908:VAL:HB	2.05	0.56
1:B:812:HIS:O	1:B:815:VAL:HG12	2.05	0.56
1:D:2586:VAL:HG13	1:D:2607:LEU:HD13	1.87	0.56
1:D:3254:GLY:O	1:D:3258:GLU:OE1	2.23	0.56
1:C:110:ARG:HD3	1:C:115:ARG:HE	1.70	0.56
1:C:2780:ASN:OD1	1:C:2781:VAL:N	2.38	0.56
1:B:553:ARG:NE	1:B:555:GLU:OE2	2.38	0.56
1:B:904:HIS:ND1	1:B:906:CYS:SG	2.73	0.56
1:B:5034:ASP:OD1	1:B:5035:GLN:N	2.38	0.56
1:D:812:HIS:O	1:D:815:VAL:HG12	2.05	0.56
1:D:1980:LEU:CD1	1:D:1991:THR:HG23	2.36	0.56
1:D:2382:GLU:OE2	1:D:2392:ARG:NH2	2.38	0.56
1:D:2625:ARG:HH12	1:D:2629:ASP:CG	2.12	0.56
1:D:2782:ASP:N	1:D:2782:ASP:OD1	2.38	0.56
1:D:4860:ARG:NH1	1:C:4630:TYR:OH	2.36	0.56
1:C:812:HIS:O	1:C:815:VAL:HG12	2.05	0.56
1:C:2781:VAL:HG23	1:C:2789:PRO:HG3	1.86	0.56
1:C:3498:ARG:O	1:C:3501:ASP:N	2.38	0.56
1:B:907:LEU:O	1:B:908:VAL:HB	2.05	0.56
1:D:1461:ASP:OD2	1:D:1468:LYS:NZ	2.37	0.56
1:A:233:ILE:O	1:A:257:ARG:NH1	2.35	0.56
1:A:384:MET:CE	1:B:167:ASP:OD1	2.54	0.56
1:A:1980:LEU:CD1	1:A:1991:THR:HG23	2.35	0.56
1:A:3137:LEU:HD23	1:A:3189:ALA:HB1	1.86	0.56
1:B:991:ASN:O	1:B:995:VAL:HG23	2.05	0.56
1:B:2780:ASN:OD1	1:B:2781:VAL:N	2.38	0.56
1:D:2781:VAL:HG23	1:D:2789:PRO:HG3	1.85	0.56
1:D:3137:LEU:HD23	1:D:3189:ALA:HB1	1.86	0.56
1:D:5034:ASP:OD1	1:D:5035:GLN:N	2.38	0.56
1:C:1461:ASP:OD2	1:C:1468:LYS:NZ	2.37	0.56
1:C:1980:LEU:CD1	1:C:1991:THR:HG23	2.36	0.56
1:C:3629:ARG:O	1:C:3633:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:HA	1:D:384:MET:SD	2.45	0.56
1:A:1497:GLY:O	1:A:1501:VAL:HG13	2.05	0.56
1:A:5034:ASP:OD1	1:A:5035:GLN:N	2.38	0.56
1:B:861:ILE:HD13	1:B:930:LYS:HD3	1.87	0.56
1:B:1497:GLY:O	1:B:1501:VAL:HG13	2.05	0.56
1:B:3327:LEU:HD12	1:B:3364:ARG:HH12	1.70	0.56
1:B:3398:PHE:HE2	1:B:3450:ASN:HB2	1.71	0.56
1:B:4768:LEU:HA	1:B:4771:ILE:HD12	1.87	0.56
1:D:897:ARG:HB2	1:D:905:PRO:HD3	1.88	0.56
1:D:3114:LYS:HD2	1:D:3125:VAL:HG21	1.88	0.56
1:C:907:LEU:O	1:C:908:VAL:HB	2.05	0.56
1:C:5034:ASP:OD1	1:C:5035:GLN:N	2.38	0.56
1:A:812:HIS:O	1:A:815:VAL:HG12	2.05	0.56
1:A:3566:SER:HB3	1:A:3569:LEU:HD12	1.86	0.56
1:A:3629:ARG:O	1:A:3633:VAL:HG23	2.06	0.56
1:D:2608:MET:O	1:D:2612[B]:ARG:HG3	2.06	0.56
1:C:991:ASN:O	1:C:995:VAL:HG23	2.05	0.56
1:A:554:LEU:HD11	1:A:1593:PRO:HG3	1.88	0.56
1:A:2761:TYR:HB3	1:A:2765:LYS:HZ3	1.70	0.56
1:B:961:MET:CE	1:B:963:ASN:CB	2.59	0.56
1:B:3435:PHE:CD2	1:B:3524:MET:HE1	2.41	0.56
1:D:991:ASN:O	1:D:995:VAL:HG23	2.05	0.56
1:D:2226:PRO:CB	1:D:2267:MET:CE	2.78	0.56
1:D:4768:LEU:HA	1:D:4771:ILE:HD12	1.87	0.56
1:C:553:ARG:NE	1:C:555:GLU:OE2	2.38	0.56
1:C:3114:LYS:HD2	1:C:3125:VAL:HG21	1.88	0.56
1:C:3398:PHE:HE2	1:C:3450:ASN:HB2	1.71	0.56
1:A:2203:MET:HE2	1:A:2235:PHE:CE1	2.41	0.56
1:A:2586:VAL:HG13	1:A:2607:LEU:HD13	1.87	0.56
1:A:3852:LYS:O	1:A:3856:LEU:HG	2.06	0.56
1:B:1157:GLU:OE1	1:B:1157:GLU:N	2.39	0.56
1:D:554:LEU:HD11	1:D:1593:PRO:HG3	1.88	0.56
1:D:3566:SER:HB3	1:D:3569:LEU:HD12	1.86	0.56
1:D:3629:ARG:O	1:D:3633:VAL:HG23	2.06	0.56
1:C:897:ARG:HB2	1:C:905:PRO:HD3	1.88	0.56
1:C:2203:MET:HE2	1:C:2235:PHE:CE1	2.41	0.56
1:A:167:ASP:OD1	1:D:384:MET:CE	2.54	0.56
1:A:991:ASN:O	1:A:995:VAL:HG23	2.05	0.56
1:A:3166:TYR:OH	1:A:3203:VAL:HG11	2.06	0.56
1:A:3372:VAL:HG12	1:A:3398:PHE:HE1	1.71	0.56
1:A:3398:PHE:HE2	1:A:3450:ASN:HB2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4768:LEU:HA	1:A:4771:ILE:HD12	1.87	0.56
1:C:125:ARG:HB3	1:C:125:ARG:HH11	1.71	0.56
1:C:499:THR:HG23	1:C:502:HIS:H	1.71	0.56
1:B:499:THR:HG23	1:B:502:HIS:H	1.71	0.55
1:B:897:ARG:HB2	1:B:905:PRO:HD3	1.87	0.55
1:B:2203:MET:HE2	1:B:2235:PHE:CE1	2.41	0.55
1:B:2608:MET:O	1:B:2612[B]:ARG:HG3	2.06	0.55
1:D:213:TYR:CE1	1:D:340:LYS:HG2	2.42	0.55
1:D:3327:LEU:HD12	1:D:3364:ARG:HH12	1.70	0.55
1:C:4651:THR:CB	1:C:4803:HIS:HE2	2.19	0.55
1:A:2780:ASN:OD1	1:A:2781:VAL:N	2.38	0.55
1:A:3327:LEU:HD12	1:A:3364:ARG:HH12	1.70	0.55
1:B:1980:LEU:CD1	1:B:1991:THR:HG23	2.36	0.55
1:B:3852:LYS:O	1:B:3856:LEU:HG	2.06	0.55
1:D:861:ILE:HD13	1:D:930:LYS:HD3	1.87	0.55
1:D:2211:MET:O	1:D:2215:LEU:HD13	2.06	0.55
1:D:4749:GLU:HB3	1:D:4753:HIS:CE1	2.41	0.55
1:C:2608:MET:O	1:C:2612[B]:ARG:HG3	2.06	0.55
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.22	0.55
1:B:3166:TYR:OH	1:B:3203:VAL:HG11	2.06	0.55
1:B:3239:MET:CG	1:B:3239:MET:HA	2.35	0.55
1:D:125:ARG:HH11	1:D:125:ARG:HB3	1.71	0.55
1:D:907:LEU:O	1:D:908:VAL:HB	2.05	0.55
1:D:928:THR:O	1:D:932:LEU:HD23	2.07	0.55
1:D:2929:PHE:CA	1:D:2932:MET:HE1	2.26	0.55
1:C:213:TYR:CE1	1:C:340:LYS:HG2	2.42	0.55
1:C:861:ILE:HD13	1:C:930:LYS:HD3	1.87	0.55
1:A:67:PHE:HB3	1:A:109:LEU:HD22	1.89	0.55
1:A:1157:GLU:OE1	1:A:1157:GLU:N	2.39	0.55
1:A:3114:LYS:HD2	1:A:3125:VAL:HG21	1.88	0.55
1:A:3435:PHE:CD2	1:A:3524:MET:HE1	2.41	0.55
1:D:3372:VAL:HG12	1:D:3398:PHE:HE1	1.71	0.55
1:D:4209:GLN:H	1:D:4209:GLN:CD	2.14	0.55
1:C:2211:MET:O	1:C:2215:LEU:HD13	2.06	0.55
1:C:3327:LEU:HD12	1:C:3364:ARG:HH12	1.70	0.55
1:A:1931:LEU:HD22	1:A:1935:VAL:HG11	1.88	0.55
1:A:4209:GLN:H	1:A:4209:GLN:CD	2.14	0.55
1:A:4860:ARG:NH1	1:D:4630:TYR:OH	2.39	0.55
1:B:928:THR:O	1:B:932:LEU:HD23	2.07	0.55
1:B:3629:ARG:O	1:B:3633:VAL:HG23	2.06	0.55
1:C:928:THR:O	1:C:932:LEU:HD23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1931:LEU:HD22	1:C:1935:VAL:HG11	1.88	0.55
1:C:3635:CYS:HA	1:C:3638:MET:HG3	1.88	0.55
1:C:4749:GLU:HB3	1:C:4753:HIS:CE1	2.41	0.55
1:A:861:ILE:HD13	1:A:930:LYS:HD3	1.87	0.55
1:A:897:ARG:HB2	1:A:905:PRO:HD3	1.88	0.55
1:A:2211:MET:O	1:A:2215:LEU:HD13	2.06	0.55
1:B:2211:MET:O	1:B:2215:LEU:HD13	2.06	0.55
1:D:499:THR:HG23	1:D:502:HIS:H	1.71	0.55
1:A:553:ARG:NE	1:A:555:GLU:OE2	2.38	0.55
1:B:67:PHE:HB3	1:B:109:LEU:HD22	1.89	0.55
1:B:4651:THR:CB	1:B:4803:HIS:HE2	2.19	0.55
1:D:3398:PHE:HE2	1:D:3450:ASN:HB2	1.71	0.55
1:C:2233:CYS:HB3	1:C:2237:CYS:HG	1.60	0.55
1:C:2929:PHE:CA	1:C:2932:MET:HE1	2.26	0.55
1:A:112:ALA:O	1:A:115:ARG:NH1	2.39	0.55
1:A:499:THR:HG23	1:A:502:HIS:H	1.71	0.55
1:B:1158:ASN:ND2	1:B:1182:ILE:O	2.40	0.55
1:B:3635:CYS:HA	1:B:3638:MET:HG3	1.88	0.55
1:D:2203:MET:HE2	1:D:2235:PHE:CE1	2.41	0.55
1:D:3852:LYS:O	1:D:3856:LEU:HG	2.06	0.55
1:D:4651:THR:CB	1:D:4803:HIS:HE2	2.19	0.55
1:C:1157:GLU:OE1	1:C:1157:GLU:N	2.39	0.55
1:C:1726:SER:O	1:C:1729:SER:OG	2.23	0.55
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.38	0.55
1:A:125:ARG:HB3	1:A:125:ARG:HH11	1.71	0.55
1:A:928:THR:O	1:A:932:LEU:HD23	2.06	0.55
1:A:2608:MET:O	1:A:2612[B]:ARG:HG3	2.06	0.55
1:B:112:ALA:O	1:B:115:ARG:NH1	2.38	0.55
1:B:2904:LEU:O	1:B:2904:LEU:HD23	2.07	0.55
1:C:1158:ASN:ND2	1:C:1182:ILE:O	2.40	0.55
1:C:3435:PHE:CD2	1:C:3524:MET:HE1	2.41	0.55
1:C:4209:GLN:H	1:C:4209:GLN:CD	2.14	0.55
1:C:4768:LEU:HA	1:C:4771:ILE:HD12	1.87	0.55
1:A:213:TYR:CE1	1:A:340:LYS:HG2	2.42	0.55
1:B:908:VAL:HG13	1:B:912:SER:HB2	1.89	0.55
1:B:4209:GLN:CD	1:B:4209:GLN:H	2.14	0.55
1:C:112:ALA:O	1:C:115:ARG:NH1	2.39	0.55
1:C:931:THR:O	1:C:935:LEU:HD23	2.07	0.55
1:A:4749:GLU:HB3	1:A:4753:HIS:CE1	2.41	0.54
1:B:554:LEU:HD11	1:B:1593:PRO:HG3	1.88	0.54
1:B:2226:PRO:CB	1:B:2267:MET:CE	2.78	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3372:VAL:HG12	1:B:3398:PHE:HE1	1.71	0.54
1:D:1931:LEU:HD22	1:D:1935:VAL:HG11	1.88	0.54
1:D:2790:MET:SD	1:D:2797:PHE:HZ	2.30	0.54
1:D:2907:PRO:HB2	1:D:2910:THR:HG23	1.89	0.54
1:D:3435:PHE:CD2	1:D:3524:MET:HE1	2.41	0.54
1:D:3635:CYS:HA	1:D:3638:MET:HG3	1.88	0.54
1:C:3166:TYR:OH	1:C:3203:VAL:HG11	2.06	0.54
1:A:2790:MET:SD	1:A:2797:PHE:HZ	2.30	0.54
1:A:2907:PRO:HB2	1:A:2910:THR:HG23	1.89	0.54
1:A:3635:CYS:HA	1:A:3638:MET:HG3	1.88	0.54
1:B:985:VAL:HG13	1:B:1039:LEU:HD22	1.89	0.54
1:B:3114:LYS:HD2	1:B:3125:VAL:HG21	1.88	0.54
1:B:3537:LYS:NZ	1:B:3607:GLU:OE2	2.33	0.54
1:D:908:VAL:HG13	1:D:912:SER:HB2	1.89	0.54
1:D:931:THR:O	1:D:935:LEU:HD23	2.07	0.54
1:D:1748:PHE:C	1:D:1758:ARG:HH12	2.16	0.54
1:C:554:LEU:HD11	1:C:1593:PRO:HG3	1.88	0.54
1:C:2194:HIS:O	1:C:2198:MET:HE2	2.08	0.54
1:C:2790:MET:SD	1:C:2797:PHE:HZ	2.30	0.54
1:C:3372:VAL:HG12	1:C:3398:PHE:HE1	1.71	0.54
1:A:384:MET:SD	1:B:167:ASP:HA	2.47	0.54
1:A:961:MET:CE	1:A:963:ASN:CB	2.59	0.54
1:A:1158:ASN:ND2	1:A:1182:ILE:O	2.40	0.54
1:A:4651:THR:CB	1:A:4803:HIS:HE2	2.19	0.54
1:B:213:TYR:CE1	1:B:340:LYS:HG2	2.42	0.54
1:B:1931:LEU:HD22	1:B:1935:VAL:HG11	1.88	0.54
1:D:67:PHE:HB3	1:D:109:LEU:HD22	1.89	0.54
1:D:2194:HIS:O	1:D:2198:MET:HE2	2.07	0.54
1:D:2761:TYR:HB3	1:D:2765:LYS:HZ3	1.73	0.54
1:A:877:ASN:O	1:A:880:GLU:HG2	2.07	0.54
1:A:931:THR:O	1:A:935:LEU:HD23	2.07	0.54
1:B:2194:HIS:O	1:B:2198:MET:HE2	2.08	0.54
1:B:2907:PRO:HB2	1:B:2910:THR:HG23	1.89	0.54
1:B:4749:GLU:HB3	1:B:4753:HIS:CE1	2.41	0.54
1:D:1045:THR:HG22	1:D:1049:TYR:CE2	2.43	0.54
1:D:1157:GLU:OE1	1:D:1157:GLU:N	2.39	0.54
1:D:3442:PHE:HE1	1:D:3511:VAL:HG12	1.73	0.54
1:C:1045:THR:HG22	1:C:1049:TYR:CE2	2.43	0.54
1:C:2907:PRO:HB2	1:C:2910:THR:HG23	1.89	0.54
1:A:167:ASP:OD1	1:D:384:MET:HE1	2.07	0.54
1:B:125:ARG:HB3	1:B:125:ARG:HH11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:THR:O	1:B:935:LEU:HD23	2.07	0.54
1:B:2961:GLN:HG3	1:B:3038:MET:HE1	1.90	0.54
1:B:3527:PRO:HD2	1:B:3573:MET:SD	2.48	0.54
1:D:2961:GLN:HG3	1:D:3038:MET:HE1	1.90	0.54
1:C:2961:GLN:HG3	1:C:3038:MET:HE1	1.90	0.54
1:C:3442:PHE:HE1	1:C:3511:VAL:HG12	1.73	0.54
1:A:1280:GLN:O	1:A:1281:ASN:CG	2.51	0.54
1:A:2874:MET:CE	1:A:2939:ARG:CB	2.75	0.54
1:A:3957:VAL:O	1:A:3961:VAL:HG23	2.08	0.54
1:B:4180:ARG:HD3	1:B:4192:ARG:HD3	1.89	0.54
1:D:2904:LEU:HD23	1:D:2904:LEU:O	2.07	0.54
1:C:1748:PHE:C	1:C:1758:ARG:HH12	2.16	0.54
1:C:3162:GLN:OE1	1:C:3218:VAL:HG23	2.08	0.54
1:C:3682:GLU:O	1:C:3685:GLU:N	2.41	0.54
1:B:1749:PRO:N	1:B:1758:ARG:HH12	2.06	0.54
1:B:2790:MET:SD	1:B:2797:PHE:HZ	2.30	0.54
1:D:985:VAL:HG13	1:D:1039:LEU:HD22	1.89	0.54
1:C:3527:PRO:HD2	1:C:3573:MET:SD	2.48	0.54
1:C:3727:ASP:O	1:C:3731:LYS:HG3	2.08	0.54
1:C:3852:LYS:O	1:C:3856:LEU:HG	2.06	0.54
1:A:1045:THR:HG22	1:A:1049:TYR:CE2	2.43	0.54
1:A:2961:GLN:HG3	1:A:3038:MET:HE1	1.90	0.54
2:E:90:ILE:HG22	2:E:91:ILE:HG13	1.90	0.54
1:B:1045:THR:HG22	1:B:1049:TYR:CE2	2.43	0.54
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.40	0.54
1:B:3957:VAL:O	1:B:3961:VAL:HG23	2.08	0.54
1:D:3162:GLN:OE1	1:D:3218:VAL:HG23	2.08	0.54
1:D:4945:ASP:OD1	1:D:4946:GLN:N	2.41	0.54
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.40	0.54
1:C:2904:LEU:O	1:C:2904:LEU:HD23	2.07	0.54
1:A:3379:LEU:HD12	1:A:3382:GLU:OE2	2.08	0.54
1:B:3442:PHE:HE1	1:B:3511:VAL:HG12	1.73	0.54
1:D:590:LEU:HG	1:D:599:VAL:HG11	1.90	0.54
1:A:590:LEU:HG	1:A:599:VAL:HG11	1.90	0.54
1:A:2194:HIS:O	1:A:2198:MET:HE2	2.07	0.54
1:A:2642:LYS:NZ	1:A:2698:MET:SD	2.81	0.54
1:A:2904:LEU:HD23	1:A:2904:LEU:O	2.07	0.54
1:A:4945:ASP:OD1	1:A:4946:GLN:N	2.41	0.54
1:B:877:ASN:O	1:B:880:GLU:HG2	2.07	0.54
1:B:1280:GLN:O	1:B:1281:ASN:CG	2.51	0.54
1:D:445:LEU:HD23	1:D:525:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.40	0.54
1:D:3786:CYS:SG	1:D:3831:SER:OG	2.65	0.54
1:C:877:ASN:O	1:C:880:GLU:HG2	2.07	0.54
1:C:2226:PRO:CB	1:C:2267:MET:CE	2.78	0.54
1:A:3527:PRO:HD2	1:A:3573:MET:SD	2.48	0.53
1:B:3727:ASP:O	1:B:3731:LYS:HG3	2.08	0.53
1:D:877:ASN:O	1:D:880:GLU:HG2	2.07	0.53
1:D:1170:MET:HE1	1:C:3471:THR:HG22	1.89	0.53
1:D:1280:GLN:O	1:D:1281:ASN:CG	2.51	0.53
1:D:3166:TYR:OH	1:D:3203:VAL:HG11	2.06	0.53
1:C:590:LEU:HG	1:C:599:VAL:HG11	1.90	0.53
1:C:2294:ASP:O	1:C:2298:VAL:HG23	2.08	0.53
1:C:2638:LYS:HE2	1:C:2694:GLU:OE1	2.08	0.53
1:A:906:CYS:HB2	1:A:913:LEU:CB	2.38	0.53
1:A:1461:ASP:OD2	1:A:1468:LYS:NZ	2.37	0.53
1:A:1748:PHE:C	1:A:1758:ARG:HH12	2.16	0.53
1:B:2627:VAL:HA	1:B:2678:LEU:HD13	1.91	0.53
1:B:2638:LYS:HE2	1:B:2694:GLU:OE1	2.08	0.53
1:B:3379:LEU:HD12	1:B:3382:GLU:OE2	2.08	0.53
1:B:3682:GLU:O	1:B:3685:GLU:N	2.41	0.53
1:D:2294:ASP:O	1:D:2298:VAL:HG23	2.08	0.53
1:D:3727:ASP:O	1:D:3731:LYS:HG3	2.08	0.53
1:C:67:PHE:HB3	1:C:109:LEU:HD22	1.89	0.53
1:C:1749:PRO:N	1:C:1758:ARG:HH12	2.06	0.53
1:C:3379:LEU:HD12	1:C:3382:GLU:OE2	2.08	0.53
1:A:1749:PRO:N	1:A:1758:ARG:HH12	2.06	0.53
1:A:2882:TYR:O	1:A:2885:THR:HG22	2.09	0.53
2:G:80:TYR:CE2	2:G:80:TYR:CD1	2.38	0.53
1:B:437:PRO:O	1:B:441:VAL:HG23	2.09	0.53
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.22	0.53
1:D:1158:ASN:ND2	1:D:1182:ILE:O	2.40	0.53
1:D:2587:TYR:OH	1:D:2629:ASP:OD2	2.24	0.53
1:C:4945:ASP:OD1	1:C:4946:GLN:N	2.41	0.53
1:A:908:VAL:HG13	1:A:912:SER:HB2	1.89	0.53
1:A:1999:ARG:HH12	1:A:3636:PHE:CA	2.18	0.53
1:A:2294:ASP:O	1:A:2298:VAL:HG23	2.08	0.53
1:A:3727:ASP:O	1:A:3731:LYS:HG3	2.08	0.53
2:F:4:VAL:HG22	2:F:74:LEU:CD2	2.39	0.53
1:B:906:CYS:HB2	1:B:913:LEU:CB	2.38	0.53
1:B:1066:GLN:O	1:B:1071:ARG:NE	2.42	0.53
1:B:1999:ARG:HH12	1:B:3636:PHE:CA	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2642:LYS:NZ	1:B:2698:MET:SD	2.81	0.53
1:B:2782:ASP:N	1:B:2782:ASP:OD1	2.38	0.53
1:D:906:CYS:HB2	1:D:913:LEU:CB	2.38	0.53
1:D:1123:VAL:HG23	1:D:1132:TRP:HB2	1.91	0.53
1:D:2882:TYR:O	1:D:2885:THR:HG22	2.09	0.53
1:C:2627:VAL:HA	1:C:2678:LEU:HD13	1.91	0.53
1:C:2761:TYR:HB3	1:C:2765:LYS:HZ3	1.73	0.53
1:C:2882:TYR:O	1:C:2885:THR:HG22	2.09	0.53
1:C:3521:GLY:CA	1:C:3524:MET:HE2	2.31	0.53
1:C:4180:ARG:HD3	1:C:4192:ARG:HD3	1.89	0.53
1:A:384:MET:HE1	1:B:167:ASP:OD1	2.09	0.53
1:A:1066:GLN:O	1:A:1071:ARG:NE	2.42	0.53
1:A:3442:PHE:HE1	1:A:3511:VAL:HG12	1.73	0.53
2:G:4:VAL:HG22	2:G:74:LEU:CD2	2.39	0.53
1:B:2011:HIS:CE1	1:B:2017:ASP:CG	2.84	0.53
1:D:69:LEU:HD23	1:D:109:LEU:CD2	2.39	0.53
1:D:553:ARG:NE	1:D:555:GLU:OE2	2.38	0.53
1:D:2642:LYS:NZ	1:D:2698:MET:SD	2.81	0.53
1:D:2969:ILE:O	1:D:2973:PHE:CD1	2.62	0.53
1:C:286:THR:HG21	1:C:481:GLU:OE1	2.09	0.53
1:C:437:PRO:O	1:C:441:VAL:HG23	2.09	0.53
1:C:906:CYS:HB2	1:C:913:LEU:CB	2.38	0.53
1:A:445:LEU:HD23	1:A:525:LEU:HD22	1.91	0.53
1:A:3682:GLU:O	1:A:3685:GLU:N	2.41	0.53
1:B:1748:PHE:C	1:B:1758:ARG:HH12	2.16	0.53
1:B:2874:MET:CE	1:B:2939:ARG:CB	2.75	0.53
1:B:4929:LEU:C	1:B:4933:GLN:OE1	2.52	0.53
1:C:2011:HIS:CE1	1:C:2017:ASP:CG	2.84	0.53
1:C:3957:VAL:O	1:C:3961:VAL:HG23	2.08	0.53
1:C:4222:VAL:HG11	1:C:4950:VAL:HA	1.90	0.53
1:A:56:GLN:O	1:A:281:ARG:NH2	2.42	0.53
1:A:652:ARG:NH1	1:A:750:LEU:O	2.42	0.53
1:A:1833:SER:HG	1:A:1836:PHE:HD1	1.56	0.53
1:A:2974:ILE:O	1:A:2978:GLU:OE1	2.27	0.53
1:A:5009:TYR:CZ	1:A:5013:MET:HE3	2.44	0.53
1:B:3372:VAL:HG12	1:B:3398:PHE:CE1	2.44	0.53
1:B:4945:ASP:OD1	1:B:4946:GLN:N	2.41	0.53
1:D:112:ALA:O	1:D:115:ARG:NH1	2.38	0.53
1:D:437:PRO:O	1:D:441:VAL:HG23	2.09	0.53
1:D:3527:PRO:HD2	1:D:3573:MET:SD	2.48	0.53
1:D:3682:GLU:O	1:D:3685:GLU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:ARG:NH1	1:C:750:LEU:O	2.42	0.53
1:C:1123:VAL:HG23	1:C:1132:TRP:HB2	1.91	0.53
1:A:2969:ILE:O	1:A:2973:PHE:CD1	2.62	0.53
2:H:4:VAL:HG22	2:H:74:LEU:CD2	2.39	0.53
2:H:90:ILE:HG22	2:H:91:ILE:HG13	1.90	0.53
2:G:90:ILE:HG22	2:G:91:ILE:HG13	1.90	0.53
2:F:90:ILE:HD11	1:B:1684:ALA:HA	1.91	0.53
1:B:2294:ASP:O	1:B:2298:VAL:HG23	2.08	0.53
1:D:652:ARG:NH1	1:D:750:LEU:O	2.42	0.53
1:C:3239:MET:CG	1:C:3239:MET:HA	2.35	0.53
1:C:3755:GLU:O	1:C:3759:GLU:OE1	2.27	0.53
1:C:4998:LYS:HB3	1:C:5003:HIS:CE1	2.44	0.53
1:A:437:PRO:O	1:A:441:VAL:HG23	2.09	0.53
1:A:3755:GLU:O	1:A:3759:GLU:OE1	2.27	0.53
1:A:4929:LEU:C	1:A:4933:GLN:OE1	2.52	0.53
1:B:286:THR:HG21	1:B:481:GLU:OE1	2.09	0.53
1:B:590:LEU:HG	1:B:599:VAL:HG11	1.90	0.53
1:B:1123:VAL:HG23	1:B:1132:TRP:HB2	1.91	0.53
1:B:2233:CYS:HA	1:B:2237:CYS:SG	2.49	0.53
1:B:2929:PHE:CA	1:B:2932:MET:HE1	2.26	0.53
1:B:3471:THR:HG22	1:C:1170:MET:HE1	1.90	0.53
1:B:4222:VAL:HG11	1:B:4950:VAL:HA	1.90	0.53
1:D:1749:PRO:N	1:D:1758:ARG:HH12	2.06	0.53
1:D:3379:LEU:HD12	1:D:3382:GLU:OE2	2.08	0.53
1:C:445:LEU:HD23	1:C:525:LEU:HD22	1.91	0.53
1:C:908:VAL:HG13	1:C:912:SER:HB2	1.89	0.53
1:C:985:VAL:HG13	1:C:1039:LEU:HD22	1.89	0.53
1:C:2642:LYS:NZ	1:C:2698:MET:SD	2.81	0.53
1:A:3239:MET:CG	1:A:3239:MET:HA	2.34	0.53
1:A:4222:VAL:HG11	1:A:4950:VAL:HA	1.90	0.53
1:B:213:TYR:CE1	1:B:340:LYS:CG	2.92	0.53
1:B:1855:GLY:O	1:B:1859:VAL:HG23	2.09	0.53
1:B:3162:GLN:OE1	1:B:3218:VAL:HG23	2.08	0.53
1:D:286:THR:HG21	1:D:481:GLU:OE1	2.09	0.53
1:D:2974:ILE:O	1:D:2978:GLU:OE1	2.27	0.53
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.91	0.53
1:C:887:ILE:CG2	1:C:959:TYR:OH	2.57	0.53
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.22	0.53
1:C:1066:GLN:O	1:C:1071:ARG:NE	2.42	0.53
1:C:2969:ILE:O	1:C:2973:PHE:CD1	2.62	0.53
1:C:4929:LEU:C	1:C:4933:GLN:OE1	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:C	1:A:35:LEU:HD12	2.35	0.52
1:A:803:LEU:HD12	1:A:804:PRO:HD2	1.91	0.52
1:A:3162:GLN:OE1	1:A:3218:VAL:HG23	2.08	0.52
1:A:4984:ASN:OD1	1:A:4986:ALA:HB3	2.09	0.52
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.91	0.52
1:B:2974:ILE:O	1:B:2978:GLU:OE1	2.27	0.52
1:D:803:LEU:HD12	1:D:804:PRO:HD2	1.91	0.52
1:D:4222:VAL:HG11	1:D:4950:VAL:HA	1.90	0.52
1:C:69:LEU:HD23	1:C:109:LEU:CD2	2.39	0.52
1:C:236:ALA:O	1:C:237:ASP:OD2	2.28	0.52
1:C:1855:GLY:O	1:C:1859:VAL:HG23	2.09	0.52
1:C:1926:LEU:HD23	1:C:1929:MET:SD	2.49	0.52
1:C:2874:MET:CE	1:C:2939:ARG:CB	2.75	0.52
1:C:4989:MET:HE1	1:C:4990:PHE:CE1	2.44	0.52
1:A:213:TYR:CE1	1:A:340:LYS:CG	2.92	0.52
1:A:228:ASP:OD2	1:B:155:LYS:HE2	2.08	0.52
1:A:985:VAL:HG13	1:A:1039:LEU:HD22	1.89	0.52
1:A:4180:ARG:HD3	1:A:4192:ARG:HD3	1.89	0.52
1:B:56:GLN:O	1:B:281:ARG:NH2	2.42	0.52
1:B:445:LEU:HD23	1:B:525:LEU:HD22	1.91	0.52
1:D:236:ALA:O	1:D:237:ASP:OD2	2.28	0.52
1:D:1066:GLN:O	1:D:1071:ARG:NE	2.42	0.52
1:D:1999:ARG:HH12	1:D:3636:PHE:CA	2.18	0.52
1:D:2233:CYS:HA	1:D:2237:CYS:SG	2.50	0.52
1:D:2572:THR:C	1:D:2618:MET:HE1	2.34	0.52
1:D:3957:VAL:O	1:D:3961:VAL:HG23	2.08	0.52
1:D:4180:ARG:HD3	1:D:4192:ARG:HD3	1.89	0.52
1:D:5009:TYR:CZ	1:D:5013:MET:HE3	2.44	0.52
1:C:2572:THR:C	1:C:2618:MET:HE1	2.34	0.52
1:A:236:ALA:O	1:A:237:ASP:OD2	2.27	0.52
1:A:973:SER:O	1:A:976:ARG:NH1	2.43	0.52
1:A:1855:GLY:O	1:A:1859:VAL:HG23	2.09	0.52
1:A:3372:VAL:HG12	1:A:3398:PHE:CE1	2.44	0.52
2:E:4:VAL:HG22	2:E:74:LEU:CD2	2.39	0.52
1:B:69:LEU:HD23	1:B:109:LEU:CD2	2.39	0.52
1:D:973:SER:O	1:D:976:ARG:NH1	2.42	0.52
1:D:2874:MET:CE	1:D:2939:ARG:CB	2.75	0.52
1:C:1280:GLN:O	1:C:1281:ASN:CG	2.51	0.52
1:C:5009:TYR:CZ	1:C:5013:MET:HE3	2.44	0.52
1:A:81:MET:HE1	1:A:147:TRP:CZ2	2.44	0.52
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1926:LEU:HD23	1:A:1929:MET:SD	2.49	0.52
1:B:3621:HIS:O	1:B:3621:HIS:ND1	2.38	0.52
1:D:34:LYS:C	1:D:35:LEU:HD12	2.35	0.52
1:D:81:MET:HE1	1:D:147:TRP:CZ2	2.44	0.52
1:D:1855:GLY:O	1:D:1859:VAL:HG23	2.09	0.52
1:D:4984:ASN:OD1	1:D:4986:ALA:HB3	2.09	0.52
1:C:803:LEU:HD12	1:C:804:PRO:HD2	1.91	0.52
1:A:1123:VAL:HG23	1:A:1132:TRP:HB2	1.91	0.52
1:B:688:LEU:HD12	1:B:776:LEU:O	2.10	0.52
1:B:1749:PRO:C	1:B:1758:ARG:NH2	2.45	0.52
1:B:2572:THR:C	1:B:2618:MET:HE1	2.34	0.52
1:B:5009:TYR:CZ	1:B:5013:MET:HE3	2.44	0.52
1:D:688:LEU:HD12	1:D:776:LEU:O	2.10	0.52
1:D:1999:ARG:HH12	1:D:3636:PHE:HD1	1.58	0.52
1:D:3755:GLU:O	1:D:3759:GLU:OE1	2.27	0.52
1:A:887:ILE:CG2	1:A:959:TYR:OH	2.58	0.52
1:A:1812:LEU:HD11	1:A:1858:ASP:HB3	1.92	0.52
1:A:2233:CYS:HA	1:A:2237:CYS:SG	2.49	0.52
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.92	0.52
2:F:90:ILE:HG22	2:F:91:ILE:HG13	1.90	0.52
1:B:236:ALA:O	1:B:237:ASP:OD2	2.28	0.52
1:B:3514:LEU:HD21	1:B:3602:VAL:HG13	1.92	0.52
1:B:4989:MET:HE1	1:B:4990:PHE:CE1	2.44	0.52
1:D:213:TYR:CE1	1:D:340:LYS:CG	2.92	0.52
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.91	0.52
1:D:887:ILE:CG2	1:D:959:TYR:OH	2.58	0.52
1:D:4118:ASP:OD1	1:D:4122:MET:N	2.42	0.52
1:D:4929:LEU:C	1:D:4933:GLN:OE1	2.52	0.52
1:C:973:SER:O	1:C:976:ARG:NH1	2.43	0.52
1:A:2627:VAL:HA	1:A:2678:LEU:HD13	1.90	0.52
1:A:4998:LYS:HB3	1:A:5003:HIS:CE1	2.44	0.52
1:B:652:ARG:NH1	1:B:750:LEU:O	2.42	0.52
1:B:803:LEU:HD12	1:B:804:PRO:HD2	1.91	0.52
1:B:973:SER:O	1:B:976:ARG:NH1	2.43	0.52
1:B:1926:LEU:HD23	1:B:1929:MET:SD	2.49	0.52
1:B:2969:ILE:O	1:B:2973:PHE:CD1	2.62	0.52
1:B:4677:LEU:HD23	1:B:4711:PHE:CZ	2.45	0.52
1:D:56:GLN:O	1:D:281:ARG:NH2	2.42	0.52
1:D:1812:LEU:HD11	1:D:1858:ASP:HB3	1.92	0.52
1:D:2627:VAL:HA	1:D:2678:LEU:HD13	1.90	0.52
1:D:2638:LYS:HE2	1:D:2694:GLU:OE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3236:VAL:O	1:D:3239:MET:HG3	2.10	0.52
1:D:4241:THR:O	1:D:4245:MET:HG3	2.10	0.52
1:C:56:GLN:O	1:C:281:ARG:NH2	2.42	0.52
1:A:69:LEU:HD23	1:A:109:LEU:CD2	2.39	0.52
1:A:2572:THR:C	1:A:2618:MET:HE1	2.34	0.52
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.15	0.52
1:A:4989:MET:HE1	1:A:4990:PHE:CE1	2.44	0.52
1:B:3755:GLU:O	1:B:3759:GLU:OE1	2.27	0.52
1:B:4984:ASN:OD1	1:B:4986:ALA:HB3	2.09	0.52
1:D:10:GLU:OE1	1:D:10:GLU:O	2.28	0.52
1:D:3532:LEU:HA	1:D:3535:LEU:HD12	1.92	0.52
1:C:688:LEU:HD12	1:C:776:LEU:O	2.10	0.52
1:C:3372:VAL:HG12	1:C:3398:PHE:CE1	2.44	0.52
1:C:3607:GLU:O	1:C:3610:GLU:HG3	2.10	0.52
1:B:1461:ASP:OD2	1:B:1468:LYS:NZ	2.37	0.52
1:D:1065:ASN:OD1	1:D:1066:GLN:N	2.43	0.52
1:D:1926:LEU:HD23	1:D:1929:MET:SD	2.49	0.52
1:D:4677:LEU:HD23	1:D:4711:PHE:CZ	2.45	0.52
1:C:213:TYR:CE1	1:C:340:LYS:CG	2.92	0.52
1:C:3236:VAL:HA	1:C:3239:MET:HG2	1.90	0.52
1:C:4677:LEU:HD23	1:C:4711:PHE:CZ	2.45	0.52
1:C:4902:GLU:O	1:C:4913:ARG:CZ	2.58	0.52
1:A:10:GLU:OE1	1:A:10:GLU:O	2.28	0.52
1:A:286:THR:HG21	1:A:481:GLU:OE1	2.09	0.52
1:B:887:ILE:CG2	1:B:959:TYR:OH	2.58	0.52
1:B:1065:ASN:OD1	1:B:1066:GLN:N	2.43	0.52
1:B:2233:CYS:HB3	1:B:2237:CYS:HG	1.62	0.52
1:B:4705:VAL:HG13	1:B:4711:PHE:HE1	1.75	0.52
1:D:3621:HIS:O	1:D:3622:LYS:HG2	2.10	0.52
1:D:4989:MET:HE1	1:D:4990:PHE:CE1	2.44	0.52
1:C:2974:ILE:O	1:C:2978:GLU:OE1	2.27	0.52
1:C:3532:LEU:HA	1:C:3535:LEU:HD12	1.92	0.52
1:C:4984:ASN:OD1	1:C:4986:ALA:HB3	2.09	0.52
1:A:688:LEU:HD12	1:A:776:LEU:O	2.10	0.51
1:A:3521:GLY:CA	1:A:3524:MET:HE2	2.31	0.51
1:A:3589:PRO:O	1:A:3593:VAL:HG13	2.11	0.51
1:B:2882:TYR:O	1:B:2885:THR:HG22	2.09	0.51
1:B:4998:LYS:HB3	1:B:5003:HIS:CE1	2.44	0.51
1:D:4045:VAL:O	1:D:4049:VAL:HG23	2.11	0.51
1:C:2233:CYS:HA	1:C:2237:CYS:SG	2.49	0.51
1:A:1065:ASN:OD1	1:A:1066:GLN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4241:THR:O	1:A:4245:MET:HG3	2.10	0.51
1:B:3607:GLU:O	1:B:3610:GLU:HG3	2.10	0.51
1:D:1749:PRO:C	1:D:1758:ARG:NH2	2.45	0.51
1:D:3372:VAL:HG12	1:D:3398:PHE:CE1	2.44	0.51
1:C:34:LYS:C	1:C:35:LEU:HD12	2.35	0.51
1:C:81:MET:HE1	1:C:147:TRP:CZ2	2.44	0.51
1:C:3169:LEU:HD12	1:C:3194:LEU:HD11	1.93	0.51
1:C:3621:HIS:O	1:C:3622:LYS:HG2	2.10	0.51
1:A:2226:PRO:CB	1:A:2267:MET:CE	2.78	0.51
1:A:3598:GLU:O	1:A:3602:VAL:HG23	2.11	0.51
1:A:4705:VAL:HG13	1:A:4711:PHE:HE1	1.75	0.51
1:C:4548:ARG:O	1:C:4552:LEU:HD13	2.11	0.51
1:A:3621:HIS:O	1:A:3622:LYS:HG2	2.10	0.51
1:D:2292:GLU:O	1:D:2296:GLU:OE1	2.29	0.51
1:D:3589:PRO:O	1:D:3593:VAL:HG13	2.11	0.51
1:D:4902:GLU:O	1:D:4913:ARG:CZ	2.58	0.51
1:C:1812:LEU:HD11	1:C:1858:ASP:HB3	1.92	0.51
1:C:2006:ILE:HD11	1:C:3641:LEU:HD11	1.93	0.51
1:C:3514:LEU:HD21	1:C:3602:VAL:HG13	1.92	0.51
1:A:2970:SER:O	1:A:2974:ILE:HG23	2.11	0.51
1:B:34:LYS:C	1:B:35:LEU:HD12	2.35	0.51
1:B:3598:GLU:O	1:B:3602:VAL:HG23	2.11	0.51
1:B:4548:ARG:O	1:B:4552:LEU:HD13	2.11	0.51
1:D:3183:VAL:O	1:D:3187:ARG:HG3	2.11	0.51
1:D:4548:ARG:O	1:D:4552:LEU:HD13	2.11	0.51
1:D:4998:LYS:HB3	1:D:5003:HIS:CE1	2.44	0.51
1:A:3372:VAL:CG1	1:A:3398:PHE:HE1	2.24	0.51
1:B:1812:LEU:HD11	1:B:1858:ASP:HB3	1.92	0.51
1:D:2006:ILE:HD11	1:D:3641:LEU:HD11	1.93	0.51
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.92	0.51
1:C:2970:SER:O	1:C:2974:ILE:HG23	2.11	0.51
1:C:4705:VAL:HG13	1:C:4711:PHE:HE1	1.75	0.51
1:A:3183:VAL:O	1:A:3187:ARG:HG3	2.11	0.51
2:G:6:THR:HG23	2:G:6:THR:O	2.11	0.51
1:B:81:MET:HE1	1:B:147:TRP:CZ2	2.45	0.51
1:B:646:PRO:HB2	1:B:648:ILE:CD1	2.41	0.51
1:B:1726:SER:O	1:B:1729:SER:OG	2.23	0.51
1:B:2292:GLU:O	1:B:2296:GLU:OE1	2.29	0.51
1:B:3532:LEU:HA	1:B:3535:LEU:HD12	1.92	0.51
1:B:3621:HIS:O	1:B:3622:LYS:HG2	2.10	0.51
1:D:3169:LEU:HD12	1:D:3194:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3607:GLU:O	1:D:3610:GLU:HG3	2.10	0.51
1:C:4241:THR:O	1:C:4245:MET:HG3	2.10	0.51
1:A:2520:HIS:O	1:A:2524:VAL:HG22	2.11	0.51
1:A:3554:GLN:OE1	1:A:3593:VAL:HG11	2.11	0.51
1:A:3607:GLU:O	1:A:3610:GLU:HG3	2.10	0.51
1:A:4548:ARG:O	1:A:4552:LEU:HD13	2.11	0.51
1:A:4677:LEU:HD23	1:A:4711:PHE:CZ	2.45	0.51
1:A:4902:GLU:O	1:A:4913:ARG:CZ	2.58	0.51
2:G:90:ILE:HD11	1:C:1684:ALA:HA	1.92	0.51
1:B:228:ASP:OD2	1:C:155:LYS:HE2	2.11	0.51
1:B:3169:LEU:HD12	1:B:3194:LEU:HD11	1.93	0.51
1:B:3554:GLN:OE1	1:B:3593:VAL:HG11	2.11	0.51
1:B:3625:SER:O	1:B:3629:ARG:HG2	2.11	0.51
1:B:4902:GLU:O	1:B:4913:ARG:CZ	2.58	0.51
1:D:646:PRO:HB2	1:D:648:ILE:CD1	2.41	0.51
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.92	0.51
1:D:3996:PHE:HD1	1:D:4016:LEU:HD11	1.76	0.51
1:C:646:PRO:HB2	1:C:648:ILE:CD1	2.41	0.51
1:C:3372:VAL:CG1	1:C:3398:PHE:HE1	2.24	0.51
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.40	0.51
1:A:3169:LEU:HD12	1:A:3194:LEU:HD11	1.93	0.51
1:A:3471:THR:HG22	1:B:1170:MET:HE1	1.92	0.51
1:A:3621:HIS:O	1:A:3621:HIS:ND1	2.38	0.51
1:B:10:GLU:OE1	1:B:10:GLU:O	2.28	0.51
1:B:2523:ASP:CB	1:B:2578:MET:HE1	2.15	0.51
1:B:4241:THR:O	1:B:4245:MET:HG3	2.10	0.51
1:D:3299:GLY:O	1:D:3300:ALA:HB2	2.11	0.51
1:D:3514:LEU:HD21	1:D:3602:VAL:HG13	1.92	0.51
1:D:4651:THR:OG1	1:D:4803:HIS:NE2	2.05	0.51
1:C:978:THR:HG1	1:C:981:GLN:CD	2.19	0.51
1:C:1065:ASN:OD1	1:C:1066:GLN:N	2.43	0.51
1:C:1999:ARG:HH12	1:C:3636:PHE:CA	2.18	0.51
1:C:3589:PRO:O	1:C:3593:VAL:HG13	2.11	0.51
1:C:3996:PHE:HD1	1:C:4016:LEU:HD11	1.76	0.51
1:A:1749:PRO:C	1:A:1758:ARG:NH2	2.45	0.51
1:A:1962:ALA:O	1:A:1966:VAL:HG23	2.11	0.51
1:A:2107:GLN:O	1:A:3694:LYS:NZ	2.36	0.51
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.92	0.51
1:B:3589:PRO:O	1:B:3593:VAL:HG13	2.11	0.51
1:C:10:GLU:OE1	1:C:10:GLU:O	2.28	0.51
1:C:3598:GLU:O	1:C:3602:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2011:HIS:CE1	1:A:2017:ASP:CG	2.84	0.50
1:A:3996:PHE:HD1	1:A:4016:LEU:HD11	1.76	0.50
1:A:4098:ASP:OD1	1:A:4099:SER:N	2.44	0.50
1:A:4678:ALA:HB1	1:A:4720:VAL:HG21	1.93	0.50
1:A:4961:CYS:SG	1:A:4983:HIS:CE1	3.04	0.50
1:B:4232:GLU:OE1	1:B:5017:ARG:NH2	2.44	0.50
1:C:2292:GLU:O	1:C:2296:GLU:OE1	2.29	0.50
1:C:4045:VAL:O	1:C:4049:VAL:HG23	2.11	0.50
1:A:646:PRO:HB2	1:A:648:ILE:CD1	2.41	0.50
1:A:3532:LEU:HA	1:A:3535:LEU:HD12	1.92	0.50
2:F:6:THR:HG23	2:F:6:THR:O	2.10	0.50
1:B:110:ARG:NH2	1:B:117:TYR:HH	2.09	0.50
1:D:4232:GLU:OE1	1:D:5017:ARG:NH2	2.45	0.50
1:C:717:ASP:OD1	1:C:720:HIS:N	2.40	0.50
1:C:1962:ALA:O	1:C:1966:VAL:HG23	2.11	0.50
1:A:2638:LYS:HE2	1:A:2694:GLU:OE1	2.08	0.50
1:A:3372:VAL:HG11	1:A:3398:PHE:CE1	2.47	0.50
1:A:4045:VAL:O	1:A:4049:VAL:HG23	2.11	0.50
1:B:820:ARG:CZ	1:B:820:ARG:HB3	2.24	0.50
1:B:4118:ASP:OD1	1:B:4122:MET:N	2.42	0.50
1:D:4649:LEU:O	1:D:4653:VAL:HG23	2.11	0.50
1:C:2520:HIS:O	1:C:2524:VAL:HG22	2.11	0.50
1:A:3514:LEU:HD21	1:A:3602:VAL:HG13	1.92	0.50
1:B:384:MET:SD	1:C:167:ASP:HA	2.52	0.50
1:B:2006:ILE:HD11	1:B:3641:LEU:HD11	1.93	0.50
1:B:2520:HIS:O	1:B:2524:VAL:HG22	2.11	0.50
1:B:3468:SER:O	1:B:3472:ALA:HB2	2.12	0.50
1:B:4661:TYR:OH	1:B:4786:ASP:OD2	2.27	0.50
1:B:4678:ALA:HB1	1:B:4720:VAL:HG21	1.93	0.50
1:D:2675:THR:HG23	1:D:2706:ILE:HG23	1.94	0.50
1:C:3372:VAL:HG11	1:C:3398:PHE:CE1	2.47	0.50
1:C:4678:ALA:HB1	1:C:4720:VAL:HG21	1.93	0.50
1:C:4961:CYS:SG	1:C:4983:HIS:CE1	3.04	0.50
1:A:796:ARG:NH1	1:A:1619:ARG:HH22	2.10	0.50
1:A:880:GLU:HG3	1:A:881:LEU:N	2.27	0.50
1:A:2006:ILE:HD11	1:A:3641:LEU:HD11	1.93	0.50
1:A:2482:ASP:C	1:A:2482:ASP:OD1	2.55	0.50
1:A:2572:THR:CG2	1:A:2579:VAL:CG2	2.83	0.50
1:B:2929:PHE:CA	1:B:2932:MET:SD	2.98	0.50
1:B:4045:VAL:O	1:B:4049:VAL:HG23	2.11	0.50
1:B:4098:ASP:OD1	1:B:4099:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4989:MET:SD	1:B:4993:MET:SD	3.10	0.50
1:D:323:LEU:HD23	1:D:323:LEU:H	1.77	0.50
1:D:880:GLU:HG3	1:D:881:LEU:N	2.27	0.50
1:D:2190:VAL:HG12	1:D:2198:MET:HE1	1.94	0.50
1:D:3468:SER:O	1:D:3472:ALA:HB2	2.12	0.50
1:D:3598:GLU:O	1:D:3602:VAL:HG23	2.11	0.50
1:C:612:VAL:HG13	1:C:2167:ILE:O	2.12	0.50
1:C:3183:VAL:O	1:C:3187:ARG:HG3	2.11	0.50
1:C:4649:LEU:O	1:C:4653:VAL:HG23	2.11	0.50
1:A:2587:TYR:OH	1:A:2629:ASP:OD2	2.24	0.50
1:A:2675:THR:HG23	1:A:2706:ILE:HG23	1.94	0.50
1:A:3468:SER:O	1:A:3472:ALA:HB2	2.12	0.50
1:A:3625:SER:O	1:A:3629:ARG:HG2	2.11	0.50
1:A:4075:GLU:CD	1:B:4736:ARG:NH1	2.69	0.50
2:H:6:THR:HG23	2:H:6:THR:O	2.10	0.50
1:B:796:ARG:NH1	1:B:1619:ARG:HH22	2.10	0.50
1:B:3521:GLY:CA	1:B:3524:MET:HE2	2.31	0.50
1:D:167:ASP:OD1	1:C:384:MET:CE	2.60	0.50
1:D:2970:SER:O	1:D:2974:ILE:HG23	2.11	0.50
1:C:323:LEU:HD23	1:C:323:LEU:H	1.77	0.50
1:C:3299:GLY:O	1:C:3300:ALA:HB2	2.11	0.50
1:C:3554:GLN:OE1	1:C:3593:VAL:HG11	2.11	0.50
1:A:72:SER:O	1:A:99:ARG:NH1	2.45	0.50
1:A:2292:GLU:O	1:A:2296:GLU:OE1	2.29	0.50
1:A:2969:ILE:O	1:A:2972:GLU:HG3	2.11	0.50
1:A:4232:GLU:OE1	1:A:5017:ARG:NH2	2.44	0.50
1:B:781:VAL:HG13	1:B:791:PHE:CZ	2.47	0.50
1:B:1962:ALA:O	1:B:1966:VAL:HG23	2.12	0.50
1:B:2524:VAL:HG23	1:B:2525:GLY:N	2.27	0.50
1:B:3169:LEU:HD21	1:B:3205:PHE:CD2	2.47	0.50
1:B:3372:VAL:HG11	1:B:3398:PHE:CE1	2.47	0.50
1:B:4649:LEU:O	1:B:4653:VAL:HG23	2.11	0.50
1:B:4961:CYS:SG	1:B:4983:HIS:CE1	3.04	0.50
1:D:1043:VAL:HA	1:D:1046:LEU:HD12	1.94	0.50
1:D:1962:ALA:O	1:D:1966:VAL:HG23	2.11	0.50
1:D:3554:GLN:OE1	1:D:3593:VAL:HG11	2.11	0.50
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.93	0.50
1:D:4989:MET:SD	1:D:4993:MET:SD	3.10	0.50
1:C:2190:VAL:HG12	1:C:2198:MET:HE1	1.94	0.50
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.93	0.50
1:C:4098:ASP:OD1	1:C:4099:SER:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:VAL:HG13	1:A:2167:ILE:O	2.12	0.50
1:A:781:VAL:HG13	1:A:791:PHE:CZ	2.47	0.50
1:A:898:ASP:HB2	1:A:901:LYS:HG3	1.94	0.50
1:A:2524:VAL:HG23	1:A:2525:GLY:N	2.27	0.50
1:A:3299:GLY:O	1:A:3300:ALA:HB2	2.11	0.50
1:A:4649:LEU:O	1:A:4653:VAL:HG23	2.11	0.50
1:A:4989:MET:SD	1:A:4993:MET:SD	3.10	0.50
2:E:6:THR:HG23	2:E:6:THR:O	2.10	0.50
1:B:384:MET:CE	1:C:167:ASP:OD1	2.60	0.50
1:B:612:VAL:HG13	1:B:2167:ILE:O	2.12	0.50
1:B:880:GLU:HG3	1:B:881:LEU:N	2.27	0.50
1:B:2970:SER:O	1:B:2974:ILE:HG23	2.11	0.50
1:B:4060:LYS:O	1:B:4064:MET:HG3	2.12	0.50
1:D:781:VAL:HG13	1:D:791:PHE:CZ	2.47	0.50
1:D:2011:HIS:CE1	1:D:2017:ASP:CG	2.84	0.50
1:D:3372:VAL:HG11	1:D:3398:PHE:CE1	2.46	0.50
1:C:3169:LEU:CD1	1:C:3194:LEU:HD11	2.41	0.50
1:C:3468:SER:O	1:C:3472:ALA:HB2	2.12	0.50
1:C:4989:MET:SD	1:C:4993:MET:SD	3.10	0.50
1:A:323:LEU:HD23	1:A:323:LEU:H	1.77	0.50
1:A:659:TYR:O	1:A:662:TRP:NE1	2.44	0.50
1:A:688:LEU:HD11	1:A:775:GLY:CA	2.42	0.50
1:B:323:LEU:H	1:B:323:LEU:HD23	1.77	0.50
1:B:3372:VAL:CG1	1:B:3398:PHE:HE1	2.24	0.50
1:B:3786:CYS:SG	1:B:3831:SER:OG	2.65	0.50
1:D:2135:LEU:HD21	1:D:3663:LEU:HD21	1.94	0.50
1:D:4098:ASP:OD1	1:D:4099:SER:N	2.44	0.50
1:C:781:VAL:HG13	1:C:791:PHE:CZ	2.47	0.50
1:A:3835:LEU:HD22	1:A:3880:PHE:CZ	2.47	0.49
1:B:2107:GLN:O	1:B:3694:LYS:NZ	2.36	0.49
1:B:2923:ALA:O	1:B:2927:LEU:HD23	2.12	0.49
1:D:72:SER:O	1:D:99:ARG:NH1	2.45	0.49
1:D:612:VAL:HG13	1:D:2167:ILE:O	2.12	0.49
1:D:796:ARG:NH1	1:D:1619:ARG:HH22	2.10	0.49
1:D:898:ASP:HB2	1:D:901:LYS:HG3	1.94	0.49
1:D:2969:ILE:O	1:D:2972:GLU:HG3	2.11	0.49
1:D:3169:LEU:CD1	1:D:3194:LEU:HD11	2.42	0.49
1:D:3239:MET:CG	1:D:3239:MET:HA	2.34	0.49
1:D:3625:SER:O	1:D:3629:ARG:HG2	2.11	0.49
1:C:898:ASP:HB2	1:C:901:LYS:HG3	1.94	0.49
1:C:4565:LEU:O	1:C:4569:LEU:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3183:VAL:O	1:B:3187:ARG:HG3	2.11	0.49
1:B:3996:PHE:HD1	1:B:4016:LEU:HD11	1.76	0.49
1:B:4835:LYS:O	1:B:4839:MET:HG2	2.12	0.49
1:D:155:LYS:HE2	1:C:228:ASP:OD2	2.11	0.49
1:D:2520:HIS:O	1:D:2524:VAL:HG22	2.11	0.49
1:D:4961:CYS:SG	1:D:4983:HIS:CE1	3.04	0.49
1:C:2675:THR:HG23	1:C:2706:ILE:HG23	1.94	0.49
1:C:2969:ILE:O	1:C:2972:GLU:HG3	2.11	0.49
1:C:3835:LEU:HD22	1:C:3880:PHE:CZ	2.47	0.49
1:C:4060:LYS:O	1:C:4064:MET:HG3	2.12	0.49
1:C:4232:GLU:OE1	1:C:5017:ARG:NH2	2.44	0.49
1:A:554:LEU:CD1	1:A:1593:PRO:HG3	2.42	0.49
1:A:913:LEU:O	1:A:918:ARG:NH2	2.45	0.49
1:A:2135:LEU:HD21	1:A:3663:LEU:HD21	1.94	0.49
1:A:3169:LEU:CD1	1:A:3194:LEU:HD11	2.42	0.49
1:A:4705:VAL:HG22	1:A:4711:PHE:HD1	1.78	0.49
1:B:667:MET:SD	1:B:790:ARG:NH2	2.85	0.49
1:B:898:ASP:HB2	1:B:901:LYS:HG3	1.94	0.49
1:B:2969:ILE:O	1:B:2972:GLU:HG3	2.11	0.49
1:B:3169:LEU:CD1	1:B:3194:LEU:HD11	2.42	0.49
1:B:3299:GLY:O	1:B:3300:ALA:HB2	2.11	0.49
1:B:4565:LEU:O	1:B:4569:LEU:HD13	2.12	0.49
1:B:4705:VAL:HG22	1:B:4711:PHE:HD1	1.78	0.49
1:D:4835:LYS:O	1:D:4839:MET:HG2	2.12	0.49
1:C:796:ARG:NH1	1:C:1619:ARG:HH22	2.10	0.49
1:C:2261:SER:O	1:C:2264:GLY:N	2.43	0.49
1:C:3169:LEU:HD21	1:C:3205:PHE:CD2	2.47	0.49
1:C:3625:SER:O	1:C:3629:ARG:HG2	2.11	0.49
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.93	0.49
1:A:2788:HIS:ND1	1:A:2790:MET:HB3	2.27	0.49
1:A:3230:LEU:HD12	1:A:3230:LEU:O	2.13	0.49
1:B:2190:VAL:HG12	1:B:2198:MET:HE1	1.94	0.49
1:B:4976:GLU:HG2	1:B:4980:LEU:HD13	1.94	0.49
1:D:887:ILE:HD11	1:D:907:LEU:HD21	1.95	0.49
1:C:72:SER:O	1:C:99:ARG:NH1	2.45	0.49
1:C:2524:VAL:HG23	1:C:2525:GLY:N	2.27	0.49
1:C:2798:SER:OG	1:C:2801:ASP:OD2	2.26	0.49
1:A:1170:MET:HE1	1:D:3471:THR:HG22	1.94	0.49
1:A:2190:VAL:HG12	1:A:2198:MET:HE1	1.94	0.49
1:A:2751:LEU:HD23	1:A:2755:ILE:HD13	1.95	0.49
1:A:4060:LYS:O	1:A:4064:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3230:LEU:HD12	1:B:3230:LEU:O	2.13	0.49
1:D:688:LEU:HD11	1:D:775:GLY:CA	2.42	0.49
1:D:1726:SER:O	1:D:1729:SER:OG	2.24	0.49
1:D:1991:THR:O	1:D:1995:THR:HG23	2.13	0.49
1:D:3169:LEU:HD21	1:D:3205:PHE:CD2	2.47	0.49
1:D:3434:LEU:HD23	1:D:3517:MET:HE2	1.94	0.49
1:C:880:GLU:HG3	1:C:881:LEU:N	2.27	0.49
1:C:2135:LEU:HD21	1:C:3663:LEU:HD21	1.94	0.49
1:C:4835:LYS:O	1:C:4839:MET:HG2	2.13	0.49
1:A:1991:THR:O	1:A:1995:THR:HG23	2.13	0.49
1:A:2693:GLN:HE22	1:A:2697:ARG:HH11	1.60	0.49
1:A:2923:ALA:O	1:A:2927:LEU:HD23	2.12	0.49
1:A:2929:PHE:CA	1:A:2932:MET:SD	2.98	0.49
1:A:3786:CYS:SG	1:A:3831:SER:OG	2.65	0.49
1:B:554:LEU:CD1	1:B:1593:PRO:HG3	2.42	0.49
1:B:688:LEU:HD11	1:B:775:GLY:CA	2.42	0.49
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.93	0.49
1:B:2693:GLN:HE22	1:B:2697:ARG:HH11	1.60	0.49
1:B:2788:HIS:ND1	1:B:2790:MET:HB3	2.27	0.49
1:B:4583:SER:OG	1:B:4585:SER:O	2.27	0.49
1:B:4732:PHE:CD2	1:B:4732:PHE:O	2.66	0.49
1:D:554:LEU:CD1	1:D:1593:PRO:HG3	2.42	0.49
1:D:667:MET:SD	1:D:790:ARG:NH2	2.86	0.49
1:D:3230:LEU:HD12	1:D:3230:LEU:O	2.12	0.49
1:D:4705:VAL:HG13	1:D:4711:PHE:HE1	1.75	0.49
1:C:554:LEU:CD1	1:C:1593:PRO:HG3	2.42	0.49
1:C:887:ILE:HD11	1:C:907:LEU:HD21	1.95	0.49
1:C:1043:VAL:HA	1:C:1046:LEU:HD12	1.94	0.49
1:C:2751:LEU:HD23	1:C:2755:ILE:HD13	1.95	0.49
1:C:2923:ALA:O	1:C:2927:LEU:HD23	2.12	0.49
1:A:2744:ASN:OD1	1:A:2745:VAL:HG23	2.13	0.49
1:B:72:SER:O	1:B:99:ARG:NH1	2.45	0.49
1:B:296:ASP:OD1	1:B:297:GLN:OE1	2.31	0.49
1:B:1991:THR:O	1:B:1995:THR:HG23	2.13	0.49
1:B:2135:LEU:HD21	1:B:3663:LEU:HD21	1.94	0.49
1:D:2482:ASP:C	1:D:2482:ASP:OD1	2.55	0.49
1:D:2744:ASN:OD1	1:D:2745:VAL:HG23	2.13	0.49
1:D:2923:ALA:O	1:D:2927:LEU:HD23	2.12	0.49
1:D:3835:LEU:HD22	1:D:3880:PHE:CZ	2.47	0.49
1:D:4976:GLU:HG2	1:D:4980:LEU:HD13	1.94	0.49
1:C:2482:ASP:C	1:C:2482:ASP:OD1	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2929:PHE:CA	1:C:2932:MET:SD	2.98	0.49
1:C:3434:LEU:HD23	1:C:3517:MET:HE2	1.95	0.49
1:C:3621:HIS:O	1:C:3621:HIS:ND1	2.38	0.49
1:A:3901:ASN:OD1	1:A:3904:ARG:NH1	2.39	0.49
1:A:4565:LEU:O	1:A:4569:LEU:HD13	2.12	0.49
1:B:979:PRO:O	1:B:983:THR:HG23	2.13	0.49
1:B:2476:ILE:HD12	1:B:2532:ALA:HB1	1.95	0.49
1:B:2751:LEU:HD23	1:B:2755:ILE:HD13	1.95	0.49
1:D:363:ASP:OD1	1:D:366:ALA:HB2	2.13	0.49
1:C:913:LEU:O	1:C:918:ARG:NH2	2.45	0.49
1:C:979:PRO:O	1:C:983:THR:HG23	2.13	0.49
1:C:2476:ILE:HD12	1:C:2532:ALA:HB1	1.95	0.49
1:C:2701:PRO:C	1:C:2702:CYS:SG	2.96	0.49
1:C:4732:PHE:CD2	1:C:4732:PHE:O	2.66	0.49
1:A:2675:THR:HB	1:A:2710:LEU:HD21	1.95	0.49
1:A:4736:ARG:NH1	1:D:4075:GLU:CD	2.70	0.49
1:B:2482:ASP:OD1	1:B:2482:ASP:C	2.55	0.49
1:B:2798:SER:OG	1:B:2801:ASP:OD2	2.26	0.49
1:B:3835:LEU:HD22	1:B:3880:PHE:CZ	2.48	0.49
1:D:4565:LEU:O	1:D:4569:LEU:HD13	2.12	0.49
1:C:1991:THR:O	1:C:1995:THR:HG23	2.12	0.49
1:C:3969:ILE:CG2	1:C:3980:LEU:HD12	2.43	0.49
1:C:4651:THR:OG1	1:C:4803:HIS:NE2	2.05	0.49
1:C:4705:VAL:HG22	1:C:4711:PHE:HD1	1.78	0.49
1:A:887:ILE:HD11	1:A:907:LEU:HD21	1.95	0.49
1:A:1743[A]:ARG:NH2	1:A:1967:ASP:OD2	2.40	0.49
1:B:360:ALA:O	1:B:361:ALA:HB3	2.13	0.49
1:B:1043:VAL:HA	1:B:1046:LEU:HD12	1.94	0.49
1:B:1810:LYS:O	1:B:1814:MET:HG3	2.13	0.49
1:B:2675:THR:HG23	1:B:2706:ILE:HG23	1.94	0.49
1:B:2701:PRO:C	1:B:2702:CYS:SG	2.96	0.49
1:D:659:TYR:O	1:D:662:TRP:NE1	2.44	0.49
1:D:1833:SER:HG	1:D:1836:PHE:HD1	1.59	0.49
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.93	0.49
1:D:2524:VAL:HG23	1:D:2525:GLY:N	2.27	0.49
1:D:4705:VAL:HG22	1:D:4711:PHE:HD1	1.78	0.49
1:C:659:TYR:O	1:C:662:TRP:NE1	2.44	0.49
1:C:2974:ILE:HG13	1:C:2975:ALA:N	2.28	0.49
1:C:3590:GLU:O	1:C:3594:ARG:HG3	2.13	0.49
1:C:4976:GLU:HG2	1:C:4980:LEU:HD13	1.94	0.49
1:A:861:ILE:HD13	1:A:930:LYS:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2751:LEU:HD23	1:D:2755:ILE:HD13	1.95	0.48
1:D:3969:ILE:CG2	1:D:3980:LEU:HD12	2.43	0.48
1:C:667:MET:SD	1:C:790:ARG:NH2	2.85	0.48
1:C:4000:MET:SD	1:C:4020:GLN:NE2	2.79	0.48
1:A:2701:PRO:C	1:A:2702:CYS:SG	2.96	0.48
1:A:3941:ASP:OD2	1:A:3941:ASP:N	2.46	0.48
1:A:4640:GLU:HB3	1:A:4641:PRO:HD3	1.95	0.48
1:B:861:ILE:HD13	1:B:930:LYS:CD	2.43	0.48
1:B:1999:ARG:HH12	1:B:3636:PHE:HD1	1.58	0.48
1:B:4640:GLU:HB3	1:B:4641:PRO:HD3	1.95	0.48
1:D:913:LEU:O	1:D:918:ARG:NH2	2.45	0.48
1:D:2481:LYS:O	1:D:2482:ASP:CG	2.57	0.48
1:D:2974:ILE:HG13	1:D:2975:ALA:N	2.28	0.48
1:C:552:ASP:OD1	1:C:553:ARG:N	2.47	0.48
1:C:4834:GLY:O	1:C:4838:VAL:HG23	2.13	0.48
1:A:360:ALA:O	1:A:361:ALA:HB3	2.13	0.48
1:A:667:MET:SD	1:A:790:ARG:NH2	2.85	0.48
1:A:898:ASP:HB2	1:A:901:LYS:CG	2.43	0.48
1:A:1043:VAL:HA	1:A:1046:LEU:HD12	1.94	0.48
1:A:1810:LYS:O	1:A:1814:MET:HG3	2.13	0.48
1:A:3442:PHE:CE1	1:A:3511:VAL:HG12	2.48	0.48
1:A:4732:PHE:O	1:A:4732:PHE:CD2	2.66	0.48
1:B:3590:GLU:O	1:B:3594:ARG:HG3	2.13	0.48
1:B:4000:MET:SD	1:B:4020:GLN:NE2	2.79	0.48
1:B:5014:TYR:HD1	6:B:5304:PNX:HAA3	1.76	0.48
1:D:167:ASP:HA	1:C:384:MET:SD	2.53	0.48
1:D:1810:LYS:O	1:D:1814:MET:HG3	2.13	0.48
1:D:3635:CYS:HA	1:D:3638:MET:HE3	1.95	0.48
1:D:4764:LEU:O	1:D:4768:LEU:HG	2.13	0.48
1:C:1810:LYS:O	1:C:1814:MET:HG3	2.13	0.48
1:C:3635:CYS:HA	1:C:3638:MET:HE3	1.95	0.48
1:C:4118:ASP:OD1	1:C:4122:MET:N	2.42	0.48
1:A:363:ASP:OD1	1:A:366:ALA:HB2	2.13	0.48
1:A:552:ASP:OD1	1:A:553:ARG:N	2.47	0.48
1:A:3169:LEU:HD21	1:A:3205:PHE:CD2	2.47	0.48
1:A:4835:LYS:O	1:A:4839:MET:HG2	2.12	0.48
1:B:2481:LYS:O	1:B:2482:ASP:CG	2.57	0.48
1:D:4060:LYS:O	1:D:4064:MET:HG3	2.12	0.48
1:D:4834:GLY:O	1:D:4838:VAL:HG23	2.13	0.48
1:D:5014:TYR:HD1	6:D:5304:PNX:HAA3	1.76	0.48
1:C:2742:THR:HG23	1:C:2814:LYS:CE	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3442:PHE:CE1	1:C:3511:VAL:HG12	2.48	0.48
1:A:3635:CYS:HA	1:A:3638:MET:HE3	1.95	0.48
1:A:3735:LEU:HG	1:A:3735:LEU:O	2.14	0.48
1:A:4976:GLU:HG2	1:A:4980:LEU:HD13	1.94	0.48
1:B:363:ASP:OD1	1:B:366:ALA:HB2	2.13	0.48
1:B:552:ASP:OD1	1:B:553:ARG:N	2.46	0.48
1:B:2223:ILE:HG23	1:B:2223:ILE:O	2.13	0.48
1:B:2534:ALA:HB1	1:B:2588:ARG:HD3	1.96	0.48
1:B:2974:ILE:HG13	1:B:2975:ALA:N	2.28	0.48
1:B:3635:CYS:HA	1:B:3638:MET:HE3	1.95	0.48
1:D:552:ASP:OD1	1:D:553:ARG:N	2.47	0.48
1:D:898:ASP:HB2	1:D:901:LYS:CG	2.43	0.48
1:D:2569:PHE:CE1	1:D:2582:MET:HE1	2.48	0.48
1:D:2701:PRO:C	1:D:2702:CYS:SG	2.96	0.48
1:D:2742:THR:HG23	1:D:2814:LYS:CE	2.41	0.48
1:D:3735:LEU:HG	1:D:3735:LEU:O	2.14	0.48
1:C:360:ALA:O	1:C:361:ALA:HB3	2.13	0.48
1:C:898:ASP:HB2	1:C:901:LYS:CG	2.43	0.48
1:C:2223:ILE:O	1:C:2223:ILE:HG23	2.13	0.48
1:C:3230:LEU:O	1:C:3230:LEU:HD12	2.13	0.48
1:A:2569:PHE:CE1	1:A:2582:MET:HE1	2.48	0.48
1:A:3321:ARG:O	1:A:3324:VAL:HG22	2.14	0.48
1:A:4661:TYR:OH	1:A:4786:ASP:OD2	2.27	0.48
1:B:717:ASP:OD1	1:B:720:HIS:N	2.40	0.48
1:B:2675:THR:HB	1:B:2710:LEU:HD21	1.95	0.48
1:B:3442:PHE:CE1	1:B:3511:VAL:HG12	2.48	0.48
1:D:360:ALA:O	1:D:361:ALA:HB3	2.13	0.48
1:D:2693:GLN:HE22	1:D:2697:ARG:HH11	1.60	0.48
1:C:2355:ARG:HG3	1:C:2355:ARG:HH11	1.79	0.48
1:C:2569:PHE:CE1	1:C:2582:MET:HE1	2.48	0.48
1:C:2742:THR:CG2	1:C:2814:LYS:HE3	2.42	0.48
1:C:2744:ASN:OD1	1:C:2745:VAL:HG23	2.13	0.48
1:A:167:ASP:OD1	1:D:384:MET:SD	2.72	0.48
1:A:953:THR:O	1:A:968:ALA:HB1	2.14	0.48
1:A:1726:SER:O	1:A:1729:SER:OG	2.24	0.48
1:A:3434:LEU:HD23	1:A:3517:MET:HE2	1.94	0.48
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.96	0.48
1:B:861:ILE:HG21	1:B:930:LYS:HD2	1.96	0.48
1:B:3434:LEU:HD23	1:B:3517:MET:HE2	1.95	0.48
1:B:3471:THR:HG22	1:C:1170:MET:CE	2.44	0.48
1:B:4834:GLY:O	1:B:4838:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ASP:OD1	1:D:297:GLN:OE1	2.31	0.48
1:D:861:ILE:HD13	1:D:930:LYS:CD	2.43	0.48
1:D:1743[A]:ARG:NH2	1:D:1967:ASP:OD2	2.39	0.48
1:D:3941:ASP:OD2	1:D:3941:ASP:N	2.47	0.48
1:D:4911:LEU:O	1:D:4914:VAL:HG22	2.14	0.48
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.15	0.48
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.39	0.48
1:C:5014:TYR:HD1	6:C:5304:PNX:HAA3	1.75	0.48
1:A:574:VAL:O	1:A:578:ILE:HG12	2.14	0.48
1:A:3651:ASN:O	1:A:3655:GLU:OE1	2.32	0.48
1:A:4764:LEU:O	1:A:4768:LEU:HG	2.13	0.48
1:A:4834:GLY:O	1:A:4838:VAL:HG23	2.13	0.48
1:B:913:LEU:O	1:B:918:ARG:NH2	2.45	0.48
1:B:978:THR:O	1:B:982:THR:HG23	2.14	0.48
1:B:3321:ARG:O	1:B:3324:VAL:HG22	2.14	0.48
1:B:4764:LEU:O	1:B:4768:LEU:HG	2.13	0.48
1:B:4911:LEU:O	1:B:4914:VAL:HG22	2.14	0.48
1:D:590:LEU:HD21	1:D:599:VAL:HB	1.96	0.48
1:D:2098:VAL:HG11	1:D:2123:LEU:HG	1.96	0.48
1:D:2122:SER:HA	1:D:3721:LEU:HD11	1.96	0.48
1:D:3365:LEU:HD11	1:D:3408:LEU:HD12	1.95	0.48
1:D:3442:PHE:CE1	1:D:3511:VAL:HG12	2.48	0.48
1:D:3651:ASN:O	1:D:3655:GLU:OE1	2.32	0.48
1:C:2098:VAL:HG11	1:C:2123:LEU:HG	1.96	0.48
1:C:2204:HIS:NE2	1:C:2205:GLU:OE2	2.47	0.48
1:C:2481:LYS:O	1:C:2482:ASP:CG	2.56	0.48
1:C:2534:ALA:HB1	1:C:2588:ARG:HD3	1.96	0.48
1:C:2788:HIS:ND1	1:C:2790:MET:HB3	2.28	0.48
1:C:3786:CYS:SG	1:C:3831:SER:OG	2.65	0.48
1:A:590:LEU:HD21	1:A:599:VAL:HB	1.96	0.48
1:A:861:ILE:HG21	1:A:930:LYS:HD2	1.96	0.48
1:A:2098:VAL:HG11	1:A:2123:LEU:HG	1.96	0.48
1:A:2476:ILE:HG13	1:A:2536:LEU:HD11	1.96	0.48
1:A:3627:GLN:O	1:A:3630:ARG:HG2	2.14	0.48
1:B:659:TYR:O	1:B:662:TRP:NE1	2.44	0.48
1:B:1112:ASP:OD1	1:B:1113:VAL:N	2.47	0.48
1:B:2098:VAL:HG11	1:B:2123:LEU:HG	1.96	0.48
1:B:2476:ILE:HG13	1:B:2536:LEU:HD11	1.96	0.48
1:B:2569:PHE:CE1	1:B:2582:MET:HE1	2.48	0.48
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.96	0.48
1:B:3969:ILE:CG2	1:B:3980:LEU:HD12	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:VAL:O	1:D:578:ILE:HG12	2.14	0.48
1:D:919:ASN:O	1:D:923:GLN:OE1	2.32	0.48
1:D:2534:ALA:HB1	1:D:2588:ARG:HD3	1.96	0.48
1:D:2675:THR:HB	1:D:2710:LEU:HD21	1.94	0.48
1:D:2788:HIS:ND1	1:D:2790:MET:HB3	2.27	0.48
1:D:4732:PHE:O	1:D:4732:PHE:CD2	2.66	0.48
1:C:590:LEU:HD21	1:C:599:VAL:HB	1.96	0.48
1:C:928:THR:O	1:C:931:THR:OG1	2.30	0.48
1:C:3735:LEU:O	1:C:3735:LEU:HG	2.14	0.48
1:A:919:ASN:O	1:A:923:GLN:OE1	2.32	0.48
1:A:979:PRO:O	1:A:983:THR:HG23	2.13	0.48
1:A:2668:SER:O	1:A:2669:GLU:HB3	2.14	0.48
1:A:2974:ILE:HG13	1:A:2975:ALA:N	2.28	0.48
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.96	0.48
1:B:2587:TYR:OH	1:B:2629:ASP:OD2	2.24	0.48
1:D:979:PRO:O	1:D:983:THR:HG23	2.13	0.48
1:D:2107:GLN:O	1:D:3694:LYS:NZ	2.36	0.48
1:D:4640:GLU:HB3	1:D:4641:PRO:HD3	1.96	0.48
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.96	0.48
1:C:941:MET:HE1	1:C:1051:TYR:CD2	2.46	0.48
1:C:953:THR:O	1:C:968:ALA:HB1	2.14	0.48
1:C:4911:LEU:O	1:C:4914:VAL:HG22	2.14	0.48
1:A:438:ILE:HG23	1:A:518:ILE:HD11	1.96	0.47
1:A:899:ASP:O	1:A:902:ARG:NE	2.45	0.47
1:A:4067:LYS:O	1:A:4070:ASP:OD1	2.33	0.47
1:B:3346:VAL:HG11	1:B:3414:ARG:HB2	1.96	0.47
1:D:1170:MET:CE	1:C:3471:THR:HG22	2.44	0.47
1:D:2329:GLU:O	1:D:2333:ASP:OD1	2.32	0.47
1:D:3627:GLN:O	1:D:3630:ARG:HG2	2.14	0.47
1:C:69:LEU:HD23	1:C:109:LEU:HD21	1.96	0.47
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.96	0.47
1:C:2392:ARG:O	1:C:2418:LEU:HD12	2.14	0.47
1:C:2693:GLN:HE22	1:C:2697:ARG:HH11	1.60	0.47
1:C:3159:ASP:O	1:C:3163:VAL:HG23	2.14	0.47
1:C:3651:ASN:O	1:C:3655:GLU:OE1	2.32	0.47
1:C:3941:ASP:OD2	1:C:3941:ASP:N	2.46	0.47
1:A:296:ASP:OD1	1:A:297:GLN:OE1	2.31	0.47
1:A:2355:ARG:HH11	1:A:2355:ARG:HG3	1.79	0.47
1:A:2373:GLY:O	1:B:130:LYS:NZ	2.44	0.47
1:A:3365:LEU:HD11	1:A:3408:LEU:HD12	1.95	0.47
1:B:221:ARG:NH2	1:B:255:HIS:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ILE:HG23	1:B:518:ILE:HD11	1.96	0.47
1:B:884:LEU:HD23	1:B:955:LEU:HD11	1.97	0.47
1:B:953:THR:O	1:B:968:ALA:HB1	2.14	0.47
1:B:2204:HIS:NE2	1:B:2205:GLU:OE2	2.47	0.47
1:B:2224:ARG:HE	1:B:2225:PHE:N	2.10	0.47
1:B:2355:ARG:HH11	1:B:2355:ARG:HG3	1.79	0.47
1:B:4067:LYS:O	1:B:4070:ASP:OD1	2.33	0.47
1:D:985:VAL:HG11	1:D:1040:CYS:HB3	1.96	0.47
1:D:2929:PHE:CA	1:D:2932:MET:SD	2.98	0.47
1:D:3346:VAL:HG11	1:D:3414:ARG:HB2	1.96	0.47
1:C:363:ASP:OD1	1:C:366:ALA:HB2	2.13	0.47
1:C:688:LEU:HD11	1:C:775:GLY:CA	2.42	0.47
1:C:978:THR:O	1:C:982:THR:HG23	2.14	0.47
1:C:1999:ARG:HH12	1:C:3636:PHE:HD1	1.58	0.47
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.80	0.47
1:A:46:LEU:CD2	1:A:125:ARG:HE	2.27	0.47
1:A:2481:LYS:O	1:A:2482:ASP:CG	2.56	0.47
1:A:4118:ASP:OD1	1:A:4122:MET:N	2.42	0.47
1:B:899:ASP:O	1:B:902:ARG:NE	2.45	0.47
1:D:1112:ASP:OD1	1:D:1113:VAL:N	2.47	0.47
1:D:2204:HIS:NE2	1:D:2205:GLU:OE2	2.47	0.47
1:D:2519:LEU:HD13	1:D:2575:ARG:HG3	1.97	0.47
1:C:2668:SER:O	1:C:2669:GLU:HB3	2.14	0.47
1:C:2675:THR:HB	1:C:2710:LEU:HD21	1.95	0.47
1:C:3398:PHE:CE2	1:C:3450:ASN:CB	2.97	0.47
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.96	0.47
1:A:978:THR:O	1:A:982:THR:HG23	2.14	0.47
1:A:1299:GLN:HG2	2:E:31:GLU:OE2	2.14	0.47
1:A:3159:ASP:O	1:A:3163:VAL:HG23	2.14	0.47
1:B:384:MET:HE1	1:C:167:ASP:OD1	2.14	0.47
1:B:898:ASP:HB2	1:B:901:LYS:CG	2.43	0.47
1:B:3365:LEU:HD11	1:B:3408:LEU:HD12	1.95	0.47
1:B:3627:GLN:O	1:B:3630:ARG:HG2	2.14	0.47
1:B:4096:ALA:O	1:B:4100:GLN:HG2	2.14	0.47
1:D:380:GLN:OE1	1:D:380:GLN:N	2.45	0.47
1:D:3166:TYR:CZ	1:D:3203:VAL:HG11	2.50	0.47
1:D:3239:MET:CB	1:D:3239:MET:HG3	2.31	0.47
1:C:3627:GLN:O	1:C:3630:ARG:HG2	2.14	0.47
1:A:928:THR:O	1:A:931:THR:OG1	2.30	0.47
1:A:3346:VAL:HG11	1:A:3414:ARG:HB2	1.96	0.47
1:A:3733:CYS:HB2	1:A:3803:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5014:TYR:HD1	6:A:5304:PNX:HAA3	1.76	0.47
2:G:2:VAL:CG2	2:G:58:GLY:HA2	2.45	0.47
1:B:3015:LEU:HD22	1:B:3025:LEU:HB3	1.96	0.47
1:B:3362:ILE:HG22	1:B:3437:MET:HB3	1.97	0.47
1:D:2414:ASN:C	1:D:2414:ASN:OD1	2.58	0.47
1:D:3362:ILE:HG22	1:D:3437:MET:HB3	1.97	0.47
1:C:1069:TRP:CE3	1:C:1602:PRO:HG2	2.50	0.47
1:C:2519:LEU:HD13	1:C:2575:ARG:HG3	1.97	0.47
1:C:4764:LEU:O	1:C:4768:LEU:HG	2.13	0.47
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.96	0.47
1:A:360:ALA:O	1:A:361:ALA:CB	2.63	0.47
1:A:384:MET:SD	1:B:167:ASP:N	2.87	0.47
1:A:2122:SER:HA	1:A:3721:LEU:HD11	1.96	0.47
1:A:2204:HIS:NE2	1:A:2205:GLU:OE2	2.47	0.47
1:A:2414:ASN:C	1:A:2414:ASN:OD1	2.58	0.47
1:A:2476:ILE:HD12	1:A:2532:ALA:HB1	1.95	0.47
1:A:2534:ALA:HB1	1:A:2588:ARG:HD3	1.96	0.47
1:A:2742:THR:HG23	1:A:2814:LYS:CE	2.41	0.47
1:A:3362:ILE:HG22	1:A:3437:MET:HB3	1.97	0.47
1:A:3477:LYS:NZ	1:A:3479:ALA:HA	2.30	0.47
1:A:4911:LEU:O	1:A:4914:VAL:HG22	2.14	0.47
2:E:2:VAL:CG2	2:E:58:GLY:HA2	2.45	0.47
1:B:880:GLU:HB2	1:B:967:PRO:HG2	1.97	0.47
1:B:2519:LEU:HD13	1:B:2575:ARG:HG3	1.97	0.47
1:D:978:THR:O	1:D:982:THR:HG23	2.14	0.47
1:D:2223:ILE:HG23	1:D:2223:ILE:O	2.13	0.47
1:D:2392:ARG:O	1:D:2418:LEU:HD12	2.14	0.47
1:D:2742:THR:CG2	1:D:2814:LYS:HE3	2.42	0.47
1:D:3159:ASP:O	1:D:3163:VAL:HG23	2.14	0.47
1:D:3321:ARG:O	1:D:3324:VAL:HG22	2.14	0.47
1:D:3590:GLU:O	1:D:3594:ARG:HG3	2.13	0.47
1:D:3621:HIS:O	1:D:3621:HIS:ND1	2.38	0.47
1:C:574:VAL:O	1:C:578:ILE:HG12	2.14	0.47
1:C:667:MET:SD	1:C:801:LYS:NZ	2.86	0.47
1:C:2122:SER:HA	1:C:3721:LEU:HD11	1.96	0.47
1:C:2329:GLU:O	1:C:2333:ASP:OD1	2.32	0.47
1:C:3321:ARG:O	1:C:3324:VAL:HG22	2.14	0.47
1:C:3346:VAL:HG11	1:C:3414:ARG:HB2	1.96	0.47
1:C:3362:ILE:HG22	1:C:3437:MET:HB3	1.97	0.47
1:C:3733:CYS:HB2	1:C:3803:SER:OG	2.14	0.47
1:A:36:CYS:SG	1:A:52:THR:HG21	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1112:ASP:OD1	1:A:1113:VAL:N	2.47	0.47
1:A:1427:ILE:O	1:A:1430:THR:HG22	2.15	0.47
1:A:2014:ASP:O	1:A:2015:GLU:HB3	2.15	0.47
1:A:2519:LEU:HD13	1:A:2575:ARG:HG3	1.97	0.47
1:A:2638:LYS:O	1:A:2698:MET:CE	2.63	0.47
1:A:2790:MET:SD	1:A:2797:PHE:CZ	3.08	0.47
1:A:3234:ASN:O	1:A:3234:ASN:OD1	2.33	0.47
1:A:3590:GLU:O	1:A:3594:ARG:HG3	2.13	0.47
1:A:3969:ILE:CG2	1:A:3980:LEU:HD12	2.43	0.47
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.96	0.47
1:B:360:ALA:O	1:B:361:ALA:CB	2.63	0.47
1:B:1069:TRP:CE3	1:B:1602:PRO:HG2	2.49	0.47
1:B:2011:HIS:O	1:B:2011:HIS:ND1	2.47	0.47
1:B:2261:SER:O	1:B:2264:GLY:N	2.43	0.47
1:B:2744:ASN:OD1	1:B:2745:VAL:HG23	2.13	0.47
1:B:2790:MET:SD	1:B:2797:PHE:CZ	3.08	0.47
1:B:3166:TYR:CZ	1:B:3203:VAL:HG11	2.50	0.47
1:B:3379:LEU:HD11	1:B:3387:ALA:O	2.15	0.47
1:B:3477:LYS:NZ	1:B:3479:ALA:HA	2.30	0.47
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.96	0.47
1:D:717:ASP:OD1	1:D:720:HIS:N	2.40	0.47
1:D:953:THR:O	1:D:968:ALA:HB1	2.14	0.47
1:D:1427:ILE:O	1:D:1430:THR:HG22	2.15	0.47
1:D:2014:ASP:O	1:D:2015:GLU:HB3	2.15	0.47
1:D:2476:ILE:HD12	1:D:2532:ALA:HB1	1.95	0.47
1:D:3015:LEU:HD22	1:D:3025:LEU:HB3	1.96	0.47
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.96	0.47
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.80	0.47
1:D:4583:SER:OG	1:D:4585:SER:O	2.27	0.47
1:C:221:ARG:NH2	1:C:255:HIS:O	2.48	0.47
1:C:296:ASP:OD1	1:C:297:GLN:OE1	2.31	0.47
1:C:380:GLN:OE1	1:C:380:GLN:N	2.45	0.47
1:C:861:ILE:HD13	1:C:930:LYS:CD	2.43	0.47
1:C:880:GLU:HB2	1:C:967:PRO:HG2	1.97	0.47
1:C:884:LEU:HD23	1:C:955:LEU:HD11	1.97	0.47
1:C:2014:ASP:O	1:C:2015:GLU:HB3	2.15	0.47
1:C:2224:ARG:HE	1:C:2225:PHE:N	2.10	0.47
1:C:3015:LEU:HD22	1:C:3025:LEU:HB3	1.96	0.47
1:C:3365:LEU:HD11	1:C:3408:LEU:HD12	1.95	0.47
1:C:4096:ALA:O	1:C:4100:GLN:HG2	2.14	0.47
1:C:4640:GLU:HB3	1:C:4641:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2392:ARG:O	1:A:2418:LEU:HD12	2.14	0.47
1:A:3166:TYR:CZ	1:A:3203:VAL:HG11	2.50	0.47
1:A:3239:MET:CB	1:A:3239:MET:HG2	2.31	0.47
1:A:3379:LEU:HD11	1:A:3387:ALA:O	2.15	0.47
2:H:2:VAL:CG2	2:H:58:GLY:HA2	2.45	0.47
2:F:2:VAL:CG2	2:F:58:GLY:HA2	2.45	0.47
1:B:577:ILE:O	1:B:579:GLN:NE2	2.48	0.47
1:B:590:LEU:HD21	1:B:599:VAL:HB	1.96	0.47
1:B:887:ILE:HD11	1:B:907:LEU:HD21	1.95	0.47
1:B:985:VAL:HG11	1:B:1040:CYS:HB3	1.96	0.47
1:B:3234:ASN:OD1	1:B:3234:ASN:O	2.33	0.47
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.80	0.47
1:D:36:CYS:SG	1:D:52:THR:HG21	2.55	0.47
1:D:46:LEU:CD2	1:D:125:ARG:HE	2.27	0.47
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.96	0.47
1:D:3372:VAL:CG1	1:D:3398:PHE:HE1	2.24	0.47
1:C:4067:LYS:O	1:C:4070:ASP:OD1	2.33	0.47
1:A:985:VAL:HG11	1:A:1040:CYS:HB3	1.96	0.47
1:A:3398:PHE:CE2	1:A:3450:ASN:CB	2.97	0.47
1:B:69:LEU:HD23	1:B:109:LEU:HD21	1.96	0.47
1:B:919:ASN:O	1:B:923:GLN:OE1	2.32	0.47
1:B:2122:SER:HA	1:B:3721:LEU:HD11	1.96	0.47
1:B:2329:GLU:O	1:B:2333:ASP:OD1	2.32	0.47
1:B:2392:ARG:O	1:B:2418:LEU:HD12	2.14	0.47
1:B:3115:VAL:HG13	1:B:3116:SER:N	2.30	0.47
1:B:3239:MET:CB	1:B:3239:MET:HG2	2.31	0.47
1:B:3651:ASN:O	1:B:3655:GLU:OE1	2.32	0.47
1:D:69:LEU:HD23	1:D:109:LEU:HD21	1.96	0.47
1:D:438:ILE:HG23	1:D:518:ILE:HD11	1.96	0.47
1:D:2146:PRO:HA	1:D:2149:VAL:HG23	1.97	0.47
1:D:2668:SER:O	1:D:2669:GLU:HB3	2.14	0.47
1:D:3100:SER:O	1:D:3104:GLU:OE1	2.33	0.47
1:D:3733:CYS:HB2	1:D:3803:SER:OG	2.14	0.47
1:D:4096:ALA:O	1:D:4100:GLN:HG2	2.14	0.47
1:C:985:VAL:HG11	1:C:1040:CYS:HB3	1.96	0.47
1:C:3166:TYR:CZ	1:C:3203:VAL:HG11	2.50	0.47
1:C:3182:TYR:O	1:C:3185:LYS:HG3	2.15	0.47
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.96	0.47
1:A:577:ILE:O	1:A:579:GLN:NE2	2.48	0.47
1:A:2434:GLY:O	1:A:2508:ARG:NE	2.43	0.47
1:B:553:ARG:O	1:B:557:SER:OG	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2414:ASN:C	1:B:2414:ASN:OD1	2.58	0.47
1:B:2572:THR:HG23	1:B:2575:ARG:HB2	1.97	0.47
1:B:2638:LYS:O	1:B:2698:MET:CE	2.63	0.47
1:B:3007:ASN:O	1:B:3011:THR:OG1	2.15	0.47
1:B:3159:ASP:O	1:B:3163:VAL:HG23	2.14	0.47
1:B:3733:CYS:HB2	1:B:3803:SER:OG	2.14	0.47
1:D:577:ILE:O	1:D:579:GLN:NE2	2.48	0.47
1:D:2476:ILE:HG13	1:D:2536:LEU:HD11	1.96	0.47
1:D:2572:THR:HG23	1:D:2575:ARG:HB2	1.97	0.47
1:D:2745:VAL:HG12	1:D:2746:ILE:N	2.30	0.47
1:D:2790:MET:SD	1:D:2797:PHE:CZ	3.08	0.47
1:D:4067:LYS:O	1:D:4070:ASP:OD1	2.33	0.47
1:C:919:ASN:O	1:C:923:GLN:OE1	2.32	0.47
1:C:1570:LYS:O	1:C:1572:ILE:HD12	2.15	0.47
1:C:2146:PRO:HA	1:C:2149:VAL:HG23	1.97	0.47
1:C:2745:VAL:HG12	1:C:2746:ILE:N	2.30	0.47
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	1.97	0.47
1:C:3100:SER:O	1:C:3104:GLU:OE1	2.33	0.47
1:C:3537:LYS:NZ	1:C:3607:GLU:OE2	2.33	0.47
1:A:509:GLU:O	1:A:513:GLU:CD	2.59	0.46
1:A:1069:TRP:CE3	1:A:1602:PRO:HG2	2.50	0.46
1:A:2329:GLU:O	1:A:2333:ASP:OD1	2.32	0.46
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.49	0.46
1:A:4096:ALA:O	1:A:4100:GLN:HG2	2.14	0.46
1:B:574:VAL:O	1:B:578:ILE:HG12	2.14	0.46
1:B:2668:SER:O	1:B:2669:GLU:HB3	2.14	0.46
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.97	0.46
1:B:3735:LEU:HG	1:B:3735:LEU:O	2.14	0.46
1:B:4848:VAL:HG11	1:B:4887:MET:HG2	1.97	0.46
1:D:861:ILE:HG21	1:D:930:LYS:HD2	1.96	0.46
1:D:1115:LEU:HD13	1:D:1123:VAL:HG11	1.97	0.46
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.49	0.46
1:D:3901:ASN:OD1	1:D:3904:ARG:NH1	2.39	0.46
1:C:1112:ASP:OD1	1:C:1113:VAL:N	2.47	0.46
1:C:2790:MET:SD	1:C:2797:PHE:CZ	3.08	0.46
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.97	0.46
1:A:2742:THR:CG2	1:A:2814:LYS:HE3	2.42	0.46
1:A:3015:LEU:HD22	1:A:3025:LEU:HB3	1.96	0.46
1:A:4747:SER:HA	1:A:4750:ILE:HG12	1.97	0.46
1:B:1115:LEU:HD13	1:B:1123:VAL:HG11	1.97	0.46
1:D:100:THR:HG21	1:D:162:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:884:LEU:HD23	1:D:955:LEU:HD11	1.97	0.46
1:D:1570:LYS:O	1:D:1572:ILE:HD12	2.15	0.46
1:D:3521:GLY:CA	1:D:3524:MET:HE2	2.31	0.46
1:C:46:LEU:CD2	1:C:125:ARG:HE	2.27	0.46
1:C:100:THR:HG21	1:C:162:LYS:HE2	1.98	0.46
1:C:577:ILE:O	1:C:579:GLN:NE2	2.48	0.46
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.49	0.46
1:A:1115:LEU:HD13	1:A:1123:VAL:HG11	1.97	0.46
1:A:2223:ILE:HG23	1:A:2223:ILE:O	2.13	0.46
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.97	0.46
1:A:4705:VAL:HG13	1:A:4711:PHE:CD1	2.51	0.46
1:B:1554:VAL:HG21	1:B:1561:VAL:CG1	2.45	0.46
1:B:2014:ASP:O	1:B:2015:GLU:HB3	2.15	0.46
1:B:3100:SER:O	1:B:3104:GLU:OE1	2.33	0.46
1:D:574:VAL:HA	1:D:577:ILE:HG12	1.98	0.46
1:D:1554:VAL:HG21	1:D:1561:VAL:CG1	2.45	0.46
1:D:2355:ARG:HH11	1:D:2355:ARG:HG3	1.79	0.46
1:D:2912:THR:HG22	1:D:2914:LYS:H	1.81	0.46
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	1.97	0.46
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.97	0.46
1:C:509:GLU:O	1:C:513:GLU:CD	2.59	0.46
1:C:1115:LEU:HD13	1:C:1123:VAL:HG11	1.97	0.46
1:C:1427:ILE:O	1:C:1430:THR:HG22	2.15	0.46
1:C:2534:ALA:HB1	1:C:2588:ARG:CD	2.46	0.46
1:A:2745:VAL:HG12	1:A:2746:ILE:N	2.30	0.46
1:A:4690:GLU:O	1:A:4691:GLN:HB2	2.16	0.46
1:A:4732:PHE:HE2	1:A:4736:ARG:HG2	1.81	0.46
1:B:46:LEU:CD2	1:B:125:ARG:HE	2.27	0.46
1:B:2211:MET:O	1:B:2214:VAL:CG1	2.64	0.46
1:B:2434:GLY:O	1:B:2508:ARG:NE	2.43	0.46
1:B:3398:PHE:CE2	1:B:3450:ASN:CB	2.97	0.46
1:B:4767:TRP:CE3	1:B:4768:LEU:CD2	2.99	0.46
1:D:1069:TRP:CE3	1:D:1602:PRO:HG2	2.49	0.46
1:D:2767:ALA:O	1:D:2771:ILE:HG12	2.16	0.46
1:D:3379:LEU:HD11	1:D:3387:ALA:O	2.15	0.46
1:C:438:ILE:HG23	1:C:518:ILE:HD11	1.96	0.46
1:C:1456:ASP:OD1	1:C:1456:ASP:N	2.47	0.46
1:C:2170:MET:HG3	1:C:2225:PHE:CE2	2.50	0.46
1:C:2476:ILE:HG13	1:C:2536:LEU:HD11	1.96	0.46
1:C:3379:LEU:HD11	1:C:3387:ALA:O	2.15	0.46
1:C:4661:TYR:OH	1:C:4786:ASP:OD2	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:LEU:O	1:A:887:ILE:HB	2.16	0.46
1:A:921:ASN:HA	1:A:924:MET:SD	2.56	0.46
1:A:1973:GLN:NE2	1:A:2005:GLN:OE1	2.44	0.46
1:A:1999:ARG:HH12	1:A:3636:PHE:HD1	1.58	0.46
1:A:3100:SER:O	1:A:3104:GLU:OE1	2.33	0.46
1:A:3182:TYR:O	1:A:3185:LYS:HG3	2.15	0.46
1:B:978:THR:HG1	1:B:981:GLN:CD	2.24	0.46
1:B:2170:MET:HG3	1:B:2225:PHE:CE2	2.50	0.46
1:B:2534:ALA:HB1	1:B:2588:ARG:CD	2.46	0.46
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.49	0.46
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	1.97	0.46
1:B:4651:THR:OG1	1:B:4803:HIS:NE2	2.05	0.46
1:D:2170:MET:HG3	1:D:2225:PHE:CE2	2.50	0.46
1:D:2233:CYS:SG	1:D:2275:VAL:CG2	3.04	0.46
1:D:2515:GLN:O	1:D:2519:LEU:HG	2.16	0.46
1:D:2638:LYS:O	1:D:2698:MET:CE	2.63	0.46
1:D:4848:VAL:HG11	1:D:4887:MET:HG2	1.96	0.46
1:C:574:VAL:HA	1:C:577:ILE:HG12	1.98	0.46
1:C:861:ILE:HG21	1:C:930:LYS:HD2	1.96	0.46
1:C:921:ASN:HA	1:C:924:MET:SD	2.56	0.46
1:C:2233:CYS:SG	1:C:2275:VAL:CG2	3.04	0.46
1:C:2515:GLN:O	1:C:2519:LEU:HG	2.16	0.46
1:C:4041:ALA:O	1:C:4045:VAL:HG23	2.16	0.46
1:C:4690:GLU:O	1:C:4691:GLN:HB2	2.16	0.46
1:A:100:THR:HG21	1:A:162:LYS:HE2	1.98	0.46
1:A:2233:CYS:SG	1:A:2275:VAL:CG2	3.04	0.46
1:A:2586:VAL:CG1	1:A:2607:LEU:HD13	2.46	0.46
1:A:2703:LEU:CD2	1:A:2706:ILE:HD12	2.46	0.46
1:A:3115:VAL:HG13	1:A:3116:SER:N	2.30	0.46
1:A:4583:SER:OG	1:A:4585:SER:O	2.27	0.46
1:A:4934:GLY:HA2	1:D:4937:ILE:HG12	1.97	0.46
1:B:884:LEU:O	1:B:887:ILE:HB	2.16	0.46
1:B:921:ASN:HA	1:B:924:MET:SD	2.56	0.46
1:B:2146:PRO:HA	1:B:2149:VAL:HG23	1.97	0.46
1:B:2742:THR:HG23	1:B:2814:LYS:CE	2.41	0.46
1:D:360:ALA:O	1:D:361:ALA:CB	2.63	0.46
1:D:2011:HIS:ND1	1:D:2011:HIS:O	2.47	0.46
1:D:3115:VAL:HG13	1:D:3116:SER:N	2.30	0.46
1:C:879:HIS:CE1	1:C:913:LEU:HD13	2.51	0.46
1:C:2414:ASN:C	1:C:2414:ASN:OD1	2.58	0.46
1:C:3234:ASN:OD1	1:C:3234:ASN:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3339:ALA:O	1:C:3343:GLN:HG2	2.16	0.46
1:C:3477:LYS:NZ	1:C:3479:ALA:HA	2.30	0.46
1:A:880:GLU:HB2	1:A:967:PRO:HG2	1.97	0.46
1:A:884:LEU:HD23	1:A:955:LEU:HD11	1.97	0.46
1:A:3530:GLN:O	1:A:3534:MET:HG2	2.16	0.46
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.80	0.46
1:A:3991:GLY:O	1:A:3995:VAL:HG23	2.16	0.46
1:B:869:ARG:HD2	1:B:870:ILE:N	2.31	0.46
1:B:2233:CYS:SG	1:B:2275:VAL:CG2	3.04	0.46
1:B:2586:VAL:CG1	1:B:2607:LEU:HD13	2.46	0.46
1:B:2703:LEU:CD2	1:B:2706:ILE:HD12	2.46	0.46
1:B:3901:ASN:OD1	1:B:3904:ARG:NH1	2.40	0.46
1:B:4075:GLU:CD	1:C:4736:ARG:NH1	2.73	0.46
1:D:509:GLU:O	1:D:513:GLU:CD	2.59	0.46
1:D:3234:ASN:OD1	1:D:3234:ASN:O	2.33	0.46
1:D:3530:GLN:O	1:D:3534:MET:HG2	2.16	0.46
1:C:884:LEU:O	1:C:887:ILE:HB	2.16	0.46
1:C:4176:PRO:O	1:C:4202:ARG:NH2	2.49	0.46
1:A:574:VAL:HA	1:A:577:ILE:HG12	1.98	0.46
1:A:2767:ALA:O	1:A:2771:ILE:HG12	2.16	0.46
1:A:3910:THR:HG23	1:A:3911:THR:HG23	1.98	0.46
1:A:4848:VAL:HG11	1:A:4887:MET:HG2	1.97	0.46
1:B:879:HIS:CE1	1:B:913:LEU:HD13	2.51	0.46
1:B:2745:VAL:HG12	1:B:2746:ILE:N	2.30	0.46
1:B:3339:ALA:O	1:B:3343:GLN:HG2	2.16	0.46
1:B:3910:THR:HG23	1:B:3911:THR:HG23	1.98	0.46
1:B:3991:GLY:O	1:B:3995:VAL:HG23	2.16	0.46
1:B:4732:PHE:HE2	1:B:4736:ARG:HG2	1.81	0.46
1:D:463:GLU:O	1:D:467:LYS:HG2	2.16	0.46
1:D:2198:MET:HB3	1:D:2203:MET:SD	2.56	0.46
1:D:2534:ALA:HB1	1:D:2588:ARG:CD	2.46	0.46
1:D:2661:TRP:HB3	1:D:2664:PHE:HD1	1.81	0.46
1:D:2908:TYR:OH	1:D:2916:LYS:HA	2.16	0.46
1:D:3910:THR:HG23	1:D:3911:THR:HG23	1.98	0.46
1:D:4661:TYR:OH	1:D:4786:ASP:OD2	2.26	0.46
1:C:360:ALA:O	1:C:361:ALA:CB	2.63	0.46
1:C:2703:LEU:CD2	1:C:2706:ILE:HD12	2.46	0.46
1:C:2767:ALA:O	1:C:2771:ILE:HG12	2.16	0.46
1:A:384:MET:SD	1:B:167:ASP:OD1	2.74	0.46
1:A:1554:VAL:HG21	1:A:1561:VAL:CG1	2.45	0.46
1:A:2170:MET:HG3	1:A:2225:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2224:ARG:HE	1:A:2225:PHE:N	2.10	0.46
1:A:2908:TYR:OH	1:A:2916:LYS:HA	2.16	0.46
1:B:36:CYS:SG	1:B:52:THR:HG21	2.55	0.46
1:B:509:GLU:O	1:B:513:GLU:CD	2.59	0.46
1:B:2203:MET:HE2	1:B:2235:PHE:HZ	1.81	0.46
1:B:2742:THR:CG2	1:B:2814:LYS:HE3	2.42	0.46
1:D:880:GLU:HB2	1:D:967:PRO:HG2	1.97	0.46
1:D:921:ASN:HA	1:D:924:MET:SD	2.56	0.46
1:D:3401:LEU:O	1:D:3405:LEU:HD13	2.16	0.46
1:D:3723:MET:HE2	1:D:3793:MET:HG2	1.98	0.46
1:D:4645:CYS:O	1:D:4649:LEU:HD13	2.16	0.46
1:D:4705:VAL:HG13	1:D:4711:PHE:CD1	2.51	0.46
1:C:2198:MET:HB3	1:C:2203:MET:SD	2.56	0.46
1:C:2586:VAL:CG1	1:C:2607:LEU:HD13	2.46	0.46
1:A:663:TYR:OH	1:A:665:GLU:OE2	2.27	0.46
1:A:4041:ALA:O	1:A:4045:VAL:HG23	2.16	0.46
1:B:4041:ALA:O	1:B:4045:VAL:HG23	2.16	0.46
1:B:4690:GLU:O	1:B:4691:GLN:HB2	2.16	0.46
1:D:167:ASP:OD1	1:C:384:MET:HE1	2.15	0.46
1:D:1821:ASP:OD1	1:D:1821:ASP:C	2.59	0.46
1:D:2233:CYS:O	1:D:2235:PHE:N	2.49	0.46
1:D:2233:CYS:SG	1:D:2275:VAL:HG23	2.57	0.46
1:D:3182:TYR:O	1:D:3185:LYS:HG3	2.15	0.46
1:D:3339:ALA:O	1:D:3343:GLN:HG2	2.16	0.46
1:D:3398:PHE:CE2	1:D:3450:ASN:CB	2.98	0.46
1:C:2638:LYS:O	1:C:2698:MET:CE	2.63	0.46
1:C:2661:TRP:HB3	1:C:2664:PHE:HD1	1.81	0.46
1:C:2912:THR:HG22	1:C:2914:LYS:H	1.81	0.46
1:C:3401:LEU:O	1:C:3405:LEU:HD13	2.16	0.46
1:C:3910:THR:HG23	1:C:3911:THR:HG23	1.98	0.46
1:A:69:LEU:HD23	1:A:109:LEU:HD21	1.96	0.45
1:A:213:TYR:HA	1:A:339:ILE:O	2.16	0.45
1:A:2011:HIS:O	1:A:2011:HIS:ND1	2.47	0.45
1:A:2146:PRO:HA	1:A:2149:VAL:HG23	1.97	0.45
1:A:2198:MET:HB3	1:A:2203:MET:SD	2.56	0.45
1:A:2303:ALA:O	1:A:2307:LEU:HD13	2.17	0.45
1:A:2515:GLN:O	1:A:2519:LEU:HG	2.16	0.45
1:A:2782:ASP:OD2	1:A:2785:LEU:HD13	2.17	0.45
1:A:3336:LYS:O	1:A:3340:VAL:HG23	2.16	0.45
1:A:3339:ALA:O	1:A:3343:GLN:HG2	2.16	0.45
1:B:463:GLU:O	1:B:467:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1427:ILE:O	1:B:1430:THR:HG22	2.15	0.45
1:B:2198:MET:HB3	1:B:2203:MET:SD	2.56	0.45
1:B:2515:GLN:O	1:B:2519:LEU:HG	2.16	0.45
1:B:2767:ALA:O	1:B:2771:ILE:HG12	2.16	0.45
1:B:2782:ASP:OD2	1:B:2785:LEU:HD13	2.17	0.45
1:B:2828:GLU:O	1:B:2829:GLY:O	2.34	0.45
1:B:2908:TYR:OH	1:B:2916:LYS:HA	2.16	0.45
1:B:2912:THR:HG22	1:B:2914:LYS:H	1.81	0.45
1:B:3723:MET:HE2	1:B:3793:MET:HG2	1.98	0.45
1:B:4176:PRO:O	1:B:4202:ARG:NH2	2.49	0.45
1:B:4705:VAL:HG13	1:B:4711:PHE:CD1	2.51	0.45
1:B:4942:GLU:O	1:B:4945:ASP:OD1	2.34	0.45
1:D:1929:MET:O	1:D:1930:LYS:HB3	2.16	0.45
1:D:2703:LEU:CD2	1:D:2706:ILE:HD12	2.46	0.45
1:D:3477:LYS:NZ	1:D:3479:ALA:HA	2.30	0.45
1:D:4041:ALA:O	1:D:4045:VAL:HG23	2.16	0.45
1:C:213:TYR:HA	1:C:339:ILE:O	2.16	0.45
1:C:869:ARG:HD2	1:C:870:ILE:N	2.31	0.45
1:C:2572:THR:HG23	1:C:2575:ARG:HB2	1.97	0.45
1:C:3115:VAL:HG13	1:C:3116:SER:N	2.30	0.45
1:A:1570:LYS:O	1:A:1572:ILE:HD12	2.15	0.45
1:A:3899:PHE:CZ	1:A:3903:LEU:HD21	2.52	0.45
1:B:100:THR:HG21	1:B:162:LYS:HE2	1.98	0.45
1:B:1570:LYS:O	1:B:1572:ILE:HD12	2.15	0.45
1:B:2233:CYS:O	1:B:2235:PHE:N	2.49	0.45
1:B:4016:LEU:O	1:B:4020:GLN:HG3	2.16	0.45
1:B:4172:GLU:OE1	1:B:4175:ARG:NH1	2.50	0.45
1:D:820:ARG:HB3	1:D:820:ARG:CZ	2.24	0.45
1:D:4148:THR:HG21	1:D:4180:ARG:NH2	2.31	0.45
1:C:2011:HIS:O	1:C:2011:HIS:ND1	2.47	0.45
1:C:3398:PHE:HE2	1:C:3450:ASN:CB	2.29	0.45
1:C:3530:GLN:O	1:C:3534:MET:HG2	2.16	0.45
1:C:4148:THR:HG21	1:C:4180:ARG:NH2	2.31	0.45
1:C:4172:GLU:OE1	1:C:4175:ARG:NH1	2.50	0.45
1:C:4732:PHE:HE2	1:C:4736:ARG:HG2	1.81	0.45
1:A:224:HIS:HA	1:A:388:LEU:HD23	1.98	0.45
1:A:260:TRP:CE3	1:A:282:ILE:HG22	2.51	0.45
1:A:463:GLU:O	1:A:467:LYS:HG2	2.16	0.45
1:A:1929:MET:O	1:A:1930:LYS:HB3	2.16	0.45
1:A:2534:ALA:HB1	1:A:2588:ARG:CD	2.46	0.45
1:A:3324:VAL:HA	1:A:3327:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4942:GLU:O	1:A:4945:ASP:OD1	2.34	0.45
2:G:25:HIS:CD2	2:G:104:LEU:HD21	2.51	0.45
1:B:213:TYR:HA	1:B:339:ILE:O	2.16	0.45
1:B:2707:ALA:HB1	1:B:3009:TYR:CD1	2.52	0.45
1:D:867:LEU:HA	1:D:870:ILE:HG22	1.98	0.45
1:D:2707:ALA:HB1	1:D:3009:TYR:CD1	2.52	0.45
1:D:3891:LEU:HD13	1:D:3899:PHE:HZ	1.79	0.45
1:D:4577:LEU:HD23	1:D:4580:TYR:CE1	2.52	0.45
1:D:4736:ARG:NH1	1:C:4075:GLU:CD	2.74	0.45
1:C:36:CYS:SG	1:C:52:THR:HG21	2.55	0.45
1:C:260:TRP:CE3	1:C:282:ILE:HG22	2.51	0.45
1:C:2233:CYS:SG	1:C:2275:VAL:HG23	2.57	0.45
1:C:4705:VAL:HG13	1:C:4711:PHE:CD1	2.51	0.45
1:A:221:ARG:NH2	1:A:255:HIS:O	2.48	0.45
1:A:2912:THR:HG22	1:A:2914:LYS:H	1.81	0.45
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.97	0.45
1:A:4172:GLU:OE1	1:A:4175:ARG:NH1	2.50	0.45
1:A:4645:CYS:O	1:A:4649:LEU:HD13	2.16	0.45
1:B:574:VAL:HA	1:B:577:ILE:HG12	1.98	0.45
1:B:927:GLU:O	1:B:931:THR:HG23	2.16	0.45
1:B:3182:TYR:O	1:B:3185:LYS:HG3	2.15	0.45
1:B:3336:LYS:O	1:B:3340:VAL:HG23	2.16	0.45
1:B:3530:GLN:O	1:B:3534:MET:HG2	2.16	0.45
1:B:4645:CYS:O	1:B:4649:LEU:HD13	2.16	0.45
1:B:4747:SER:HA	1:B:4750:ILE:HG12	1.98	0.45
1:D:1791:VAL:O	1:D:1792:ALA:HB3	2.16	0.45
1:D:2828:GLU:O	1:D:2829:GLY:O	2.34	0.45
1:D:3409:TYR:O	1:D:3412:LEU:N	2.50	0.45
1:D:4176:PRO:O	1:D:4202:ARG:NH2	2.49	0.45
1:D:4690:GLU:O	1:D:4691:GLN:HB2	2.16	0.45
1:D:4747:SER:HA	1:D:4750:ILE:HG12	1.97	0.45
1:C:867:LEU:HA	1:C:870:ILE:HG22	1.98	0.45
1:C:927:GLU:O	1:C:931:THR:HG23	2.16	0.45
1:C:985:VAL:HA	1:C:1039:LEU:HD22	1.98	0.45
1:C:1929:MET:O	1:C:1930:LYS:HB3	2.16	0.45
1:C:2280:VAL:O	1:C:2280:VAL:HG22	2.16	0.45
1:C:2782:ASP:OD2	1:C:2785:LEU:HD13	2.17	0.45
1:C:4016:LEU:O	1:C:4020:GLN:HG3	2.16	0.45
1:A:365:LYS:O	1:A:369:LEU:HG	2.17	0.45
1:A:759:ILE:O	1:A:759:ILE:HG23	2.17	0.45
1:A:869:ARG:HD2	1:A:870:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:HIS:CE1	1:A:913:LEU:HD13	2.51	0.45
1:A:1272:LEU:HD22	1:A:1289:LEU:HD11	1.98	0.45
1:A:1821:ASP:OD1	1:A:1821:ASP:C	2.59	0.45
1:A:1866:ILE:HG12	1:A:1939:MET:HE1	1.98	0.45
1:A:2211:MET:O	1:A:2214:VAL:CG1	2.64	0.45
1:A:2233:CYS:SG	1:A:2275:VAL:HG23	2.56	0.45
1:A:2254:LEU:CD1	1:A:2276:ALA:HB1	2.47	0.45
1:A:2261:SER:O	1:A:2264:GLY:N	2.43	0.45
1:A:2572:THR:HG23	1:A:2575:ARG:HB2	1.97	0.45
1:A:3036:LYS:O	1:A:3039:ILE:HG22	2.16	0.45
1:A:3401:LEU:O	1:A:3405:LEU:HD13	2.16	0.45
1:A:4577:LEU:HD23	1:A:4580:TYR:CE1	2.52	0.45
1:A:4902:GLU:O	1:A:4913:ARG:NH2	2.50	0.45
2:F:25:HIS:HD2	2:F:104:LEU:HD21	1.82	0.45
1:B:365:LYS:O	1:B:369:LEU:HG	2.17	0.45
1:B:880:GLU:O	1:B:884:LEU:HD13	2.17	0.45
1:B:941:MET:SD	1:B:1051:TYR:HE1	2.32	0.45
1:B:1272:LEU:HD22	1:B:1289:LEU:HD11	1.98	0.45
1:B:2233:CYS:SG	1:B:2275:VAL:HG23	2.56	0.45
1:D:2280:VAL:O	1:D:2280:VAL:HG22	2.16	0.45
1:D:2782:ASP:OD2	1:D:2785:LEU:HD13	2.17	0.45
1:D:4172:GLU:OE1	1:D:4175:ARG:NH1	2.50	0.45
1:C:553:ARG:NH2	1:C:555:GLU:OE2	2.50	0.45
1:C:880:GLU:O	1:C:884:LEU:HD13	2.17	0.45
1:C:1791:VAL:O	1:C:1792:ALA:HB3	2.16	0.45
1:C:2107:GLN:O	1:C:3694:LYS:NZ	2.36	0.45
1:C:2211:MET:O	1:C:2214:VAL:CG1	2.64	0.45
1:C:4645:CYS:O	1:C:4649:LEU:HD13	2.16	0.45
1:C:4848:VAL:HG11	1:C:4887:MET:HG2	1.97	0.45
1:A:2661:TRP:HB3	1:A:2664:PHE:HD1	1.81	0.45
2:H:25:HIS:CD2	2:H:104:LEU:HD21	2.51	0.45
2:F:25:HIS:CD2	2:F:104:LEU:HD21	2.51	0.45
1:B:260:TRP:CE3	1:B:282:ILE:HG22	2.51	0.45
1:B:553:ARG:NH2	1:B:555:GLU:OE2	2.50	0.45
1:B:1821:ASP:OD1	1:B:1821:ASP:C	2.59	0.45
1:B:1866:ILE:HG12	1:B:1939:MET:HE1	1.98	0.45
1:B:2572:THR:CG2	1:B:2579:VAL:CG2	2.83	0.45
1:D:1272:LEU:HD22	1:D:1289:LEU:HD11	1.98	0.45
1:D:2303:ALA:O	1:D:2307:LEU:HD13	2.17	0.45
1:D:3036:LYS:O	1:D:3039:ILE:HG22	2.16	0.45
1:C:224:HIS:HA	1:C:388:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:ILE:HG23	1:C:759:ILE:O	2.17	0.45
1:C:1272:LEU:HD22	1:C:1289:LEU:HD11	1.98	0.45
1:C:1554:VAL:HG21	1:C:1561:VAL:CG1	2.45	0.45
1:A:2886:TRP:O	1:A:2890:LYS:HG2	2.17	0.45
1:A:3086:GLU:OE2	1:A:3093:ARG:NH1	2.50	0.45
1:A:3254:GLY:C	1:A:3258:GLU:OE1	2.60	0.45
1:B:1943:LEU:HD12	1:B:2101:MET:HE1	1.99	0.45
1:B:2303:ALA:O	1:B:2307:LEU:HD13	2.17	0.45
1:B:2886:TRP:O	1:B:2890:LYS:HG2	2.17	0.45
1:D:365:LYS:O	1:D:369:LEU:HG	2.17	0.45
1:D:985:VAL:HA	1:D:1039:LEU:HD22	1.98	0.45
1:D:2244:ARG:NH2	1:D:2283:ASN:OD1	2.50	0.45
1:D:3213:TYR:CD1	1:D:3302:PRO:HG2	2.52	0.45
1:D:3324:VAL:HA	1:D:3327:LEU:HG	1.99	0.45
1:D:3390:GLY:HA2	1:D:3393:LEU:HD13	1.99	0.45
1:D:3414:ARG:HH22	1:D:3472:ALA:CB	2.30	0.45
1:D:3899:PHE:CZ	1:D:3903:LEU:HD21	2.52	0.45
1:D:3991:GLY:O	1:D:3995:VAL:HG23	2.16	0.45
1:C:463:GLU:O	1:C:467:LYS:HG2	2.16	0.45
1:C:941:MET:SD	1:C:1051:TYR:HE1	2.32	0.45
1:C:1105:ALA:O	1:C:1189:LEU:N	2.50	0.45
1:C:1866:ILE:HG12	1:C:1939:MET:HE1	1.98	0.45
1:C:2233:CYS:O	1:C:2235:PHE:N	2.49	0.45
1:C:2254:LEU:CD1	1:C:2276:ALA:HB1	2.47	0.45
1:C:2908:TYR:OH	1:C:2916:LYS:HA	2.16	0.45
1:C:3409:TYR:O	1:C:3412:LEU:N	2.50	0.45
1:C:3899:PHE:CZ	1:C:3903:LEU:HD21	2.52	0.45
1:C:3991:GLY:O	1:C:3995:VAL:HG23	2.16	0.45
1:C:4747:SER:HA	1:C:4750:ILE:HG12	1.98	0.45
1:A:717:ASP:OD1	1:A:720:HIS:N	2.40	0.45
1:A:985:VAL:HA	1:A:1039:LEU:HD22	1.98	0.45
1:A:3106:MET:O	1:A:3110:LEU:HD23	2.17	0.45
1:A:3254:GLY:O	1:A:3255:GLY:C	2.60	0.45
1:A:3566:SER:CB	1:A:3569:LEU:HD12	2.47	0.45
2:E:25:HIS:HD2	2:E:104:LEU:HD21	1.82	0.45
1:B:2254:LEU:CD1	1:B:2276:ALA:HB1	2.47	0.45
1:B:3628:ARG:HD2	1:B:3632:VAL:HG13	1.99	0.45
1:D:759:ILE:HG23	1:D:759:ILE:O	2.17	0.45
1:D:1105:ALA:O	1:D:1189:LEU:N	2.50	0.45
1:D:2586:VAL:CG1	1:D:2607:LEU:HD13	2.46	0.45
1:D:3086:GLU:OE2	1:D:3093:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2244:ARG:NH2	1:C:2283:ASN:OD1	2.50	0.45
1:C:2828:GLU:O	1:C:2829:GLY:O	2.34	0.45
1:C:3390:GLY:HA2	1:C:3393:LEU:HD13	1.99	0.45
1:C:3566:SER:CB	1:C:3569:LEU:HD12	2.47	0.45
1:A:2203:MET:HE2	1:A:2235:PHE:HZ	1.81	0.45
1:A:2233:CYS:O	1:A:2235:PHE:N	2.49	0.45
1:A:3166:TYR:CE2	1:A:3239:MET:HE2	2.52	0.45
1:A:3802:ILE:HD11	1:A:3883:ASP:O	2.17	0.45
1:A:4016:LEU:O	1:A:4020:GLN:HG3	2.16	0.45
2:G:25:HIS:HD2	2:G:104:LEU:HD21	1.81	0.45
1:B:759:ILE:HG23	1:B:759:ILE:O	2.17	0.45
1:B:1873:GLU:OE1	1:B:1873:GLU:N	2.50	0.45
1:B:1929:MET:O	1:B:1930:LYS:HB3	2.16	0.45
1:B:2661:TRP:HB3	1:B:2664:PHE:HD1	1.81	0.45
1:B:3166:TYR:CE2	1:B:3239:MET:HE2	2.52	0.45
1:B:3398:PHE:HE2	1:B:3450:ASN:CB	2.30	0.45
1:D:260:TRP:CE3	1:D:282:ILE:HG22	2.51	0.45
1:D:2224:ARG:HE	1:D:2225:PHE:N	2.10	0.45
1:D:4732:PHE:HE2	1:D:4736:ARG:HG2	1.81	0.45
1:D:4902:GLU:O	1:D:4913:ARG:NH2	2.50	0.45
1:C:2303:ALA:O	1:C:2307:LEU:HD13	2.17	0.45
1:C:2685:SER:O	1:C:2689:LYS:HG2	2.17	0.45
1:C:3213:TYR:CD1	1:C:3302:PRO:HG2	2.52	0.45
1:C:3324:VAL:HA	1:C:3327:LEU:HG	1.99	0.45
1:C:3414:ARG:HH22	1:C:3472:ALA:CB	2.30	0.45
1:C:3802:ILE:HD11	1:C:3883:ASP:O	2.17	0.45
1:C:4577:LEU:HD23	1:C:4580:TYR:CE1	2.52	0.45
1:C:4821:LYS:O	1:C:4825:THR:HG23	2.17	0.45
1:C:4942:GLU:O	1:C:4945:ASP:OD1	2.34	0.45
1:A:380:GLN:OE1	1:A:380:GLN:N	2.45	0.45
1:A:622:THR:HA	1:A:626:LEU:HD13	1.99	0.45
1:A:1791:VAL:O	1:A:1792:ALA:HB3	2.16	0.45
1:A:2904:LEU:O	1:A:2906:VAL:HG22	2.17	0.45
1:A:3213:TYR:CD1	1:A:3302:PRO:HG2	2.52	0.45
1:A:3414:ARG:HH22	1:A:3472:ALA:CB	2.30	0.45
1:A:4176:PRO:O	1:A:4202:ARG:NH2	2.49	0.45
1:A:4821:LYS:O	1:A:4825:THR:HG23	2.17	0.45
1:B:155:LYS:HD2	1:B:156:GLN:N	2.32	0.45
1:B:345:LEU:HD12	1:B:387:ALA:HB1	1.99	0.45
1:B:363:ASP:OD1	1:B:363:ASP:C	2.60	0.45
1:B:820:ARG:CZ	1:B:820:ARG:CB	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:GLY:HA3	1:B:1143:TRP:CE3	2.52	0.45
1:B:2685:SER:O	1:B:2689:LYS:HG2	2.17	0.45
1:B:3230:LEU:HD12	1:B:3232:LEU:HG	1.99	0.45
1:B:3401:LEU:O	1:B:3405:LEU:HD13	2.16	0.45
1:B:3409:TYR:O	1:B:3412:LEU:N	2.50	0.45
1:B:3566:SER:CB	1:B:3569:LEU:HD12	2.47	0.45
1:B:3899:PHE:CZ	1:B:3903:LEU:HD21	2.52	0.45
1:D:221:ARG:NH2	1:D:255:HIS:O	2.47	0.45
1:D:879:HIS:CE1	1:D:913:LEU:HD13	2.51	0.45
1:D:2303:ALA:O	1:D:2307:LEU:CD1	2.65	0.45
1:D:3254:GLY:C	1:D:3258:GLU:OE1	2.60	0.45
1:D:3537:LYS:NZ	1:D:3607:GLU:OE2	2.33	0.45
1:D:3580:PRO:O	1:D:3583:GLU:OE2	2.35	0.45
1:D:3891:LEU:CB	1:D:3899:PHE:CE2	3.00	0.45
1:D:3966:THR:HG23	1:D:4029:SER:OG	2.17	0.45
1:D:4095:LYS:O	1:D:4098:ASP:OD1	2.35	0.45
1:C:365:LYS:O	1:C:369:LEU:HG	2.17	0.45
1:C:2303:ALA:O	1:C:2307:LEU:CD1	2.65	0.45
1:C:3107:VAL:O	1:C:3111:ARG:HG2	2.17	0.45
1:A:155:LYS:HD2	1:A:156:GLN:N	2.32	0.44
1:A:336:PRO:HA	1:A:337:PRO:HD3	1.91	0.44
1:A:345:LEU:HD12	1:A:387:ALA:HB1	2.00	0.44
1:A:880:GLU:O	1:A:884:LEU:HD13	2.17	0.44
1:A:927:GLU:O	1:A:931:THR:HG23	2.16	0.44
1:A:2707:ALA:HB1	1:A:3009:TYR:CD1	2.52	0.44
1:A:3327:LEU:O	1:A:3403:ARG:NH2	2.50	0.44
1:A:3409:TYR:O	1:A:3412:LEU:N	2.50	0.44
1:B:2280:VAL:HG22	1:B:2280:VAL:O	2.16	0.44
1:B:3036:LYS:O	1:B:3039:ILE:HG22	2.16	0.44
1:B:3254:GLY:C	1:B:3258:GLU:OE1	2.60	0.44
1:B:3324:VAL:HA	1:B:3327:LEU:HG	1.99	0.44
1:B:3414:ARG:HH22	1:B:3472:ALA:CB	2.30	0.44
1:B:4148:THR:HG21	1:B:4180:ARG:NH2	2.31	0.44
1:D:155:LYS:HD2	1:D:156:GLN:N	2.32	0.44
1:D:363:ASP:OD1	1:D:363:ASP:C	2.60	0.44
1:D:1515:VAL:O	1:D:1531:ALA:O	2.36	0.44
1:D:1805:GLU:HG2	1:D:1806:ALA:N	2.33	0.44
1:D:2261:SER:O	1:D:2264:GLY:N	2.43	0.44
1:D:3435:PHE:HD2	1:D:3524:MET:HE1	1.82	0.44
1:D:3546:ASP:O	1:D:3549:VAL:HG22	2.17	0.44
1:D:4016:LEU:O	1:D:4020:GLN:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:ARG:HB3	1:C:820:ARG:CZ	2.24	0.44
1:C:2203:MET:HE2	1:C:2235:PHE:HZ	1.81	0.44
1:C:2675:THR:CG2	1:C:2706:ILE:HG23	2.48	0.44
1:C:3723:MET:HE2	1:C:3793:MET:HG2	1.98	0.44
1:A:363:ASP:OD1	1:A:363:ASP:C	2.60	0.44
1:A:1126:GLY:HA3	1:A:1143:TRP:CE3	2.52	0.44
1:A:1515:VAL:O	1:A:1531:ALA:O	2.36	0.44
2:H:7:ILE:HA	1:D:719:LEU:HD11	1.99	0.44
1:B:224:HIS:HA	1:B:388:LEU:HD23	1.98	0.44
1:B:1742:THR:O	1:B:1960:ALA:HB2	2.18	0.44
1:B:1805:GLU:HG2	1:B:1806:ALA:N	2.33	0.44
1:B:3106:MET:O	1:B:3110:LEU:HD23	2.17	0.44
1:B:3842:LEU:HD23	1:B:3874:VAL:CG1	2.47	0.44
1:B:3941:ASP:OD2	1:B:3941:ASP:N	2.46	0.44
1:B:4095:LYS:O	1:B:4098:ASP:OD1	2.35	0.44
1:D:884:LEU:O	1:D:887:ILE:HB	2.16	0.44
1:D:3465:ASN:OD1	1:D:3467:MET:CG	2.60	0.44
1:D:4942:GLU:O	1:D:4945:ASP:OD1	2.34	0.44
1:C:363:ASP:OD1	1:C:363:ASP:C	2.60	0.44
1:C:553:ARG:O	1:C:557:SER:OG	2.29	0.44
1:C:1821:ASP:OD1	1:C:1821:ASP:C	2.59	0.44
1:C:3036:LYS:O	1:C:3039:ILE:HG22	2.16	0.44
1:C:3580:PRO:O	1:C:3583:GLU:OE2	2.35	0.44
1:C:3966:THR:HG23	1:C:4029:SER:OG	2.17	0.44
1:C:4094:GLN:HG3	1:C:4108:ILE:HG21	1.99	0.44
1:C:4583:SER:OG	1:C:4585:SER:O	2.27	0.44
1:A:941:MET:SD	1:A:1051:TYR:HE1	2.32	0.44
1:A:2244:ARG:NH2	1:A:2283:ASN:OD1	2.50	0.44
1:A:3723:MET:HE2	1:A:3793:MET:HG2	1.98	0.44
1:A:4094:GLN:HG3	1:A:4108:ILE:HG21	2.00	0.44
1:A:4937:ILE:HG12	1:B:4934:GLY:HA2	1.99	0.44
1:B:985:VAL:HA	1:B:1039:LEU:HD22	1.98	0.44
1:B:2214:VAL:HG11	1:B:2228:MET:CE	2.48	0.44
1:B:2303:ALA:O	1:B:2307:LEU:CD1	2.65	0.44
1:B:3107:VAL:O	1:B:3111:ARG:HG2	2.17	0.44
1:B:3802:ILE:HD11	1:B:3883:ASP:O	2.17	0.44
1:B:3966:THR:HG23	1:B:4029:SER:OG	2.17	0.44
1:B:4902:GLU:O	1:B:4913:ARG:NH2	2.50	0.44
1:D:76:ARG:O	1:D:80:GLU:HG2	2.18	0.44
1:D:213:TYR:HA	1:D:339:ILE:O	2.16	0.44
1:D:622:THR:HA	1:D:626:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1866:ILE:HG12	1:D:1939:MET:HE1	1.98	0.44
1:D:1943:LEU:HD12	1:D:2101:MET:HE1	1.99	0.44
1:D:2791:LEU:HD13	1:D:2791:LEU:HA	1.89	0.44
1:D:3802:ILE:HD11	1:D:3883:ASP:O	2.17	0.44
1:D:4821:LYS:O	1:D:4825:THR:HG23	2.17	0.44
1:C:2572:THR:CG2	1:C:2579:VAL:CG2	2.83	0.44
1:C:3842:LEU:HD23	1:C:3874:VAL:CG1	2.47	0.44
1:C:4093:PHE:O	1:C:4097:MET:HG2	2.17	0.44
1:C:4943:LEU:O	1:C:4947:GLN:HG2	2.17	0.44
1:A:553:ARG:NH2	1:A:555:GLU:OE2	2.50	0.44
1:A:3230:LEU:HD12	1:A:3232:LEU:HG	1.99	0.44
1:A:3528:THR:HG23	1:A:3573:MET:SD	2.58	0.44
1:A:3546:ASP:O	1:A:3549:VAL:HG22	2.17	0.44
1:A:3842:LEU:HD23	1:A:3874:VAL:CG1	2.47	0.44
1:A:4820:VAL:HG11	1:B:4839:MET:CE	2.47	0.44
2:E:25:HIS:CD2	2:E:104:LEU:HD21	2.51	0.44
2:H:25:HIS:HD2	2:H:104:LEU:HD21	1.82	0.44
1:B:1791:VAL:O	1:B:1792:ALA:HB3	2.16	0.44
1:B:3327:LEU:O	1:B:3403:ARG:NH2	2.50	0.44
1:D:869:ARG:HD2	1:D:870:ILE:N	2.31	0.44
1:D:927:GLU:O	1:D:931:THR:HG23	2.16	0.44
1:D:959:TYR:CD2	1:D:966:LYS:HE2	2.50	0.44
1:D:1456:ASP:OD1	1:D:1456:ASP:N	2.47	0.44
1:D:4093:PHE:O	1:D:4097:MET:HG2	2.17	0.44
1:D:4094:GLN:HG3	1:D:4108:ILE:HG21	1.99	0.44
1:D:4943:LEU:O	1:D:4947:GLN:HG2	2.18	0.44
1:C:984:LEU:HD23	1:C:988:LEU:HD23	2.00	0.44
1:C:1515:VAL:O	1:C:1531:ALA:O	2.35	0.44
1:C:1873:GLU:N	1:C:1873:GLU:OE1	2.50	0.44
1:C:2707:ALA:HB1	1:C:3009:TYR:CD1	2.52	0.44
1:C:2904:LEU:O	1:C:2906:VAL:HG22	2.17	0.44
1:C:3254:GLY:C	1:C:3258:GLU:OE1	2.60	0.44
1:C:3336:LYS:O	1:C:3340:VAL:HG23	2.16	0.44
1:C:4029:SER:HA	1:C:4032:GLU:HG3	2.00	0.44
1:A:2675:THR:CG2	1:A:2706:ILE:HG23	2.47	0.44
1:A:2828:GLU:O	1:A:2829:GLY:O	2.34	0.44
1:A:3107:VAL:O	1:A:3111:ARG:HG2	2.17	0.44
1:A:3398:PHE:HE2	1:A:3450:ASN:CB	2.30	0.44
1:A:4778:TRP:O	1:A:4782:VAL:HG23	2.18	0.44
1:B:380:GLN:OE1	1:B:380:GLN:N	2.45	0.44
1:B:961:MET:SD	1:B:963:ASN:HB2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2675:THR:CG2	1:B:2706:ILE:HG23	2.47	0.44
1:B:2904:LEU:O	1:B:2906:VAL:HG22	2.17	0.44
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.51	0.44
1:B:3086:GLU:OE2	1:B:3093:ARG:NH1	2.50	0.44
1:B:3604:TYR:CD1	1:B:3608:GLN:OE1	2.71	0.44
1:B:4093:PHE:O	1:B:4097:MET:HG2	2.17	0.44
1:B:4094:GLN:HG3	1:B:4108:ILE:HG21	2.00	0.44
1:B:4977:THR:OG1	1:B:5029:ARG:NH2	2.51	0.44
1:D:880:GLU:O	1:D:884:LEU:HD13	2.17	0.44
1:D:3166:TYR:CE2	1:D:3239:MET:HE2	2.52	0.44
1:D:3628:ARG:HD2	1:D:3632:VAL:HG13	1.99	0.44
1:D:3842:LEU:HD23	1:D:3874:VAL:CG1	2.47	0.44
1:D:4029:SER:HA	1:D:4032:GLU:HG3	2.00	0.44
1:D:4977:THR:OG1	1:D:5029:ARG:NH2	2.51	0.44
1:C:663:TYR:OH	1:C:665:GLU:OE2	2.27	0.44
1:C:1126:GLY:HA3	1:C:1143:TRP:CE3	2.52	0.44
1:C:3086:GLU:OE2	1:C:3093:ARG:NH1	2.50	0.44
1:C:3435:PHE:HD2	1:C:3524:MET:HE1	1.82	0.44
1:C:3528:THR:HG23	1:C:3573:MET:SD	2.58	0.44
1:C:3546:ASP:O	1:C:3549:VAL:HG22	2.17	0.44
1:A:1170:MET:CE	1:D:3471:THR:HG22	2.47	0.44
1:A:1805:GLU:HG2	1:A:1806:ALA:N	2.33	0.44
1:A:2280:VAL:O	1:A:2280:VAL:HG22	2.16	0.44
1:A:3580:PRO:O	1:A:3583:GLU:OE2	2.35	0.44
1:B:867:LEU:HA	1:B:870:ILE:HG22	1.98	0.44
1:B:984:LEU:HD23	1:B:988:LEU:HD23	2.00	0.44
1:B:3875:MET:HE1	1:B:3954:ALA:HA	2.00	0.44
1:B:4077:PHE:O	1:B:4081:VAL:HG23	2.18	0.44
1:B:4732:PHE:CE2	1:B:4736:ARG:HG2	2.53	0.44
1:D:345:LEU:HD12	1:D:387:ALA:HB1	2.00	0.44
1:D:553:ARG:NH2	1:D:555:GLU:OE2	2.50	0.44
1:D:3106:MET:O	1:D:3110:LEU:HD23	2.17	0.44
1:D:3343:GLN:HE22	1:D:3410:PRO:HB2	1.83	0.44
1:D:3971:GLY:N	1:D:3972:PRO:HA	2.33	0.44
1:D:4778:TRP:O	1:D:4782:VAL:HG23	2.18	0.44
1:C:345:LEU:HD12	1:C:387:ALA:HB1	2.00	0.44
1:C:4902:GLU:O	1:C:4913:ARG:NH2	2.50	0.44
1:C:4977:THR:OG1	1:C:5029:ARG:NH2	2.51	0.44
1:A:155:LYS:HE2	1:D:228:ASP:OD2	2.17	0.44
1:A:345:LEU:HD12	1:A:387:ALA:CB	2.48	0.44
1:A:1873:GLU:OE1	1:A:1873:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3984:ARG:NH1	1:B:160:GLY:O	2.48	0.44
1:A:4767:TRP:CE3	1:A:4768:LEU:CD2	2.99	0.44
1:B:1067:SER:O	1:B:1071:ARG:HG3	2.18	0.44
1:D:224:HIS:HA	1:D:388:LEU:HD23	1.98	0.44
1:D:598:LYS:O	1:D:602:VAL:HG23	2.18	0.44
1:D:1742:THR:O	1:D:1960:ALA:HB2	2.18	0.44
1:D:3327:LEU:O	1:D:3403:ARG:NH2	2.50	0.44
1:D:3336:LYS:O	1:D:3340:VAL:HG23	2.17	0.44
1:D:3566:SER:CB	1:D:3569:LEU:HD12	2.47	0.44
1:C:622:THR:HA	1:C:626:LEU:HD13	1.99	0.44
1:C:646:PRO:HB2	1:C:648:ILE:HD13	2.00	0.44
1:C:1805:GLU:HG2	1:C:1806:ALA:N	2.33	0.44
1:C:2886:TRP:O	1:C:2890:LYS:HG2	2.17	0.44
1:C:3455:GLU:O	1:C:3459:VAL:HG23	2.17	0.44
1:A:730:VAL:HG23	1:A:1476:MET:SD	2.58	0.44
1:A:867:LEU:HA	1:A:870:ILE:HG22	1.98	0.44
1:A:1067:SER:O	1:A:1071:ARG:HG3	2.18	0.44
1:A:1943:LEU:HD12	1:A:2101:MET:HE1	1.99	0.44
1:A:2303:ALA:O	1:A:2307:LEU:CD1	2.65	0.44
1:A:2929:PHE:CD1	1:A:2932:MET:SD	3.11	0.44
1:A:3343:GLN:HE22	1:A:3410:PRO:HB2	1.83	0.44
1:A:3628:ARG:HD2	1:A:3632:VAL:HG13	1.99	0.44
1:A:4977:THR:OG1	1:A:5029:ARG:NH2	2.51	0.44
2:H:103:LEU:HD21	2:H:106:LEU:HD11	2.00	0.44
1:B:76:ARG:O	1:B:80:GLU:HG2	2.18	0.44
1:B:259:LEU:HD11	1:B:397:GLU:HG2	2.00	0.44
1:B:730:VAL:HG23	1:B:1476:MET:SD	2.58	0.44
1:B:3390:GLY:HA2	1:B:3393:LEU:HD13	1.99	0.44
1:B:3971:GLY:N	1:B:3972:PRO:HA	2.33	0.44
1:B:4098:ASP:OD1	1:B:4098:ASP:C	2.61	0.44
1:B:4943:LEU:O	1:B:4947:GLN:HG2	2.17	0.44
1:D:345:LEU:HD12	1:D:387:ALA:CB	2.48	0.44
1:D:2904:LEU:O	1:D:2906:VAL:HG22	2.17	0.44
1:D:2929:PHE:CD1	1:D:2932:MET:SD	3.11	0.44
1:D:3455:GLU:O	1:D:3459:VAL:HG23	2.17	0.44
1:D:3504:SER:O	1:D:3507:THR:OG1	2.30	0.44
1:D:3789:GLU:OE1	1:D:3789:GLU:N	2.51	0.44
1:D:4767:TRP:CE3	1:D:4768:LEU:CD2	2.99	0.44
1:C:1943:LEU:HD12	1:C:2101:MET:HE1	1.99	0.44
1:C:2214:VAL:HG11	1:C:2228:MET:CE	2.48	0.44
1:C:2330:ARG:O	1:C:2333:ASP:OD1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2527:LEU:O	1:C:2531:ARG:HG3	2.18	0.44
1:C:3254:GLY:O	1:C:3255:GLY:C	2.60	0.44
1:A:783:PHE:HB2	1:A:787:VAL:HG21	2.00	0.44
1:A:2330:ARG:O	1:A:2333:ASP:OD1	2.36	0.44
1:A:3390:GLY:HA2	1:A:3393:LEU:HD13	1.99	0.44
1:A:4095:LYS:O	1:A:4098:ASP:OD1	2.35	0.44
1:A:4098:ASP:OD1	1:A:4098:ASP:C	2.61	0.44
1:B:266:ARG:O	1:B:270:SER:OG	2.34	0.44
1:B:345:LEU:HD12	1:B:387:ALA:CB	2.48	0.44
1:B:1515:VAL:O	1:B:1531:ALA:O	2.36	0.44
1:B:2926:LEU:O	1:B:2930:LEU:HD13	2.18	0.44
1:B:3343:GLN:HE22	1:B:3410:PRO:HB2	1.83	0.44
1:B:4577:LEU:HD23	1:B:4580:TYR:CE1	2.52	0.44
1:D:1694:LEU:O	1:D:1698:LEU:HG	2.18	0.44
1:D:4098:ASP:OD1	1:D:4098:ASP:C	2.61	0.44
6:D:5304:PNX:HAK1	6:D:5304:PNX:HAA1	2.00	0.44
1:C:155:LYS:HD2	1:C:156:GLN:N	2.32	0.44
1:C:345:LEU:HD12	1:C:387:ALA:CB	2.48	0.44
1:C:1067:SER:O	1:C:1071:ARG:HG3	2.18	0.44
1:C:2929:PHE:CD1	1:C:2932:MET:SD	3.11	0.44
1:C:3327:LEU:O	1:C:3403:ARG:NH2	2.50	0.44
1:C:3429:ALA:HA	1:C:3432:GLU:OE1	2.18	0.44
1:C:3875:MET:HE1	1:C:3954:ALA:HA	2.00	0.44
1:C:4767:TRP:HE3	1:C:4768:LEU:HD23	1.80	0.44
1:A:1077:ALA:HB2	1:A:1190:PRO:HG2	2.00	0.43
1:A:2926:LEU:O	1:A:2930:LEU:HD13	2.18	0.43
1:A:3604:TYR:CD1	1:A:3608:GLN:OE1	2.71	0.43
1:A:4182:GLU:HB2	1:A:4983:HIS:CD2	2.53	0.43
2:F:31:GLU:OE2	1:B:1299:GLN:HG2	2.18	0.43
1:B:3455:GLU:O	1:B:3459:VAL:HG23	2.17	0.43
1:B:4778:TRP:O	1:B:4782:VAL:HG23	2.18	0.43
1:D:646:PRO:HB2	1:D:648:ILE:HD13	2.00	0.43
1:D:667:MET:SD	1:D:801:LYS:NZ	2.85	0.43
1:D:2434:GLY:O	1:D:2508:ARG:NE	2.43	0.43
1:D:3107:VAL:O	1:D:3111:ARG:HG2	2.17	0.43
1:D:3254:GLY:O	1:D:3255:GLY:C	2.60	0.43
1:D:3429:ALA:HA	1:D:3432:GLU:OE1	2.18	0.43
1:D:3528:THR:HG23	1:D:3573:MET:SD	2.58	0.43
1:C:76:ARG:O	1:C:80:GLU:HG2	2.18	0.43
1:C:309:THR:O	1:C:309:THR:HG22	2.18	0.43
1:C:3166:TYR:CE2	1:C:3239:MET:HE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3212:GLU:OE2	1:C:3213:TYR:CZ	2.71	0.43
1:C:3343:GLN:HE22	1:C:3410:PRO:HB2	1.83	0.43
1:C:3891:LEU:CB	1:C:3899:PHE:CE2	3.00	0.43
1:C:4095:LYS:O	1:C:4098:ASP:OD1	2.35	0.43
1:C:4182:GLU:HB2	1:C:4983:HIS:CD2	2.53	0.43
1:C:4732:PHE:CE2	1:C:4736:ARG:HG2	2.53	0.43
6:C:5304:PNX:HAA1	6:C:5304:PNX:HAK1	2.00	0.43
1:A:259:LEU:HD11	1:A:397:GLU:HG2	2.00	0.43
1:A:1694:LEU:O	1:A:1698:LEU:HG	2.18	0.43
1:A:1999:ARG:NH1	1:A:3635:CYS:C	2.76	0.43
1:A:2214:VAL:HG11	1:A:2228:MET:CE	2.48	0.43
1:A:3212:GLU:OE2	1:A:3213:TYR:CZ	2.72	0.43
1:A:4093:PHE:O	1:A:4097:MET:HG2	2.17	0.43
2:H:31:GLU:OE2	1:D:1299:GLN:HG2	2.18	0.43
2:G:105:LYS:C	2:G:106:LEU:HD12	2.43	0.43
1:B:598:LYS:O	1:B:602:VAL:HG23	2.18	0.43
1:B:615:ARG:NH2	1:B:1676:LEU:O	2.50	0.43
1:B:646:PRO:HB2	1:B:648:ILE:HD13	2.00	0.43
1:B:1694:LEU:O	1:B:1698:LEU:HG	2.18	0.43
1:B:2527:LEU:O	1:B:2531:ARG:HG3	2.18	0.43
1:B:2929:PHE:CD1	1:B:2932:MET:SD	3.11	0.43
1:B:3789:GLU:N	1:B:3789:GLU:OE1	2.51	0.43
1:B:3891:LEU:CB	1:B:3899:PHE:CE2	3.00	0.43
1:B:4029:SER:HA	1:B:4032:GLU:HG3	2.00	0.43
1:D:220:LEU:C	1:D:220:LEU:HD12	2.44	0.43
1:D:730:VAL:HG23	1:D:1476:MET:SD	2.58	0.43
1:D:1126:GLY:HA3	1:D:1143:TRP:CE3	2.52	0.43
1:D:1705:GLY:HA3	1:D:1836:PHE:CD2	2.53	0.43
1:D:1873:GLU:OE1	1:D:1873:GLU:N	2.50	0.43
1:D:2254:LEU:CD1	1:D:2276:ALA:HB1	2.47	0.43
1:D:2675:THR:CG2	1:D:2706:ILE:HG23	2.47	0.43
1:D:2685:SER:O	1:D:2689:LYS:HG2	2.17	0.43
1:D:2798:SER:OG	1:D:2801:ASP:OD2	2.26	0.43
1:D:2926:LEU:O	1:D:2930:LEU:HD13	2.18	0.43
1:D:3104:GLU:OE2	1:D:3167:ARG:HB3	2.19	0.43
1:D:3604:TYR:CD1	1:D:3608:GLN:OE1	2.71	0.43
1:C:1045:THR:HG22	1:C:1049:TYR:CZ	2.53	0.43
1:C:1705:GLY:HA3	1:C:1836:PHE:CD2	2.53	0.43
1:C:2514:ASN:OD1	1:C:2517:PHE:HB3	2.19	0.43
1:C:3559:LEU:O	1:C:3560:GLN:C	2.61	0.43
1:C:3628:ARG:HD2	1:C:3632:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4778:TRP:O	1:C:4782:VAL:HG23	2.18	0.43
1:C:4945:ASP:OD1	1:C:4945:ASP:C	2.61	0.43
1:A:598:LYS:O	1:A:602:VAL:HG23	2.18	0.43
1:A:646:PRO:HB2	1:A:648:ILE:HD13	2.00	0.43
1:A:978:THR:HG1	1:A:981:GLN:CD	2.26	0.43
1:A:1980:LEU:CD2	1:A:1995:THR:HG22	2.48	0.43
1:A:3604:TYR:CE1	1:A:3608:GLN:OE1	2.72	0.43
1:A:3789:GLU:OE1	1:A:3789:GLU:N	2.51	0.43
2:E:88:PRO:O	2:E:90:ILE:HD12	2.19	0.43
2:F:103:LEU:HD21	2:F:106:LEU:HD11	2.00	0.43
1:B:783:PHE:HB2	1:B:787:VAL:HG21	2.00	0.43
1:B:1743[A]:ARG:NH2	1:B:1967:ASP:OD2	2.40	0.43
1:B:2514:ASN:OD1	1:B:2517:PHE:HB3	2.18	0.43
1:B:2791:LEU:HD13	1:B:2791:LEU:HA	1.89	0.43
1:B:3213:TYR:CD1	1:B:3302:PRO:HG2	2.52	0.43
1:B:4061:PHE:HA	1:B:4064:MET:HE3	2.01	0.43
1:B:4945:ASP:OD1	1:B:4945:ASP:C	2.61	0.43
1:D:309:THR:O	1:D:309:THR:HG22	2.18	0.43
1:D:1077:ALA:HB2	1:D:1190:PRO:HG2	2.00	0.43
1:D:1999:ARG:NH1	1:D:3635:CYS:C	2.76	0.43
1:D:2886:TRP:O	1:D:2890:LYS:HG2	2.17	0.43
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.51	0.43
1:D:3574:ALA:HA	1:D:3577:ARG:NH2	2.33	0.43
1:D:4182:GLU:HB2	1:D:4983:HIS:CD2	2.53	0.43
1:D:4673:ARG:O	1:D:4676:GLU:HG3	2.18	0.43
1:D:4732:PHE:CE2	1:D:4736:ARG:HG2	2.53	0.43
1:C:116:MET:HG2	1:C:139:GLU:HA	2.00	0.43
1:C:336:PRO:HA	1:C:337:PRO:HD3	1.91	0.43
1:C:2092:GLN:O	1:C:2092:GLN:HG2	2.19	0.43
1:C:3604:TYR:CE1	1:C:3608:GLN:OE1	2.72	0.43
1:A:2527:LEU:O	1:A:2531:ARG:HG3	2.18	0.43
1:A:2801:ASP:OD1	1:A:2802:LYS:N	2.52	0.43
1:A:3130:THR:O	1:A:3134:VAL:HG23	2.19	0.43
1:A:3966:THR:HG23	1:A:4029:SER:OG	2.17	0.43
1:A:4029:SER:HA	1:A:4032:GLU:HG3	2.00	0.43
1:A:4651:THR:OG1	1:A:4803:HIS:NE2	2.05	0.43
1:A:4655:PHE:CE2	1:A:4659:ILE:HD11	2.54	0.43
1:A:4732:PHE:CE2	1:A:4736:ARG:HG2	2.53	0.43
1:B:116:MET:HG2	1:B:139:GLU:HA	2.00	0.43
1:B:928:THR:O	1:B:931:THR:OG1	2.30	0.43
1:B:2330:ARG:O	1:B:2333:ASP:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2393:ASP:OD1	1:B:2418:LEU:N	2.52	0.43
1:B:2801:ASP:OD1	1:B:2802:LYS:N	2.52	0.43
1:B:3162:GLN:O	1:B:3166:TYR:CD2	2.72	0.43
1:B:3580:PRO:O	1:B:3583:GLU:OE2	2.35	0.43
1:B:4060:LYS:O	1:B:4063:ASP:OD1	2.37	0.43
1:B:4821:LYS:O	1:B:4825:THR:HG23	2.17	0.43
1:D:941:MET:SD	1:D:1051:TYR:HE1	2.32	0.43
1:D:2330:ARG:O	1:D:2333:ASP:OD1	2.36	0.43
1:D:2816:MET:HG3	1:D:2878:LEU:HD13	2.01	0.43
1:D:4655:PHE:CE2	1:D:4659:ILE:HD11	2.54	0.43
1:C:959:TYR:CD2	1:C:966:LYS:HE2	2.50	0.43
1:C:3686:GLU:O	1:C:3687:GLU:HB2	2.18	0.43
1:C:3789:GLU:OE1	1:C:3789:GLU:N	2.51	0.43
1:C:4061:PHE:HA	1:C:4064:MET:HE3	2.00	0.43
1:A:76:ARG:O	1:A:80:GLU:HG2	2.18	0.43
1:A:667:MET:SD	1:A:801:LYS:NZ	2.86	0.43
1:A:3455:GLU:O	1:A:3459:VAL:HG23	2.17	0.43
1:A:3686:GLU:O	1:A:3687:GLU:HB2	2.18	0.43
1:A:3891:LEU:CB	1:A:3899:PHE:CE2	3.00	0.43
1:A:4077:PHE:O	1:A:4081:VAL:HG23	2.18	0.43
1:B:1005:TRP:HB3	1:B:1021:LEU:CD1	2.48	0.43
1:B:1077:ALA:HB2	1:B:1190:PRO:HG2	2.00	0.43
1:B:3574:ALA:HA	1:B:3577:ARG:NH2	2.33	0.43
1:B:4182:GLU:HB2	1:B:4983:HIS:CD2	2.53	0.43
6:B:5304:PNX:HAK1	6:B:5304:PNX:HAA1	2.00	0.43
1:D:615:ARG:NH2	1:D:1676:LEU:O	2.49	0.43
1:D:2393:ASP:OD1	1:D:2418:LEU:N	2.52	0.43
1:D:4717:ASP:OD2	1:D:4723:LYS:NZ	2.35	0.43
1:C:598:LYS:O	1:C:602:VAL:HG23	2.18	0.43
1:C:730:VAL:HG23	1:C:1476:MET:SD	2.58	0.43
1:C:1980:LEU:CD2	1:C:1995:THR:HG22	2.48	0.43
1:C:2393:ASP:OD1	1:C:2418:LEU:N	2.52	0.43
1:C:2736:ASP:OD1	1:C:2736:ASP:O	2.36	0.43
1:C:3162:GLN:O	1:C:3166:TYR:CD2	2.72	0.43
1:A:310:LYS:O	1:A:350:HIS:NE2	2.51	0.43
1:A:985:VAL:HG13	1:A:1039:LEU:HD23	2.00	0.43
1:A:2393:ASP:OD1	1:A:2418:LEU:N	2.52	0.43
1:A:3429:ALA:HA	1:A:3432:GLU:OE1	2.18	0.43
1:A:3971:GLY:N	1:A:3972:PRO:HA	2.33	0.43
1:A:4943:LEU:O	1:A:4947:GLN:HG2	2.17	0.43
2:E:24:VAL:HG12	2:E:103:LEU:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:ASP:OD1	2:H:14:THR:HG23	2.19	0.43
2:H:88:PRO:O	2:H:90:ILE:HD12	2.19	0.43
2:G:24:VAL:HG12	2:G:103:LEU:HA	2.01	0.43
2:G:88:PRO:O	2:G:90:ILE:HD12	2.19	0.43
2:G:103:LEU:HD21	2:G:106:LEU:HD11	2.00	0.43
2:F:11:ASP:OD1	2:F:14:THR:HG23	2.19	0.43
1:B:622:THR:HA	1:B:626:LEU:HD13	1.99	0.43
1:B:874:LEU:O	1:B:878:ILE:HG12	2.19	0.43
1:B:1804:LEU:HD13	1:B:1853:ILE:HD12	2.00	0.43
1:B:2092:GLN:O	1:B:2092:GLN:HG2	2.19	0.43
1:B:2736:ASP:OD1	1:B:2736:ASP:O	2.36	0.43
1:B:2992:GLU:O	1:B:2996:LYS:HG2	2.19	0.43
1:D:874:LEU:O	1:D:878:ILE:HG12	2.19	0.43
1:D:961:MET:SD	1:D:963:ASN:HB2	2.57	0.43
1:D:1126:GLY:O	1:D:1142:PRO:HA	2.19	0.43
1:D:1804:LEU:HD13	1:D:1853:ILE:HD12	2.00	0.43
1:D:2514:ASN:OD1	1:D:2517:PHE:HB3	2.19	0.43
1:D:3104:GLU:O	1:D:3107:VAL:HG22	2.19	0.43
1:D:3398:PHE:HE2	1:D:3450:ASN:CB	2.30	0.43
1:D:3442:PHE:HZ	1:D:3609:THR:HG1	1.66	0.43
1:D:3623:LEU:HD12	1:D:3624:LEU:N	2.34	0.43
1:D:3686:GLU:O	1:D:3687:GLU:HB2	2.18	0.43
1:D:4705:VAL:O	1:D:4708:THR:OG1	2.35	0.43
1:C:1694:LEU:O	1:C:1698:LEU:HG	2.18	0.43
1:C:1742:THR:O	1:C:1960:ALA:HB2	2.18	0.43
1:C:3106:MET:O	1:C:3110:LEU:HD23	2.17	0.43
1:C:3230:LEU:HD12	1:C:3232:LEU:HG	1.99	0.43
1:C:3574:ALA:HA	1:C:3577:ARG:NH2	2.33	0.43
1:C:3604:TYR:CD1	1:C:3608:GLN:OE1	2.71	0.43
1:A:1742:THR:O	1:A:1960:ALA:HB2	2.18	0.43
1:A:2514:ASN:OD1	1:A:2517:PHE:HB3	2.18	0.43
1:A:3104:GLU:O	1:A:3107:VAL:HG22	2.19	0.43
1:A:3435:PHE:HD2	1:A:3524:MET:HE1	1.82	0.43
1:A:3442:PHE:HZ	1:A:3609:THR:HG1	1.66	0.43
1:A:3465:ASN:OD1	1:A:3467:MET:CG	2.60	0.43
1:A:3640:PRO:HB2	1:A:3642:TYR:CE1	2.54	0.43
6:A:5304:PNX:HAK1	6:A:5304:PNX:HAA1	2.00	0.43
2:H:105:LYS:C	2:H:106:LEU:HD12	2.43	0.43
2:F:105:LYS:C	2:F:106:LEU:HD12	2.43	0.43
1:B:1045:THR:HG22	1:B:1049:TYR:CZ	2.53	0.43
1:B:1705:GLY:HA3	1:B:1836:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3429:ALA:HA	1:B:3432:GLU:OE1	2.18	0.43
1:B:3528:THR:HG23	1:B:3573:MET:SD	2.58	0.43
1:B:3546:ASP:O	1:B:3549:VAL:HG22	2.17	0.43
1:B:3604:TYR:CE1	1:B:3608:GLN:OE1	2.72	0.43
1:B:3693:LYS:HA	1:B:3693:LYS:HE2	2.01	0.43
1:D:984:LEU:HD23	1:D:988:LEU:HD23	2.00	0.43
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.37	0.43
1:D:2092:GLN:HG2	1:D:2092:GLN:O	2.19	0.43
1:D:2203:MET:HE2	1:D:2235:PHE:HZ	1.81	0.43
1:C:310:LYS:O	1:C:350:HIS:NE2	2.51	0.43
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.37	0.43
1:C:1999:ARG:NH1	1:C:3635:CYS:C	2.76	0.43
1:C:2816:MET:HG3	1:C:2878:LEU:HD13	2.01	0.43
1:C:2986:VAL:O	1:C:2986:VAL:HG13	2.19	0.43
1:C:3640:PRO:HB2	1:C:3642:TYR:CE1	2.54	0.43
1:C:4077:PHE:O	1:C:4081:VAL:HG23	2.18	0.43
1:C:4098:ASP:OD1	1:C:4098:ASP:C	2.61	0.43
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.37	0.43
1:A:1804:LEU:HD13	1:A:1853:ILE:HD12	2.00	0.43
1:A:3623:LEU:HD12	1:A:3624:LEU:N	2.34	0.43
1:A:3693:LYS:HE2	1:A:3693:LYS:HA	2.01	0.43
1:A:4673:ARG:O	1:A:4676:GLU:HG3	2.18	0.43
1:A:4677:LEU:HD23	1:A:4711:PHE:HE1	1.83	0.43
2:H:24:VAL:HG12	2:H:103:LEU:HA	2.01	0.43
1:B:484:LEU:HD12	1:B:526:LEU:HD12	2.01	0.43
1:B:2244:ARG:NH2	1:B:2283:ASN:OD1	2.50	0.43
1:B:3104:GLU:OE2	1:B:3167:ARG:HB3	2.19	0.43
1:D:259:LEU:HD11	1:D:397:GLU:HG2	2.00	0.43
1:D:985:VAL:HG13	1:D:1039:LEU:HD23	2.00	0.43
1:D:1005:TRP:HB3	1:D:1021:LEU:CD1	2.48	0.43
1:D:1067:SER:O	1:D:1071:ARG:HG3	2.18	0.43
1:D:2211:MET:O	1:D:2214:VAL:CG1	2.64	0.43
1:D:2801:ASP:OD1	1:D:2802:LYS:N	2.52	0.43
1:D:3673:MET:HE2	1:D:3725:TYR:HE1	1.84	0.43
1:D:4000:MET:SD	1:D:4020:GLN:NE2	2.79	0.43
1:C:259:LEU:HD11	1:C:397:GLU:HG2	2.00	0.43
1:C:2801:ASP:OD1	1:C:2802:LYS:N	2.52	0.43
1:C:2992:GLU:O	1:C:2996:LYS:HG2	2.19	0.43
1:C:3104:GLU:O	1:C:3107:VAL:HG22	2.19	0.43
1:C:3583:GLU:HB3	1:C:3585:ASP:OD1	2.19	0.43
1:C:3971:GLY:N	1:C:3972:PRO:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD12	1:A:220:LEU:C	2.44	0.43
1:A:266:ARG:O	1:A:270:SER:OG	2.34	0.43
1:A:984:LEU:HD23	1:A:988:LEU:HD23	2.00	0.43
1:A:1705:GLY:HA3	1:A:1836:PHE:CD2	2.53	0.43
1:A:2800:LYS:O	1:A:2804:ILE:HG13	2.19	0.43
1:A:2816:MET:HG3	1:A:2878:LEU:HD13	2.01	0.43
1:A:3391:GLU:O	1:A:3395:ARG:HD2	2.19	0.43
1:A:3777:GLU:OE1	1:A:3777:GLU:N	2.47	0.43
1:A:4071:ILE:O	1:A:4074:SER:OG	2.35	0.43
1:B:309:THR:HG22	1:B:309:THR:O	2.18	0.43
1:B:310:LYS:O	1:B:350:HIS:NE2	2.51	0.43
1:B:1126:GLY:O	1:B:1142:PRO:HA	2.19	0.43
1:B:1999:ARG:NH1	1:B:3635:CYS:C	2.76	0.43
1:B:3212:GLU:OE2	1:B:3213:TYR:CZ	2.72	0.43
1:B:3682:GLU:O	1:B:3686:GLU:OE2	2.37	0.43
1:B:3725:TYR:O	1:B:3729:MET:HG3	2.19	0.43
1:D:1045:THR:HG22	1:D:1049:TYR:CZ	2.53	0.43
1:D:1828:ASP:N	1:D:1828:ASP:OD1	2.52	0.43
1:D:1980:LEU:CD2	1:D:1995:THR:HG22	2.48	0.43
1:D:3693:LYS:HE2	1:D:3693:LYS:HA	2.01	0.43
1:D:3777:GLU:OE1	1:D:3777:GLU:N	2.47	0.43
1:D:3875:MET:HE1	1:D:3954:ALA:HA	2.00	0.43
1:D:4071:ILE:O	1:D:4074:SER:OG	2.35	0.43
1:D:4946:GLN:O	1:D:4950:VAL:HG23	2.19	0.43
1:C:1077:ALA:HB2	1:C:1190:PRO:HG2	2.01	0.43
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.51	0.43
1:C:3104:GLU:OE2	1:C:3167:ARG:HB3	2.19	0.43
1:A:116:MET:HG2	1:A:139:GLU:HA	2.00	0.43
1:A:820:ARG:HB3	1:A:820:ARG:CZ	2.24	0.43
1:A:2685:SER:O	1:A:2689:LYS:HG2	2.17	0.43
1:A:2736:ASP:O	1:A:2736:ASP:OD1	2.36	0.43
1:A:3104:GLU:OE2	1:A:3167:ARG:HB3	2.19	0.43
1:A:3673:MET:HE2	1:A:3725:TYR:HE1	1.84	0.43
1:A:4148:THR:HG21	1:A:4180:ARG:NH2	2.31	0.43
1:A:4182:GLU:HB2	1:A:4983:HIS:NE2	2.34	0.43
2:F:24:VAL:HG12	2:F:103:LEU:HA	2.01	0.43
1:B:236:ALA:C	1:B:237:ASP:OD2	2.62	0.43
1:B:1440:PHE:CZ	1:B:1563:GLN:HG3	2.54	0.43
1:B:1828:ASP:OD1	1:B:1828:ASP:N	2.52	0.43
1:B:2800:LYS:O	1:B:2804:ILE:HG13	2.19	0.43
1:B:3686:GLU:O	1:B:3687:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4901:ILE:HG13	1:B:4913:ARG:NH2	2.34	0.43
1:D:167:ASP:OD1	1:C:384:MET:SD	2.77	0.43
1:D:2736:ASP:O	1:D:2736:ASP:OD1	2.36	0.43
1:D:2800:LYS:O	1:D:2804:ILE:HG13	2.19	0.43
1:D:3162:GLN:O	1:D:3166:TYR:CD2	2.72	0.43
1:D:3175:LEU:O	1:D:3175:LEU:HD23	2.19	0.43
1:D:3212:GLU:OE2	1:D:3213:TYR:CZ	2.71	0.43
1:D:3230:LEU:HD12	1:D:3232:LEU:HG	1.99	0.43
1:D:4781:GLY:O	1:D:4785:THR:HG23	2.19	0.43
1:C:874:LEU:O	1:C:878:ILE:HG12	2.19	0.43
1:C:2725:LYS:HE3	1:C:2734:ASN:O	2.19	0.43
1:C:3239:MET:CB	1:C:3239:MET:HG2	2.31	0.43
1:C:3891:LEU:HD13	1:C:3899:PHE:HZ	1.79	0.43
1:C:4655:PHE:CE2	1:C:4659:ILE:HD11	2.54	0.43
1:C:4673:ARG:O	1:C:4676:GLU:HG3	2.18	0.43
1:C:4781:GLY:O	1:C:4785:THR:HG23	2.19	0.43
1:A:236:ALA:C	1:A:237:ASP:OD2	2.62	0.42
1:A:908:VAL:O	1:A:909:ASN:HB2	2.19	0.42
1:A:1105:ALA:HB2	1:A:1191:VAL:HG11	2.00	0.42
1:A:1143:TRP:HB2	1:A:1147:ASP:HB2	2.01	0.42
1:A:3162:GLN:O	1:A:3166:TYR:CD2	2.72	0.42
1:A:3583:GLU:HB3	1:A:3585:ASP:OD1	2.19	0.42
1:A:4000:MET:SD	1:A:4020:GLN:NE2	2.79	0.42
1:A:4060:LYS:O	1:A:4063:ASP:OD1	2.37	0.42
1:A:4901:ILE:HG13	1:A:4913:ARG:NH2	2.34	0.42
2:E:11:ASP:OD1	2:E:14:THR:HG23	2.19	0.42
2:E:105:LYS:C	2:E:106:LEU:HD12	2.43	0.42
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.37	0.42
1:B:1756:ASN:OD1	1:B:2040:ALA:HB2	2.19	0.42
1:B:3239:MET:CB	1:B:3239:MET:HG3	2.31	0.42
1:B:3380:ARG:NH1	1:B:3391:GLU:OE2	2.50	0.42
1:D:1084:GLN:C	1:D:1155:LEU:HD22	2.44	0.42
1:D:2527:LEU:O	1:D:2531:ARG:HG3	2.18	0.42
1:D:2572:THR:CG2	1:D:2579:VAL:CG2	2.83	0.42
1:D:3868:ARG:HG2	1:D:3869:GLN:N	2.34	0.42
1:D:4061:PHE:HA	1:D:4064:MET:HE3	2.01	0.42
1:D:4077:PHE:O	1:D:4081:VAL:HG23	2.18	0.42
1:C:236:ALA:C	1:C:237:ASP:OD2	2.62	0.42
1:C:484:LEU:HD12	1:C:526:LEU:HD12	2.01	0.42
1:C:783:PHE:HB2	1:C:787:VAL:HG21	2.00	0.42
1:C:961:MET:SD	1:C:963:ASN:HB2	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1436:SER:OG	1:C:1565:GLU:HB2	2.19	0.42
1:C:2185:ILE:HG21	1:C:2203:MET:HE1	2.01	0.42
1:C:2969:ILE:O	1:C:2973:PHE:HD1	2.02	0.42
1:C:3682:GLU:O	1:C:3686:GLU:OE2	2.37	0.42
1:C:3693:LYS:HE2	1:C:3693:LYS:HA	2.01	0.42
1:A:961:MET:HE1	1:A:963:ASN:CG	2.41	0.42
1:A:1005:TRP:HB3	1:A:1021:LEU:CD1	2.48	0.42
1:A:1045:THR:HG22	1:A:1049:TYR:CZ	2.54	0.42
1:A:1436:SER:OG	1:A:1565:GLU:HB2	2.19	0.42
1:A:1756:ASN:OD1	1:A:2040:ALA:HB2	2.19	0.42
1:A:2992:GLU:O	1:A:2996:LYS:HG2	2.19	0.42
1:A:4946:GLN:O	1:A:4950:VAL:HG23	2.19	0.42
2:G:31:GLU:OE2	1:C:1299:GLN:HG2	2.19	0.42
1:B:1105:ALA:HB2	1:B:1191:VAL:HG11	2.00	0.42
1:B:1105:ALA:O	1:B:1189:LEU:N	2.50	0.42
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.52	0.42
1:B:3573:MET:CB	1:B:3577:ARG:NH1	2.73	0.42
1:B:3623:LEU:HD12	1:B:3624:LEU:N	2.34	0.42
1:B:3734:HIS:O	1:B:3735:LEU:C	2.62	0.42
1:B:4673:ARG:O	1:B:4676:GLU:HG3	2.18	0.42
1:B:4674:GLU:OE2	1:B:4775:TYR:OH	2.35	0.42
1:D:928:THR:O	1:D:931:THR:OG1	2.30	0.42
1:D:3604:TYR:CE1	1:D:3608:GLN:OE1	2.72	0.42
1:D:3725:TYR:O	1:D:3729:MET:HG3	2.19	0.42
1:D:4231:MET:O	1:D:4235:VAL:HG23	2.20	0.42
1:C:1005:TRP:HB3	1:C:1021:LEU:CD1	2.48	0.42
1:C:2208:MET:O	1:C:2212:VAL:HG22	2.19	0.42
1:C:2434:GLY:O	1:C:2508:ARG:NE	2.43	0.42
1:C:3725:TYR:O	1:C:3729:MET:HG3	2.19	0.42
1:C:4060:LYS:O	1:C:4063:ASP:OD1	2.37	0.42
1:C:4182:GLU:HB2	1:C:4983:HIS:NE2	2.34	0.42
1:A:553:ARG:O	1:A:557:SER:OG	2.29	0.42
1:A:893:TYR:HD1	1:A:907:LEU:O	2.03	0.42
1:A:921:ASN:O	1:A:924:MET:HG2	2.19	0.42
1:A:2986:VAL:HG13	1:A:2986:VAL:O	2.19	0.42
1:A:3071:LEU:O	1:A:3075:LEU:HG	2.19	0.42
1:A:3197:LEU:CD2	1:A:3201:MET:HE3	2.41	0.42
1:A:3471:THR:HG22	1:B:1170:MET:CE	2.49	0.42
1:B:667:MET:SD	1:B:801:LYS:NZ	2.86	0.42
1:B:921:ASN:O	1:B:924:MET:HG2	2.19	0.42
1:B:2700:MET:O	1:B:2702:CYS:SG	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3130:THR:O	1:B:3134:VAL:HG23	2.19	0.42
1:B:3254:GLY:O	1:B:3255:GLY:C	2.60	0.42
1:D:492:ASP:O	1:D:496:VAL:HG13	2.19	0.42
1:D:2214:VAL:HG11	1:D:2228:MET:CE	2.48	0.42
1:D:4182:GLU:HB2	1:D:4983:HIS:NE2	2.34	0.42
1:C:220:LEU:C	1:C:220:LEU:HD12	2.44	0.42
1:C:266:ARG:O	1:C:270:SER:OG	2.34	0.42
1:C:1743[A]:ARG:NH2	1:C:1967:ASP:OD2	2.39	0.42
1:C:2865:VAL:HG11	1:C:2928:LYS:HE2	2.02	0.42
1:C:2926:LEU:O	1:C:2930:LEU:HD13	2.18	0.42
1:C:3197:LEU:HD23	1:C:3197:LEU:O	2.20	0.42
1:C:3879:GLU:HG2	1:C:3880:PHE:N	2.35	0.42
1:C:4021:LYS:N	1:C:4139:ILE:HD13	2.35	0.42
1:C:4563:ARG:NH2	1:C:4815:ASP:OD1	2.53	0.42
1:A:1084:GLN:C	1:A:1155:LEU:HD22	2.44	0.42
1:A:3559:LEU:O	1:A:3560:GLN:C	2.61	0.42
2:F:24:VAL:HG21	2:F:59:TRP:HZ3	1.85	0.42
1:B:2373:GLY:O	1:C:130:LYS:NZ	2.49	0.42
1:B:2816:MET:HG3	1:B:2878:LEU:HD13	2.01	0.42
1:B:4021:LYS:N	1:B:4139:ILE:HD13	2.35	0.42
1:B:4182:GLU:HB2	1:B:4983:HIS:NE2	2.34	0.42
1:B:4231:MET:O	1:B:4235:VAL:HG23	2.20	0.42
1:D:783:PHE:HB2	1:D:787:VAL:HG21	2.00	0.42
1:D:921:ASN:O	1:D:924:MET:HG2	2.19	0.42
1:D:1194:LEU:HD23	1:D:1198:GLN:O	2.19	0.42
1:D:1434:TYR:HB2	1:D:1572:ILE:HG21	2.01	0.42
1:D:3640:PRO:HB2	1:D:3642:TYR:CE1	2.54	0.42
1:D:4945:ASP:OD1	1:D:4945:ASP:C	2.61	0.42
1:C:908:VAL:O	1:C:909:ASN:HB2	2.19	0.42
1:C:1194:LEU:HD23	1:C:1198:GLN:O	2.19	0.42
1:C:1828:ASP:OD1	1:C:1828:ASP:N	2.52	0.42
1:C:2612[B]:ARG:NH1	1:C:2613:TYR:OH	2.53	0.42
1:A:998:ARG:HG2	1:A:998:ARG:HH11	1.84	0.42
1:A:3682:GLU:O	1:A:3686:GLU:OE2	2.37	0.42
1:A:3734:HIS:O	1:A:3735:LEU:C	2.62	0.42
1:A:3875:MET:HE1	1:A:3954:ALA:HA	2.00	0.42
1:A:4781:GLY:O	1:A:4785:THR:HG23	2.19	0.42
1:A:4945:ASP:OD1	1:A:4945:ASP:C	2.61	0.42
2:E:103:LEU:HD21	2:E:106:LEU:HD11	2.00	0.42
2:G:11:ASP:OD1	2:G:14:THR:HG23	2.19	0.42
1:B:893:TYR:HD1	1:B:907:LEU:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2628:PHE:CZ	1:B:2734:ASN:CG	2.94	0.42
1:B:2703:LEU:HD22	1:B:2706:ILE:HD12	2.02	0.42
1:B:3071:LEU:O	1:B:3075:LEU:HG	2.19	0.42
1:B:3175:LEU:O	1:B:3175:LEU:HD23	2.19	0.42
1:B:3879:GLU:HG2	1:B:3880:PHE:N	2.35	0.42
1:B:4781:GLY:O	1:B:4785:THR:HG23	2.19	0.42
1:D:116:MET:HG2	1:D:139:GLU:HA	2.00	0.42
1:D:236:ALA:C	1:D:237:ASP:OD2	2.62	0.42
1:D:266:ARG:O	1:D:270:SER:OG	2.34	0.42
1:D:998:ARG:HG2	1:D:998:ARG:HH11	1.84	0.42
1:D:1143:TRP:HB2	1:D:1147:ASP:HB2	2.01	0.42
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.52	0.42
1:C:1084:GLN:C	1:C:1155:LEU:HD22	2.44	0.42
1:C:1105:ALA:HB2	1:C:1191:VAL:HG11	2.00	0.42
1:C:1143:TRP:HB2	1:C:1147:ASP:HB2	2.01	0.42
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.52	0.42
1:C:2667:THR:HG21	1:C:2672:LEU:HG	2.01	0.42
1:C:3294:PRO:HB2	1:C:3297:PRO:HD2	2.01	0.42
1:C:3435:PHE:CD2	1:C:3524:MET:CE	3.03	0.42
1:C:3573:MET:CB	1:C:3577:ARG:NH1	2.73	0.42
1:C:3673:MET:HE2	1:C:3725:TYR:HE1	1.84	0.42
1:C:4717:ASP:OD2	1:C:4723:LYS:NZ	2.35	0.42
1:C:4946:GLN:O	1:C:4950:VAL:HG23	2.19	0.42
1:A:309:THR:O	1:A:309:THR:HG22	2.18	0.42
1:A:484:LEU:HD12	1:A:526:LEU:HD12	2.01	0.42
1:A:492:ASP:O	1:A:496:VAL:HG13	2.19	0.42
1:A:2700:MET:O	1:A:2702:CYS:SG	2.78	0.42
1:A:2703:LEU:HD22	1:A:2706:ILE:HD12	2.02	0.42
1:A:3725:TYR:O	1:A:3729:MET:HG3	2.19	0.42
1:A:3879:GLU:HG2	1:A:3880:PHE:N	2.35	0.42
1:A:4021:LYS:N	1:A:4139:ILE:HD13	2.35	0.42
1:A:4061:PHE:HA	1:A:4064:MET:HE3	2.00	0.42
1:B:220:LEU:C	1:B:220:LEU:HD12	2.44	0.42
1:B:908:VAL:O	1:B:909:ASN:HB2	2.19	0.42
1:B:1436:SER:OG	1:B:1565:GLU:HB2	2.20	0.42
1:B:1727:ARG:O	1:B:1731:LEU:HG	2.20	0.42
1:B:1868:PRO:O	1:B:1872:THR:OG1	2.28	0.42
1:B:2667:THR:HG21	1:B:2672:LEU:HG	2.01	0.42
1:B:2977:LEU:HD23	1:B:3056:LEU:HD11	2.02	0.42
1:B:3435:PHE:CD2	1:B:3524:MET:CE	3.03	0.42
1:B:3435:PHE:HD2	1:B:3524:MET:HE1	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3640:PRO:HB2	1:B:3642:TYR:CE1	2.54	0.42
1:B:4717:ASP:OD2	1:B:4723:LYS:NZ	2.35	0.42
1:D:908:VAL:O	1:D:909:ASN:HB2	2.19	0.42
1:D:1927:LEU:HD22	1:D:2101:MET:SD	2.60	0.42
1:D:3610:GLU:OE1	1:D:3611:HIS:CD2	2.73	0.42
1:D:4060:LYS:O	1:D:4063:ASP:OD1	2.37	0.42
1:C:921:ASN:O	1:C:924:MET:HG2	2.20	0.42
1:C:1804:LEU:HD13	1:C:1853:ILE:HD12	2.00	0.42
1:C:2628:PHE:CZ	1:C:2734:ASN:CG	2.94	0.42
1:C:3391:GLU:O	1:C:3395:ARG:HD2	2.19	0.42
1:A:954:LYS:HG2	1:A:957:LYS:HZ1	1.84	0.42
1:A:1440:PHE:CZ	1:A:1563:GLN:HG3	2.54	0.42
1:A:1828:ASP:N	1:A:1828:ASP:OD1	2.52	0.42
1:A:1992:ALA:O	1:A:1995:THR:OG1	2.29	0.42
1:A:2092:GLN:HG2	1:A:2092:GLN:O	2.19	0.42
1:A:2545:GLU:HG2	1:A:2546:MET:N	2.35	0.42
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.52	0.42
1:A:2638:LYS:C	1:A:2698:MET:HE2	2.45	0.42
1:A:3386:GLU:O	1:A:3389:GLU:O	2.38	0.42
1:A:3574:ALA:HA	1:A:3577:ARG:NH2	2.33	0.42
1:A:3673:MET:HE2	1:A:3725:TYR:CE1	2.55	0.42
2:F:88:PRO:O	2:F:90:ILE:HD12	2.19	0.42
1:B:278:GLN:HG3	1:B:328:LYS:NZ	2.35	0.42
1:B:873:LYS:O	1:B:876:GLU:HG2	2.20	0.42
1:B:1194:LEU:HD23	1:B:1198:GLN:O	2.19	0.42
1:B:1276:THR:O	1:B:1279:SER:OG	2.27	0.42
1:B:1927:LEU:HD22	1:B:2101:MET:SD	2.60	0.42
1:B:2208:MET:O	1:B:2212:VAL:HG22	2.19	0.42
1:D:69:LEU:CD2	1:D:109:LEU:HD21	2.50	0.42
1:D:2208:MET:O	1:D:2212:VAL:HG22	2.19	0.42
1:D:3130:THR:O	1:D:3134:VAL:HG23	2.19	0.42
1:D:3604:TYR:CD1	1:D:3604:TYR:C	2.98	0.42
1:D:3660:ALA:HB3	1:D:3661:TRP:HD1	1.85	0.42
1:D:3899:PHE:HE2	1:D:3903:LEU:HD11	1.85	0.42
1:C:69:LEU:CD2	1:C:109:LEU:HD21	2.50	0.42
1:C:1126:GLY:O	1:C:1142:PRO:HA	2.19	0.42
1:C:1927:LEU:HD22	1:C:2101:MET:SD	2.60	0.42
1:C:3175:LEU:HD23	1:C:3175:LEU:O	2.19	0.42
1:C:3734:HIS:O	1:C:3735:LEU:C	2.62	0.42
1:C:4179:GLY:CA	1:C:4197:ILE:HD11	2.50	0.42
1:A:167:ASP:N	1:D:384:MET:SD	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASP:CG	1:B:156:GLN:HE22	2.27	0.42
1:A:468:LEU:O	1:A:472:ARG:HG2	2.20	0.42
1:A:874:LEU:O	1:A:878:ILE:HG12	2.19	0.42
1:A:1194:LEU:HD23	1:A:1198:GLN:O	2.19	0.42
1:A:1927:LEU:HD22	1:A:2101:MET:SD	2.60	0.42
1:A:2798:SER:OG	1:A:2801:ASP:OD2	2.26	0.42
1:A:4999:ASP:OD1	1:A:5000:GLU:N	2.53	0.42
1:B:1434:TYR:HB2	1:B:1572:ILE:HG21	2.01	0.42
1:B:3197:LEU:CD2	1:B:3201:MET:HE3	2.41	0.42
1:D:1756:ASN:OD1	1:D:2040:ALA:HB2	2.19	0.42
1:D:2313:LEU:HB3	1:D:2318:TYR:HB2	2.02	0.42
1:D:2992:GLU:O	1:D:2996:LYS:HG2	2.19	0.42
1:D:3682:GLU:O	1:D:3686:GLU:OE2	2.37	0.42
1:C:292:ALA:HB2	1:C:312:THR:HG22	2.02	0.42
1:C:468:LEU:O	1:C:472:ARG:HG2	2.20	0.42
1:C:873:LYS:O	1:C:876:GLU:HG2	2.20	0.42
1:C:2001:PRO:O	1:C:2005:GLN:HG3	2.20	0.42
1:C:2545:GLU:HG2	1:C:2546:MET:N	2.35	0.42
1:C:3458:PHE:CE2	1:C:3464:ILE:HD11	2.54	0.42
1:C:3673:MET:HE2	1:C:3725:TYR:CE1	2.55	0.42
1:A:869:ARG:NH2	1:A:947:GLU:OE2	2.52	0.42
1:A:1126:GLY:O	1:A:1142:PRO:HA	2.19	0.42
1:A:1434:TYR:HB2	1:A:1572:ILE:HG21	2.01	0.42
1:A:3294:PRO:HB2	1:A:3297:PRO:HD2	2.01	0.42
1:A:4843:LEU:HD21	1:D:4827:LEU:HD21	2.02	0.42
1:B:292:ALA:HB2	1:B:312:THR:HG22	2.02	0.42
1:B:309:THR:O	1:B:309:THR:CG2	2.68	0.42
1:B:468:LEU:O	1:B:472:ARG:HG2	2.20	0.42
1:B:516:LYS:O	1:B:519:VAL:HG22	2.20	0.42
1:B:1286:MET:HE2	1:B:1464:PHE:HB3	2.02	0.42
1:B:3103:ILE:O	1:B:3107:VAL:HG13	2.20	0.42
1:B:3148:ALA:O	1:B:3151:GLN:NE2	2.53	0.42
1:B:3673:MET:HE2	1:B:3725:TYR:HE1	1.84	0.42
1:B:4187:SER:O	1:B:4188:ARG:HB2	2.20	0.42
1:B:4705:VAL:HG23	1:B:4775:TYR:HD2	1.85	0.42
1:D:292:ALA:HB2	1:D:312:THR:HG22	2.02	0.42
1:D:309:THR:O	1:D:309:THR:CG2	2.68	0.42
1:D:516:LYS:O	1:D:519:VAL:HG22	2.20	0.42
1:D:887:ILE:HD13	1:D:887:ILE:HA	1.87	0.42
1:D:893:TYR:HD1	1:D:907:LEU:O	2.03	0.42
1:D:1105:ALA:HB2	1:D:1191:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1265:ASP:OD1	1:D:1266:THR:N	2.53	0.42
1:D:1440:PHE:CZ	1:D:1563:GLN:HG3	2.54	0.42
1:D:2545:GLU:HG2	1:D:2546:MET:N	2.35	0.42
1:D:3148:ALA:O	1:D:3151:GLN:NE2	2.53	0.42
1:D:3321:ARG:HA	1:D:3324:VAL:HG22	2.02	0.42
1:D:3583:GLU:HB3	1:D:3585:ASP:OD1	2.19	0.42
1:D:4021:LYS:N	1:D:4139:ILE:HD13	2.35	0.42
1:D:4070:ASP:OD1	1:D:4070:ASP:C	2.63	0.42
1:D:4179:GLY:CA	1:D:4197:ILE:HD11	2.50	0.42
1:C:961:MET:HE1	1:C:963:ASN:CG	2.41	0.42
1:C:1434:TYR:HB2	1:C:1572:ILE:HG21	2.01	0.42
1:C:2700:MET:O	1:C:2702:CYS:SG	2.78	0.42
1:C:2977:LEU:HD23	1:C:3056:LEU:HD11	2.02	0.42
1:C:3623:LEU:HD12	1:C:3624:LEU:N	2.34	0.42
1:A:484:LEU:HD11	1:A:526:LEU:HD11	2.02	0.42
1:A:3604:TYR:CD1	1:A:3604:TYR:C	2.98	0.42
1:A:4179:GLY:HA3	1:A:4197:ILE:HD11	2.02	0.42
2:E:24:VAL:HG21	2:E:59:TRP:HZ3	1.85	0.42
1:B:384:MET:SD	1:C:167:ASP:OD1	2.78	0.42
1:B:484:LEU:HD11	1:B:526:LEU:HD11	2.02	0.42
1:B:2045:GLN:C	1:B:2046:LEU:HD12	2.45	0.42
1:B:2865:VAL:HG11	1:B:2928:LYS:HE2	2.02	0.42
1:B:3391:GLU:O	1:B:3395:ARG:HD2	2.19	0.42
1:B:3559:LEU:O	1:B:3560:GLN:C	2.61	0.42
1:B:3604:TYR:CD1	1:B:3604:TYR:C	2.98	0.42
1:B:3997:ALA:HB1	1:B:4057:MET:SD	2.60	0.42
1:B:4655:PHE:CE2	1:B:4659:ILE:HD11	2.54	0.42
1:D:310:LYS:O	1:D:350:HIS:NE2	2.51	0.42
1:D:484:LEU:HD12	1:D:526:LEU:HD12	2.01	0.42
1:D:2441:HIS:CE1	1:D:2442:LEU:HD12	2.55	0.42
1:D:2612[B]:ARG:NH1	1:D:2613:TYR:OH	2.53	0.42
1:D:3197:LEU:HD23	1:D:3197:LEU:O	2.20	0.42
1:D:3478:MET:O	1:D:3478:MET:HG3	2.19	0.42
1:D:3734:HIS:O	1:D:3735:LEU:C	2.62	0.42
1:D:4069:LYS:O	1:D:4072:VAL:HG22	2.20	0.42
1:C:484:LEU:HD11	1:C:526:LEU:HD11	2.02	0.42
1:C:484:LEU:CD1	1:C:526:LEU:CD1	2.98	0.42
1:C:1440:PHE:CZ	1:C:1563:GLN:HG3	2.54	0.42
1:C:1756:ASN:OD1	1:C:2040:ALA:HB2	2.19	0.42
1:C:2800:LYS:O	1:C:2804:ILE:HG13	2.19	0.42
1:C:2946:LEU:N	1:C:2948:THR:HG23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3478:MET:O	1:C:3478:MET:HG3	2.19	0.42
1:C:4999:ASP:OD1	1:C:5000:GLU:N	2.53	0.42
1:A:1265:ASP:OD1	1:A:1266:THR:N	2.53	0.41
1:A:1684:ALA:HA	2:E:90:ILE:HD11	2.02	0.41
1:A:2045:GLN:C	1:A:2046:LEU:HD12	2.45	0.41
1:A:2495:VAL:HG22	1:A:2498:HIS:CE1	2.55	0.41
1:A:2667:THR:HG21	1:A:2672:LEU:HG	2.01	0.41
1:A:3111:ARG:O	1:A:3112:LEU:HB2	2.20	0.41
1:A:3148:ALA:O	1:A:3151:GLN:NE2	2.53	0.41
1:A:3175:LEU:O	1:A:3175:LEU:HD23	2.19	0.41
1:A:3321:ARG:HA	1:A:3324:VAL:HG22	2.02	0.41
1:A:3997:ALA:HB1	1:A:4057:MET:SD	2.60	0.41
1:A:4231:MET:O	1:A:4235:VAL:HG23	2.20	0.41
1:B:484:LEU:CD1	1:B:526:LEU:CD1	2.98	0.41
1:B:998:ARG:HG2	1:B:998:ARG:HH11	1.84	0.41
1:B:3077:ALA:O	1:B:3081:MET:HG2	2.20	0.41
1:B:3104:GLU:O	1:B:3107:VAL:HG22	2.19	0.41
1:B:3633:VAL:O	1:B:3637:ARG:HD3	2.20	0.41
1:B:4179:GLY:CA	1:B:4197:ILE:HD11	2.50	0.41
1:B:4179:GLY:HA3	1:B:4197:ILE:HD11	2.02	0.41
1:D:484:LEU:HD11	1:D:526:LEU:HD11	2.02	0.41
1:D:1819:VAL:HG22	1:D:1926:LEU:HD21	2.02	0.41
1:D:2185:ILE:HG21	1:D:2203:MET:HE1	2.01	0.41
1:D:2495:VAL:HG22	1:D:2498:HIS:CE1	2.55	0.41
1:D:3294:PRO:HB2	1:D:3297:PRO:HD2	2.02	0.41
1:D:3458:PHE:CE2	1:D:3464:ILE:HD11	2.54	0.41
1:D:4999:ASP:OD1	1:D:5000:GLU:N	2.53	0.41
1:C:492:ASP:O	1:C:496:VAL:HG13	2.19	0.41
1:C:926:GLY:O	1:C:930:LYS:HG3	2.20	0.41
1:C:998:ARG:HG2	1:C:998:ARG:HH11	1.84	0.41
1:C:1265:ASP:OD1	1:C:1266:THR:N	2.53	0.41
1:C:1727:ARG:O	1:C:1731:LEU:HG	2.20	0.41
1:C:2117:VAL:O	1:C:2120:MET:HG2	2.21	0.41
1:C:2135:LEU:HD12	1:C:3658:LYS:HG3	2.02	0.41
1:C:2313:LEU:HB3	1:C:2318:TYR:HB2	2.02	0.41
1:C:2487:GLN:NE2	1:C:2545:GLU:OE1	2.53	0.41
1:C:3660:ALA:HB3	1:C:3661:TRP:HD1	1.85	0.41
1:C:4231:MET:O	1:C:4235:VAL:HG23	2.20	0.41
1:C:4705:VAL:O	1:C:4708:THR:OG1	2.35	0.41
1:A:885:THR:HA	1:A:888:GLU:OE1	2.20	0.41
1:A:2001:PRO:O	1:A:2005:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2374:SER:OG	1:A:2378:ALA:HB3	2.21	0.41
1:A:2444:GLN:OE1	1:A:2444:GLN:N	2.53	0.41
1:A:3504:SER:O	1:A:3507:THR:OG1	2.30	0.41
1:A:3610:GLU:OE1	1:A:3611:HIS:CD2	2.73	0.41
1:A:3899:PHE:HE2	1:A:3903:LEU:HD11	1.85	0.41
1:A:4705:VAL:HG23	1:A:4775:TYR:HD2	1.85	0.41
2:G:24:VAL:HG21	2:G:59:TRP:HZ3	1.85	0.41
1:B:384:MET:SD	1:C:167:ASP:N	2.93	0.41
1:B:492:ASP:O	1:B:496:VAL:HG13	2.19	0.41
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	2.03	0.41
1:B:2202:GLY:HA2	1:B:2205:GLU:OE1	2.20	0.41
1:B:2487:GLN:NE2	1:B:2545:GLU:OE1	2.53	0.41
1:B:2495:VAL:HG22	1:B:2498:HIS:CE1	2.55	0.41
1:B:2725:LYS:HE3	1:B:2734:ASN:O	2.19	0.41
1:B:2986:VAL:O	1:B:2986:VAL:HG13	2.19	0.41
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	2.02	0.41
1:B:3111:ARG:HH21	1:B:3178:THR:CB	2.33	0.41
1:B:3916:ILE:HD12	1:B:3916:ILE:H	1.86	0.41
1:B:4069:LYS:O	1:B:4072:VAL:HG22	2.21	0.41
1:D:336:PRO:HA	1:D:337:PRO:HD3	1.91	0.41
1:D:873:LYS:O	1:D:876:GLU:HG2	2.20	0.41
1:D:1085:SER:N	1:D:1155:LEU:HD22	2.35	0.41
1:D:1727:ARG:O	1:D:1731:LEU:HG	2.20	0.41
1:D:3386:GLU:O	1:D:3389:GLU:O	2.38	0.41
1:D:3391:GLU:O	1:D:3395:ARG:HD2	2.19	0.41
1:D:3409:TYR:N	1:D:3410:PRO:HD2	2.35	0.41
1:D:3997:ALA:HB1	1:D:4057:MET:SD	2.60	0.41
1:D:4024:VAL:HG11	1:D:4142:ASN:HB3	2.02	0.41
1:D:4705:VAL:HG23	1:D:4775:TYR:HD2	1.85	0.41
1:C:1992:ALA:O	1:C:1995:THR:OG1	2.29	0.41
1:C:2182:ILE:CG2	1:C:2186:MET:HE3	2.50	0.41
1:C:2441:HIS:CE1	1:C:2442:LEU:HD12	2.55	0.41
1:C:3239:MET:CB	1:C:3239:MET:HG3	2.31	0.41
1:C:4024:VAL:HG11	1:C:4142:ASN:HB3	2.02	0.41
1:A:292:ALA:HB2	1:A:312:THR:HG22	2.02	0.41
1:A:399:GLN:O	1:A:403:MET:HG3	2.21	0.41
1:A:1085:SER:N	1:A:1155:LEU:HD22	2.35	0.41
1:A:1568:LYS:HB2	1:A:1572:ILE:O	2.20	0.41
1:A:1727:ARG:O	1:A:1731:LEU:HG	2.20	0.41
1:A:2185:ILE:HG21	1:A:2203:MET:HE1	2.01	0.41
1:A:2208:MET:O	1:A:2212:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2625:ARG:O	1:A:2628:PHE:HB3	2.21	0.41
1:A:4069:LYS:O	1:A:4072:VAL:HG22	2.20	0.41
1:A:4187:SER:O	1:A:4188:ARG:HB2	2.20	0.41
1:B:1999:ARG:NH1	1:B:3636:PHE:CD1	2.76	0.41
1:B:2313:LEU:HB3	1:B:2318:TYR:HB2	2.02	0.41
1:B:2374:SER:OG	1:B:2378:ALA:HB3	2.21	0.41
1:B:2444:GLN:OE1	1:B:2444:GLN:N	2.54	0.41
1:B:3478:MET:O	1:B:3478:MET:HG3	2.19	0.41
1:B:3583:GLU:HB3	1:B:3585:ASP:OD1	2.19	0.41
1:B:3610:GLU:OE1	1:B:3611:HIS:CD2	2.73	0.41
1:B:3660:ALA:HB3	1:B:3661:TRP:HD1	1.85	0.41
1:B:3673:MET:HE2	1:B:3725:TYR:CE1	2.55	0.41
1:B:4677:LEU:HD23	1:B:4711:PHE:HE1	1.83	0.41
1:B:4946:GLN:O	1:B:4950:VAL:HG23	2.19	0.41
1:D:2202:GLY:HA2	1:D:2205:GLU:OE1	2.20	0.41
1:D:2700:MET:O	1:D:2702:CYS:SG	2.78	0.41
1:D:3899:PHE:CE2	1:D:3903:LEU:HD11	2.55	0.41
1:D:4901:ILE:HG13	1:D:4913:ARG:NH2	2.34	0.41
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	2.03	0.41
1:C:2703:LEU:HD22	1:C:2706:ILE:HD12	2.02	0.41
1:C:3071:LEU:O	1:C:3075:LEU:HG	2.19	0.41
1:C:3148:ALA:O	1:C:3151:GLN:NE2	2.53	0.41
1:C:3610:GLU:OE1	1:C:3611:HIS:CD2	2.73	0.41
1:C:3628:ARG:HH11	1:C:3632:VAL:HG11	1.85	0.41
1:C:3899:PHE:CE2	1:C:3903:LEU:HD11	2.55	0.41
1:C:4677:LEU:HD23	1:C:4711:PHE:HE1	1.83	0.41
1:C:5000:GLU:HA	1:C:5003:HIS:CD2	2.56	0.41
1:A:501:ALA:O	1:A:505:GLU:HG3	2.20	0.41
1:A:516:LYS:O	1:A:519:VAL:HG22	2.20	0.41
1:A:873:LYS:O	1:A:876:GLU:HG2	2.20	0.41
1:A:2487:GLN:NE2	1:A:2545:GLU:OE1	2.53	0.41
1:A:2977:LEU:HD23	1:A:3056:LEU:HD11	2.02	0.41
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	2.02	0.41
1:A:3137:LEU:HD23	1:A:3189:ALA:CB	2.50	0.41
2:F:4:VAL:HG22	2:F:74:LEU:HD22	2.03	0.41
1:B:501:ALA:O	1:B:505:GLU:HG3	2.20	0.41
1:B:926:GLY:O	1:B:930:LYS:HG3	2.20	0.41
1:B:1084:GLN:C	1:B:1155:LEU:HD22	2.44	0.41
1:B:1552:VAL:HG11	1:B:1562:ILE:HD13	2.02	0.41
1:B:1992:ALA:O	1:B:1995:THR:OG1	2.29	0.41
1:B:2452:ARG:HG3	1:C:175:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2545:GLU:HG2	1:B:2546:MET:N	2.35	0.41
1:D:399:GLN:O	1:D:403:MET:HG3	2.21	0.41
1:D:1088:TRP:O	1:D:1152:MET:HA	2.21	0.41
1:D:2638:LYS:C	1:D:2698:MET:HE2	2.45	0.41
1:D:2725:LYS:HE3	1:D:2734:ASN:O	2.19	0.41
1:D:3879:GLU:HG2	1:D:3880:PHE:N	2.34	0.41
1:C:2045:GLN:C	1:C:2046:LEU:HD12	2.45	0.41
1:C:3130:THR:O	1:C:3134:VAL:HG23	2.19	0.41
1:C:3386:GLU:O	1:C:3389:GLU:O	2.38	0.41
1:C:3633:VAL:O	1:C:3637:ARG:HD3	2.20	0.41
1:C:4069:LYS:O	1:C:4072:VAL:HG22	2.20	0.41
1:C:4070:ASP:OD1	1:C:4070:ASP:C	2.63	0.41
1:C:4187:SER:O	1:C:4188:ARG:HB2	2.20	0.41
1:C:4901:ILE:HG13	1:C:4913:ARG:NH2	2.34	0.41
1:A:156:GLN:HE22	1:D:385:ASP:CG	2.27	0.41
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	2.03	0.41
1:A:2182:ILE:CG2	1:A:2186:MET:HE3	2.50	0.41
1:A:2330:ARG:HA	1:A:2333:ASP:OD1	2.21	0.41
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.51	0.41
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.85	0.41
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.35	0.41
1:A:3435:PHE:CD2	1:A:3524:MET:CE	3.03	0.41
1:A:3660:ALA:HB3	1:A:3661:TRP:HD1	1.85	0.41
1:A:3891:LEU:HD13	1:A:3899:PHE:HZ	1.79	0.41
1:A:4179:GLY:CA	1:A:4197:ILE:HD11	2.50	0.41
1:B:125:ARG:NH1	1:B:125:ARG:CB	2.84	0.41
1:B:221:ARG:NH1	1:B:255:HIS:O	2.54	0.41
1:B:869:ARG:NH2	1:B:947:GLU:OE2	2.52	0.41
1:B:1143:TRP:HB2	1:B:1147:ASP:HB2	2.01	0.41
1:B:1265:ASP:OD1	1:B:1266:THR:N	2.53	0.41
1:B:2182:ILE:CG2	1:B:2186:MET:HE3	2.50	0.41
1:B:2612[B]:ARG:NH1	1:B:2613:TYR:OH	2.53	0.41
1:B:2625:ARG:O	1:B:2628:PHE:HB3	2.21	0.41
1:B:3294:PRO:HB2	1:B:3297:PRO:HD2	2.01	0.41
1:B:3458:PHE:CE2	1:B:3464:ILE:HD11	2.54	0.41
1:B:4705:VAL:HG23	1:B:4775:TYR:CD2	2.56	0.41
1:D:885:THR:HA	1:D:888:GLU:OE1	2.20	0.41
1:D:1568:LYS:HB2	1:D:1572:ILE:O	2.21	0.41
1:D:2117:VAL:O	1:D:2120:MET:HG2	2.21	0.41
1:D:2865:VAL:HG11	1:D:2928:LYS:HE2	2.02	0.41
1:D:3380:ARG:NH1	1:D:3391:GLU:OE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3559:LEU:O	1:D:3560:GLN:C	2.61	0.41
1:C:125:ARG:NH1	1:C:125:ARG:CB	2.84	0.41
1:C:2330:ARG:HA	1:C:2333:ASP:OD1	2.21	0.41
1:C:2916:LYS:O	1:C:2917:ALA:C	2.64	0.41
1:C:3077:ALA:O	1:C:3081:MET:HG2	2.20	0.41
1:C:3103:ILE:O	1:C:3107:VAL:HG13	2.20	0.41
1:C:3380:ARG:NH2	1:C:3391:GLU:OE2	2.52	0.41
1:C:3997:ALA:HB1	1:C:4057:MET:SD	2.60	0.41
1:C:4767:TRP:CE3	1:C:4768:LEU:CD2	2.99	0.41
1:A:631:LEU:HD23	1:A:631:LEU:HA	1.96	0.41
1:A:820:ARG:CZ	1:A:820:ARG:CB	2.80	0.41
1:A:973:SER:O	1:A:976:ARG:NH2	2.54	0.41
1:A:1286:MET:HE2	1:A:1464:PHE:HB3	2.02	0.41
1:A:1819:VAL:HG22	1:A:1926:LEU:HD21	2.03	0.41
1:A:2476:ILE:HD11	1:A:2536:LEU:HG	2.03	0.41
1:A:2894:LEU:O	1:A:2897:LYS:HG2	2.21	0.41
1:A:2946:LEU:N	1:A:2948:THR:HG23	2.35	0.41
1:A:2969:ILE:O	1:A:2973:PHE:HD1	2.03	0.41
1:A:3197:LEU:HD23	1:A:3197:LEU:O	2.20	0.41
2:H:90:ILE:HD11	1:D:1684:ALA:HA	2.02	0.41
2:F:11:ASP:OD2	2:F:11:ASP:C	2.64	0.41
1:B:399:GLN:O	1:B:403:MET:HG3	2.21	0.41
1:B:975:VAL:HG11	1:B:1044:ARG:HA	2.03	0.41
1:B:2638:LYS:C	1:B:2698:MET:HE2	2.45	0.41
1:B:3434:LEU:O	1:B:3438:VAL:HG13	2.21	0.41
1:B:3729:MET:HB3	1:B:3770:LEU:HD11	2.03	0.41
1:B:3899:PHE:CE2	1:B:3903:LEU:HD11	2.55	0.41
1:B:3899:PHE:HE2	1:B:3903:LEU:HD11	1.85	0.41
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	2.03	0.41
1:D:2045:GLN:C	1:D:2046:LEU:HD12	2.45	0.41
1:D:2182:ILE:CG2	1:D:2186:MET:HE3	2.50	0.41
1:D:2444:GLN:OE1	1:D:2444:GLN:N	2.54	0.41
1:D:2946:LEU:N	1:D:2948:THR:HG23	2.35	0.41
1:D:2977:LEU:HD23	1:D:3056:LEU:HD11	2.02	0.41
1:D:2986:VAL:O	1:D:2986:VAL:HG13	2.19	0.41
1:D:3628:ARG:HH11	1:D:3632:VAL:HG11	1.85	0.41
1:D:3633:VAL:O	1:D:3637:ARG:HD3	2.20	0.41
1:D:3673:MET:HE2	1:D:3725:TYR:CE1	2.55	0.41
1:D:3916:ILE:H	1:D:3916:ILE:HD12	1.85	0.41
1:D:4989:MET:O	1:D:4993:MET:HG3	2.21	0.41
1:C:2202:GLY:HA2	1:C:2205:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2495:VAL:HG22	1:C:2498:HIS:CE1	2.55	0.41
1:C:3409:TYR:N	1:C:3410:PRO:HD2	2.35	0.41
1:A:484:LEU:CD1	1:A:526:LEU:CD1	2.98	0.41
1:A:1552:VAL:HG11	1:A:1562:ILE:HD13	2.03	0.41
1:A:2117:VAL:O	1:A:2120:MET:HG2	2.21	0.41
1:A:2513:GLU:OE1	1:A:2513:GLU:N	2.54	0.41
1:A:2916:LYS:O	1:A:2917:ALA:C	2.64	0.41
1:A:3077:ALA:O	1:A:3081:MET:HG2	2.20	0.41
1:A:3899:PHE:CE2	1:A:3903:LEU:HD11	2.55	0.41
1:B:69:LEU:CD2	1:B:109:LEU:HD21	2.50	0.41
1:B:961:MET:HE1	1:B:963:ASN:CG	2.41	0.41
1:B:1085:SER:N	1:B:1155:LEU:HD22	2.35	0.41
1:B:1568:LYS:HB2	1:B:1572:ILE:O	2.21	0.41
1:B:1973:GLN:NE2	1:B:2005:GLN:OE1	2.44	0.41
1:B:2135:LEU:HD12	1:B:3658:LYS:HG3	2.02	0.41
1:B:2330:ARG:HA	1:B:2333:ASP:OD1	2.21	0.41
1:B:2819:TRP:C	1:B:2820:GLU:HG3	2.46	0.41
1:B:3137:LEU:HD23	1:B:3189:ALA:CB	2.50	0.41
1:B:3197:LEU:HD23	1:B:3197:LEU:O	2.20	0.41
1:B:3499:ARG:HD3	1:B:3499:ARG:C	2.46	0.41
1:B:3891:LEU:HD13	1:B:3899:PHE:HZ	1.79	0.41
1:B:4070:ASP:OD1	1:B:4070:ASP:C	2.63	0.41
1:B:4930:ALA:CA	1:B:4933:GLN:OE1	2.69	0.41
1:D:278:GLN:HG3	1:D:328:LYS:NZ	2.35	0.41
1:D:501:ALA:O	1:D:505:GLU:HG3	2.20	0.41
1:D:869:ARG:NH2	1:D:947:GLU:OE2	2.52	0.41
1:D:973:SER:O	1:D:976:ARG:NH2	2.54	0.41
1:D:2135:LEU:HD12	1:D:3658:LYS:HG3	2.02	0.41
1:D:2330:ARG:HA	1:D:2333:ASP:OD1	2.21	0.41
1:D:2667:THR:HG21	1:D:2672:LEU:HG	2.02	0.41
1:D:2916:LYS:O	1:D:2917:ALA:C	2.64	0.41
1:D:3071:LEU:O	1:D:3075:LEU:HG	2.19	0.41
1:D:3103:ILE:O	1:D:3107:VAL:HG13	2.20	0.41
1:D:3499:ARG:HD3	1:D:3499:ARG:C	2.46	0.41
1:D:4161:ARG:HH11	1:D:4161:ARG:HD2	1.54	0.41
1:D:4563:ARG:NH2	1:D:4815:ASP:OD1	2.53	0.41
1:C:887:ILE:HD13	1:C:887:ILE:HA	1.87	0.41
1:C:1021:LEU:HD23	1:C:1021:LEU:O	2.21	0.41
1:C:3465:ASN:OD1	1:C:3467:MET:CG	2.60	0.41
1:C:3604:TYR:CD1	1:C:3604:TYR:C	2.98	0.41
1:C:3660:ALA:O	1:C:3664:THR:OG1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLY:O	1:D:3984:ARG:NH1	2.49	0.41
1:A:278:GLN:HG3	1:A:328:LYS:NZ	2.35	0.41
1:A:1088:TRP:O	1:A:1152:MET:HA	2.21	0.41
1:A:1105:ALA:O	1:A:1189:LEU:N	2.50	0.41
1:A:1805:GLU:O	1:A:1808:ARG:HG2	2.21	0.41
1:A:2442:LEU:HD23	1:A:2447:LYS:CE	2.51	0.41
1:A:2819:TRP:C	1:A:2820:GLU:HG3	2.46	0.41
1:A:2905:LEU:HD23	1:A:2905:LEU:HA	1.98	0.41
1:A:3103:ILE:O	1:A:3107:VAL:HG13	2.20	0.41
1:A:3434:LEU:O	1:A:3438:VAL:HG13	2.21	0.41
1:B:2001:PRO:O	1:B:2005:GLN:HG3	2.20	0.41
1:B:2699:ALA:O	1:B:2702:CYS:HB3	2.21	0.41
1:B:3321:ARG:HA	1:B:3324:VAL:HG22	2.02	0.41
1:B:4063:ASP:OD1	1:B:4063:ASP:C	2.64	0.41
1:B:4999:ASP:OD1	1:B:5000:GLU:N	2.53	0.41
1:B:5000:GLU:HA	1:B:5003:HIS:CD2	2.56	0.41
1:D:468:LEU:O	1:D:472:ARG:HG2	2.20	0.41
1:D:484:LEU:CD1	1:D:526:LEU:CD1	2.98	0.41
1:D:553:ARG:O	1:D:557:SER:OG	2.29	0.41
1:D:926:GLY:O	1:D:930:LYS:HG3	2.20	0.41
1:D:1436:SER:OG	1:D:1565:GLU:HB2	2.20	0.41
1:D:1805:GLU:O	1:D:1808:ARG:HG2	2.21	0.41
1:D:1973:GLN:NE2	1:D:2005:GLN:OE1	2.44	0.41
1:D:2628:PHE:CZ	1:D:2734:ASN:CG	2.94	0.41
1:D:2703:LEU:HD22	1:D:2706:ILE:HD12	2.02	0.41
1:D:3077:ALA:O	1:D:3081:MET:HG2	2.20	0.41
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.85	0.41
1:D:3435:PHE:CD2	1:D:3524:MET:CE	3.03	0.41
1:D:3604:TYR:O	1:D:3608:GLN:OE1	2.39	0.41
1:D:4179:GLY:HA3	1:D:4197:ILE:HD11	2.02	0.41
1:D:4767:TRP:HE3	1:D:4768:LEU:HD23	1.80	0.41
1:D:5000:GLU:HA	1:D:5003:HIS:CD2	2.56	0.41
1:C:874:LEU:HD21	1:C:1046:LEU:HG	2.03	0.41
1:C:885:THR:HA	1:C:888:GLU:OE1	2.20	0.41
1:C:1085:SER:N	1:C:1155:LEU:HD22	2.35	0.41
1:C:1568:LYS:HB2	1:C:1572:ILE:O	2.20	0.41
1:C:2374:SER:OG	1:C:2378:ALA:HB3	2.20	0.41
1:C:3111:ARG:HH21	1:C:3178:THR:CB	2.33	0.41
1:C:3197:LEU:CD2	1:C:3201:MET:HE3	2.41	0.41
1:C:3336:LYS:HG3	1:C:3337:ARG:N	2.36	0.41
1:C:4705:VAL:HG23	1:C:4775:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4989:MET:O	1:C:4993:MET:HG3	2.21	0.41
1:A:69:LEU:CD2	1:A:109:LEU:HD21	2.50	0.41
1:A:117:TYR:O	1:A:138:GLN:N	2.51	0.41
1:A:160:GLY:O	1:D:3984:ARG:NH2	2.52	0.41
1:A:823:LEU:HD13	1:A:1626:TRP:CE3	2.56	0.41
1:A:926:GLY:O	1:A:930:LYS:HG3	2.20	0.41
1:A:943:ASP:CG	1:A:946:ALA:HB3	2.46	0.41
1:A:1021:LEU:O	1:A:1021:LEU:HD23	2.21	0.41
1:A:2202:GLY:HA2	1:A:2205:GLU:OE1	2.20	0.41
1:A:2253:HIS:O	1:A:2254:LEU:C	2.63	0.41
1:A:2261:SER:O	1:A:2262:GLY:C	2.64	0.41
1:A:2313:LEU:HB3	1:A:2318:TYR:HB2	2.02	0.41
1:A:2725:LYS:HE3	1:A:2734:ASN:O	2.19	0.41
1:A:2865:VAL:HG11	1:A:2928:LYS:HE2	2.02	0.41
1:A:3336:LYS:HG3	1:A:3337:ARG:N	2.36	0.41
1:A:3384:LYS:H	1:A:3387:ALA:HB3	1.86	0.41
1:A:3458:PHE:HE2	1:A:3464:ILE:HD11	1.82	0.41
1:A:3573:MET:CB	1:A:3577:ARG:NH1	2.73	0.41
1:A:3604:TYR:O	1:A:3608:GLN:OE1	2.39	0.41
1:A:3628:ARG:HH11	1:A:3632:VAL:HG11	1.85	0.41
1:A:3633:VAL:O	1:A:3637:ARG:HD3	2.20	0.41
1:A:3969:ILE:HD11	1:A:4029:SER:HB2	2.02	0.41
1:A:4024:VAL:HG11	1:A:4142:ASN:HB3	2.02	0.41
1:A:4839:MET:CE	1:D:4820:VAL:HG11	2.50	0.41
1:A:5000:GLU:HA	1:A:5003:HIS:CD2	2.56	0.41
2:H:24:VAL:HG21	2:H:59:TRP:HZ3	1.85	0.41
1:B:117:TYR:O	1:B:138:GLN:N	2.51	0.41
1:B:365:LYS:HD3	1:B:369:LEU:HD21	2.03	0.41
1:B:823:LEU:HD13	1:B:1626:TRP:CE3	2.56	0.41
1:B:885:THR:HA	1:B:888:GLU:OE1	2.21	0.41
1:B:973:SER:O	1:B:976:ARG:NH2	2.54	0.41
1:B:985:VAL:HG13	1:B:1039:LEU:HD23	2.00	0.41
1:B:2185:ILE:HG21	1:B:2203:MET:HE1	2.01	0.41
1:B:2441:HIS:CE1	1:B:2442:LEU:HD12	2.55	0.41
1:B:2442:LEU:HD23	1:B:2447:LYS:CE	2.51	0.41
1:B:2476:ILE:HD11	1:B:2536:LEU:HG	2.02	0.41
1:B:2946:LEU:N	1:B:2948:THR:HG23	2.35	0.41
1:B:2969:ILE:O	1:B:2973:PHE:HD1	2.02	0.41
1:B:3062:PRO:O	1:B:3065:VAL:HG22	2.21	0.41
1:B:3101:GLU:HA	1:B:3104:GLU:OE1	2.21	0.41
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3282:PRO:C	1:B:3286:GLU:OE1	2.63	0.41
1:B:3384:LYS:H	1:B:3387:ALA:HB3	1.86	0.41
1:B:3386:GLU:O	1:B:3389:GLU:O	2.38	0.41
1:B:3628:ARG:HH11	1:B:3632:VAL:HG11	1.85	0.41
1:B:3868:ARG:HG2	1:B:3869:GLN:N	2.34	0.41
1:B:3969:ILE:HD11	1:B:4029:SER:HB2	2.02	0.41
1:D:130:LYS:NZ	1:C:2373:GLY:O	2.50	0.41
1:D:874:LEU:HD21	1:D:1046:LEU:HG	2.03	0.41
1:D:877:ASN:O	1:D:880:GLU:CG	2.69	0.41
1:D:1712:TYR:CG	1:D:1840:PRO:HB3	2.56	0.41
1:D:2374:SER:OG	1:D:2378:ALA:HB3	2.21	0.41
1:D:2442:LEU:HD23	1:D:2447:LYS:CE	2.51	0.41
1:D:2487:GLN:NE2	1:D:2545:GLU:OE1	2.53	0.41
1:D:3111:ARG:O	1:D:3112:LEU:HB2	2.20	0.41
1:D:3111:ARG:HH21	1:D:3178:THR:CB	2.33	0.41
1:D:3380:ARG:NH2	1:D:3391:GLU:OE2	2.52	0.41
1:D:3434:LEU:O	1:D:3438:VAL:HG13	2.21	0.41
1:D:3545:THR:HG23	1:D:3548:GLU:H	1.86	0.41
1:D:4063:ASP:OD1	1:D:4063:ASP:C	2.64	0.41
1:D:4705:VAL:HG23	1:D:4775:TYR:CD2	2.56	0.41
1:C:399:GLN:O	1:C:403:MET:HG3	2.21	0.41
1:C:985:VAL:HG13	1:C:1039:LEU:HD23	2.00	0.41
1:C:1088:TRP:O	1:C:1152:MET:HA	2.21	0.41
1:C:2442:LEU:HD23	1:C:2447:LYS:CE	2.51	0.41
1:C:2444:GLN:OE1	1:C:2444:GLN:N	2.53	0.41
1:C:2625:ARG:O	1:C:2628:PHE:HB3	2.21	0.41
1:C:2762:THR:HA	1:C:2765:LYS:HE2	2.03	0.41
1:C:2928:LYS:O	1:C:2932:MET:HE3	2.21	0.41
1:C:3062:PRO:O	1:C:3065:VAL:HG22	2.21	0.41
1:C:3101:GLU:HA	1:C:3104:GLU:OE1	2.21	0.41
1:C:3111:ARG:O	1:C:3112:LEU:HB2	2.20	0.41
1:C:3434:LEU:O	1:C:3438:VAL:HG13	2.21	0.41
1:A:221:ARG:NH1	1:A:255:HIS:O	2.54	0.41
1:A:1926:LEU:HA	1:A:1929:MET:SD	2.61	0.41
1:A:2369[B]:ARG:HD3	1:A:2369[B]:ARG:HA	1.92	0.41
1:A:2441:HIS:CE1	1:A:2442:LEU:HD12	2.55	0.41
1:A:3545:THR:HG23	1:A:3548:GLU:H	1.86	0.41
1:A:4063:ASP:OD1	1:A:4063:ASP:C	2.64	0.41
1:A:4705:VAL:HG23	1:A:4775:TYR:CD2	2.56	0.41
1:B:866:HIS:CD2	1:B:867:LEU:CD2	3.04	0.41
1:B:1980:LEU:HD21	1:B:1995:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2762:THR:HA	1:B:2765:LYS:HE2	2.03	0.41
1:B:2792:ARG:HB3	1:B:2793:PRO:HD2	2.03	0.41
1:D:943:ASP:CG	1:D:946:ALA:HB3	2.46	0.41
1:D:975:VAL:HG11	1:D:1044:ARG:HA	2.03	0.41
1:D:1241:SER:HA	1:D:1603:VAL:HG22	2.03	0.41
1:D:1478:ASP:HB2	1:D:1484:HIS:CE1	2.56	0.41
1:D:1748:PHE:HA	1:D:1749:PRO:HD3	1.92	0.41
1:D:2625:ARG:O	1:D:2628:PHE:HB3	2.21	0.41
1:D:3336:LYS:HG3	1:D:3337:ARG:N	2.36	0.41
1:D:3666:ASP:OD1	1:D:3666:ASP:O	2.39	0.41
1:C:501:ALA:O	1:C:505:GLU:HG3	2.20	0.41
1:C:516:LYS:O	1:C:519:VAL:HG22	2.20	0.41
1:C:615:ARG:NH2	1:C:1676:LEU:O	2.50	0.41
1:C:879:HIS:HE1	1:C:913:LEU:HD13	1.86	0.41
1:C:973:SER:O	1:C:976:ARG:NH2	2.54	0.41
1:C:1241:SER:HA	1:C:1603:VAL:HG22	2.03	0.41
1:C:1712:TYR:CG	1:C:1840:PRO:HB3	2.56	0.41
1:C:2253:HIS:O	1:C:2254:LEU:C	2.63	0.41
1:C:2638:LYS:C	1:C:2698:MET:HE2	2.45	0.41
1:C:3244:PRO:HD2	1:C:3249:LEU:HD21	2.03	0.41
1:C:3282:PRO:C	1:C:3286:GLU:OE1	2.63	0.41
1:C:3899:PHE:HE2	1:C:3903:LEU:HD11	1.85	0.41
1:C:4705:VAL:HG23	1:C:4775:TYR:HD2	1.85	0.41
1:A:125:ARG:NH1	1:A:125:ARG:CB	2.84	0.40
1:A:515:TRP:O	1:A:519:VAL:HG13	2.21	0.40
1:A:1241:SER:HA	1:A:1603:VAL:HG22	2.03	0.40
1:A:3101:GLU:HA	1:A:3104:GLU:OE1	2.21	0.40
1:A:3111:ARG:HH21	1:A:3178:THR:CB	2.33	0.40
1:A:3666:ASP:O	1:A:3666:ASP:OD1	2.40	0.40
1:A:3729:MET:HB3	1:A:3770:LEU:HD11	2.03	0.40
1:A:3868:ARG:HG2	1:A:3869:GLN:N	2.34	0.40
1:A:4748:LEU:O	1:A:4751:THR:OG1	2.35	0.40
1:A:4876:CYS:HA	1:A:4882:CYS:HB2	2.04	0.40
2:E:4:VAL:HG22	2:E:74:LEU:HD22	2.03	0.40
2:G:11:ASP:OD2	2:G:11:ASP:C	2.64	0.40
2:G:50:LEU:HA	2:G:50:LEU:HD12	1.89	0.40
1:B:1478:ASP:HB2	1:B:1484:HIS:CE1	2.56	0.40
1:B:1984:PHE:HA	1:B:1991:THR:HG21	2.03	0.40
1:B:2784:GLU:OE2	1:B:2785:LEU:HD12	2.21	0.40
1:B:3302:PRO:HA	1:B:3303:PRO:HD3	2.00	0.40
1:D:721:LEU:CD1	1:D:1476:MET:HE1	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:HIS:NE2	1:D:742:ASP:OD2	2.55	0.40
1:D:1286:MET:HE2	1:D:1464:PHE:HB3	2.02	0.40
1:D:2319:PRO:HG2	1:D:2392:ARG:HA	2.03	0.40
1:D:3062:PRO:O	1:D:3065:VAL:HG22	2.21	0.40
1:D:3244:PRO:HD2	1:D:3249:LEU:HD21	2.03	0.40
1:D:4187:SER:O	1:D:4188:ARG:HB2	2.20	0.40
1:C:221:ARG:NH1	1:C:255:HIS:O	2.54	0.40
1:C:626:LEU:N	1:C:627:PRO:HD2	2.37	0.40
1:C:820:ARG:CZ	1:C:820:ARG:CB	2.80	0.40
1:C:869:ARG:NH2	1:C:947:GLU:OE2	2.52	0.40
1:C:1819:VAL:HG22	1:C:1926:LEU:HD21	2.03	0.40
1:C:1856:ASP:O	1:C:1860:LYS:HG3	2.21	0.40
1:C:3321:ARG:HA	1:C:3324:VAL:HG22	2.02	0.40
1:C:3604:TYR:CE1	1:C:3608:GLN:CD	3.00	0.40
1:C:3868:ARG:HG2	1:C:3869:GLN:N	2.34	0.40
1:A:1008:SER:HB3	1:A:1017:ARG:HB3	2.03	0.40
1:A:2319:PRO:HG2	1:A:2392:ARG:HA	2.03	0.40
1:A:2628:PHE:CZ	1:A:2734:ASN:CG	2.94	0.40
1:A:2699:ALA:O	1:A:2702:CYS:HB3	2.21	0.40
1:A:3499:ARG:C	1:A:3499:ARG:HD3	2.46	0.40
1:A:3622:LYS:HB2	1:A:3625:SER:HB3	2.03	0.40
1:A:3916:ILE:H	1:A:3916:ILE:HD12	1.85	0.40
1:A:4989:MET:O	1:A:4993:MET:HG3	2.21	0.40
1:B:891:TRP:CE3	1:B:903:LEU:HA	2.56	0.40
1:B:1021:LEU:O	1:B:1021:LEU:HD23	2.21	0.40
1:B:2319:PRO:HG2	1:B:2392:ARG:HA	2.03	0.40
1:B:2894:LEU:O	1:B:2897:LYS:HG2	2.21	0.40
1:B:3604:TYR:CE1	1:B:3608:GLN:CD	3.00	0.40
1:B:4024:VAL:HG11	1:B:4142:ASN:HB3	2.03	0.40
1:D:125:ARG:NH1	1:D:125:ARG:CB	2.84	0.40
1:D:906:CYS:HA	1:D:914:PRO:HD3	2.04	0.40
1:D:1984:PHE:HA	1:D:1991:THR:HG21	2.03	0.40
1:D:2001:PRO:O	1:D:2005:GLN:HG3	2.20	0.40
1:D:2476:ILE:HD11	1:D:2536:LEU:HG	2.03	0.40
1:D:3183:VAL:HG12	1:D:3187:ARG:HE	1.87	0.40
1:C:309:THR:O	1:C:309:THR:CG2	2.68	0.40
1:C:1286:MET:HE2	1:C:1464:PHE:HB3	2.02	0.40
1:C:2513:GLU:OE1	1:C:2513:GLU:N	2.54	0.40
1:C:2699:ALA:O	1:C:2702:CYS:HB3	2.21	0.40
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.86	0.40
1:C:3916:ILE:H	1:C:3916:ILE:HD12	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:O	1:A:309:THR:CG2	2.68	0.40
1:A:941:MET:HE1	1:A:1051:TYR:CD2	2.46	0.40
1:A:2135:LEU:HD12	1:A:3658:LYS:HG3	2.02	0.40
1:A:2240:CYS:SG	1:A:2250:MET:HG3	2.62	0.40
1:A:2784:GLU:OE2	1:A:2785:LEU:HD12	2.21	0.40
1:A:3458:PHE:CE2	1:A:3464:ILE:HD11	2.54	0.40
1:B:221:ARG:NE	1:B:253:CYS:O	2.55	0.40
1:B:515:TRP:O	1:B:519:VAL:HG13	2.21	0.40
1:B:736:HIS:NE2	1:B:742:ASP:OD2	2.55	0.40
1:B:993:HIS:NE2	1:B:1022:VAL:O	2.53	0.40
1:B:1241:SER:HA	1:B:1603:VAL:HG22	2.03	0.40
1:B:1926:LEU:HA	1:B:1929:MET:SD	2.61	0.40
1:B:2117:VAL:O	1:B:2120:MET:HG2	2.21	0.40
1:B:2240:CYS:SG	1:B:2250:MET:HG3	2.62	0.40
1:B:2513:GLU:N	1:B:2513:GLU:OE1	2.54	0.40
1:B:2928:LYS:O	1:B:2932:MET:HE3	2.21	0.40
1:B:3111:ARG:O	1:B:3112:LEU:HB2	2.20	0.40
1:B:3336:LYS:HG3	1:B:3337:ARG:N	2.36	0.40
1:B:3409:TYR:N	1:B:3410:PRO:HD2	2.35	0.40
1:D:870:ILE:HD12	1:D:870:ILE:HA	1.98	0.40
1:D:993:HIS:NE2	1:D:1022:VAL:O	2.53	0.40
1:D:1926:LEU:HA	1:D:1929:MET:SD	2.61	0.40
1:D:2240:CYS:SG	1:D:2250:MET:HG3	2.62	0.40
1:D:2969:ILE:O	1:D:2973:PHE:HD1	2.02	0.40
1:D:3003:LEU:HB2	1:D:3004:PRO:HD3	2.02	0.40
1:D:3532:LEU:HD23	1:D:3535:LEU:HD12	2.03	0.40
1:D:4003:LEU:HA	1:D:4009:GLN:OE1	2.22	0.40
1:C:891:TRP:CE3	1:C:903:LEU:HA	2.57	0.40
1:C:893:TYR:CD1	1:C:907:LEU:O	2.75	0.40
1:C:893:TYR:HD1	1:C:907:LEU:O	2.03	0.40
1:C:2476:ILE:HD11	1:C:2536:LEU:HG	2.03	0.40
1:C:3499:ARG:C	1:C:3499:ARG:HD3	2.46	0.40
1:C:3532:LEU:HD23	1:C:3535:LEU:HD12	2.02	0.40
1:A:350:HIS:O	1:A:354:GLY:N	2.49	0.40
1:A:874:LEU:HD21	1:A:1046:LEU:HG	2.03	0.40
1:A:975:VAL:HG11	1:A:1044:ARG:HA	2.03	0.40
1:A:1478:ASP:HB2	1:A:1484:HIS:CE1	2.56	0.40
1:A:1712:TYR:CG	1:A:1840:PRO:HB3	2.56	0.40
1:A:2630:VAL:N	1:A:2631:PRO:CD	2.85	0.40
1:A:3239:MET:CB	1:A:3239:MET:HG3	2.31	0.40
1:A:4710:SER:O	1:A:4711:PHE:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:ASP:CG	1:C:156:GLN:HE22	2.30	0.40
1:B:4844:LEU:O	1:B:4847:VAL:HG22	2.21	0.40
1:B:4989:MET:O	1:B:4993:MET:HG3	2.21	0.40
1:D:167:ASP:N	1:C:384:MET:SD	2.95	0.40
1:D:823:LEU:HD13	1:D:1626:TRP:CE3	2.56	0.40
1:D:899:ASP:O	1:D:902:ARG:NE	2.45	0.40
1:D:2253:HIS:O	1:D:2254:LEU:C	2.63	0.40
1:D:3197:LEU:HD21	1:D:3201:MET:CE	2.44	0.40
1:D:3969:ILE:HD11	1:D:4029:SER:HB2	2.02	0.40
1:D:4666:VAL:N	1:D:4667:PRO:CD	2.85	0.40
1:D:4844:LEU:O	1:D:4847:VAL:HG22	2.21	0.40
1:C:866:HIS:CD2	1:C:867:LEU:CD2	3.04	0.40
1:C:1805:GLU:O	1:C:1808:ARG:HG2	2.21	0.40
1:C:2319:PRO:HG2	1:C:2392:ARG:HA	2.03	0.40
1:C:2520:HIS:HA	1:C:2523:ASP:OD2	2.22	0.40
1:C:2784:GLU:OE2	1:C:2785:LEU:HD12	2.21	0.40
1:C:2819:TRP:C	1:C:2820:GLU:HG3	2.46	0.40
1:C:3003:LEU:HB2	1:C:3004:PRO:HD3	2.02	0.40
1:C:3545:THR:HG23	1:C:3548:GLU:H	1.86	0.40
1:C:3729:MET:HB3	1:C:3770:LEU:HD11	2.03	0.40
1:A:736:HIS:NE2	1:A:742:ASP:OD2	2.55	0.40
1:A:866:HIS:CD2	1:A:867:LEU:CD2	3.04	0.40
1:A:891:TRP:CE3	1:A:903:LEU:HA	2.56	0.40
1:A:973:SER:O	1:A:976:ARG:CZ	2.70	0.40
1:A:2165:LEU:HD21	1:A:2177:LEU:HD22	2.04	0.40
1:A:3239:MET:CA	1:A:3239:MET:HG2	2.46	0.40
1:A:4767:TRP:HE3	1:A:4768:LEU:HD23	1.80	0.40
1:A:4848:VAL:HG13	1:A:4886:HIS:HB3	2.03	0.40
1:A:4951:LYS:O	1:A:4955:GLU:OE1	2.40	0.40
1:B:1698:LEU:HD22	1:B:1712:TYR:CE2	2.57	0.40
1:B:2888:ARG:O	1:B:2892:GLN:HG2	2.22	0.40
1:B:3548:GLU:O	1:B:3551:GLU:HG3	2.22	0.40
1:B:3622:LYS:HB2	1:B:3625:SER:HB3	2.03	0.40
1:B:4118:ASP:OD1	1:B:4121:GLU:N	2.55	0.40
1:B:4904:PRO:HB3	1:B:4913:ARG:HD3	2.04	0.40
1:B:4937:ILE:HG12	1:C:4934:GLY:HA2	2.03	0.40
1:D:961:MET:HE1	1:D:963:ASN:CG	2.41	0.40
1:D:2442:LEU:HD23	1:D:2447:LYS:HE3	2.03	0.40
1:D:2784:GLU:OE2	1:D:2785:LEU:HD12	2.21	0.40
1:D:3101:GLU:HA	1:D:3104:GLU:OE1	2.21	0.40
1:D:3604:TYR:CE1	1:D:3608:GLN:CD	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4047:MET:HE3	1:D:4047:MET:HB3	1.99	0.40
1:D:4754:ASN:OD1	1:D:4755:GLU:N	2.55	0.40
1:D:4848:VAL:HG13	1:D:4886:HIS:HB3	2.03	0.40
1:C:278:GLN:HG3	1:C:328:LYS:NZ	2.35	0.40
1:C:365:LYS:HD3	1:C:369:LEU:HD21	2.03	0.40
1:C:943:ASP:CG	1:C:946:ALA:HB3	2.46	0.40
1:C:4003:LEU:HA	1:C:4009:GLN:OE1	2.22	0.40
1:C:4666:VAL:N	1:C:4667:PRO:CD	2.85	0.40
1:C:4743:MET:HE2	1:C:4748:LEU:HD11	2.04	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	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	43	65
1	B	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	43	65
1	C	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	43	65
1	D	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	43	65
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17960/20580 (87%)	17480 (97%)	448 (2%)	32 (0%)	44	65

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	908	VAL

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Mol	Chain	Res	Type
1	A	2829	GLY
1	A	3239	MET
1	A	3300	ALA
1	B	908	VAL
1	B	2829	GLY
1	B	3239	MET
1	B	3300	ALA
1	D	908	VAL
1	D	2829	GLY
1	D	3239	MET
1	D	3300	ALA
1	C	908	VAL
1	C	2829	GLY
1	C	3239	MET
1	C	3300	ALA
1	A	55	ALA
1	A	1930	LYS
1	B	55	ALA
1	B	1930	LYS
1	D	55	ALA
1	D	1930	LYS
1	C	55	ALA
1	C	1930	LYS
1	A	1036	ARG
1	B	1036	ARG
1	D	1036	ARG
1	C	1036	ARG
1	A	361	ALA
1	B	361	ALA
1	D	361	ALA
1	C	361	ALA

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3836/4276 (90%)	3825 (100%)	11 (0%)	86	94
1	B	3836/4276 (90%)	3825 (100%)	11 (0%)	86	94
1	C	3836/4276 (90%)	3824 (100%)	12 (0%)	86	94
1	D	3836/4276 (90%)	3824 (100%)	12 (0%)	86	94
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15700/17464 (90%)	15654 (100%)	46 (0%)	84	94

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	MET
1	A	820	ARG
1	A	1036	ARG
1	A	1559	GLN
1	A	2177	LEU
1	A	2308	GLN
1	A	2444	GLN
1	A	2870[A]	GLU
1	A	2870[B]	GLU
1	A	3014	CYS
1	A	3557	LEU
1	B	384	MET
1	B	820	ARG
1	B	1036	ARG
1	B	1559	GLN
1	B	2177	LEU
1	B	2308	GLN
1	B	2444	GLN
1	B	2870[A]	GLU
1	B	2870[B]	GLU
1	B	3014	CYS
1	B	3557	LEU
1	D	384	MET
1	D	820	ARG

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Mol	Chain	Res	Type
1	D	1036	ARG
1	D	1559	GLN
1	D	2177	LEU
1	D	2308	GLN
1	D	2444	GLN
1	D	2870[A]	GLU
1	D	2870[B]	GLU
1	D	3014	CYS
1	D	3239	MET
1	D	3557	LEU
1	C	384	MET
1	C	820	ARG
1	C	1036	ARG
1	C	1559	GLN
1	C	2177	LEU
1	C	2308	GLN
1	C	2444	GLN
1	C	2870[A]	GLU
1	C	2870[B]	GLU
1	C	3014	CYS
1	C	3239	MET
1	C	3557	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	461	HIS
1	A	720	HIS
1	A	838	HIS
1	A	879	HIS
1	A	889	GLN
1	A	911	HIS
1	A	921	ASN
1	A	1041	GLN
1	A	1130	GLN
1	A	1299	GLN
1	A	1300	HIS
1	A	1688	HIS
1	A	1824	GLN
1	A	1938	GLN
1	A	2011	HIS

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Mol	Chain	Res	Type
1	A	2161	GLN
1	A	2253	HIS
1	A	2324	ASN
1	A	2883	HIS
1	A	2933	ASN
1	A	3030	HIS
1	A	3605	HIS
1	A	3611	HIS
1	A	3867	ASN
1	A	3927	GLN
1	A	3978	GLN
1	A	4043	GLN
1	A	4109	GLN
1	A	4204	GLN
1	A	4650	HIS
1	A	4836	GLN
1	A	5003	HIS
1	B	105	HIS
1	B	461	HIS
1	B	720	HIS
1	B	838	HIS
1	B	879	HIS
1	B	889	GLN
1	B	911	HIS
1	B	921	ASN
1	B	1041	GLN
1	B	1130	GLN
1	B	1299	GLN
1	B	1300	HIS
1	B	1459	GLN
1	B	1688	HIS
1	B	1824	GLN
1	B	1938	GLN
1	B	2011	HIS
1	B	2161	GLN
1	B	2253	HIS
1	B	2324	ASN
1	B	2734	ASN
1	B	2883	HIS
1	B	2933	ASN
1	B	3030	HIS
1	B	3560	GLN

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Mol	Chain	Res	Type
1	B	3605	HIS
1	B	3611	HIS
1	B	3651	ASN
1	B	3867	ASN
1	B	3927	GLN
1	B	3978	GLN
1	B	4043	GLN
1	B	4109	GLN
1	B	4204	GLN
1	B	4650	HIS
1	B	5003	HIS
1	D	105	HIS
1	D	520	ASN
1	D	720	HIS
1	D	838	HIS
1	D	860	GLN
1	D	866	HIS
1	D	879	HIS
1	D	889	GLN
1	D	911	HIS
1	D	1041	GLN
1	D	1130	GLN
1	D	1299	GLN
1	D	1300	HIS
1	D	1688	HIS
1	D	1824	GLN
1	D	1938	GLN
1	D	2011	HIS
1	D	2161	GLN
1	D	2253	HIS
1	D	2324	ASN
1	D	2734	ASN
1	D	2883	HIS
1	D	2933	ASN
1	D	2991	HIS
1	D	3030	HIS
1	D	3605	HIS
1	D	3611	HIS
1	D	3651	ASN
1	D	3867	ASN
1	D	3927	GLN
1	D	3978	GLN

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Mol	Chain	Res	Type
1	D	4043	GLN
1	D	4109	GLN
1	D	4204	GLN
1	D	4650	HIS
1	D	5003	HIS
1	C	105	HIS
1	C	197	GLN
1	C	720	HIS
1	C	838	HIS
1	C	879	HIS
1	C	889	GLN
1	C	911	HIS
1	C	921	ASN
1	C	963	ASN
1	C	1041	GLN
1	C	1130	GLN
1	C	1299	GLN
1	C	1300	HIS
1	C	1688	HIS
1	C	1824	GLN
1	C	1938	GLN
1	C	2011	HIS
1	C	2161	GLN
1	C	2194	HIS
1	C	2253	HIS
1	C	2734	ASN
1	C	2772	GLN
1	C	2883	HIS
1	C	2933	ASN
1	C	3030	HIS
1	C	3605	HIS
1	C	3611	HIS
1	C	3651	ASN
1	C	3867	ASN
1	C	3927	GLN
1	C	3978	GLN
1	C	4043	GLN
1	C	4109	GLN
1	C	4204	GLN
1	C	4650	HIS
1	C	5003	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
6	PNX	A	5304	-	21,21,21	0.38	0	30,30,30	0.53	0
3	ATP	D	5301	-	32,33,33	0.30	0	48,52,52	0.77	2 (4%)
3	ATP	C	5301	-	32,33,33	0.30	0	48,52,52	0.77	2 (4%)
6	PNX	C	5304	-	21,21,21	0.39	0	30,30,30	0.52	0
3	ATP	A	5301	-	32,33,33	0.30	0	48,52,52	0.77	2 (4%)
3	ATP	B	5301	-	32,33,33	0.30	0	48,52,52	0.77	2 (4%)
6	PNX	D	5304	-	21,21,21	0.38	0	30,30,30	0.53	0
6	PNX	B	5304	-	21,21,21	0.38	0	30,30,30	0.53	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
6	PNX	A	5304	-	-	5/7/7/7	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	D	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	6/22/38/38	0/3/3/3
6	PNX	C	5304	-	-	5/7/7/7	0/2/2/2
3	ATP	A	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	6/22/38/38	0/3/3/3
6	PNX	D	5304	-	-	5/7/7/7	0/2/2/2
6	PNX	B	5304	-	-	5/7/7/7	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5301	ATP	O3'-C3'-C4'	-2.09	105.09	111.08
3	C	5301	ATP	O3'-C3'-C4'	-2.07	105.12	111.08
3	A	5301	ATP	O3'-C3'-C4'	-2.07	105.13	111.08
3	B	5301	ATP	O3'-C3'-C4'	-2.06	105.15	111.08
3	C	5301	ATP	O3'-C3'-C2'	-2.05	105.25	111.82
3	B	5301	ATP	O3'-C3'-C2'	-2.05	105.26	111.82
3	A	5301	ATP	O3'-C3'-C2'	-2.05	105.26	111.82
3	D	5301	ATP	O3'-C3'-C2'	-2.04	105.27	111.82

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	PB-O3B-PG-O3G
3	B	5301	ATP	PB-O3B-PG-O3G
3	D	5301	ATP	PB-O3B-PG-O3G
3	C	5301	ATP	PB-O3B-PG-O3G
6	B	5304	PNX	CAH-CAI-CAK-N1
6	D	5304	PNX	CAH-CAI-CAK-N1
6	C	5304	PNX	CAH-CAI-CAK-N1
6	A	5304	PNX	CAH-CAI-CAK-N1
6	A	5304	PNX	CAI-CAH-CAJ-CAM
6	B	5304	PNX	CAI-CAH-CAJ-CAM
6	D	5304	PNX	CAI-CAH-CAJ-CAM
6	C	5304	PNX	CAI-CAH-CAJ-CAM
6	A	5304	PNX	CAH-CAJ-CAM-CAA
6	A	5304	PNX	CAH-CAJ-CAM-OAD

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Mol	Chain	Res	Type	Atoms
6	B	5304	PNX	CAH-CAJ-CAM-CAA
6	B	5304	PNX	CAH-CAJ-CAM-OAD
6	D	5304	PNX	CAH-CAJ-CAM-CAA
6	D	5304	PNX	CAH-CAJ-CAM-OAD
6	C	5304	PNX	CAH-CAJ-CAM-CAA
6	C	5304	PNX	CAH-CAJ-CAM-OAD
3	A	5301	ATP	C3'-C4'-C5'-O5'
3	B	5301	ATP	C3'-C4'-C5'-O5'
3	D	5301	ATP	C3'-C4'-C5'-O5'
3	C	5301	ATP	C3'-C4'-C5'-O5'
6	D	5304	PNX	CAJ-CAH-CAI-CAK
6	B	5304	PNX	CAJ-CAH-CAI-CAK
6	C	5304	PNX	CAJ-CAH-CAI-CAK
6	A	5304	PNX	CAJ-CAH-CAI-CAK
3	A	5301	ATP	O4'-C1'-N9-C8
3	B	5301	ATP	O4'-C1'-N9-C8
3	D	5301	ATP	O4'-C1'-N9-C8
3	C	5301	ATP	O4'-C1'-N9-C8
3	A	5301	ATP	O4'-C1'-N9-C4
3	B	5301	ATP	O4'-C1'-N9-C4
3	D	5301	ATP	O4'-C1'-N9-C4
3	C	5301	ATP	O4'-C1'-N9-C4
3	A	5301	ATP	O4'-C4'-C5'-O5'
3	B	5301	ATP	O4'-C4'-C5'-O5'
3	D	5301	ATP	O4'-C4'-C5'-O5'
3	C	5301	ATP	O4'-C4'-C5'-O5'
3	A	5301	ATP	PG-O3B-PB-O1B
3	B	5301	ATP	PG-O3B-PB-O1B
3	D	5301	ATP	PG-O3B-PB-O1B
3	C	5301	ATP	PG-O3B-PB-O1B

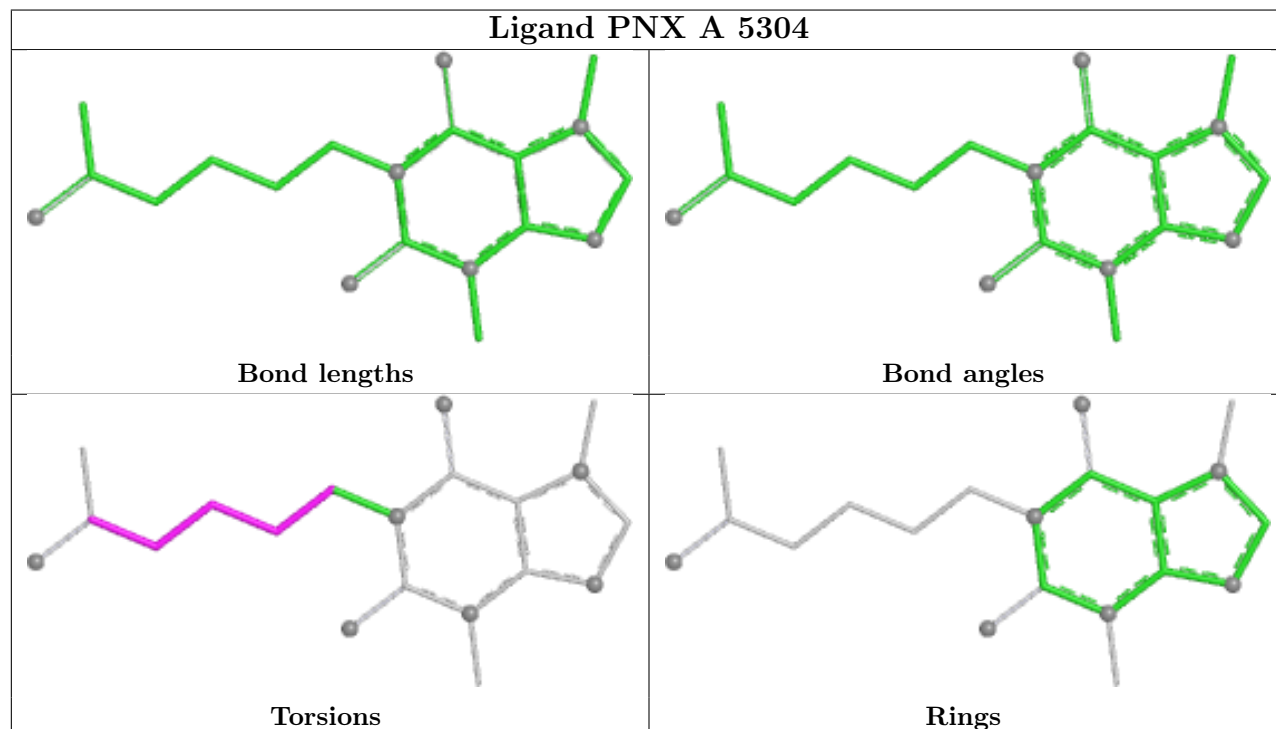
There are no ring outliers.

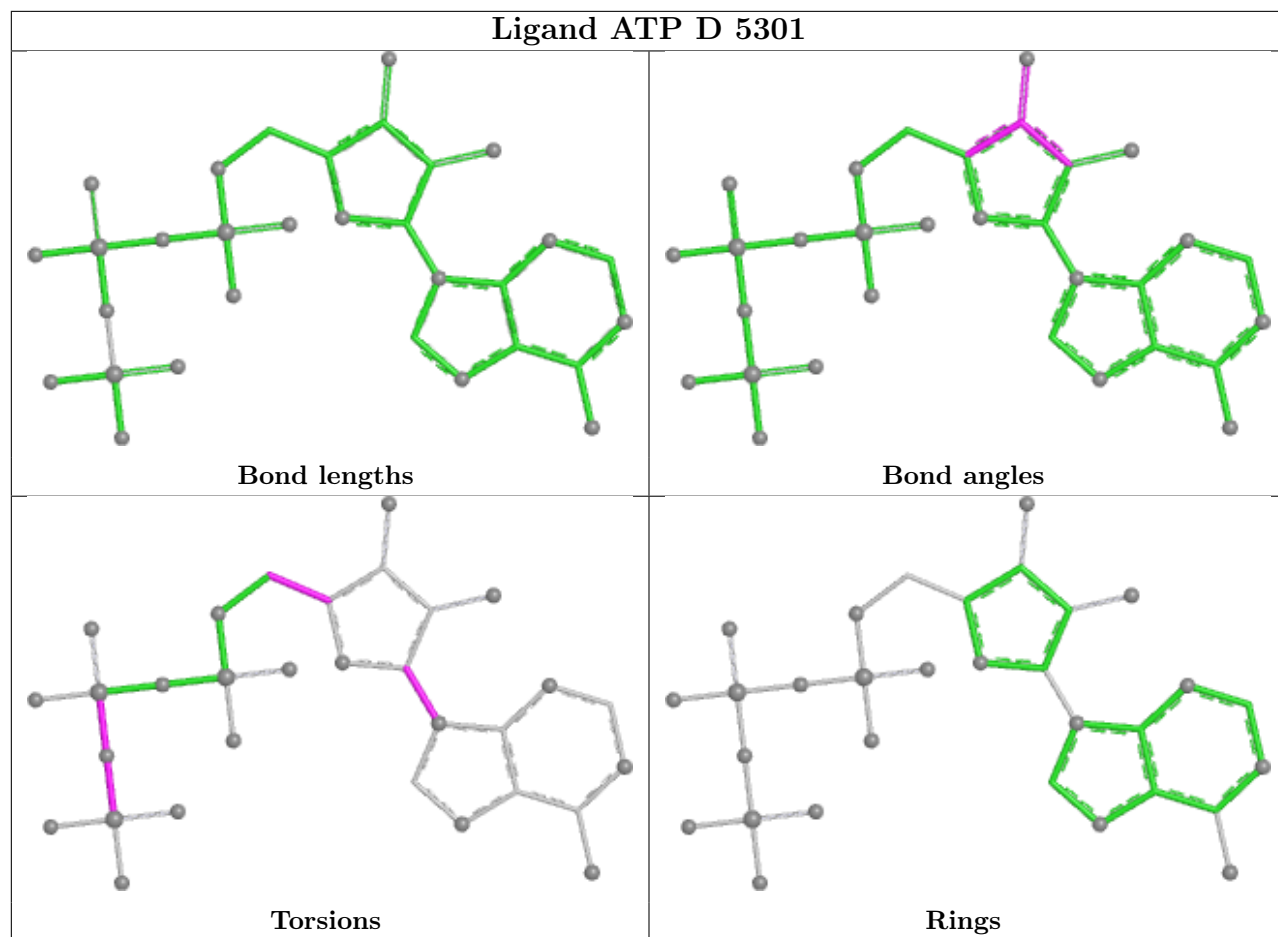
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5304	PNX	3	0
6	C	5304	PNX	3	0
6	D	5304	PNX	3	0
6	B	5304	PNX	3	0

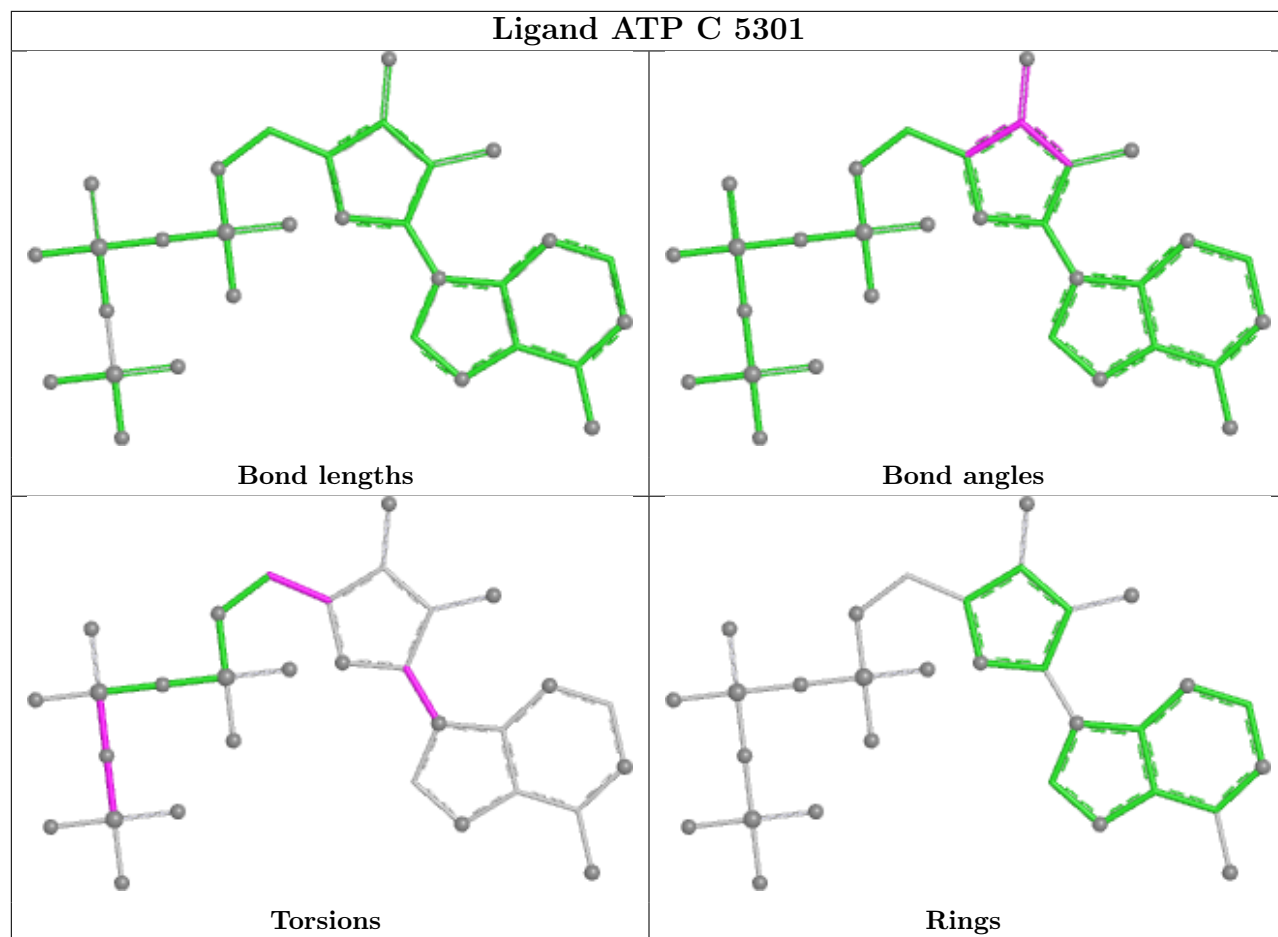
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

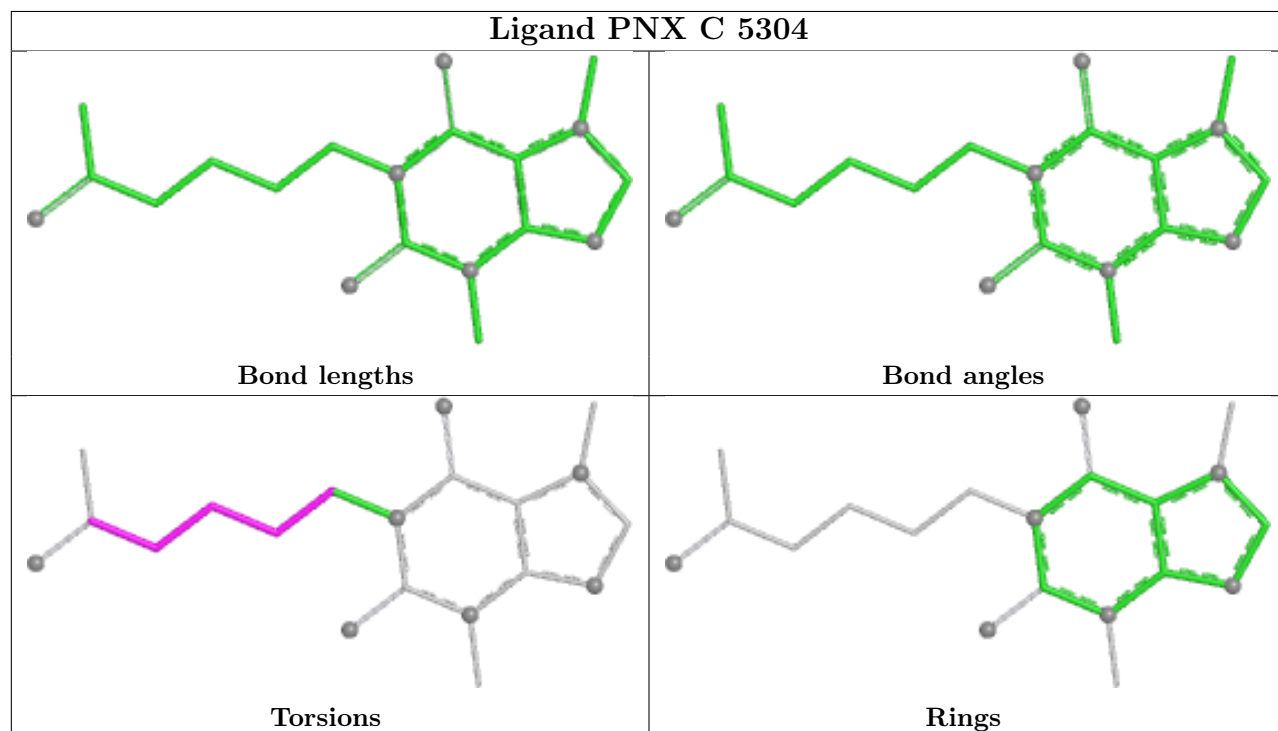


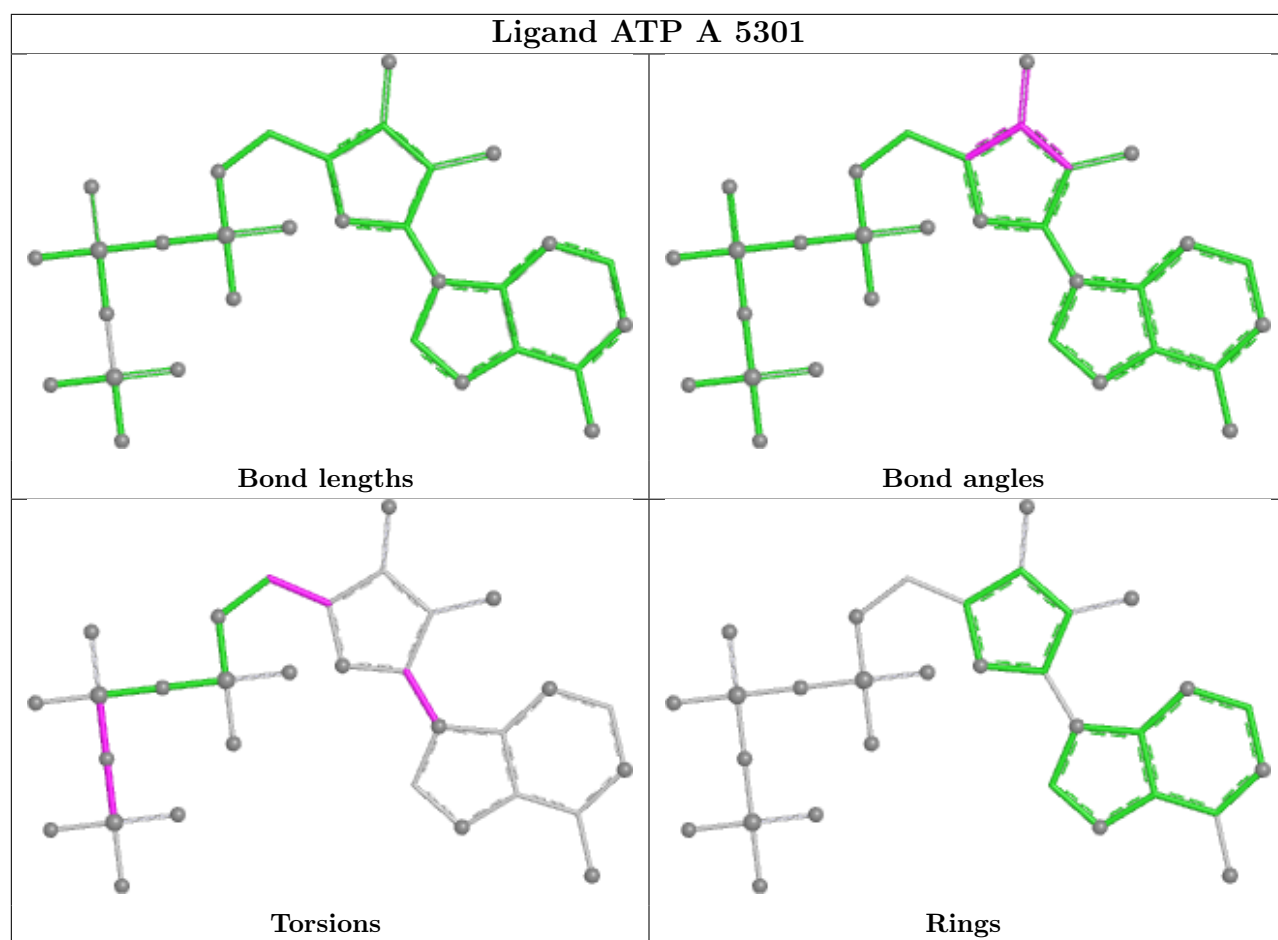


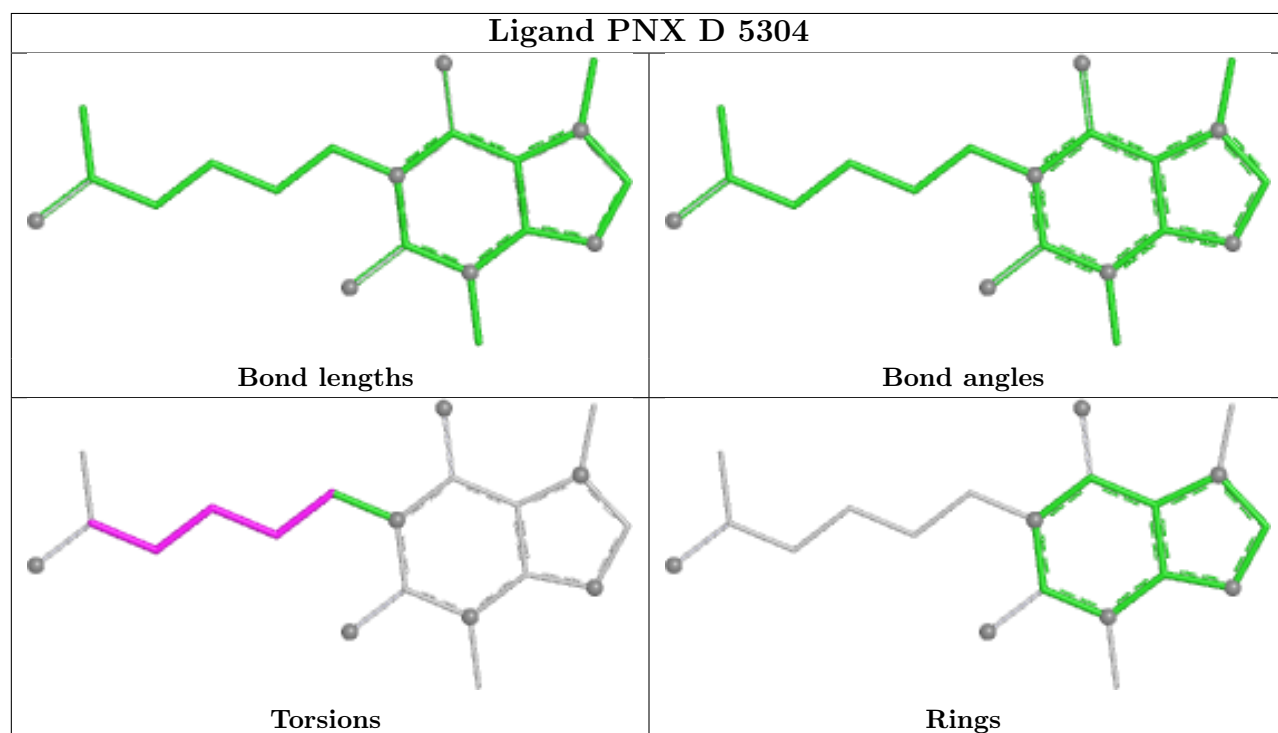
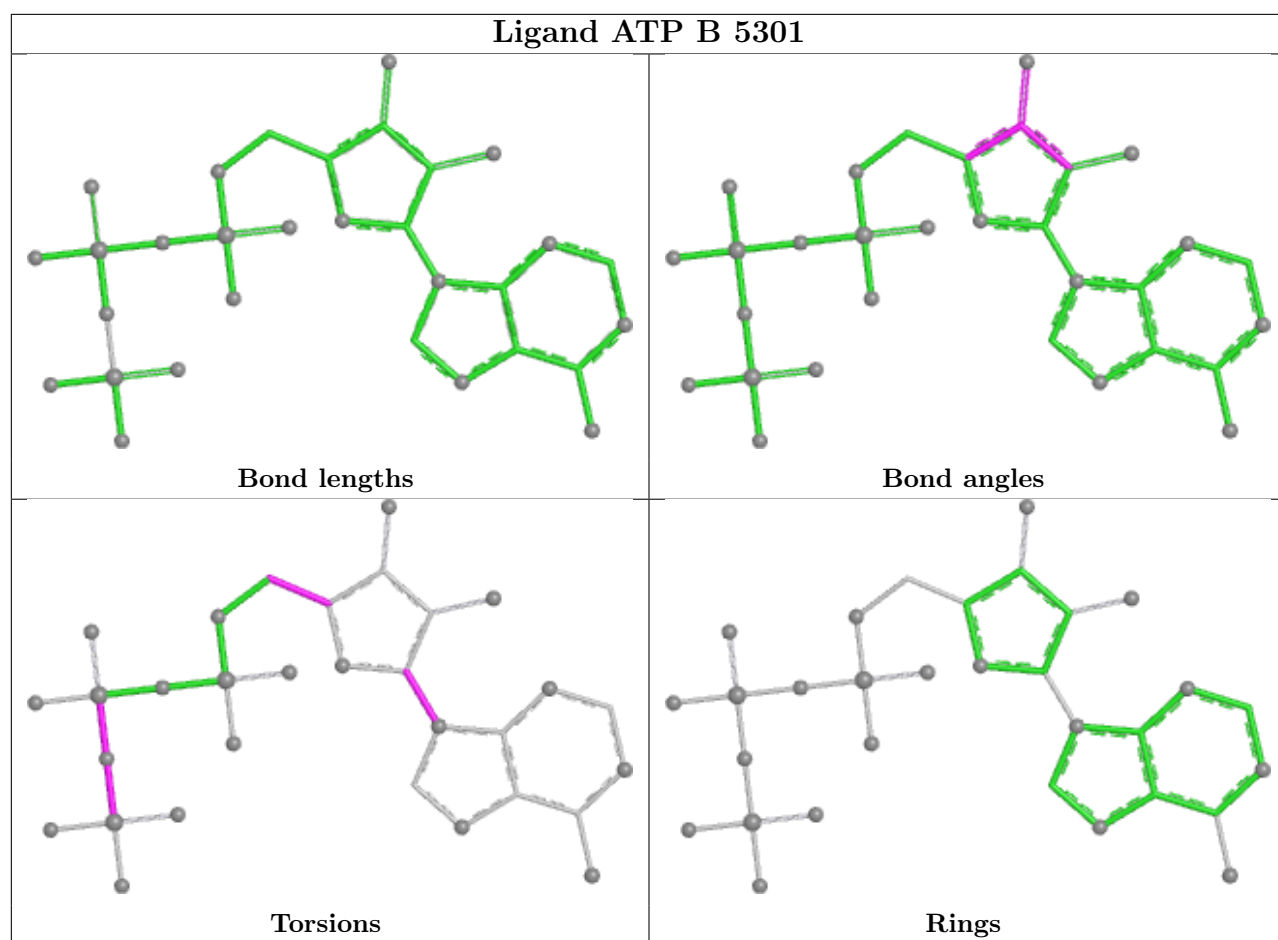
Ligand ATP C 5301

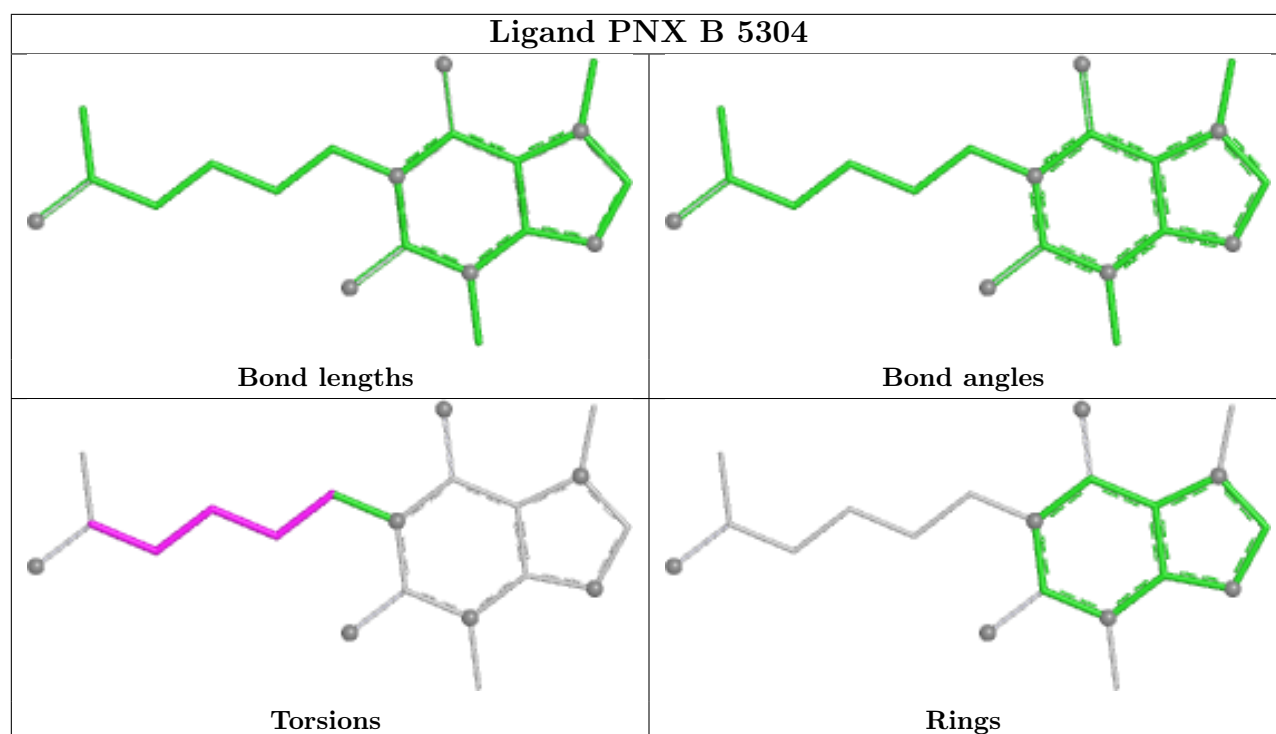


Ligand PNX C 5304









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.

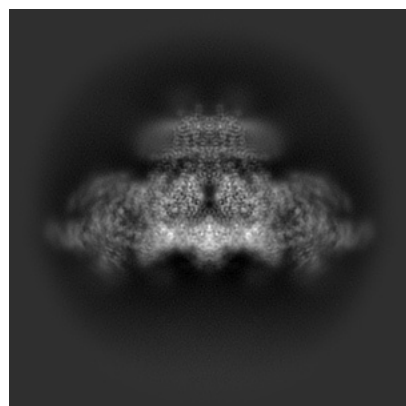
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47385. These allow visual inspection of the internal detail of the map and identification of artifacts.

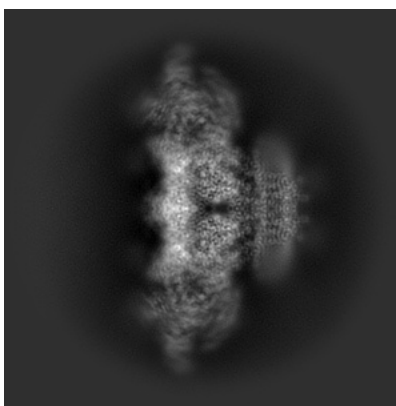
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

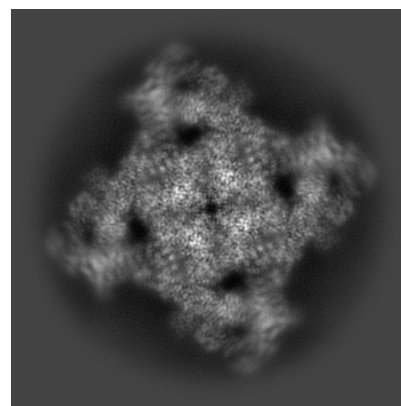
6.1.1 Primary map



X

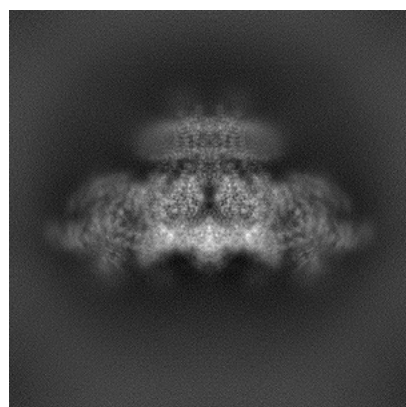


Y

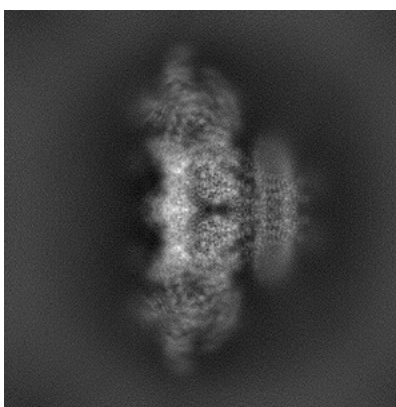


Z

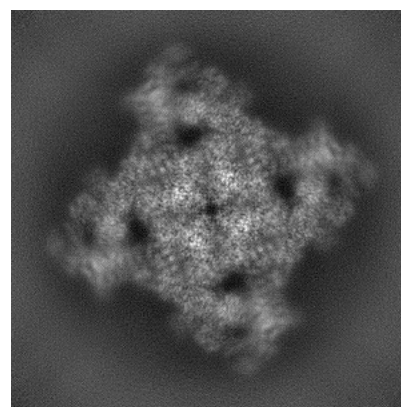
6.1.2 Raw map



X



Y

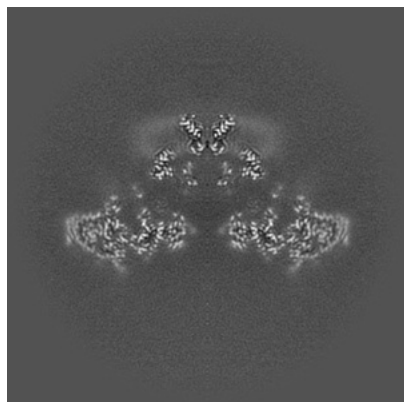


Z

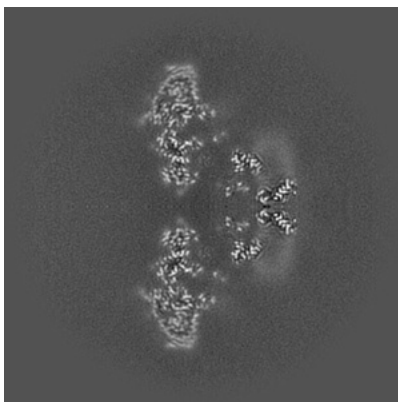
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

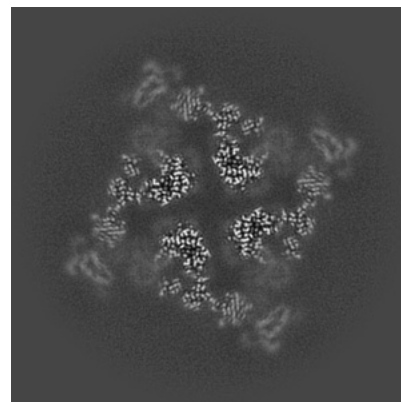
6.2.1 Primary map



X Index: 256

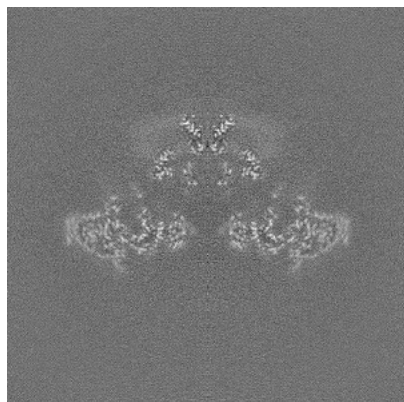


Y Index: 256

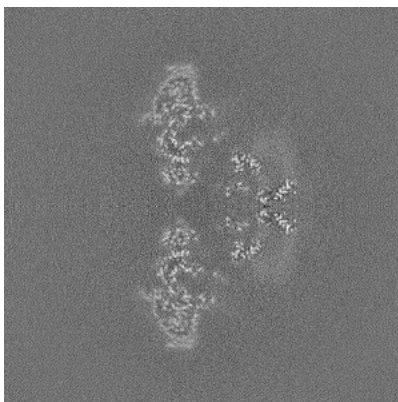


Z Index: 256

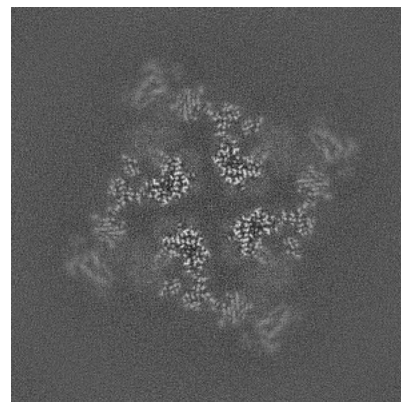
6.2.2 Raw map



X Index: 256



Y Index: 256

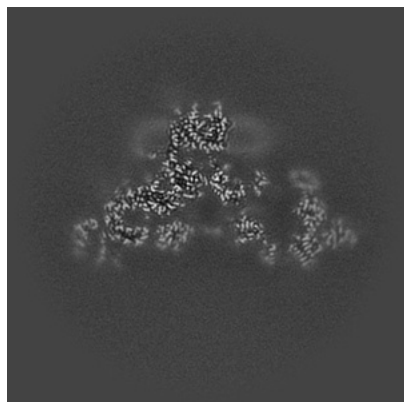


Z Index: 256

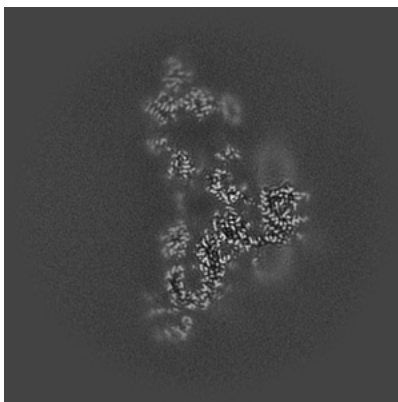
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

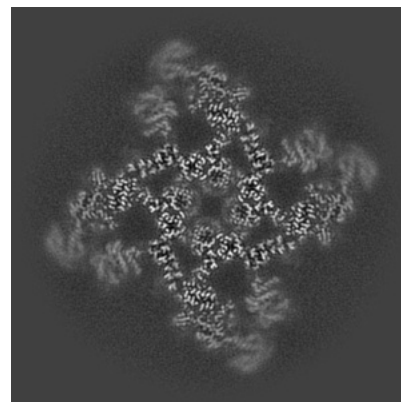
6.3.1 Primary map



X Index: 239

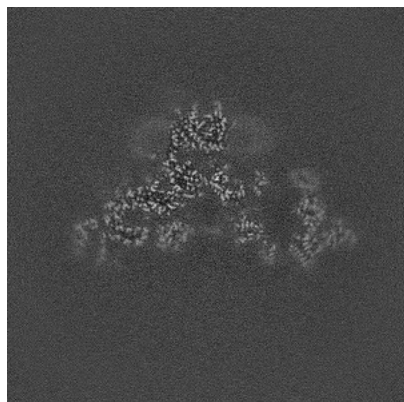


Y Index: 273



Z Index: 229

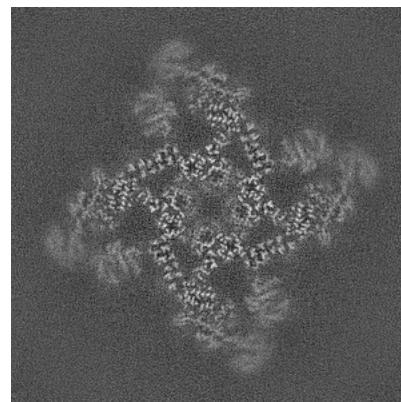
6.3.2 Raw map



X Index: 239



Y Index: 239

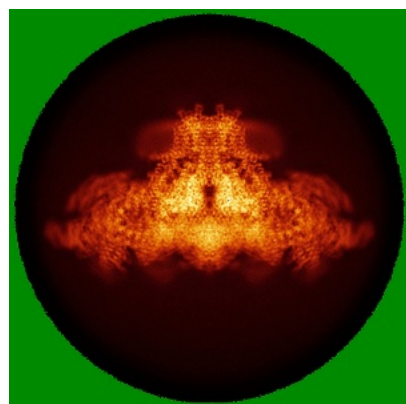


Z Index: 229

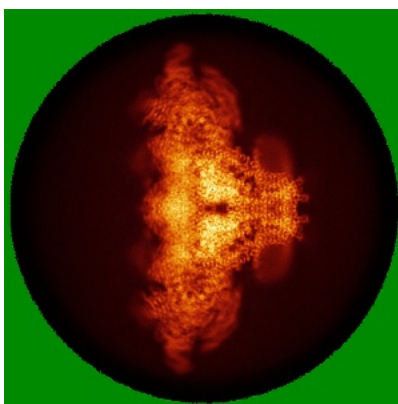
The images above show the largest variance slices of the map in three orthogonal directions.

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

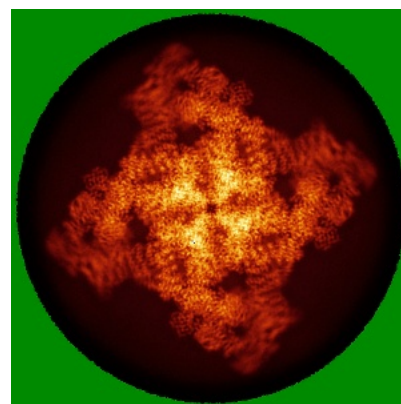
6.4.1 Primary map



X

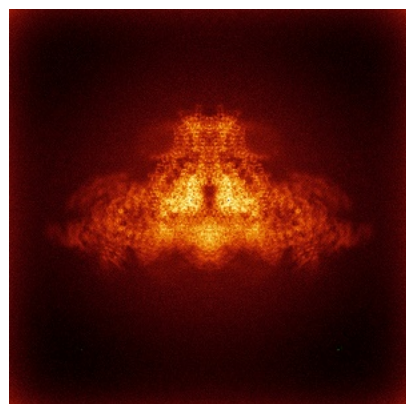


Y

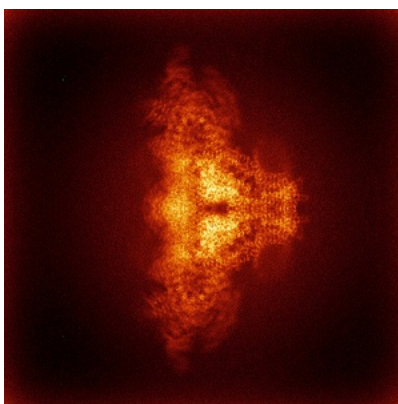


Z

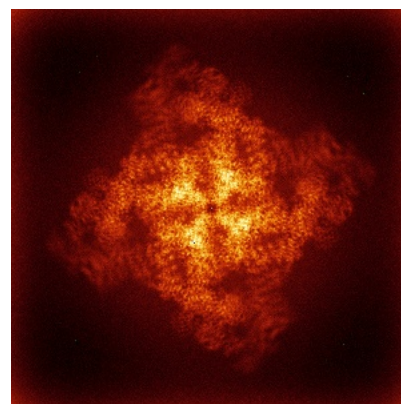
6.4.2 Raw map



X



Y

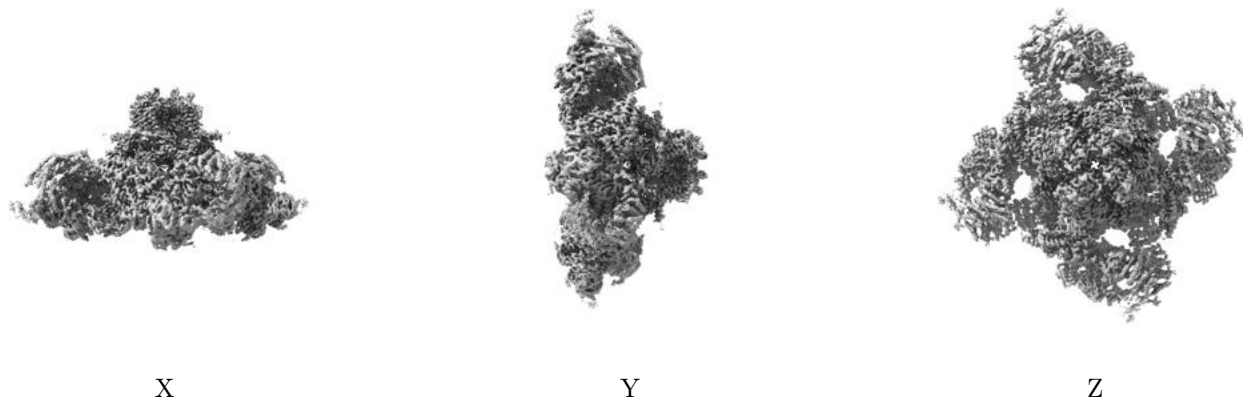


Z

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.

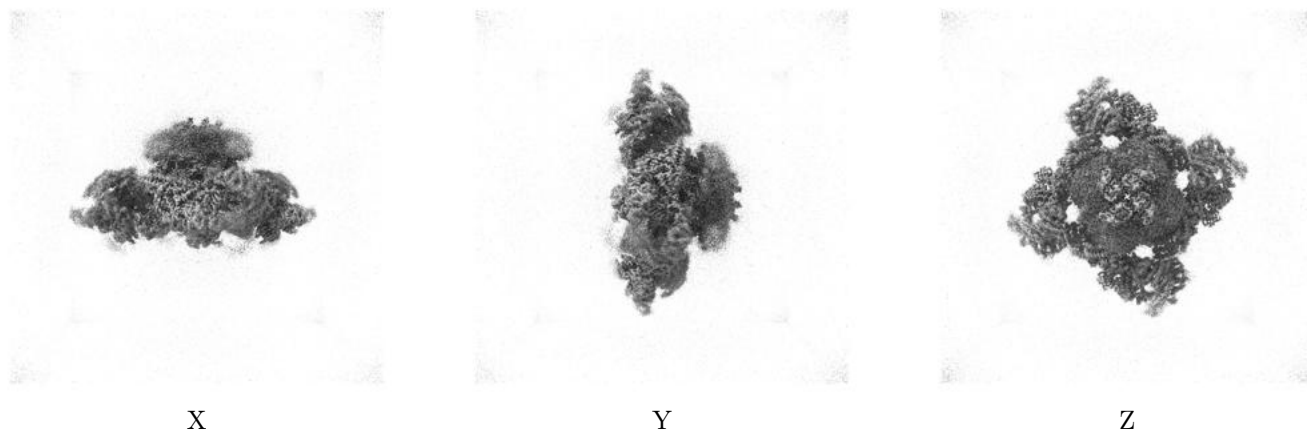
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

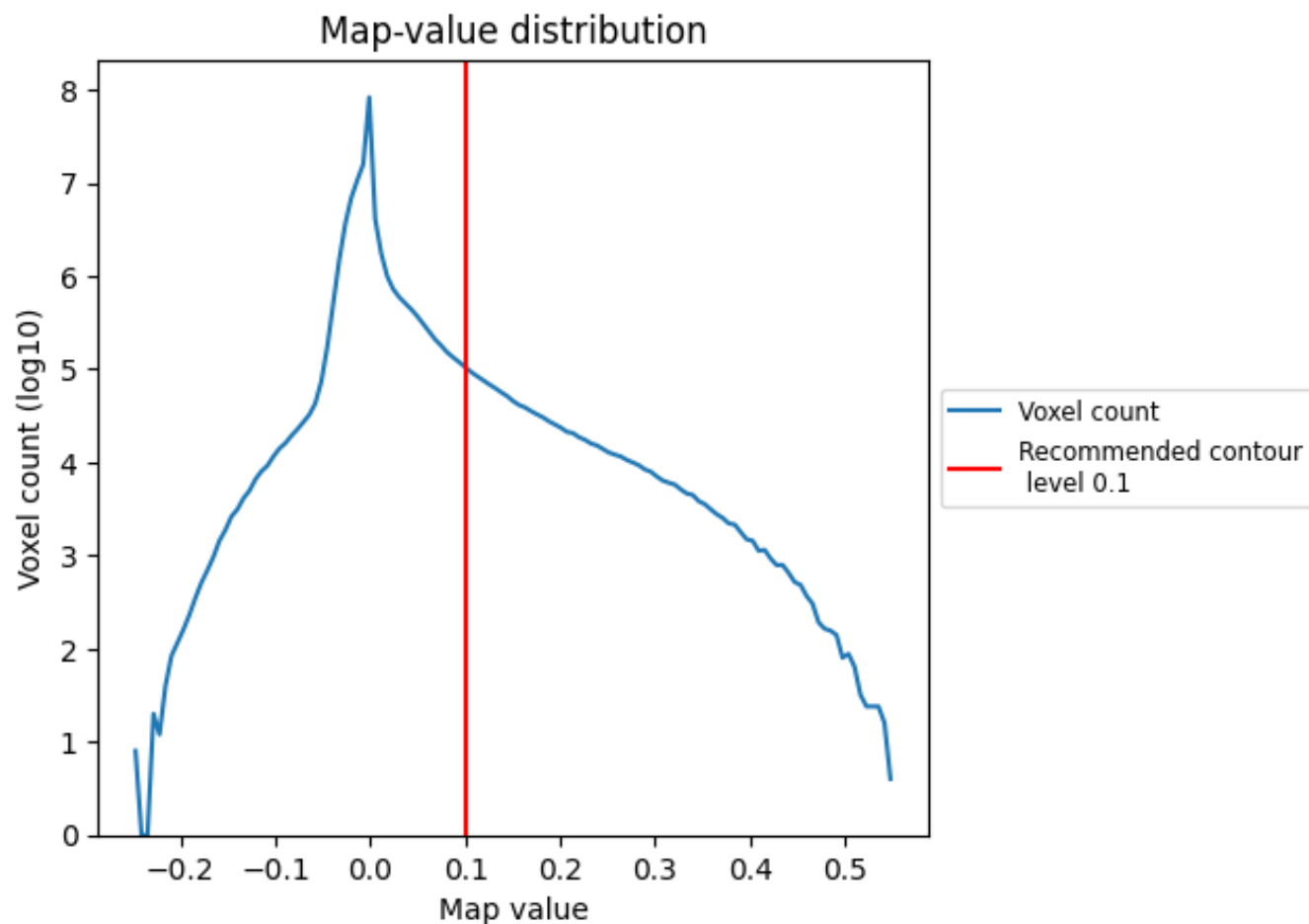
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

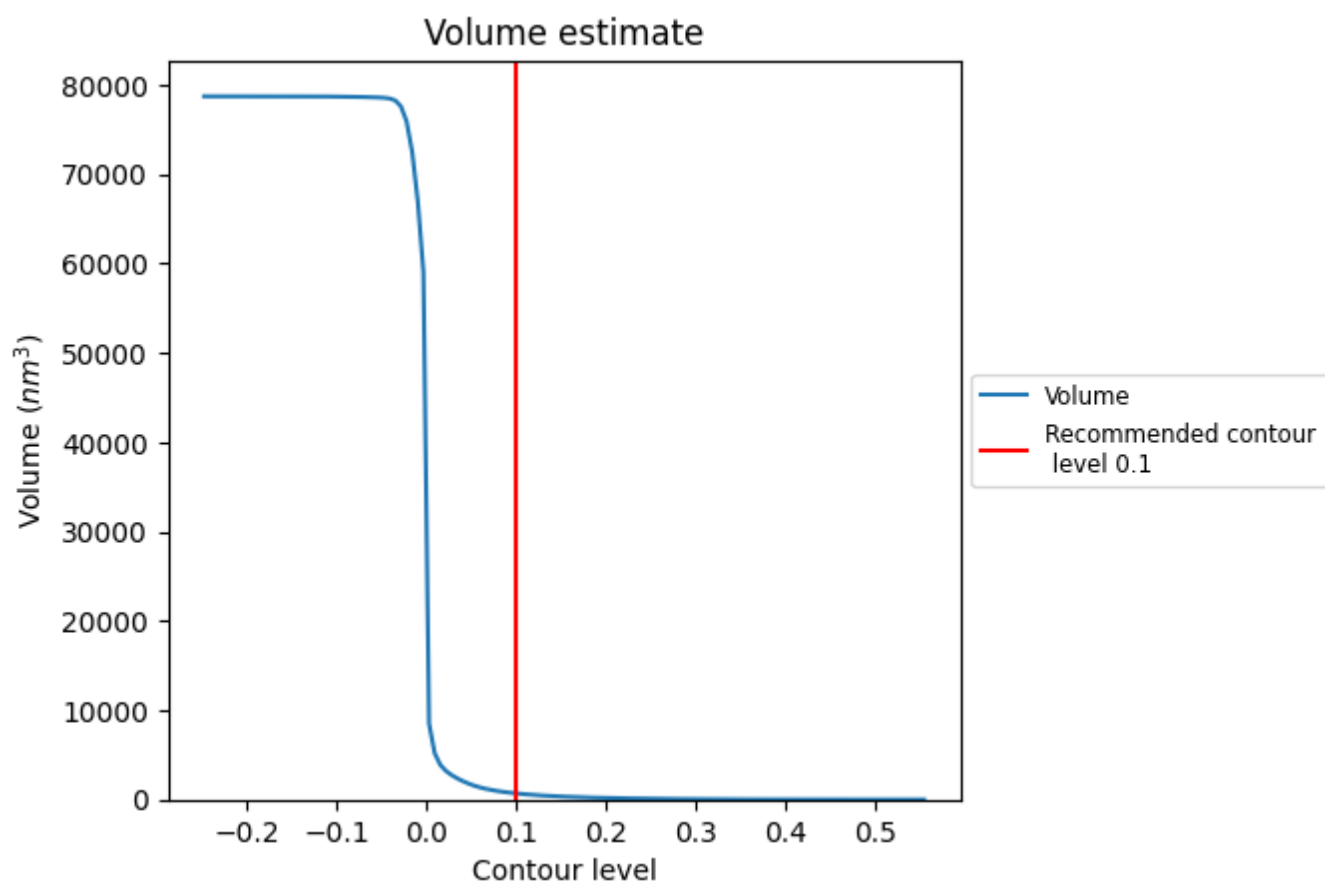
This section contains the results of statistical analysis of the map.

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.

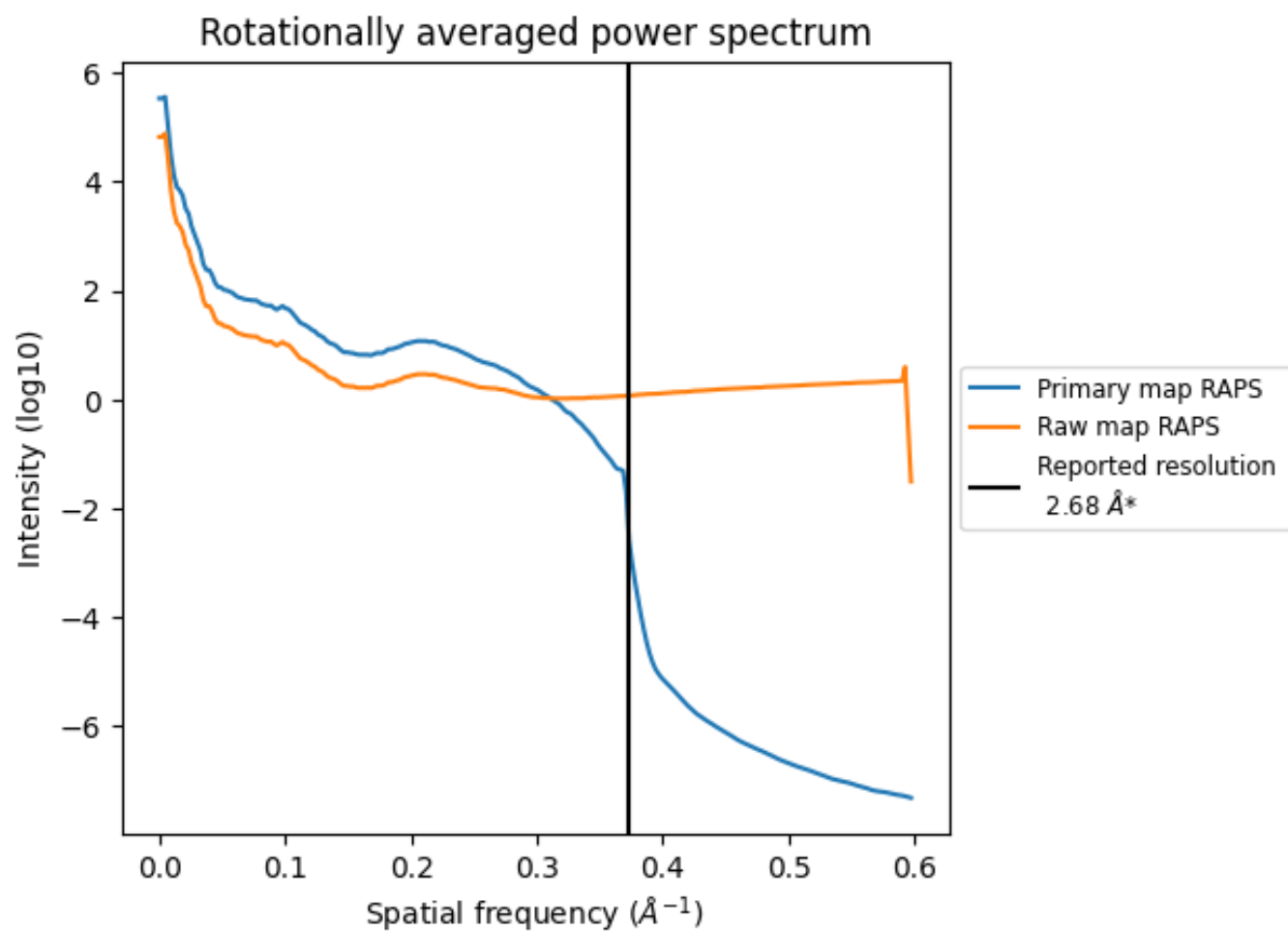
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 692 nm³; this corresponds to an approximate mass of 625 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 ⓘ

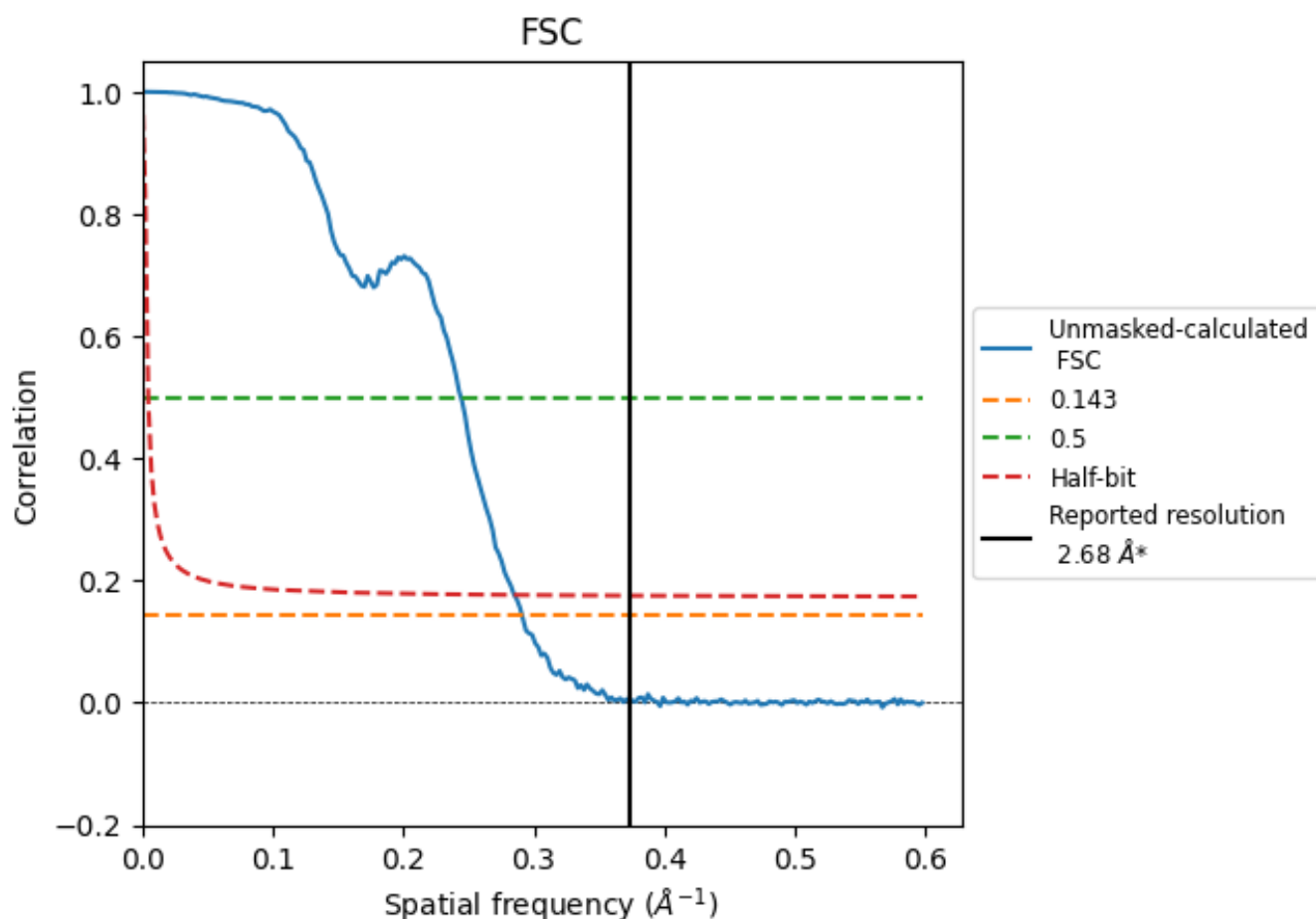


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

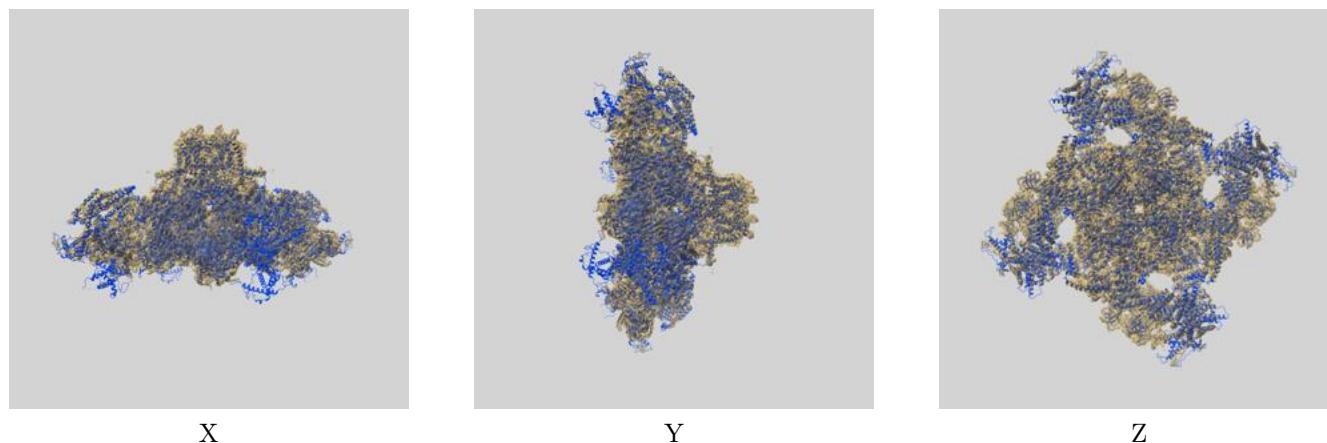
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.10	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

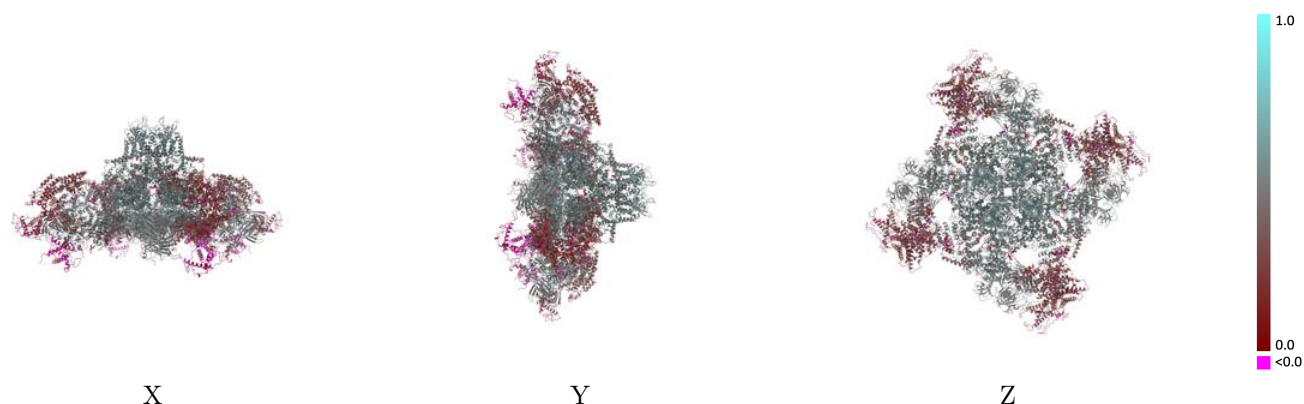
This section contains information regarding the fit between EMDB map EMD-47385 and PDB model 9E18. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



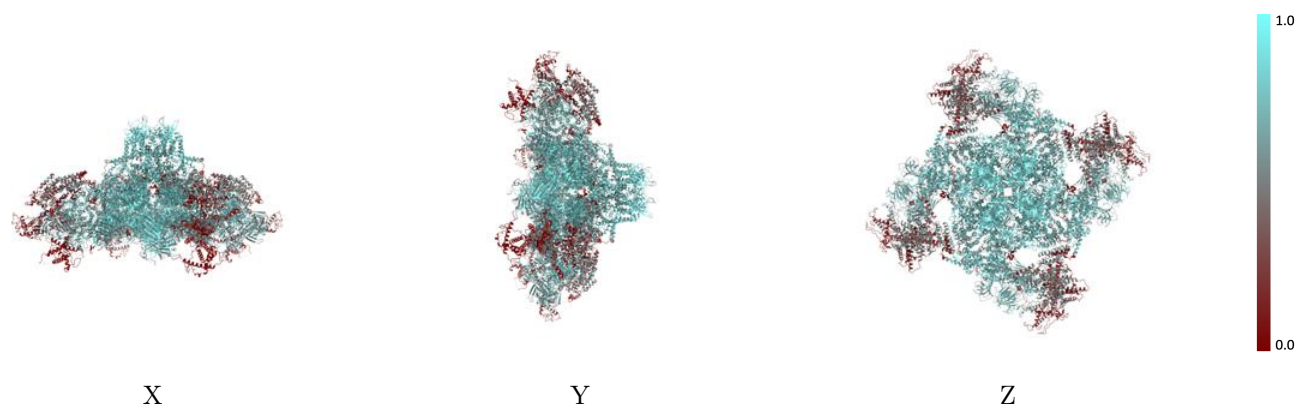
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



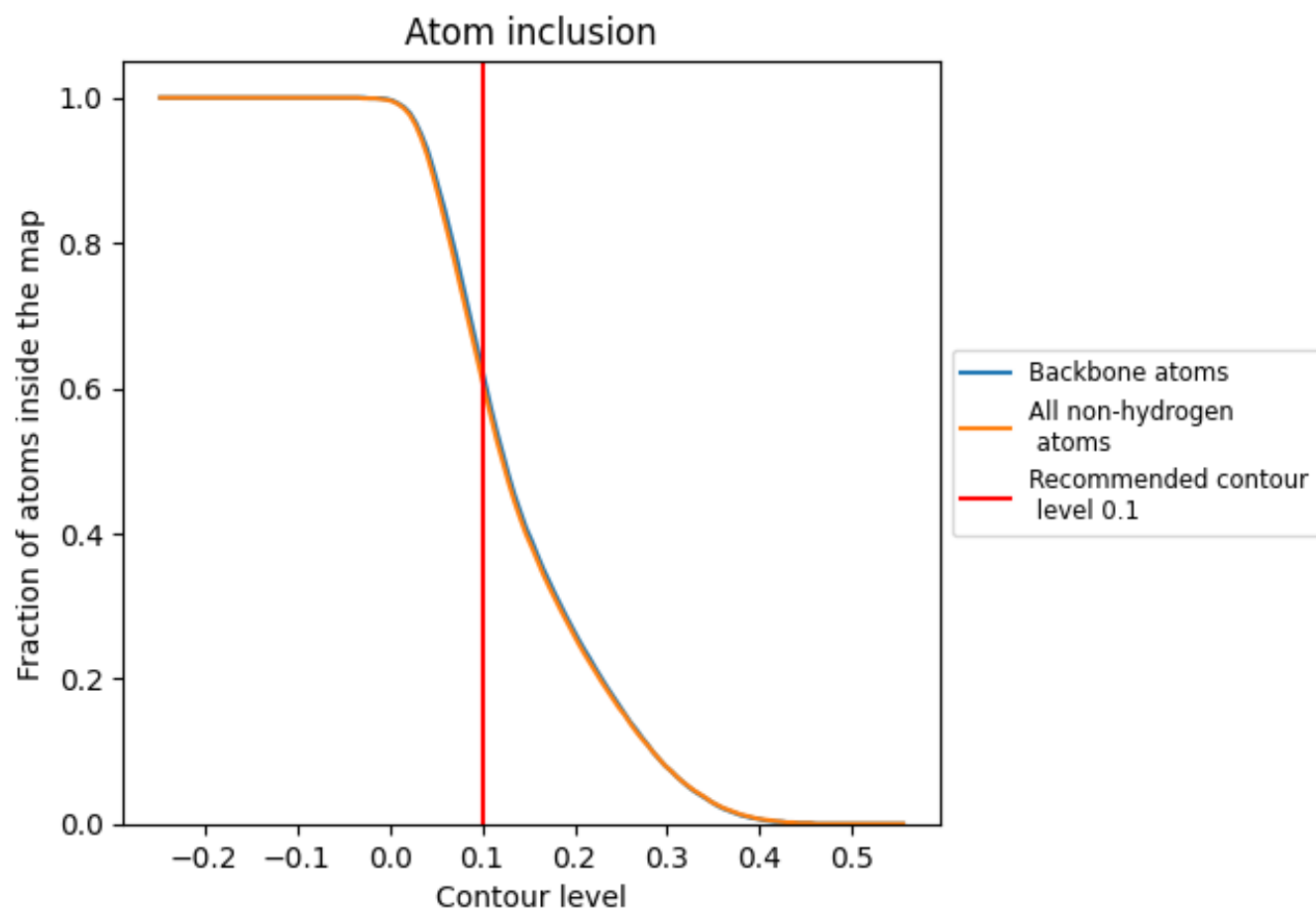
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 61% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6110	0.4160
A	0.6180	0.4140
B	0.6180	0.4150
C	0.6180	0.4140
D	0.6180	0.4140
E	0.6470	0.5000
F	0.6500	0.4970
G	0.6430	0.4940
H	0.6470	0.4960

