



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:11 PM UTC

PDB ID : 9E1H / pdb_00009e1h
EMDB ID : EMD-47394
Title : Structure of RyR1 in the primed state in the presence of oxopyricid
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 3.26 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

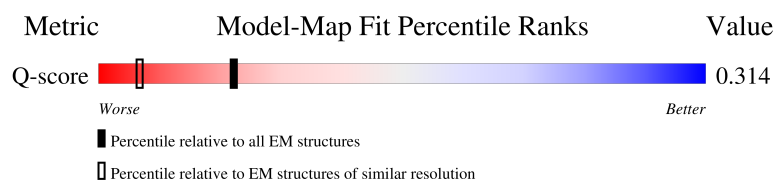
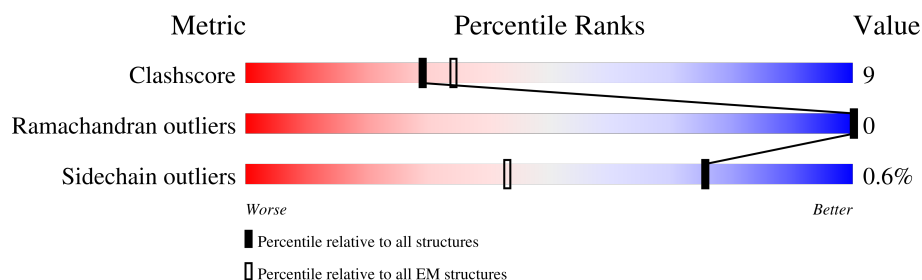
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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	14557 (2.76 - 3.76)

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	74% 67% 31% ..
2	F	108	73% 66% 31% ..
2	G	108	73% 68% 31% ..
2	H	108	75% 67% 31% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144120 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.

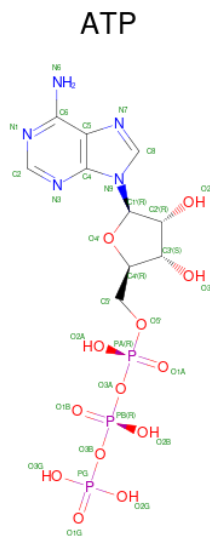
- Molecule 1 is a protein called Ryanodine receptor 1.

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 31	C 10	N 5	O 13	P 3	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0

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

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

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

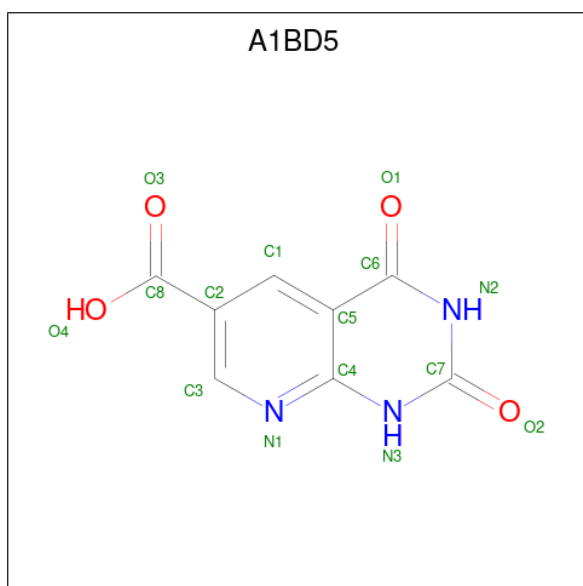
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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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 oxopyridic (CCD ID: A1BD5) (formula: $C_8H_5N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			15	8	3	4	
6	B	1	Total	C	N	O	0
			15	8	3	4	
6	D	1	Total	C	N	O	0
			15	8	3	4	
6	C	1	Total	C	N	O	0
			15	8	3	4	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	B	1	Total	O	0
			1	1	

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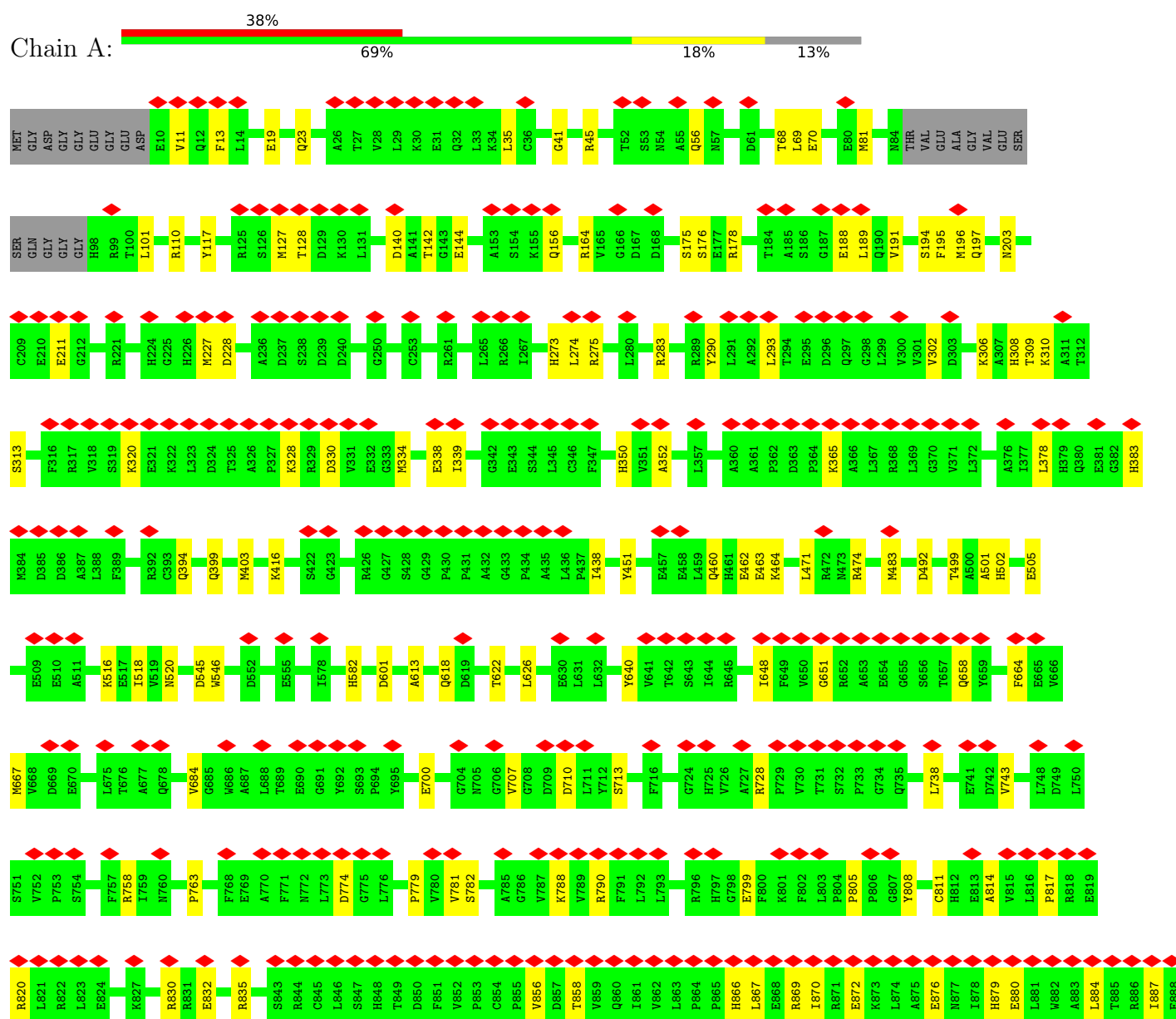
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Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	O	0
			1	1	
7	C	1	Total	O	0
			1	1	

3 Residue-property plots

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

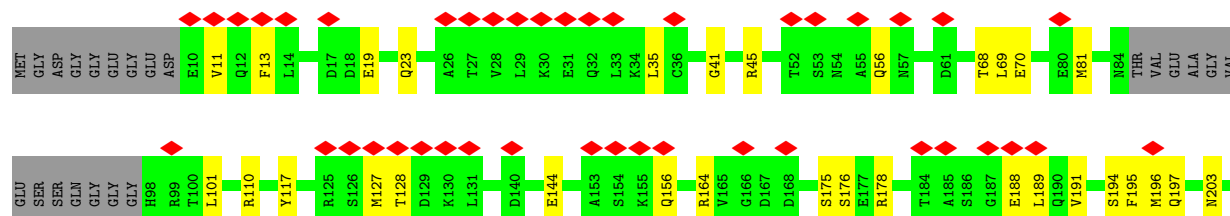
• Molecule 1: Ryanodine receptor 1



Q889	G890	W891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	M924	S925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	M941	A942	D943	E944	K945	A946	E947	D948																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
M949	L950	K951	K952	T953	K954	L955	P956	K957	T958	P1023	Y959	M960	M961	S962	M963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	R987	L988	E989	E990	N991	A997	R998	D999	R1000	V1001	A1002	Q1003	G1004	M1005	S1006	Y1007	S1008	A1009	V1010	Q1011	D1012																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
I1013	P1014	A1015	R1016	R1017	N1018	P1019	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	D1027	L1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	I1053	E1054	P1055	P1056	D1057	R998	Q1058	E1059	P1060	S1061	Q1062	V1063	E1064	M1065	Q1066	S1067	R1068	V1069	D1070	R1071	V1072																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
E1078	K1079	G1086	E1093	A1094	V1095	T1096	E1099	M1100	R1101	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	F1124	N1125	H1127	A1128	W1132	F1139	Q1144	S1145	G1146	D1147	G1150	D1154	L1155	T1156	E1157	T1163	L1164	N1165	E1167	V1168	L1169	M1170	S1171	D1172	G1174	S1175	E1176																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									

L2905	T2906	P2907	V2908	D2909	T2910	L2911	T2912	T2913	T2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	G2922	A2923	Q2924	E2925	L2926	R2927	K2928	F2929	L2930	Q2931	W2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	GLY	L2940	D2941	T2942	T2943	S2944	S2945	R2946	R2947	T2948	S2949	S2950	L2951	E2952	L2953	R2954	F2955	K2956	F2957	G2958	F2959	L2960	Q2961	L2962	L2963	L2964																																																												
THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	V2886	Q2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904																																																													
L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLY	GLY	ARG	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	E2784																																																													
F2664	G2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	K2676	K2677	L2678	F2679	V2680	G2681	I2682	F2683	D2684	S2685	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	Q2693	E2694	L2695	V2696	R2697	M2698	A2699	M2700	C2701	C2702	L2703	C2704	A2705	L2706	A2707	G2708	A2709	L2710	F2711	P2712	D2713	Y2714	V2715	D2716	Y2717	A2718	S2719	S2720	S2721	K2722	E2723	E2724																																																														
K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	R2738	F2739	E2740	T2742	L2743	N2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	M2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	Q2778	E2779	N2780	L2781	D2782	E2783	E2784																																																														
L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLY	GLY	ARG	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	E2784																																																													
THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	V2886	Q2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904																																																													
L2167	M2170	E2175	Q2176	L2177	T2185	M2186	F2191	N2196	L2197	M2198	M2203	T2206	V2207	M2208	E2209	V2212	L2215	Q2216	Q2217	Q2218	E2219	T2220	K2221	E2222	I2223	R2224	F2225	M2228	V2229	T2230	F2235	Y2238	T2242	S2243	R2244	M2250	Y2256	E2259	M2260	S2261	I2263	Q2264	L2265	L2266	L2267	L2268	L2269	L2270	L2271	L2272	L2273	L2274	L2275	L2276	L2277	L2278	L2279	L2280	L2281	L2282	L2283	L2284	L2285	L2286	L2287	L2288	L2289	L2290	L2291	L2292	L2293	L2294	L2295	L2296	L2297	L2298	L2299	L2300	L2301	L2302	L2303	L2304	L2305	L2306	L2307	L2308	L2309	L2310	L2311	M2312	L2313	L2314	A2315	K2316	G2317	D2320	I2321	G2327	K2330	Y2331	L2332	R2336	E2348	R2355	K2359	K2360	P2361	E2362	C2363	F2364	L2368	R2369	G2370	E2371	G2372	G2373	S2374	G2375	L2376	L2377
SER	SER	ARG	LEU	ARG	SER	LEU	GLY	THR	VAL	ARG	LEU	R1999	S2000	P2001	P2002	Q2003	E2004	Q2005	L2006	N2007	M2008	L2009	GLU	LEU	H2011	F2012	K2013	D2014	E2015	A2016	D2017	E2018	E2019	D2020	C2021	E2025	R2028	Q2029	D2030	L2031	Q2032	D2033	D2037	Q2045	L2046	GLY	GLY	GLY	GLY	GLY	PRO	GLY	GLY	THR	SER	LEU																																																																

H3734	R2965	L3025	P3085	Q3145	F3205	E3265	N3325	A3385	V3445	V3505	G3565	Q3627	H3734
L3735	W2966	G3026	E3086	H3146	L3206	K3266	N3326	E3386	S3446	Q3506	S3566	R3628	L3735
E3736	W2967	S3027	T3087	I3147	E3207	P3267	L3327	A3387	K3447	T3507	P3567	R3629	E3736
GLU	D2968	G3028	V3088	A3148	P3208	K3268	G3328	E3388	S3448	S3508	S3568	R3630	GLU
GLY	T2969	G3029	K3089	Q3149	K3209	H3269	I3329	E3389	N3449	L3509	L3569	A3631	GLY
GLU	S2970	H3030	A3090	H3150	L3210	T3270	D3330	G3390	K3450	I3510	R3570	V3632	GLU
ASN	Q2971	A3031	G3091	Q3151	N3211	E3271	E3331	E3391	F3451	V3511	M3573	V3633	ASN
GLY	E2972	S3032	L3092	F3152	K3212	T3272	A3332	L3392	K3452	A3512	A3574	A3634	GLY
GLU	F2973	N3033	R3093	G3153	Y3213	T3273	T3333	L3393	R3453	T3513	L3575	C3635	GLU
ALA	T2974	K3034	S3094	D3154	K3214	L3274	W3334	V3394	E3454	L3514	L3576	F3636	ALA
GLU	A2975	E3035	P3095	D3155	A3215	P3275	M3335	R3395	E3455	K3515	Y3576	R3637	GLU
GLU	H2976	K3036	P3096	V3156	C3216	K3276	K3336	D3396	Q3456	K3516	G3578	M3638	GLU
GLU	E2977	E3037	E3097	V3157	S3217	L3277	K3337	E3397	K3457	L3517	G3579	Y3642	GLU
GLU	L2978	M3038	S3098	L3158	V3218	K3278	R3338	F3398	N3458	K3518	L3579	Y3642	GLU
GLU	A2979	I3039	A3099	D3159	Y3219	S3279	A3339	S3399	F3458	P3519	P3580	D3666	GLU
GLU	V2980	T3040	S3100	D3160	T3220	V3280	V3340	V3399	V3459	I3520	G3581	D3666	GLU
GLU	V2981	S3041	E3101	D3161	T3221	L3281	F3341	L3401	Q3461	G3521	R3582	D3666	GLU
GLU	S2982	L3042	D3102	V3162	K3222	P3282	A3342	C3402	N3462	L3522	E3583	E3670	GLU
GLU	S2983	F3043	T3103	V3163	S3223	R3283	Q3343	R3403	E3463	M3523	E3584	D3671	GLU
GLU	G2984	C3044	E3104	S3164	P3224	K3284	P3344	D3404	I3464	M3524	L3575	R3672	GLU
GLU	R2985	K3045	K3105	G3165	R3225	W3285	I3345	L3405	N3465	C3525	A3586	M3673	GLU
GLU	W2986	L3046	M3106	V3166	E3226	S3286	V3346	V3406	N3466	A3526	D3587	D3676	GLU
GLU	E2987	A3047	V3107	R3167	R3227	R3287	S3347	A3407	M3467	P3527	P3588	E3670	GLU
GLU	K2988	A3048	E3108	T3168	A3228	G3288	A3348	L3408	S3468	T3528	P3589	E3671	GLU
GLU	S2989	L3049	N3109	L3169	L3229	P3289	R3349	Y3409	F3469	D3529	E3590	E3672	GLU
GLU	P2990	V3050	L3110	C3170	G3230	K3290	R3350	P3410	L3470	Q3530	K3591	Q3683	GLU
GLU	H2991	R3051	R3111	S3171	G3231	A3291	P3351	L3411	T3471	D3531	L3592	E3685	GLU
GLU	E2992	H3052	L3112	I3172	L3232	P3292	E3352	L3412	A3472	L3532	V3593	E3686	GLU
GLU	Q2993	R3053	G3113	Y3173	P3233	P3293	L3353	T3413	D3473	I3533	R3594	E3687	GLU
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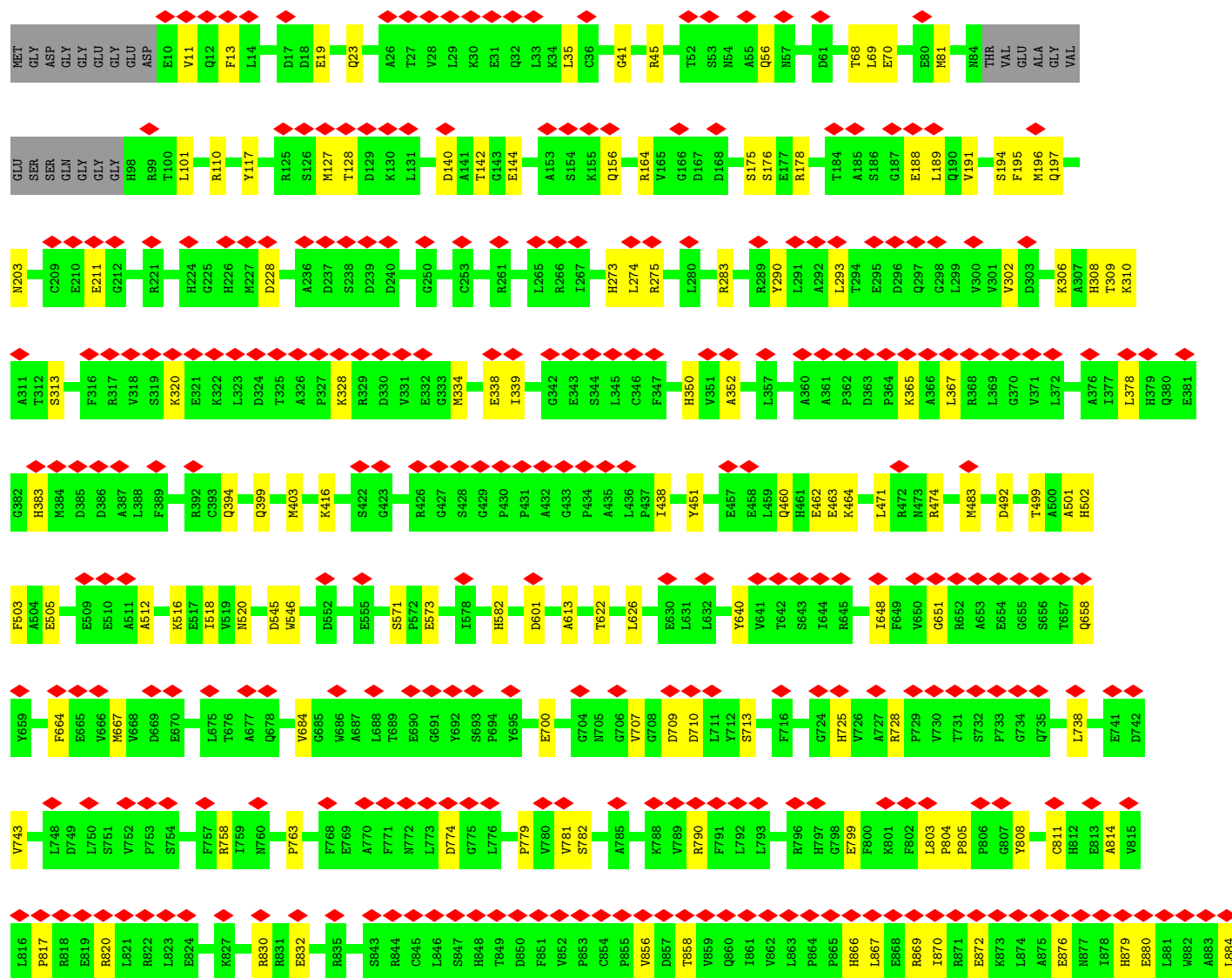


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GLU	S1279	E1176	R1071	Q1011	E947	I887	R818	D749	F664	H383	H502	F503	A504	E505	E509	E510	A511	A512	K516	E517	I518	N520	D545	V546	D552	E555	I578	H582	D601	A613	Q618	T622	L626	E630	L631	L632	Y640	V641	T642	S643	I644	R645	I648	F649	V650	G651	R652	A653	E654	G655	S656	T657	Q658	H308	K309	K310	A311	T312	
ALA	Q1280	T1177	V1072	D1012	D948	E888	E819	D749	E665	H384	H503	F504	A505	E506	E510	E511	A512	K517	E518	N521	D546	V547	D553	E556	I579	H583	D602	A614	Q619	T623	L627	E631	L632	Y641	V642	T643	S644	I645	R646	I649	F650	V651	G652	R653	A654	E655	G656	S657	T658	Q659	H309	K310	A312	T313					
GLY	N1281	A1178	V1079	I1013	N949	Q889	R820	S751	V667	D386	E509	E510	A511	A512	K517	E518	N520	D546	V547	D553	E556	I579	H583	D602	A614	Q619	T623	L627	E631	L632	Y641	V642	T643	S644	I645	R646	I649	F650	V651	G652	R653	A654	E655	G656	S657	T658	Q659	H309	K310	A312	T313								
LYS	S1282	R1180	G1086	R1016	K951	G890	L821	V752	V668	L388	E509	E510	A511	A512	K517	E518	N520	D546	V547	D553	E556	I579	H583	D602	A614	Q619	T623	L627	E631	L632	Y641	V642	T643	S644	I645	R646	I649	F650	V651	G652	R653	A654	E655	G656	S657	T658	Q659	H309	K310	A312	T313								
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THR	E1285	E1183	E1093	R1017	T953	Y893	E824	F757	L675	R392	K516	E517	I518	N520	D546	V547	D553	E556	I579	H583	D602	A614	Q619	T623	L627	E631	L632	Y641	V642	T643	S644	I645	R646	I649	F650	V651	G652	R653	A654	E655	G656	S657	T658	Q659	H309	K310	A312	T313											
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LYS	L1287	G1185	T1096	R1020	P956	V896	R830	I759	A677	Q394	K516	E517	I518	N520	D546	V547	D553	E556	I579	H583	D602	A614	Q619	T623	L627	E631	L632	Y641	V642	T643	S644	I645	R646	I649	F650	V651	G652	R653	A654	E655	G656	S657	T658	Q659	H309	K310	A312	T313											
GLU	F1288	D1186	T1096	L1021	P956	V896	R830	I759	A677	Q394	K516	E517	I518	N520	D546	V547	D553	E556	I579	H583	D602	A614	Q619	T623	L627	E631	L632	Y641	V642	T643	S644	I645	R646	I649	F650	V651	G652	R653	A654	E655	G656	S657	T658	Q659	H309	K310	A312	T313											
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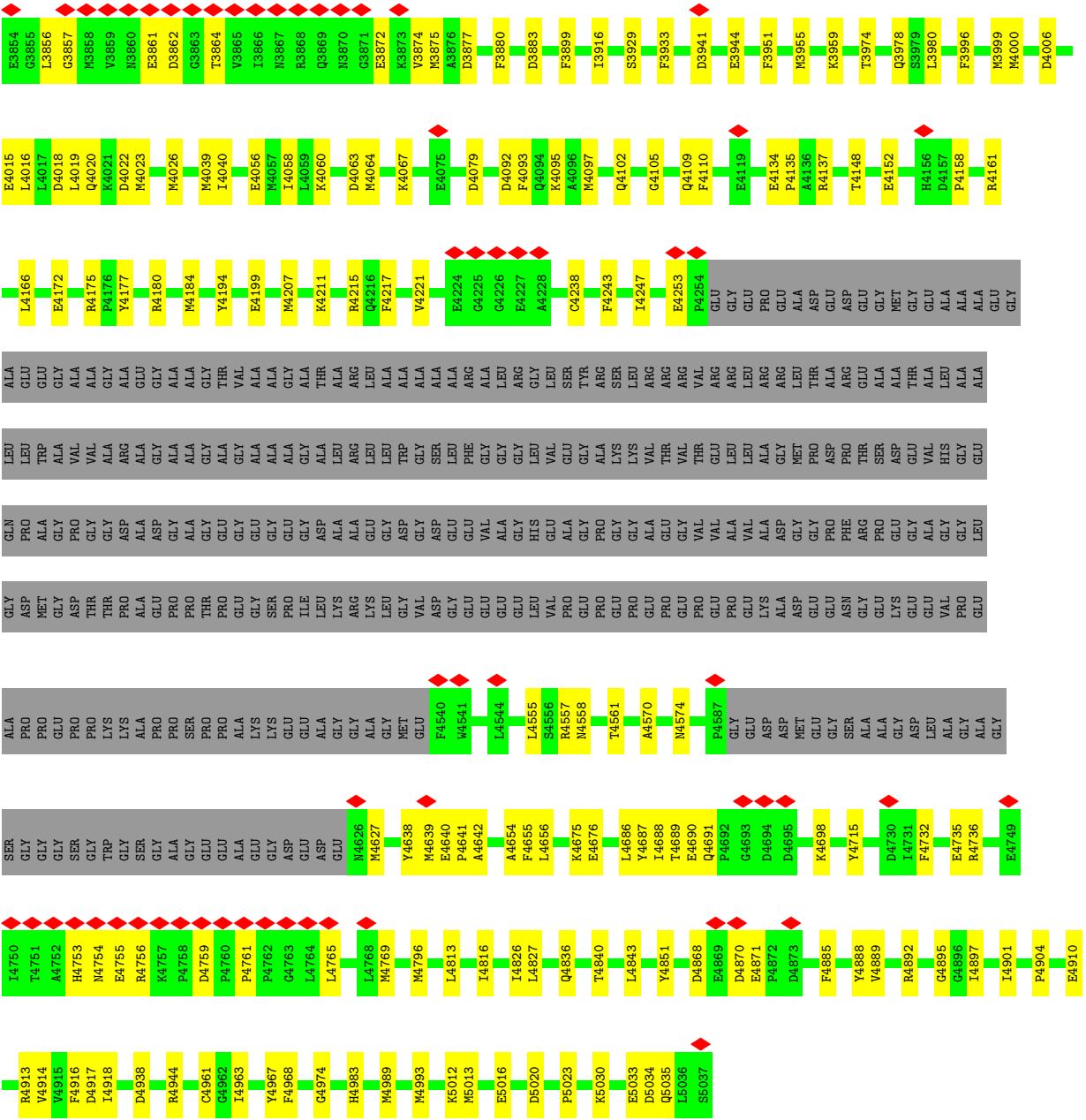




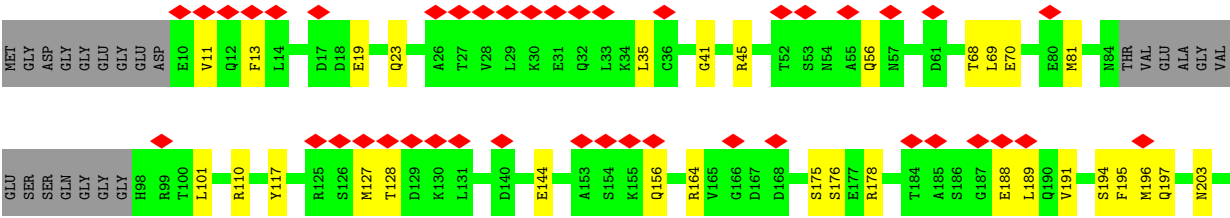


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					E3433	V3373	L3313	L3253	T3133	L3071	L3071	N3012
					L3434	E3374	S3314	G3254	V3134	A3072	A3072	H3013
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● Molecule 1: Ryanodine receptor 1

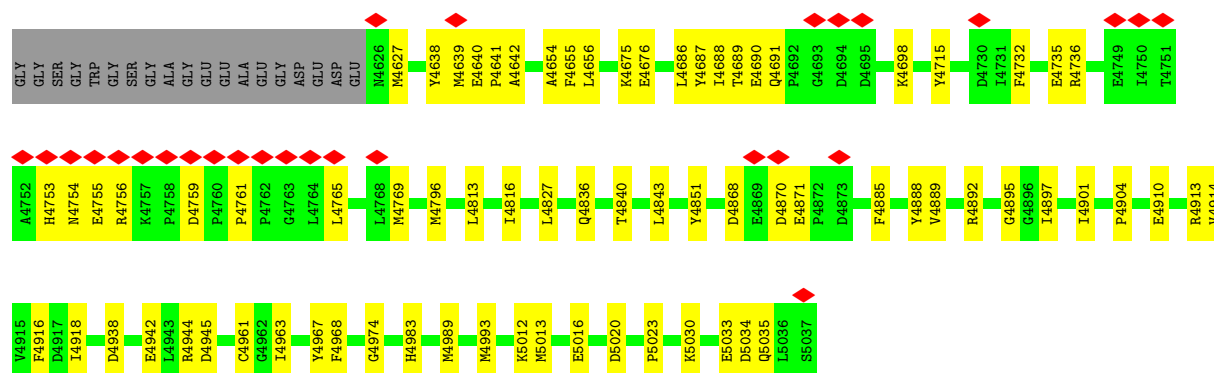


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A883	L884	T885	R886	L887	E888	Q889	G890	W891	T892	F893	G894	P895	V896	R897	D898	D899	N900	K901	R902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	N916	E917	R918	N919	Y920	N921	L922	Q923	P924	N925	G926	E927	T928	L929	K930	T931	L932	L933	A934	L935	C937	H938	V939	G940	H941	A942	
D943	E944	K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	M960	M961	S962	N963	G964	Y965	K966	P967	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	L983	L984	V985	D986	R987	L988	A989	E990	N991	A997	R998	D999	R1000	A1001	A1002	G1004	W1005	S1006		
Y1007	S1008	A1009	V1010	Q1011	D1012	I1013	P1014	A1015	R1016	M1017	R1018	P1019	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	M1035	L1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	M1052	I1053	E1054	P1055	P1056	D1057	Q1058	E1059	P1060	S1061	Q1062	V1063	E1064	N1065	Q1066
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C209	E210	E211	G212	R221	H224	G225	H226	M227	D228	A236	D237	S238	D239	D240	G250	C253	R261	L265	R266	L267	H273	L274	L275	L280	R283	R289	Y290	A292	L293	T294	E295	D296	Q297	G298	L299	V300	V301	V302	D303	K306	H308	T309	K310	A311	T312														
S313	F316	R317	V318	S319	K320	E321	K322	L323	D324	T325	A326	P327	K328	R329	D330	V331	E332	G333	M334	E338	I339	G342	E343	S344	L345	C346	F347	H350	V351	A352	L357	A360	A361	P362	D363	P364	K365	A366	L367	R368	L369	G370	V371	L372	A376	I377	L378	H379	Q380	E381	G382	H383							
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E505	E509	E510	A511	A512	K516	E517	I518	V519	N520	D545	W546	D552	E555	S571	F572	E573	I578	H582	L589	D601	A613	Q618	T622	L626	E630	L631	L632	Y640	V641	T642	S643	I644	R645	L648	F649	V650	G651	R652	A653	E654	G655	S656																	
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E741	D742	V743	L748	D749	L750	S751	V752	P753	S754	F757	R758	I759	N760	P763	F768	E769	A770	F771	N772	L773	D774	G775	S776	P779	W780	V781	S782	A785	K788	V789	R790	F791	L792	L793	R796	H797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	C811	H812	E813									
A814	W815	L816	P817	R818	E819	R820	L821	R822	L823	E824	K827	R830	R831	E832	R835	S843	R844	C845	L846	S847	H848	T849	D850	F851	W852	P853	C854	P855	D857	T858	W859	Q860	L861	V862	L863	P864	P865	H866	L867	E868	R869	T870	R871	R872	K873	L874	A875	E876	N877	T878	H879	L881	W882						

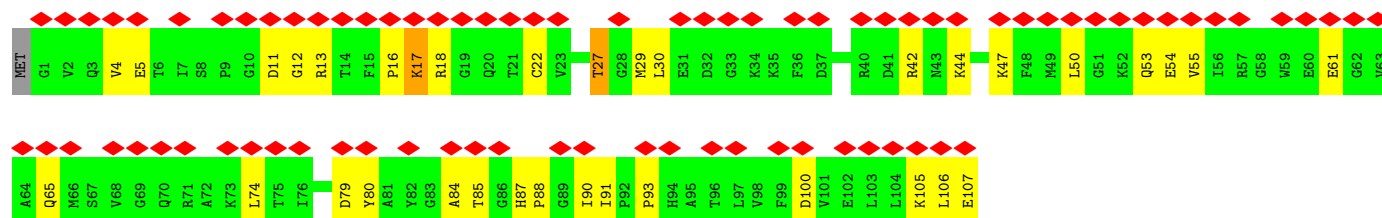
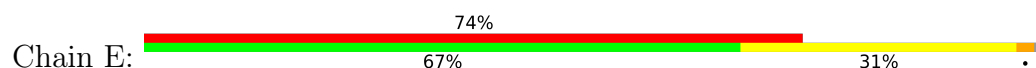


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	Y2655	C2656	L2657	P2658	T2659	Q2660	W2661	A2662	N2663	F2664	G2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	T2675	R2676	K2677	L2678	Y2679	W2680	G2681	L2682	F2683	D2684	S2685	L2686	A2687	H2688	K2689	K2690	Y2691	D2692	P2693	E2694	L2695	Y2696	R2697	M2698	A2699	M2700	P2701	C2702	L2703	C2704	A2705	I2706	A2707	G2708	A2709	L2710	P2711	P2712	D2713		
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	N2774	W2775	S2776	Y2777	G2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	I2804	Y2805	K2806	N2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	
	THR	GLU	LYS	LYS	THR	ARG	LYS	SER	GLN	THR	ALA	GLN	THR	TYR	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	N2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	T2891	Q2892	E2893				
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	R2954	P2955	A2956	P2957	G2958	P2959	L2960	Q2961	Q2962	L2963	L2964	R2965	W2966	M2967	D2968	I2969	S2970	Q2971	E2972	I2973	L2974	A2975	H2976	L2977	E2978	A2979	V2980	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	H2991	E2992	Q2993	E2994	I2995	K2996	P2997	P2998	A2999	K3000	I3001	L3002	L3003	P3004	L3005	I3006	Q3007	Q3008	Y3009	F3010	T3011	N3012	H3013		
	C3014	L3015	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	G3029	H3030	A3031	S3032	N3033	K3034	E3035	K3036	E3037	M3038	L3039	T3040	S3041	L3042	F3043	C3044	K3045	L3046	A3047	A3048	L3049	V3050	R3051	H3052	R3053	V3054	S3055	L3056	F3057	G3058	T3059	D3060	A3061	A3062	A3063	V3064	V3065	N3066	C3067	L3068	H3069	I3070	L3071	A3072	R3073	
	S3074	L3075	D3076	A3077	R3078	T3079	V3080	M3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	K3089	A3090	G3091	L3092	R3093	S3094	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	L3103	E3104	K3105	M3106	V3107	E3108	N3109	R3110	L3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	Y3131	T3132	T3133	
	V3134	A3135	L3136	L3137	P3138	V3139	L3140	T3141	T3142	L3143	F3144	K3145	H3146	I3147	A3148	K3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	I3157	L3158	D3159	D3160	V3161	Q3162	V3163	S3164	K3165	Y3166	R3167	T3168	L3169	C3170	S3171	I3172	S3173	L3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181	Y3182	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	G3191	E3192	C3193	
	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	G3213	N3214	A3215	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	L3229	Y3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	C3240	P3241	D3242	I3243	P3244	V3245	L3246	D3247	R3248	L3249	M3250	A3251	D3252	L3253	
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	S3314	L3315	L3316	G3317	N3318	L3319	L3320	R3321	L3322	L3323	V3324	N3325	L3326	L3327	G3328	I3329	D3330	E3331	A3332	T3333	V3334	M3335	K3336	L3337	L3338	A3339	V3340	F3341	A3342	K3343	R3344	V3345	V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	L3354	L3355	S3356	H3357	F3358	L3359	P3360	T3361	G3362	L3363	R3364	R3365	K3366	K3367	R3368	A3369	G3370	L3371	V3372	V3373	

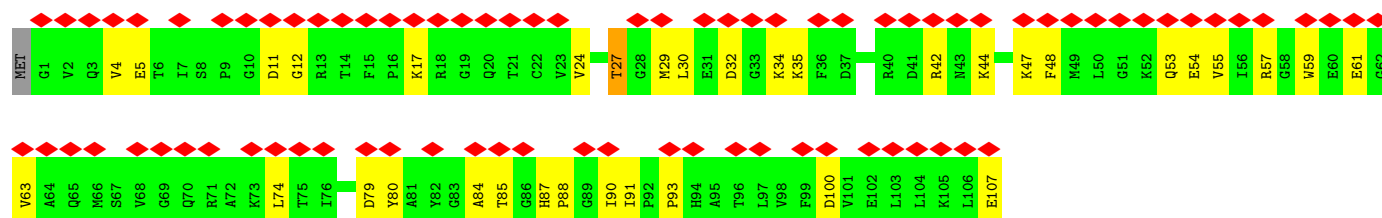
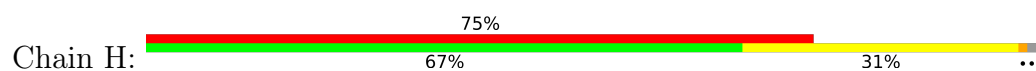




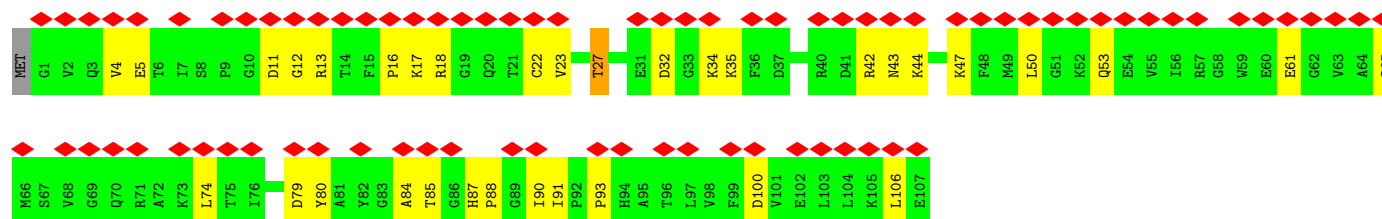
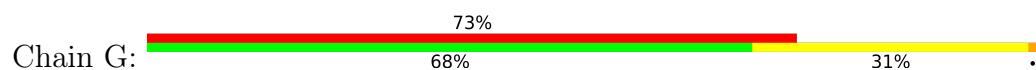
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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

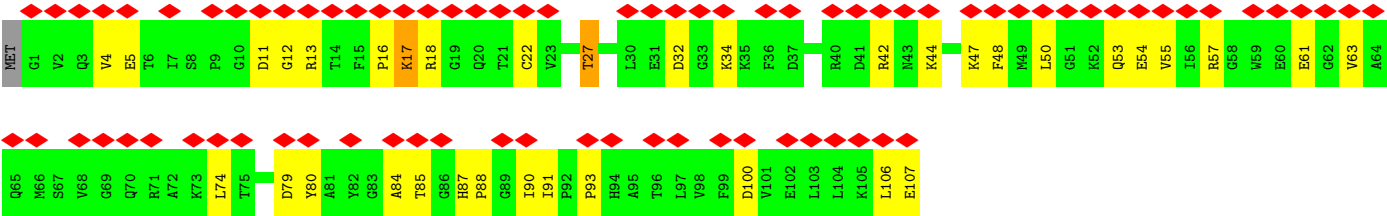


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14467	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	0.395	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	423.424, 423.424, 423.424	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, ATP, A1BD5

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	0.25	0/35977	0.35	2/48726 (0.0%)
1	B	0.25	0/35977	0.35	2/48726 (0.0%)
1	C	0.25	0/35977	0.35	2/48726 (0.0%)
1	D	0.25	0/35977	0.35	2/48726 (0.0%)
2	E	0.23	0/850	0.42	0/1146
2	F	0.23	0/850	0.46	0/1146
2	G	0.23	0/850	0.41	0/1146
2	H	0.23	0/850	0.41	0/1146
All	All	0.25	0/147308	0.36	8/199488 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2639	MET	CB-CG-SD	5.15	128.16	112.70
1	C	2639	MET	CB-CG-SD	5.14	128.12	112.70
1	A	2639	MET	CB-CG-SD	5.14	128.11	112.70
1	B	2639	MET	CB-CG-SD	5.13	128.09	112.70
1	A	3603	LEU	CA-CB-CG	5.01	133.84	116.30
1	B	3603	LEU	CA-CB-CG	5.01	133.82	116.30
1	D	3603	LEU	CA-CB-CG	5.01	133.82	116.30
1	C	3603	LEU	CA-CB-CG	5.00	133.81	116.30

There are no chirality outliers.

There are no planarity outliers.

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	34797	644	0
1	B	35150	0	34797	646	0
1	C	35150	0	34797	643	0
1	D	35150	0	34797	650	0
2	E	831	0	831	32	0
2	F	831	0	831	32	0
2	G	831	0	831	27	0
2	H	831	0	831	22	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	15	0	0	0	0
6	B	15	0	0	0	0
6	C	15	0	0	0	0
6	D	15	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
All	All	144120	0	142560	2658	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 9.

All (2658) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2765:LYS:HZ3	1:A:2857:PRO:HB2	1.38	0.85
1:B:2765:LYS:HZ2	1:B:2860:PRO:HA	1.41	0.85
2:F:18:ARG:HH21	2:F:50:LEU:HD22	1.43	0.83
1:D:3539:ARG:HH12	1:D:3542:LEU:HD22	1.43	0.83
2:E:61:GLU:OE2	2:E:61:GLU:N	2.12	0.82
1:A:3539:ARG:HH12	1:A:3542:LEU:HD22	1.43	0.82
1:C:2765:LYS:HZ3	1:C:2857:PRO:HB2	1.43	0.82
1:B:3539:ARG:HH12	1:B:3542:LEU:HD22	1.43	0.82
2:G:18:ARG:HH21	2:G:50:LEU:HD22	1.44	0.81
2:E:18:ARG:HH21	2:E:50:LEU:HD22	1.43	0.81
1:C:3539:ARG:HH12	1:C:3542:LEU:HD22	1.43	0.80
2:H:61:GLU:OE1	2:H:61:GLU:N	2.14	0.79
2:F:61:GLU:OE1	2:F:61:GLU:N	2.12	0.79
2:F:90:ILE:HG22	2:F:91:ILE:HG13	1.63	0.79
1:D:2765:LYS:HZ3	1:D:2857:PRO:HB2	1.47	0.78
2:G:61:GLU:OE1	2:G:61:GLU:N	2.11	0.77
1:A:1280:GLN:O	1:A:1281:ASN:ND2	2.20	0.75
1:D:1280:GLN:O	1:D:1281:ASN:ND2	2.20	0.75
1:B:1280:GLN:O	1:B:1281:ASN:ND2	2.20	0.75
1:C:1280:GLN:O	1:C:1281:ASN:ND2	2.20	0.74
1:A:127:MET:H	1:A:127:MET:HE3	1.53	0.73
1:C:127:MET:HE3	1:C:127:MET:H	1.53	0.73
1:A:1684:ALA:HA	2:E:90:ILE:HD11	1.70	0.73
1:A:1996:ARG:HH21	1:A:1999:ARG:HE	1.37	0.73
1:B:1996:ARG:HH21	1:B:1999:ARG:HE	1.37	0.73
1:B:127:MET:HE3	1:B:127:MET:H	1.53	0.73
1:C:891:TRP:HA	1:C:902:ARG:HB3	1.71	0.73
1:D:891:TRP:HA	1:D:902:ARG:HB3	1.71	0.72
1:D:1601:MET:HA	1:D:1601:MET:HE3	1.71	0.72
1:C:1601:MET:HA	1:C:1601:MET:HE3	1.71	0.72
1:D:127:MET:H	1:D:127:MET:HE3	1.53	0.72
1:B:891:TRP:HA	1:B:902:ARG:HB3	1.71	0.72
1:A:891:TRP:HA	1:A:902:ARG:HB3	1.71	0.72
1:A:1601:MET:HA	1:A:1601:MET:HE3	1.71	0.72
1:B:1601:MET:HA	1:B:1601:MET:HE3	1.71	0.72
1:D:1996:ARG:HH21	1:D:1999:ARG:HE	1.37	0.71
1:C:3442:PHE:HE1	1:C:3511:VAL:HG12	1.56	0.71
1:D:3442:PHE:HE1	1:D:3511:VAL:HG12	1.56	0.71
1:C:1996:ARG:HH21	1:C:1999:ARG:HE	1.37	0.71
1:B:3442:PHE:HE1	1:B:3511:VAL:HG12	1.56	0.71
1:C:972:LEU:HD13	1:C:1044:ARG:HB3	1.73	0.71
1:B:972:LEU:HD13	1:B:1044:ARG:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4938:ASP:OD1	1:D:4944:ARG:NH1	2.23	0.70
1:B:1636:MET:HE1	1:B:1649:ASP:HA	1.74	0.70
1:A:972:LEU:HD13	1:A:1044:ARG:HB3	1.73	0.70
1:A:3442:PHE:HE1	1:A:3511:VAL:HG12	1.56	0.70
1:A:1636:MET:HE1	1:A:1649:ASP:HA	1.74	0.70
1:C:3324:VAL:HG11	1:C:3361:THR:HG22	1.74	0.70
2:H:90:ILE:HD11	1:D:1684:ALA:HA	1.74	0.70
1:A:1170:MET:HA	1:A:1170:MET:HE3	1.75	0.69
1:A:3324:VAL:HG11	1:A:3361:THR:HG22	1.74	0.69
1:C:1170:MET:HA	1:C:1170:MET:HE3	1.75	0.69
1:C:1636:MET:HE1	1:C:1649:ASP:HA	1.74	0.69
1:B:2165:LEU:HD11	1:B:2177:LEU:HD23	1.74	0.69
1:B:3324:VAL:HG11	1:B:3361:THR:HG22	1.74	0.69
1:D:3324:VAL:HG11	1:D:3361:THR:HG22	1.74	0.69
1:D:972:LEU:HD13	1:D:1044:ARG:HB3	1.73	0.69
1:D:1636:MET:HE1	1:D:1649:ASP:HA	1.73	0.69
1:D:2165:LEU:HD11	1:D:2177:LEU:HD23	1.74	0.69
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.57	0.69
1:C:23:GLN:NE2	1:C:203:ASN:OD1	2.26	0.69
2:F:90:ILE:HD11	1:B:1684:ALA:HA	1.75	0.68
1:B:1170:MET:HA	1:B:1170:MET:HE3	1.75	0.68
1:D:1170:MET:HA	1:D:1170:MET:HE3	1.75	0.68
1:C:2230:THR:HB	1:C:2267:MET:HE3	1.76	0.68
1:A:23:GLN:NE2	1:A:203:ASN:OD1	2.26	0.68
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.57	0.68
1:A:1066:GLN:HB2	1:A:1071:ARG:HE	1.58	0.68
1:B:4944:ARG:NH1	1:C:4938:ASP:OD1	2.26	0.68
1:C:3359:ILE:HG23	1:C:3437:MET:HE1	1.75	0.68
1:B:2230:THR:HB	1:B:2267:MET:HE3	1.76	0.68
1:C:4967:TYR:OH	1:C:5033:GLU:OE2	2.12	0.68
1:A:2230:THR:HB	1:A:2267:MET:HE3	1.75	0.68
1:D:2230:THR:HB	1:D:2267:MET:HE3	1.76	0.68
2:G:87:HIS:HB3	2:G:90:ILE:HB	1.75	0.68
1:B:23:GLN:NE2	1:B:203:ASN:OD1	2.26	0.68
1:D:1066:GLN:HB2	1:D:1071:ARG:HE	1.58	0.68
1:D:925:SER:O	1:D:928:THR:OG1	2.12	0.68
1:B:1066:GLN:HB2	1:B:1071:ARG:HE	1.58	0.68
1:D:23:GLN:NE2	1:D:203:ASN:OD1	2.26	0.68
1:C:2165:LEU:HD11	1:C:2177:LEU:HD23	1.74	0.68
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.57	0.67
1:A:3359:ILE:HG23	1:A:3437:MET:HE1	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:925:SER:O	1:B:928:THR:OG1	2.12	0.67
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.57	0.67
1:D:2754:PHE:HE2	1:D:2813:LEU:HD11	1.59	0.67
1:D:3359:ILE:HG23	1:D:3437:MET:HE1	1.75	0.67
1:D:4938:ASP:OD1	1:C:4944:ARG:NH1	2.26	0.67
1:A:925:SER:O	1:A:928:THR:OG1	2.12	0.67
1:C:925:SER:O	1:C:928:THR:OG1	2.12	0.67
1:A:2165:LEU:HD11	1:A:2177:LEU:HD23	1.74	0.67
1:A:4967:TYR:OH	1:A:5033:GLU:OE2	2.12	0.67
1:C:2754:PHE:HE2	1:C:2813:LEU:HD11	1.60	0.67
1:B:3359:ILE:HG23	1:B:3437:MET:HE1	1.75	0.67
1:C:3169:LEU:HD12	1:C:3194:LEU:HD11	1.77	0.67
2:G:90:ILE:HD11	1:C:1684:ALA:HA	1.76	0.67
1:C:1066:GLN:HB2	1:C:1071:ARG:HE	1.58	0.67
1:A:2742:THR:HG21	1:A:2814:LYS:HB3	1.76	0.67
1:B:2737:PRO:HD2	1:B:2891:LYS:HD3	1.76	0.67
1:B:2754:PHE:HE2	1:B:2813:LEU:HD11	1.59	0.67
1:D:1980:LEU:HD11	1:D:1994:ARG:HB3	1.77	0.67
1:C:2737:PRO:HD2	1:C:2891:LYS:HD3	1.76	0.67
1:C:3594:ARG:NH2	1:C:3597:GLN:OE1	2.28	0.67
1:B:3169:LEU:HD12	1:B:3194:LEU:HD11	1.77	0.67
1:B:4967:TYR:OH	1:B:5033:GLU:OE2	2.12	0.67
1:C:1980:LEU:HD11	1:C:1994:ARG:HB3	1.77	0.67
1:B:2742:THR:HG21	1:B:2814:LYS:HB3	1.76	0.66
1:A:3594:ARG:NH2	1:A:3597:GLN:OE1	2.28	0.66
1:D:2737:PRO:HD2	1:D:2891:LYS:HD3	1.76	0.66
1:D:3169:LEU:HD12	1:D:3194:LEU:HD11	1.77	0.66
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.69	0.66
1:C:2902:HIS:HB3	1:C:2905:LEU:HG	1.78	0.66
1:A:2737:PRO:HD2	1:A:2891:LYS:HD3	1.76	0.66
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.29	0.66
1:D:2902:HIS:HB3	1:D:2905:LEU:HG	1.78	0.66
1:D:4627:MET:HE3	1:D:4627:MET:H	1.59	0.66
1:D:957:LYS:HA	1:D:960:MET:HE2	1.78	0.66
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.29	0.66
1:D:2765:LYS:HZ2	1:D:2860:PRO:HA	1.60	0.66
1:D:4967:TYR:OH	1:D:5033:GLU:OE2	2.12	0.66
1:C:858:THR:HB	1:C:930:LYS:HD2	1.77	0.66
1:A:858:THR:HB	1:A:930:LYS:HD2	1.77	0.66
1:A:2754:PHE:HE2	1:A:2813:LEU:HD11	1.60	0.66
1:B:858:THR:HB	1:B:930:LYS:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:943:ASP:HB2	1:C:1050:GLY:HA3	1.77	0.66
1:A:4627:MET:H	1:A:4627:MET:HE3	1.59	0.66
2:G:18:ARG:HG2	2:G:18:ARG:HH11	1.61	0.66
1:C:830:ARG:NH2	1:C:832:GLU:OE2	2.29	0.66
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.14	0.65
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.69	0.65
2:E:18:ARG:HG2	2:E:18:ARG:HH11	1.61	0.65
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.69	0.65
1:B:3594:ARG:NH2	1:B:3597:GLN:OE1	2.28	0.65
1:B:4627:MET:HE3	1:B:4627:MET:H	1.59	0.65
1:D:3594:ARG:NH2	1:D:3597:GLN:OE1	2.28	0.65
1:A:876:GLU:HG2	1:A:918:ARG:HD3	1.78	0.65
1:B:4654:ALA:C	1:B:4796:MET:HE1	2.22	0.65
1:A:957:LYS:HA	1:A:960:MET:HE2	1.78	0.65
1:A:1980:LEU:HD11	1:A:1994:ARG:HB3	1.77	0.65
1:A:2902:HIS:HB3	1:A:2905:LEU:HG	1.78	0.65
1:A:3169:LEU:HD12	1:A:3194:LEU:HD11	1.77	0.65
1:B:987:ARG:HH12	1:B:1056:PRO:HD2	1.61	0.65
1:D:830:ARG:NH2	1:D:832:GLU:OE2	2.29	0.65
1:D:858:THR:HB	1:D:930:LYS:HD2	1.77	0.65
1:C:3599:VAL:O	1:C:3603:LEU:HD12	1.97	0.65
1:C:4654:ALA:C	1:C:4796:MET:HE1	2.22	0.65
1:A:830:ARG:NH2	1:A:832:GLU:OE2	2.30	0.65
1:D:943:ASP:HB2	1:D:1050:GLY:HA3	1.77	0.65
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.14	0.65
1:C:2742:THR:HG21	1:C:2814:LYS:HB3	1.76	0.65
2:F:5:GLU:OE1	2:F:5:GLU:N	2.29	0.65
1:B:1980:LEU:HD11	1:B:1994:ARG:HB3	1.77	0.65
1:B:2902:HIS:HB3	1:B:2905:LEU:HG	1.78	0.65
1:C:957:LYS:HA	1:C:960:MET:HE2	1.78	0.65
1:C:2170:MET:HE1	1:C:2228:MET:HG2	1.78	0.65
1:C:2779:GLU:HG3	1:C:2792:ARG:HG2	1.78	0.65
1:A:2170:MET:HE1	1:A:2228:MET:HG2	1.78	0.65
1:A:2191:PHE:HA	1:A:2198:MET:HE2	1.79	0.65
1:A:3594:ARG:CZ	1:A:3594:ARG:HA	2.27	0.65
1:B:830:ARG:NH2	1:B:832:GLU:OE2	2.30	0.65
1:B:943:ASP:HB2	1:B:1050:GLY:HA3	1.77	0.65
1:D:2191:PHE:HA	1:D:2198:MET:HE2	1.79	0.65
1:D:2742:THR:HG21	1:D:2814:LYS:HB3	1.76	0.65
1:D:2779:GLU:HG3	1:D:2792:ARG:HG2	1.78	0.65
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.29	0.65
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.69	0.65
1:B:2191:PHE:HA	1:B:2198:MET:HE2	1.79	0.65
1:B:3599:VAL:O	1:B:3603:LEU:HD12	1.97	0.65
1:C:4627:MET:HE3	1:C:4627:MET:H	1.59	0.65
1:A:4654:ALA:C	1:A:4796:MET:HE1	2.22	0.65
1:D:3599:VAL:O	1:D:3603:LEU:HD12	1.97	0.65
1:C:987:ARG:HH12	1:C:1056:PRO:HD2	1.61	0.65
1:A:4944:ARG:NH1	1:B:4938:ASP:OD1	2.29	0.65
2:E:5:GLU:N	2:E:5:GLU:OE2	2.30	0.65
1:B:957:LYS:HA	1:B:960:MET:HE2	1.78	0.65
1:B:3594:ARG:CZ	1:B:3594:ARG:HA	2.27	0.65
1:D:4654:ALA:C	1:D:4796:MET:HE1	2.21	0.65
1:A:987:ARG:HH12	1:A:1056:PRO:HD2	1.61	0.64
1:A:2779:GLU:HG3	1:A:2792:ARG:HG2	1.79	0.64
1:D:987:ARG:HH12	1:D:1056:PRO:HD2	1.60	0.64
2:H:5:GLU:N	2:H:5:GLU:OE2	2.30	0.64
1:D:876:GLU:HG2	1:D:918:ARG:HD3	1.78	0.64
1:C:3594:ARG:HA	1:C:3594:ARG:CZ	2.27	0.64
2:G:5:GLU:N	2:G:5:GLU:OE2	2.30	0.64
2:F:18:ARG:HG2	2:F:18:ARG:HH11	1.61	0.64
1:B:2170:MET:HE1	1:B:2228:MET:HG2	1.78	0.64
1:B:3414:ARG:HE	1:B:3472:ALA:HB3	1.62	0.64
1:B:4676:GLU:OE2	1:B:4698:LYS:NZ	2.31	0.64
1:C:2191:PHE:HA	1:C:2198:MET:HE2	1.79	0.64
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.71	0.64
1:A:943:ASP:HB2	1:A:1050:GLY:HA3	1.77	0.64
1:A:4676:GLU:OE2	1:A:4698:LYS:NZ	2.31	0.64
1:C:876:GLU:HG2	1:C:918:ARG:HD3	1.78	0.64
1:A:943:ASP:OD2	1:A:945:LYS:NZ	2.31	0.64
1:B:876:GLU:HG2	1:B:918:ARG:HD3	1.78	0.64
1:B:2779:GLU:HG3	1:B:2792:ARG:HG2	1.78	0.64
1:D:3594:ARG:CZ	1:D:3594:ARG:HA	2.27	0.64
1:A:3599:VAL:O	1:A:3603:LEU:HD12	1.97	0.64
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.14	0.64
1:B:2644:LEU:HD13	1:B:2678:LEU:HD21	1.79	0.64
1:D:2170:MET:HE1	1:D:2228:MET:HG2	1.78	0.64
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.71	0.64
1:A:3329:ILE:HD11	1:A:3332:ALA:HB2	1.80	0.64
1:B:2624:ARG:HD3	1:B:2910:THR:HB	1.80	0.64
1:D:1981:MET:HA	1:D:1981:MET:HE3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3959:LYS:NZ	1:D:4022:ASP:OD2	2.31	0.64
1:C:943:ASP:OD2	1:C:945:LYS:NZ	2.31	0.64
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.14	0.64
1:C:3414:ARG:HE	1:C:3472:ALA:HB3	1.62	0.64
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.29	0.63
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.29	0.63
1:B:2777:TYR:HB3	1:B:2791:LEU:HD23	1.80	0.63
1:D:2624:ARG:HD3	1:D:2910:THR:HB	1.80	0.63
1:D:4676:GLU:OE2	1:D:4698:LYS:NZ	2.31	0.63
1:B:943:ASP:OD2	1:B:945:LYS:NZ	2.31	0.63
1:D:460:GLN:N	1:D:463:GLU:OE2	2.31	0.63
1:A:394:GLN:OE1	1:A:394:GLN:N	2.32	0.63
1:A:460:GLN:N	1:A:463:GLU:OE2	2.31	0.63
1:C:2644:LEU:HD13	1:C:2678:LEU:HD21	1.79	0.63
1:C:4676:GLU:OE2	1:C:4698:LYS:NZ	2.31	0.63
1:D:3414:ARG:HE	1:D:3472:ALA:HB3	1.62	0.63
1:B:56:GLN:O	1:B:309:THR:OG1	2.16	0.63
1:B:394:GLN:OE1	1:B:394:GLN:N	2.32	0.63
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.71	0.63
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.71	0.63
1:C:2153:MET:HA	1:C:2153:MET:HE3	1.81	0.63
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.29	0.63
1:B:2153:MET:HA	1:B:2153:MET:HE3	1.81	0.63
1:D:3329:ILE:HD11	1:D:3332:ALA:HB2	1.79	0.63
1:C:56:GLN:O	1:C:309:THR:OG1	2.16	0.63
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.29	0.63
2:F:27:THR:HG23	2:F:100:ASP:HB3	1.81	0.63
1:D:2153:MET:HE3	1:D:2153:MET:HA	1.81	0.63
1:A:2155:LEU:HD11	1:A:2198:MET:HE1	1.81	0.63
1:A:3959:LYS:NZ	1:A:4022:ASP:OD2	2.31	0.63
1:A:5034:ASP:OD1	1:A:5035:GLN:N	2.32	0.63
2:G:27:THR:HG23	2:G:100:ASP:HB3	1.81	0.63
1:B:1981:MET:HA	1:B:1981:MET:HE3	1.80	0.63
1:D:56:GLN:O	1:D:309:THR:OG1	2.16	0.63
1:D:2777:TYR:HB3	1:D:2791:LEU:HD23	1.80	0.63
1:C:2155:LEU:HD11	1:C:2198:MET:HE1	1.81	0.63
1:A:2153:MET:HA	1:A:2153:MET:HE3	1.81	0.62
1:A:2644:LEU:HD13	1:A:2678:LEU:HD21	1.79	0.62
1:A:2777:TYR:HB3	1:A:2791:LEU:HD23	1.80	0.62
1:B:2650:ARG:NH1	1:B:2651:CYS:SG	2.72	0.62
1:D:5034:ASP:OD1	1:D:5035:GLN:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5034:ASP:OD1	1:C:5035:GLN:N	2.32	0.62
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.34	0.62
1:D:2155:LEU:HD11	1:D:2198:MET:HE1	1.81	0.62
1:D:2644:LEU:HD13	1:D:2678:LEU:HD21	1.79	0.62
1:A:2624:ARG:HD3	1:A:2910:THR:HB	1.80	0.62
1:A:2650:ARG:NH1	1:A:2651:CYS:SG	2.73	0.62
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.64	0.62
1:A:3414:ARG:HE	1:A:3472:ALA:HB3	1.62	0.62
1:B:2155:LEU:HD11	1:B:2198:MET:HE1	1.81	0.62
1:D:483:MET:HE2	1:D:483:MET:N	2.14	0.62
1:D:2309:SER:HB2	1:D:2314:LEU:HD21	1.81	0.62
1:D:2650:ARG:NH1	1:D:2651:CYS:SG	2.72	0.62
1:D:876:GLU:OE2	1:D:918:ARG:NH1	2.32	0.62
1:C:188:GLU:OE2	1:C:188:GLU:N	2.33	0.62
1:C:2970:SER:HA	1:C:2973:PHE:CE2	2.34	0.62
1:C:3329:ILE:HD11	1:C:3332:ALA:HB2	1.79	0.62
1:A:188:GLU:N	1:A:188:GLU:OE2	2.33	0.62
1:D:943:ASP:OD2	1:D:945:LYS:NZ	2.31	0.62
1:C:460:GLN:N	1:C:463:GLU:OE2	2.31	0.62
1:A:1981:MET:HA	1:A:1981:MET:HE3	1.80	0.62
1:B:483:MET:HE2	1:B:483:MET:N	2.14	0.62
1:B:3329:ILE:HD11	1:B:3332:ALA:HB2	1.79	0.62
1:A:919:ASN:HA	1:A:922:LEU:HD23	1.82	0.62
1:A:2309:SER:HB2	1:A:2314:LEU:HD21	1.81	0.62
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.64	0.62
1:C:483:MET:N	1:C:483:MET:HE2	2.14	0.62
1:B:876:GLU:OE2	1:B:918:ARG:NH1	2.32	0.62
1:C:1981:MET:HA	1:C:1981:MET:HE3	1.80	0.62
1:C:2777:TYR:HB3	1:C:2791:LEU:HD23	1.80	0.62
1:A:483:MET:HE2	1:A:483:MET:N	2.14	0.62
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.64	0.62
1:C:799:GLU:OE1	1:C:1623:ARG:NH2	2.33	0.62
1:C:2288:LEU:O	1:C:3849:ARG:NH1	2.31	0.62
1:C:2650:ARG:NH1	1:C:2651:CYS:SG	2.73	0.62
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.34	0.61
1:B:176:SER:OG	1:B:178:ARG:NH1	2.30	0.61
1:D:394:GLN:OE1	1:D:394:GLN:N	2.32	0.61
1:A:876:GLU:OE2	1:A:918:ARG:NH1	2.32	0.61
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.64	0.61
1:A:56:GLN:O	1:A:309:THR:OG1	2.16	0.61
1:A:4836:GLN:O	1:A:4840:THR:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1427:ILE:HG23	1:C:1428:LEU:HD22	1.83	0.61
1:A:799:GLU:OE1	1:A:1623:ARG:NH2	2.33	0.61
2:F:47:LYS:NZ	2:F:107:GLU:OE2	2.32	0.61
1:B:799:GLU:OE1	1:B:1623:ARG:NH2	2.33	0.61
1:B:1427:ILE:HG23	1:B:1428:LEU:HD22	1.82	0.61
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	1.83	0.61
1:B:4836:GLN:O	1:B:4840:THR:HG23	2.01	0.61
1:B:5034:ASP:OD1	1:B:5035:GLN:N	2.32	0.61
1:C:876:GLU:OE2	1:C:918:ARG:NH1	2.32	0.61
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	1.83	0.61
1:B:3623:LEU:HD12	1:B:3624:LEU:N	2.16	0.61
1:D:176:SER:OG	1:D:178:ARG:NH1	2.30	0.61
1:D:4172:GLU:OE1	1:D:4175:ARG:NH1	2.34	0.61
1:A:4172:GLU:OE1	1:A:4175:ARG:NH1	2.34	0.61
1:B:3959:LYS:NZ	1:B:4022:ASP:OD2	2.31	0.61
1:C:176:SER:OG	1:C:178:ARG:NH1	2.30	0.61
1:C:990:GLU:OE2	1:C:1025:ARG:NH2	2.34	0.61
1:C:2309:SER:HB2	1:C:2314:LEU:HD21	1.81	0.61
1:B:1062:GLN:NE2	1:B:1064:GLU:OE1	2.30	0.61
1:C:2624:ARG:HD3	1:C:2910:THR:HB	1.80	0.61
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	1.83	0.61
1:A:2288:LEU:O	1:A:3849:ARG:NH1	2.31	0.61
1:B:919:ASN:HA	1:B:922:LEU:HD23	1.82	0.61
1:D:799:GLU:OE1	1:D:1623:ARG:NH2	2.33	0.61
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	1.83	0.61
1:D:2970:SER:HA	1:D:2973:PHE:CE2	2.34	0.61
1:C:3623:LEU:HD12	1:C:3624:LEU:N	2.16	0.61
1:C:4172:GLU:OE1	1:C:4175:ARG:NH1	2.34	0.61
1:A:990:GLU:OE2	1:A:1025:ARG:NH2	2.34	0.61
1:A:3623:LEU:HD12	1:A:3624:LEU:N	2.16	0.61
1:C:394:GLN:N	1:C:394:GLN:OE1	2.32	0.61
1:B:4172:GLU:OE1	1:B:4175:ARG:NH1	2.34	0.61
2:G:90:ILE:HG22	2:G:91:ILE:HG13	1.82	0.60
1:B:188:GLU:N	1:B:188:GLU:OE2	2.33	0.60
1:B:3400:VAL:HG23	1:B:3403:ARG:HH21	1.67	0.60
1:D:990:GLU:OE2	1:D:1025:ARG:NH2	2.34	0.60
1:D:4836:GLN:O	1:D:4840:THR:HG23	2.01	0.60
1:B:2309:SER:HB2	1:B:2314:LEU:HD21	1.81	0.60
1:D:188:GLU:N	1:D:188:GLU:OE2	2.33	0.60
1:D:1427:ILE:HG23	1:D:1428:LEU:HD22	1.82	0.60
1:C:919:ASN:HA	1:C:922:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:HIS:HB3	2:H:90:ILE:HB	1.83	0.60
1:B:399:GLN:O	1:B:403:MET:HG2	2.02	0.60
1:D:3623:LEU:HD12	1:D:3624:LEU:N	2.16	0.60
1:D:4687:TYR:O	1:D:4691:GLN:NE2	2.34	0.60
1:C:399:GLN:O	1:C:403:MET:HG2	2.01	0.60
1:D:399:GLN:O	1:D:403:MET:HG2	2.02	0.60
1:C:4836:GLN:O	1:C:4840:THR:HG23	2.01	0.60
2:E:42:ARG:HE	2:E:44:LYS:HE3	1.65	0.60
1:C:156:GLN:OE1	1:C:156:GLN:N	2.34	0.60
1:B:4687:TYR:O	1:B:4691:GLN:NE2	2.35	0.60
1:D:156:GLN:OE1	1:D:156:GLN:N	2.34	0.60
1:A:3951:PHE:O	1:A:3955:MET:HG3	2.02	0.60
1:A:4687:TYR:O	1:A:4691:GLN:NE2	2.34	0.60
1:C:3400:VAL:HG23	1:C:3403:ARG:HH21	1.67	0.60
1:C:3951:PHE:O	1:C:3955:MET:HG3	2.02	0.60
1:C:4687:TYR:O	1:C:4691:GLN:NE2	2.34	0.60
1:A:1062:GLN:NE2	1:A:1064:GLU:OE1	2.30	0.60
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.19	0.60
1:C:2108:GLU:O	1:C:3694:LYS:NZ	2.35	0.60
1:A:1427:ILE:HG23	1:A:1428:LEU:HD22	1.83	0.60
1:B:990:GLU:OE2	1:B:1025:ARG:NH2	2.34	0.60
1:D:3951:PHE:O	1:D:3955:MET:HG3	2.02	0.60
1:C:302:VAL:HB	1:C:306:LYS:HE3	1.84	0.60
1:C:3959:LYS:NZ	1:C:4022:ASP:OD2	2.31	0.60
1:A:2191:PHE:HD1	1:A:2198:MET:HE3	1.67	0.59
2:H:27:THR:HG23	2:H:100:ASP:HB3	1.83	0.59
1:C:3504:SER:HG	1:C:3507:THR:HG1	1.45	0.59
1:A:3400:VAL:HG23	1:A:3403:ARG:HH21	1.67	0.59
1:C:1619:ARG:NH2	1:C:1622:GLU:OE1	2.35	0.59
1:D:919:ASN:HA	1:D:922:LEU:HD23	1.82	0.59
1:D:1619:ARG:NH2	1:D:1622:GLU:OE1	2.35	0.59
1:C:2191:PHE:HD1	1:C:2198:MET:HE3	1.67	0.59
1:C:2765:LYS:HZ2	1:C:2860:PRO:HA	1.66	0.59
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.36	0.59
1:D:3412:LEU:HD11	1:D:3434:LEU:HD21	1.85	0.59
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.36	0.59
1:A:3412:LEU:HD11	1:A:3434:LEU:HD21	1.85	0.59
1:B:302:VAL:HB	1:B:306:LYS:HE3	1.84	0.59
1:D:545:ASP:OD1	1:D:582:HIS:NE2	2.32	0.59
1:D:4064:MET:HE1	1:D:4110:PHE:HD2	1.67	0.59
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.19	0.59
1:A:1619:ARG:NH2	1:A:1622:GLU:OE1	2.35	0.59
1:A:2108:GLU:O	1:A:3694:LYS:NZ	2.35	0.59
1:A:2128:TYR:OH	1:A:3676:ASP:OD2	2.20	0.59
1:A:2175:GLU:HG3	1:A:2228:MET:HB3	1.85	0.59
1:B:1870:VAL:HA	1:B:2090:LYS:HZ3	1.68	0.59
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.85	0.59
1:B:4064:MET:HE1	1:B:4110:PHE:HD2	1.67	0.59
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.36	0.59
1:D:2175:GLU:HG3	1:D:2228:MET:HB3	1.85	0.59
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.19	0.59
1:C:3412:LEU:HD11	1:C:3434:LEU:HD21	1.85	0.59
1:B:460:GLN:N	1:B:463:GLU:OE2	2.30	0.59
1:B:3951:PHE:O	1:B:3955:MET:HG3	2.02	0.59
1:D:3400:VAL:HG23	1:D:3403:ARG:HH21	1.67	0.59
1:C:970:LEU:HD23	1:C:1045:THR:HG23	1.85	0.59
1:C:1870:VAL:HA	1:C:2090:LYS:HZ3	1.68	0.59
1:D:3296:LEU:HG	1:D:3297:PRO:HD3	1.85	0.59
1:D:3530:GLN:N	1:D:3530:GLN:OE1	2.36	0.59
1:A:302:VAL:HB	1:A:306:LYS:HE3	1.84	0.59
2:E:27:THR:HG23	2:E:100:ASP:HB3	1.83	0.59
2:E:87:HIS:HB3	2:E:90:ILE:HB	1.84	0.59
1:B:970:LEU:HD23	1:B:1045:THR:HG23	1.85	0.59
1:C:4064:MET:HE1	1:C:4110:PHE:HD2	1.67	0.59
1:A:399:GLN:O	1:A:403:MET:HG2	2.02	0.58
1:A:4064:MET:HE1	1:A:4110:PHE:HD2	1.67	0.58
1:B:2191:PHE:HD1	1:B:2198:MET:HE3	1.67	0.58
1:B:2288:LEU:O	1:B:3849:ARG:NH1	2.31	0.58
1:B:5012:LYS:NZ	1:B:5016:GLU:OE2	2.33	0.58
1:C:545:ASP:OD1	1:C:582:HIS:NE2	2.32	0.58
1:A:4901:ILE:HG13	1:A:4913:ARG:NH2	2.18	0.58
1:B:4901:ILE:HG13	1:B:4913:ARG:NH2	2.18	0.58
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.36	0.58
1:B:1619:ARG:NH2	1:B:1622:GLU:OE1	2.36	0.58
1:D:1062:GLN:NE2	1:D:1064:GLU:OE1	2.30	0.58
1:A:3530:GLN:N	1:A:3530:GLN:OE1	2.36	0.58
1:D:2191:PHE:HD1	1:D:2198:MET:HE3	1.67	0.58
1:B:2456:ILE:O	1:B:2459:SER:OG	2.17	0.58
1:D:302:VAL:HB	1:D:306:LYS:HE3	1.84	0.58
1:D:2128:TYR:OH	1:D:3676:ASP:OD2	2.20	0.58
1:B:3530:GLN:OE1	1:B:3530:GLN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3530:GLN:OE1	1:C:3530:GLN:N	2.36	0.58
1:D:127:MET:HE3	1:D:127:MET:N	2.19	0.58
1:A:156:GLN:OE1	1:A:156:GLN:N	2.34	0.58
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.85	0.58
1:B:156:GLN:N	1:B:156:GLN:OE1	2.34	0.58
1:B:3412:LEU:HD11	1:B:3434:LEU:HD21	1.85	0.58
1:B:197:GLN:OE1	1:B:197:GLN:N	2.30	0.58
1:C:211:GLU:CD	1:C:211:GLU:H	2.12	0.58
1:C:1062:GLN:NE2	1:C:1064:GLU:OE1	2.30	0.58
1:C:4901:ILE:HG13	1:C:4913:ARG:NH2	2.18	0.58
1:A:3296:LEU:HG	1:A:3297:PRO:HD3	1.85	0.58
1:B:2128:TYR:OH	1:B:3676:ASP:OD2	2.20	0.58
1:C:3017:PHE:O	1:C:3036:LYS:NZ	2.37	0.58
1:B:1031:THR:O	1:B:1035:ASN:ND2	2.36	0.57
1:B:3270:ILE:HA	1:B:3274:LEU:HD12	1.86	0.57
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.21	0.57
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.85	0.57
1:B:211:GLU:H	1:B:211:GLU:CD	2.12	0.57
1:B:3296:LEU:HG	1:B:3297:PRO:HD3	1.85	0.57
1:D:970:LEU:HD23	1:D:1045:THR:HG23	1.85	0.57
1:C:3296:LEU:HG	1:C:3297:PRO:HD3	1.85	0.57
1:A:176:SER:OG	1:A:178:ARG:NH1	2.30	0.57
1:A:211:GLU:CD	1:A:211:GLU:H	2.12	0.57
1:B:127:MET:HE3	1:B:127:MET:N	2.19	0.57
1:D:3270:ILE:HA	1:D:3274:LEU:HD12	1.86	0.57
1:D:4901:ILE:HG13	1:D:4913:ARG:NH2	2.18	0.57
1:C:127:MET:HE3	1:C:127:MET:N	2.19	0.57
1:C:309:THR:O	1:C:313:SER:OG	2.18	0.57
1:A:545:ASP:OD1	1:A:582:HIS:NE2	2.32	0.57
1:A:2410:PRO:HB3	1:A:2415:ARG:HB3	1.86	0.57
1:B:2410:PRO:HB3	1:B:2415:ARG:HB3	1.86	0.57
1:B:2456:ILE:O	1:B:2460:LEU:HD22	2.05	0.57
1:D:2456:ILE:O	1:D:2460:LEU:HD22	2.05	0.57
1:C:2456:ILE:O	1:C:2460:LEU:HD22	2.05	0.57
1:A:970:LEU:HD23	1:A:1045:THR:HG23	1.85	0.57
1:A:3550:ARG:HG2	1:A:3594:ARG:NH1	2.20	0.57
1:B:3017:PHE:O	1:B:3036:LYS:NZ	2.37	0.57
1:C:2175:GLU:HG3	1:C:2228:MET:HB3	1.85	0.57
1:D:1031:THR:O	1:D:1035:ASN:ND2	2.36	0.57
1:D:2108:GLU:O	1:D:3694:LYS:NZ	2.35	0.57
1:C:3550:ARG:HG2	1:C:3594:ARG:NH1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.37	0.57
1:D:197:GLN:OE1	1:D:197:GLN:N	2.30	0.57
1:A:2881:ASN:HA	1:A:2884:ASN:ND2	2.20	0.57
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	1.87	0.57
1:B:3442:PHE:CE1	1:B:3511:VAL:HG12	2.39	0.57
1:D:1870:VAL:HA	1:D:2090:LYS:HZ3	1.68	0.57
1:D:2116:LEU:O	1:D:2120:MET:HG2	2.05	0.57
1:D:2410:PRO:HB3	1:D:2415:ARG:HB3	1.86	0.57
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.86	0.57
1:C:2881:ASN:HA	1:C:2884:ASN:ND2	2.20	0.57
1:A:2679:PHE:HB2	1:A:2706:ILE:HG21	1.87	0.57
1:D:211:GLU:CD	1:D:211:GLU:H	2.12	0.57
1:D:1987:SER:HB2	1:D:1994:ARG:HH22	1.70	0.57
1:D:2679:PHE:HB2	1:D:2706:ILE:HG21	1.87	0.57
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.23	0.57
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	1.87	0.56
1:B:2175:GLU:HG3	1:B:2228:MET:HB3	1.85	0.56
1:B:3550:ARG:HG2	1:B:3594:ARG:NH1	2.20	0.56
1:C:2116:LEU:O	1:C:2120:MET:HG2	2.05	0.56
1:C:2128:TYR:OH	1:C:3676:ASP:OD2	2.20	0.56
1:C:4555:LEU:HD21	1:C:4656:LEU:HD22	1.87	0.56
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.88	0.56
1:A:4137:ARG:NH2	1:A:4199:GLU:OE2	2.38	0.56
1:B:984:LEU:O	1:B:988:LEU:HG	2.05	0.56
1:B:2108:GLU:O	1:B:3694:LYS:NZ	2.35	0.56
1:B:2679:PHE:HB2	1:B:2706:ILE:HG21	1.87	0.56
1:B:2881:ASN:HA	1:B:2884:ASN:ND2	2.20	0.56
1:D:3017:PHE:O	1:D:3036:LYS:NZ	2.37	0.56
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.23	0.56
1:C:3850:GLN:NE2	1:C:3872:GLU:OE1	2.32	0.56
1:B:545:ASP:OD1	1:B:582:HIS:NE2	2.32	0.56
1:B:856:VAL:H	1:B:991:ASN:ND2	2.03	0.56
1:D:984:LEU:O	1:D:988:LEU:HG	2.05	0.56
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.87	0.56
1:D:2881:ASN:HA	1:D:2884:ASN:ND2	2.20	0.56
1:D:4006:ASP:N	1:D:4006:ASP:OD1	2.38	0.56
1:D:5012:LYS:NZ	1:D:5016:GLU:OE2	2.33	0.56
1:C:856:VAL:H	1:C:991:ASN:ND2	2.03	0.56
1:C:3270:ILE:HA	1:C:3274:LEU:HD12	1.86	0.56
1:C:4006:ASP:N	1:C:4006:ASP:OD1	2.38	0.56
1:A:516:LYS:O	1:A:520:ASN:ND2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:O	1:A:988:LEU:HG	2.05	0.56
1:A:3752:SER:OG	1:A:3755:GLU:OE1	2.23	0.56
1:C:2679:PHE:HB2	1:C:2706:ILE:HG21	1.87	0.56
1:C:3366:ARG:NH1	1:C:3440:GLU:OE1	2.34	0.56
1:A:2116:LEU:O	1:A:2120:MET:HG2	2.05	0.56
1:A:3270:ILE:HA	1:A:3274:LEU:HD12	1.86	0.56
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.39	0.56
1:A:4639:MET:HA	1:A:4642:ALA:HB3	1.87	0.56
1:B:2765:LYS:HZ3	1:B:2857:PRO:HB2	1.70	0.56
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.23	0.56
1:D:4137:ARG:NH2	1:D:4199:GLU:OE2	2.38	0.56
1:C:1999:ARG:HG2	1:C:3635:CYS:HB3	1.88	0.56
1:A:1987:SER:HB2	1:A:1994:ARG:HH22	1.70	0.56
1:B:2116:LEU:O	1:B:2120:MET:HG2	2.05	0.56
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.87	0.56
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.23	0.56
1:B:4006:ASP:OD1	1:B:4006:ASP:N	2.38	0.56
1:D:19:GLU:HG2	1:D:68:THR:HG22	1.88	0.56
1:D:856:VAL:H	1:D:991:ASN:ND2	2.03	0.56
1:D:3550:ARG:HG2	1:D:3594:ARG:NH1	2.20	0.56
1:C:983:THR:O	1:C:987:ARG:HG3	2.06	0.56
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.88	0.56
1:B:1990:GLU:OE1	1:B:1994:ARG:NH2	2.39	0.56
1:B:2867:LEU:HB2	1:B:2928:LYS:HZ3	1.71	0.56
1:B:4989:MET:O	1:B:4993:MET:HG3	2.06	0.56
1:C:1031:THR:O	1:C:1035:ASN:ND2	2.36	0.56
1:C:4639:MET:HA	1:C:4642:ALA:HB3	1.87	0.56
1:A:2456:ILE:O	1:A:2460:LEU:HD22	2.05	0.56
1:A:4060:LYS:O	1:A:4064:MET:HG3	2.06	0.56
1:A:4989:MET:O	1:A:4993:MET:HG3	2.06	0.56
1:B:1987:SER:HB2	1:B:1994:ARG:HH22	1.70	0.56
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.41	0.56
1:D:1990:GLU:OE1	1:D:1994:ARG:NH2	2.39	0.56
1:C:1272:LEU:HD22	1:C:1289:LEU:HD11	1.87	0.56
1:A:462:GLU:OE2	1:A:462:GLU:N	2.27	0.56
1:A:5012:LYS:NZ	1:A:5016:GLU:OE2	2.33	0.56
1:D:2867:LEU:HB2	1:D:2928:LYS:HZ3	1.71	0.56
1:D:3413:ILE:HD12	1:D:3509:LEU:HD23	1.88	0.56
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.41	0.56
1:C:1987:SER:HB2	1:C:1994:ARG:HH22	1.70	0.56
1:C:4137:ARG:NH2	1:C:4199:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5012:LYS:NZ	1:C:5016:GLU:OE2	2.33	0.56
1:A:872:GLU:HA	1:A:922:LEU:HD11	1.88	0.55
1:A:1990:GLU:OE1	1:A:1994:ARG:NH2	2.39	0.55
1:B:950:LEU:HD13	1:B:970:LEU:HD11	1.88	0.55
1:B:4137:ARG:NH2	1:B:4199:GLU:OE2	2.38	0.55
1:B:4639:MET:HA	1:B:4642:ALA:HB3	1.87	0.55
1:C:4989:MET:O	1:C:4993:MET:HG3	2.06	0.55
1:A:950:LEU:HD13	1:A:970:LEU:HD11	1.88	0.55
1:A:985:VAL:HG22	1:A:1043:VAL:HG21	1.89	0.55
1:B:4555:LEU:HD21	1:B:4656:LEU:HD22	1.87	0.55
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.87	0.55
1:C:4207:MET:HE2	1:C:4207:MET:HA	1.89	0.55
1:C:4686:LEU:HD12	1:C:4690:GLU:HG3	1.89	0.55
1:A:127:MET:HE3	1:A:127:MET:N	2.19	0.55
1:A:1999:ARG:HG2	1:A:3635:CYS:HB3	1.88	0.55
2:G:18:ARG:HG2	2:G:18:ARG:NH1	2.21	0.55
1:B:2751:LEU:HD13	1:B:2823:ILE:HD13	1.87	0.55
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.19	0.55
1:D:1272:LEU:HD22	1:D:1289:LEU:HD11	1.87	0.55
1:C:1990:GLU:OE1	1:C:1994:ARG:NH2	2.39	0.55
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.87	0.55
1:A:983:THR:O	1:A:987:ARG:HG3	2.06	0.55
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.88	0.55
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.41	0.55
1:B:3261:ALA:HB1	1:B:3265:GLU:HG3	1.88	0.55
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.88	0.55
1:D:4989:MET:O	1:D:4993:MET:HG3	2.06	0.55
1:C:3261:ALA:HB1	1:C:3265:GLU:HG3	1.88	0.55
1:A:19:GLU:HG2	1:A:68:THR:HG22	1.88	0.55
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.39	0.55
1:A:2639:MET:HE3	1:A:2640:PRO:N	2.22	0.55
1:B:2639:MET:HE3	1:B:2640:PRO:N	2.22	0.55
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.39	0.55
1:D:2751:LEU:HD13	1:D:2823:ILE:HD13	1.87	0.55
1:D:3850:GLN:NE2	1:D:3872:GLU:OE1	2.32	0.55
1:D:4060:LYS:O	1:D:4064:MET:HG3	2.06	0.55
1:D:4686:LEU:HD12	1:D:4690:GLU:HG3	1.88	0.55
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.41	0.55
1:B:983:THR:O	1:B:987:ARG:HG3	2.06	0.55
1:B:2029:GLN:NE2	1:B:2033:ASP:OD1	2.40	0.55
1:D:700:GLU:OE2	1:D:1458:HIS:NE2	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	1.87	0.55
1:D:4207:MET:HE2	1:D:4207:MET:HA	1.89	0.55
1:A:1031:THR:O	1:A:1035:ASN:ND2	2.36	0.55
1:A:1272:LEU:HD22	1:A:1289:LEU:HD11	1.88	0.55
1:B:462:GLU:OE2	1:B:462:GLU:N	2.27	0.55
1:B:4207:MET:HE2	1:B:4207:MET:HA	1.89	0.55
1:D:228:ASP:OD1	1:D:228:ASP:N	2.40	0.55
1:D:1999:ARG:HG2	1:D:3635:CYS:HB3	1.88	0.55
1:C:984:LEU:O	1:C:988:LEU:HG	2.05	0.55
1:C:2029:GLN:NE2	1:C:2033:ASP:OD1	2.40	0.55
1:A:856:VAL:H	1:A:991:ASN:ND2	2.04	0.55
2:G:50:LEU:H	2:G:50:LEU:HD12	1.71	0.55
1:B:4060:LYS:O	1:B:4064:MET:HG3	2.06	0.55
1:C:4060:LYS:O	1:C:4064:MET:HG3	2.06	0.55
1:A:2029:GLN:NE2	1:A:2033:ASP:OD1	2.40	0.55
1:A:3413:ILE:HD12	1:A:3509:LEU:HD23	1.89	0.55
1:A:4555:LEU:HD21	1:A:4656:LEU:HD22	1.87	0.55
1:B:19:GLU:HG2	1:B:68:THR:HG22	1.88	0.55
1:B:516:LYS:O	1:B:520:ASN:ND2	2.34	0.55
1:D:3638:MET:HE2	1:D:3638:MET:HA	1.89	0.55
1:D:4904:PRO:HB3	1:D:4913:ARG:HG2	1.89	0.55
1:C:516:LYS:O	1:C:520:ASN:ND2	2.34	0.55
1:C:950:LEU:HD13	1:C:970:LEU:HD11	1.88	0.55
1:A:228:ASP:OD1	1:A:228:ASP:N	2.40	0.55
1:A:3261:ALA:HB1	1:A:3265:GLU:HG3	1.88	0.55
1:A:4006:ASP:N	1:A:4006:ASP:OD1	2.38	0.55
1:B:4056:GLU:HG2	1:B:4166:LEU:HD13	1.89	0.55
1:B:4686:LEU:HD12	1:B:4690:GLU:HG3	1.89	0.55
1:D:309:THR:O	1:D:313:SER:OG	2.18	0.55
1:C:19:GLU:HG2	1:C:68:THR:HG22	1.88	0.55
1:D:950:LEU:HD13	1:D:970:LEU:HD11	1.88	0.54
1:C:2751:LEU:HD13	1:C:2823:ILE:HD13	1.87	0.54
1:A:2456:ILE:O	1:A:2459:SER:OG	2.17	0.54
1:A:2751:LEU:HD13	1:A:2823:ILE:HD13	1.87	0.54
1:A:3623:LEU:HD12	1:A:3624:LEU:H	1.72	0.54
1:A:4056:GLU:HG2	1:A:4166:LEU:HD13	1.89	0.54
1:B:3623:LEU:HD12	1:B:3624:LEU:H	1.72	0.54
1:D:2929:PHE:HA	1:D:2932:MET:SD	2.47	0.54
1:C:872:GLU:HA	1:C:922:LEU:HD11	1.88	0.54
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.23	0.54
1:B:3356:SER:OG	1:B:3357:HIS:ND1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:983:THR:O	1:D:987:ARG:HG3	2.06	0.54
1:D:985:VAL:HG22	1:D:1043:VAL:HG21	1.89	0.54
1:D:2029:GLN:NE2	1:D:2033:ASP:OD1	2.40	0.54
1:D:4639:MET:HA	1:D:4642:ALA:HB3	1.87	0.54
1:C:3413:ILE:HD12	1:C:3509:LEU:HD23	1.88	0.54
1:B:309:THR:O	1:B:313:SER:OG	2.18	0.54
1:B:1999:ARG:HG2	1:B:3635:CYS:HB3	1.88	0.54
1:B:3638:MET:HA	1:B:3638:MET:HE2	1.89	0.54
1:C:985:VAL:HG22	1:C:1043:VAL:HG21	1.89	0.54
1:C:3442:PHE:CE1	1:C:3511:VAL:HG12	2.39	0.54
1:D:872:GLU:HA	1:D:922:LEU:HD11	1.88	0.54
1:D:3261:ALA:HB1	1:D:3265:GLU:HG3	1.88	0.54
1:C:2456:ILE:O	1:C:2459:SER:OG	2.17	0.54
1:C:2819:TRP:CG	1:C:2877:GLN:HE22	2.26	0.54
1:A:2149:VAL:O	1:A:2153:MET:HG2	2.08	0.54
1:A:2736:ASP:O	1:A:2738:ARG:NH1	2.40	0.54
1:A:2924:GLN:O	1:A:2928:LYS:HG2	2.08	0.54
1:A:2929:PHE:HA	1:A:2932:MET:SD	2.47	0.54
1:B:985:VAL:HG22	1:B:1043:VAL:HG21	1.89	0.54
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.39	0.54
1:B:1272:LEU:HD22	1:B:1289:LEU:HD11	1.87	0.54
1:B:2736:ASP:O	1:B:2738:ARG:NH1	2.40	0.54
1:D:3673:MET:HE1	1:D:3728:ILE:HD13	1.89	0.54
1:D:3723:MET:HE2	1:D:3793:MET:SD	2.47	0.54
1:A:483:MET:HE2	1:A:483:MET:H	1.72	0.54
1:A:1870:VAL:HA	1:A:2090:LYS:HZ3	1.71	0.54
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.23	0.54
1:A:4207:MET:HA	1:A:4207:MET:HE2	1.89	0.54
1:B:2587:TYR:O	1:B:2590:SER:OG	2.18	0.54
1:B:3413:ILE:HD12	1:B:3509:LEU:HD23	1.88	0.54
1:B:3955:MET:HB3	1:B:4019:LEU:HD22	1.89	0.54
1:D:483:MET:HE2	1:D:483:MET:H	1.72	0.54
1:D:4555:LEU:HD21	1:D:4656:LEU:HD22	1.87	0.54
1:C:1996:ARG:NH2	1:C:1999:ARG:HE	2.05	0.54
1:C:2587:TYR:O	1:C:2590:SER:OG	2.18	0.54
1:C:2924:GLN:O	1:C:2928:LYS:HG2	2.08	0.54
1:C:3723:MET:HE2	1:C:3793:MET:SD	2.48	0.54
1:C:4056:GLU:HG2	1:C:4166:LEU:HD13	1.89	0.54
1:A:197:GLN:OE1	1:A:197:GLN:N	2.30	0.54
1:A:1996:ARG:NH2	1:A:1999:ARG:HE	2.05	0.54
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3673:MET:HE1	1:B:3728:ILE:HD13	1.89	0.54
1:D:2924:GLN:O	1:D:2928:LYS:HG2	2.08	0.54
1:D:4688:ILE:HG23	1:D:4732:PHE:CD1	2.43	0.54
1:C:462:GLU:OE2	1:C:462:GLU:N	2.27	0.54
1:C:2639:MET:HE3	1:C:2640:PRO:N	2.22	0.54
1:C:2929:PHE:HA	1:C:2932:MET:SD	2.47	0.54
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.88	0.54
1:A:4686:LEU:HD12	1:A:4690:GLU:HG3	1.89	0.54
2:F:18:ARG:HG2	2:F:18:ARG:NH1	2.21	0.54
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.21	0.54
1:D:622:THR:HG23	1:D:626:LEU:HD12	1.90	0.54
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.90	0.54
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.88	0.54
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.90	0.54
1:A:1289:LEU:HD12	1:A:1562:ILE:HD11	1.90	0.54
1:B:2149:VAL:O	1:B:2153:MET:HG2	2.08	0.54
1:D:3955:MET:HB3	1:D:4019:LEU:HD22	1.89	0.54
1:C:228:ASP:OD1	1:C:228:ASP:N	2.40	0.54
1:C:3955:MET:HB3	1:C:4019:LEU:HD22	1.89	0.54
1:A:622:THR:HG23	1:A:626:LEU:HD12	1.90	0.53
1:A:2867:LEU:HB2	1:A:2928:LYS:HZ3	1.72	0.53
1:A:3535:LEU:O	1:A:3539:ARG:HG2	2.08	0.53
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.89	0.53
1:B:2819:TRP:CG	1:B:2877:GLN:HE22	2.26	0.53
1:C:275:ARG:HH21	1:C:328:LYS:HG3	1.74	0.53
1:C:3638:MET:HE2	1:C:3638:MET:HA	1.90	0.53
1:A:2519:LEU:HD13	1:A:2575:ARG:HG3	1.90	0.53
1:A:2765:LYS:NZ	1:A:2860:PRO:HA	2.23	0.53
1:A:2819:TRP:CG	1:A:2877:GLN:HE22	2.26	0.53
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.41	0.53
1:A:3723:MET:HE2	1:A:3793:MET:SD	2.47	0.53
1:B:2929:PHE:HA	1:B:2932:MET:SD	2.47	0.53
1:D:1996:ARG:NH2	1:D:1999:ARG:HE	2.05	0.53
1:D:2736:ASP:O	1:D:2738:ARG:NH1	2.40	0.53
1:D:4056:GLU:HG2	1:D:4166:LEU:HD13	1.89	0.53
1:C:3673:MET:HE1	1:C:3728:ILE:HD13	1.89	0.53
1:A:3955:MET:HB3	1:A:4019:LEU:HD22	1.89	0.53
1:B:1289:LEU:HD12	1:B:1562:ILE:HD11	1.90	0.53
1:D:1289:LEU:HD12	1:D:1562:ILE:HD11	1.90	0.53
1:D:2149:VAL:O	1:D:2153:MET:HG2	2.08	0.53
1:D:2382:GLU:O	1:D:2386:ILE:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2639:MET:HE3	1:D:2640:PRO:N	2.22	0.53
1:D:2819:TRP:CG	1:D:2877:GLN:HE22	2.26	0.53
1:C:2736:ASP:O	1:C:2738:ARG:NH1	2.40	0.53
1:C:3623:LEU:HD12	1:C:3624:LEU:H	1.72	0.53
1:A:3442:PHE:CE1	1:A:3511:VAL:HG12	2.39	0.53
1:B:872:GLU:HA	1:B:922:LEU:HD11	1.88	0.53
1:B:2660:GLY:HA3	1:B:2666:VAL:HG22	1.91	0.53
1:B:2924:GLN:O	1:B:2928:LYS:HG2	2.08	0.53
1:B:3723:MET:HE2	1:B:3793:MET:SD	2.48	0.53
1:D:516:LYS:O	1:D:520:ASN:ND2	2.34	0.53
1:D:2522:LEU:HD13	1:D:2582:MET:HE1	1.91	0.53
1:D:3442:PHE:CE1	1:D:3511:VAL:HG12	2.39	0.53
1:C:2382:GLU:O	1:C:2386:ILE:HG23	2.09	0.53
1:C:2522:LEU:HD13	1:C:2582:MET:HE1	1.90	0.53
1:A:4759:ASP:O	1:A:4761:PRO:HD3	2.09	0.53
1:B:483:MET:HE2	1:B:483:MET:H	1.72	0.53
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.41	0.53
1:D:2519:LEU:HD13	1:D:2575:ARG:HG3	1.90	0.53
1:D:4759:ASP:O	1:D:4761:PRO:HD3	2.09	0.53
1:A:4910:GLU:O	1:A:4914:VAL:HG13	2.09	0.53
2:E:18:ARG:HG2	2:E:18:ARG:NH1	2.21	0.53
1:B:228:ASP:OD1	1:B:228:ASP:N	2.40	0.53
1:B:3535:LEU:O	1:B:3539:ARG:HG2	2.08	0.53
1:D:2587:TYR:O	1:D:2590:SER:OG	2.18	0.53
1:C:2660:GLY:HA3	1:C:2666:VAL:HG22	1.91	0.53
1:C:2765:LYS:NZ	1:C:2860:PRO:HA	2.23	0.53
1:C:2867:LEU:HB2	1:C:2928:LYS:HZ3	1.73	0.53
1:A:2660:GLY:HA3	1:A:2666:VAL:HG22	1.91	0.53
1:A:4688:ILE:HG23	1:A:4732:PHE:CD1	2.43	0.53
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.89	0.53
1:D:1078:GLU:OE2	1:D:1654:SER:OG	2.19	0.53
1:D:2660:GLY:HA3	1:D:2666:VAL:HG22	1.91	0.53
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.41	0.53
1:A:3638:MET:HE2	1:A:3638:MET:HA	1.89	0.53
1:B:2382:GLU:O	1:B:2386:ILE:HG23	2.09	0.53
1:B:4910:GLU:O	1:B:4914:VAL:HG13	2.09	0.53
1:D:3623:LEU:HD12	1:D:3624:LEU:H	1.72	0.53
1:D:4910:GLU:O	1:D:4914:VAL:HG13	2.09	0.53
1:D:4963:ILE:HD13	1:D:5030:LYS:HE3	1.91	0.53
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.41	0.53
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3673:MET:HE1	1:A:3728:ILE:HD13	1.89	0.53
2:H:79:ASP:OD2	2:H:80:TYR:N	2.42	0.53
2:G:16:PRO:HG3	2:G:106:LEU:HD11	1.89	0.53
1:B:2003:GLN:NE2	1:B:2007:ASN:OD1	2.42	0.53
1:B:2522:LEU:HD13	1:B:2582:MET:HE1	1.90	0.53
1:B:3366:ARG:NH1	1:B:3440:GLU:OE1	2.34	0.53
1:B:4627:MET:H	1:B:4627:MET:CE	2.22	0.53
1:C:3389:GLU:N	1:C:3389:GLU:OE2	2.42	0.53
2:E:4:VAL:HG22	2:E:74:LEU:HD22	1.91	0.53
2:F:50:LEU:HD12	2:F:50:LEU:H	1.72	0.53
1:B:622:THR:HG23	1:B:626:LEU:HD12	1.90	0.53
1:B:2519:LEU:HD13	1:B:2575:ARG:HG3	1.90	0.53
1:D:2765:LYS:NZ	1:D:2860:PRO:HA	2.23	0.53
1:D:2813:LEU:HD13	1:D:2816:MET:SD	2.49	0.53
1:C:483:MET:HE2	1:C:483:MET:H	1.73	0.53
1:C:2819:TRP:CD1	1:C:2877:GLN:HE22	2.27	0.53
1:C:4688:ILE:HG23	1:C:4732:PHE:CD1	2.43	0.53
1:C:4759:ASP:O	1:C:4761:PRO:HD3	2.09	0.53
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.27	0.52
1:B:3389:GLU:N	1:B:3389:GLU:OE2	2.42	0.52
1:B:3528:THR:HG23	1:B:3573:MET:HE3	1.91	0.52
1:B:4759:ASP:O	1:B:4761:PRO:HD3	2.09	0.52
1:D:2288:LEU:O	1:D:3849:ARG:NH1	2.31	0.52
1:D:3528:THR:HG23	1:D:3573:MET:HE3	1.91	0.52
1:A:3528:THR:HG23	1:A:3573:MET:HE3	1.91	0.52
1:A:4769:MET:SD	1:A:4769:MET:N	2.73	0.52
1:B:275:ARG:HH21	1:B:328:LYS:HG3	1.74	0.52
1:D:2186:MET:HE2	1:D:2235:PHE:HA	1.92	0.52
1:C:2149:VAL:O	1:C:2153:MET:HG2	2.08	0.52
1:C:2792:ARG:NH2	1:C:2798:SER:OG	2.43	0.52
1:A:3389:GLU:N	1:A:3389:GLU:OE2	2.42	0.52
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.41	0.52
1:D:3389:GLU:N	1:D:3389:GLU:OE2	2.42	0.52
1:C:283:ARG:NH1	1:C:290:TYR:OH	2.42	0.52
1:C:2186:MET:HE2	1:C:2235:PHE:HA	1.91	0.52
1:C:4910:GLU:O	1:C:4914:VAL:HG13	2.09	0.52
1:A:283:ARG:NH1	1:A:290:TYR:OH	2.43	0.52
1:A:923:GLN:O	1:A:927:GLU:HG2	2.10	0.52
1:B:2813:LEU:HD13	1:B:2816:MET:SD	2.49	0.52
1:B:4688:ILE:HG23	1:B:4732:PHE:CD1	2.43	0.52
1:D:275:ARG:HH21	1:D:328:LYS:HG3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3366:ARG:NH1	1:D:3440:GLU:OE1	2.34	0.52
1:D:3535:LEU:O	1:D:3539:ARG:HG2	2.08	0.52
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.23	0.52
1:C:622:THR:HG23	1:C:626:LEU:HD12	1.90	0.52
1:C:2309:SER:OG	1:C:2321:ILE:O	2.20	0.52
1:C:3288:GLY:HA2	1:C:3303:PRO:HB3	1.92	0.52
1:C:3528:THR:HG23	1:C:3573:MET:HE3	1.91	0.52
1:A:293:LEU:HD13	1:A:378:LEU:HD12	1.91	0.52
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.42	0.52
1:A:913:LEU:HD11	1:A:918:ARG:HE	1.75	0.52
1:A:2186:MET:HE2	1:A:2235:PHE:HA	1.92	0.52
1:A:2813:LEU:HD13	1:A:2816:MET:SD	2.50	0.52
2:G:4:VAL:HG22	2:G:74:LEU:HD22	1.92	0.52
1:D:923:GLN:O	1:D:927:GLU:HG2	2.10	0.52
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.27	0.52
1:D:2309:SER:OG	1:D:2321:ILE:O	2.20	0.52
1:D:2456:ILE:O	1:D:2459:SER:OG	2.17	0.52
1:D:3545:THR:HG22	1:D:3548:GLU:HG3	1.91	0.52
1:C:308:HIS:CE1	1:C:310:LYS:HB3	2.45	0.52
1:A:1175:SER:OG	1:A:1180:ARG:NH1	2.43	0.52
1:A:2382:GLU:O	1:A:2386:ILE:HG23	2.09	0.52
1:A:4963:ILE:HD13	1:A:5030:LYS:HE3	1.91	0.52
2:E:44:LYS:HD2	2:E:44:LYS:O	2.10	0.52
1:B:923:GLN:O	1:B:927:GLU:HG2	2.10	0.52
1:B:1996:ARG:NH2	1:B:1999:ARG:HE	2.05	0.52
1:B:2751:LEU:O	1:B:2755:ILE:HG12	2.10	0.52
1:B:2819:TRP:CD1	1:B:2877:GLN:HE22	2.27	0.52
1:D:913:LEU:HD11	1:D:918:ARG:HE	1.75	0.52
1:D:1175:SER:OG	1:D:1180:ARG:NH1	2.43	0.52
1:D:2792:ARG:NH2	1:D:2798:SER:OG	2.43	0.52
1:C:293:LEU:HD13	1:C:378:LEU:HD12	1.91	0.52
1:C:2637:ALA:C	1:C:2640:PRO:HD2	2.35	0.52
1:A:4627:MET:H	1:A:4627:MET:CE	2.22	0.52
2:H:44:LYS:HD2	2:H:44:LYS:O	2.10	0.52
1:B:308:HIS:CE1	1:B:310:LYS:HB3	2.45	0.52
1:B:884:LEU:O	1:B:887:ILE:HG22	2.10	0.52
1:B:913:LEU:HD11	1:B:918:ARG:HE	1.75	0.52
1:D:2637:ALA:C	1:D:2640:PRO:HD2	2.35	0.52
1:C:2003:GLN:NE2	1:C:2007:ASN:OD1	2.42	0.52
1:C:2519:LEU:HD13	1:C:2575:ARG:HG3	1.90	0.52
1:C:3535:LEU:O	1:C:3539:ARG:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4640:GLU:HB3	1:C:4641:PRO:HD3	1.92	0.52
1:C:4963:ILE:HD13	1:C:5030:LYS:HE3	1.91	0.52
1:A:275:ARG:HH21	1:A:328:LYS:HG3	1.74	0.52
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.41	0.52
2:E:16:PRO:HG3	2:E:106:LEU:HD11	1.91	0.52
2:G:22:CYS:SG	2:G:50:LEU:HD11	2.50	0.52
2:F:79:ASP:OD1	2:F:80:TYR:N	2.43	0.52
1:B:4963:ILE:HD13	1:B:5030:LYS:HE3	1.91	0.52
1:D:867:LEU:HG	1:D:929:LEU:HD13	1.92	0.52
1:D:2382:GLU:OE1	1:D:2385:ARG:NH1	2.38	0.52
1:C:1547:LYS:NZ	1:C:1642:PRO:O	2.43	0.52
1:C:2751:LEU:O	1:C:2755:ILE:HG12	2.10	0.52
1:C:3443:ILE:HG12	1:C:3605:HIS:CD2	2.45	0.52
1:A:308:HIS:CE1	1:A:310:LYS:HB3	2.45	0.52
1:A:2587:TYR:O	1:A:2590:SER:OG	2.18	0.52
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.92	0.52
2:E:22:CYS:SG	2:E:50:LEU:HD11	2.50	0.52
1:B:1547:LYS:NZ	1:B:1642:PRO:O	2.43	0.52
1:B:2001:PRO:HB3	1:B:3864:THR:HB	1.92	0.52
1:B:2309:SER:OG	1:B:2321:ILE:O	2.20	0.52
1:B:2792:ARG:NH2	1:B:2798:SER:OG	2.43	0.52
1:D:283:ARG:NH1	1:D:290:TYR:OH	2.42	0.52
1:C:2382:GLU:OE1	1:C:2385:ARG:NH1	2.38	0.52
1:C:4627:MET:H	1:C:4627:MET:CE	2.22	0.52
1:A:2522:LEU:HD13	1:A:2582:MET:HE1	1.90	0.52
1:A:3443:ILE:HG12	1:A:3605:HIS:CD2	2.45	0.52
2:E:79:ASP:OD2	2:E:80:TYR:N	2.43	0.52
1:B:1175:SER:OG	1:B:1180:ARG:NH1	2.43	0.52
1:B:1861:GLN:O	1:B:1865:MET:HE3	2.11	0.52
1:B:2573:GLU:OE2	1:B:2615:ARG:NE	2.42	0.52
1:B:3718:GLU:HG3	1:B:3723:MET:HE1	1.92	0.52
1:D:2819:TRP:CD1	1:D:2877:GLN:HE22	2.27	0.52
1:C:867:LEU:HG	1:C:929:LEU:HD13	1.92	0.52
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.21	0.52
1:C:1289:LEU:HD12	1:C:1562:ILE:HD11	1.90	0.52
1:A:309:THR:O	1:A:313:SER:OG	2.18	0.51
1:A:3455:GLU:OE2	1:A:3508:SER:OG	2.28	0.51
1:A:3718:GLU:HG3	1:A:3723:MET:HE1	1.93	0.51
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.92	0.51
1:B:3443:ILE:HG12	1:B:3605:HIS:CD2	2.45	0.51
1:D:2812:SER:O	1:D:2816:MET:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3288:GLY:HA2	1:D:3303:PRO:HB3	1.92	0.51
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.92	0.51
1:C:952:LYS:HD3	1:C:970:LEU:HA	1.92	0.51
1:C:2813:LEU:HD13	1:C:2816:MET:SD	2.50	0.51
1:C:3545:THR:HG22	1:C:3548:GLU:HG3	1.91	0.51
1:A:1547:LYS:NZ	1:A:1642:PRO:O	2.43	0.51
1:A:2637:ALA:C	1:A:2640:PRO:HD2	2.35	0.51
1:A:2792:ARG:NH2	1:A:2798:SER:OG	2.43	0.51
2:F:4:VAL:HG22	2:F:74:LEU:HD22	1.92	0.51
1:B:975:VAL:HG12	1:B:1044:ARG:HH11	1.75	0.51
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.27	0.51
1:B:2186:MET:HE2	1:B:2235:PHE:HA	1.92	0.51
1:B:3916:ILE:HG22	1:B:3980:LEU:HD21	1.93	0.51
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.41	0.51
1:A:3545:THR:HG22	1:A:3548:GLU:HG3	1.91	0.51
1:A:4640:GLU:HB3	1:A:4641:PRO:HD3	1.92	0.51
2:G:79:ASP:OD2	2:G:80:TYR:N	2.42	0.51
1:B:3288:GLY:HA2	1:B:3303:PRO:HB3	1.92	0.51
1:D:293:LEU:HD13	1:D:378:LEU:HD12	1.91	0.51
1:D:1547:LYS:NZ	1:D:1642:PRO:O	2.43	0.51
1:D:1861:GLN:O	1:D:1865:MET:HE3	2.10	0.51
1:D:2751:LEU:O	1:D:2755:ILE:HG12	2.10	0.51
1:D:4640:GLU:HB3	1:D:4641:PRO:HD3	1.92	0.51
1:C:923:GLN:O	1:C:927:GLU:HG2	2.10	0.51
1:C:1175:SER:OG	1:C:1180:ARG:NH1	2.43	0.51
1:C:3356:SER:OG	1:C:3357:HIS:ND1	2.38	0.51
1:C:3377:GLU:HA	1:C:3380:ARG:HG2	1.92	0.51
1:A:2155:LEU:HD21	1:A:2198:MET:HE1	1.92	0.51
1:A:2812:SER:O	1:A:2816:MET:HE3	2.10	0.51
1:A:2819:TRP:CD1	1:A:2877:GLN:HE22	2.27	0.51
1:A:3182:TYR:HA	1:A:3185:LYS:HE3	1.93	0.51
1:B:293:LEU:HD13	1:B:378:LEU:HD12	1.91	0.51
1:D:70:GLU:OE2	1:D:110:ARG:NE	2.38	0.51
1:D:451:TYR:CZ	1:D:474:ARG:HD2	2.46	0.51
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.42	0.51
1:D:975:VAL:HG12	1:D:1044:ARG:HH11	1.75	0.51
1:D:3916:ILE:HG22	1:D:3980:LEU:HD21	1.93	0.51
1:C:913:LEU:HD11	1:C:918:ARG:HE	1.75	0.51
1:C:2001:PRO:HB3	1:C:3864:THR:HB	1.92	0.51
1:C:2327:GLY:O	1:C:2331:TYR:HD1	1.94	0.51
1:C:3916:ILE:HG22	1:C:3980:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:GLU:OE2	1:A:1458:HIS:NE2	2.33	0.51
1:B:952:LYS:HD3	1:B:970:LEU:HA	1.93	0.51
1:B:3106:MET:SD	1:B:3129:LEU:HA	2.51	0.51
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.44	0.51
1:D:127:MET:H	1:D:127:MET:CE	2.21	0.51
1:D:2155:LEU:HD21	1:D:2198:MET:HE1	1.92	0.51
1:D:3455:GLU:OE2	1:D:3508:SER:OG	2.28	0.51
1:C:975:VAL:HG12	1:C:1044:ARG:HH11	1.75	0.51
1:C:3455:GLU:OE2	1:C:3508:SER:OG	2.28	0.51
1:A:975:VAL:HG12	1:A:1044:ARG:HH11	1.75	0.51
1:A:2751:LEU:O	1:A:2755:ILE:HG12	2.10	0.51
1:B:2637:ALA:C	1:B:2640:PRO:HD2	2.35	0.51
1:B:3391:GLU:HG3	1:B:3395:ARG:HE	1.76	0.51
1:D:308:HIS:CE1	1:D:310:LYS:HB3	2.45	0.51
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.27	0.51
1:C:5013:MET:HE1	1:C:5020:ASP:HB2	1.93	0.51
1:A:127:MET:H	1:A:127:MET:CE	2.22	0.51
1:A:451:TYR:CZ	1:A:474:ARG:HD2	2.46	0.51
1:A:884:LEU:O	1:A:887:ILE:HG22	2.10	0.51
1:A:2749:GLU:HG3	1:A:2752:ASP:HB2	1.93	0.51
1:A:3862:ASP:OD1	1:A:3862:ASP:N	2.44	0.51
1:B:451:TYR:CZ	1:B:474:ARG:HD2	2.46	0.51
1:D:3182:TYR:HA	1:D:3185:LYS:HE3	1.93	0.51
1:D:5013:MET:HE1	1:D:5020:ASP:HB2	1.93	0.51
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.93	0.51
1:B:1293:LEU:HD11	1:B:1594:ARG:HD3	1.93	0.51
1:B:2327:GLY:O	1:B:2331:TYR:HD1	1.94	0.51
1:D:2749:GLU:HG3	1:D:2752:ASP:HB2	1.93	0.51
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.42	0.51
1:C:884:LEU:O	1:C:887:ILE:HG22	2.10	0.51
1:C:1293:LEU:HD11	1:C:1594:ARG:HD3	1.93	0.51
1:C:1861:GLN:O	1:C:1865:MET:HE3	2.10	0.51
1:C:2155:LEU:HD21	1:C:2198:MET:HE1	1.92	0.51
1:A:2166:LEU:HD11	1:A:2206:THR:HG23	1.93	0.51
1:A:3916:ILE:HG22	1:A:3980:LEU:HD21	1.93	0.51
1:A:4063:ASP:OD1	1:A:4064:MET:N	2.44	0.51
1:A:4843:LEU:HD21	1:D:4827:LEU:HD21	1.93	0.51
1:B:867:LEU:HG	1:B:929:LEU:HD13	1.92	0.51
1:B:2382:GLU:OE1	1:B:2385:ARG:NH1	2.38	0.51
1:B:3590:GLU:O	1:B:3594:ARG:HG2	2.11	0.51
1:B:5013:MET:HE1	1:B:5020:ASP:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1492:CYS:SG	1:D:1494:MET:HG3	2.51	0.51
1:D:2001:PRO:HB3	1:D:3864:THR:HB	1.92	0.51
1:D:3443:ILE:HG12	1:D:3605:HIS:CD2	2.45	0.51
1:D:3718:GLU:HG3	1:D:3723:MET:HE1	1.93	0.51
1:C:929:LEU:HA	1:C:932:LEU:HD12	1.93	0.51
1:A:1861:GLN:O	1:A:1865:MET:HE3	2.10	0.51
1:A:2001:PRO:HB3	1:A:3864:THR:HB	1.92	0.51
1:A:2327:GLY:O	1:A:2331:TYR:HD1	1.94	0.51
1:A:5013:MET:HE1	1:A:5020:ASP:HB2	1.93	0.51
2:F:44:LYS:HD2	2:F:44:LYS:O	2.11	0.51
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.93	0.51
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.44	0.51
1:B:2166:LEU:HD11	1:B:2206:THR:HG23	1.93	0.51
1:B:2812:SER:O	1:B:2816:MET:HE3	2.10	0.51
1:D:2311:PRO:HA	1:D:2314:LEU:HD23	1.93	0.51
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.93	0.51
1:C:2166:LEU:HD11	1:C:2206:THR:HG23	1.93	0.51
1:C:2495:VAL:HG22	1:C:2498:HIS:CE1	2.46	0.51
1:C:3260:GLY:HA2	1:C:3325:ASN:ND2	2.26	0.51
1:A:2495:VAL:HG22	1:A:2498:HIS:CE1	2.46	0.50
1:A:3202:PRO:HB2	1:A:3216:CYS:SG	2.51	0.50
1:B:127:MET:H	1:B:127:MET:CE	2.21	0.50
1:B:2155:LEU:HD21	1:B:2198:MET:HE1	1.92	0.50
1:B:2514:ASN:OD1	1:B:2514:ASN:N	2.45	0.50
1:B:3182:TYR:HA	1:B:3185:LYS:HE3	1.92	0.50
1:B:3545:THR:HG22	1:B:3548:GLU:HG3	1.91	0.50
1:B:4063:ASP:OD1	1:B:4064:MET:N	2.44	0.50
1:B:4064:MET:HE1	1:B:4110:PHE:CD2	2.46	0.50
1:B:4640:GLU:HB3	1:B:4641:PRO:HD3	1.92	0.50
1:D:884:LEU:O	1:D:887:ILE:HG22	2.10	0.50
1:D:2003:GLN:NE2	1:D:2007:ASN:OD1	2.42	0.50
1:D:2495:VAL:HG22	1:D:2498:HIS:CE1	2.46	0.50
1:D:2812:SER:OG	1:D:2882:TYR:OH	2.15	0.50
1:D:3357:HIS:O	1:D:3361:THR:HG23	2.11	0.50
1:C:1997:GLU:O	1:C:2000:SER:OG	2.27	0.50
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.44	0.50
1:C:3240:CYS:HB3	1:C:3243:ILE:HG12	1.93	0.50
1:A:2479:LEU:HB2	1:A:2541:PHE:HZ	1.77	0.50
2:H:4:VAL:HG22	2:H:74:LEU:HD22	1.93	0.50
1:B:3719:ASP:O	1:B:3723:MET:HE3	2.12	0.50
1:D:462:GLU:OE2	1:D:462:GLU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2166:LEU:HD11	1:D:2206:THR:HG23	1.93	0.50
1:D:3240:CYS:HB3	1:D:3243:ILE:HG12	1.93	0.50
1:D:4064:MET:HE1	1:D:4110:PHE:CD2	2.46	0.50
1:C:451:TYR:CZ	1:C:474:ARG:HD2	2.46	0.50
1:C:3357:HIS:O	1:C:3361:THR:HG23	2.11	0.50
1:C:3719:ASP:O	1:C:3723:MET:HE3	2.12	0.50
1:C:4064:MET:HE1	1:C:4110:PHE:CD2	2.46	0.50
1:A:3106:MET:SD	1:A:3129:LEU:HA	2.51	0.50
1:A:3590:GLU:O	1:A:3594:ARG:HG2	2.11	0.50
1:A:3872:GLU:HG3	1:A:3874:VAL:H	1.77	0.50
2:E:50:LEU:H	2:E:50:LEU:HD12	1.75	0.50
1:D:952:LYS:HD3	1:D:970:LEU:HA	1.93	0.50
1:D:2224:ARG:HG2	1:D:2225:PHE:CD2	2.47	0.50
1:D:3872:GLU:HG3	1:D:3874:VAL:H	1.77	0.50
1:C:3106:MET:SD	1:C:3129:LEU:HA	2.51	0.50
1:C:3391:GLU:HG3	1:C:3395:ARG:HE	1.76	0.50
1:A:952:LYS:HD3	1:A:970:LEU:HA	1.93	0.50
1:A:3260:GLY:HA2	1:A:3325:ASN:ND2	2.26	0.50
1:B:2479:LEU:HB2	1:B:2541:PHE:HZ	1.76	0.50
1:B:3202:PRO:HB2	1:B:3216:CYS:SG	2.51	0.50
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.93	0.50
1:D:2514:ASN:OD1	1:D:2514:ASN:N	2.45	0.50
1:D:3202:PRO:HB2	1:D:3216:CYS:SG	2.51	0.50
1:C:1492:CYS:SG	1:C:1494:MET:HG3	2.51	0.50
1:C:2479:LEU:HB2	1:C:2541:PHE:HZ	1.77	0.50
1:C:2749:GLU:HG3	1:C:2752:ASP:HB2	1.93	0.50
1:A:1492:CYS:SG	1:A:1494:MET:HG3	2.51	0.50
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	1.92	0.50
1:A:3391:GLU:HG3	1:A:3395:ARG:HE	1.76	0.50
1:B:2462:PRO:HG2	1:B:2465:ASP:HB2	1.93	0.50
1:B:3260:GLY:HA2	1:B:3325:ASN:ND2	2.27	0.50
1:D:1252:HIS:O	1:D:1275:ARG:NH1	2.45	0.50
1:D:2538:THR:O	1:D:2542:SER:HB2	2.11	0.50
1:D:3604:TYR:O	1:D:3607:GLU:HG3	2.12	0.50
1:C:3718:GLU:HG3	1:C:3723:MET:HE1	1.93	0.50
1:A:867:LEU:HG	1:A:929:LEU:HD13	1.92	0.50
1:A:2155:LEU:HD11	1:A:2198:MET:CE	2.42	0.50
2:G:44:LYS:HD2	2:G:44:LYS:O	2.12	0.50
1:B:2495:VAL:HG22	1:B:2498:HIS:CE1	2.46	0.50
1:D:2462:PRO:HG2	1:D:2465:ASP:HB2	1.93	0.50
1:D:2573:GLU:OE2	1:D:2615:ARG:NE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3356:SER:OG	1:D:3357:HIS:ND1	2.38	0.50
1:D:4063:ASP:OD1	1:D:4064:MET:N	2.44	0.50
1:C:2514:ASN:OD1	1:C:2514:ASN:N	2.44	0.50
1:C:2812:SER:O	1:C:2816:MET:HE3	2.10	0.50
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.45	0.50
1:A:3266:MET:O	1:A:3266:MET:HG2	2.12	0.50
1:B:929:LEU:HA	1:B:932:LEU:HD12	1.93	0.50
1:B:1252:HIS:O	1:B:1275:ARG:NH1	2.45	0.50
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	1.93	0.50
1:D:2327:GLY:O	1:D:2331:TYR:HD1	1.94	0.50
1:D:2827:ARG:NH2	1:D:2935:TYR:OH	2.45	0.50
1:D:3266:MET:O	1:D:3266:MET:HG2	2.12	0.50
1:D:3391:GLU:HG3	1:D:3395:ARG:HE	1.76	0.50
1:D:3719:ASP:O	1:D:3723:MET:HE3	2.12	0.50
1:C:601:ASP:OD1	1:C:1665:HIS:ND1	2.41	0.50
1:C:2462:PRO:HG2	1:C:2465:ASP:HB2	1.93	0.50
1:C:3539:ARG:NH1	1:C:3542:LEU:HD22	2.21	0.50
1:C:3862:ASP:N	1:C:3862:ASP:OD1	2.44	0.50
1:C:4063:ASP:OD1	1:C:4064:MET:N	2.44	0.50
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.21	0.50
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.44	0.50
1:A:2538:THR:O	1:A:2542:SER:HB2	2.11	0.50
1:B:2827:ARG:NH2	1:B:2935:TYR:OH	2.45	0.50
1:D:127:MET:SD	1:D:128:THR:HG23	2.52	0.50
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.44	0.50
1:D:2781:VAL:HA	1:D:2789:PRO:HB2	1.93	0.50
1:C:2224:ARG:HG2	1:C:2225:PHE:CD2	2.47	0.50
1:C:3182:TYR:HA	1:C:3185:LYS:HE3	1.92	0.50
1:C:3604:TYR:O	1:C:3607:GLU:HG3	2.12	0.50
1:C:3872:GLU:HG3	1:C:3874:VAL:H	1.77	0.50
1:A:2514:ASN:OD1	1:A:2514:ASN:N	2.44	0.50
1:A:3357:HIS:O	1:A:3361:THR:HG23	2.11	0.50
1:A:3556:ASN:HB3	1:A:3559:LEU:HD13	1.94	0.50
2:G:79:ASP:OD2	2:G:80:TYR:HD2	1.95	0.50
2:F:79:ASP:OD1	2:F:80:TYR:HD1	1.95	0.50
1:B:2311:PRO:HA	1:B:2314:LEU:HD23	1.93	0.50
1:B:3240:CYS:HB3	1:B:3243:ILE:HG12	1.93	0.50
1:D:2155:LEU:HD11	1:D:2198:MET:CE	2.42	0.50
1:D:3629:ARG:HA	1:D:3632:VAL:HG22	1.94	0.50
1:C:127:MET:SD	1:C:128:THR:HG23	2.52	0.50
1:C:758:ARG:HG2	1:C:763:PRO:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1252:HIS:O	1:C:1275:ARG:NH1	2.45	0.50
1:C:3556:ASN:HB3	1:C:3559:LEU:HD13	1.94	0.50
1:A:127:MET:SD	1:A:128:THR:HG23	2.52	0.49
1:B:1492:CYS:SG	1:B:1494:MET:HG3	2.51	0.49
1:B:1997:GLU:O	1:B:2000:SER:OG	2.28	0.49
1:B:2538:THR:O	1:B:2542:SER:HB2	2.11	0.49
1:B:3872:GLU:HG3	1:B:3874:VAL:H	1.77	0.49
1:D:3433:GLU:HG3	1:D:3437:MET:HE3	1.94	0.49
1:D:3590:GLU:O	1:D:3594:ARG:HG2	2.11	0.49
1:D:3604:TYR:O	1:D:3608:GLN:HG2	2.13	0.49
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.44	0.49
1:C:11:VAL:HG11	1:C:164:ARG:HD3	1.94	0.49
1:A:1293:LEU:HD11	1:A:1594:ARG:HD3	1.93	0.49
1:A:3366:ARG:NH1	1:A:3440:GLU:OE1	2.34	0.49
1:A:3433:GLU:HG3	1:A:3437:MET:HE3	1.94	0.49
1:B:11:VAL:HG11	1:B:164:ARG:HD3	1.94	0.49
1:D:929:LEU:HA	1:D:932:LEU:HD12	1.93	0.49
1:D:2208:MET:HE1	1:D:2250:MET:HE1	1.94	0.49
1:D:2250:MET:O	1:D:2250:MET:HE3	2.12	0.49
1:D:3106:MET:SD	1:D:3129:LEU:HA	2.51	0.49
1:D:3233:PRO:HB2	1:D:3238:GLU:HB2	1.94	0.49
1:D:3556:ASN:HB3	1:D:3559:LEU:HD13	1.94	0.49
1:D:4627:MET:H	1:D:4627:MET:CE	2.22	0.49
1:C:127:MET:H	1:C:127:MET:CE	2.22	0.49
1:C:1031:THR:HG22	1:C:1035:ASN:HD21	1.78	0.49
1:C:2781:VAL:HA	1:C:2789:PRO:HB2	1.93	0.49
1:C:3590:GLU:O	1:C:3594:ARG:HG2	2.11	0.49
1:A:2208:MET:HE1	1:A:2250:MET:HE1	1.95	0.49
1:A:2311:PRO:HA	1:A:2314:LEU:HD23	1.93	0.49
1:B:283:ARG:NH1	1:B:290:TYR:OH	2.42	0.49
1:B:2155:LEU:HD11	1:B:2198:MET:CE	2.42	0.49
1:B:2781:VAL:HA	1:B:2789:PRO:HB2	1.93	0.49
1:D:320:LYS:NZ	1:D:383:HIS:O	2.32	0.49
1:C:2827:ARG:NH2	1:C:2935:TYR:OH	2.45	0.49
1:C:3433:GLU:HG3	1:C:3437:MET:HE3	1.95	0.49
1:A:2462:PRO:HG2	1:A:2465:ASP:HB2	1.93	0.49
1:A:3332:ALA:HB3	1:A:3403:ARG:NH1	2.28	0.49
1:A:3719:ASP:O	1:A:3723:MET:HE3	2.12	0.49
1:B:127:MET:SD	1:B:128:THR:HG23	2.52	0.49
1:B:3266:MET:HG2	1:B:3266:MET:O	2.12	0.49
1:B:3357:HIS:O	1:B:3361:THR:HG23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3260:GLY:HA2	1:D:3325:ASN:ND2	2.27	0.49
1:D:3539:ARG:NH1	1:D:3542:LEU:HD22	2.21	0.49
1:C:197:GLN:OE1	1:C:197:GLN:N	2.30	0.49
1:C:2155:LEU:HD11	1:C:2198:MET:CE	2.42	0.49
1:C:2311:PRO:HA	1:C:2314:LEU:HD23	1.93	0.49
1:C:2538:THR:O	1:C:2542:SER:HB2	2.11	0.49
1:C:3233:PRO:HB2	1:C:3238:GLU:HB2	1.94	0.49
1:C:3266:MET:O	1:C:3266:MET:HG2	2.12	0.49
1:C:3332:ALA:HB3	1:C:3403:ARG:NH1	2.28	0.49
1:A:3629:ARG:HA	1:A:3632:VAL:HG22	1.94	0.49
1:A:4064:MET:HE1	1:A:4110:PHE:CD2	2.46	0.49
1:B:3604:TYR:O	1:B:3608:GLN:HG2	2.13	0.49
1:C:2477:PRO:HB3	1:C:2487:GLN:HG2	1.95	0.49
1:C:3202:PRO:HB2	1:C:3216:CYS:SG	2.51	0.49
1:C:3449:HIS:C	1:C:3449:HIS:ND1	2.71	0.49
1:A:2827:ARG:NH2	1:A:2935:TYR:OH	2.45	0.49
1:A:3240:CYS:HB3	1:A:3243:ILE:HG12	1.93	0.49
1:A:4736:ARG:NH2	1:D:4079:ASP:OD2	2.36	0.49
1:B:2546:MET:HE2	1:B:2546:MET:HA	1.95	0.49
1:B:3604:TYR:O	1:B:3607:GLU:HG3	2.12	0.49
1:D:3332:ALA:HB3	1:D:3403:ARG:NH1	2.28	0.49
1:C:499:THR:HG23	1:C:502:HIS:H	1.77	0.49
1:C:3604:TYR:O	1:C:3608:GLN:HG2	2.12	0.49
1:A:1163:THR:HG22	1:A:1168:VAL:HA	1.95	0.49
1:A:2781:VAL:HA	1:A:2789:PRO:HB2	1.93	0.49
1:B:417:GLY:O	1:B:420:SER:OG	2.28	0.49
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.42	0.49
1:B:758:ARG:HG2	1:B:763:PRO:HA	1.94	0.49
1:B:3332:ALA:HB3	1:B:3403:ARG:NH1	2.28	0.49
1:D:1293:LEU:HD11	1:D:1594:ARG:HD3	1.93	0.49
1:C:3629:ARG:HA	1:C:3632:VAL:HG22	1.94	0.49
1:A:684:VAL:HG22	1:A:781:VAL:HG12	1.95	0.49
1:A:2382:GLU:OE1	1:A:2385:ARG:NH1	2.38	0.49
1:A:2546:MET:HA	1:A:2546:MET:HE2	1.95	0.49
1:A:3604:TYR:O	1:A:3607:GLU:HG3	2.12	0.49
2:H:79:ASP:OD2	2:H:80:TYR:HD1	1.96	0.49
2:F:22:CYS:SG	2:F:50:LEU:HD11	2.53	0.49
1:B:1170:MET:HE1	1:B:1176:GLU:HA	1.95	0.49
1:B:3449:HIS:ND1	1:B:3449:HIS:C	2.71	0.49
1:D:499:THR:HG23	1:D:502:HIS:H	1.77	0.49
1:D:2479:LEU:HB2	1:D:2541:PHE:HZ	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2812:SER:OG	1:C:2882:TYR:OH	2.15	0.49
1:A:758:ARG:HG2	1:A:763:PRO:HA	1.94	0.49
1:A:2003:GLN:NE2	1:A:2007:ASN:OD1	2.42	0.49
1:A:2250:MET:O	1:A:2250:MET:HE3	2.12	0.49
1:A:3539:ARG:HH11	1:A:3539:ARG:HA	1.78	0.49
1:A:3604:TYR:O	1:A:3608:GLN:HG2	2.13	0.49
1:B:2477:PRO:HB3	1:B:2487:GLN:HG2	1.95	0.49
1:B:2765:LYS:NZ	1:B:2859:PRO:O	2.44	0.49
1:B:3433:GLU:HG3	1:B:3437:MET:HE3	1.95	0.49
1:A:929:LEU:HA	1:A:932:LEU:HD12	1.93	0.49
1:A:1170:MET:HE1	1:A:1176:GLU:HA	1.95	0.49
1:A:2224:ARG:HG2	1:A:2225:PHE:CD2	2.47	0.49
1:B:700:GLU:OE2	1:B:1458:HIS:NE2	2.33	0.49
1:D:1753:LYS:HB3	1:D:1758:ARG:HA	1.95	0.49
1:C:1163:THR:HG22	1:C:1168:VAL:HA	1.95	0.49
1:C:2773:ASN:OD1	1:C:2786:LYS:NZ	2.37	0.49
1:B:273:HIS:CE1	1:B:334:MET:HE2	2.48	0.48
1:B:499:THR:HG23	1:B:502:HIS:H	1.77	0.48
1:B:667:MET:SD	1:B:790:ARG:NH2	2.86	0.48
1:B:2224:ARG:HG2	1:B:2225:PHE:CD2	2.47	0.48
1:B:3556:ASN:HB3	1:B:3559:LEU:HD13	1.94	0.48
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.95	0.48
1:A:601:ASP:OD1	1:A:1665:HIS:ND1	2.41	0.48
1:A:3233:PRO:HB2	1:A:3238:GLU:HB2	1.94	0.48
1:A:3941:ASP:OD1	1:A:3941:ASP:N	2.46	0.48
1:B:2208:MET:HE1	1:B:2250:MET:HE1	1.94	0.48
1:B:4092:ASP:HA	1:B:4095:LYS:HG2	1.95	0.48
1:D:667:MET:SD	1:D:790:ARG:NH2	2.86	0.48
1:D:684:VAL:HG22	1:D:781:VAL:HG12	1.95	0.48
1:D:758:ARG:HG2	1:D:763:PRO:HA	1.94	0.48
1:D:866:HIS:CE1	1:D:941:MET:HG2	2.49	0.48
1:C:1170:MET:HE1	1:C:1176:GLU:HA	1.95	0.48
1:C:2208:MET:HE1	1:C:2250:MET:HE1	1.95	0.48
1:C:2250:MET:HE3	1:C:2250:MET:O	2.12	0.48
1:A:2440:MET:HE3	1:A:2441:HIS:N	2.29	0.48
1:A:4079:ASP:OD2	1:B:4736:ARG:NH2	2.35	0.48
2:E:79:ASP:OD2	2:E:80:TYR:HD1	1.96	0.48
1:B:41:GLY:O	1:B:45:ARG:NH1	2.47	0.48
1:B:1031:THR:HG22	1:B:1035:ASN:HD21	1.78	0.48
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.95	0.48
1:B:3629:ARG:HA	1:B:3632:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:VAL:HG11	1:D:164:ARG:HD3	1.94	0.48
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.95	0.48
1:D:4015:GLU:HA	1:D:4018:ASP:OD2	2.14	0.48
1:C:667:MET:SD	1:C:790:ARG:NH2	2.86	0.48
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.31	0.48
1:C:3539:ARG:HA	1:C:3539:ARG:HH11	1.78	0.48
1:C:4015:GLU:HA	1:C:4018:ASP:OD2	2.14	0.48
1:A:1031:THR:HG22	1:A:1035:ASN:HD21	1.78	0.48
1:A:2816:MET:HB3	1:A:2816:MET:HE2	1.66	0.48
1:A:3449:HIS:C	1:A:3449:HIS:ND1	2.71	0.48
1:A:3539:ARG:NH1	1:A:3542:LEU:HD22	2.21	0.48
1:B:684:VAL:HG22	1:B:781:VAL:HG12	1.95	0.48
1:B:2440:MET:HE3	1:B:2441:HIS:N	2.29	0.48
1:B:2765:LYS:NZ	1:B:2857:PRO:HB2	2.27	0.48
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.31	0.48
1:D:1170:MET:HE1	1:D:1176:GLU:HA	1.95	0.48
1:A:273:HIS:CE1	1:A:334:MET:HE2	2.49	0.48
1:A:1983:ALA:O	1:A:1987:SER:OG	2.28	0.48
1:A:1997:GLU:O	1:A:2000:SER:OG	2.27	0.48
1:A:3850:GLN:NE2	1:A:3872:GLU:OE1	2.33	0.48
2:H:11:ASP:OD2	2:H:12:GLY:N	2.47	0.48
1:D:273:HIS:CE1	1:D:334:MET:HE2	2.49	0.48
1:D:2440:MET:HE3	1:D:2441:HIS:N	2.29	0.48
1:D:3105:LYS:O	1:D:3108:GLU:HG3	2.14	0.48
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.46	0.48
1:C:2384:ILE:O	1:C:2387:SER:OG	2.28	0.48
1:A:499:THR:HG23	1:A:502:HIS:H	1.77	0.48
1:A:3226:GLU:C	1:A:3228:ALA:H	2.21	0.48
1:B:2250:MET:O	1:B:2250:MET:HE3	2.12	0.48
1:B:2668:SER:C	1:B:2670:GLU:H	2.22	0.48
1:B:3105:LYS:O	1:B:3108:GLU:HG3	2.14	0.48
1:D:1163:THR:HG22	1:D:1168:VAL:HA	1.95	0.48
1:C:2440:MET:HE3	1:C:2441:HIS:N	2.29	0.48
1:C:3226:GLU:C	1:C:3228:ALA:H	2.21	0.48
1:C:3263:TYR:N	1:C:3326:ASN:OD1	2.47	0.48
1:A:2477:PRO:HB3	1:A:2487:GLN:HG2	1.95	0.48
1:B:3201:MET:SD	1:B:3202:PRO:HD2	2.54	0.48
1:B:3455:GLU:OE2	1:B:3508:SER:OG	2.28	0.48
1:B:4000:MET:HE1	1:B:4058:ILE:HG12	1.95	0.48
1:B:4015:GLU:HA	1:B:4018:ASP:OD2	2.14	0.48
1:D:1024:TYR:CZ	1:D:1032:LYS:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1031:THR:HG22	1:D:1035:ASN:HD21	1.78	0.48
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.41	0.48
1:D:3263:TYR:N	1:D:3326:ASN:OD1	2.47	0.48
1:D:3449:HIS:C	1:D:3449:HIS:ND1	2.71	0.48
1:A:11:VAL:HG11	1:A:164:ARG:HD3	1.94	0.48
1:A:3256:LEU:HD11	1:A:3322:ILE:HD11	1.96	0.48
1:A:4000:MET:HE1	1:A:4058:ILE:HG12	1.95	0.48
2:F:11:ASP:OD2	2:F:12:GLY:N	2.47	0.48
1:B:3539:ARG:HA	1:B:3539:ARG:HH11	1.78	0.48
1:C:41:GLY:O	1:C:45:ARG:NH1	2.46	0.48
1:C:273:HIS:CE1	1:C:334:MET:HE2	2.49	0.48
1:C:700:GLU:OE2	1:C:1458:HIS:NE2	2.33	0.48
1:C:2123:LEU:O	1:C:2127:GLN:HG2	2.14	0.48
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.95	0.48
1:A:3263:TYR:N	1:A:3326:ASN:OD1	2.47	0.48
1:A:4888:TYR:HD1	1:B:4918:ILE:CD1	2.27	0.48
2:H:48:PHE:HZ	2:H:63:VAL:HG21	1.79	0.48
1:B:1163:THR:HG22	1:B:1168:VAL:HA	1.94	0.48
1:B:1753:LYS:HB3	1:B:1758:ARG:HA	1.95	0.48
1:B:3233:PRO:HB2	1:B:3238:GLU:HB2	1.94	0.48
1:B:3291:ALA:O	1:B:3293:PRO:HD3	2.14	0.48
1:B:4754:ASN:HB3	1:B:4756:ARG:HH21	1.79	0.48
1:D:2546:MET:HA	1:D:2546:MET:HE2	1.95	0.48
1:C:1024:TYR:CZ	1:C:1032:LYS:HG3	2.49	0.48
1:C:3201:MET:SD	1:C:3202:PRO:HD2	2.54	0.48
1:A:41:GLY:O	1:A:45:ARG:NH1	2.46	0.48
1:A:667:MET:SD	1:A:790:ARG:NH2	2.86	0.48
1:A:1078:GLU:OE2	1:A:1654:SER:OG	2.19	0.48
1:A:2185:ILE:HG21	1:A:2203:MET:HE1	1.95	0.48
1:A:2573:GLU:OE2	1:A:2615:ARG:NE	2.42	0.48
1:A:2773:ASN:OD1	1:A:2786:LYS:NZ	2.37	0.48
1:B:866:HIS:CE1	1:B:941:MET:HG2	2.49	0.48
1:D:1079:LYS:HA	1:D:1189:LEU:HD11	1.96	0.48
1:D:3291:ALA:O	1:D:3293:PRO:HD3	2.14	0.48
1:D:3539:ARG:HH11	1:D:3539:ARG:HA	1.78	0.48
1:D:4016:LEU:O	1:D:4020:GLN:HG3	2.14	0.48
1:D:4177:TYR:CE1	1:D:4199:GLU:HG3	2.49	0.48
1:D:4754:ASN:HB3	1:D:4756:ARG:HH21	1.79	0.48
1:C:684:VAL:HG22	1:C:781:VAL:HG12	1.95	0.48
1:C:866:HIS:CE1	1:C:941:MET:HG2	2.49	0.48
1:C:3105:LYS:O	1:C:3108:GLU:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:NZ	1:A:383:HIS:O	2.32	0.47
1:A:1024:TYR:CZ	1:A:1032:LYS:HG3	2.49	0.47
1:A:3105:LYS:O	1:A:3108:GLU:HG3	2.14	0.47
1:A:4092:ASP:HA	1:A:4095:LYS:HG2	1.95	0.47
1:A:4754:ASN:HB3	1:A:4756:ARG:HH21	1.79	0.47
1:B:774:ASP:OD2	1:B:1470:ARG:NH2	2.36	0.47
1:B:2185:ILE:HG21	1:B:2203:MET:HE1	1.95	0.47
1:B:2755:ILE:HD12	1:B:2813:LEU:HG	1.96	0.47
1:B:3256:LEU:HD11	1:B:3322:ILE:HD11	1.96	0.47
1:B:4177:TYR:CE1	1:B:4199:GLU:HG3	2.49	0.47
1:D:601:ASP:OD1	1:D:1665:HIS:ND1	2.41	0.47
1:D:2477:PRO:HB3	1:D:2487:GLN:HG2	1.95	0.47
1:D:4092:ASP:HA	1:D:4095:LYS:HG2	1.95	0.47
1:C:2546:MET:HE2	1:C:2546:MET:HA	1.95	0.47
1:A:1079:LYS:HA	1:A:1189:LEU:HD11	1.95	0.47
1:A:2393:ASP:OD1	1:A:2418:LEU:N	2.47	0.47
1:A:2782:ASP:N	1:A:2782:ASP:OD1	2.47	0.47
1:A:3291:ALA:O	1:A:3293:PRO:HD3	2.14	0.47
1:A:4177:TYR:CE1	1:A:4199:GLU:HG3	2.49	0.47
1:A:4888:TYR:HD1	1:B:4918:ILE:HD11	1.79	0.47
1:B:403:MET:HE1	1:B:451:TYR:CZ	2.50	0.47
1:D:41:GLY:O	1:D:45:ARG:NH1	2.47	0.47
1:D:2386:ILE:HG22	1:D:2392:ARG:CZ	2.45	0.47
1:D:2393:ASP:OD1	1:D:2418:LEU:N	2.47	0.47
1:D:3201:MET:SD	1:D:3202:PRO:HD2	2.54	0.47
1:D:3226:GLU:C	1:D:3228:ALA:H	2.21	0.47
1:C:2386:ILE:HG22	1:C:2392:ARG:CZ	2.45	0.47
1:C:2573:GLU:OE2	1:C:2615:ARG:NE	2.42	0.47
2:F:16:PRO:HG3	2:F:106:LEU:HD11	1.95	0.47
1:B:1024:TYR:CZ	1:B:1032:LYS:HG3	2.49	0.47
1:D:1983:ALA:O	1:D:1987:SER:OG	2.28	0.47
1:D:3442:PHE:CD2	1:D:3514:LEU:HD22	2.49	0.47
1:D:3686:GLU:N	1:D:3686:GLU:OE2	2.47	0.47
1:D:4000:MET:HE1	1:D:4058:ILE:HG12	1.95	0.47
1:C:70:GLU:OE2	1:C:110:ARG:NE	2.38	0.47
1:C:1753:LYS:HB3	1:C:1758:ARG:HA	1.95	0.47
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.46	0.47
1:A:3686:GLU:N	1:A:3686:GLU:OE2	2.47	0.47
1:B:70:GLU:OE2	1:B:110:ARG:NE	2.38	0.47
1:B:2209:GLU:HA	1:B:2212:VAL:HG22	1.97	0.47
1:B:2754:PHE:CE2	1:B:2813:LEU:HD11	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3226:GLU:C	1:B:3228:ALA:H	2.21	0.47
1:D:2185:ILE:HG21	1:D:2203:MET:HE1	1.95	0.47
1:D:3535:LEU:O	1:D:3538:THR:OG1	2.28	0.47
1:D:4813:LEU:O	1:D:4816:ILE:HG12	2.15	0.47
1:C:2393:ASP:OD1	1:C:2418:LEU:N	2.47	0.47
1:C:3686:GLU:N	1:C:3686:GLU:OE2	2.47	0.47
1:C:4092:ASP:HA	1:C:4095:LYS:HG2	1.95	0.47
1:C:4813:LEU:O	1:C:4816:ILE:HG12	2.15	0.47
1:A:403:MET:HE1	1:A:451:TYR:CZ	2.50	0.47
1:A:866:HIS:CE1	1:A:941:MET:HG2	2.49	0.47
1:A:2095:GLN:HG3	1:A:2127:GLN:HB3	1.97	0.47
1:B:2095:GLN:HG3	1:B:2127:GLN:HB3	1.97	0.47
1:B:3686:GLU:OE2	1:B:3686:GLU:N	2.47	0.47
1:B:3941:ASP:OD1	1:B:3941:ASP:N	2.46	0.47
1:D:2384:ILE:O	1:D:2387:SER:OG	2.28	0.47
1:D:3734:HIS:CG	1:D:3735:LEU:N	2.82	0.47
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.47	0.47
1:C:4968:PHE:O	1:C:4974:GLY:HA3	2.15	0.47
1:A:3114:LYS:HE3	1:A:3123:LYS:HD2	1.97	0.47
1:A:3362:ILE:HG22	1:A:3437:MET:HB3	1.97	0.47
1:A:4813:LEU:O	1:A:4816:ILE:HG12	2.15	0.47
1:B:3362:ILE:HG22	1:B:3437:MET:HB3	1.97	0.47
1:B:3734:HIS:CG	1:B:3735:LEU:N	2.82	0.47
1:B:4769:MET:SD	1:B:4769:MET:N	2.73	0.47
1:C:2185:ILE:HG21	1:C:2203:MET:HE1	1.95	0.47
1:C:4754:ASN:HB3	1:C:4756:ARG:HH21	1.79	0.47
1:A:70:GLU:OE2	1:A:110:ARG:NE	2.38	0.47
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.43	0.47
1:A:1753:LYS:HB3	1:A:1758:ARG:HA	1.95	0.47
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.31	0.47
1:A:4016:LEU:O	1:A:4020:GLN:HG3	2.14	0.47
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.43	0.47
1:B:1079:LYS:HA	1:B:1189:LEU:HD11	1.95	0.47
1:B:1819:VAL:O	1:B:1929:MET:HE1	2.15	0.47
1:B:2123:LEU:O	1:B:2127:GLN:HG2	2.14	0.47
1:B:3114:LYS:HE3	1:B:3123:LYS:HD2	1.97	0.47
1:B:4888:TYR:HD1	1:C:4918:ILE:CD1	2.28	0.47
1:D:2095:GLN:HG3	1:D:2127:GLN:HB3	1.97	0.47
1:D:2123:LEU:O	1:D:2127:GLN:HG2	2.14	0.47
1:D:2527:LEU:HD11	1:D:2582:MET:HA	1.97	0.47
1:D:2773:ASN:OD1	1:D:2786:LYS:NZ	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3443:ILE:HG12	1:D:3605:HIS:HD2	1.80	0.47
1:D:4968:PHE:O	1:D:4974:GLY:HA3	2.15	0.47
1:C:2209:GLU:HA	1:C:2212:VAL:HG22	1.97	0.47
1:C:2755:ILE:HD12	1:C:2813:LEU:HG	1.96	0.47
1:C:3256:LEU:HD11	1:C:3322:ILE:HD11	1.96	0.47
1:C:3362:ILE:HG22	1:C:3437:MET:HB3	1.97	0.47
1:C:3442:PHE:CD2	1:C:3514:LEU:HD22	2.49	0.47
1:C:4016:LEU:O	1:C:4020:GLN:HG3	2.14	0.47
1:C:4769:MET:SD	1:C:4769:MET:N	2.73	0.47
1:A:1819:VAL:O	1:A:1929:MET:HE1	2.15	0.47
1:A:2755:ILE:HD12	1:A:2813:LEU:HG	1.97	0.47
1:A:4015:GLU:HA	1:A:4018:ASP:OD2	2.14	0.47
1:B:2386:ILE:HG22	1:B:2392:ARG:CZ	2.45	0.47
1:B:2773:ASN:OD1	1:B:2786:LYS:NZ	2.37	0.47
1:B:2782:ASP:N	1:B:2782:ASP:OD1	2.47	0.47
1:D:403:MET:HE1	1:D:451:TYR:CZ	2.50	0.47
1:D:571:SER:OG	1:D:573:GLU:OE1	2.25	0.47
1:D:2001:PRO:O	1:D:2005:GLN:HG3	2.15	0.47
1:D:2668:SER:C	1:D:2670:GLU:H	2.22	0.47
1:D:3717:ASP:OD1	1:D:3717:ASP:N	2.48	0.47
1:C:35:LEU:HD11	1:C:189:LEU:HD13	1.97	0.47
1:C:2095:GLN:HG3	1:C:2127:GLN:HB3	1.97	0.47
1:C:3291:ALA:O	1:C:3293:PRO:HD3	2.14	0.47
1:C:3734:HIS:CG	1:C:3735:LEU:N	2.82	0.47
1:C:4000:MET:HE1	1:C:4058:ILE:HG12	1.95	0.47
1:A:2209:GLU:HA	1:A:2212:VAL:HG22	1.97	0.47
1:A:2464:ASP:OD1	1:A:2465:ASP:N	2.48	0.47
1:A:3201:MET:SD	1:A:3202:PRO:HD2	2.54	0.47
1:A:3734:HIS:CG	1:A:3735:LEU:N	2.82	0.47
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.97	0.47
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.97	0.47
1:B:3850:GLN:NE2	1:B:3872:GLU:OE1	2.33	0.47
1:B:4079:ASP:OD2	1:C:4736:ARG:NH2	2.36	0.47
1:D:950:LEU:HD23	1:D:950:LEU:HA	1.81	0.47
1:C:2668:SER:C	1:C:2670:GLU:H	2.22	0.47
1:A:2123:LEU:O	1:A:2127:GLN:HG2	2.14	0.47
1:A:3579:LEU:HB2	1:A:3582:ARG:HG2	1.97	0.47
1:B:35:LEU:HD11	1:B:189:LEU:HD13	1.97	0.47
1:B:110:ARG:NH2	1:B:117:TYR:OH	2.48	0.47
1:B:2020:ASP:OD1	1:B:2020:ASP:N	2.42	0.47
1:B:4968:PHE:O	1:B:4974:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ARG:NH2	1:D:117:TYR:OH	2.48	0.47
1:D:4918:ILE:CD1	1:C:4888:TYR:HD1	2.27	0.47
1:C:2527:LEU:HD11	1:C:2582:MET:HA	1.97	0.47
1:C:3443:ILE:HG12	1:C:3605:HIS:HD2	1.80	0.47
1:C:3765:TYR:CD2	1:C:4753:HIS:HA	2.50	0.47
1:A:3442:PHE:CD2	1:A:3514:LEU:HD22	2.49	0.46
1:A:3717:ASP:OD1	1:A:3717:ASP:N	2.48	0.46
1:A:3996:PHE:CD2	1:A:4020:GLN:HG2	2.51	0.46
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.97	0.46
1:B:3263:TYR:N	1:B:3326:ASN:OD1	2.47	0.46
1:B:3442:PHE:CD2	1:B:3514:LEU:HD22	2.49	0.46
1:D:438:ILE:HG23	1:D:518:ILE:HD11	1.98	0.46
1:D:3362:ILE:HG22	1:D:3437:MET:HB3	1.97	0.46
1:C:1079:LYS:HA	1:C:1189:LEU:HD11	1.96	0.46
1:C:4158:PRO:HA	1:C:4161:ARG:HD3	1.97	0.46
2:H:90:ILE:HG22	2:H:91:ILE:HG13	1.97	0.46
1:B:2757:LYS:O	1:B:2761:TYR:HB2	2.15	0.46
1:B:2812:SER:OG	1:B:2882:TYR:OH	2.15	0.46
1:B:4158:PRO:HA	1:B:4161:ARG:HD3	1.97	0.46
1:B:4813:LEU:O	1:B:4816:ILE:HG12	2.15	0.46
1:D:2101:MET:HE3	1:D:2105:TRP:CE3	2.50	0.46
1:D:3256:LEU:HD11	1:D:3322:ILE:HD11	1.96	0.46
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.98	0.46
1:C:2464:ASP:OD1	1:C:2465:ASP:N	2.48	0.46
1:C:2754:PHE:CE2	1:C:2813:LEU:HD11	2.47	0.46
1:A:1168:VAL:HG11	1:A:1176:GLU:HG2	1.98	0.46
1:A:2668:SER:C	1:A:2670:GLU:H	2.22	0.46
1:A:3443:ILE:HG12	1:A:3605:HIS:HD2	1.80	0.46
2:G:32:ASP:OD2	2:G:34:LYS:NZ	2.46	0.46
2:F:87:HIS:HB3	2:F:90:ILE:HB	1.96	0.46
1:B:438:ILE:HG23	1:B:518:ILE:HD11	1.98	0.46
1:B:3765:TYR:CD2	1:B:4753:HIS:HA	2.50	0.46
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.44	0.46
1:B:4655:PHE:N	1:B:4796:MET:HE1	2.30	0.46
1:D:3114:LYS:HE3	1:D:3123:LYS:HD2	1.97	0.46
1:C:438:ILE:HG23	1:C:518:ILE:HD11	1.98	0.46
1:C:2101:MET:HE3	1:C:2105:TRP:CE3	2.50	0.46
1:A:1753:LYS:HD3	1:A:1759:ARG:N	2.31	0.46
1:A:2386:ILE:HG22	1:A:2392:ARG:CZ	2.45	0.46
1:A:4655:PHE:N	1:A:4796:MET:HE1	2.30	0.46
1:B:1753:LYS:HD3	1:B:1759:ARG:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2393:ASP:OD1	1:B:2418:LEU:N	2.47	0.46
1:B:3996:PHE:CD2	1:B:4020:GLN:HG2	2.51	0.46
1:D:1753:LYS:HD3	1:D:1759:ARG:N	2.31	0.46
1:D:2219:GLU:N	1:D:2219:GLU:OE2	2.49	0.46
1:D:4238:CYS:SG	1:D:4989:MET:HG2	2.56	0.46
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.98	0.46
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.98	0.46
1:A:4968:PHE:O	1:A:4974:GLY:HA3	2.15	0.46
2:G:11:ASP:OD1	2:G:12:GLY:N	2.49	0.46
1:B:601:ASP:OD1	1:B:1665:HIS:ND1	2.41	0.46
1:B:1008:SER:HB3	1:B:1017:ARG:HB3	1.98	0.46
1:B:2001:PRO:O	1:B:2005:GLN:HG3	2.15	0.46
1:B:3579:LEU:HB2	1:B:3582:ARG:HG2	1.97	0.46
1:B:4016:LEU:O	1:B:4020:GLN:HG3	2.14	0.46
1:D:2755:ILE:HD12	1:D:2813:LEU:HG	1.97	0.46
1:D:4655:PHE:N	1:D:4796:MET:HE1	2.29	0.46
1:D:4769:MET:SD	1:D:4769:MET:N	2.73	0.46
1:C:1753:LYS:HD3	1:C:1759:ARG:N	2.31	0.46
1:C:4238:CYS:SG	1:C:4989:MET:HG2	2.56	0.46
1:A:2527:LEU:HD11	1:A:2582:MET:HA	1.97	0.46
1:A:2757:LYS:O	1:A:2761:TYR:HB2	2.15	0.46
1:A:2986:VAL:HG22	1:A:2988:LYS:H	1.81	0.46
2:E:11:ASP:OD1	2:E:12:GLY:N	2.49	0.46
1:B:2464:ASP:OD1	1:B:2465:ASP:N	2.48	0.46
1:B:2502:MET:HE2	1:B:2502:MET:N	2.31	0.46
1:B:2986:VAL:HG22	1:B:2988:LYS:H	1.81	0.46
1:B:4238:CYS:SG	1:B:4989:MET:HG2	2.56	0.46
1:D:3765:TYR:CD2	1:D:4753:HIS:HA	2.50	0.46
1:D:3996:PHE:CD2	1:D:4020:GLN:HG2	2.51	0.46
1:C:110:ARG:NH2	1:C:117:TYR:OH	2.48	0.46
1:C:4177:TYR:CE1	1:C:4199:GLU:HG3	2.49	0.46
1:A:438:ILE:HG23	1:A:518:ILE:HD11	1.98	0.46
1:A:866:HIS:CG	1:A:941:MET:HG2	2.51	0.46
1:A:2001:PRO:O	1:A:2005:GLN:HG3	2.15	0.46
1:B:194:SER:OG	1:B:195:PHE:N	2.49	0.46
1:B:1168:VAL:HG11	1:B:1176:GLU:HG2	1.98	0.46
1:B:2101:MET:HE3	1:B:2105:TRP:CE3	2.50	0.46
1:B:2512:ILE:HG21	1:B:2518:LEU:HD13	1.97	0.46
1:D:2209:GLU:HA	1:D:2212:VAL:HG22	1.97	0.46
1:D:2757:LYS:O	1:D:2761:TYR:HB2	2.15	0.46
1:C:710:ASP:OD1	1:C:713:SER:OG	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1819:VAL:O	1:C:1929:MET:HE1	2.15	0.46
1:C:2502:MET:HE2	1:C:2502:MET:N	2.31	0.46
1:C:2641:LEU:HD12	1:C:2698:MET:HE1	1.98	0.46
1:C:3734:HIS:CG	1:C:3735:LEU:H	2.34	0.46
1:A:2219:GLU:N	1:A:2219:GLU:OE2	2.49	0.46
1:A:2384:ILE:O	1:A:2387:SER:OG	2.28	0.46
1:A:2974:ILE:HG13	1:A:2975:ALA:N	2.31	0.46
1:A:3373:VAL:HG12	1:A:3398:PHE:HZ	1.81	0.46
2:F:18:ARG:NH2	2:F:50:LEU:HD22	2.22	0.46
1:B:2641:LEU:HD12	1:B:2698:MET:HE1	1.98	0.46
1:D:866:HIS:O	1:D:869:ARG:HG3	2.16	0.46
1:D:1997:GLU:O	1:D:2000:SER:OG	2.27	0.46
1:D:2974:ILE:HG13	1:D:2975:ALA:N	2.31	0.46
1:C:403:MET:HE1	1:C:451:TYR:CZ	2.50	0.46
1:C:571:SER:OG	1:C:573:GLU:OE1	2.25	0.46
1:C:1168:VAL:HG11	1:C:1176:GLU:HG2	1.98	0.46
1:C:2001:PRO:O	1:C:2005:GLN:HG3	2.15	0.46
1:C:3579:LEU:HB2	1:C:3582:ARG:HG2	1.97	0.46
1:A:110:ARG:NH2	1:A:117:TYR:OH	2.48	0.46
1:A:4238:CYS:SG	1:A:4989:MET:HG2	2.56	0.46
1:B:2219:GLU:OE2	1:B:2219:GLU:N	2.49	0.46
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	1.98	0.46
1:B:3373:VAL:HG12	1:B:3398:PHE:HZ	1.81	0.46
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.97	0.46
1:D:957:LYS:O	1:D:960:MET:HG2	2.16	0.46
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	1.97	0.46
1:C:866:HIS:CG	1:C:941:MET:HG2	2.51	0.46
1:C:2219:GLU:N	1:C:2219:GLU:OE2	2.49	0.46
1:C:2768:PHE:HB2	1:C:2857:PRO:HG2	1.98	0.46
1:C:3941:ASP:N	1:C:3941:ASP:OD1	2.46	0.46
1:A:894:GLY:HA3	1:A:903:LEU:HB3	1.98	0.46
1:A:1864:LYS:NZ	1:A:1871:PHE:O	2.45	0.46
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	1.98	0.46
1:A:3765:TYR:CD2	1:A:4753:HIS:HA	2.50	0.46
1:A:4686:LEU:HD23	1:A:4687:TYR:CE2	2.52	0.46
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.45	0.46
1:B:3856:LEU:HD12	1:B:3857:GLY:N	2.31	0.46
1:D:1168:VAL:HG11	1:D:1176:GLU:HG2	1.98	0.46
1:D:1819:VAL:O	1:D:1929:MET:HE1	2.15	0.46
1:D:2858:GLN:HB2	1:D:2859:PRO:HD3	1.98	0.46
1:C:350:HIS:CE1	1:C:352:ALA:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2522:LEU:HD13	1:C:2582:MET:CE	2.46	0.46
1:C:2757:LYS:O	1:C:2761:TYR:HB2	2.16	0.46
1:C:3734:HIS:O	1:C:3736:GLU:HG3	2.16	0.46
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.97	0.46
1:A:2101:MET:HE3	1:A:2105:TRP:CE3	2.50	0.45
1:A:2212:VAL:HG11	1:A:2256:TYR:CE2	2.52	0.45
1:B:866:HIS:O	1:B:869:ARG:HG3	2.16	0.45
1:B:3734:HIS:CG	1:B:3735:LEU:H	2.34	0.45
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.98	0.45
1:D:3269:VAL:HA	1:D:3273:THR:HB	1.98	0.45
1:D:3373:VAL:HG12	1:D:3398:PHE:HZ	1.81	0.45
1:D:3579:LEU:HB2	1:D:3582:ARG:HG2	1.97	0.45
1:D:3734:HIS:CG	1:D:3735:LEU:H	2.34	0.45
1:C:866:HIS:O	1:C:869:ARG:HG3	2.16	0.45
1:C:3996:PHE:CD2	1:C:4020:GLN:HG2	2.50	0.45
1:A:2012:PHE:CZ	1:A:2031:LEU:HD23	2.51	0.45
2:G:84:ALA:O	2:G:93:PRO:HB3	2.17	0.45
1:B:866:HIS:CG	1:B:941:MET:HG2	2.51	0.45
1:B:2527:LEU:HD11	1:B:2582:MET:HA	1.97	0.45
1:D:35:LEU:HD11	1:D:189:LEU:HD13	1.97	0.45
1:D:1226:PHE:O	1:D:1827:ARG:NH2	2.50	0.45
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.99	0.45
1:D:2522:LEU:HD13	1:D:2582:MET:CE	2.46	0.45
1:D:4158:PRO:HA	1:D:4161:ARG:HD3	1.97	0.45
1:C:3856:LEU:HD12	1:C:3857:GLY:N	2.31	0.45
1:A:774:ASP:OD2	1:A:1470:ARG:NH2	2.36	0.45
1:A:3734:HIS:CG	1:A:3735:LEU:H	2.34	0.45
1:A:4892:ARG:NH1	1:B:4895:GLY:O	2.44	0.45
1:B:2212:VAL:HG11	1:B:2256:TYR:CE2	2.52	0.45
1:D:866:HIS:CG	1:D:941:MET:HG2	2.51	0.45
1:D:2012:PHE:CZ	1:D:2031:LEU:HD23	2.51	0.45
1:D:2464:ASP:OD1	1:D:2465:ASP:N	2.48	0.45
1:D:2502:MET:N	1:D:2502:MET:HE2	2.31	0.45
1:D:3003:LEU:HB2	1:D:3004:PRO:HD3	1.98	0.45
1:D:3875:MET:HE3	1:D:3875:MET:HB3	1.75	0.45
1:D:4868:ASP:OD1	1:D:4870:ASP:N	2.50	0.45
1:C:3114:LYS:HE3	1:C:3123:LYS:HD2	1.97	0.45
1:C:4655:PHE:N	1:C:4796:MET:HE1	2.30	0.45
1:A:35:LEU:HD11	1:A:189:LEU:HD13	1.97	0.45
1:A:957:LYS:O	1:A:960:MET:HG2	2.16	0.45
1:A:4158:PRO:HA	1:A:4161:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2758:PHE:CE2	1:B:2926:LEU:HD12	2.52	0.45
1:B:4686:LEU:HD23	1:B:4687:TYR:CE2	2.52	0.45
1:B:4827:LEU:HD21	1:C:4843:LEU:HD21	1.99	0.45
1:D:194:SER:OG	1:D:195:PHE:N	2.49	0.45
1:D:613:ALA:HB2	1:D:1676:LEU:HD12	1.98	0.45
1:C:1078:GLU:OE2	1:C:1654:SER:OG	2.19	0.45
1:C:2758:PHE:CE2	1:C:2926:LEU:HD12	2.52	0.45
1:A:194:SER:OG	1:A:195:PHE:N	2.49	0.45
1:A:1008:SER:HB3	1:A:1017:ARG:HB3	1.98	0.45
1:A:1297:PHE:CE2	1:A:1525:GLY:HA2	2.52	0.45
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.99	0.45
1:A:2502:MET:N	1:A:2502:MET:HE2	2.31	0.45
1:A:2754:PHE:CE2	1:A:2813:LEU:HD11	2.47	0.45
1:A:2758:PHE:CE2	1:A:2926:LEU:HD12	2.52	0.45
2:E:61:GLU:O	2:E:65:GLN:HG3	2.16	0.45
2:E:105:LYS:HZ2	2:E:105:LYS:HB3	1.82	0.45
2:G:18:ARG:NH2	2:G:50:LEU:HD22	2.22	0.45
2:G:88:PRO:HB2	1:C:1680:ARG:HH12	1.82	0.45
1:B:1297:PHE:CE2	1:B:1525:GLY:HA2	2.52	0.45
1:B:2012:PHE:CZ	1:B:2031:LEU:HD23	2.51	0.45
1:B:2208:MET:HE1	1:B:2250:MET:SD	2.57	0.45
1:B:2758:PHE:HE2	1:B:2926:LEU:HD12	1.82	0.45
1:D:2208:MET:HE1	1:D:2250:MET:SD	2.57	0.45
1:C:938:HIS:HB3	1:C:1054:GLU:HB3	1.99	0.45
1:C:1008:SER:HB3	1:C:1017:ARG:HB3	1.98	0.45
1:C:3445:TRP:NE1	1:C:3455:GLU:OE1	2.46	0.45
1:A:2641:LEU:HD12	1:A:2698:MET:HE1	1.98	0.45
1:A:3130:THR:HA	1:A:3133:THR:HG22	1.98	0.45
1:B:3535:LEU:O	1:B:3538:THR:OG1	2.28	0.45
1:B:3734:HIS:O	1:B:3736:GLU:HG3	2.16	0.45
1:B:4885:PHE:O	1:B:4889:VAL:HG22	2.17	0.45
1:D:2641:LEU:HD12	1:D:2698:MET:HE1	1.98	0.45
1:D:2758:PHE:HE2	1:D:2926:LEU:HD12	1.82	0.45
1:D:2782:ASP:N	1:D:2782:ASP:OD1	2.47	0.45
1:D:2986:VAL:HG22	1:D:2988:LYS:H	1.81	0.45
1:D:3856:LEU:HD12	1:D:3857:GLY:N	2.31	0.45
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.99	0.45
1:C:3762:ARG:CZ	1:C:4755:GLU:HB2	2.47	0.45
1:A:866:HIS:O	1:A:869:ARG:HG3	2.16	0.45
1:A:1226:PHE:O	1:A:1827:ARG:NH2	2.50	0.45
1:A:2758:PHE:HE2	1:A:2926:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2812:SER:OG	1:A:2882:TYR:OH	2.15	0.45
1:A:2858:GLN:HB2	1:A:2859:PRO:HD3	1.99	0.45
1:A:3856:LEU:HD12	1:A:3857:GLY:N	2.31	0.45
1:B:3539:ARG:NH1	1:B:3542:LEU:HD22	2.21	0.45
1:D:2512:ILE:HG21	1:D:2518:LEU:HD13	1.97	0.45
1:D:2768:PHE:HB2	1:D:2857:PRO:HG2	1.98	0.45
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.44	0.45
1:D:3941:ASP:OD1	1:D:3941:ASP:N	2.46	0.45
1:D:4736:ARG:NH2	1:C:4079:ASP:OD2	2.36	0.45
1:C:194:SER:OG	1:C:195:PHE:N	2.49	0.45
1:C:2986:VAL:HG22	1:C:2988:LYS:H	1.81	0.45
1:C:3373:VAL:HG12	1:C:3398:PHE:HZ	1.81	0.45
1:C:3535:LEU:O	1:C:3538:THR:OG1	2.28	0.45
1:A:710:ASP:OD1	1:A:713:SER:OG	2.26	0.45
1:A:2208:MET:HE1	1:A:2250:MET:SD	2.57	0.45
1:A:2768:PHE:HB2	1:A:2857:PRO:HG2	1.97	0.45
1:A:3762:ARG:CZ	1:A:4755:GLU:HB2	2.47	0.45
1:A:4217:PHE:O	1:A:4221:VAL:HG22	2.17	0.45
2:F:84:ALA:O	2:F:93:PRO:HB3	2.17	0.45
1:B:350:HIS:CE1	1:B:352:ALA:HB3	2.51	0.45
1:B:957:LYS:O	1:B:960:MET:HG2	2.16	0.45
1:B:2747:ILE:HD11	1:B:2814:LYS:HD3	1.99	0.45
1:B:2768:PHE:HB2	1:B:2857:PRO:HG2	1.97	0.45
1:D:2212:VAL:HG11	1:D:2256:TYR:CE2	2.52	0.45
1:D:3501:ASP:OD1	1:D:3501:ASP:N	2.50	0.45
1:C:1226:PHE:O	1:C:1827:ARG:NH2	2.50	0.45
1:C:2974:ILE:HG13	1:C:2975:ALA:N	2.31	0.45
1:C:3717:ASP:N	1:C:3717:ASP:OD1	2.48	0.45
1:C:4868:ASP:OD1	1:C:4870:ASP:N	2.50	0.45
1:A:350:HIS:CE1	1:A:352:ALA:HB3	2.51	0.45
2:E:11:ASP:OD1	2:E:11:ASP:C	2.60	0.45
2:H:84:ALA:O	2:H:93:PRO:HB3	2.17	0.45
1:B:894:GLY:HA3	1:B:903:LEU:HB3	1.98	0.45
1:D:350:HIS:CE1	1:D:352:ALA:HB3	2.52	0.45
1:D:2747:ILE:HD11	1:D:2814:LYS:HD3	1.99	0.45
1:D:4686:LEU:HD23	1:D:4687:TYR:CE2	2.52	0.45
1:D:4918:ILE:HD11	1:C:4888:TYR:HD1	1.82	0.45
1:C:2256:TYR:HD2	1:C:2256:TYR:O	2.00	0.45
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.97	0.45
1:C:2858:GLN:HB2	1:C:2859:PRO:HD3	1.98	0.45
1:C:3249:LEU:HD21	1:C:3273:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4885:PHE:O	1:C:4889:VAL:HG22	2.17	0.45
1:A:365:LYS:HE3	1:A:365:LYS:HB3	1.74	0.45
1:A:2821:TRP:HH2	1:A:2877:GLN:HB3	1.82	0.45
1:A:3628:ARG:HG3	1:A:3631:ALA:HB3	1.99	0.45
1:A:4868:ASP:OD1	1:A:4870:ASP:N	2.50	0.45
2:E:11:ASP:OD1	2:E:13:ARG:N	2.32	0.45
2:E:29:MET:HE2	2:E:29:MET:HB3	1.81	0.45
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.99	0.45
1:B:3628:ARG:HG3	1:B:3631:ALA:HB3	1.99	0.45
1:B:3762:ARG:CZ	1:B:4755:GLU:HB2	2.47	0.45
1:D:2867:LEU:HD21	1:D:2871:LEU:HB3	1.99	0.45
1:C:144:GLU:HG3	1:C:175:SER:HB3	1.99	0.45
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.99	0.45
1:C:4686:LEU:HD23	1:C:4687:TYR:CE2	2.52	0.45
1:A:2747:ILE:HD11	1:A:2814:LYS:HD3	1.99	0.44
1:A:3269:VAL:HA	1:A:3273:THR:HB	1.98	0.44
1:B:144:GLU:HG3	1:B:175:SER:HB3	1.99	0.44
1:B:613:ALA:HB2	1:B:1676:LEU:HD12	1.99	0.44
1:B:3130:THR:HA	1:B:3133:THR:HG22	1.98	0.44
1:D:460:GLN:HB2	1:D:463:GLU:OE1	2.18	0.44
1:C:1297:PHE:CE2	1:C:1525:GLY:HA2	2.52	0.44
1:C:2208:MET:HE1	1:C:2250:MET:SD	2.57	0.44
1:C:2212:VAL:HG11	1:C:2256:TYR:CE2	2.52	0.44
1:C:2764:GLU:HG3	1:C:2857:PRO:HB3	2.00	0.44
1:C:3628:ARG:HG3	1:C:3631:ALA:HB3	1.99	0.44
1:A:399:GLN:HG2	1:A:403:MET:HE2	1.99	0.44
1:A:1025:ARG:H	1:A:1025:ARG:HD2	1.82	0.44
2:H:11:ASP:OD2	2:H:11:ASP:C	2.60	0.44
1:B:1226:PHE:O	1:B:1827:ARG:NH2	2.50	0.44
1:B:2823:ILE:HA	1:B:2937:VAL:HA	2.00	0.44
1:D:275:ARG:NH1	1:D:338:GLU:OE2	2.50	0.44
1:D:399:GLN:HG2	1:D:403:MET:HE2	1.99	0.44
1:D:1025:ARG:H	1:D:1025:ARG:HD2	1.82	0.44
1:C:275:ARG:NH1	1:C:338:GLU:OE2	2.50	0.44
1:C:3130:THR:HA	1:C:3133:THR:HG22	1.98	0.44
1:C:4217:PHE:O	1:C:4221:VAL:HG22	2.17	0.44
1:A:3734:HIS:O	1:A:3736:GLU:HG3	2.16	0.44
2:G:11:ASP:OD1	2:G:11:ASP:C	2.60	0.44
2:F:11:ASP:OD2	2:F:11:ASP:C	2.60	0.44
1:B:399:GLN:HG2	1:B:403:MET:HE2	1.99	0.44
1:B:1805:GLU:H	1:B:1805:GLU:CD	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2821:TRP:HD1	1:B:2939:ARG:HA	1.83	0.44
1:B:4868:ASP:OD1	1:B:4870:ASP:N	2.50	0.44
1:D:938:HIS:HB3	1:D:1054:GLU:HB3	1.99	0.44
1:D:1008:SER:HB3	1:D:1017:ARG:HB3	1.98	0.44
1:D:3445:TRP:NE1	1:D:3455:GLU:OE1	2.46	0.44
1:D:3762:ARG:CZ	1:D:4755:GLU:HB2	2.47	0.44
1:D:4843:LEU:HD21	1:C:4827:LEU:HD21	1.99	0.44
1:C:2012:PHE:CZ	1:C:2031:LEU:HD23	2.51	0.44
1:C:2623:LEU:O	1:C:2627:VAL:HG23	2.18	0.44
1:C:3003:LEU:HB2	1:C:3004:PRO:HD3	1.98	0.44
1:A:2821:TRP:HD1	1:A:2939:ARG:HA	1.83	0.44
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.33	0.44
1:A:3137:LEU:HD21	1:A:3190:LEU:HD23	2.00	0.44
1:A:3534:MET:C	1:A:3534:MET:HE2	2.43	0.44
2:G:61:GLU:O	2:G:65:GLN:HG3	2.17	0.44
1:B:938:HIS:HB3	1:B:1054:GLU:HB3	1.99	0.44
1:B:961:MET:H	1:B:961:MET:HG2	1.58	0.44
1:B:2479:LEU:HD22	1:B:2480:GLY:H	1.83	0.44
1:B:2522:LEU:HD13	1:B:2582:MET:CE	2.46	0.44
1:B:2641:LEU:HD23	1:B:2641:LEU:HA	1.88	0.44
1:B:3249:LEU:HD21	1:B:3273:THR:HG23	1.99	0.44
1:B:3269:VAL:HA	1:B:3273:THR:HB	1.98	0.44
1:D:1823:GLY:O	1:D:1825:HIS:ND1	2.47	0.44
1:D:2256:TYR:O	1:D:2256:TYR:HD2	2.00	0.44
1:D:2758:PHE:CE2	1:D:2926:LEU:HD12	2.52	0.44
1:D:2793:PRO:HA	1:D:2855:TYR:CG	2.53	0.44
1:D:3130:THR:HA	1:D:3133:THR:HG22	1.98	0.44
1:D:4039:MET:HG2	1:D:4040:ILE:N	2.33	0.44
1:C:399:GLN:HG2	1:C:403:MET:HE2	1.99	0.44
1:C:460:GLN:HB2	1:C:463:GLU:OE1	2.18	0.44
1:C:501:ALA:O	1:C:505:GLU:HG3	2.18	0.44
1:C:613:ALA:HB2	1:C:1676:LEU:HD12	1.99	0.44
1:C:2747:ILE:HD11	1:C:2814:LYS:HD3	1.99	0.44
1:C:2755:ILE:CD1	1:C:2813:LEU:HG	2.48	0.44
1:C:2758:PHE:HE2	1:C:2926:LEU:HD12	1.82	0.44
1:A:4885:PHE:O	1:A:4889:VAL:HG22	2.17	0.44
1:B:901:LYS:HA	1:B:901:LYS:HD2	1.81	0.44
1:B:976:ARG:HA	1:B:1044:ARG:HH12	1.83	0.44
1:B:1970:GLN:HG2	1:B:3642:TYR:HA	2.00	0.44
1:B:2755:ILE:CD1	1:B:2813:LEU:HG	2.48	0.44
1:B:4039:MET:HG2	1:B:4040:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1206:GLN:HA	1:D:1227:ALA:O	2.18	0.44
1:D:1297:PHE:CE2	1:D:1525:GLY:HA2	2.52	0.44
1:D:1575:LEU:HD13	1:D:1579:MET:HE3	2.00	0.44
1:D:1970:GLN:HG2	1:D:3642:TYR:HA	2.00	0.44
1:D:2755:ILE:CD1	1:D:2813:LEU:HG	2.48	0.44
1:D:3310:ASP:HA	1:D:3350:ARG:HH12	1.83	0.44
1:D:3734:HIS:O	1:D:3736:GLU:HG3	2.16	0.44
1:C:957:LYS:O	1:C:960:MET:HG2	2.16	0.44
1:C:4039:MET:HG2	1:C:4040:ILE:N	2.33	0.44
1:A:613:ALA:HB2	1:A:1676:LEU:HD12	1.99	0.44
1:A:774:ASP:CG	1:A:1470:ARG:HH22	2.24	0.44
1:A:2522:LEU:HD13	1:A:2582:MET:CE	2.46	0.44
1:A:2755:ILE:CD1	1:A:2813:LEU:HG	2.48	0.44
1:B:2740:VAL:HG21	1:B:2819:TRP:NE1	2.33	0.44
1:B:3376:GLU:OE2	1:B:3450:ASN:ND2	2.51	0.44
1:B:3534:MET:C	1:B:3534:MET:HE2	2.43	0.44
1:B:3717:ASP:N	1:B:3717:ASP:OD1	2.48	0.44
1:D:501:ALA:O	1:D:505:GLU:HG3	2.18	0.44
1:D:2623:LEU:O	1:D:2627:VAL:HG23	2.18	0.44
1:D:3249:LEU:HD21	1:D:3273:THR:HG23	1.99	0.44
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.31	0.44
1:C:950:LEU:HD23	1:C:950:LEU:HA	1.81	0.44
1:C:1575:LEU:HD13	1:C:1579:MET:HE3	2.00	0.44
1:C:1805:GLU:CD	1:C:1805:GLU:H	2.26	0.44
1:C:2178:MET:HE2	1:C:2178:MET:HB2	1.92	0.44
1:A:460:GLN:HB2	1:A:463:GLU:OE1	2.18	0.44
1:A:2793:PRO:HA	1:A:2855:TYR:CG	2.53	0.44
2:H:88:PRO:HB2	1:D:1680:ARG:HH12	1.82	0.44
1:B:460:GLN:HB2	1:B:463:GLU:OE1	2.18	0.44
1:B:1575:LEU:HD13	1:B:1579:MET:HE3	2.00	0.44
1:B:2974:ILE:HG13	1:B:2975:ALA:N	2.31	0.44
1:B:3443:ILE:HG12	1:B:3605:HIS:HD2	1.80	0.44
1:B:4892:ARG:NH1	1:C:4895:GLY:O	2.44	0.44
1:D:2716:ASP:OD1	1:D:2716:ASP:N	2.51	0.44
1:D:2754:PHE:CE2	1:D:2813:LEU:HD11	2.47	0.44
1:D:3628:ARG:HG3	1:D:3631:ALA:HB3	1.99	0.44
1:C:1970:GLN:HG2	1:C:3642:TYR:HA	2.00	0.44
1:C:2479:LEU:HD22	1:C:2480:GLY:H	1.83	0.44
1:C:2765:LYS:HD3	1:C:2765:LYS:HA	1.70	0.44
1:C:2821:TRP:HD1	1:C:2939:ARG:HA	1.82	0.44
1:C:2867:LEU:HD21	1:C:2871:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3501:ASP:OD1	1:C:3501:ASP:N	2.50	0.44
1:A:144:GLU:HG3	1:A:175:SER:HB3	1.99	0.44
1:A:1780:PRO:HG2	2:E:42:ARG:HD3	2.00	0.44
1:A:2764:GLU:HG3	1:A:2857:PRO:HB3	2.00	0.44
1:A:3310:ASP:HA	1:A:3350:ARG:HH12	1.83	0.44
1:A:4039:MET:HG2	1:A:4040:ILE:N	2.33	0.44
1:A:5030:LYS:HB2	1:A:5030:LYS:HE2	1.78	0.44
1:B:835:ARG:NH2	1:B:1210:SER:O	2.35	0.44
1:B:1000:ARG:HA	1:B:1003:GLN:OE1	2.18	0.44
1:B:2858:GLN:HB2	1:B:2859:PRO:HD3	1.98	0.44
1:B:3607:GLU:OE2	1:B:3608:GLN:NE2	2.48	0.44
1:B:3836:MET:HE3	1:B:3836:MET:HB2	1.82	0.44
1:D:2821:TRP:HD1	1:D:2939:ARG:HA	1.83	0.44
1:D:3534:MET:HE2	1:D:3534:MET:C	2.43	0.44
1:C:1000:ARG:HA	1:C:1003:GLN:OE1	2.18	0.44
1:C:3255:GLY:O	1:C:3258:GLU:HG3	2.18	0.44
1:C:3534:MET:C	1:C:3534:MET:HE2	2.43	0.44
1:A:3209:GLN:HG2	1:A:3210:LEU:HG	2.00	0.44
1:A:3376:GLU:OE2	1:A:3450:ASN:ND2	2.51	0.44
1:A:3835:LEU:HD22	1:A:3880:PHE:HZ	1.83	0.44
2:E:47:LYS:NZ	2:E:107:GLU:OE2	2.34	0.44
2:G:23:VAL:HG22	2:G:47:LYS:HD3	1.99	0.44
1:B:2516:ASP:N	1:B:2516:ASP:OD1	2.51	0.44
1:D:144:GLU:HG3	1:D:175:SER:HB3	2.00	0.44
1:D:2740:VAL:HG21	1:D:2819:TRP:NE1	2.33	0.44
1:D:3378:GLN:HA	1:D:3381:LEU:HD23	2.00	0.44
1:D:3590:GLU:H	1:D:3590:GLU:CD	2.26	0.44
1:C:365:LYS:HE3	1:C:365:LYS:HB3	1.74	0.44
1:C:3269:VAL:HA	1:C:3273:THR:HB	1.98	0.44
1:C:3376:GLU:OE2	1:C:3450:ASN:ND2	2.51	0.44
1:A:938:HIS:HB3	1:A:1054:GLU:HB3	1.99	0.43
1:A:950:LEU:HD23	1:A:950:LEU:HA	1.81	0.43
1:A:1575:LEU:HD13	1:A:1579:MET:HE3	2.00	0.43
1:A:1805:GLU:CD	1:A:1805:GLU:H	2.26	0.43
1:A:3249:LEU:HD21	1:A:3273:THR:HG23	1.99	0.43
1:A:3255:GLY:O	1:A:3258:GLU:HG3	2.18	0.43
1:A:4026:MET:HE2	1:A:4026:MET:HB3	1.81	0.43
1:A:4253:GLU:HG3	1:A:4557:ARG:HH21	1.83	0.43
1:B:3835:LEU:HD22	1:B:3880:PHE:HZ	1.83	0.43
1:B:4897:ILE:O	1:B:4901:ILE:HG12	2.18	0.43
1:D:403:MET:HE1	1:D:451:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1805:GLU:H	1:D:1805:GLU:CD	2.26	0.43
1:D:1943:LEU:HB2	1:D:2123:LEU:HD21	2.00	0.43
1:C:817:PRO:O	1:C:820:ARG:NH2	2.51	0.43
1:C:2694:GLU:HA	1:C:2697:ARG:NH1	2.33	0.43
1:A:501:ALA:O	1:A:505:GLU:HG3	2.18	0.43
1:A:817:PRO:O	1:A:820:ARG:NH2	2.51	0.43
1:A:2823:ILE:HA	1:A:2937:VAL:HA	2.00	0.43
1:A:3284:TRP:HB3	1:A:3305:THR:HG21	2.00	0.43
1:B:275:ARG:NH1	1:B:338:GLU:OE2	2.50	0.43
1:B:2623:LEU:O	1:B:2627:VAL:HG23	2.18	0.43
1:B:2764:GLU:HG3	1:B:2857:PRO:HB3	2.00	0.43
1:B:2765:LYS:HD3	1:B:2765:LYS:HA	1.70	0.43
1:B:2821:TRP:HB3	1:B:2937:VAL:HG22	2.01	0.43
1:B:3137:LEU:HD21	1:B:3190:LEU:HD23	2.00	0.43
1:B:4712:PRO:O	1:B:4718:LYS:NZ	2.42	0.43
1:D:140:ASP:OD1	1:D:142:THR:OG1	2.30	0.43
1:D:1465:ASP:OD1	1:D:1468:LYS:HG2	2.18	0.43
1:C:2823:ILE:HA	1:C:2937:VAL:HA	2.00	0.43
1:C:3378:GLN:HA	1:C:3381:LEU:HD23	2.00	0.43
1:C:4253:GLU:HG3	1:C:4557:ARG:HH21	1.83	0.43
1:A:1465:ASP:OD1	1:A:1468:LYS:HG2	2.18	0.43
1:A:1943:LEU:HB2	1:A:2123:LEU:HD21	2.00	0.43
1:A:2867:LEU:HD21	1:A:2871:LEU:HB3	1.99	0.43
2:F:32:ASP:OD2	2:F:34:LYS:NZ	2.47	0.43
1:B:501:ALA:O	1:B:505:GLU:HG3	2.18	0.43
1:B:2821:TRP:HH2	1:B:2877:GLN:HB3	1.83	0.43
1:B:3209:GLN:HG2	1:B:3210:LEU:HG	2.00	0.43
1:D:328:LYS:HE3	1:D:328:LYS:HB3	1.75	0.43
1:D:817:PRO:O	1:D:820:ARG:NH2	2.51	0.43
1:D:1099:GLU:CD	1:D:1125:ASN:HD21	2.26	0.43
1:D:4217:PHE:O	1:D:4221:VAL:HG22	2.17	0.43
1:D:4813:LEU:HD23	1:D:4813:LEU:HA	1.79	0.43
1:D:4897:ILE:O	1:D:4901:ILE:HG12	2.18	0.43
1:C:1943:LEU:HB2	1:C:2123:LEU:HD21	2.00	0.43
1:C:2821:TRP:HH2	1:C:2877:GLN:HB3	1.83	0.43
1:C:2821:TRP:HB3	1:C:2937:VAL:HG22	2.01	0.43
1:C:4897:ILE:O	1:C:4901:ILE:HG12	2.18	0.43
1:A:2538:THR:HG23	1:A:2541:PHE:H	1.83	0.43
1:A:2694:GLU:HA	1:A:2697:ARG:NH1	2.33	0.43
2:E:90:ILE:HG22	2:E:91:ILE:HG13	1.99	0.43
1:B:817:PRO:O	1:B:820:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:ILE:HG12	1:B:1051:TYR:HE2	1.84	0.43
1:B:1025:ARG:H	1:B:1025:ARG:HD2	1.82	0.43
1:B:1823:GLY:O	1:B:1825:HIS:ND1	2.47	0.43
1:B:2256:TYR:HD2	1:B:2256:TYR:O	2.00	0.43
1:B:4888:TYR:HD1	1:C:4918:ILE:HD11	1.83	0.43
1:D:664:PHE:HB3	1:D:811:CYS:SG	2.59	0.43
1:D:2479:LEU:HD22	1:D:2480:GLY:H	1.83	0.43
1:C:1465:ASP:OD1	1:C:1468:LYS:HG2	2.18	0.43
1:C:4184:MET:HE2	1:C:4184:MET:HB2	1.92	0.43
1:A:870:ILE:HG12	1:A:1051:TYR:HE2	1.84	0.43
1:A:1206:GLN:HA	1:A:1227:ALA:O	2.18	0.43
1:A:2256:TYR:O	1:A:2256:TYR:HD2	2.00	0.43
1:A:2430:ILE:HB	1:A:2502:MET:HE1	2.00	0.43
1:A:2479:LEU:HD22	1:A:2480:GLY:H	1.83	0.43
1:A:3823:LYS:HD3	1:A:3823:LYS:HA	1.83	0.43
1:B:2867:LEU:HD21	1:B:2871:LEU:HB3	1.99	0.43
1:B:3255:GLY:O	1:B:3258:GLU:HG3	2.18	0.43
1:B:3875:MET:HE3	1:B:3875:MET:HB3	1.76	0.43
1:D:2821:TRP:HB3	1:D:2937:VAL:HG22	2.00	0.43
1:D:3209:GLN:HG2	1:D:3210:LEU:HG	2.00	0.43
1:D:3255:GLY:O	1:D:3258:GLU:HG3	2.18	0.43
1:D:3880:PHE:HA	1:D:3883:ASP:OD2	2.19	0.43
1:D:4023:MET:HE2	1:D:4023:MET:HB3	1.86	0.43
1:D:4885:PHE:O	1:D:4889:VAL:HG22	2.17	0.43
1:C:976:ARG:HA	1:C:1044:ARG:HH12	1.83	0.43
1:C:1025:ARG:H	1:C:1025:ARG:HD2	1.82	0.43
1:C:3284:TRP:HB3	1:C:3305:THR:HG21	2.00	0.43
1:A:2516:ASP:OD1	1:A:2516:ASP:N	2.51	0.43
1:A:2740:VAL:HG21	1:A:2819:TRP:NE1	2.33	0.43
1:A:3183:VAL:O	1:A:3187:ARG:HG3	2.19	0.43
1:A:3501:ASP:N	1:A:3501:ASP:OD1	2.50	0.43
1:A:3688:GLU:C	1:A:3690:VAL:H	2.27	0.43
2:F:48:PHE:HZ	2:F:63:VAL:HG21	1.84	0.43
2:F:88:PRO:HB2	1:B:1680:ARG:HH12	1.83	0.43
1:B:1231[B]:GLN:H	1:B:1231[B]:GLN:HG3	1.56	0.43
1:B:1465:ASP:OD1	1:B:1468:LYS:HG2	2.18	0.43
1:B:3310:ASP:HA	1:B:3350:ARG:HH12	1.83	0.43
1:B:3705:PHE:HA	1:B:3708:THR:HG22	2.01	0.43
1:B:3880:PHE:HA	1:B:3883:ASP:OD2	2.19	0.43
1:B:4067:LYS:NZ	1:B:4102:GLN:O	2.51	0.43
1:B:4093:PHE:CE2	1:B:4097:MET:HE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4217:PHE:O	1:B:4221:VAL:HG22	2.17	0.43
1:B:4253:GLU:HG3	1:B:4557:ARG:NH2	2.34	0.43
1:D:416:LYS:HE3	1:D:416:LYS:HB2	1.84	0.43
1:D:976:ARG:HA	1:D:1044:ARG:HH12	1.83	0.43
1:D:2516:ASP:OD1	1:D:2516:ASP:N	2.51	0.43
1:D:2694:GLU:HA	1:D:2697:ARG:NH1	2.33	0.43
1:D:2764:GLU:HG3	1:D:2857:PRO:HB3	2.00	0.43
1:D:4961:CYS:HB3	1:D:4983:HIS:CE1	2.54	0.43
1:C:403:MET:HE1	1:C:451:TYR:CE1	2.53	0.43
1:C:664:PHE:HB3	1:C:811:CYS:SG	2.59	0.43
1:C:1099:GLU:CD	1:C:1125:ASN:HD21	2.26	0.43
1:C:1206:GLN:HA	1:C:1227:ALA:O	2.18	0.43
1:C:2793:PRO:HA	1:C:2855:TYR:CG	2.53	0.43
1:C:3137:LEU:HD21	1:C:3190:LEU:HD23	2.00	0.43
1:C:4253:GLU:HG3	1:C:4557:ARG:NH2	2.34	0.43
1:A:275:ARG:NH1	1:A:338:GLU:OE2	2.50	0.43
1:A:1970:GLN:HG2	1:A:3642:TYR:HA	2.00	0.43
1:A:2462:PRO:HB2	1:A:2464:ASP:OD1	2.19	0.43
1:A:2600:ARG:O	1:A:2604:GLU:HG3	2.19	0.43
1:A:2677:LYS:HB3	1:A:2677:LYS:HE2	1.85	0.43
1:A:2821:TRP:HB3	1:A:2937:VAL:HG22	2.00	0.43
1:A:3384:LYS:HD2	1:A:3386:GLU:HB3	2.01	0.43
1:A:4895:GLY:O	1:D:4892:ARG:NH1	2.44	0.43
1:A:4918:ILE:CD1	1:D:4888:TYR:HD1	2.31	0.43
2:G:11:ASP:OD1	2:G:13:ARG:N	2.32	0.43
1:B:2430:ILE:HB	1:B:2502:MET:HE1	2.00	0.43
1:B:2600:ARG:O	1:B:2604:GLU:HG3	2.19	0.43
1:B:2793:PRO:HA	1:B:2855:TYR:CG	2.53	0.43
1:B:3378:GLN:HA	1:B:3381:LEU:HD23	2.00	0.43
1:B:4961:CYS:HB3	1:B:4983:HIS:CE1	2.54	0.43
1:D:196:MET:SD	1:D:196:MET:N	2.92	0.43
1:D:1249:PRO:HA	1:D:1250:PRO:HD3	1.95	0.43
1:D:2462:PRO:HB2	1:D:2464:ASP:OD1	2.19	0.43
1:D:3183:VAL:O	1:D:3187:ARG:HG3	2.19	0.43
1:D:3284:TRP:HB3	1:D:3305:THR:HG21	2.00	0.43
1:D:4638:TYR:O	1:D:4641:PRO:HD2	2.19	0.43
1:C:416:LYS:HE3	1:C:416:LYS:HB2	1.84	0.43
1:C:2244:ARG:H	1:C:3861:GLU:CD	2.27	0.43
1:C:2600:ARG:O	1:C:2604:GLU:HG3	2.19	0.43
1:C:2740:VAL:HG21	1:C:2819:TRP:NE1	2.33	0.43
1:A:2238:TYR:O	1:A:2242:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3880:PHE:HA	1:A:3883:ASP:OD2	2.19	0.43
2:E:84:ALA:O	2:E:93:PRO:HB3	2.17	0.43
2:H:42:ARG:HD3	1:D:1780:PRO:HG2	2.01	0.43
2:H:57:ARG:HD3	2:H:80:TYR:HA	2.00	0.43
2:F:11:ASP:OD2	2:F:13:ARG:N	2.35	0.43
1:B:664:PHE:HB3	1:B:811:CYS:SG	2.59	0.43
1:B:1424:PRO:HA	1:B:1427:ILE:HG22	2.01	0.43
1:B:1864:LYS:NZ	1:B:1871:PHE:O	2.45	0.43
1:B:1943:LEU:HB2	1:B:2123:LEU:HD21	2.00	0.43
1:B:2694:GLU:HA	1:B:2697:ARG:NH1	2.33	0.43
1:B:2768:PHE:O	1:B:2771:ILE:HG22	2.19	0.43
1:B:3462:ASN:OD1	1:B:3462:ASN:N	2.52	0.43
1:B:3501:ASP:N	1:B:3501:ASP:OD1	2.50	0.43
1:B:3590:GLU:H	1:B:3590:GLU:CD	2.26	0.43
1:D:1447:CYS:HB3	1:D:1555:LEU:HB3	2.00	0.43
1:D:2538:THR:HG23	1:D:2541:PHE:H	1.83	0.43
1:D:3112:LEU:HA	1:D:3112:LEU:HD13	1.85	0.43
1:D:3137:LEU:HD21	1:D:3190:LEU:HD23	2.00	0.43
1:D:4253:GLU:HG3	1:D:4557:ARG:HH21	1.83	0.43
1:D:4627:MET:HE3	1:D:4627:MET:N	2.30	0.43
1:C:3590:GLU:CD	1:C:3590:GLU:H	2.26	0.43
1:C:3880:PHE:HA	1:C:3883:ASP:OD2	2.19	0.43
1:A:196:MET:SD	1:A:196:MET:N	2.92	0.43
1:A:664:PHE:HB3	1:A:811:CYS:SG	2.59	0.43
1:A:924:MET:O	1:A:928:THR:HG23	2.19	0.43
1:A:3478:MET:O	1:A:3478:MET:SD	2.77	0.43
1:A:3695:PRO:HB3	1:A:3699:HIS:HB3	2.01	0.43
1:A:4093:PHE:CE2	1:A:4097:MET:HE3	2.54	0.43
1:A:4840:THR:HG22	1:D:4826:ILE:HD13	2.00	0.43
2:H:32:ASP:OD2	2:H:34:LYS:NZ	2.45	0.43
2:F:44:LYS:HD2	2:F:44:LYS:C	2.44	0.43
1:B:196:MET:N	1:B:196:MET:SD	2.92	0.43
1:B:403:MET:HE1	1:B:451:TYR:CE1	2.53	0.43
1:B:1206:GLN:HA	1:B:1227:ALA:O	2.18	0.43
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	2.00	0.43
1:D:880:GLU:HG3	1:D:910:PHE:HB3	2.01	0.43
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.52	0.43
1:D:2430:ILE:HB	1:D:2502:MET:HE1	2.00	0.43
1:D:3376:GLU:OE2	1:D:3450:ASN:ND2	2.51	0.43
1:D:3835:LEU:HD22	1:D:3880:PHE:HZ	1.83	0.43
1:C:1424:PRO:HA	1:C:1427:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1447:CYS:HB3	1:C:1555:LEU:HB3	2.00	0.43
1:C:1748:PHE:HB2	1:C:1758:ARG:NH2	2.34	0.43
1:C:2238:TYR:O	1:C:2242:ILE:HG13	2.19	0.43
1:C:2527:LEU:HD12	1:C:2527:LEU:HA	1.87	0.43
1:C:3382:GLU:OE1	1:C:3382:GLU:N	2.52	0.43
1:C:3525:CYS:SG	1:C:3599:VAL:HG21	2.59	0.43
1:C:3835:LEU:HD22	1:C:3880:PHE:HZ	1.83	0.43
1:C:4243:PHE:CE2	1:C:4247:ILE:HD11	2.54	0.43
1:A:738:LEU:HD23	1:A:738:LEU:HA	1.86	0.43
1:A:976:ARG:HA	1:A:1044:ARG:HH12	1.83	0.43
1:A:1000:ARG:HA	1:A:1003:GLN:OE1	2.18	0.43
1:A:1055:PRO:HA	1:A:1056:PRO:HD3	1.95	0.43
1:A:1099:GLU:CD	1:A:1125:ASN:HD21	2.26	0.43
1:A:3378:GLN:HA	1:A:3381:LEU:HD23	2.00	0.43
1:B:2527:LEU:HA	1:B:2527:LEU:HD12	1.87	0.43
1:B:3384:LYS:HD2	1:B:3386:GLU:HB3	2.01	0.43
1:D:961:MET:HE2	1:D:965:TYR:O	2.19	0.43
1:D:3634:ALA:HA	1:D:3637:ARG:HG2	2.01	0.43
1:C:81:MET:C	1:C:81:MET:HE2	2.44	0.43
1:C:2008:MET:HE1	1:C:2020:ASP:OD2	2.19	0.43
1:C:3689:GLU:C	1:C:3691:GLU:H	2.27	0.43
1:C:4961:CYS:HB3	1:C:4983:HIS:CE1	2.54	0.43
1:A:664:PHE:CZ	1:A:779:PRO:HB3	2.54	0.42
1:A:880:GLU:HG3	1:A:910:PHE:HB3	2.01	0.42
1:A:1575:LEU:HD23	1:A:1575:LEU:HA	1.84	0.42
1:A:1748:PHE:HB2	1:A:1758:ARG:NH2	2.34	0.42
1:A:2604:GLU:HG2	1:A:2639:MET:HG3	2.01	0.42
1:A:3277:LEU:HD23	1:A:3277:LEU:HA	1.90	0.42
1:A:3590:GLU:CD	1:A:3590:GLU:H	2.26	0.42
2:F:57:ARG:HE	2:F:57:ARG:HB2	1.56	0.42
1:B:2462:PRO:HB2	1:B:2464:ASP:OD1	2.19	0.42
1:B:2604:GLU:HG2	1:B:2639:MET:HG3	2.01	0.42
1:B:3689:GLU:C	1:B:3691:GLU:H	2.27	0.42
1:B:4638:TYR:O	1:B:4641:PRO:HD2	2.19	0.42
1:D:924:MET:O	1:D:928:THR:HG23	2.19	0.42
1:D:1000:ARG:HA	1:D:1003:GLN:OE1	2.18	0.42
1:D:2238:TYR:O	1:D:2242:ILE:HG13	2.19	0.42
1:D:2604:GLU:HG2	1:D:2639:MET:HG3	2.01	0.42
1:D:2641:LEU:HA	1:D:2641:LEU:HD23	1.88	0.42
1:D:4253:GLU:HG3	1:D:4557:ARG:NH2	2.34	0.42
1:D:4961:CYS:HA	1:D:5023:PRO:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:961:MET:HE2	1:C:965:TYR:O	2.19	0.42
1:C:2516:ASP:OD1	1:C:2516:ASP:N	2.51	0.42
1:C:2599:GLN:O	1:C:2603:ILE:HG13	2.19	0.42
1:A:81:MET:C	1:A:81:MET:HE2	2.44	0.42
1:A:403:MET:HE1	1:A:451:TYR:CE1	2.53	0.42
1:A:2599:GLN:O	1:A:2603:ILE:HG13	2.19	0.42
1:A:2881:ASN:HA	1:A:2884:ASN:HD21	1.83	0.42
1:A:4253:GLU:HG3	1:A:4557:ARG:NH2	2.34	0.42
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.44	0.42
1:A:4627:MET:HE3	1:A:4627:MET:N	2.30	0.42
1:B:81:MET:C	1:B:81:MET:HE2	2.44	0.42
1:B:1299:GLN:NE2	1:B:1545:ASN:OD1	2.53	0.42
1:B:1926:LEU:O	1:B:1929:MET:HB2	2.19	0.42
1:B:2310:CYS:O	1:B:2314:LEU:HD22	2.19	0.42
1:B:2765:LYS:NZ	1:B:2860:PRO:HA	2.23	0.42
1:B:3132:THR:HG22	1:B:3137:LEU:HD13	2.01	0.42
1:B:3944:GLU:OE1	1:B:3946:GLN:N	2.50	0.42
1:D:2008:MET:HE1	1:D:2020:ASP:OD2	2.19	0.42
1:D:2768:PHE:O	1:D:2771:ILE:HG22	2.19	0.42
1:D:2785:LEU:C	1:D:2786:LYS:HG3	2.44	0.42
1:D:2821:TRP:HH2	1:D:2877:GLN:HB3	1.82	0.42
1:D:2823:ILE:HA	1:D:2937:VAL:HA	2.00	0.42
1:D:4243:PHE:CE2	1:D:4247:ILE:HD11	2.54	0.42
1:C:618:GLN:OE1	1:C:1678:ASN:ND2	2.43	0.42
1:C:2604:GLU:HG2	1:C:2639:MET:HG3	2.01	0.42
1:C:3209:GLN:HG2	1:C:3210:LEU:HG	2.00	0.42
1:C:3310:ASP:HA	1:C:3350:ARG:HH12	1.83	0.42
1:C:3478:MET:O	1:C:3478:MET:SD	2.77	0.42
1:C:3634:ALA:HA	1:C:3637:ARG:HG2	2.01	0.42
1:A:140:ASP:OD1	1:A:142:THR:OG1	2.30	0.42
1:A:328:LYS:HE3	1:A:328:LYS:HB3	1.75	0.42
1:A:961:MET:HE2	1:A:965:TYR:O	2.19	0.42
1:A:4961:CYS:HB3	1:A:4983:HIS:CE1	2.54	0.42
1:B:4253:GLU:HG3	1:B:4557:ARG:HH21	1.83	0.42
1:D:471:LEU:HA	1:D:474:ARG:HE	1.85	0.42
1:D:901:LYS:HD2	1:D:901:LYS:HA	1.81	0.42
1:D:1299:GLN:NE2	1:D:1545:ASN:OD1	2.53	0.42
1:D:2599:GLN:O	1:D:2603:ILE:HG13	2.19	0.42
1:D:2765:LYS:HD3	1:D:2765:LYS:HA	1.70	0.42
1:D:2990:PRO:HG2	1:D:2991:HIS:CE1	2.55	0.42
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3462:ASN:OD1	1:D:3462:ASN:N	2.52	0.42
1:D:3999:MET:HE3	1:D:3999:MET:HB3	1.82	0.42
1:C:471:LEU:HA	1:C:474:ARG:HE	1.85	0.42
1:C:2102:VAL:HG13	1:C:2120:MET:HE2	2.01	0.42
1:C:2263:ILE:HD12	1:C:2263:ILE:HA	1.92	0.42
1:C:2462:PRO:HB2	1:C:2464:ASP:OD1	2.19	0.42
1:C:2768:PHE:O	1:C:2771:ILE:HG22	2.19	0.42
1:C:3462:ASN:OD1	1:C:3462:ASN:N	2.52	0.42
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.45	0.42
1:A:648:ILE:HD13	1:A:811:CYS:HB3	2.01	0.42
1:A:667:MET:HE3	1:A:743:VAL:HG22	2.01	0.42
1:A:1037:ASP:O	1:A:1041:GLN:HG2	2.20	0.42
1:A:1658:ASP:N	1:A:1658:ASP:OD1	2.52	0.42
1:A:2527:LEU:HD12	1:A:2527:LEU:HA	1.87	0.42
1:A:3705:PHE:HA	1:A:3708:THR:HG22	2.01	0.42
1:A:4097:MET:HE2	1:A:4097:MET:HB2	1.71	0.42
1:A:4638:TYR:O	1:A:4641:PRO:HD2	2.19	0.42
2:H:47:LYS:NZ	2:H:107:GLU:OE2	2.30	0.42
2:F:57:ARG:HD3	2:F:80:TYR:HA	2.01	0.42
1:B:879:HIS:NE2	1:B:921:ASN:HB2	2.35	0.42
1:B:1447:CYS:HB3	1:B:1555:LEU:HB3	2.00	0.42
1:B:2238:TYR:O	1:B:2242:ILE:HG13	2.19	0.42
1:B:2998:PHE:HA	1:B:3002:LEU:HD23	2.02	0.42
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.02	0.42
1:D:2102:VAL:HG13	1:D:2120:MET:HE2	2.01	0.42
1:D:2600:ARG:O	1:D:2604:GLU:HG3	2.19	0.42
1:D:3594:ARG:HA	1:D:3594:ARG:NH1	2.35	0.42
1:D:3688:GLU:C	1:D:3690:VAL:H	2.27	0.42
1:C:1930:LYS:HE2	1:C:1930:LYS:HB2	1.91	0.42
1:C:3688:GLU:C	1:C:3690:VAL:H	2.27	0.42
1:C:3999:MET:HE3	1:C:3999:MET:HB3	1.82	0.42
1:C:4134:GLU:HB3	1:C:4135:PRO:HD3	2.02	0.42
1:A:188:GLU:H	1:A:188:GLU:CD	2.28	0.42
1:A:922:LEU:HD13	1:A:922:LEU:HA	1.89	0.42
1:A:1447:CYS:HB3	1:A:1555:LEU:HB3	2.00	0.42
1:A:2623:LEU:O	1:A:2627:VAL:HG23	2.18	0.42
1:A:2990:PRO:HG2	1:A:2991:HIS:CE1	2.55	0.42
1:A:3367:LYS:HE3	1:A:3367:LYS:HB2	1.86	0.42
1:A:4897:ILE:O	1:A:4901:ILE:HG12	2.18	0.42
2:G:42:ARG:HD3	1:C:1780:PRO:HG2	2.02	0.42
1:B:336:PRO:HA	1:B:337:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:961:MET:HE2	1:B:965:TYR:O	2.19	0.42
1:B:1055:PRO:HA	1:B:1056:PRO:HD3	1.95	0.42
1:B:1099:GLU:CD	1:B:1125:ASN:HD21	2.26	0.42
1:B:1999:ARG:HG3	1:B:3635:CYS:C	2.45	0.42
1:B:2102:VAL:HG13	1:B:2120:MET:HE2	2.01	0.42
1:B:2307:LEU:HD21	1:B:2362:GLU:HB2	2.02	0.42
1:B:3183:VAL:O	1:B:3187:ARG:HG3	2.19	0.42
1:B:3688:GLU:C	1:B:3690:VAL:H	2.27	0.42
1:D:1926:LEU:O	1:D:1929:MET:HB2	2.19	0.42
1:D:1999:ARG:HG3	1:D:3635:CYS:C	2.45	0.42
1:D:2020:ASP:OD1	1:D:2020:ASP:N	2.42	0.42
1:D:3695:PRO:HB3	1:D:3699:HIS:HB3	2.01	0.42
1:C:640:TYR:CE2	1:C:1636:MET:HB3	2.55	0.42
1:C:709:ASP:OD1	1:C:725:HIS:ND1	2.48	0.42
1:C:1926:LEU:O	1:C:1929:MET:HB2	2.19	0.42
1:C:2430:ILE:HB	1:C:2502:MET:HE1	2.00	0.42
1:C:2785:LEU:C	1:C:2786:LYS:HG3	2.44	0.42
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.02	0.42
1:C:4675:LYS:HG3	1:C:4715:TYR:CE1	2.55	0.42
1:C:4961:CYS:HA	1:C:5023:PRO:O	2.19	0.42
1:A:13:PHE:CE1	1:A:164:ARG:HG2	2.55	0.42
1:A:835:ARG:NH2	1:A:1210:SER:O	2.35	0.42
1:A:1926:LEU:O	1:A:1929:MET:HB2	2.19	0.42
1:A:2785:LEU:C	1:A:2786:LYS:HG3	2.44	0.42
1:A:4675:LYS:HG3	1:A:4715:TYR:CE1	2.55	0.42
1:B:788:LYS:HB2	1:B:788:LYS:HE3	1.82	0.42
1:B:924:MET:O	1:B:928:THR:HG23	2.19	0.42
1:B:1748:PHE:HB2	1:B:1758:ARG:NH2	2.34	0.42
1:B:2008:MET:HE1	1:B:2020:ASP:OD2	2.19	0.42
1:B:3525:CYS:SG	1:B:3599:VAL:HG21	2.59	0.42
1:B:4243:PHE:CE2	1:B:4247:ILE:HD11	2.54	0.42
1:B:4675:LYS:HG3	1:B:4715:TYR:CE1	2.55	0.42
1:D:1424:PRO:HA	1:D:1427:ILE:HG22	2.01	0.42
1:D:3478:MET:SD	1:D:3478:MET:O	2.77	0.42
1:D:3525:CYS:SG	1:D:3599:VAL:HG21	2.59	0.42
1:D:4093:PHE:CE2	1:D:4097:MET:HE3	2.54	0.42
1:D:4675:LYS:HG3	1:D:4715:TYR:CE1	2.55	0.42
1:C:2150:GLU:H	1:C:2150:GLU:CD	2.27	0.42
1:C:3183:VAL:O	1:C:3187:ARG:HG3	2.19	0.42
1:C:3384:LYS:HD2	1:C:3386:GLU:HB3	2.01	0.42
1:C:3594:ARG:HA	1:C:3594:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3944:GLU:H	1:C:3944:GLU:HG3	1.74	0.42
1:C:4093:PHE:CE2	1:C:4097:MET:HE3	2.54	0.42
1:A:640:TYR:CE2	1:A:1636:MET:HB3	2.55	0.42
1:A:970:LEU:HG	1:A:972:LEU:HD21	2.02	0.42
1:A:2008:MET:HE1	1:A:2020:ASP:OD2	2.19	0.42
1:A:2998:PHE:HA	1:A:3002:LEU:HD23	2.01	0.42
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	2.02	0.42
1:A:4961:CYS:HA	1:A:5023:PRO:O	2.19	0.42
1:B:2694:GLU:HA	1:B:2697:ARG:HH12	1.85	0.42
1:B:3478:MET:SD	1:B:3478:MET:O	2.77	0.42
1:B:4047:MET:HE3	1:B:4047:MET:HB3	1.78	0.42
1:D:1032:LYS:HE3	1:D:1032:LYS:HB2	1.88	0.42
1:D:1037:ASP:O	1:D:1041:GLN:HG2	2.20	0.42
1:D:2307:LEU:HD21	1:D:2362:GLU:HB2	2.02	0.42
1:D:2624:ARG:O	1:D:2627:VAL:HB	2.20	0.42
1:D:3384:LYS:HD2	1:D:3386:GLU:HB3	2.01	0.42
1:C:196:MET:N	1:C:196:MET:SD	2.92	0.42
1:C:664:PHE:CZ	1:C:779:PRO:HB3	2.54	0.42
1:C:870:ILE:HG12	1:C:1051:TYR:HE2	1.84	0.42
1:C:924:MET:O	1:C:928:THR:HG23	2.19	0.42
1:C:2998:PHE:HA	1:C:3002:LEU:HD23	2.01	0.42
1:C:3705:PHE:HA	1:C:3708:THR:HG22	2.01	0.42
1:C:4638:TYR:O	1:C:4641:PRO:HD2	2.19	0.42
1:A:2765:LYS:HD3	1:A:2765:LYS:HA	1.70	0.42
1:A:3462:ASN:OD1	1:A:3462:ASN:N	2.52	0.42
1:A:4902:GLU:O	1:A:4913:ARG:NH1	2.52	0.42
1:B:648:ILE:HD13	1:B:811:CYS:HB3	2.02	0.42
1:B:2538:THR:HG23	1:B:2541:PHE:H	1.83	0.42
1:B:2816:MET:HB3	1:B:2816:MET:HE2	1.66	0.42
1:D:640:TYR:CE2	1:D:1636:MET:HB3	2.55	0.42
1:D:870:ILE:HG12	1:D:1051:TYR:HE2	1.84	0.42
1:D:937:CYS:N	1:D:1056:PRO:HG3	2.35	0.42
1:D:970:LEU:HG	1:D:972:LEU:HD21	2.02	0.42
1:D:2256:TYR:O	1:D:2259:GLU:HG3	2.20	0.42
1:D:4060:LYS:HD2	1:D:4060:LYS:HA	1.91	0.42
1:C:13:PHE:CE1	1:C:164:ARG:HG2	2.55	0.42
1:C:970:LEU:HG	1:C:972:LEU:HD21	2.02	0.42
1:C:1055:PRO:HA	1:C:1056:PRO:HD3	1.95	0.42
1:C:2307:LEU:HD21	1:C:2362:GLU:HB2	2.02	0.42
1:C:2310:CYS:O	1:C:2314:LEU:HD22	2.19	0.42
1:C:2538:THR:HG23	1:C:2541:PHE:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2694:GLU:HA	1:C:2697:ARG:HH12	1.85	0.42
1:C:2907:PRO:HB2	1:C:2910:THR:HG23	2.02	0.42
1:C:4851:TYR:HD1	1:C:4916:PHE:CE1	2.38	0.42
1:A:471:LEU:HA	1:A:474:ARG:HE	1.85	0.42
1:A:901:LYS:HA	1:A:901:LYS:HD2	1.82	0.42
1:A:1424:PRO:HA	1:A:1427:ILE:HG22	2.01	0.42
1:A:1864:LYS:HE3	1:A:1872:THR:HA	2.02	0.42
1:A:2256:TYR:O	1:A:2259:GLU:HG3	2.20	0.42
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	2.02	0.42
1:A:2907:PRO:HB2	1:A:2910:THR:HG23	2.02	0.42
1:A:3525:CYS:SG	1:A:3599:VAL:HG21	2.59	0.42
1:A:4790:LEU:HD23	1:A:4790:LEU:HA	1.90	0.42
2:H:54:GLU:OE1	2:H:55:VAL:HG13	2.20	0.42
1:B:188:GLU:H	1:B:188:GLU:CD	2.28	0.42
1:B:664:PHE:CZ	1:B:779:PRO:HB3	2.54	0.42
1:B:2150:GLU:H	1:B:2150:GLU:CD	2.27	0.42
1:B:2907:PRO:HB2	1:B:2910:THR:HG23	2.02	0.42
1:B:2912:THR:HG23	1:B:2914:LYS:HG3	2.02	0.42
1:B:3382:GLU:OE1	1:B:3382:GLU:N	2.52	0.42
1:B:4023:MET:HE2	1:B:4023:MET:HB3	1.86	0.42
1:B:4134:GLU:HB3	1:B:4135:PRO:HD3	2.02	0.42
1:B:4874:MET:HE3	1:B:4874:MET:HB3	1.90	0.42
1:D:774:ASP:CG	1:D:1470:ARG:HH22	2.24	0.42
1:D:879:HIS:NE2	1:D:921:ASN:HB2	2.35	0.42
1:D:1748:PHE:HB2	1:D:1758:ARG:NH2	2.34	0.42
1:D:2881:ASN:HA	1:D:2884:ASN:HD21	1.83	0.42
1:D:3852:LYS:HE3	1:D:3852:LYS:HB3	1.91	0.42
1:C:1299:GLN:NE2	1:C:1545:ASN:OD1	2.53	0.42
1:A:69:LEU:HD13	1:A:101:LEU:HD11	2.02	0.42
1:A:651:GLY:N	1:A:658:GLN:OE1	2.53	0.42
1:A:2574:HIS:CD2	1:A:2574:HIS:H	2.38	0.42
1:A:3607:GLU:OE2	1:A:3608:GLN:NE2	2.48	0.42
1:A:3621:HIS:O	1:A:3622:LYS:HG3	2.20	0.42
1:A:3762:ARG:HD3	1:A:4754:ASN:HA	2.02	0.42
1:A:4091:LYS:HE2	1:A:4091:LYS:HB2	1.89	0.42
1:A:4243:PHE:CE2	1:A:4247:ILE:HD11	2.54	0.42
1:A:4735:GLU:H	1:A:4735:GLU:CD	2.28	0.42
1:B:13:PHE:CE1	1:B:164:ARG:HG2	2.55	0.42
1:B:471:LEU:HA	1:B:474:ARG:HE	1.85	0.42
1:B:640:TYR:CE2	1:B:1636:MET:HB3	2.55	0.42
1:B:2191:PHE:CE2	1:B:2242:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3594:ARG:HA	1:B:3594:ARG:NH1	2.35	0.42
1:B:3695:PRO:HB3	1:B:3699:HIS:HB3	2.01	0.42
1:D:13:PHE:CE1	1:D:164:ARG:HG2	2.55	0.42
1:D:81:MET:HE2	1:D:81:MET:C	2.44	0.42
1:D:738:LEU:HA	1:D:738:LEU:HD23	1.86	0.42
1:D:1668:ARG:HG3	1:D:1671:ARG:NH2	2.35	0.42
1:D:2310:CYS:O	1:D:2314:LEU:HD22	2.19	0.42
1:D:4558:ASN:HB3	1:D:4561:THR:OG1	2.20	0.42
1:C:1488:LYS:HE3	1:C:1488:LYS:HB2	1.85	0.42
1:C:1999:ARG:HG3	1:C:3635:CYS:C	2.45	0.42
1:C:3132:THR:HG22	1:C:3137:LEU:HD13	2.01	0.42
1:C:3308:THR:H	1:C:3311:HIS:HD1	1.67	0.42
1:C:3695:PRO:HB3	1:C:3699:HIS:HB3	2.01	0.42
1:C:4148:THR:HG21	1:C:4180:ARG:HH21	1.85	0.42
1:C:5030:LYS:HB2	1:C:5030:LYS:HE2	1.78	0.42
1:A:788:LYS:HE3	1:A:788:LYS:HB2	1.82	0.41
1:A:805:PRO:HG2	1:A:808:TYR:CD1	2.55	0.41
1:A:1999:ARG:HG3	1:A:3635:CYS:C	2.45	0.41
1:A:2624:ARG:O	1:A:2627:VAL:HB	2.20	0.41
1:A:2768:PHE:O	1:A:2771:ILE:HG22	2.19	0.41
1:A:3230:LEU:HD23	1:A:3230:LEU:H	1.85	0.41
1:A:3382:GLU:OE1	1:A:3382:GLU:N	2.52	0.41
1:A:3731:LYS:HA	1:A:3734:HIS:CE1	2.55	0.41
1:A:4047:MET:HE3	1:A:4047:MET:HB3	1.78	0.41
1:B:176:SER:HG	1:B:178:ARG:HH11	1.61	0.41
1:B:3367:LYS:HE3	1:B:3367:LYS:HB2	1.86	0.41
1:B:4148:THR:HG21	1:B:4180:ARG:HH21	1.85	0.41
1:B:4184:MET:HE2	1:B:4184:MET:HB2	1.92	0.41
1:D:709:ASP:OD1	1:D:725:HIS:ND1	2.48	0.41
1:D:2150:GLU:H	1:D:2150:GLU:CD	2.27	0.41
1:D:3006:ILE:HG23	1:D:3010:PHE:CD2	2.55	0.41
1:D:3342:ALA:O	1:D:3345:ILE:HG12	2.21	0.41
1:D:4148:THR:HG21	1:D:4180:ARG:HH21	1.85	0.41
1:D:4917:ASP:OD2	1:C:4888:TYR:OH	2.25	0.41
1:C:2793:PRO:O	1:C:2797:PHE:N	2.53	0.41
1:C:4067:LYS:NZ	1:C:4102:GLN:O	2.51	0.41
1:C:4558:ASN:HB3	1:C:4561:THR:OG1	2.20	0.41
1:A:1299:GLN:NE2	1:A:1545:ASN:OD1	2.53	0.41
1:A:2019:GLU:H	1:A:2019:GLU:CD	2.28	0.41
1:A:2765:LYS:HZ1	1:A:2860:PRO:HA	1.85	0.41
1:A:3132:THR:HG22	1:A:3137:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3689:GLU:C	1:A:3691:GLU:H	2.27	0.41
1:A:3933:PHE:HD2	1:A:3951:PHE:CE2	2.38	0.41
1:A:4558:ASN:HB3	1:A:4561:THR:OG1	2.20	0.41
2:G:13:ARG:HB2	2:G:13:ARG:CZ	2.51	0.41
2:F:42:ARG:HD3	1:B:1780:PRO:HG2	2.02	0.41
1:B:667:MET:HE3	1:B:743:VAL:HG22	2.01	0.41
1:B:880:GLU:HG3	1:B:910:PHE:HB3	2.01	0.41
1:B:937:CYS:N	1:B:1056:PRO:HG3	2.35	0.41
1:B:970:LEU:HG	1:B:972:LEU:HD21	2.02	0.41
1:B:1690:ASP:OD2	1:B:1693:GLN:NE2	2.53	0.41
1:B:3230:LEU:HD23	1:B:3230:LEU:H	1.85	0.41
1:B:3762:ARG:HD3	1:B:4754:ASN:HA	2.02	0.41
1:B:3933:PHE:HD2	1:B:3951:PHE:CE2	2.39	0.41
1:D:651:GLY:N	1:D:658:GLN:OE1	2.53	0.41
1:D:1694:LEU:O	1:D:1698:LEU:HG	2.21	0.41
1:D:2694:GLU:HA	1:D:2697:ARG:HH12	1.85	0.41
1:D:2907:PRO:HB2	1:D:2910:THR:HG23	2.02	0.41
1:D:3762:ARG:HD3	1:D:4754:ASN:HA	2.02	0.41
1:D:4895:GLY:O	1:C:4892:ARG:NH1	2.44	0.41
1:C:835:ARG:NH2	1:C:1210:SER:O	2.35	0.41
1:C:2624:ARG:O	1:C:2627:VAL:HB	2.20	0.41
1:C:3762:ARG:HD3	1:C:4754:ASN:HA	2.02	0.41
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.44	0.41
1:A:1694:LEU:O	1:A:1698:LEU:HG	2.21	0.41
1:A:1823:GLY:O	1:A:1825:HIS:ND1	2.47	0.41
1:A:2263:ILE:HD12	1:A:2263:ILE:HA	1.92	0.41
1:B:463:GLU:HG2	1:B:464:LYS:N	2.35	0.41
1:B:651:GLY:N	1:B:658:GLN:OE1	2.53	0.41
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.52	0.41
1:B:1668:ARG:HG3	1:B:1671:ARG:NH2	2.35	0.41
1:B:2599:GLN:O	1:B:2603:ILE:HG13	2.19	0.41
1:B:2785:LEU:C	1:B:2786:LYS:HG3	2.44	0.41
1:B:3465:ASN:C	1:B:3467:MET:H	2.28	0.41
1:D:803:LEU:HD12	1:D:804:PRO:HD2	2.02	0.41
1:D:1864:LYS:HE3	1:D:1872:THR:HA	2.02	0.41
1:D:1926:LEU:HB3	1:D:1939:MET:SD	2.60	0.41
1:D:2244:ARG:H	1:D:3861:GLU:CD	2.27	0.41
1:D:2677:LYS:HE2	1:D:2677:LYS:HB3	1.85	0.41
1:D:3465:ASN:C	1:D:3467:MET:H	2.28	0.41
1:C:2191:PHE:CE2	1:C:2242:ILE:HD11	2.55	0.41
1:C:2801:ASP:HA	1:C:2804:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3621:HIS:O	1:C:3622:LYS:HG3	2.20	0.41
1:C:3974:THR:O	1:C:3978:GLN:HG2	2.20	0.41
1:A:2123:LEU:HD12	1:A:2123:LEU:HA	1.95	0.41
1:A:2793:PRO:O	1:A:2797:PHE:N	2.53	0.41
1:A:3594:ARG:HA	1:A:3594:ARG:NH1	2.35	0.41
1:A:3634:ALA:HA	1:A:3637:ARG:HG2	2.01	0.41
2:F:54:GLU:OE2	2:F:55:VAL:HG13	2.20	0.41
1:B:274:LEU:HB3	1:B:339:ILE:HD12	2.03	0.41
1:B:365:LYS:HB3	1:B:365:LYS:HE3	1.74	0.41
1:B:2244:ARG:H	1:B:3861:GLU:CD	2.27	0.41
1:B:2256:TYR:O	1:B:2259:GLU:HG3	2.20	0.41
1:B:4902:GLU:O	1:B:4913:ARG:NH1	2.52	0.41
1:D:367:LEU:HD12	1:D:367:LEU:HA	1.89	0.41
1:D:805:PRO:HG2	1:D:808:TYR:CD1	2.55	0.41
1:D:2574:HIS:CD2	1:D:2574:HIS:H	2.38	0.41
1:D:3051:ARG:HA	1:D:3131:TYR:CE1	2.56	0.41
1:D:3308:THR:H	1:D:3311:HIS:HD1	1.67	0.41
1:D:3689:GLU:C	1:D:3691:GLU:H	2.27	0.41
1:D:3705:PHE:HA	1:D:3708:THR:HG22	2.01	0.41
1:C:648:ILE:HD13	1:C:811:CYS:HB3	2.01	0.41
1:C:667:MET:HE3	1:C:743:VAL:HG22	2.01	0.41
1:C:981:GLN:O	1:C:985:VAL:HG23	2.20	0.41
1:C:2881:ASN:HA	1:C:2884:ASN:HD21	1.83	0.41
1:C:3465:ASN:C	1:C:3467:MET:H	2.28	0.41
1:A:990:GLU:HA	1:A:1024:TYR:CG	2.56	0.41
1:A:2102:VAL:HG13	1:A:2120:MET:HE2	2.01	0.41
1:A:2307:LEU:HD21	1:A:2362:GLU:HB2	2.02	0.41
1:A:2310:CYS:O	1:A:2314:LEU:HD22	2.19	0.41
1:A:2775:TRP:CD2	1:A:2786:LYS:HE3	2.56	0.41
1:A:3006:ILE:HG23	1:A:3010:PHE:CD2	2.55	0.41
1:A:3445:TRP:NE1	1:A:3455:GLU:OE1	2.46	0.41
1:B:2793:PRO:O	1:B:2797:PHE:N	2.53	0.41
1:B:2819:TRP:C	1:B:2820:GLU:HG3	2.46	0.41
1:B:2990:PRO:HG2	1:B:2991:HIS:CE1	2.55	0.41
1:B:3051:ARG:HA	1:B:3131:TYR:CE1	2.56	0.41
1:B:4627:MET:HE3	1:B:4627:MET:N	2.30	0.41
1:D:664:PHE:CZ	1:D:779:PRO:HB3	2.54	0.41
1:D:3132:THR:HG22	1:D:3137:LEU:HD13	2.01	0.41
1:D:3508:SER:HB3	1:D:3511:VAL:HG22	2.02	0.41
1:D:4184:MET:HE2	1:D:4184:MET:HB2	1.92	0.41
1:C:458:GLU:H	1:C:458:GLU:HG3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:803:LEU:HD12	1:C:804:PRO:HD2	2.02	0.41
1:C:901:LYS:HG3	1:C:903:LEU:HG	2.03	0.41
1:C:961:MET:H	1:C:961:MET:HG2	1.59	0.41
1:C:1668:ARG:HG3	1:C:1671:ARG:NH2	2.35	0.41
1:C:3162:GLN:OE1	1:C:3218:VAL:HG13	2.21	0.41
1:C:3875:MET:HE3	1:C:3875:MET:HB3	1.75	0.41
1:C:3933:PHE:HD2	1:C:3951:PHE:CE2	2.38	0.41
1:A:981:GLN:O	1:A:985:VAL:HG23	2.20	0.41
1:A:3342:ALA:O	1:A:3345:ILE:HG12	2.20	0.41
1:A:4148:THR:HG21	1:A:4180:ARG:HH21	1.85	0.41
1:B:2419:GLY:O	1:B:2423:MET:SD	2.79	0.41
1:B:2624:ARG:O	1:B:2627:VAL:HB	2.20	0.41
1:B:3112:LEU:HD13	1:B:3112:LEU:HA	1.85	0.41
1:B:4851:TYR:HD1	1:B:4916:PHE:CE1	2.38	0.41
1:B:4904:PRO:CB	1:B:4913:ARG:HG2	2.51	0.41
1:D:365:LYS:HB3	1:D:365:LYS:HE3	1.74	0.41
1:D:710:ASP:OD1	1:D:713:SER:OG	2.26	0.41
1:D:2628:PHE:HZ	1:D:2910:THR:HG21	1.86	0.41
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.86	0.41
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	2.03	0.41
1:D:3230:LEU:H	1:D:3230:LEU:HD23	1.85	0.41
1:D:3731:LYS:HA	1:D:3734:HIS:CE1	2.56	0.41
1:D:3974:THR:O	1:D:3978:GLN:HG2	2.20	0.41
1:D:4134:GLU:HB3	1:D:4135:PRO:HD3	2.01	0.41
1:C:463:GLU:HG2	1:C:464:LYS:N	2.35	0.41
1:C:1032:LYS:HE3	1:C:1032:LYS:HB2	1.88	0.41
1:C:2628:PHE:HZ	1:C:2910:THR:HG21	1.86	0.41
1:C:4765:LEU:O	1:C:4769:MET:HE1	2.21	0.41
1:A:1183:GLU:CD	1:A:1183:GLU:H	2.29	0.41
1:A:1680:ARG:HH12	2:E:88:PRO:HB2	1.84	0.41
1:A:2191:PHE:CE2	1:A:2242:ILE:HD11	2.55	0.41
1:A:2383:ALA:HA	1:A:2386:ILE:HG12	2.03	0.41
1:A:2419:GLY:O	1:A:2422:ILE:N	2.54	0.41
1:A:2754:PHE:HB2	1:A:2935:TYR:CZ	2.55	0.41
1:A:3944:GLU:OE1	1:A:3946:GLN:N	2.50	0.41
1:A:4874:MET:HE3	1:A:4874:MET:HB3	1.90	0.41
2:E:29:MET:HG2	2:E:30:LEU:O	2.21	0.41
1:B:981:GLN:O	1:B:985:VAL:HG23	2.20	0.41
1:B:1434:TYR:OH	1:B:1436:SER:HB3	2.21	0.41
1:B:1820:ARG:O	1:B:1824:GLN:HG2	2.20	0.41
1:B:2019:GLU:CD	1:B:2019:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2092:GLN:HE21	1:B:2092:GLN:HB3	1.69	0.41
1:B:2412:GLU:C	1:B:2414:ASN:H	2.28	0.41
1:B:3445:TRP:NE1	1:B:3455:GLU:OE1	2.46	0.41
1:B:4010:ILE:O	1:B:4014:LYS:HG3	2.21	0.41
1:B:4735:GLU:H	1:B:4735:GLU:CD	2.28	0.41
1:D:274:LEU:HB3	1:D:339:ILE:HD12	2.03	0.41
1:D:1726:SER:O	1:D:1729:SER:OG	2.37	0.41
1:D:2191:PHE:CE2	1:D:2242:ILE:HD11	2.55	0.41
1:D:2419:GLY:O	1:D:2422:ILE:N	2.54	0.41
1:D:2998:PHE:HA	1:D:3002:LEU:HD23	2.01	0.41
1:D:3836:MET:HE3	1:D:3836:MET:HB2	1.82	0.41
1:D:3933:PHE:HD2	1:D:3951:PHE:CE2	2.39	0.41
1:D:4067:LYS:NZ	1:D:4102:GLN:O	2.51	0.41
1:D:4735:GLU:H	1:D:4735:GLU:CD	2.28	0.41
1:C:274:LEU:HB3	1:C:339:ILE:HD12	2.03	0.41
1:C:879:HIS:NE2	1:C:921:ASN:HB2	2.35	0.41
1:C:1690:ASP:OD2	1:C:1693:GLN:NE2	2.53	0.41
1:C:1820:ARG:O	1:C:1824:GLN:HG2	2.20	0.41
1:C:2019:GLU:H	1:C:2019:GLU:CD	2.28	0.41
1:A:879:HIS:NE2	1:A:921:ASN:HB2	2.35	0.41
1:A:937:CYS:N	1:A:1056:PRO:HG3	2.35	0.41
1:A:1808:ARG:HB2	1:A:1854:PHE:CE1	2.56	0.41
1:A:2150:GLU:H	1:A:2150:GLU:CD	2.27	0.41
1:A:2336:ARG:HG3	1:A:2431:ASP:OD2	2.21	0.41
1:A:2412:GLU:C	1:A:2414:ASN:H	2.28	0.41
1:A:4010:ILE:O	1:A:4014:LYS:HG3	2.21	0.41
2:H:24:VAL:HG21	2:H:59:TRP:HZ3	1.86	0.41
1:B:69:LEU:HD13	1:B:101:LEU:HD11	2.02	0.41
1:B:330:ASP:OD1	1:B:330:ASP:N	2.54	0.41
1:B:710:ASP:OD1	1:B:713:SER:OG	2.26	0.41
1:B:1037:ASP:O	1:B:1041:GLN:HG2	2.20	0.41
1:B:2419:GLY:O	1:B:2422:ILE:N	2.54	0.41
1:B:2775:TRP:CD2	1:B:2786:LYS:HE3	2.56	0.41
1:B:3634:ALA:HA	1:B:3637:ARG:HG2	2.01	0.41
1:B:3731:LYS:HA	1:B:3734:HIS:CE1	2.56	0.41
1:B:3974:THR:O	1:B:3978:GLN:HG2	2.20	0.41
1:B:4961:CYS:HA	1:B:5023:PRO:O	2.19	0.41
1:D:667:MET:HE3	1:D:743:VAL:HG22	2.01	0.41
1:D:990:GLU:HA	1:D:1024:TYR:CG	2.56	0.41
1:D:1690:ASP:OD2	1:D:1693:GLN:NE2	2.53	0.41
1:D:2017:ASP:OD1	1:D:2017:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2412:GLU:C	1:D:2414:ASN:H	2.28	0.41
1:D:2419:GLY:O	1:D:2423:MET:SD	2.79	0.41
1:D:2754:PHE:HB2	1:D:2935:TYR:CZ	2.56	0.41
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	2.02	0.41
1:D:2816:MET:HE2	1:D:2816:MET:HB3	1.66	0.41
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.54	0.41
1:D:3607:GLU:OE2	1:D:3608:GLN:NE2	2.48	0.41
1:D:4765:LEU:O	1:D:4769:MET:HE1	2.20	0.41
1:C:69:LEU:HD13	1:C:101:LEU:HD11	2.02	0.41
1:C:328:LYS:HB3	1:C:328:LYS:HE3	1.75	0.41
1:C:651:GLY:N	1:C:658:GLN:OE1	2.53	0.41
1:C:937:CYS:N	1:C:1056:PRO:HG3	2.35	0.41
1:C:2336:ARG:HG3	1:C:2431:ASP:OD2	2.21	0.41
1:C:2412:GLU:C	1:C:2414:ASN:H	2.28	0.41
1:C:2641:LEU:HA	1:C:2641:LEU:HD23	1.88	0.41
1:C:2713:ASP:OD1	1:C:2713:ASP:N	2.52	0.41
1:C:2816:MET:HB3	1:C:2816:MET:HE2	1.66	0.41
1:C:2819:TRP:C	1:C:2820:GLU:HG3	2.46	0.41
1:C:3731:LYS:HA	1:C:3734:HIS:CE1	2.56	0.41
1:A:330:ASP:N	1:A:330:ASP:OD1	2.54	0.41
1:A:416:LYS:HE3	1:A:416:LYS:HB2	1.84	0.41
1:A:1690:ASP:OD2	1:A:1693:GLN:NE2	2.53	0.41
1:A:1926:LEU:HB3	1:A:1939:MET:SD	2.60	0.41
1:A:2628:PHE:HZ	1:A:2910:THR:HG21	1.86	0.41
1:A:2713:ASP:OD1	1:A:2713:ASP:N	2.52	0.41
1:A:2716:ASP:OD1	1:A:2716:ASP:N	2.51	0.41
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.86	0.41
1:A:3329:ILE:O	1:A:3403:ARG:NH2	2.54	0.41
1:A:3465:ASN:C	1:A:3467:MET:H	2.28	0.41
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.54	0.41
1:A:4942:GLU:HA	1:A:4945:ASP:OD2	2.21	0.41
2:F:13:ARG:HB2	2:F:13:ARG:CZ	2.51	0.41
1:B:306:LYS:HE3	1:B:306:LYS:HB2	1.94	0.41
1:B:803:LEU:HD12	1:B:804:PRO:HD2	2.02	0.41
1:B:805:PRO:HG2	1:B:808:TYR:CD1	2.55	0.41
1:B:1634:LEU:HD23	1:B:1634:LEU:HA	1.90	0.41
1:B:1864:LYS:HE3	1:B:1872:THR:HA	2.02	0.41
1:B:2574:HIS:CD2	1:B:2574:HIS:H	2.38	0.41
1:B:2628:PHE:HZ	1:B:2910:THR:HG21	1.86	0.41
1:B:2754:PHE:HB2	1:B:2935:TYR:CZ	2.56	0.41
1:B:3342:ALA:O	1:B:3345:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3508:SER:HB3	1:B:3511:VAL:HG22	2.02	0.41
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.54	0.41
1:B:4765:LEU:O	1:B:4769:MET:HE1	2.20	0.41
1:B:4942:GLU:HA	1:B:4945:ASP:OD2	2.21	0.41
1:D:503:PHE:HD2	1:D:512:ALA:HA	1.86	0.41
1:D:1820:ARG:O	1:D:1824:GLN:HG2	2.20	0.41
1:D:2019:GLU:H	1:D:2019:GLU:CD	2.28	0.41
1:D:2258:LEU:HD23	1:D:2258:LEU:HA	1.89	0.41
1:D:2819:TRP:C	1:D:2820:GLU:HG3	2.46	0.41
1:D:2912:THR:HG23	1:D:2914:LYS:HG3	2.02	0.41
1:D:3162:GLN:OE1	1:D:3218:VAL:HG13	2.21	0.41
1:D:3621:HIS:O	1:D:3622:LYS:HG3	2.20	0.41
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.44	0.41
1:D:4689:THR:OG1	1:D:4690:GLU:OE1	2.34	0.41
1:D:4851:TYR:HD1	1:D:4916:PHE:CE1	2.38	0.41
1:C:1037:ASP:O	1:C:1041:GLN:HG2	2.20	0.41
1:C:1658:ASP:OD1	1:C:1658:ASP:N	2.52	0.41
1:C:1694:LEU:O	1:C:1698:LEU:HG	2.21	0.41
1:C:1808:ARG:HB2	1:C:1854:PHE:CE1	2.56	0.41
1:C:1864:LYS:HE3	1:C:1872:THR:HA	2.02	0.41
1:C:1926:LEU:HB3	1:C:1939:MET:SD	2.60	0.41
1:C:2256:TYR:O	1:C:2259:GLU:HG3	2.20	0.41
1:C:2298:VAL:HG21	1:C:2334:PHE:CE2	2.56	0.41
1:C:2419:GLY:O	1:C:2423:MET:SD	2.79	0.41
1:C:2675:THR:HB	1:C:2710:LEU:HD21	2.03	0.41
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.86	0.41
1:C:2775:TRP:CD2	1:C:2786:LYS:HE3	2.56	0.41
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	2.02	0.41
1:C:2912:THR:HG23	1:C:2914:LYS:HG3	2.02	0.41
1:C:3006:ILE:HG23	1:C:3010:PHE:CD2	2.55	0.41
1:C:3051:ARG:HA	1:C:3131:TYR:CE1	2.56	0.41
1:C:3230:LEU:HD23	1:C:3230:LEU:H	1.85	0.41
1:C:3342:ALA:O	1:C:3345:ILE:HG12	2.20	0.41
1:C:4010:ILE:O	1:C:4014:LYS:HG3	2.21	0.41
1:A:274:LEU:HB3	1:A:339:ILE:HD12	2.03	0.41
1:A:2479:LEU:HD22	1:A:2480:GLY:N	2.36	0.41
1:A:2531:ARG:HG2	1:A:2585:THR:HG21	2.03	0.41
1:A:2694:GLU:HA	1:A:2697:ARG:HH12	1.85	0.41
1:A:2912:THR:HG23	1:A:2914:LYS:HG3	2.02	0.41
1:A:3974:THR:O	1:A:3978:GLN:HG2	2.20	0.41
1:A:4765:LEU:O	1:A:4769:MET:HE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:PHE:HD2	1:B:512:ALA:HA	1.86	0.41
1:B:1694:LEU:O	1:B:1698:LEU:HG	2.21	0.41
1:B:2675:THR:HB	1:B:2710:LEU:HD21	2.02	0.41
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.86	0.41
1:B:3199:ALA:HB2	1:B:3279:SER:OG	2.21	0.41
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.83	0.41
1:D:463:GLU:HG2	1:D:464:LYS:N	2.36	0.41
1:D:648:ILE:HD13	1:D:811:CYS:HB3	2.02	0.41
1:D:981:GLN:O	1:D:985:VAL:HG23	2.20	0.41
1:D:1808:ARG:HB2	1:D:1854:PHE:CE1	2.56	0.41
1:D:1999:ARG:HG3	1:D:3635:CYS:O	2.21	0.41
1:D:4026:MET:HE2	1:D:4026:MET:HB3	1.81	0.41
1:C:367:LEU:HD12	1:C:367:LEU:HA	1.89	0.41
1:C:503:PHE:HD2	1:C:512:ALA:HA	1.86	0.41
1:C:805:PRO:HG2	1:C:808:TYR:CD1	2.55	0.41
1:C:880:GLU:HG3	1:C:910:PHE:HB3	2.01	0.41
1:C:924:MET:HE3	1:C:924:MET:HB3	1.93	0.41
1:C:990:GLU:HG3	1:C:1024:TYR:HB3	2.03	0.41
1:C:1183:GLU:H	1:C:1183:GLU:CD	2.29	0.41
1:C:2383:ALA:HA	1:C:2386:ILE:HG12	2.03	0.41
1:C:2419:GLY:O	1:C:2422:ILE:N	2.54	0.41
1:C:2574:HIS:CD2	1:C:2574:HIS:H	2.38	0.41
1:C:2990:PRO:HG2	1:C:2991:HIS:CE1	2.55	0.41
1:A:990:GLU:HG3	1:A:1024:TYR:HB3	2.03	0.40
1:A:1434:TYR:OH	1:A:1436:SER:HB3	2.21	0.40
1:A:1820:ARG:O	1:A:1824:GLN:HG2	2.20	0.40
1:A:2419:GLY:O	1:A:2423:MET:SD	2.79	0.40
1:A:2907:PRO:O	1:A:2910:THR:OG1	2.39	0.40
1:A:3199:ALA:HB2	1:A:3279:SER:OG	2.21	0.40
1:A:3508:SER:HB3	1:A:3511:VAL:HG22	2.02	0.40
1:A:3535:LEU:O	1:A:3538:THR:OG1	2.28	0.40
1:A:4904:PRO:CB	1:A:4913:ARG:HG2	2.51	0.40
1:B:1488:LYS:HE3	1:B:1488:LYS:HB2	1.85	0.40
1:B:1926:LEU:HB3	1:B:1939:MET:SD	2.60	0.40
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	2.03	0.40
1:B:3308:THR:H	1:B:3311:HIS:HD1	1.67	0.40
1:B:3329:ILE:O	1:B:3403:ARG:NH2	2.54	0.40
1:D:69:LEU:HD13	1:D:101:LEU:HD11	2.02	0.40
1:D:886:ARG:HB3	1:D:891:TRP:HB2	2.03	0.40
1:D:924:MET:HE3	1:D:924:MET:HB3	1.92	0.40
1:D:1575:LEU:HA	1:D:1575:LEU:HD23	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2775:TRP:CD2	1:D:2786:LYS:HE3	2.56	0.40
1:D:2793:PRO:O	1:D:2797:PHE:N	2.53	0.40
1:D:3329:ILE:O	1:D:3403:ARG:NH2	2.54	0.40
1:D:3733:CYS:HB2	1:D:3803:SER:OG	2.21	0.40
1:D:4105:GLY:O	1:D:4109:GLN:HG2	2.21	0.40
1:C:1434:TYR:OH	1:C:1436:SER:HB3	2.21	0.40
1:C:4047:MET:HB3	1:C:4047:MET:HE3	1.78	0.40
1:C:4689:THR:OG1	1:C:4690:GLU:OE1	2.34	0.40
1:A:2244:ARG:H	1:A:3861:GLU:CD	2.27	0.40
1:A:3051:ARG:HA	1:A:3131:TYR:CE1	2.55	0.40
1:A:3733:CYS:HB2	1:A:3803:SER:OG	2.21	0.40
2:F:17:LYS:HE3	2:F:17:LYS:HB3	1.81	0.40
1:B:901:LYS:HG3	1:B:903:LEU:HG	2.03	0.40
1:B:2123:LEU:HD12	1:B:2123:LEU:HA	1.95	0.40
1:B:2298:VAL:HG21	1:B:2334:PHE:CE2	2.56	0.40
1:B:3194:LEU:HD12	1:B:3194:LEU:HA	1.86	0.40
1:B:3232:LEU:HA	1:B:3233:PRO:HD3	1.89	0.40
1:B:3546:ASP:O	1:B:3550:ARG:HG3	2.22	0.40
1:D:2867:LEU:HD21	1:D:2871:LEU:HD23	2.03	0.40
1:D:3459:VAL:HG11	1:D:3503:TYR:HD1	1.87	0.40
1:C:589:LEU:HD12	1:C:589:LEU:HA	1.92	0.40
1:C:990:GLU:HA	1:C:1024:TYR:CG	2.56	0.40
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.51	0.40
1:C:4105:GLY:O	1:C:4109:GLN:HG2	2.21	0.40
1:C:4735:GLU:CD	1:C:4735:GLU:H	2.28	0.40
1:A:1668:ARG:HG3	1:A:1671:ARG:NH2	2.35	0.40
1:A:2017:ASP:OD1	1:A:2017:ASP:N	2.53	0.40
1:A:2759:ALA:HB1	1:A:2806:ARG:HA	2.04	0.40
1:A:2819:TRP:C	1:A:2820:GLU:HG3	2.46	0.40
1:A:3256:LEU:HD21	1:A:3269:VAL:HG11	2.04	0.40
1:A:4023:MET:HE2	1:A:4023:MET:HB3	1.86	0.40
1:A:4134:GLU:HB3	1:A:4135:PRO:HD3	2.02	0.40
2:E:54:GLU:OE2	2:E:55:VAL:HG13	2.22	0.40
1:B:2881:ASN:HA	1:B:2884:ASN:HD21	1.84	0.40
1:B:3733:CYS:HB2	1:B:3803:SER:OG	2.21	0.40
1:B:4558:ASN:HB3	1:B:4561:THR:OG1	2.20	0.40
1:D:1183:GLU:H	1:D:1183:GLU:CD	2.29	0.40
1:D:1858:ASP:O	1:D:1862:ILE:HG13	2.22	0.40
1:D:2390:PRO:C	1:D:2392:ARG:H	2.29	0.40
1:D:2675:THR:HB	1:D:2710:LEU:HD21	2.03	0.40
1:D:3232:LEU:HA	1:D:3233:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3528:THR:HG23	1:D:3573:MET:CE	2.52	0.40
1:D:3944:GLU:H	1:D:3944:GLU:HG3	1.74	0.40
1:C:330:ASP:OD1	1:C:330:ASP:N	2.54	0.40
1:C:1999:ARG:HG3	1:C:3635:CYS:O	2.21	0.40
1:C:2479:LEU:HD22	1:C:2480:GLY:N	2.36	0.40
1:C:3955:MET:HE3	1:C:4015:GLU:HG2	2.04	0.40
1:C:4023:MET:HE2	1:C:4023:MET:HB3	1.86	0.40
1:C:4060:LYS:HD2	1:C:4060:LYS:HA	1.91	0.40
1:A:463:GLU:HG2	1:A:464:LYS:N	2.36	0.40
1:A:1999:ARG:HG3	1:A:3635:CYS:O	2.21	0.40
1:A:3308:THR:H	1:A:3311:HIS:HD1	1.67	0.40
1:A:3528:THR:HG23	1:A:3573:MET:CE	2.52	0.40
1:A:3621:HIS:C	1:A:3622:LYS:HG3	2.47	0.40
1:A:4827:LEU:HD21	1:B:4843:LEU:HD21	2.02	0.40
1:A:4851:TYR:HD1	1:A:4916:PHE:CE1	2.38	0.40
2:E:13:ARG:CZ	2:E:13:ARG:HB2	2.51	0.40
2:H:29:MET:HG2	2:H:30:LEU:O	2.21	0.40
1:B:908:VAL:HG13	1:B:909:ASN:H	1.87	0.40
1:B:990:GLU:HA	1:B:1024:TYR:CG	2.56	0.40
1:B:1118:ASP:OD1	1:B:1118:ASP:N	2.55	0.40
1:B:2263:ILE:HD12	1:B:2263:ILE:HA	1.92	0.40
1:B:2390:PRO:C	1:B:2392:ARG:H	2.29	0.40
1:B:2663:ASN:ND2	1:B:2663:ASN:O	2.55	0.40
1:B:2785:LEU:O	1:B:2786:LYS:HG3	2.22	0.40
1:B:3368:ARG:O	1:B:3372:VAL:HG23	2.22	0.40
1:B:3528:THR:HG23	1:B:3573:MET:CE	2.52	0.40
1:B:3621:HIS:O	1:B:3622:LYS:HG3	2.20	0.40
1:D:901:LYS:HG3	1:D:903:LEU:HG	2.03	0.40
1:D:922:LEU:HD13	1:D:922:LEU:HA	1.89	0.40
1:D:2263:ILE:HD12	1:D:2263:ILE:HA	1.92	0.40
1:D:2298:VAL:HG21	1:D:2334:PHE:CE2	2.56	0.40
1:D:2663:ASN:ND2	1:D:2663:ASN:O	2.55	0.40
1:D:2785:LEU:O	1:D:2786:LYS:HG3	2.22	0.40
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.91	0.40
1:C:2020:ASP:OD1	1:C:2020:ASP:N	2.42	0.40
1:C:2754:PHE:HB2	1:C:2935:TYR:CZ	2.56	0.40
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.54	0.40
1:C:3633:VAL:HG12	1:C:3637:ARG:HE	1.87	0.40
1:C:3733:CYS:HB2	1:C:3803:SER:OG	2.21	0.40
1:A:2785:LEU:O	1:A:2786:LYS:HG3	2.22	0.40
1:A:3162:GLN:OE1	1:A:3218:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3240:CYS:HB3	1:A:3243:ILE:CG1	2.51	0.40
1:A:3531:ASP:HA	1:A:3534:MET:SD	2.62	0.40
2:E:17:LYS:HE3	2:E:17:LYS:HB3	1.80	0.40
2:E:44:LYS:HD2	2:E:44:LYS:C	2.46	0.40
1:B:950:LEU:HD23	1:B:950:LEU:HA	1.81	0.40
1:B:1183:GLU:H	1:B:1183:GLU:CD	2.29	0.40
1:B:2336:ARG:HG3	1:B:2431:ASP:OD2	2.21	0.40
1:B:3449:HIS:C	1:B:3449:HIS:HD1	2.29	0.40
1:B:3633:VAL:HG12	1:B:3637:ARG:HE	1.87	0.40
1:B:3955:MET:HE3	1:B:4015:GLU:HG2	2.04	0.40
1:B:4826:ILE:HD13	1:C:4840:THR:HG22	2.03	0.40
1:D:1118:ASP:OD1	1:D:1118:ASP:N	2.55	0.40
1:D:1286:MET:HE3	1:D:1286:MET:HB3	1.88	0.40
1:D:3693:LYS:HA	1:D:3693:LYS:HD2	1.89	0.40
1:D:3955:MET:HE3	1:D:4015:GLU:HG2	2.04	0.40
1:D:4097:MET:HB2	1:D:4097:MET:HE2	1.71	0.40
1:D:4211:LYS:O	1:D:4215:ARG:HG3	2.22	0.40
1:C:774:ASP:CG	1:C:1470:ARG:HH22	2.24	0.40
1:C:886:ARG:HB3	1:C:891:TRP:HB2	2.03	0.40
1:C:2126:ARG:NH2	1:C:2133:GLU:OE2	2.52	0.40
1:C:2390:PRO:C	1:C:2392:ARG:H	2.29	0.40
1:C:3400:VAL:HG23	1:C:3403:ARG:NH2	2.35	0.40
1:C:3459:VAL:HG11	1:C:3503:TYR:HD1	1.87	0.40
1:C:3528:THR:HG23	1:C:3573:MET:CE	2.52	0.40
1:C:4942:GLU:HA	1:C:4945:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	4247 (97%)	138 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	C	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
1	D	4385/5037 (87%)	4247 (97%)	138 (3%)	0	100	100
2	E	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	G	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17960/20580 (87%)	17398 (97%)	562 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3836/4276 (90%)	3815 (100%)	21 (0%)	81	82
1	B	3836/4276 (90%)	3816 (100%)	20 (0%)	81	82
1	C	3836/4276 (90%)	3815 (100%)	21 (0%)	81	82
1	D	3836/4276 (90%)	3817 (100%)	19 (0%)	81	82
2	E	89/90 (99%)	85 (96%)	4 (4%)	24	52
2	F	89/90 (99%)	85 (96%)	4 (4%)	24	52
2	G	89/90 (99%)	83 (93%)	6 (7%)	15	41
2	H	89/90 (99%)	84 (94%)	5 (6%)	19	46
All	All	15700/17464 (90%)	15600 (99%)	100 (1%)	76	81

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	VAL
1	A	227	MET

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Mol	Chain	Res	Type
1	A	898	ASP
1	A	945	LYS
1	A	957	LYS
1	A	959	TYR
1	A	960	MET
1	A	1428	LEU
1	A	1538	THR
1	A	2037	ASP
1	A	2267	MET
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2490	MET
1	A	2608	MET
1	A	3038	MET
1	A	3409	TYR
1	A	3449	HIS
1	A	3759	GLU
1	A	3899	PHE
1	A	4871	GLU
2	E	17	LYS
2	E	27	THR
2	E	53	GLN
2	E	85	THR
2	H	17	LYS
2	H	27	THR
2	H	35	LYS
2	H	53	GLN
2	H	85	THR
2	G	17	LYS
2	G	27	THR
2	G	35	LYS
2	G	43	ASN
2	G	53	GLN
2	G	85	THR
2	F	17	LYS
2	F	27	THR
2	F	53	GLN
2	F	85	THR
1	B	191	VAL
1	B	227	MET
1	B	898	ASP
1	B	945	LYS

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Mol	Chain	Res	Type
1	B	957	LYS
1	B	959	TYR
1	B	960	MET
1	B	1538	THR
1	B	2037	ASP
1	B	2267	MET
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2490	MET
1	B	2608	MET
1	B	3038	MET
1	B	3409	TYR
1	B	3449	HIS
1	B	3759	GLU
1	B	3899	PHE
1	B	4871	GLU
1	D	191	VAL
1	D	898	ASP
1	D	945	LYS
1	D	957	LYS
1	D	959	TYR
1	D	960	MET
1	D	1428	LEU
1	D	1538	THR
1	D	2037	ASP
1	D	2267	MET
1	D	2369[A]	ARG
1	D	2369[B]	ARG
1	D	2490	MET
1	D	3038	MET
1	D	3409	TYR
1	D	3449	HIS
1	D	3759	GLU
1	D	3899	PHE
1	D	4871	GLU
1	C	191	VAL
1	C	227	MET
1	C	898	ASP
1	C	945	LYS
1	C	957	LYS
1	C	959	TYR
1	C	960	MET

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Mol	Chain	Res	Type
1	C	1428	LEU
1	C	1538	THR
1	C	2037	ASP
1	C	2267	MET
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2490	MET
1	C	2608	MET
1	C	3038	MET
1	C	3409	TYR
1	C	3449	HIS
1	C	3759	GLU
1	C	3899	PHE
1	C	4871	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	HIS
1	A	241	GLN
1	A	593	HIS
1	A	911	HIS
1	A	921	ASN
1	A	949	ASN
1	A	963	ASN
1	A	991	ASN
1	A	1011	GLN
1	A	1066	GLN
1	A	1229	ASN
1	A	1420	ASN
1	A	2127	GLN
1	A	2260	ASN
1	A	2291	GLN
1	A	2498	HIS
1	A	2877	GLN
1	A	2883	HIS
1	A	3211	ASN
1	A	3355	HIS
1	A	3704	HIS
1	A	3914	ASN
1	A	4009	GLN
1	A	4054	ASN

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Mol	Chain	Res	Type
1	A	4120	ASN
1	A	4133	GLN
1	A	4156	HIS
1	A	4162	ASN
1	A	4836	GLN
2	E	20	GLN
2	E	43	ASN
2	H	43	ASN
2	G	20	GLN
2	G	43	ASN
2	F	20	GLN
2	F	43	ASN
2	F	65	GLN
1	B	224	HIS
1	B	241	GLN
1	B	461	HIS
1	B	593	HIS
1	B	838	HIS
1	B	911	HIS
1	B	921	ASN
1	B	963	ASN
1	B	991	ASN
1	B	1011	GLN
1	B	1066	GLN
1	B	1229	ASN
1	B	1420	ASN
1	B	2245	GLN
1	B	2260	ASN
1	B	2291	GLN
1	B	2877	GLN
1	B	2883	HIS
1	B	3180	ASN
1	B	3355	HIS
1	B	3704	HIS
1	B	3914	ASN
1	B	4009	GLN
1	B	4054	ASN
1	B	4120	ASN
1	B	4156	HIS
1	B	4162	ASN
1	B	4836	GLN
1	D	224	HIS

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Mol	Chain	Res	Type
1	D	241	GLN
1	D	593	HIS
1	D	838	HIS
1	D	911	HIS
1	D	921	ASN
1	D	949	ASN
1	D	963	ASN
1	D	991	ASN
1	D	1011	GLN
1	D	1066	GLN
1	D	1229	ASN
1	D	1420	ASN
1	D	1719	HIS
1	D	2253	HIS
1	D	2260	ASN
1	D	2291	GLN
1	D	2756	ASN
1	D	2877	GLN
1	D	2883	HIS
1	D	3355	HIS
1	D	3704	HIS
1	D	3914	ASN
1	D	4009	GLN
1	D	4054	ASN
1	D	4120	ASN
1	D	4133	GLN
1	D	4156	HIS
1	D	4162	ASN
1	D	4836	GLN
1	C	224	HIS
1	C	241	GLN
1	C	593	HIS
1	C	838	HIS
1	C	911	HIS
1	C	921	ASN
1	C	949	ASN
1	C	963	ASN
1	C	991	ASN
1	C	1011	GLN
1	C	1066	GLN
1	C	1229	ASN
1	C	1719	HIS

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Mol	Chain	Res	Type
1	C	1938	GLN
1	C	2253	HIS
1	C	2260	ASN
1	C	2291	GLN
1	C	2877	GLN
1	C	2883	HIS
1	C	3180	ASN
1	C	3355	HIS
1	C	3704	HIS
1	C	3914	ASN
1	C	4009	GLN
1	C	4120	ASN
1	C	4156	HIS
1	C	4162	ASN
1	C	4836	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 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	A1BD5	A	5304	-	16,16,16	0.97	0	21,23,23	0.73	0
6	A1BD5	D	5304	-	16,16,16	0.96	0	21,23,23	0.73	0
6	A1BD5	C	5304	-	16,16,16	0.96	0	21,23,23	0.73	0
3	ATP	D	5301	-	32,33,33	0.32	0	48,52,52	0.41	0
6	A1BD5	B	5304	-	16,16,16	0.96	0	21,23,23	0.73	0
3	ATP	A	5301	-	32,33,33	0.32	0	48,52,52	0.41	0
3	ATP	B	5301	-	32,33,33	0.32	0	48,52,52	0.41	0
3	ATP	C	5301	-	32,33,33	0.32	0	48,52,52	0.42	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	A1BD5	A	5304	-	-	0/4/4/4	0/2/2/2
6	A1BD5	D	5304	-	-	0/4/4/4	0/2/2/2
6	A1BD5	C	5304	-	-	0/4/4/4	0/2/2/2
3	ATP	D	5301	-	-	10/22/38/38	0/3/3/3
6	A1BD5	B	5304	-	-	0/4/4/4	0/2/2/2
3	ATP	A	5301	-	-	10/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	10/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	10/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	PB-O3B-PG-O2G
3	A	5301	ATP	C5'-O5'-PA-O1A
3	A	5301	ATP	C5'-O5'-PA-O2A
3	A	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	PB-O3B-PG-O2G
3	B	5301	ATP	C5'-O5'-PA-O1A
3	B	5301	ATP	C5'-O5'-PA-O2A
3	B	5301	ATP	C5'-O5'-PA-O3A
3	D	5301	ATP	PB-O3B-PG-O2G
3	D	5301	ATP	C5'-O5'-PA-O1A

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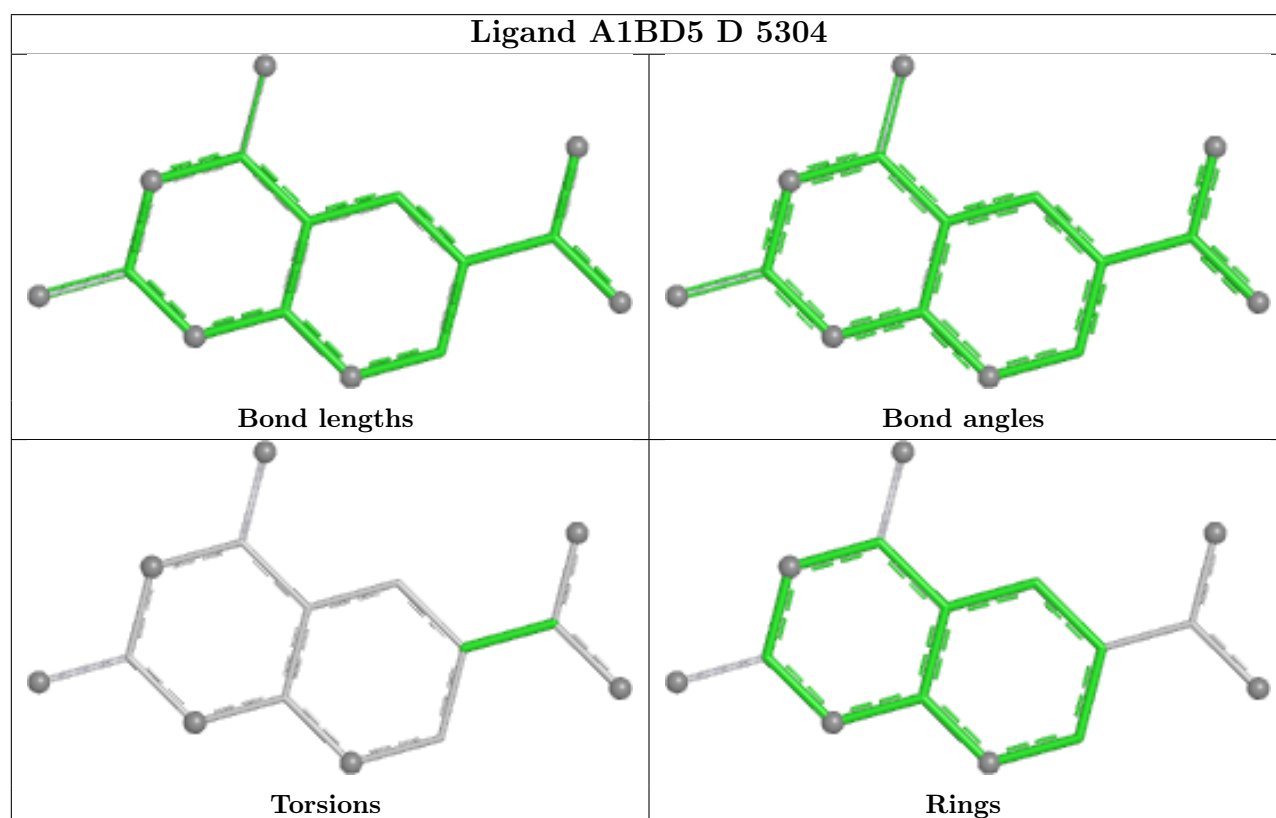
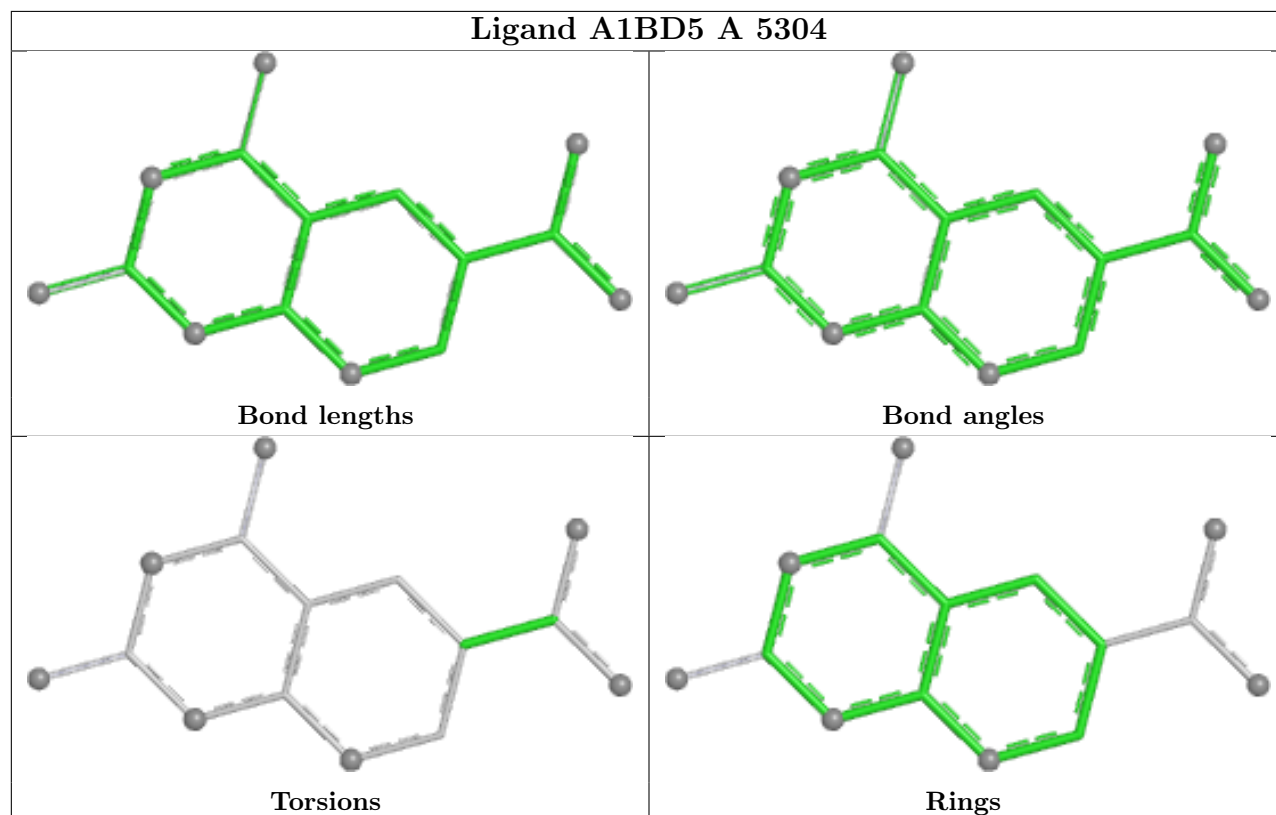
Mol	Chain	Res	Type	Atoms
3	D	5301	ATP	C5'-O5'-PA-O2A
3	D	5301	ATP	C5'-O5'-PA-O3A
3	C	5301	ATP	PB-O3B-PG-O2G
3	C	5301	ATP	C5'-O5'-PA-O1A
3	C	5301	ATP	C5'-O5'-PA-O2A
3	C	5301	ATP	C5'-O5'-PA-O3A
3	B	5301	ATP	O4'-C4'-C5'-O5'
3	A	5301	ATP	PB-O3B-PG-O3G
3	B	5301	ATP	PB-O3B-PG-O3G
3	D	5301	ATP	PB-O3B-PG-O3G
3	C	5301	ATP	PB-O3B-PG-O3G
3	A	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	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'
3	A	5301	ATP	C4'-C5'-O5'-PA
3	B	5301	ATP	C4'-C5'-O5'-PA
3	D	5301	ATP	C4'-C5'-O5'-PA
3	C	5301	ATP	C4'-C5'-O5'-PA
3	A	5301	ATP	PB-O3B-PG-O1G
3	B	5301	ATP	PB-O3B-PG-O1G
3	D	5301	ATP	PB-O3B-PG-O1G
3	C	5301	ATP	PB-O3B-PG-O1G
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

There are no ring outliers.

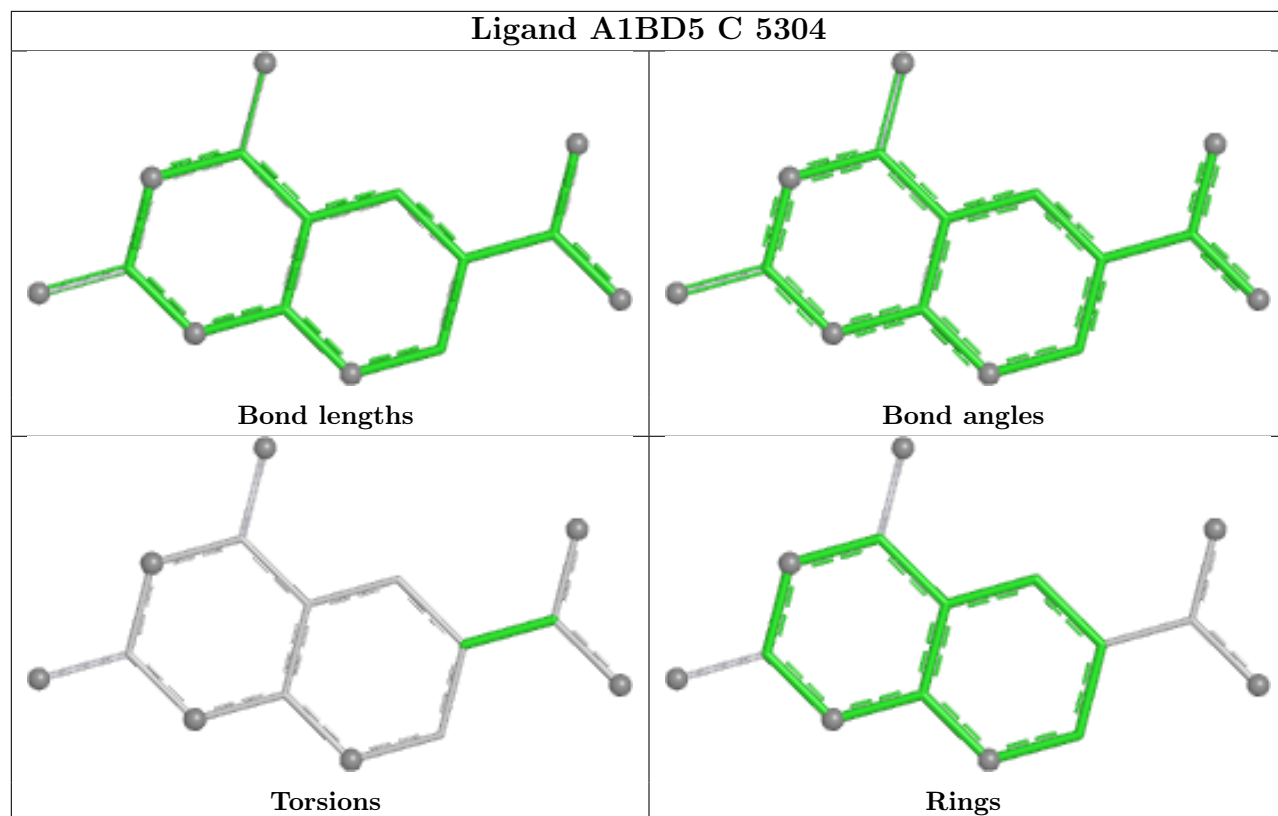
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

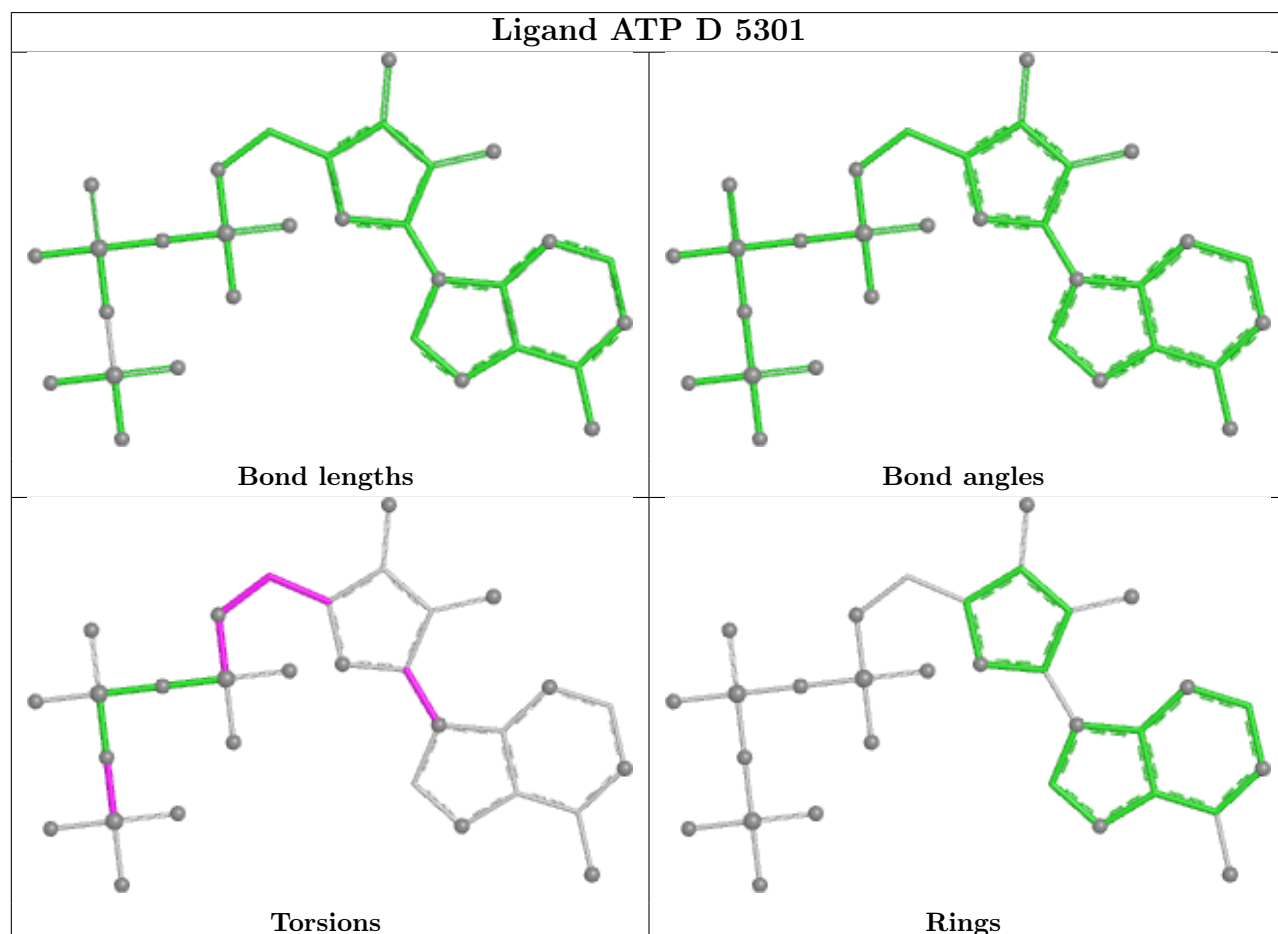
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



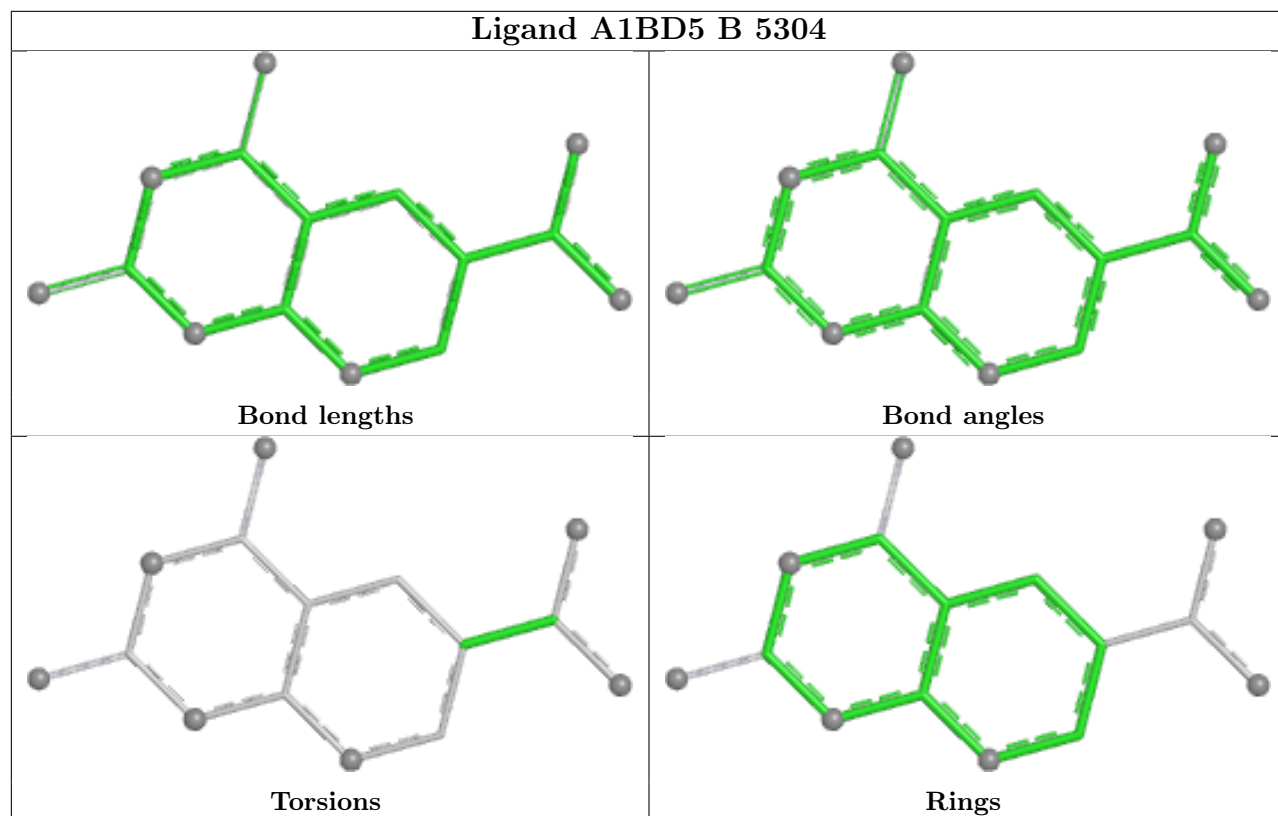
Ligand A1BD5 C 5304



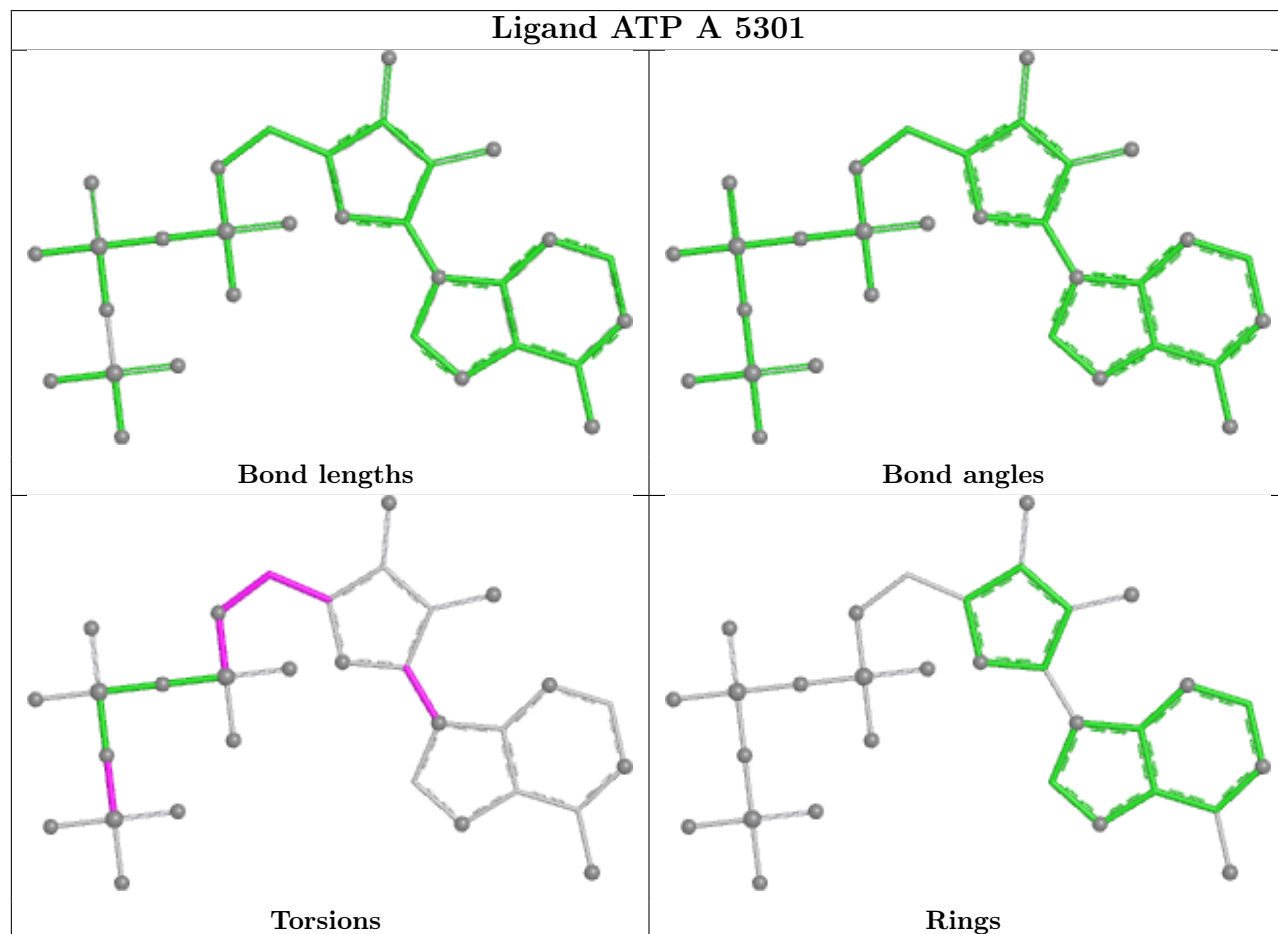
Ligand ATP D 5301

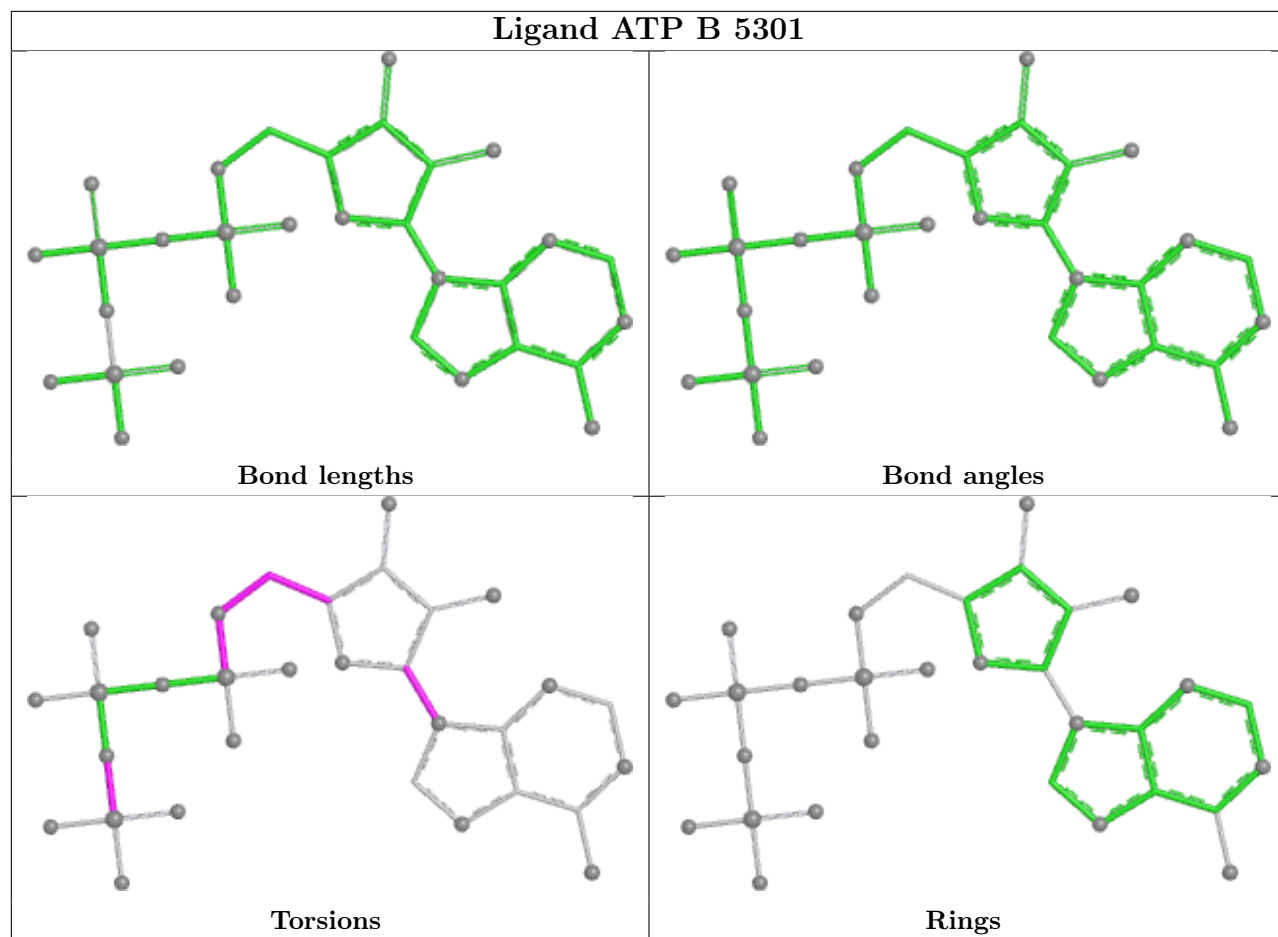


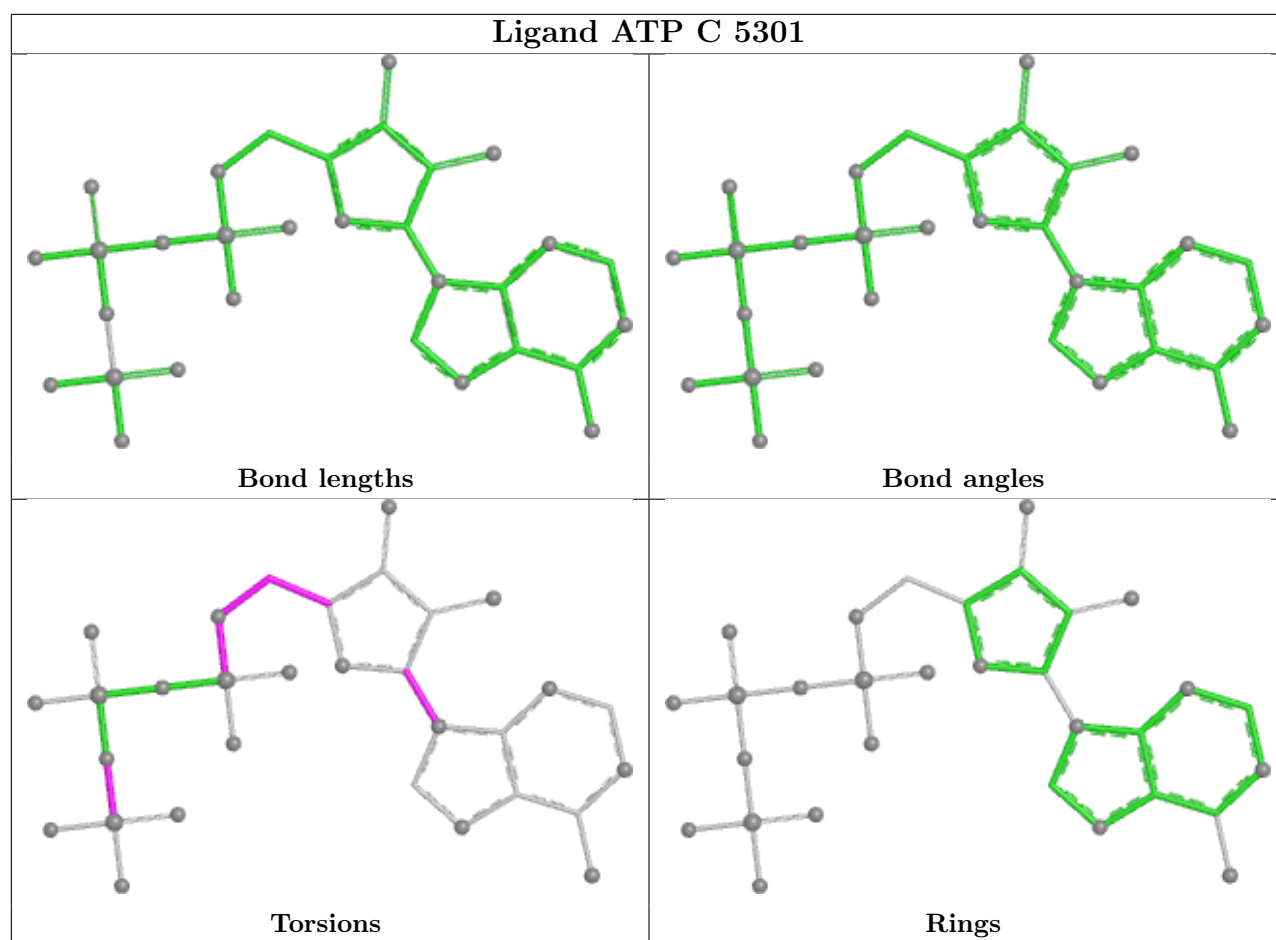
Ligand A1BD5 B 5304



Ligand ATP A 5301







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.

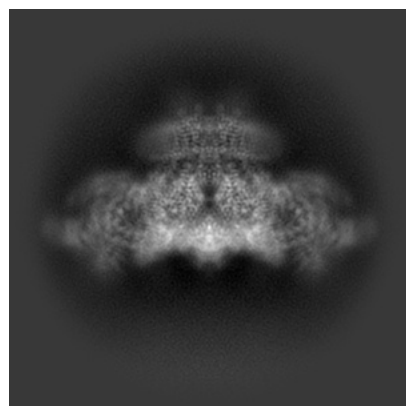
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47394. These allow visual inspection of the internal detail of the map and identification of artifacts.

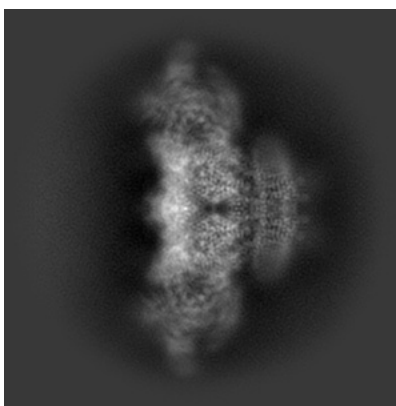
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

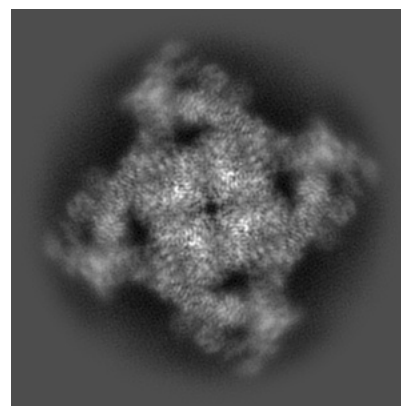
6.1.1 Primary map



X

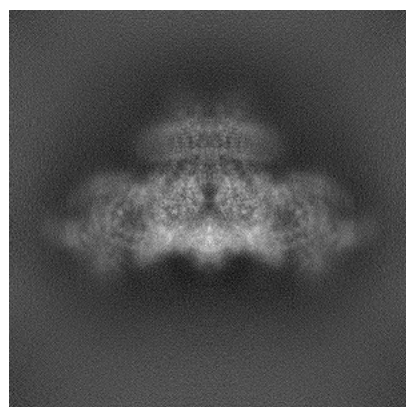


Y

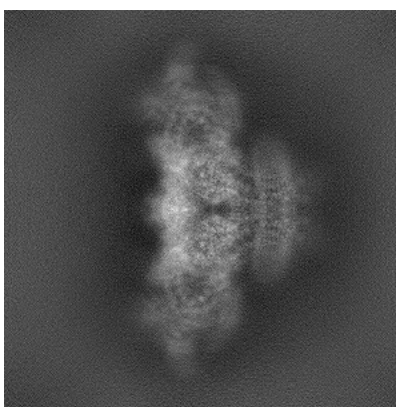


Z

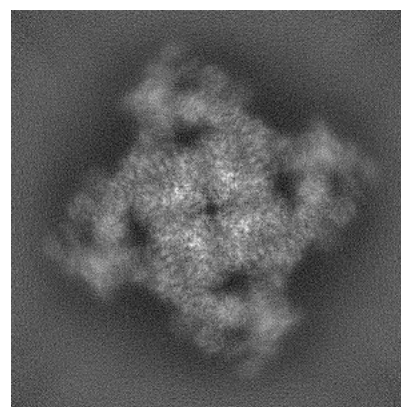
6.1.2 Raw map



X



Y

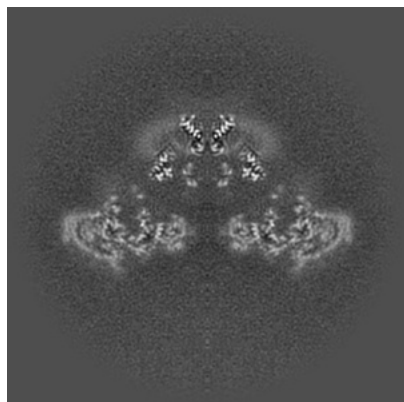


Z

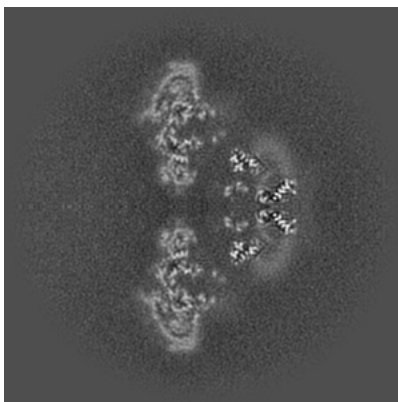
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

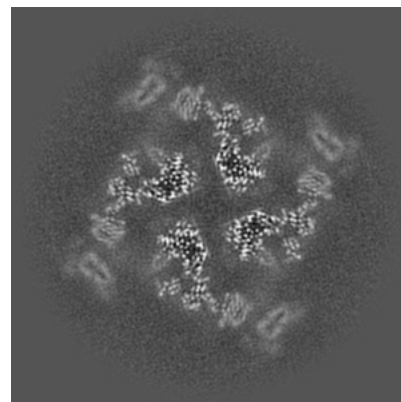
6.2.1 Primary map



X Index: 256

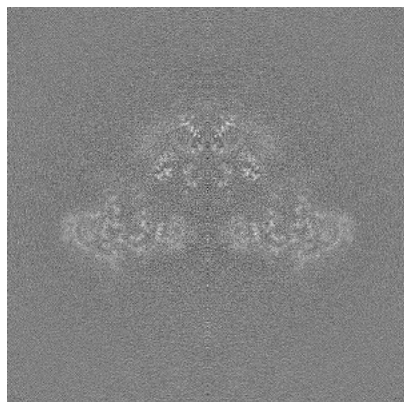


Y Index: 256

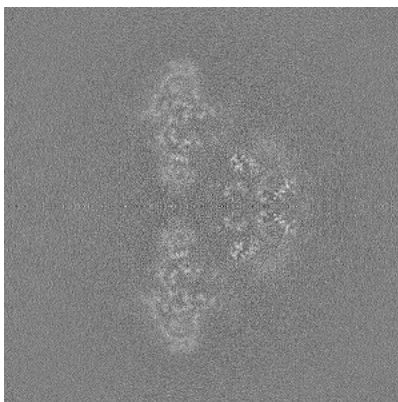


Z Index: 256

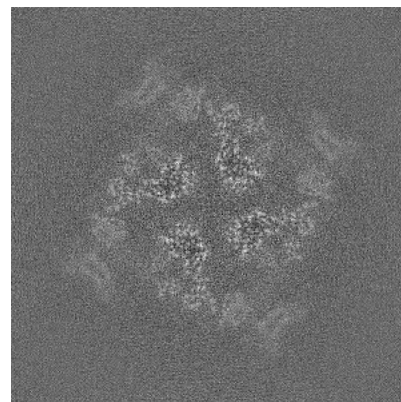
6.2.2 Raw map



X Index: 256



Y Index: 256

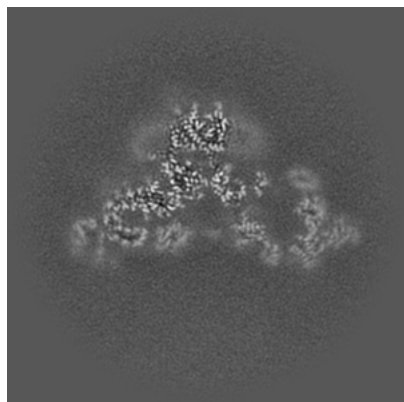


Z Index: 256

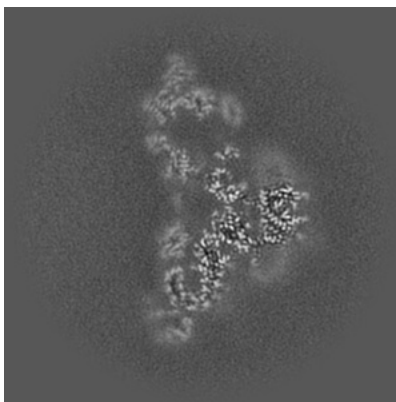
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

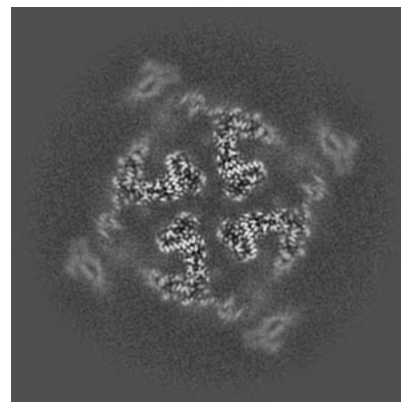
6.3.1 Primary map



X Index: 239

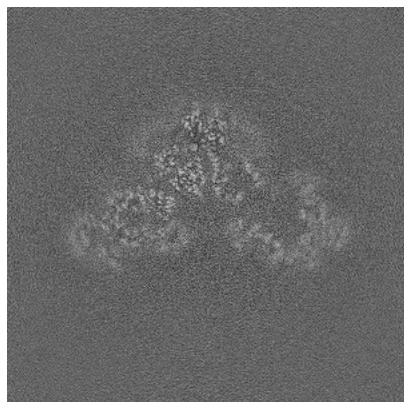


Y Index: 273

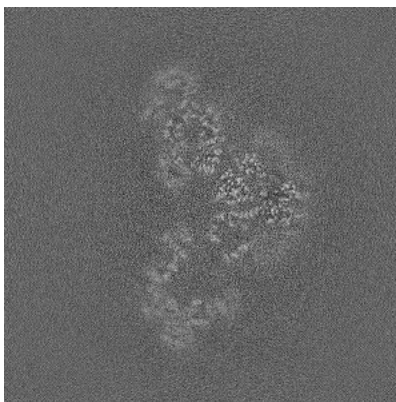


Z Index: 265

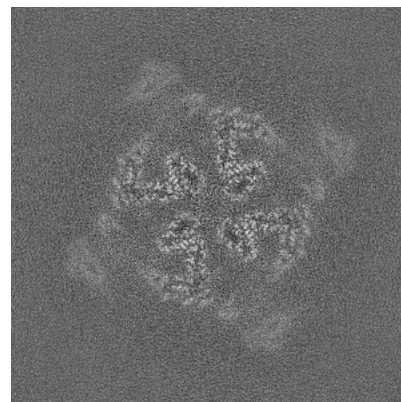
6.3.2 Raw map



X Index: 244



Y Index: 244

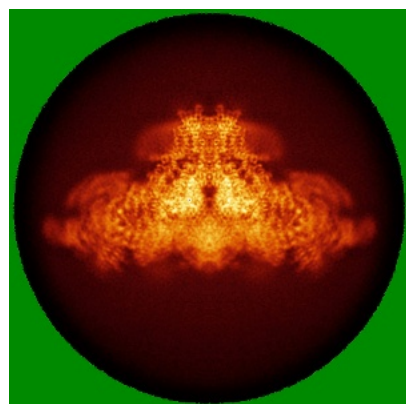


Z Index: 266

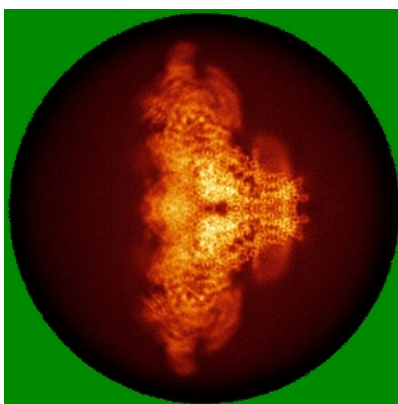
The images above show the largest variance slices of the map in three orthogonal directions.

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

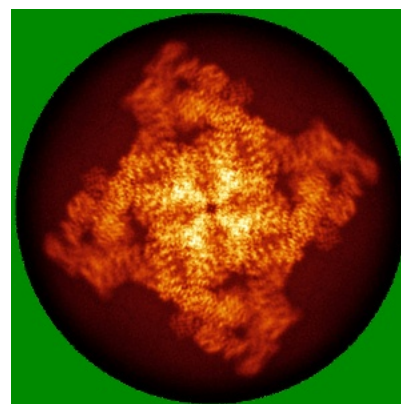
6.4.1 Primary map



X

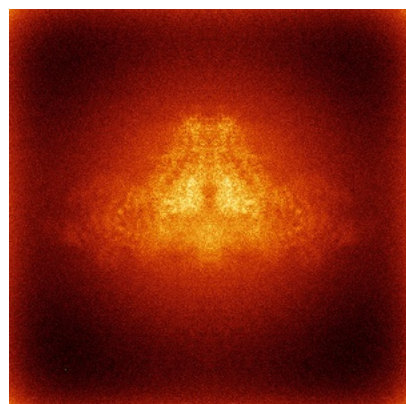


Y

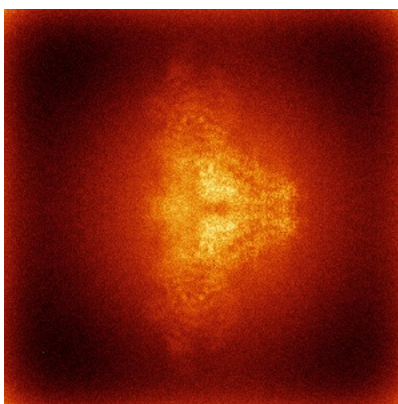


Z

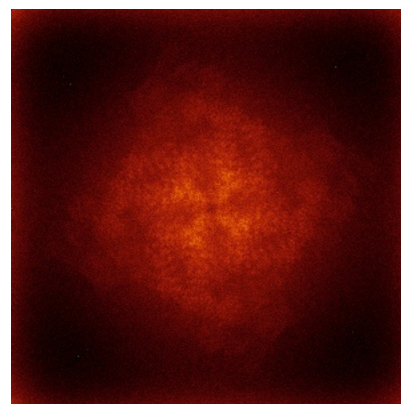
6.4.2 Raw map



X



Y

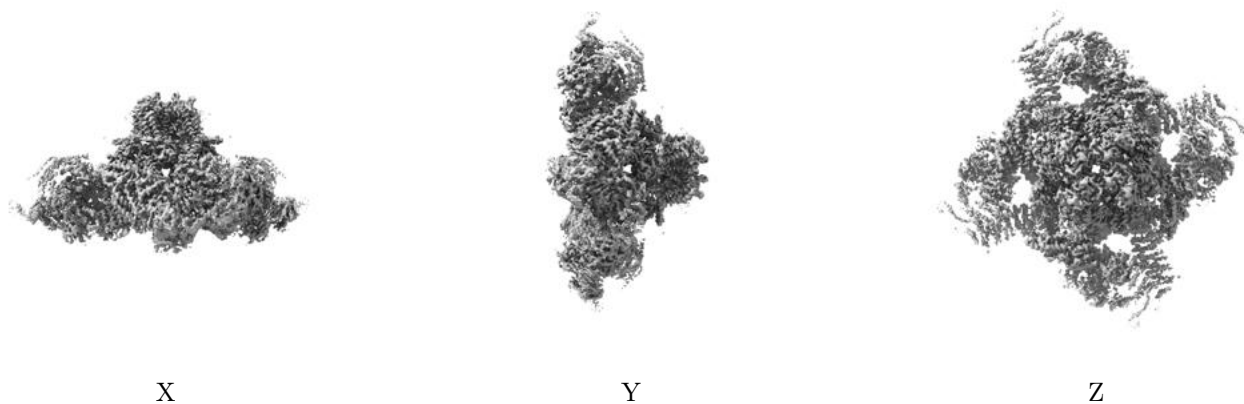


Z

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.

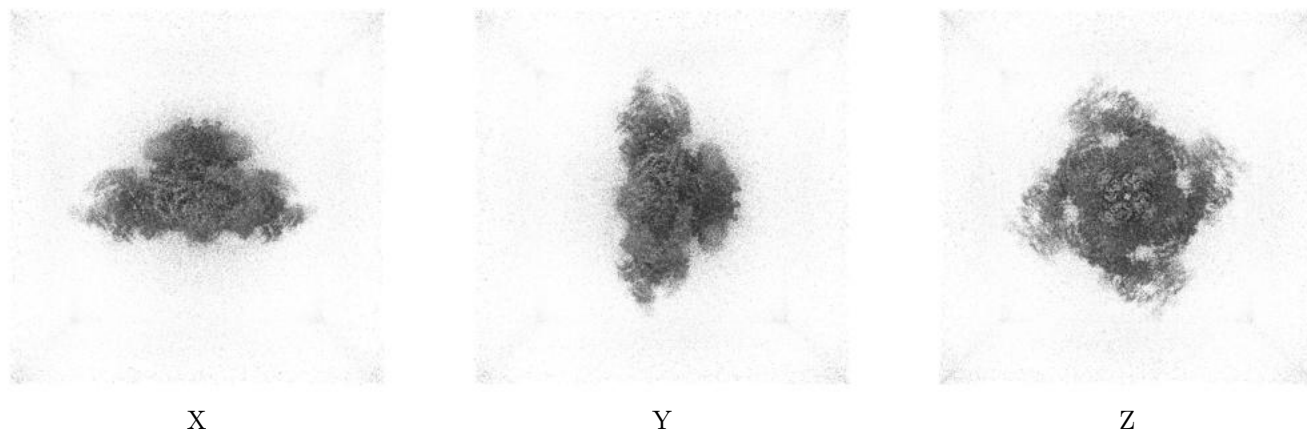
6.5 Orthogonal surface views [i](#)

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.

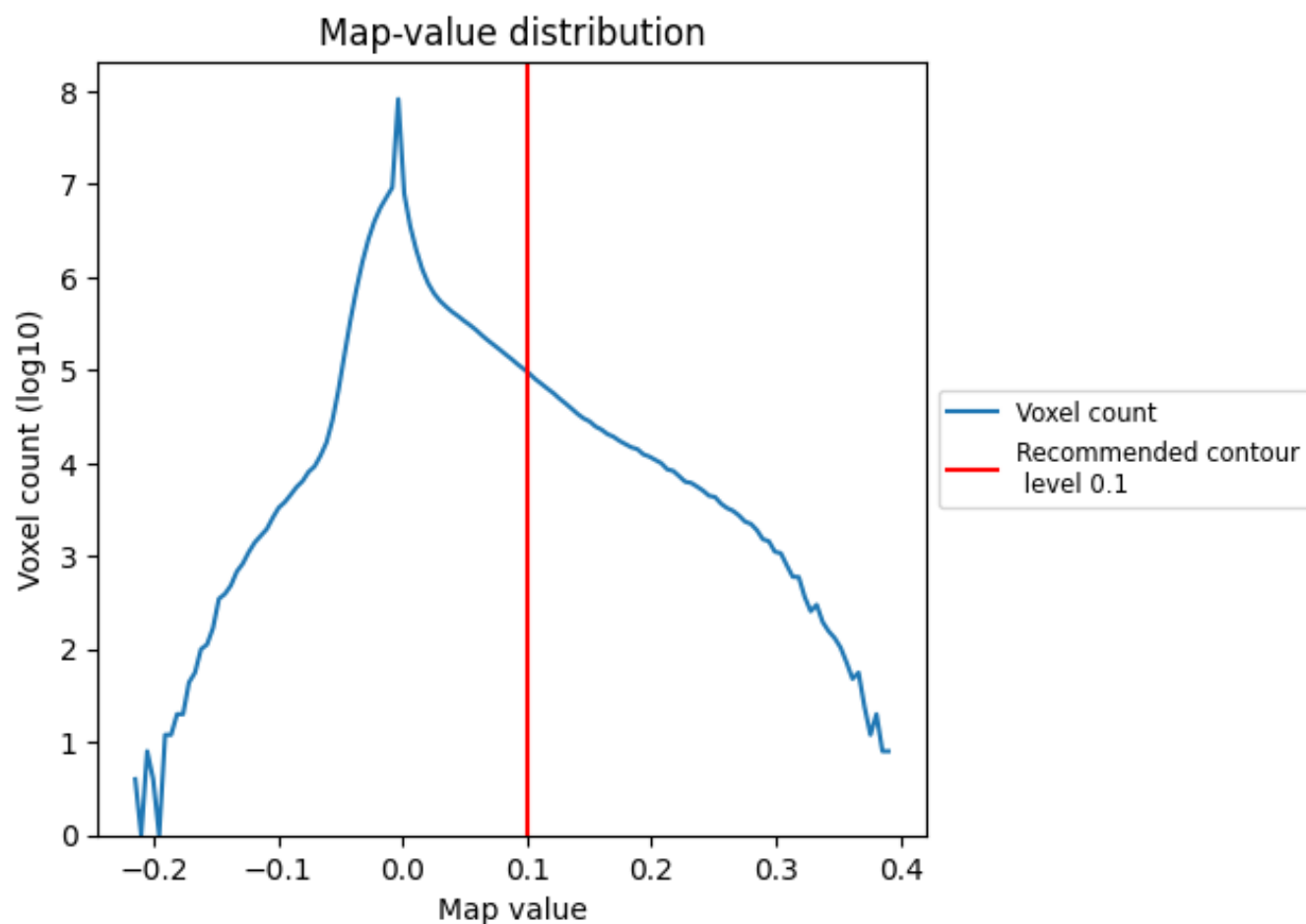
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

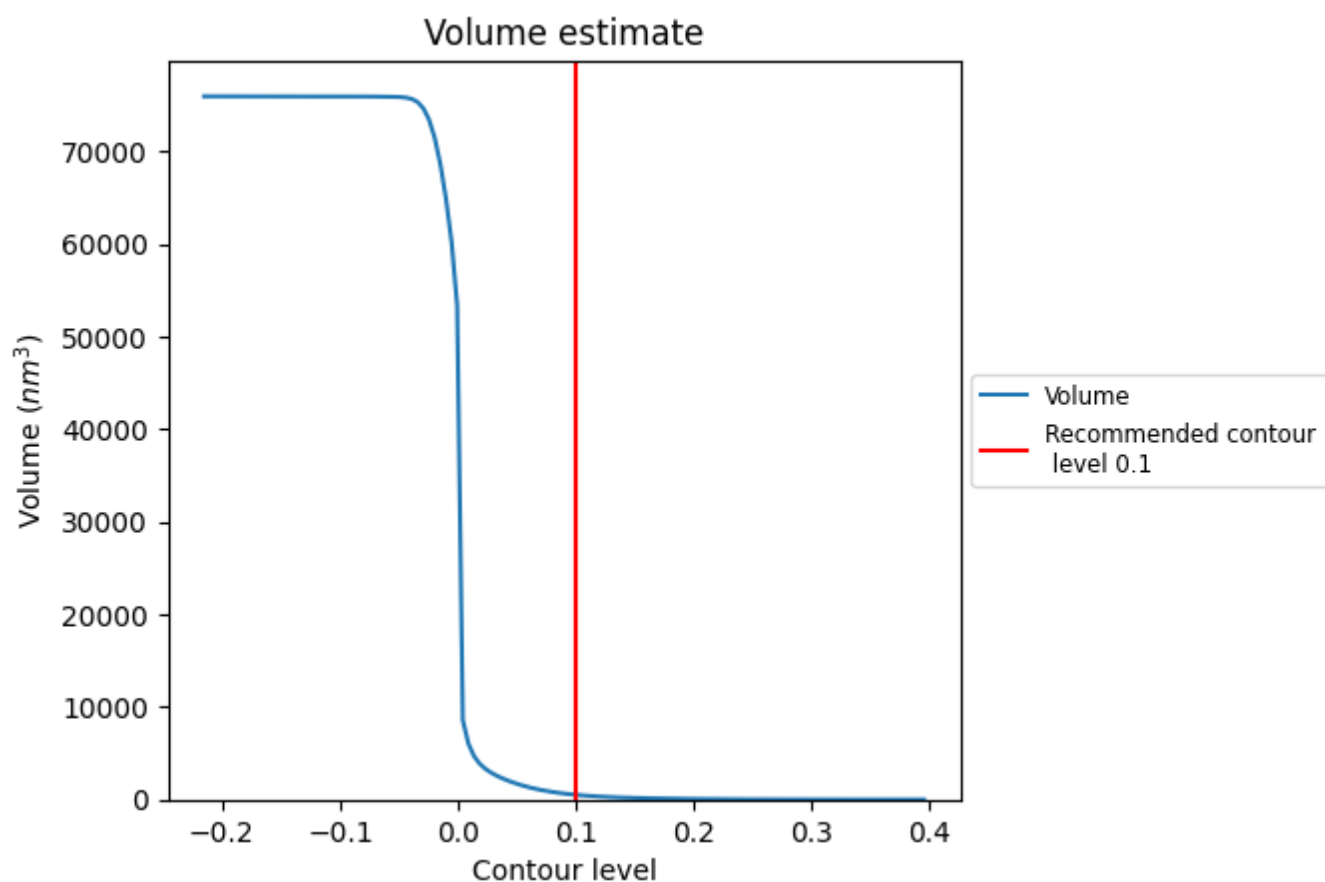
This section contains the results of statistical analysis of the map.

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.

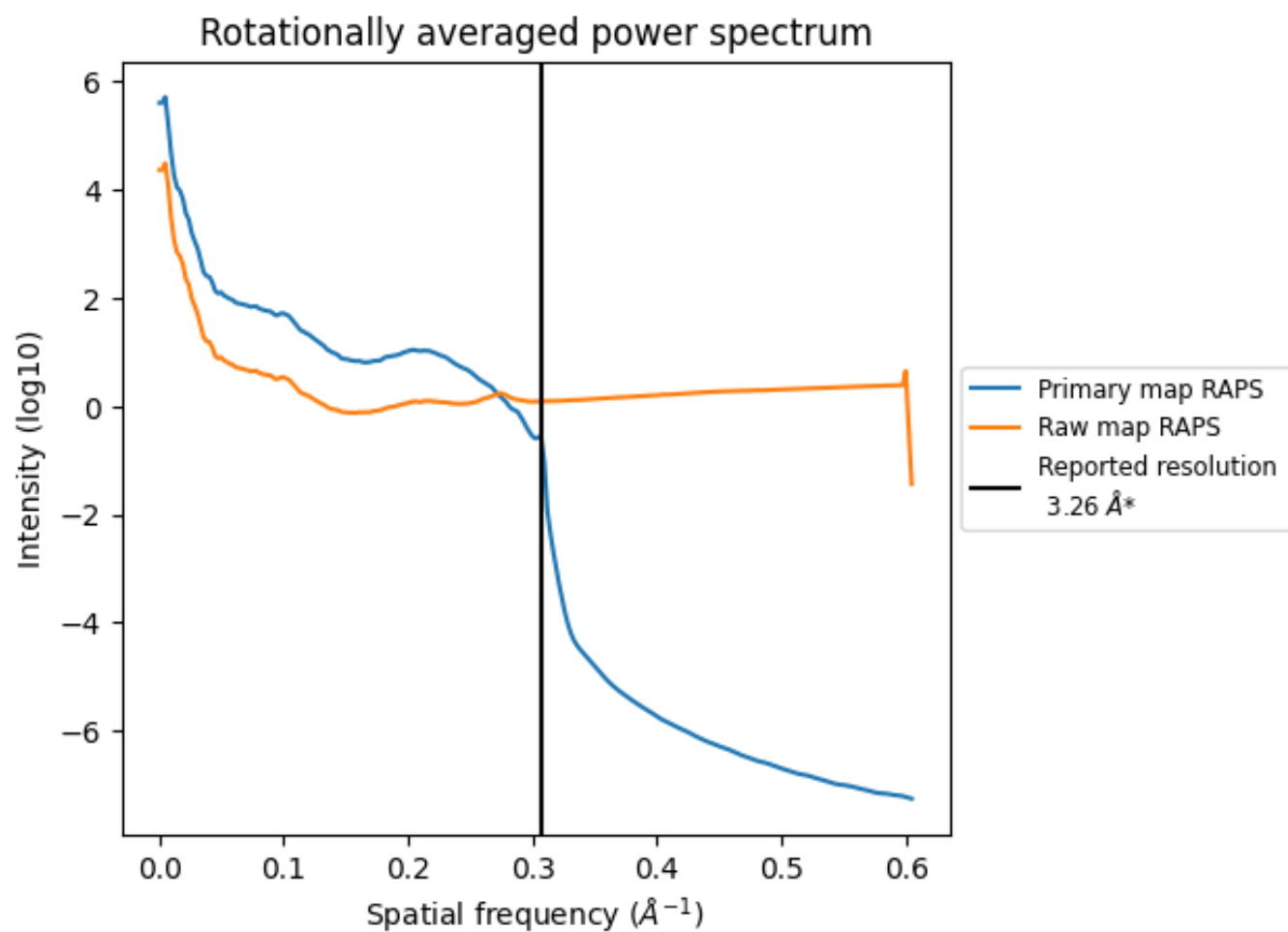
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 512 nm³; this corresponds to an approximate mass of 463 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 ⓘ

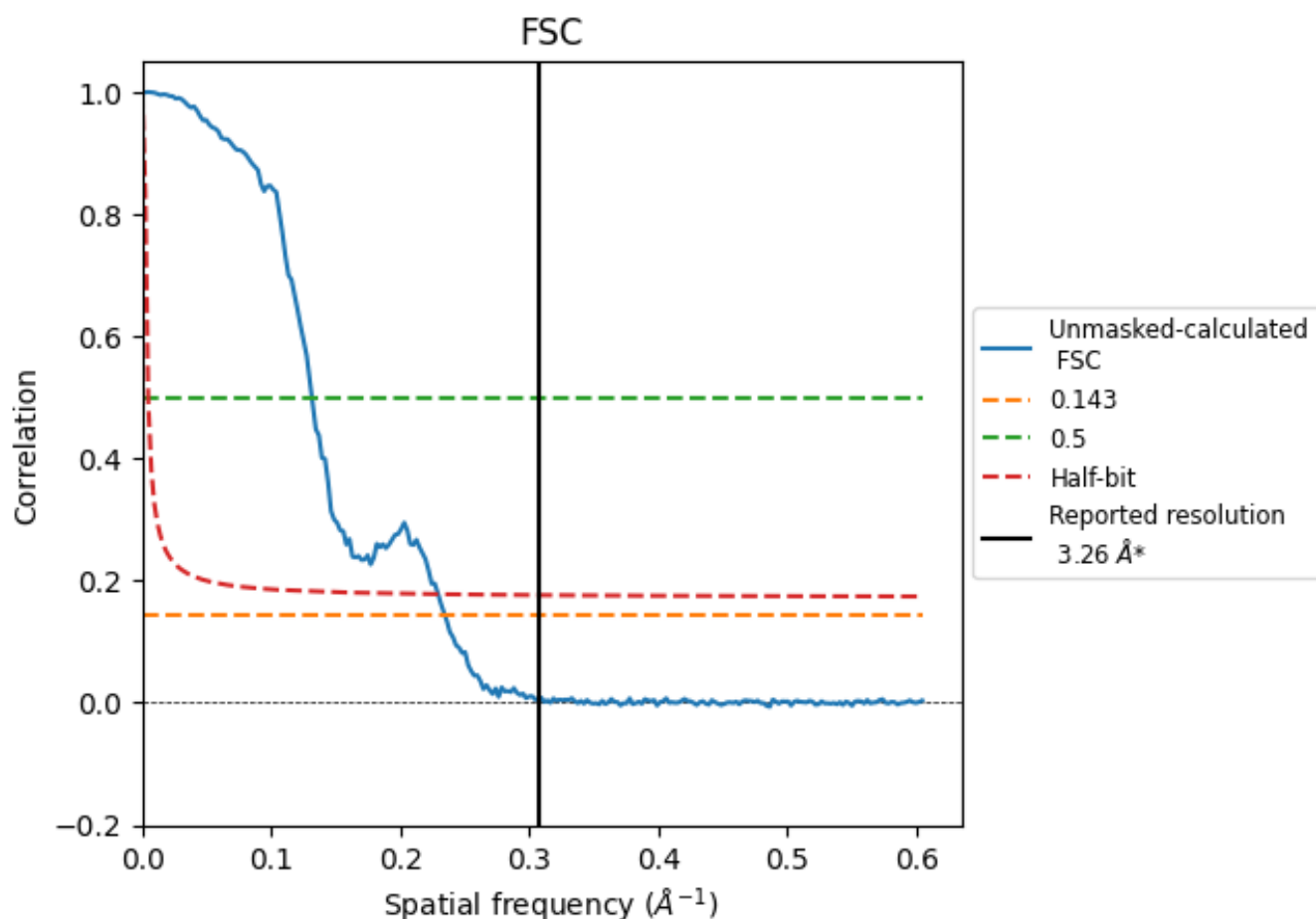


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

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 0.307 Å⁻¹

8.2 Resolution estimates [i](#)

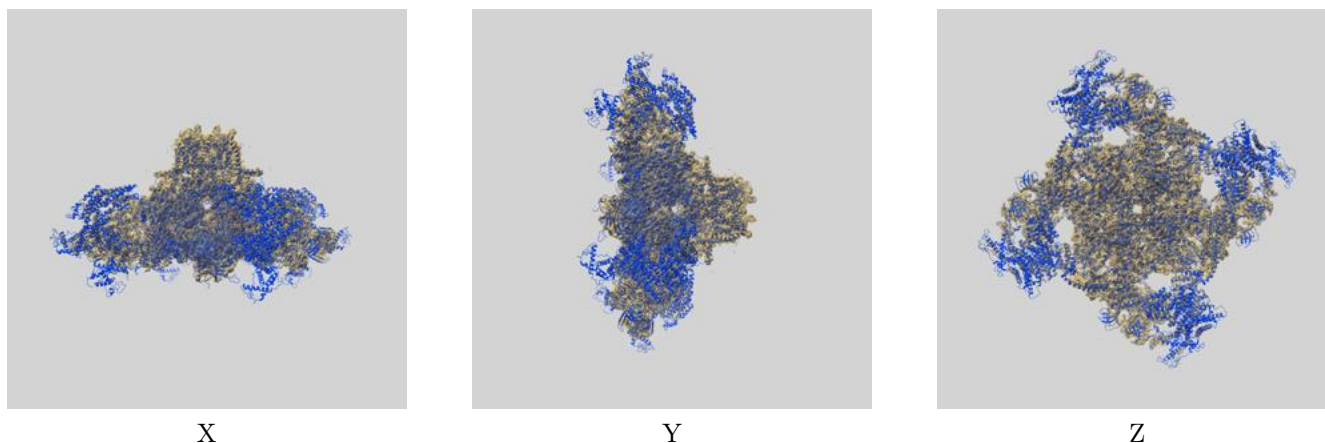
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	7.60	4.36

*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 4.26 differs from the reported value 3.26 by more than 10 %

9 Map-model fit [i](#)

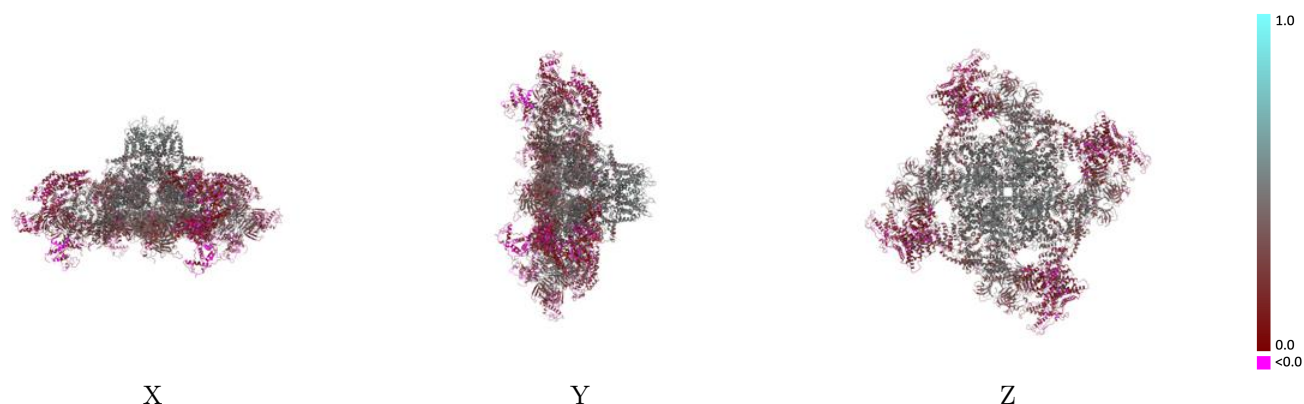
This section contains information regarding the fit between EMDB map EMD-47394 and PDB model 9E1H. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



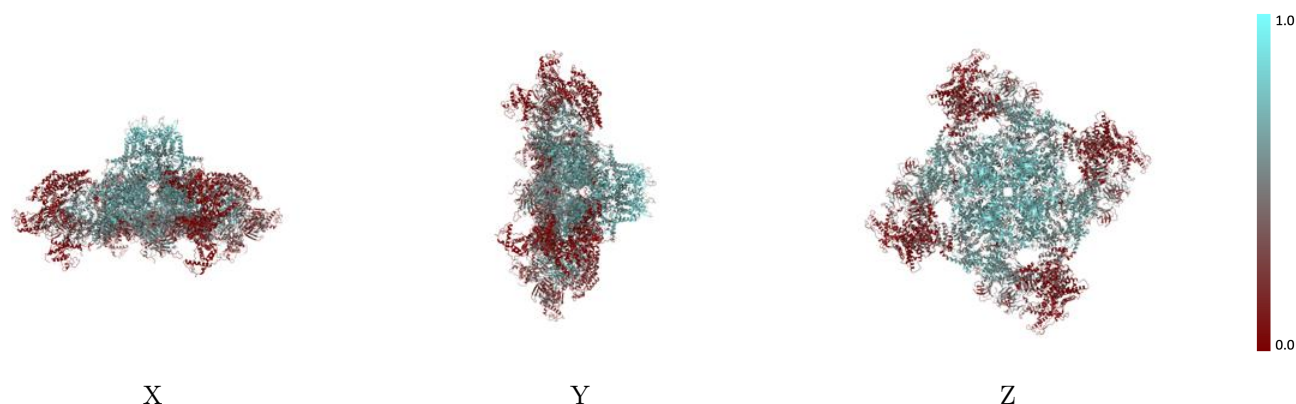
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



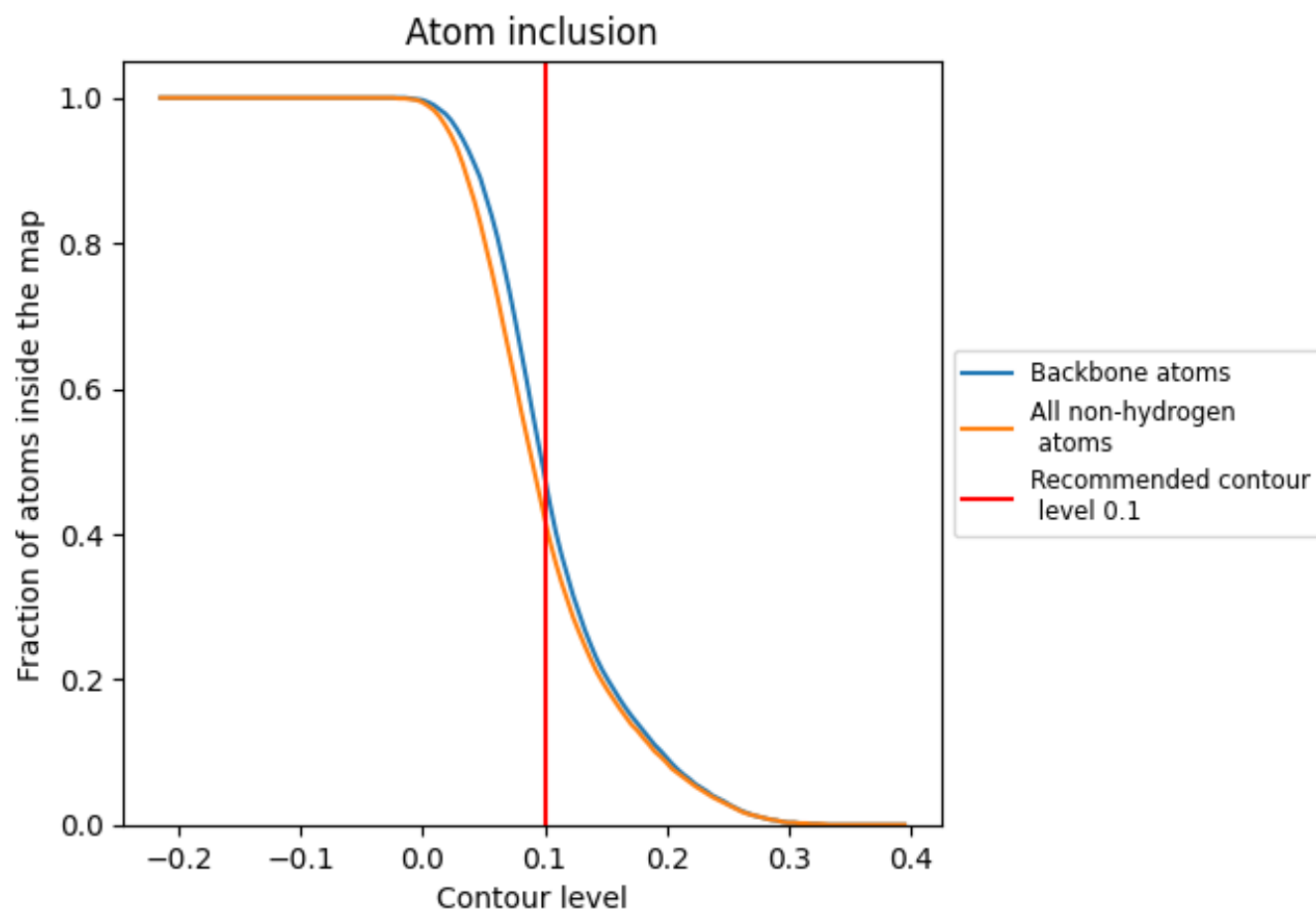
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 48% of all backbone atoms, 42% 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	0.4210	0.3140
A	0.4340	0.3130
B	0.4350	0.3130
C	0.4340	0.3130
D	0.4340	0.3130
E	0.2440	0.3570
F	0.2440	0.3560
G	0.2470	0.3530
H	0.2420	0.3560

