



## Full wwPDB EM Validation Report ⓘ

Jun 16, 2025 – 03:00 PM EDT

PDB ID : 9E1E / pdb\_00009e1e  
EMDB ID : EMD-47391  
Title : Structure of RyR1 in the primed state in the presence of uracil  
Authors : Miotto, M.C.; Marks, A.R.  
Deposited on : 2024-10-21  
Resolution : 2.92 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

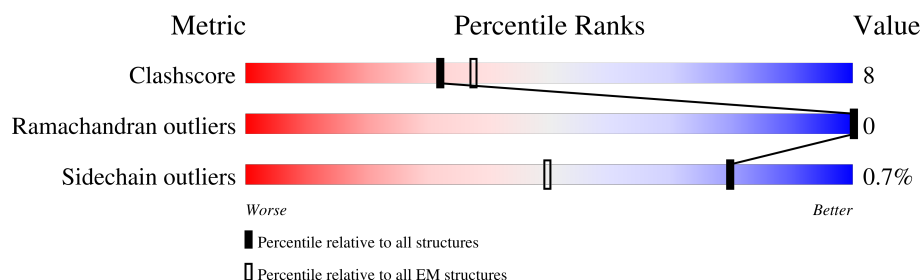
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.92 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	<div> <div>29%</div> <div>70%</div> <div>17%</div> <div>13%</div> </div>
1	B	5037	<div> <div>29%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div>
1	C	5037	<div> <div>29%</div> <div>69%</div> <div>18%</div> <div>13%</div> </div>
1	D	5037	<div> <div>29%</div> <div>71%</div> <div>16%</div> <div>13%</div> </div>
2	E	108	<div> <div>30%</div> <div>69%</div> <div>29%</div> <div>..</div> </div>
2	F	108	<div> <div>28%</div> <div>73%</div> <div>25%</div> <div>..</div> </div>
2	G	108	<div> <div>29%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
2	H	108	<div> <div>28%</div> <div>74%</div> <div>23%</div> <div>..</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 144088 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.

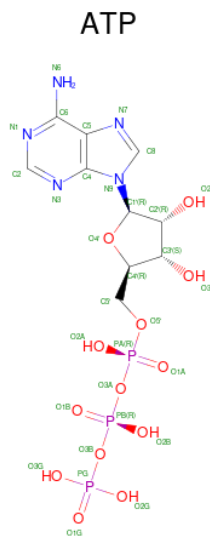
- Molecule 1 is a protein called Ryanodine receptor 1.

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: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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:  $\text{Zn}$ ).

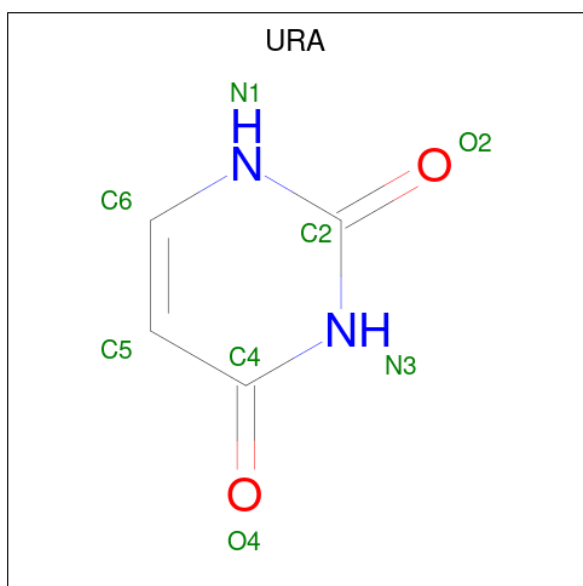
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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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 URACIL (CCD ID: URA) (formula:  $C_4H_4N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).

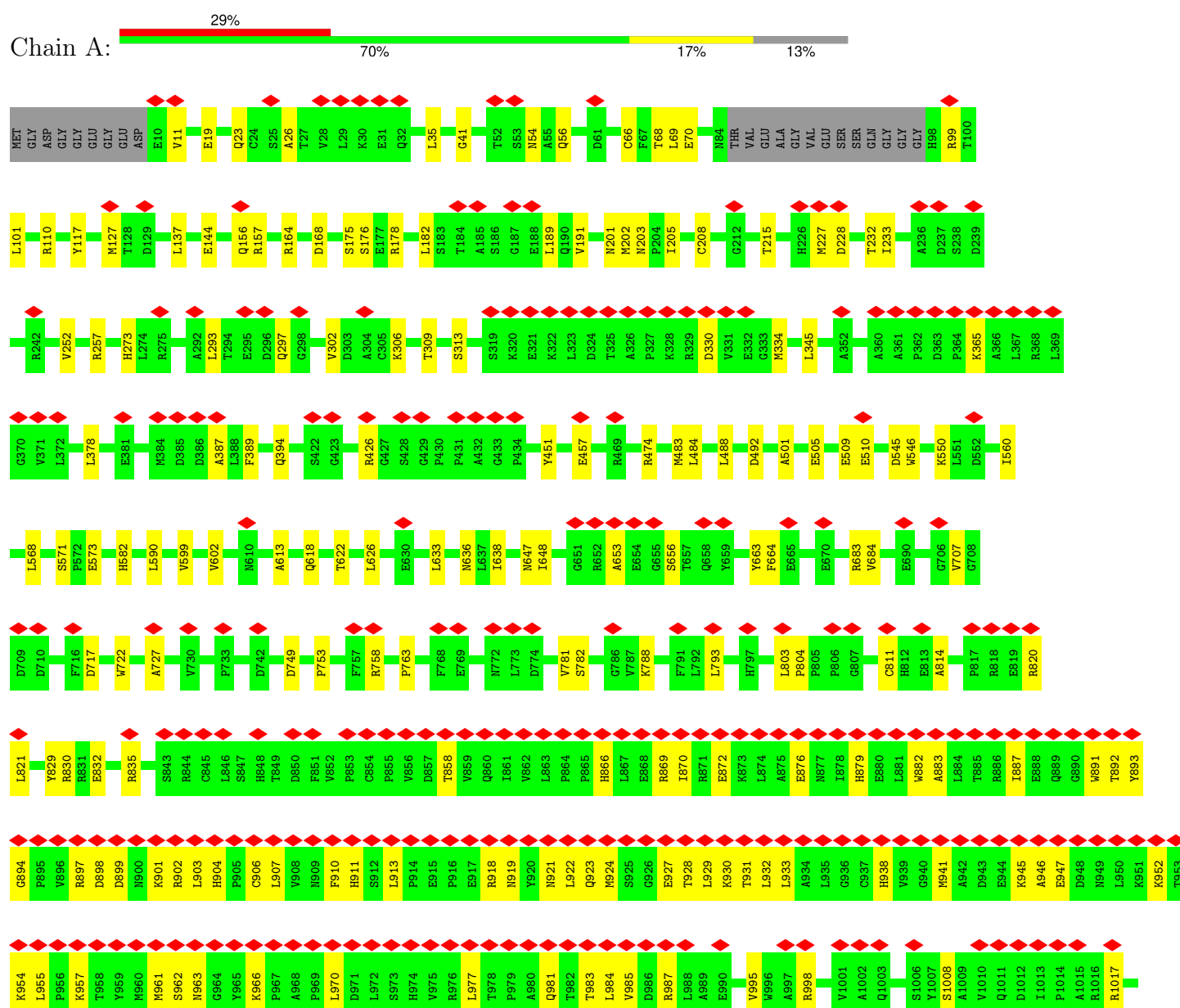


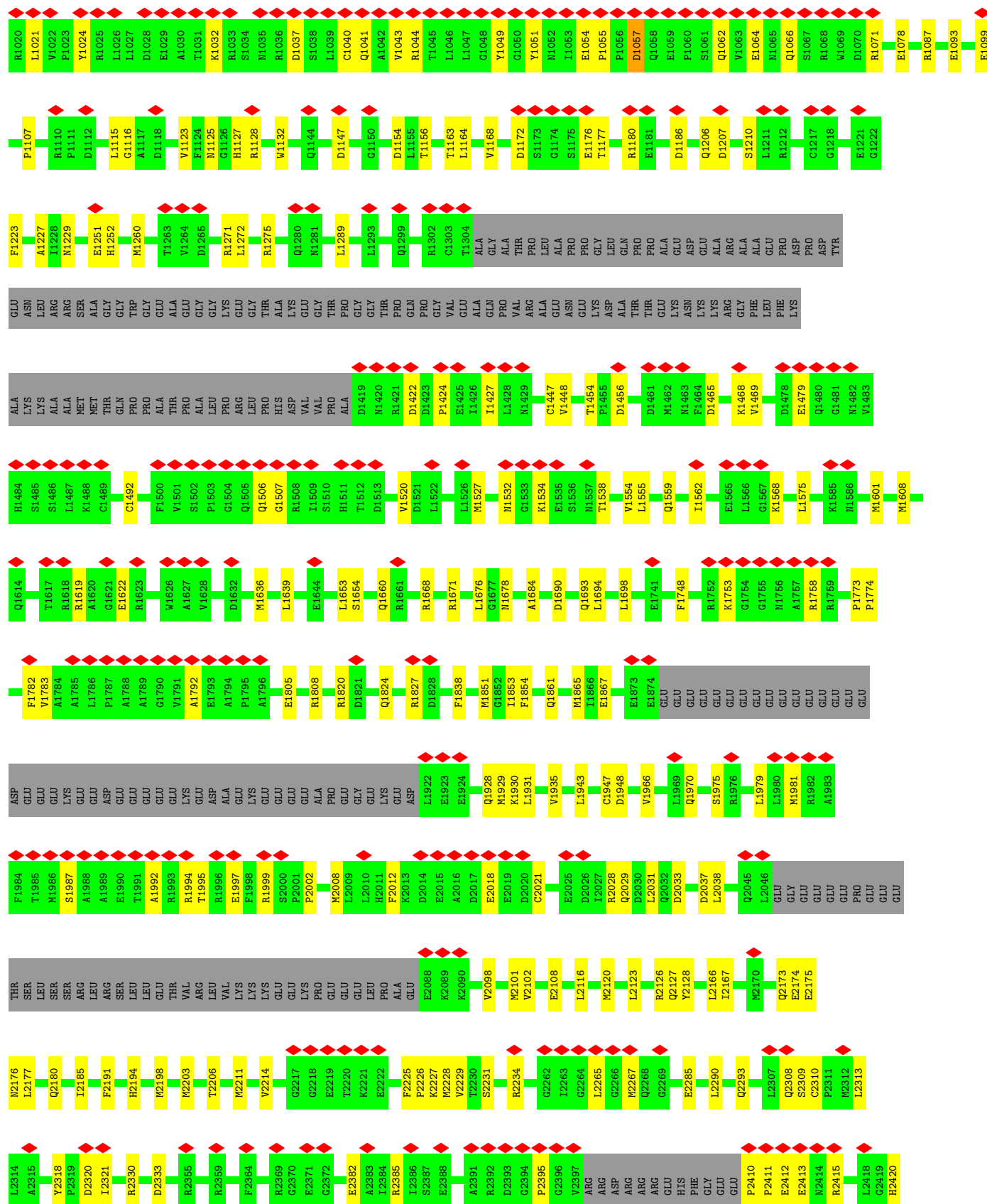
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			8	4	2	2	
6	B	1	Total	C	N	O	0
			8	4	2	2	
6	D	1	Total	C	N	O	0
			8	4	2	2	
6	C	1	Total	C	N	O	0
			8	4	2	2	

### 3 Residue-property plots

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

#### • Molecule 1: Ryanodine receptor 1

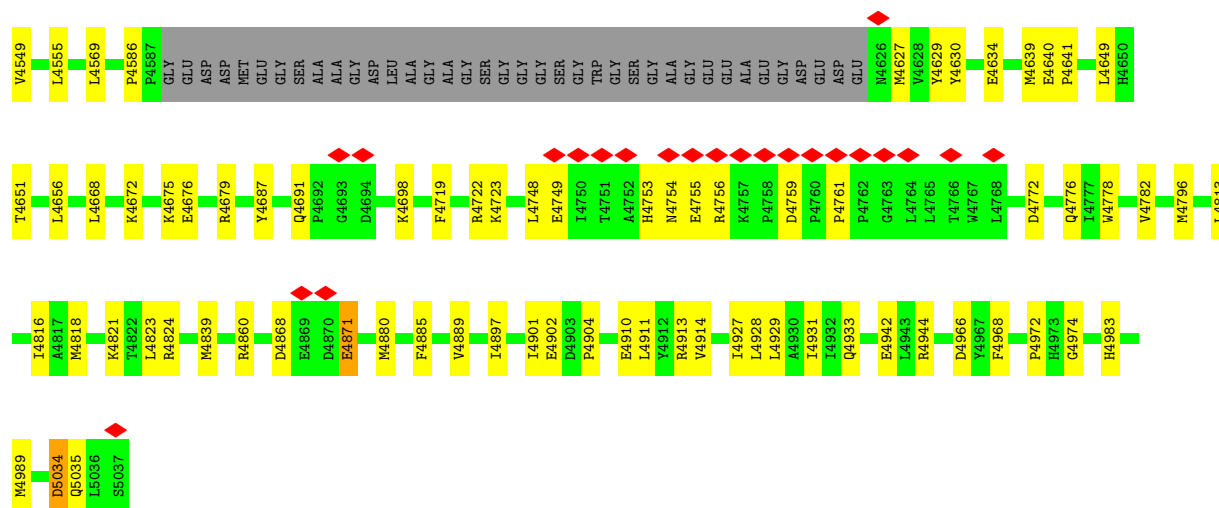




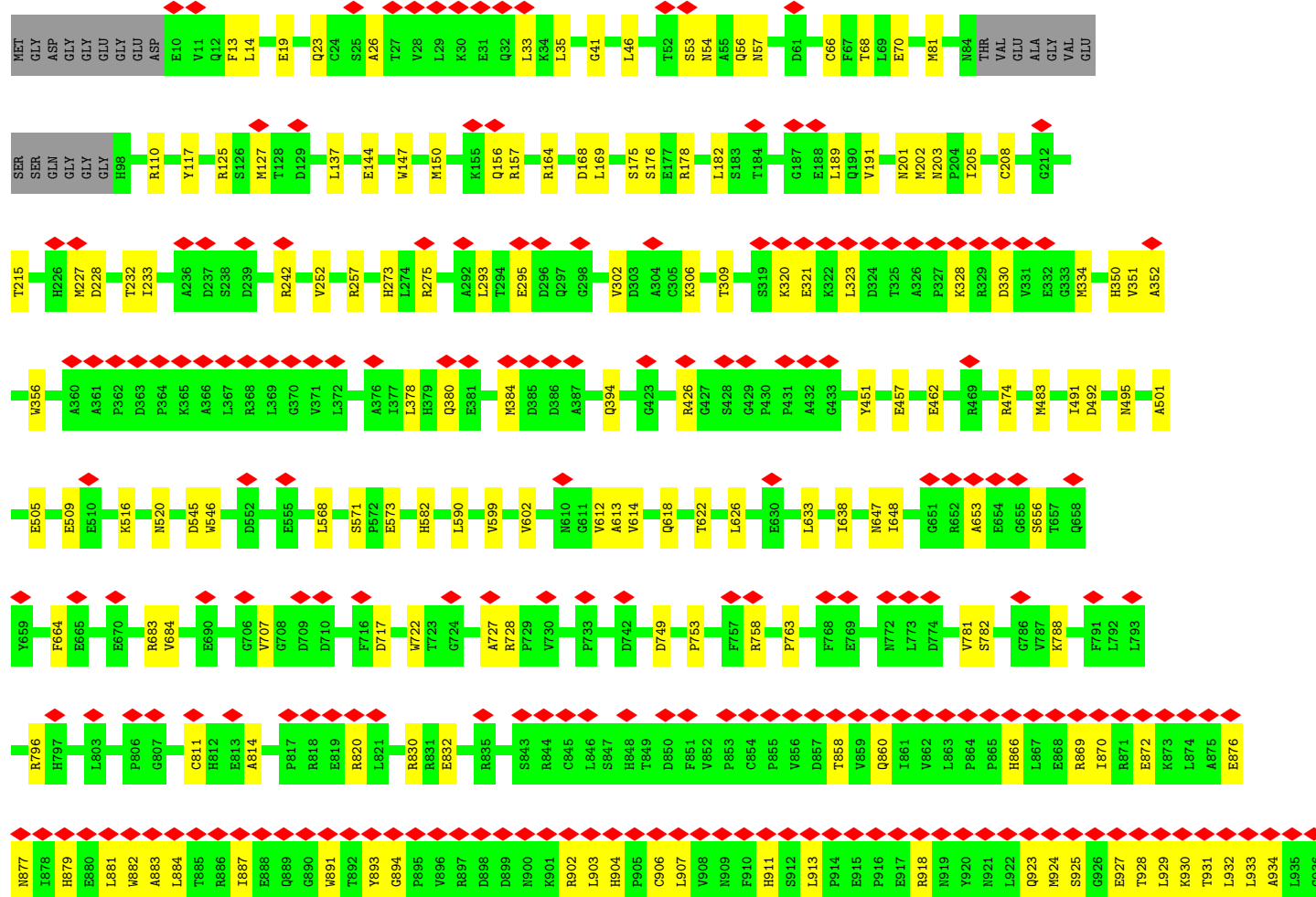
D3242	D3243	D3244	D3245	D3246	D3247	D3248	D3249	D3250	D3251	D3252	D3253	D3254	D3255	D3256	D3257	D3258	D3259	D3260	D3261	D3262	D3263	D3264	D3265	D3266	D3267	D3268	D3269	D3270	D3271	D3272	D3273	D3274	D3275	D3276	D3277	D3278	D3279	D3280	D3281	D3282	D3283	D3284	D3285	D3286	D3287	D3288	D3289	D3290	D3291	D3292	D3293	D3294	D3295	D3296	D3297	D3298	D3299	D3300	D3301	D3302				
Y3182	V3183	E3184	K3185	K3186	R3187	P3188	A3189	K3190	G3191	E3192	C3193	L3194	A3195	R3196	L3197	A3198	A3199	A3200	M3201	P3202	V3203	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	L3219	R3220	T3221	K3222	P3223	P3224	R3225	G3226	R3227	A3228	I3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	C3240						
ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	V3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	F3144	Q3145	H3146	T3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	T3157	L3158	D3159	D3160	V3161	Q3162	G3165	V3166	R3167	T3168	L3169	T3172	V3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181								
Y2541	S2542	H2441	Q2444	P2462	D2463	D2464	D2465	L2466	L2474	Q2475	L2476	P2477	T2478	L2479	G2480	K2481	D2482	A2484	L2485	V2486	Q2487	S2493	F2494	V2495	H2498	K2499	M2502	E2513	N2514	D2515	D2516	L2519	H2520	V2523	V2524	G2525	F2526	L2527	F2528	D2529	M2530	R2531	A2534	S2535	L2536	D2537	T2538																	
F2541	S2542	H2546	A2547	L2550	K2564	F2569	A2570	G2571	T2572	H2573	H2574	R2575	A2576	I2577	M2578	N2582	L2583	H2584	T2585	V2586	R2587	R2588	L2589	S2590	R2591	G2592	R2593	S2594	Q2599	R2600	I2603	E2604	E2605	C2606	L2607	M2608	C2611	I2614	R2615	F2619	L2622	L2623	R2624	R2625	L2626	V2627	F2628																	
D2629	V2630	P2631	L2632	L2633	N2634	E2635	F2636	A2637	N2638	M2639	P2640	L2641	K2642	L2643	L2644	T2645	H2646	I2647	M2648	E2649	C2651	Y2655	C2656	L2657	P2658	T2659	W2661	G2662	N2663	T2664	Q2665	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	T2675	R2676	K2677	L2678	P2679	W2680	Q2681	L2682	F2683	D2684	H2688	K2689	K2690	Y2691	D2692									
Q2693	E2694	L2695	Y2696	R2697	M2698	A2699	P2700	M2701	C2702	L2703	C2704	A2705	L2706	A2707	G2708	A2709	L2710	P2711	P2712	D2713	Y2714	V2715	D2716	A2717	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	W2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	W2744	V2745	I2746	L2747	P2748	E2749	K2750	L2751	D2752					
S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	T2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	E2803	L2804	Y2805	R2806	W2807	P2808	I2809	K2810	E2811	S2812						
L2813	K2814	A2815	W2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	A2825	A2826	R2827	E2828	G2829	GLU	GLU	ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	Y2856	Q2857	P2858	P2859	P2860	L2861	L2862	S2863	Q2864	T2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872						
A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	E2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	Q2922	A2923	Q2924	E2925	L2926	L2927	K2928	Y2929	L2930	Q2931	M2932					
N2933	G2934	Y2935	A2936	T2937	R2938	A2939	GLY	LEU	ASP	MET	GLU	L2946	D2947	T2948	S2949	S2950	L2951	E2952	K2953	R2954	F2955	A2956	F2957	G2958	F2959	L2960	Q2961	Q2962	L2963	L2964	R2965	W2966	M2967	D2968	L2969	S2970	Q2971	E2972	T2973	L2974	A2975	H2976	L2977	E2978	A2979	V2980	S2981	S2982	S2983	Q2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992						
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ALA	ARG	THR	GLN	VAL	K3123	G3124	V3125	G3126	Q3127	N3128	L3129	T3130	V3131	T3132	T3133	V3134	A3135	L3136	L3137	P3138	V3139	L3140	F3144	Q3145	H3146	T3147	A3148	Q3149	H3150	Q3151	F3152	G3153	D3154	D3155	V3156	T3157	L3158	D3159	D3160	V3161	Q3162	G3165	V3166	R3167	T3168	L3169	T3172	V3173	S3174	L3175	G3176	T3177	T3178	K3179	N3180	T3181								
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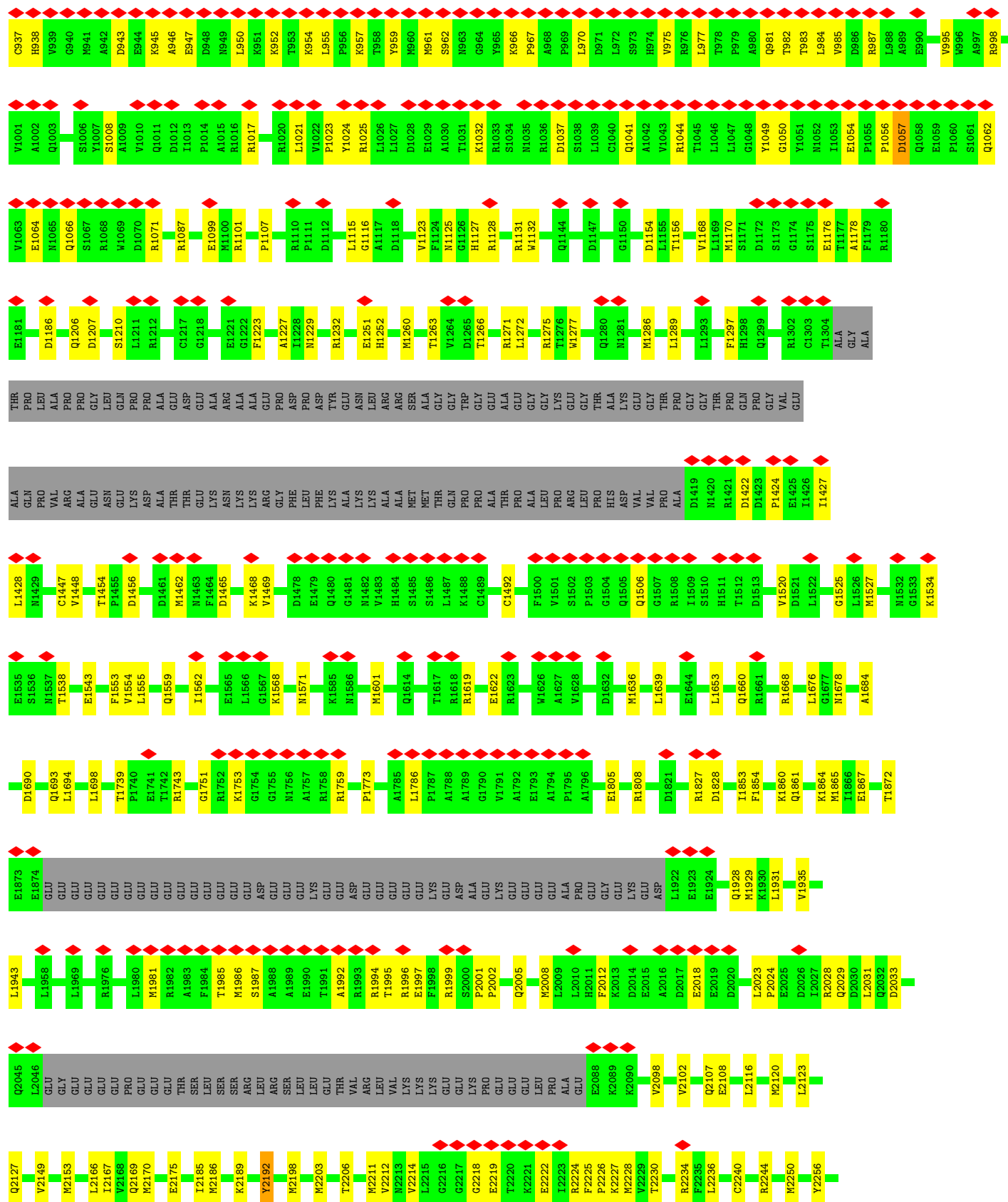






• Molecule 1: Ryanodine receptor 1

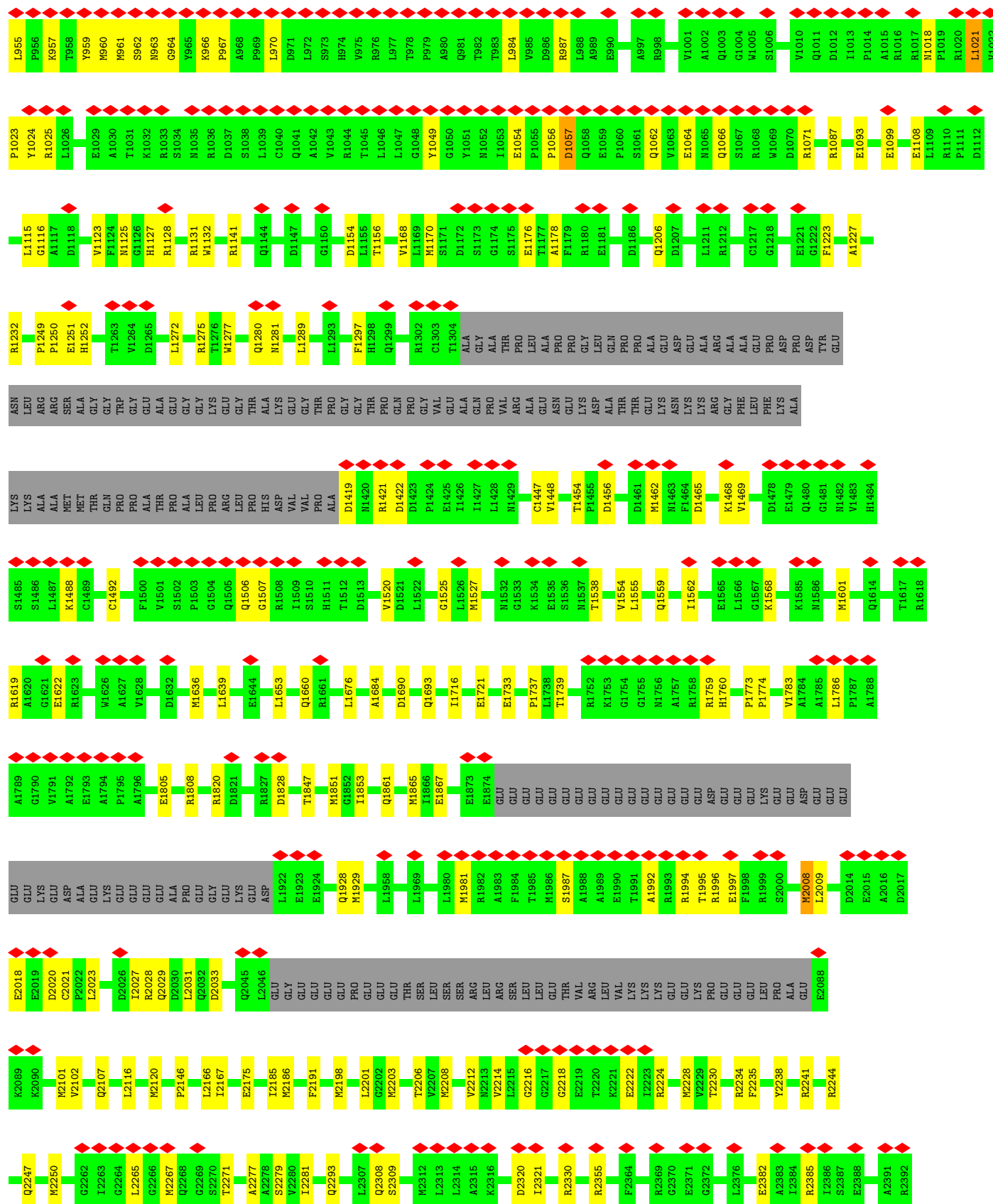




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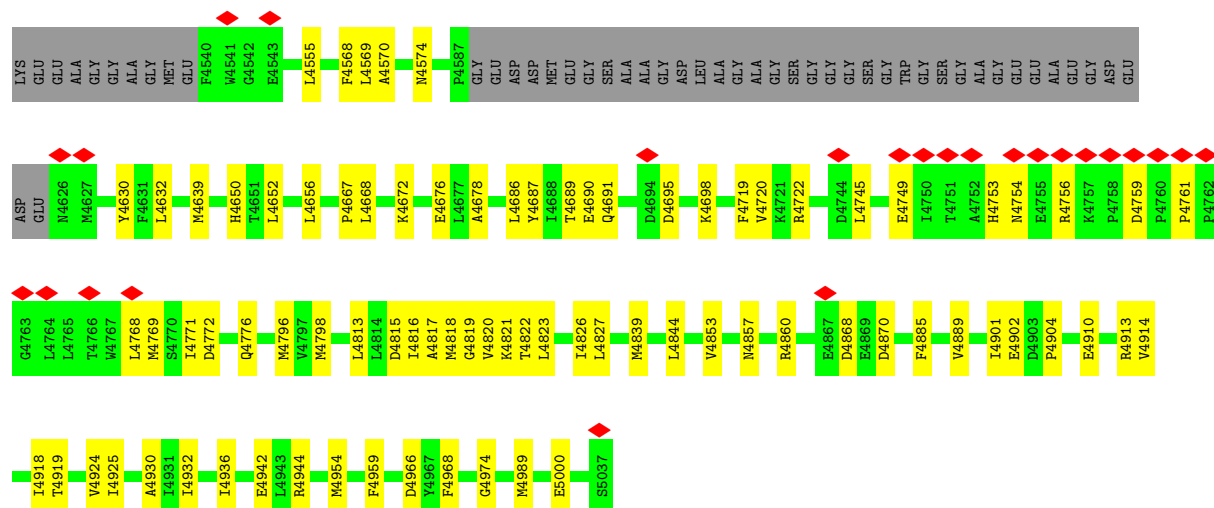




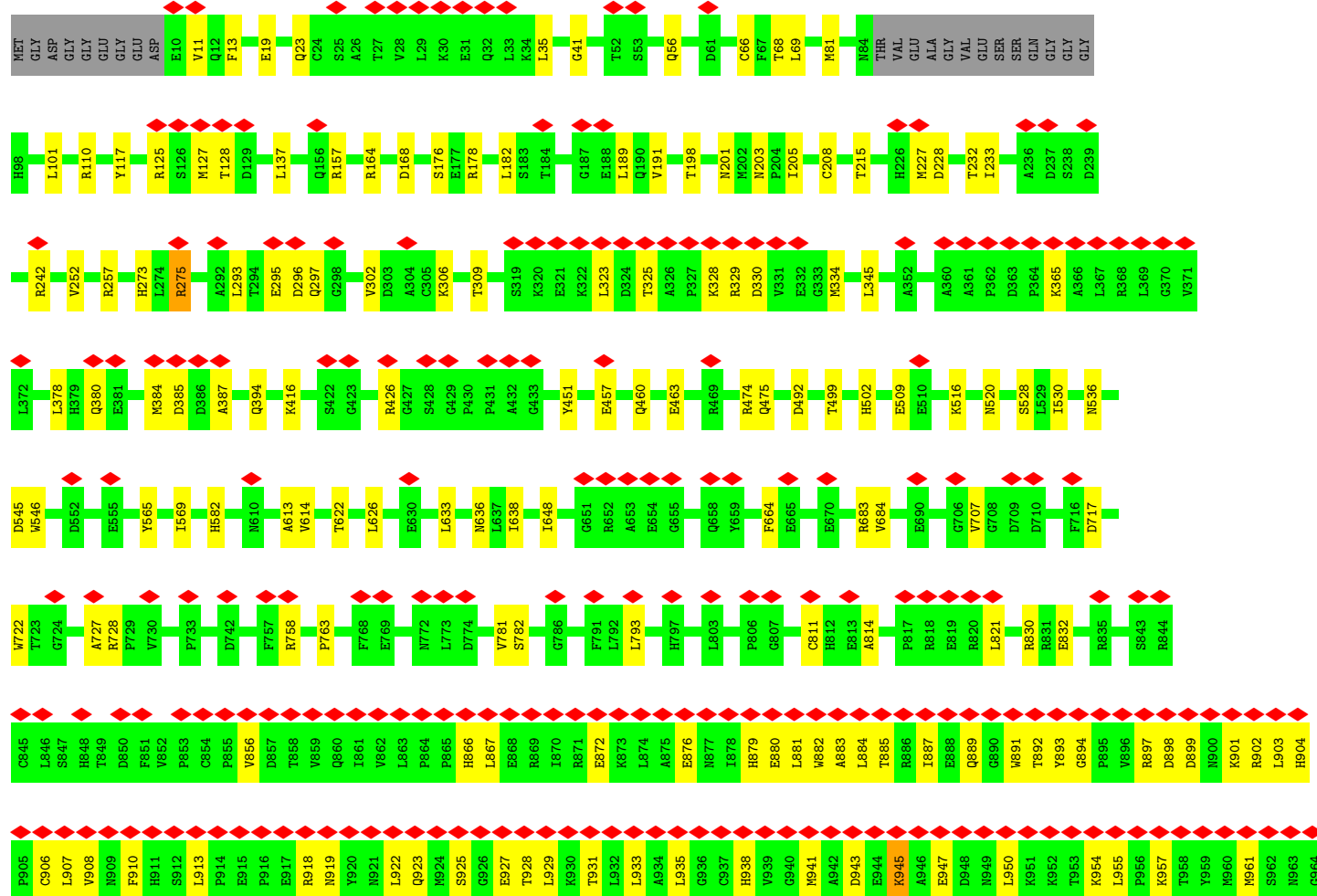
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D2393	G2394	P2395	G2396	V2397	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	P2410	P2411	E2412	E2413	N2414	R2415	L2418	G2419	A2420	A2421	T2422	M2423	W2440	T2456	S2459	L2460	D2464	D2465	L2466	L2474	Q2475	T2476	F2477	T2478	L2479	K2480	K2481	D2482	G2483	A2484	L2485	V2486	Q2487	W2490	S2493													
F2494	D2497	L2498	K2499	M2502	E2513	N2514	Q2515	D2516	L2519	L2522	D2523	F2526	P2528	D2529	M2530	R2531	A2534	S2535	L2536	D2537	T2538	A2539	T2540	S2542	E2545	M2546	A2547	L2550	T2562	F2569	A2570	G2571	T2572	M2573	H2574	R2575	A2576	L2577	D2580	S2581	M2582	L2583	H2584	T2585	V2586																	
Y2587	R2588	S2589	R2591	Q2592	R2593	S2594	R2600	I2603	E2604	L2607	M2608	A2609	L2610	C2611	I2614	R2615	M2618	L2619	K2620	H2621	L2622	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	P2631	L2632	L2633	N2634	E2635	F2636	A2637	M2638	P2640	L2641	K2642	L2643	L2644	Y2648	E2649	R2650	C2651	Y2655	L2657	P2658													

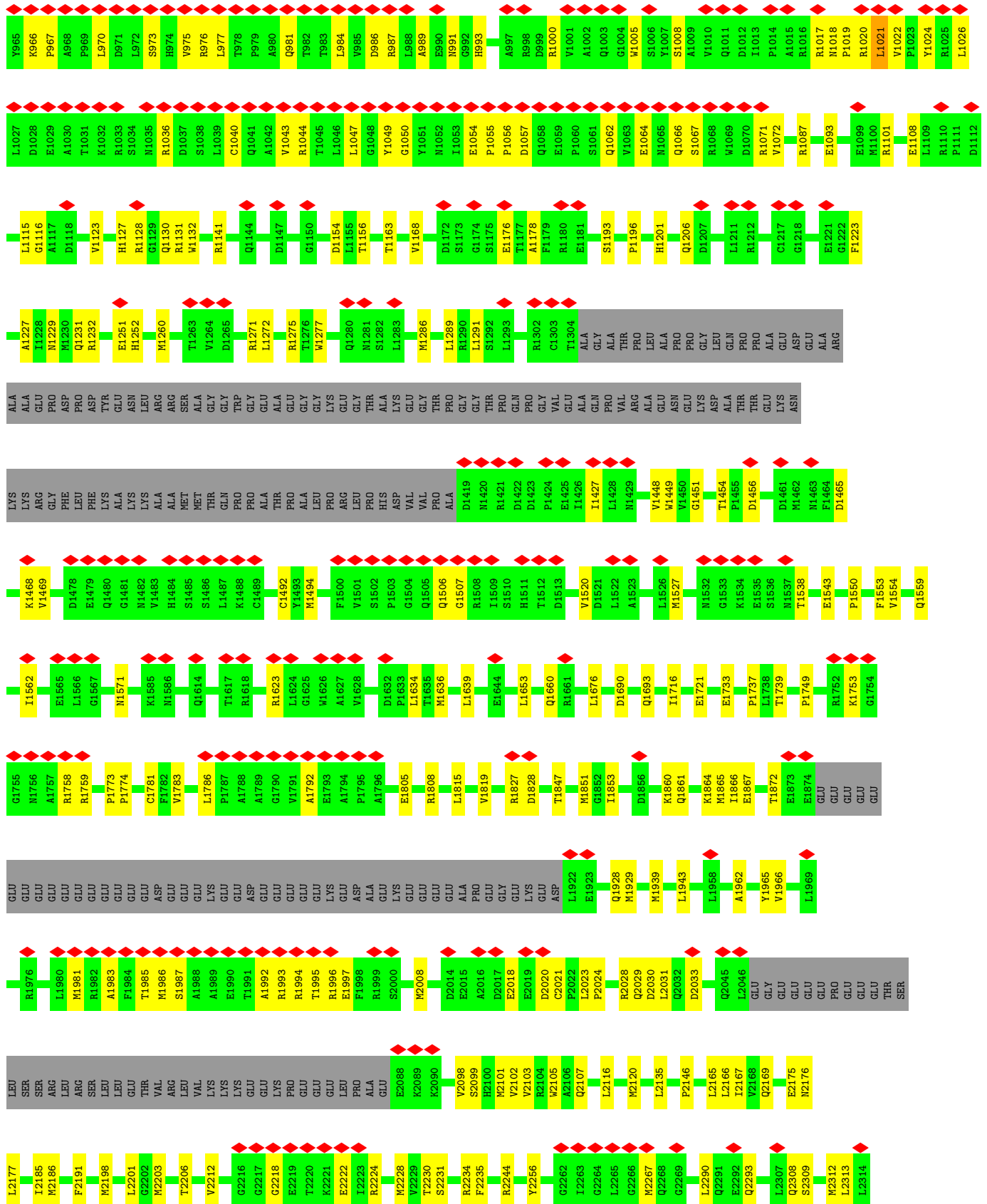


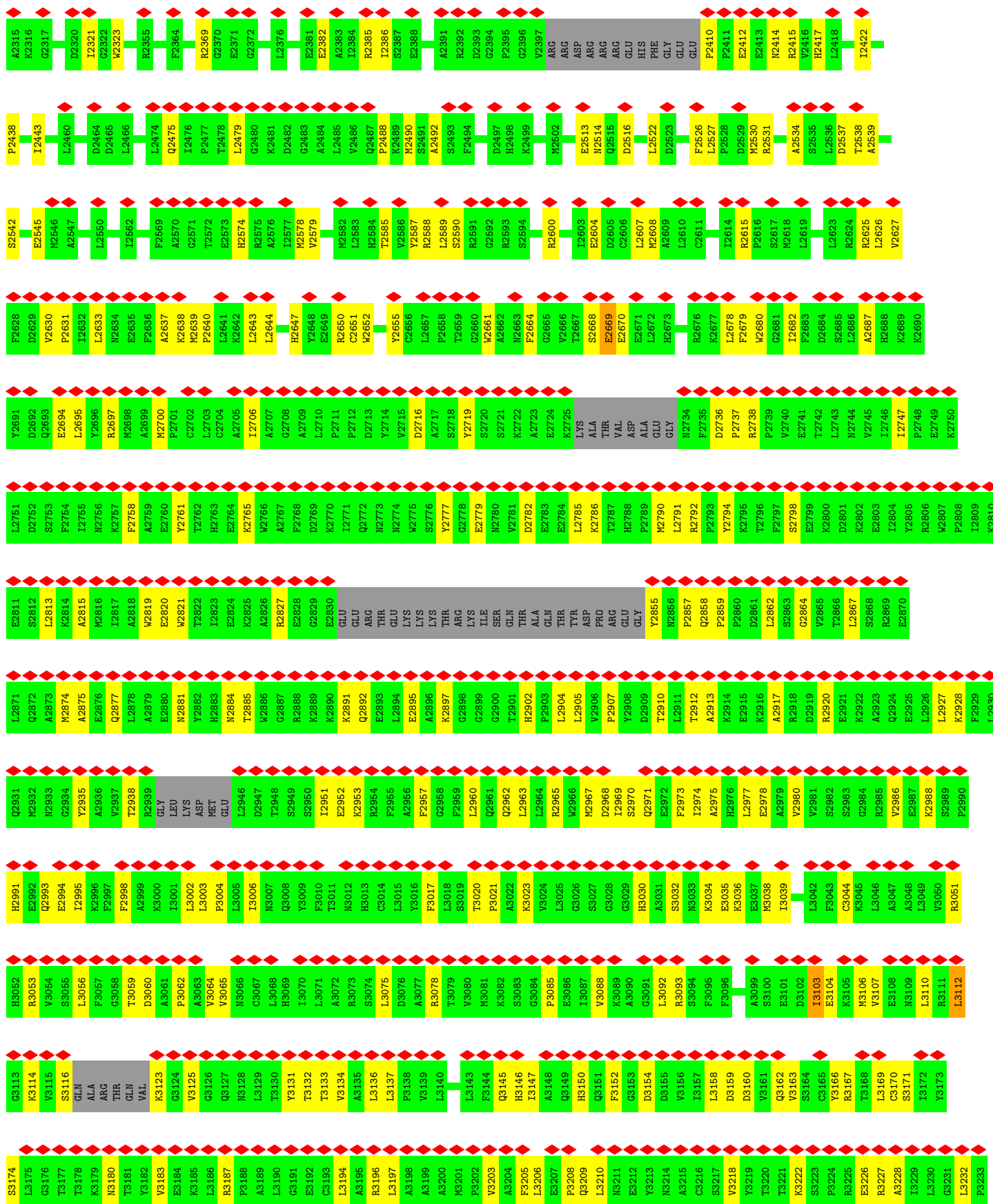




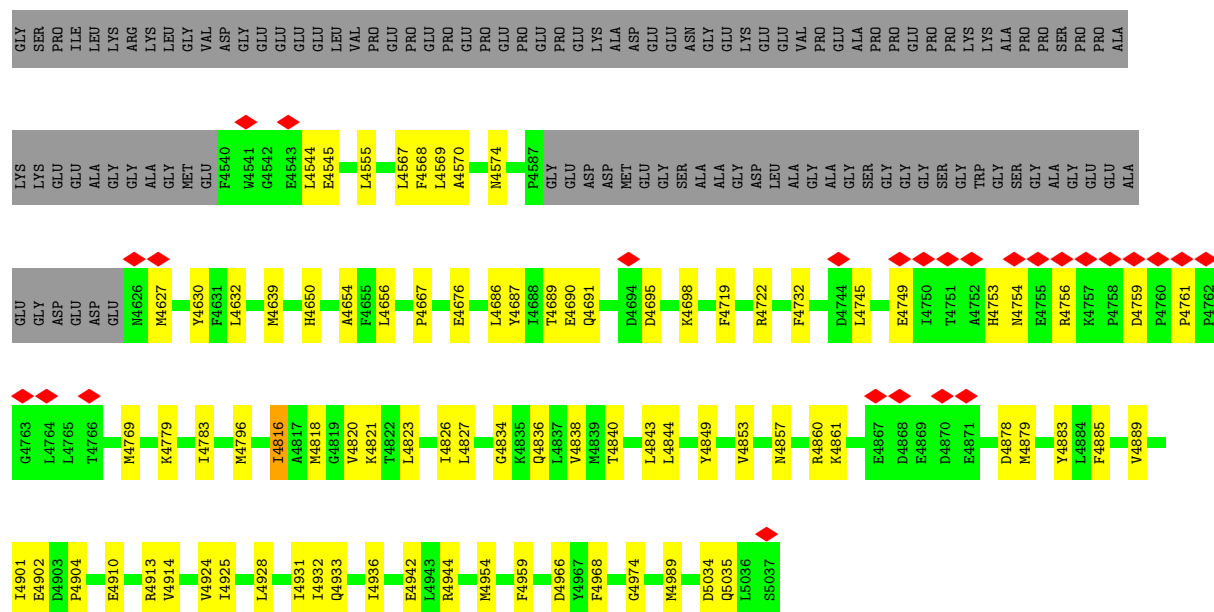
• Molecule 1: Ryanodine receptor 1



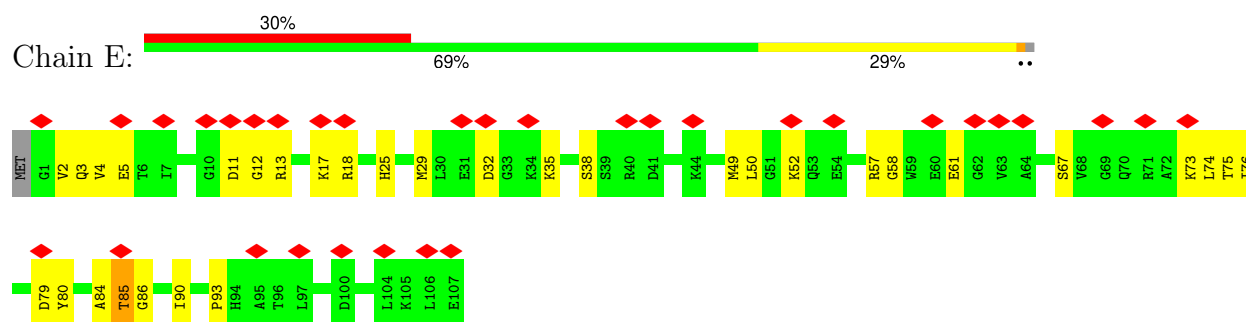




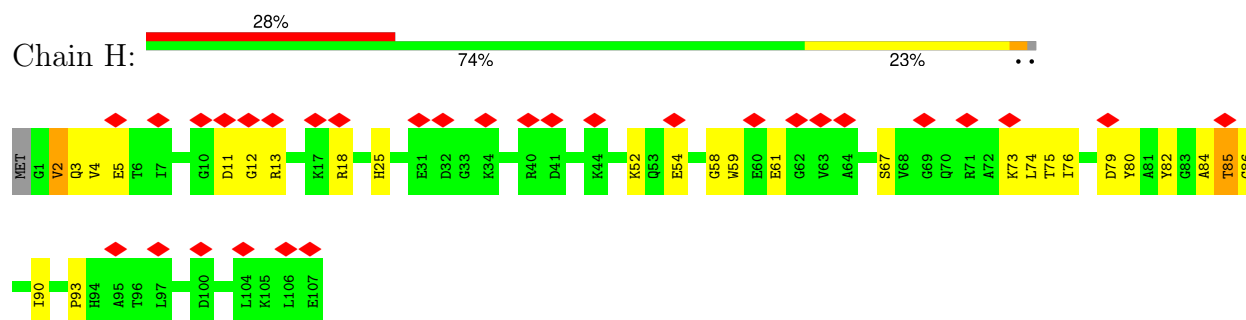




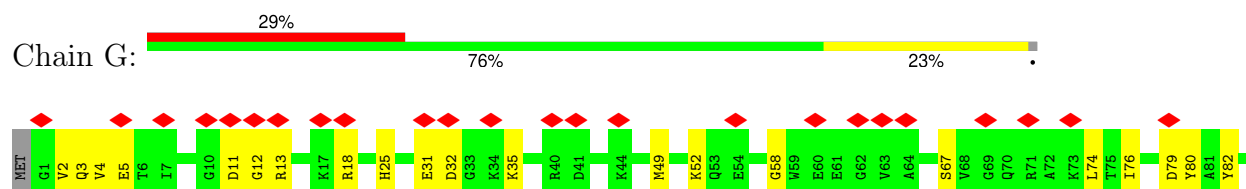
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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

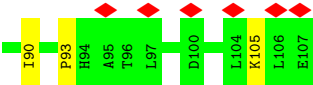
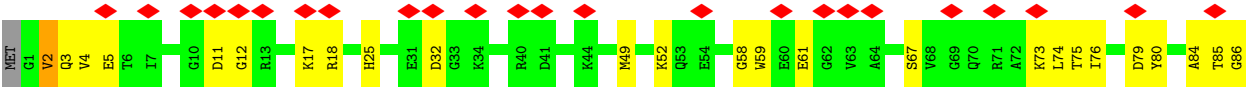


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A





• 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	33584	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	0.482	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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	0.17	0/35977	0.34	2/48726 (0.0%)
1	B	0.17	0/35977	0.34	0/48726
1	C	0.16	0/35977	0.34	2/48726 (0.0%)
1	D	0.15	0/35977	0.31	1/48726 (0.0%)
2	E	0.17	0/850	0.36	0/1146
2	F	0.18	0/850	0.40	0/1146
2	G	0.18	0/850	0.39	0/1146
2	H	0.17	0/850	0.36	0/1146
All	All	0.16	0/147308	0.33	5/199488 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2669	GLU	CA-CB-CG	5.61	125.32	114.10
1	C	2971	GLN	CA-CB-CG	5.30	124.70	114.10
1	D	1783	VAL	N-CA-C	-5.25	108.16	113.20
1	A	1783	VAL	N-CA-C	-5.21	108.20	113.20
1	A	3534	MET	CB-CG-SD	5.12	128.06	112.70

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	570	0
1	B	35150	0	34797	609	0
1	C	35150	0	34797	639	0
1	D	35150	0	34797	542	0
2	E	831	0	831	19	0
2	F	831	0	831	18	0
2	G	831	0	831	16	0
2	H	831	0	831	17	0
3	A	31	0	12	1	0
3	B	31	0	12	1	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	8	0	3	0	0
6	B	8	0	3	0	0
6	C	8	0	3	0	0
6	D	8	0	3	0	0
All	All	144088	0	142572	2402	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 8.

All (2402) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2647:HIS:HE2	1:C:2655:TYR:HH	1.18	0.89
1:C:893:TYR:HB2	1:C:961:MET:HE2	1.53	0.89
1:C:3254:GLY:HA2	1:C:3318:ASN:HD21	1.40	0.86
1:D:957:LYS:H	1:D:957:LYS:HD2	1.41	0.84
1:B:3233:PRO:HD2	1:B:3239:MET:HE1	1.59	0.82
1:D:3573:MET:HB3	1:D:3577:ARG:HH21	1.43	0.81
1:D:3550:ARG:HD3	1:D:3594:ARG:HH22	1.44	0.81
1:D:894:GLY:HA3	1:D:903:LEU:HB3	1.63	0.81
1:B:2765:LYS:HZ3	1:B:2857:PRO:HB2	1.44	0.81
1:C:1520:VAL:HG12	1:C:1527:MET:HG2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:GLU:HG2	1:A:918:ARG:HD3	1.65	0.79
1:A:1520:VAL:HG12	1:A:1527:MET:HG2	1.65	0.79
1:B:876:GLU:HG2	1:B:918:ARG:HD3	1.66	0.78
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.16	0.77
1:B:1996:ARG:HH21	1:B:1999:ARG:HE	1.31	0.77
1:B:2293:GLN:OE1	1:B:2293:GLN:N	2.18	0.77
1:C:2023:LEU:HD12	1:C:2024:PRO:HD2	1.66	0.77
1:B:2230:THR:HB	1:B:2267:MET:HE1	1.67	0.76
1:D:1520:VAL:HG12	1:D:1527:MET:HG2	1.67	0.76
1:C:1067:SER:O	1:C:1071:ARG:NH2	2.18	0.76
1:A:2765:LYS:HZ3	1:A:2857:PRO:HB2	1.50	0.76
1:D:1280:GLN:O	1:D:1281:ASN:ND2	2.19	0.76
1:B:4821:LYS:HD3	1:B:4821:LYS:H	1.51	0.75
1:D:2694:GLU:HA	1:D:2697:ARG:HH12	1.51	0.75
1:A:2293:GLN:OE1	1:A:2293:GLN:N	2.18	0.75
1:C:3132:THR:HA	1:C:3136:LEU:HB3	1.69	0.75
1:D:876:GLU:HG2	1:D:918:ARG:HD3	1.68	0.74
1:A:2441:HIS:HA	1:A:2444:GLN:HE21	1.52	0.74
1:A:3530:GLN:N	1:A:3530:GLN:OE1	2.20	0.74
1:C:876:GLU:HG2	1:C:918:ARG:HD3	1.69	0.74
1:A:3110:LEU:HD11	1:A:3182:TYR:HB2	1.67	0.74
1:B:3530:GLN:OE1	1:B:3530:GLN:N	2.20	0.74
1:B:3535:LEU:HD13	1:B:3552:PHE:HE1	1.53	0.73
1:A:4821:LYS:HD3	1:A:4821:LYS:H	1.53	0.73
1:B:893:TYR:HB2	1:B:961:MET:HE1	1.68	0.73
1:C:3107:VAL:HG21	1:C:3171:SER:HB2	1.69	0.73
1:B:2694:GLU:HA	1:B:2697:ARG:HH12	1.52	0.73
1:A:2694:GLU:HA	1:A:2697:ARG:HH12	1.52	0.73
1:B:2627:VAL:HG22	1:B:2678:LEU:HB2	1.71	0.73
1:C:384:MET:HE3	1:C:384:MET:H	1.52	0.73
1:A:4209:GLN:OE1	1:A:4209:GLN:N	2.20	0.72
1:D:3528:THR:HG23	1:D:3573:MET:HE3	1.70	0.72
1:A:2779:GLU:HG3	1:A:2792:ARG:HG2	1.70	0.72
1:B:3527:PRO:HA	1:B:3530:GLN:HE22	1.53	0.72
1:D:2293:GLN:OE1	1:D:2293:GLN:N	2.19	0.72
2:G:52:LYS:HE2	2:G:52:LYS:HA	1.72	0.72
1:B:2175:GLU:HG3	1:B:2228:MET:HB2	1.71	0.72
1:C:973:SER:O	1:C:976:ARG:NH1	2.21	0.72
1:C:3550:ARG:HE	1:C:3594:ARG:HH12	1.37	0.72
1:C:4161:ARG:HE	1:C:4161:ARG:H	1.38	0.72
1:D:4186:ALA:O	1:D:4188:ARG:NH1	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3329:ILE:HD11	1:D:3332:ALA:HB2	1.71	0.71
1:D:2186:MET:HE1	1:D:2234:ARG:HH12	1.54	0.71
1:D:3233:PRO:O	1:D:3234:ASN:ND2	2.21	0.71
1:C:2779:GLU:HG3	1:C:2792:ARG:HG2	1.71	0.71
1:A:3329:ILE:HD11	1:A:3332:ALA:HB2	1.72	0.71
1:B:2779:GLU:HG3	1:B:2792:ARG:HG2	1.71	0.71
1:D:2198:MET:H	1:D:2198:MET:HE2	1.53	0.71
2:F:52:LYS:HE2	2:F:52:LYS:HA	1.72	0.71
1:D:955:LEU:O	1:D:966:LYS:NZ	2.24	0.71
1:C:4186:ALA:O	1:C:4188:ARG:NH1	2.21	0.71
1:A:3623:LEU:HD12	1:A:3624:LEU:HG	1.73	0.70
1:C:2737:PRO:HD2	1:C:2891:LYS:HD3	1.71	0.70
1:C:3208:PRO:HB2	1:C:3237:GLU:HG3	1.73	0.70
1:C:955:LEU:O	1:C:966:LYS:NZ	2.23	0.70
1:D:2779:GLU:HG3	1:D:2792:ARG:HG2	1.73	0.70
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.24	0.70
1:C:23:GLN:NE2	1:C:203:ASN:OD1	2.24	0.70
1:C:2608:MET:HE2	1:C:2639:MET:HE1	1.74	0.70
1:B:3132:THR:HA	1:B:3136:LEU:HB3	1.72	0.70
1:A:2479:LEU:O	1:A:2897:LYS:NZ	2.24	0.70
1:B:3412:LEU:HD11	1:B:3434:LEU:HD21	1.74	0.70
1:D:2737:PRO:HD2	1:D:2891:LYS:HD3	1.72	0.70
1:A:3527:PRO:HA	1:A:3530:GLN:HE22	1.57	0.70
1:B:227:MET:HE2	1:B:227:MET:H	1.57	0.69
1:B:380:GLN:OE1	1:B:380:GLN:N	2.22	0.69
1:B:3039:ILE:HD11	1:B:3071:LEU:HD22	1.73	0.69
1:D:872:GLU:HA	1:D:922:LEU:HD11	1.74	0.69
1:B:3110:LEU:HD11	1:B:3182:TYR:HB2	1.74	0.69
1:B:3702:VAL:HG13	1:B:3778:MET:HE3	1.73	0.69
1:A:2867:LEU:HB2	1:A:2928:LYS:HZ3	1.57	0.69
1:D:3514:LEU:HD21	1:D:3602:VAL:HG13	1.74	0.69
1:D:3702:VAL:HG13	1:D:3778:MET:HE3	1.74	0.69
1:C:3078:ARG:NH2	1:C:3150:HIS:O	2.26	0.69
1:B:2812:SER:HG	1:B:2882:TYR:HH	1.32	0.69
1:B:3329:ILE:HD11	1:B:3332:ALA:HB2	1.73	0.69
1:C:2650:ARG:NH1	1:C:2651:CYS:SG	2.66	0.69
1:A:3758:MET:HE2	1:A:3758:MET:HA	1.73	0.69
1:D:3758:MET:HA	1:D:3758:MET:HE2	1.75	0.69
1:C:2230:THR:HB	1:C:2267:MET:HE1	1.75	0.69
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.56	0.69
1:D:2186:MET:HE2	1:D:2235:PHE:HD1	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4634:GLU:HG2	1:B:4639:MET:HE2	1.74	0.69
1:C:457:GLU:N	1:C:457:GLU:OE2	2.24	0.69
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.57	0.68
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.56	0.68
1:B:891:TRP:HA	1:B:902:ARG:HB3	1.75	0.68
1:B:2867:LEU:HB2	1:B:2928:LYS:HZ3	1.58	0.68
1:A:3702:VAL:HG13	1:A:3778:MET:HE3	1.74	0.68
1:B:3128:ASN:O	1:B:3132:THR:HG23	1.93	0.68
1:B:4630:TYR:OH	1:C:4860:ARG:NH1	2.26	0.68
1:A:156:GLN:OE1	1:A:156:GLN:N	2.23	0.68
1:B:23:GLN:NE2	1:B:203:ASN:OD1	2.27	0.68
1:B:3477:LYS:HB3	1:C:1141:ARG:HD3	1.74	0.68
1:D:2781:VAL:HA	1:D:2789:PRO:HB2	1.76	0.68
1:B:2479:LEU:O	1:B:2897:LYS:NZ	2.26	0.68
1:B:2737:PRO:HD2	1:B:2891:LYS:HD3	1.76	0.68
1:C:3445:TRP:NE1	1:C:3455:GLU:OE1	2.26	0.68
1:A:2781:VAL:HA	1:A:2789:PRO:HB2	1.76	0.68
1:D:510:GLU:OE1	1:D:510:GLU:N	2.24	0.68
1:A:23:GLN:NE2	1:A:203:ASN:OD1	2.26	0.68
1:A:1260:MET:HE3	1:A:1271:ARG:HE	1.59	0.68
1:C:380:GLN:OE1	1:C:380:GLN:N	2.22	0.68
1:B:54:ASN:HA	1:B:56:GLN:HE22	1.59	0.67
1:C:1981:MET:N	1:C:1981:MET:SD	2.67	0.67
1:A:3412:LEU:HD11	1:A:3434:LEU:HD21	1.76	0.67
1:A:835:ARG:NH2	1:A:1093:GLU:OE1	2.27	0.67
1:D:23:GLN:NE2	1:D:203:ASN:OD1	2.26	0.67
1:C:866:HIS:HB2	1:C:941:MET:HE3	1.75	0.67
1:C:2513:GLU:N	1:C:2513:GLU:OE2	2.27	0.67
1:A:1792:ALA:O	1:A:2176:ASN:ND2	2.28	0.67
1:B:2577:ILE:H	1:B:2577:ILE:HD12	1.59	0.67
1:C:2534:ALA:HA	1:C:2588:ARG:HH21	1.60	0.67
1:B:3449:HIS:HB2	1:B:3453:ARG:NH2	2.10	0.67
1:C:3262:ARG:HD2	1:C:3329:ILE:HD11	1.77	0.67
1:B:879:HIS:HA	1:B:882:TRP:CD1	2.30	0.66
1:A:3528:THR:HG23	1:A:3573:MET:HE3	1.78	0.66
1:A:4839:MET:HA	1:A:4839:MET:HE3	1.76	0.66
1:B:2781:VAL:HA	1:B:2789:PRO:HB2	1.77	0.66
1:A:858:THR:HB	1:A:930:LYS:HD2	1.77	0.66
1:C:3194:LEU:HD13	1:C:3276:MET:HB3	1.76	0.66
1:C:3579:LEU:HB3	1:C:3582:ARG:HG2	1.77	0.66
1:B:858:THR:HB	1:B:930:LYS:HD2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.61	0.66
1:C:2638:LYS:HE2	1:C:2695:LEU:HD13	1.77	0.66
1:A:2642:LYS:HE2	1:A:2642:LYS:HA	1.77	0.66
1:C:2765:LYS:NZ	1:C:2859:PRO:O	2.28	0.66
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.29	0.66
1:C:2765:LYS:HZ3	1:C:2857:PRO:HB2	1.60	0.66
1:B:394:GLN:OE1	1:B:394:GLN:N	2.29	0.66
1:C:297:GLN:OE1	1:C:297:GLN:N	2.27	0.66
1:A:879:HIS:HA	1:A:882:TRP:CD1	2.31	0.66
1:A:3324:VAL:HG11	1:A:3361:THR:HG22	1.78	0.66
1:D:2479:LEU:O	1:D:2897:LYS:NZ	2.28	0.66
1:D:3456:GLN:OE1	1:D:3456:GLN:N	2.27	0.66
1:C:3545:THR:HG23	1:C:3547:GLU:H	1.60	0.66
1:B:2816:MET:HE1	1:B:2930:LEU:HD11	1.79	0.65
1:D:3579:LEU:HB2	1:D:3582:ARG:HG2	1.77	0.65
1:C:3702:VAL:HG13	1:C:3778:MET:HE3	1.76	0.65
1:C:4689:THR:OG1	1:C:4690:GLU:OE1	2.12	0.65
1:B:2410:PRO:HB3	1:B:2415:ARG:HB2	1.79	0.65
1:A:2420:HIS:HA	1:A:2423:MET:HE3	1.79	0.65
1:B:3389:GLU:N	1:B:3389:GLU:OE2	2.28	0.65
1:A:4634:GLU:HG2	1:A:4639:MET:HE2	1.78	0.65
1:B:384:MET:HE3	1:B:384:MET:H	1.60	0.65
1:B:2519:LEU:HD13	1:B:2575:ARG:HG3	1.77	0.65
1:C:622:THR:HG23	1:C:626:LEU:HD12	1.77	0.65
1:C:4820:VAL:HG12	1:C:4823:LEU:H	1.61	0.65
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.30	0.65
1:A:2410:PRO:HB3	1:A:2415:ARG:HB2	1.77	0.65
1:A:866:HIS:CD2	1:A:941:MET:HG2	2.32	0.65
1:A:2175:GLU:HG3	1:A:2228:MET:HB3	1.79	0.65
1:B:2679:PHE:HB2	1:B:2706:ILE:HG21	1.78	0.65
1:D:2244:ARG:NH2	1:D:3859:VAL:O	2.30	0.65
1:D:3467:MET:HA	1:D:3467:MET:HE2	1.78	0.65
1:D:4039:MET:HE2	1:D:4039:MET:HA	1.79	0.65
1:B:3945:GLU:OE1	1:B:3949:ARG:NH2	2.30	0.64
1:D:2765:LYS:NZ	1:D:2859:PRO:O	2.30	0.64
1:C:2479:LEU:O	1:C:2897:LYS:NZ	2.29	0.64
1:C:2627:VAL:HG22	1:C:2678:LEU:HB2	1.78	0.64
1:A:2644:LEU:HD13	1:A:2678:LEU:HD21	1.80	0.64
1:D:4821:LYS:HD3	1:D:4821:LYS:H	1.60	0.64
1:B:1260:MET:HE3	1:B:1271:ARG:HE	1.62	0.64
1:B:275:ARG:HH21	1:B:328:LYS:NZ	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3414:ARG:NH1	1:C:3414:ARG:HB2	2.12	0.64
1:D:156:GLN:OE1	1:D:156:GLN:N	2.22	0.64
1:D:457:GLU:OE2	1:D:457:GLU:N	2.24	0.64
1:B:2475:GLN:HG2	1:B:2488:PRO:HG3	1.80	0.64
1:D:2309:SER:OG	1:D:2321:ILE:O	2.15	0.64
1:C:1024:TYR:OH	1:C:1036:ARG:NH2	2.29	0.64
1:D:2650:ARG:NH1	1:D:2651:CYS:SG	2.71	0.64
1:C:984:LEU:HD21	1:C:1056:PRO:HD2	1.79	0.64
1:C:3085:PRO:HG2	1:C:3088:VAL:HB	1.79	0.64
1:B:1985:THR:OG1	1:B:1986:MET:SD	2.52	0.64
1:B:3114:LYS:HD2	1:B:3125:VAL:HG11	1.79	0.64
1:C:872:GLU:HA	1:C:922:LEU:HD11	1.79	0.64
1:A:2534:ALA:HA	1:A:2588:ARG:HH21	1.62	0.64
1:A:2737:PRO:HD2	1:A:2891:LYS:HD3	1.79	0.64
1:D:622:THR:HG23	1:D:626:LEU:HD12	1.78	0.64
1:C:2522:LEU:HA	1:C:2526:PHE:HB2	1.80	0.63
1:C:3533:ILE:HD12	1:C:3596:VAL:HG23	1.80	0.63
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.30	0.63
1:B:925:SER:O	1:B:928:THR:OG1	2.15	0.63
1:C:2694:GLU:HA	1:C:2697:ARG:HH12	1.63	0.63
1:B:955:LEU:O	1:B:966:LYS:NZ	2.30	0.63
1:B:3723:MET:HE2	1:B:3793:MET:HG2	1.80	0.63
1:C:3256:LEU:HD13	1:C:3266:MET:HE3	1.80	0.63
1:C:4209:GLN:OE1	1:C:4209:GLN:N	2.23	0.63
1:A:1975:SER:O	1:A:1979:LEU:HD12	1.98	0.63
1:A:1987:SER:HB2	1:A:1994:ARG:HH22	1.63	0.63
1:B:4818:MET:N	1:B:4818:MET:SD	2.71	0.63
1:C:4137:ARG:NH2	1:C:4199:GLU:OE2	2.31	0.63
1:B:2765:LYS:NZ	1:B:2859:PRO:O	2.32	0.63
1:D:4689:THR:OG1	1:D:4690:GLU:OE1	2.17	0.63
1:A:4860:ARG:NH2	1:D:4630:TYR:OH	2.31	0.63
1:C:3103:ILE:HD11	1:C:3137:LEU:HD21	1.80	0.63
1:B:46:LEU:HD23	1:B:125:ARG:HH21	1.64	0.63
1:C:2222:GLU:O	1:C:2224:ARG:NH1	2.32	0.63
1:A:2765:LYS:NZ	1:A:2859:PRO:O	2.26	0.63
1:B:2777:TYR:HB3	1:B:2791:LEU:HD23	1.81	0.63
1:D:394:GLN:OE1	1:D:394:GLN:N	2.32	0.63
1:D:2029:GLN:NE2	1:D:2033:ASP:OD1	2.31	0.63
1:D:2633:LEU:HD22	1:D:2695:LEU:HD11	1.81	0.63
1:C:929:LEU:HD23	1:C:929:LEU:H	1.63	0.63
1:A:893:TYR:HB3	1:A:962:SER:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.16	0.62
1:B:275:ARG:HH21	1:B:328:LYS:HZ3	1.46	0.62
1:D:2222:GLU:O	1:D:2224:ARG:NH2	2.32	0.62
1:C:394:GLN:N	1:C:394:GLN:OE1	2.32	0.62
1:C:919:ASN:HA	1:C:922:LEU:HD23	1.81	0.62
1:C:2960:LEU:HD21	1:C:3039:ILE:HB	1.81	0.62
1:A:3414:ARG:NH1	1:A:3414:ARG:HB2	2.15	0.62
1:B:869:ARG:HH11	1:B:870:ILE:HB	1.64	0.62
1:B:2902:HIS:HB3	1:B:2905:LEU:HG	1.81	0.62
1:B:1520:VAL:HG12	1:B:1527:MET:HG2	1.82	0.62
1:A:894:GLY:HA3	1:A:903:LEU:HB3	1.81	0.62
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.82	0.62
1:B:156:GLN:OE1	1:B:156:GLN:N	2.22	0.62
1:B:2244:ARG:HE	1:B:3858:MET:HE3	1.65	0.62
1:D:56:GLN:OE1	1:D:56:GLN:N	2.26	0.62
1:C:925:SER:O	1:C:928:THR:OG1	2.15	0.62
1:B:894:GLY:HA3	1:B:903:LEU:HB3	1.81	0.62
1:B:4039:MET:HE2	1:B:4039:MET:HA	1.81	0.62
1:B:622:THR:HG23	1:B:626:LEU:HD12	1.81	0.62
1:D:4796:MET:HE2	1:D:4796:MET:HA	1.80	0.62
1:C:1792:ALA:O	1:C:2176:ASN:ND2	2.33	0.62
1:A:945:LYS:HD2	1:A:946:ALA:N	2.15	0.62
1:B:2827:ARG:NH2	1:B:2935:TYR:OH	2.33	0.62
1:D:2175:GLU:HG3	1:D:2228:MET:HB3	1.82	0.62
1:D:3250:MET:HE2	1:D:3277:LEU:HD13	1.81	0.62
1:C:891:TRP:HA	1:C:902:ARG:HB3	1.82	0.62
1:A:1981:MET:HA	1:A:1981:MET:HE3	1.80	0.61
1:B:3227:ARG:HG3	1:B:3232:LEU:HD12	1.82	0.61
1:D:891:TRP:HA	1:D:902:ARG:HB3	1.82	0.61
1:C:2902:HIS:HB3	1:C:2905:LEU:HG	1.82	0.61
1:A:2116:LEU:O	1:A:2120:MET:HG2	2.00	0.61
1:A:2309:SER:OG	1:A:2321:ILE:O	2.18	0.61
1:A:3599:VAL:O	1:A:3603:LEU:HD22	2.00	0.61
1:A:4137:ARG:NH2	1:A:4199:GLU:OE2	2.33	0.61
1:B:2023:LEU:HD23	1:B:2024:PRO:HD2	1.80	0.61
1:D:462:GLU:OE2	1:D:462:GLU:N	2.23	0.61
1:C:3592:ILE:O	1:C:3596:VAL:HG12	2.00	0.61
1:C:4087:LEU:HB2	1:C:4122:MET:HE2	1.80	0.61
1:A:394:GLN:OE1	1:A:394:GLN:N	2.34	0.61
1:A:830:ARG:NH2	1:A:832:GLU:OE2	2.33	0.61
1:A:2812:SER:OG	1:A:2882:TYR:OH	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1506:GLN:CD	1:C:1507:GLY:H	2.07	0.61
1:B:4689:THR:OG1	1:B:4690:GLU:OE1	2.17	0.61
1:D:545:ASP:OD1	1:D:582:HIS:NE2	2.29	0.61
1:C:3577:ARG:NH1	1:C:3577:ARG:HA	2.14	0.61
1:B:952:LYS:HD3	1:B:970:LEU:HA	1.81	0.61
1:A:3996:PHE:O	1:A:4000:MET:HG3	2.00	0.61
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.34	0.61
1:D:2230:THR:HB	1:D:2267:MET:HE1	1.81	0.61
1:D:2271:THR:HG21	1:D:2330:ARG:HH22	1.65	0.61
1:C:3017:PHE:O	1:C:3036:LYS:NZ	2.33	0.61
1:A:622:THR:HG23	1:A:626:LEU:HD12	1.81	0.61
1:B:4137:ARG:NH2	1:B:4199:GLU:OE2	2.33	0.61
1:D:2534:ALA:HA	1:D:2588:ARG:HH21	1.66	0.61
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.64	0.61
1:C:3114:LYS:HD2	1:C:3125:VAL:HG11	1.82	0.61
2:E:11:ASP:OD2	2:E:12:GLY:N	2.34	0.61
1:B:4628:VAL:HG21	1:C:4860:ARG:HH22	1.66	0.61
1:C:1108:GLU:OE1	1:C:1108:GLU:N	2.27	0.61
1:A:3454:GLU:HA	1:A:3457:ASN:ND2	2.16	0.61
1:B:3455:GLU:OE2	1:B:3508:SER:OG	2.15	0.60
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.34	0.60
1:C:4039:MET:HA	1:C:4039:MET:HE2	1.81	0.60
1:B:866:HIS:O	1:B:869:ARG:NH1	2.34	0.60
1:D:893:TYR:CE1	1:D:905:PRO:HA	2.36	0.60
1:D:4137:ARG:NH2	1:D:4199:GLU:OE2	2.35	0.60
1:C:4185:GLY:O	1:C:4188:ARG:NH2	2.34	0.60
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.83	0.60
1:A:2821:TRP:HH2	1:A:2877:GLN:HB3	1.67	0.60
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.36	0.60
1:B:56:GLN:O	1:B:309:THR:OG1	2.17	0.60
1:B:462:GLU:HG3	1:B:3710:LEU:HD13	1.84	0.60
1:D:1108:GLU:OE1	1:D:1108:GLU:N	2.25	0.60
1:D:2792:ARG:NH2	1:D:2798:SER:OG	2.34	0.60
1:D:3455:GLU:OE2	1:D:3508:SER:OG	2.19	0.60
1:C:1987:SER:HB2	1:C:1994:ARG:HH22	1.66	0.60
1:A:2624:ARG:NH1	1:A:2910:THR:O	2.34	0.60
1:D:928:THR:O	1:D:931:THR:OG1	2.18	0.60
2:F:11:ASP:OD2	2:F:12:GLY:N	2.34	0.60
1:B:943:ASP:HB2	1:B:1050:GLY:HA3	1.83	0.60
1:D:4853:VAL:O	1:D:4857:ASN:ND2	2.34	0.60
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2777:TYR:HB3	1:A:2791:LEU:HD23	1.82	0.60
1:B:4067:LYS:NZ	1:B:4102:GLN:O	2.35	0.60
1:A:891:TRP:HA	1:A:902:ARG:HB3	1.82	0.60
1:A:2382:GLU:OE1	1:A:2385:ARG:NH1	2.34	0.60
1:A:2792:ARG:NH2	1:A:2798:SER:OG	2.34	0.60
1:A:3531:ASP:O	1:A:3535:LEU:HG	2.02	0.60
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.65	0.60
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.83	0.60
1:D:2902:HIS:HB3	1:D:2905:LEU:HG	1.84	0.60
1:D:919:ASN:HA	1:D:922:LEU:HD23	1.84	0.60
1:C:3239:MET:HE2	1:C:3239:MET:HA	1.84	0.60
1:B:984:LEU:HD21	1:B:1056:PRO:HD2	1.84	0.60
1:B:2186:MET:O	1:B:2192:TYR:OH	2.17	0.60
1:B:2821:TRP:HH2	1:B:2877:GLN:HB3	1.66	0.60
1:D:830:ARG:NH2	1:D:832:GLU:OE2	2.35	0.60
1:D:3176:GLY:O	1:D:3179:LYS:NZ	2.35	0.60
1:D:3527:PRO:HG2	1:D:3573:MET:HE2	1.83	0.60
1:C:4823:LEU:HA	1:C:4826:ILE:HD12	1.84	0.60
1:A:56:GLN:O	1:A:309:THR:OG1	2.17	0.59
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.75	0.59
1:A:3449:HIS:HB2	1:A:3453:ARG:CZ	2.32	0.59
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.66	0.59
1:B:3648:ARG:O	1:B:3652:MET:HG3	2.01	0.59
1:D:1997:GLU:HB2	1:D:2008:MET:HE1	1.84	0.59
1:D:3222:LYS:O	1:D:3227:ARG:NH2	2.31	0.59
1:C:989:ALA:HB3	1:C:1036:ARG:HH21	1.67	0.59
1:C:4158:PRO:O	1:C:4161:ARG:NH2	2.35	0.59
1:A:4901:ILE:HG13	1:A:4913:ARG:NH2	2.16	0.59
1:D:110:ARG:NH2	1:D:117:TYR:OH	2.35	0.59
1:C:3545:THR:HG22	1:C:3548:GLU:HG3	1.83	0.59
1:A:887:ILE:HG12	1:A:907:LEU:HD11	1.83	0.59
1:B:2116:LEU:O	1:B:2120:MET:HG2	2.02	0.59
1:D:638:ILE:HD11	1:D:1636:MET:HE2	1.84	0.59
1:C:2827:ARG:NH2	1:C:2935:TYR:OH	2.35	0.59
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.85	0.59
1:B:1808:ARG:HD3	1:B:1853:ILE:HG22	1.84	0.59
1:C:728:ARG:NH2	1:C:1543:GLU:OE2	2.31	0.59
1:B:3844:LEU:HD11	1:B:3936:TYR:HB2	1.84	0.59
1:D:3716:LEU:HD11	1:D:3793:MET:HE2	1.84	0.59
1:C:3249:LEU:HD23	1:C:3277:LEU:HD21	1.85	0.59
1:A:110:ARG:NH2	1:A:117:TYR:OH	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.19	0.59
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.35	0.59
1:A:4241:THR:HG22	1:A:4245:MET:HE3	1.85	0.59
1:C:127:MET:HE3	1:C:127:MET:H	1.66	0.59
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.84	0.59
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.66	0.59
2:H:52:LYS:HD3	2:H:52:LYS:N	2.18	0.59
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.85	0.59
1:B:4676:GLU:OE2	1:B:4698:LYS:NZ	2.36	0.59
1:D:468:LEU:HD22	1:D:472:ARG:HH12	1.67	0.59
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.38	0.59
1:D:4172:GLU:OE1	1:D:4175:ARG:NH1	2.36	0.59
1:C:880:GLU:O	1:C:884:LEU:N	2.33	0.59
1:B:56:GLN:HE21	1:B:57:ASN:HD22	1.49	0.58
1:D:2644:LEU:HD13	1:D:2678:LEU:HD21	1.85	0.58
1:C:2029:GLN:NE2	1:C:2033:ASP:OD1	2.35	0.58
1:A:955:LEU:O	1:A:966:LYS:NZ	2.27	0.58
1:B:3940:LYS:O	1:B:4002:LYS:NZ	2.32	0.58
1:D:3599:VAL:O	1:D:3603:LEU:HD12	2.03	0.58
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.85	0.58
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.36	0.58
1:B:2907:PRO:O	1:B:2910:THR:OG1	2.21	0.58
1:C:2794:TYR:H	1:C:2855:TYR:HB2	1.68	0.58
1:A:2650:ARG:NH1	1:A:2651:CYS:SG	2.77	0.58
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.39	0.58
1:B:2224:ARG:HE	1:B:2224:ARG:H	1.50	0.58
1:C:2224:ARG:H	1:C:2224:ARG:HD2	1.67	0.58
1:C:3169:LEU:HD13	1:C:3197:LEU:HD22	1.85	0.58
1:A:54:ASN:HA	1:A:56:GLN:HE22	1.68	0.58
1:A:1619:ARG:NH2	1:A:1622:GLU:OE1	2.37	0.58
1:A:2330:ARG:HA	1:A:2333:ASP:OD2	2.03	0.58
1:A:2679:PHE:HB2	1:A:2706:ILE:HG21	1.86	0.58
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.84	0.58
1:D:2607:LEU:HD23	1:D:2639:MET:HE1	1.86	0.58
1:D:3453:ARG:HA	1:D:3456:GLN:HE22	1.68	0.58
1:D:3996:PHE:O	1:D:4000:MET:HG3	2.03	0.58
1:C:4687:TYR:O	1:C:4691:GLN:NE2	2.36	0.58
1:B:227:MET:HE2	1:B:227:MET:N	2.19	0.58
1:C:1819:VAL:HG11	1:C:1865:MET:HG2	1.85	0.58
1:C:2165:LEU:HD11	1:C:2177:LEU:HD23	1.84	0.58
1:A:1808:ARG:HD3	1:A:1853:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:11:ASP:OD2	2:F:67:SER:OG	2.22	0.58
1:B:56:GLN:CD	1:B:56:GLN:H	2.10	0.58
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.84	0.58
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.85	0.58
1:C:1427:ILE:HD13	1:C:1571:ASN:HA	1.86	0.58
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.86	0.58
1:A:4676:GLU:OE2	1:A:4698:LYS:NZ	2.37	0.58
1:D:215:THR:HG22	1:D:273:HIS:HA	1.86	0.58
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.86	0.58
1:C:227:MET:H	1:C:227:MET:HE2	1.69	0.58
1:C:426:ARG:NH2	1:C:509:GLU:OE2	2.36	0.58
1:C:545:ASP:OD1	1:C:582:HIS:NE2	2.29	0.58
1:A:928:THR:O	1:A:931:THR:OG1	2.22	0.58
1:B:2650:ARG:NH1	1:B:2651:CYS:SG	2.77	0.58
1:D:2907:PRO:O	1:D:2910:THR:OG1	2.21	0.58
1:C:69:LEU:HD13	1:C:101:LEU:HD11	1.86	0.58
1:B:1987:SER:HB2	1:B:1994:ARG:HH22	1.67	0.58
1:C:11:VAL:HG11	1:C:164:ARG:HD3	1.84	0.58
1:C:110:ARG:NH2	1:C:117:TYR:OH	2.36	0.58
1:C:2962:GLN:HE22	1:C:2965:ARG:NH1	2.02	0.58
1:B:4901:ILE:HG13	1:B:4913:ARG:NH2	2.18	0.57
1:D:984:LEU:HD21	1:D:1056:PRO:HD2	1.85	0.57
1:C:1066:GLN:HB2	1:C:1071:ARG:HH21	1.69	0.57
1:C:2968:ASP:OD2	1:C:2969:ILE:N	2.37	0.57
1:A:2827:ARG:NH2	1:A:2935:TYR:OH	2.37	0.57
1:A:3169:LEU:HD12	1:A:3194:LEU:HD11	1.85	0.57
1:B:830:ARG:NH2	1:B:832:GLU:OE2	2.35	0.57
1:B:3202:PRO:HB2	1:B:3216:CYS:SG	2.43	0.57
1:C:4818:MET:SD	1:C:4818:MET:N	2.77	0.57
1:B:110:ARG:NH2	1:B:117:TYR:OH	2.37	0.57
1:B:2644:LEU:HD13	1:B:2678:LEU:HD21	1.85	0.57
1:B:3107:VAL:HG21	1:B:3171:SER:HB2	1.87	0.57
1:B:4687:TYR:O	1:B:4691:GLN:NE2	2.37	0.57
1:B:4722:ARG:HH11	1:B:4748:LEU:HD22	1.68	0.57
1:C:2957:PHE:CD2	1:C:3038:MET:HE1	2.39	0.57
1:C:2974:ILE:O	1:C:2978:GLU:N	2.30	0.57
1:B:2792:ARG:NH2	1:B:2798:SER:OG	2.37	0.57
1:B:3103:ILE:HD11	1:B:3137:LEU:HD21	1.86	0.57
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.86	0.57
1:D:2224:ARG:HE	1:D:2224:ARG:H	1.51	0.57
1:A:4630:TYR:OH	1:B:4860:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:11:ASP:OD2	2:G:12:GLY:N	2.37	0.57
1:B:869:ARG:NH1	1:B:870:ILE:HB	2.19	0.57
1:B:2970:SER:HA	1:B:2973:PHE:CD2	2.39	0.57
1:B:3172:ILE:HD12	1:B:3190:LEU:HD22	1.86	0.57
1:B:321:GLU:HG2	1:C:329:ARG:HH22	1.68	0.57
1:B:955:LEU:HD12	1:B:967:PRO:HD2	1.86	0.57
1:B:983:THR:O	1:B:987:ARG:HG3	2.05	0.57
1:A:3723:MET:HE3	1:A:3793:MET:HG2	1.86	0.57
1:B:2170:MET:HG2	1:B:2214:VAL:HG22	1.85	0.57
1:D:11:VAL:HG11	1:D:164:ARG:HD3	1.86	0.57
1:D:835:ARG:NH2	1:D:1093:GLU:OE1	2.30	0.57
1:D:3514:LEU:HD23	1:D:3606:LEU:HD11	1.85	0.57
1:C:1749:PRO:HB2	1:C:1758:ARG:HH11	1.70	0.57
1:C:3577:ARG:HH12	1:C:3582:ARG:HB3	1.68	0.57
1:C:4853:VAL:O	1:C:4857:ASN:ND2	2.36	0.57
1:A:1066:GLN:HB2	1:A:1071:ARG:HE	1.69	0.57
1:C:3268:HIS:CD2	1:C:3272:ILE:HD12	2.40	0.57
1:C:4090:LYS:HG2	1:C:4123:ILE:HD11	1.87	0.57
1:A:1792:ALA:HA	1:A:2173:GLN:HG3	1.87	0.57
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.38	0.57
1:A:3850:GLN:NE2	1:A:3872:GLU:OE1	2.34	0.57
1:A:4152:GLU:OE1	1:A:4194:TYR:OH	2.21	0.57
2:E:49:MET:HG2	2:E:52:LYS:HG2	1.87	0.57
2:G:32:ASP:OD2	2:G:32:ASP:N	2.38	0.57
1:D:3545:THR:HG22	1:D:3548:GLU:HG3	1.87	0.57
1:C:4749:GLU:HB3	1:C:4753:HIS:CE1	2.40	0.57
1:C:4844:LEU:HD21	1:C:4924:VAL:HG13	1.85	0.57
2:H:11:ASP:OD2	2:H:12:GLY:N	2.38	0.56
1:B:977:LEU:HG	1:B:1044:ARG:NH1	2.20	0.56
1:D:3850:GLN:NE2	1:D:3872:GLU:OE1	2.37	0.56
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.38	0.56
1:A:961:MET:HE1	1:A:963:ASN:HB3	1.87	0.56
1:D:1987:SER:HB2	1:D:1994:ARG:HH22	1.69	0.56
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.23	0.56
1:C:295:GLU:OE2	1:C:295:GLU:N	2.36	0.56
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.86	0.56
1:C:3162:GLN:HE21	1:C:3203:VAL:HG11	1.71	0.56
1:A:869:ARG:NH1	1:A:870:ILE:HB	2.20	0.56
1:A:2185:ILE:HD13	1:A:2203:MET:SD	2.45	0.56
1:A:4687:TYR:O	1:A:4691:GLN:NE2	2.39	0.56
1:B:295:GLU:OE2	1:B:295:GLU:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2224:ARG:H	1:D:2224:ARG:NE	2.03	0.56
1:D:4822:THR:O	1:D:4826:ILE:HD12	2.05	0.56
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.23	0.56
1:C:2309:SER:OG	1:C:2321:ILE:O	2.17	0.56
1:C:4063:ASP:OD1	1:C:4064:MET:N	2.39	0.56
1:A:869:ARG:HH11	1:A:870:ILE:HB	1.70	0.56
1:A:3371:LYS:NZ	1:A:3375:GLU:OE2	2.37	0.56
1:B:3017:PHE:O	1:B:3036:LYS:NZ	2.38	0.56
1:D:3017:PHE:O	1:D:3036:LYS:NZ	2.38	0.56
1:C:3758:MET:HE2	1:C:3758:MET:HA	1.88	0.56
1:C:4172:GLU:OE1	1:C:4175:ARG:NH1	2.39	0.56
1:A:56:GLN:CD	1:A:56:GLN:H	2.14	0.56
1:A:2794:TYR:H	1:A:2855:TYR:HB2	1.70	0.56
1:B:215:THR:HG22	1:B:273:HIS:HA	1.87	0.56
1:B:571:SER:OG	1:B:573:GLU:OE1	2.22	0.56
1:D:3324:VAL:HG11	1:D:3361:THR:HG22	1.86	0.56
1:D:4901:ILE:HG13	1:D:4913:ARG:NH2	2.20	0.56
1:C:3539:ARG:HH12	1:C:3542:LEU:HD22	1.71	0.56
1:C:4769:MET:SD	1:C:4769:MET:N	2.64	0.56
1:A:2265:LEU:HA	1:A:2330:ARG:NH1	2.20	0.56
1:A:2519:LEU:HD13	1:A:2575:ARG:HG3	1.86	0.56
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	1.86	0.56
1:A:4155:PRO:O	1:A:4161:ARG:NH2	2.36	0.56
1:B:614:VAL:HG22	1:B:2169:GLN:HG3	1.86	0.56
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.86	0.56
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.39	0.56
1:A:3709:ALA:HB2	1:A:3782:MET:HE2	1.88	0.56
1:B:1062:GLN:NE2	1:B:1064:GLU:OE1	2.31	0.56
1:B:3343:GLN:OE1	1:B:3414:ARG:NH1	2.38	0.56
1:D:866:HIS:CD2	1:D:941:MET:HG2	2.41	0.56
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.17	0.56
1:C:1449:TRP:HB3	1:C:1494:MET:HE3	1.88	0.56
1:C:2166:LEU:HD11	1:C:2206:THR:HG23	1.87	0.56
1:C:4207:MET:HG3	1:C:4208:PRO:HD2	1.88	0.56
1:A:930:LYS:HA	1:A:933:LEU:HD12	1.87	0.56
1:B:1066:GLN:HB2	1:B:1071:ARG:HE	1.70	0.56
1:D:2765:LYS:HZ3	1:D:2857:PRO:HB2	1.71	0.56
1:C:2679:PHE:HB2	1:C:2706:ILE:HG21	1.86	0.56
1:A:545:ASP:OD1	1:A:582:HIS:NE2	2.30	0.56
1:C:866:HIS:CD2	1:C:941:MET:HG2	2.41	0.56
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3455:GLU:OE2	1:C:3508:SER:OG	2.23	0.56
1:A:19:GLU:HB3	1:A:205:ILE:HB	1.86	0.56
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.86	0.56
1:C:3644:LEU:HD12	1:C:3645:PRO:HD2	1.88	0.56
1:C:4188:ARG:HH11	1:C:4188:ARG:HG2	1.71	0.56
1:A:2881:ASN:HA	1:A:2884:ASN:ND2	2.21	0.55
1:B:26:ALA:HB2	1:B:182:LEU:HD21	1.87	0.55
1:B:3284:TRP:HB3	1:B:3305:THR:HG21	1.88	0.55
1:D:2102:VAL:HG13	1:D:2120:MET:HB2	1.88	0.55
1:D:3550:ARG:HD3	1:D:3594:ARG:NH2	2.19	0.55
1:C:2633:LEU:HG	1:C:2695:LEU:HD21	1.87	0.55
1:C:3755:GLU:HA	1:C:3758:MET:HB2	1.87	0.55
1:A:2907:PRO:O	1:A:2910:THR:OG1	2.23	0.55
1:D:127:MET:N	1:D:127:MET:SD	2.80	0.55
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.39	0.55
1:D:858:THR:HB	1:D:930:LYS:HD2	1.89	0.55
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.25	0.55
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.89	0.55
1:C:2687:ALA:O	1:C:2993:GLN:NE2	2.38	0.55
1:A:2902:HIS:HB3	1:A:2905:LEU:HG	1.88	0.55
1:A:3523:ASN:OD1	1:A:3582:ARG:NH2	2.38	0.55
1:B:1751:GLY:HA3	1:B:1759:ARG:HH12	1.71	0.55
1:C:56:GLN:O	1:C:309:THR:OG1	2.23	0.55
1:C:1749:PRO:HB2	1:C:1758:ARG:NH1	2.21	0.55
1:C:3246:LEU:HD11	1:C:3281:LEU:HD21	1.88	0.55
1:C:4067:LYS:NZ	1:C:4102:GLN:O	2.37	0.55
1:A:638:ILE:HD11	1:A:1636:MET:HE2	1.88	0.55
1:B:2382:GLU:OE1	1:B:2385:ARG:NH1	2.37	0.55
1:B:3535:LEU:HD13	1:B:3552:PHE:CE1	2.38	0.55
1:D:14:LEU:HD13	1:D:202:MET:HE2	1.89	0.55
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.40	0.55
1:C:3269:VAL:HA	1:C:3273:THR:HB	1.89	0.55
2:G:82:TYR:HA	1:C:1786:LEU:HD21	1.87	0.55
1:B:1251:GLU:OE2	1:B:1251:GLU:N	2.36	0.55
1:D:168:ASP:OD1	1:D:201:ASN:ND2	2.40	0.55
1:D:952:LYS:HD3	1:D:970:LEU:HA	1.89	0.55
1:C:4006:ASP:N	1:C:4006:ASP:OD1	2.38	0.55
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.24	0.55
1:B:3081:MET:HE3	1:B:3092:LEU:HD23	1.88	0.55
1:B:3162:GLN:O	1:B:3166:TYR:HB2	2.07	0.55
1:B:3365:LEU:HD23	1:B:3405:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2590:SER:O	1:C:2600:ARG:NH1	2.40	0.55
1:B:545:ASP:OD1	1:B:582:HIS:NE2	2.30	0.55
1:B:3842:LEU:HB2	1:B:3929:SER:HB2	1.89	0.55
1:C:3166:TYR:O	1:C:3170:CYS:HB2	2.06	0.55
1:C:4555:LEU:HD21	1:C:4656:LEU:HD22	1.89	0.55
1:C:4966:ASP:OD2	1:C:4966:ASP:N	2.40	0.55
1:A:3535:LEU:O	1:A:3539:ARG:HG2	2.07	0.55
1:A:4006:ASP:N	1:A:4006:ASP:OD1	2.40	0.55
1:B:2166:LEU:HD11	1:B:2206:THR:HG23	1.89	0.55
1:D:866:HIS:HB2	1:D:941:MET:HE3	1.88	0.55
1:C:894:GLY:HA3	1:C:903:LEU:HB3	1.88	0.55
1:C:2777:TYR:HB3	1:C:2791:LEU:HD23	1.88	0.55
1:C:4241:THR:HG22	1:C:4245:MET:HE3	1.89	0.55
1:A:233:ILE:O	1:A:257:ARG:NH1	2.40	0.54
1:A:1251:GLU:OE1	1:A:1251:GLU:N	2.36	0.54
1:B:2382:GLU:O	1:B:2386:ILE:HG23	2.06	0.54
1:B:2881:ASN:HA	1:B:2884:ASN:ND2	2.22	0.54
1:B:3587:ASP:HA	1:B:3592:ILE:HD11	1.89	0.54
1:B:4006:ASP:OD1	1:B:4006:ASP:N	2.38	0.54
1:D:4820:VAL:HG13	1:D:4823:LEU:HB2	1.89	0.54
1:C:1057:ASP:OD1	1:C:1057:ASP:N	2.37	0.54
1:B:150:MET:HG2	1:B:169:LEU:HD23	1.89	0.54
1:B:2973:PHE:CE1	1:B:2995:ILE:HG12	2.41	0.54
1:D:233:ILE:O	1:D:257:ARG:NH1	2.40	0.54
1:D:2970:SER:HA	1:D:2973:PHE:CE1	2.41	0.54
1:D:4687:TYR:O	1:D:4691:GLN:NE2	2.40	0.54
1:C:3553:LEU:HD13	1:C:3596:VAL:HG13	1.90	0.54
1:C:3844:LEU:HD11	1:C:3936:TYR:HB2	1.89	0.54
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.26	0.54
1:C:1451:GLY:HA3	1:C:1494:MET:HG2	1.89	0.54
1:A:1062:GLN:NE2	1:A:1064:GLU:OE1	2.33	0.54
2:E:13:ARG:HB3	2:E:13:ARG:NH1	2.23	0.54
1:B:1929:MET:HE2	1:B:1931:LEU:HD11	1.90	0.54
1:B:2794:TYR:H	1:B:2855:TYR:HB2	1.72	0.54
1:B:4759:ASP:O	1:B:4761:PRO:HD3	2.07	0.54
1:D:961:MET:SD	1:D:962:SER:N	2.80	0.54
1:D:2198:MET:HG3	1:D:2203:MET:SD	2.46	0.54
1:A:3377:GLU:HA	1:A:3380:ARG:HG2	1.90	0.54
1:B:1024:TYR:HB3	1:B:1025:ARG:NH1	2.21	0.54
1:D:1057:ASP:OD1	1:D:1057:ASP:N	2.36	0.54
1:D:1759:ARG:NH1	1:D:1759:ARG:HA	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ASP:HB2	1:C:297:GLN:OE1	2.07	0.54
1:A:2411:PRO:HD2	1:A:2415:ARG:HG3	1.88	0.54
1:A:4067:LYS:NZ	1:A:4102:GLN:O	2.38	0.54
1:B:457:GLU:OE2	1:B:457:GLU:N	2.29	0.54
1:B:1690:ASP:OD2	1:B:1693:GLN:NE2	2.40	0.54
1:B:3850:GLN:NE2	1:B:3872:GLU:OE1	2.38	0.54
1:D:426:ARG:NH2	1:D:509:GLU:OE2	2.41	0.54
1:D:4942:GLU:OE1	1:C:4944:ARG:NH1	2.41	0.54
1:C:2116:LEU:O	1:C:2120:MET:HG2	2.07	0.54
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.40	0.54
1:A:3940:LYS:O	1:A:4002:LYS:NZ	2.34	0.54
1:A:4063:ASP:OD1	1:A:4064:MET:N	2.41	0.54
1:D:910:PHE:HA	1:D:913:LEU:HD23	1.88	0.54
1:C:3276:MET:O	1:C:3280:TYR:N	2.36	0.54
1:D:19:GLU:HB3	1:D:205:ILE:HB	1.89	0.54
1:D:1619:ARG:NH2	1:D:1622:GLU:OE1	2.40	0.54
1:C:3599:VAL:O	1:C:3603:LEU:HD12	2.08	0.54
1:A:4759:ASP:O	1:A:4761:PRO:HD3	2.08	0.54
1:B:3377:GLU:HA	1:B:3380:ARG:HG2	1.88	0.54
1:B:4241:THR:HG22	1:B:4245:MET:HE3	1.90	0.54
1:D:4240:ASP:OD2	1:D:4672:LYS:NZ	2.38	0.54
1:C:384:MET:H	1:C:384:MET:CE	2.20	0.54
1:C:1985:THR:OG1	1:C:1986:MET:SD	2.65	0.54
1:A:3570:ARG:NH1	1:A:3570:ARG:HB2	2.23	0.54
2:G:58:GLY:HA3	2:G:76:ILE:HD13	1.89	0.54
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.41	0.54
1:A:3132:THR:HG23	1:A:3136:LEU:HD23	1.90	0.53
1:B:233:ILE:O	1:B:257:ARG:NH1	2.41	0.53
1:B:728:ARG:NH2	1:B:1543:GLU:OE2	2.31	0.53
1:D:1062:GLN:NE2	1:D:1064:GLU:OE1	2.32	0.53
1:D:1559:GLN:H	1:D:1559:GLN:CD	2.15	0.53
1:C:897:ARG:NH2	1:C:899:ASP:OD1	2.41	0.53
1:A:3842:LEU:HB2	1:A:3929:SER:HB2	1.90	0.53
2:E:58:GLY:HA3	2:E:76:ILE:HD12	1.90	0.53
1:B:2583:LEU:HD11	1:B:2614:ILE:HD13	1.89	0.53
1:B:2626:LEU:O	1:B:2630:VAL:HG12	2.08	0.53
1:C:2892:GLN:NE2	1:C:2895:GLU:OE2	2.41	0.53
1:A:1690:ASP:OD2	1:A:1693:GLN:NE2	2.41	0.53
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.42	0.53
1:A:3758:MET:HE3	1:A:4719:PHE:CE1	2.43	0.53
1:B:1462:MET:HE2	1:B:1462:MET:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3543:LYS:N	1:B:3543:LYS:HD2	2.24	0.53
1:B:4063:ASP:OD1	1:B:4064:MET:N	2.41	0.53
1:D:297:GLN:N	1:D:297:GLN:OE1	2.38	0.53
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.91	0.53
1:C:3556:ASN:HB3	1:C:3559:LEU:HD13	1.89	0.53
1:A:2002:PRO:HD3	1:A:3638:MET:HE1	1.90	0.53
1:B:4910:GLU:O	1:B:4914:VAL:HG13	2.08	0.53
1:D:4241:THR:HG22	1:D:4245:MET:HE3	1.90	0.53
1:C:215:THR:HG22	1:C:273:HIS:HA	1.91	0.53
1:C:1260:MET:HE3	1:C:1271:ARG:HE	1.72	0.53
1:A:1177:THR:OG1	1:A:1180:ARG:NH1	2.37	0.53
1:A:4910:GLU:O	1:A:4914:VAL:HG13	2.09	0.53
1:B:3123:LYS:HG3	1:B:3125:VAL:H	1.73	0.53
1:D:1462:MET:HE2	1:D:1462:MET:HA	1.90	0.53
1:D:2116:LEU:O	1:D:2120:MET:HG2	2.09	0.53
1:C:2607:LEU:HG	1:C:2643:LEU:HD21	1.91	0.53
1:C:3316:LEU:HD21	1:C:3346:VAL:HG23	1.91	0.53
2:G:11:ASP:OD2	2:G:67:SER:OG	2.26	0.53
1:B:2411:PRO:HD2	1:B:2415:ARG:HG3	1.90	0.53
1:D:2758:PHE:HA	1:D:2761:TYR:HB2	1.90	0.53
1:D:3250:MET:HE1	1:D:3315:LEU:HB2	1.90	0.53
1:C:1251:GLU:OE1	1:C:1251:GLU:N	2.40	0.53
1:C:2862:LEU:HD13	1:C:2864:GLY:H	1.72	0.53
1:C:3359:ILE:HD12	1:C:3434:LEU:HD13	1.90	0.53
1:A:215:THR:HG22	1:A:273:HIS:HA	1.91	0.53
1:A:987:ARG:HB3	1:A:987:ARG:NH1	2.24	0.53
1:A:3539:ARG:HB2	1:A:3549:VAL:HG12	1.91	0.53
1:A:4569:LEU:HD21	1:A:4649:LEU:HD23	1.90	0.53
1:D:2794:TYR:H	1:D:2855:TYR:HB2	1.74	0.53
1:D:3132:THR:HG23	1:D:3136:LEU:HD23	1.90	0.53
1:C:2792:ARG:NH2	1:C:2798:SER:OG	2.41	0.53
1:C:2951:ILE:HD11	1:C:3032:SER:HB2	1.90	0.53
1:C:3540:TYR:HB3	1:C:3604:TYR:CD1	2.44	0.53
1:A:168:ASP:OD1	1:A:201:ASN:ND2	2.41	0.53
1:A:457:GLU:OE1	1:A:457:GLU:N	2.42	0.53
1:B:684:VAL:HG22	1:B:781:VAL:HG12	1.91	0.53
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.41	0.53
1:D:3530:GLN:OE1	1:D:3530:GLN:N	2.30	0.53
1:C:887:ILE:HD13	1:C:907:LEU:HD21	1.89	0.53
1:C:1819:VAL:HA	1:C:1929:MET:HE1	1.91	0.53
1:C:3366:ARG:NH1	1:C:3440:GLU:OE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:LYS:HD3	1:A:970:LEU:HA	1.90	0.53
1:A:1506:GLN:OE1	1:A:1507:GLY:N	2.42	0.53
1:A:3449:HIS:O	1:A:3453:ARG:HD2	2.08	0.53
1:B:19:GLU:HB3	1:B:205:ILE:HB	1.89	0.53
1:B:2423:MET:HG3	1:B:2498:HIS:NE2	2.24	0.53
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.91	0.53
1:B:2736:ASP:O	1:B:2738:ARG:NH1	2.42	0.53
1:D:1066:GLN:HB2	1:D:1071:ARG:HE	1.72	0.53
1:D:4749:GLU:HB3	1:D:4753:HIS:CE1	2.44	0.53
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.91	0.53
1:C:3194:LEU:HD21	1:C:3272:ILE:HG23	1.91	0.53
1:C:4901:ILE:HG13	1:C:4913:ARG:NH2	2.23	0.53
1:B:647:ASN:ND2	1:B:820:ARG:O	2.31	0.53
1:B:3371:LYS:NZ	1:B:3375:GLU:OE2	2.39	0.53
1:D:3133:THR:HG23	1:D:3134:VAL:HG23	1.91	0.53
1:A:176:SER:OG	1:A:178:ARG:NH1	2.41	0.52
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.92	0.52
1:A:4722:ARG:HH11	1:A:4748:LEU:HD22	1.73	0.52
1:B:3366:ARG:NH1	1:B:3440:GLU:OE1	2.35	0.52
1:C:2790:MET:N	1:C:2790:MET:SD	2.82	0.52
1:C:3850:GLN:NE2	1:C:3872:GLU:OE1	2.40	0.52
1:C:3937:TYR:OH	1:C:3944:GLU:OE2	2.27	0.52
1:B:1559:GLN:CD	1:B:1559:GLN:H	2.17	0.52
1:D:932:LEU:H	1:D:932:LEU:HD12	1.75	0.52
1:C:2867:LEU:HB2	1:C:2928:LYS:HZ3	1.74	0.52
1:C:3359:ILE:HG23	1:C:3437:MET:HE1	1.91	0.52
1:C:3729:MET:HE1	1:C:3778:MET:HE1	1.92	0.52
1:A:227:MET:H	1:A:227:MET:HE2	1.75	0.52
1:A:1861:GLN:O	1:A:1865:MET:HE3	2.09	0.52
1:B:638:ILE:HD11	1:B:1636:MET:HE2	1.90	0.52
1:B:3296:LEU:HD12	1:B:3296:LEU:H	1.74	0.52
1:D:1419:ASP:HA	1:D:1421:ARG:NH2	2.24	0.52
1:D:4006:ASP:N	1:D:4006:ASP:OD1	2.41	0.52
1:D:4759:ASP:O	1:D:4761:PRO:HD3	2.09	0.52
1:C:1062:GLN:NE2	1:C:1064:GLU:OE1	2.33	0.52
1:C:3368:ARG:HH11	1:C:3368:ARG:HG3	1.75	0.52
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.27	0.52
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.42	0.52
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.42	0.52
1:D:2736:ASP:OD1	1:D:2736:ASP:N	2.41	0.52
1:D:2747:ILE:HD12	1:D:2748:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2821:TRP:HH2	1:D:2877:GLN:HB3	1.75	0.52
1:C:2538:THR:O	1:C:2542:SER:HB2	2.10	0.52
1:A:684:VAL:HG22	1:A:781:VAL:HG12	1.92	0.52
1:A:2697:ARG:HB3	1:A:2697:ARG:NH1	2.24	0.52
1:A:3233:PRO:HB2	1:A:3238:GLU:HB2	1.91	0.52
1:B:228:ASP:OD1	1:B:228:ASP:N	2.42	0.52
1:B:2224:ARG:H	1:B:2224:ARG:NE	2.06	0.52
1:B:2490:MET:HE1	1:B:2546:MET:HE2	1.91	0.52
1:B:2747:ILE:HD12	1:B:2748:PRO:HD2	1.91	0.52
1:D:684:VAL:HG22	1:D:781:VAL:HG12	1.91	0.52
1:D:2244:ARG:NH2	1:D:3858:MET:SD	2.83	0.52
1:C:19:GLU:HB3	1:C:205:ILE:HB	1.90	0.52
1:C:2986:VAL:HG22	1:C:2988:LYS:H	1.74	0.52
1:A:983:THR:O	1:A:987:ARG:HG3	2.09	0.52
1:A:3455:GLU:OE2	1:A:3508:SER:OG	2.22	0.52
1:A:4966:ASP:OD2	1:A:4966:ASP:N	2.40	0.52
1:B:1861:GLN:O	1:B:1865:MET:HE3	2.10	0.52
1:D:3233:PRO:C	1:D:3234:ASN:HD22	2.15	0.52
1:C:901:LYS:HG3	1:C:903:LEU:HG	1.90	0.52
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.41	0.52
1:C:2293:GLN:OE1	1:C:2293:GLN:N	2.19	0.52
1:C:2514:ASN:ND2	1:C:2516:ASP:OD1	2.42	0.52
1:C:3133:THR:HG23	1:C:3134:VAL:HG23	1.90	0.52
1:B:2490:MET:HE3	1:B:2545:GLU:HB2	1.92	0.52
1:B:2694:GLU:HA	1:B:2697:ARG:NH1	2.24	0.52
1:B:3414:ARG:NH1	1:B:3414:ARG:HB2	2.24	0.52
1:D:3946:GLN:OE1	1:D:3949:ARG:NH2	2.43	0.52
1:C:3196:ARG:HH12	1:C:3341:PHE:HE1	1.57	0.52
1:B:2219:GLU:OE2	1:B:2219:GLU:N	2.38	0.52
1:B:3130:THR:HA	1:B:3133:THR:HG22	1.90	0.52
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.92	0.52
1:D:2308:GLN:OE1	1:D:2309:SER:N	2.42	0.52
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.28	0.52
1:D:4185:GLY:O	1:D:4188:ARG:NH2	2.42	0.52
1:C:233:ILE:O	1:C:257:ARG:NH1	2.43	0.52
1:A:3667:HIS:ND1	1:A:3667:HIS:O	2.38	0.52
1:B:928:THR:O	1:B:931:THR:OG1	2.28	0.52
1:B:3181:THR:O	1:B:3185:LYS:HG2	2.10	0.52
1:D:2736:ASP:O	1:D:2738:ARG:NH1	2.43	0.52
1:D:4966:ASP:N	1:D:4966:ASP:OD1	2.37	0.52
1:C:884:LEU:O	1:C:887:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3114:LYS:HE3	1:A:3123:LYS:HD2	1.92	0.52
2:F:90:ILE:HD11	1:B:1684:ALA:HA	1.91	0.52
1:B:293:LEU:HD13	1:B:378:LEU:HD12	1.91	0.52
1:B:1424:PRO:HA	1:B:1427:ILE:HG22	1.92	0.52
1:B:3226:GLU:C	1:B:3228:ALA:H	2.18	0.52
1:B:3528:THR:HG23	1:B:3573:MET:HE3	1.92	0.52
1:C:2991:HIS:HB3	1:C:2994:GLU:HB2	1.92	0.52
1:C:3110:LEU:C	1:C:3112:LEU:H	2.18	0.52
2:E:11:ASP:OD2	2:E:67:SER:OG	2.27	0.51
1:B:384:MET:H	1:B:384:MET:CE	2.22	0.51
1:D:2827:ARG:NH2	1:D:2935:TYR:OH	2.43	0.51
1:D:4555:LEU:HD21	1:D:4656:LEU:HD22	1.92	0.51
1:D:4722:ARG:HG2	1:D:4722:ARG:HH11	1.73	0.51
1:C:516:LYS:O	1:C:520:ASN:ND2	2.34	0.51
1:C:2382:GLU:O	1:C:2386:ILE:HG23	2.10	0.51
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.42	0.51
1:A:2538:THR:HG23	1:A:2541:PHE:H	1.75	0.51
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.42	0.51
1:A:3157:ILE:HA	1:A:3161:VAL:HG23	1.92	0.51
1:A:3359:ILE:HG23	1:A:3437:MET:HE1	1.93	0.51
1:B:2629:ASP:O	1:B:2632:ILE:HG22	2.09	0.51
1:D:22:LEU:HD23	1:D:202:MET:HG2	1.91	0.51
1:D:2519:LEU:HD13	1:D:2575:ARG:HG3	1.91	0.51
1:D:2777:TYR:HB3	1:D:2791:LEU:HD23	1.92	0.51
1:D:5000:GLU:OE1	1:D:5000:GLU:N	2.42	0.51
1:C:3034:LYS:O	1:C:3034:LYS:NZ	2.39	0.51
1:C:3051:ARG:HG2	1:C:3051:ARG:HH11	1.75	0.51
1:C:3329:ILE:O	1:C:3403:ARG:NH2	2.42	0.51
1:A:227:MET:HE2	1:A:227:MET:N	2.25	0.51
1:A:3235:SER:OG	1:A:3237:GLU:OE1	2.28	0.51
1:A:4821:LYS:H	1:A:4821:LYS:CD	2.23	0.51
1:B:2285:GLU:HG3	1:B:3858:MET:HG3	1.91	0.51
1:B:2751:LEU:O	1:B:2755:ILE:HG12	2.09	0.51
1:D:116:MET:HG2	1:D:139:GLU:HA	1.91	0.51
1:D:2355:ARG:HH11	1:D:2355:ARG:HG3	1.75	0.51
1:C:986:ASP:HA	1:C:1036:ARG:NH2	2.26	0.51
1:C:1983:ALA:O	1:C:1987:SER:OG	2.28	0.51
1:C:2678:LEU:O	1:C:2682:ILE:HG22	2.09	0.51
1:C:3171:SER:O	1:C:3174:SER:OG	2.28	0.51
1:C:4745:LEU:HD12	1:C:4745:LEU:H	1.76	0.51
1:A:1684:ALA:HA	2:E:90:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:961:MET:SD	1:D:963:ASN:N	2.76	0.51
1:D:3400:VAL:HG23	1:D:3403:ARG:NH2	2.25	0.51
1:C:1759:ARG:NH1	1:C:1759:ARG:HB2	2.25	0.51
1:C:2231:SER:HA	1:C:2234:ARG:NH2	2.25	0.51
1:C:2821:TRP:HH2	1:C:2877:GLN:HB3	1.75	0.51
1:C:3335:MET:HE3	1:C:3403:ARG:HH12	1.75	0.51
1:C:3514:LEU:O	1:C:3518:LEU:N	2.43	0.51
1:A:3757:GLU:O	1:A:3761:GLN:HG2	2.11	0.51
2:H:4:VAL:HG22	2:H:74:LEU:HD22	1.92	0.51
1:B:1759:ARG:H	1:B:1759:ARG:CD	2.23	0.51
1:B:2754:PHE:HE2	1:B:2813:LEU:HD11	1.76	0.51
1:D:176:SER:OG	1:D:178:ARG:NH1	2.39	0.51
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.92	0.51
1:D:3573:MET:HB3	1:D:3577:ARG:NH2	2.18	0.51
1:C:684:VAL:HG22	1:C:781:VAL:HG12	1.91	0.51
1:C:954:LYS:HB3	1:C:966:LYS:HE3	1.93	0.51
1:C:993:HIS:NE2	1:C:1022:VAL:O	2.41	0.51
1:C:3517:MET:O	1:C:3517:MET:HG3	2.11	0.51
1:C:3862:ASP:N	1:C:3862:ASP:OD1	2.42	0.51
1:C:4152:GLU:OE1	1:C:4194:TYR:OH	2.26	0.51
1:D:4138:ASP:O	1:D:4142:ASN:ND2	2.36	0.51
1:D:4209:GLN:OE1	1:D:4209:GLN:N	2.30	0.51
1:D:4745:LEU:H	1:D:4745:LEU:HD12	1.75	0.51
1:D:4818:MET:N	1:D:4818:MET:SD	2.83	0.51
1:C:293:LEU:HD13	1:C:378:LEU:HD12	1.92	0.51
1:C:943:ASP:HB2	1:C:1050:GLY:HA3	1.93	0.51
1:A:228:ASP:OD1	1:A:228:ASP:N	2.44	0.51
1:A:2751:LEU:O	1:A:2755:ILE:HG12	2.11	0.51
1:A:4902:GLU:O	1:A:4913:ARG:NH1	2.40	0.51
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.43	0.51
1:B:3588:ASP:O	1:B:3592:ILE:HG12	2.11	0.51
1:C:3021:PRO:HD3	1:C:3030:HIS:NE2	2.25	0.51
1:C:4567:LEU:HD11	1:C:4816:ILE:HG23	1.93	0.51
1:B:426:ARG:NH2	1:B:509:GLU:OE2	2.44	0.51
1:B:961:MET:SD	1:B:962:SER:N	2.84	0.51
1:B:4821:LYS:H	1:B:4821:LYS:CD	2.23	0.51
1:D:3459:VAL:HG13	1:D:3464:ILE:HB	1.92	0.51
1:D:4918:ILE:HD12	1:D:4919:THR:N	2.26	0.51
1:C:2244:ARG:NH2	1:C:3859:VAL:O	2.44	0.51
1:C:3159:ASP:HB2	1:C:3222:LYS:HE2	1.93	0.51
1:A:571:SER:OG	1:A:573:GLU:OE1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2627:VAL:HG21	1:A:2674:LEU:HD12	1.91	0.51
2:F:4:VAL:HG22	2:F:74:LEU:HD22	1.93	0.51
1:D:228:ASP:OD1	1:D:228:ASP:N	2.44	0.51
1:D:3226:GLU:C	1:D:3228:ALA:H	2.18	0.51
1:C:4759:ASP:O	1:C:4761:PRO:HD3	2.11	0.51
1:B:3169:LEU:HD21	1:B:3205:PHE:CD1	2.46	0.51
1:B:4695:ASP:OD1	1:B:4695:ASP:N	2.37	0.51
1:D:3114:LYS:HE3	1:D:3123:LYS:HD2	1.93	0.51
1:D:4904:PRO:HG3	1:D:4913:ARG:HG2	1.92	0.51
1:C:1289:LEU:HD12	1:C:1562:ILE:HD11	1.92	0.51
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.43	0.51
1:A:1057:ASP:OD1	1:A:1057:ASP:N	2.35	0.50
1:A:5034:ASP:OD2	1:A:5035:GLN:NE2	2.44	0.50
1:B:2002:PRO:HD3	1:B:3638:MET:HE1	1.93	0.50
1:B:2376:LEU:HG	1:B:2469:ILE:HD11	1.93	0.50
1:B:3667:HIS:O	1:B:3667:HIS:ND1	2.40	0.50
1:D:2514:ASN:ND2	1:D:2516:ASP:OD1	2.44	0.50
1:C:2668:SER:C	1:C:2670:GLU:H	2.18	0.50
1:C:3686:GLU:OE1	1:C:3686:GLU:N	2.44	0.50
1:A:910:PHE:HA	1:A:913:LEU:HD23	1.93	0.50
1:A:1559:GLN:H	1:A:1559:GLN:CD	2.19	0.50
1:A:3400:VAL:HG23	1:A:3403:ARG:HH21	1.76	0.50
2:G:31:GLU:OE2	2:G:96:THR:HB	2.10	0.50
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.92	0.50
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.43	0.50
1:B:3535:LEU:O	1:B:3539:ARG:HG2	2.10	0.50
1:B:3943:ILE:HD11	1:B:3999:MET:HE1	1.93	0.50
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.21	0.50
1:D:901:LYS:HG3	1:D:903:LEU:HG	1.93	0.50
1:D:960:MET:HE2	1:D:964:GLY:HA2	1.94	0.50
1:D:1251:GLU:OE1	1:D:1251:GLU:N	2.37	0.50
1:D:1737:PRO:HB2	1:D:1739:THR:HG23	1.92	0.50
1:D:3172:ILE:HG21	1:D:3194:LEU:HB2	1.93	0.50
1:D:4063:ASP:OD1	1:D:4064:MET:N	2.45	0.50
1:C:565:TYR:CZ	1:C:569:ILE:HD11	2.47	0.50
1:C:943:ASP:OD2	1:C:945:LYS:NZ	2.45	0.50
1:C:2661:TRP:HB3	1:C:2664:PHE:HB2	1.93	0.50
1:C:3946:GLN:HE22	1:C:3949:ARG:HH12	1.58	0.50
1:A:954:LYS:HB3	1:A:966:LYS:HE3	1.92	0.50
1:A:2661:TRP:HB3	1:A:2664:PHE:HB2	1.93	0.50
2:H:11:ASP:OD2	2:H:67:SER:OG	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:MET:N	1:B:127:MET:SD	2.74	0.50
1:D:3376:GLU:OE1	1:D:3448:SER:OG	2.27	0.50
1:D:4914:VAL:O	1:D:4918:ILE:HG13	2.10	0.50
1:C:3709:ALA:HB2	1:C:3782:MET:HE2	1.93	0.50
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.45	0.50
1:A:2872:GLN:O	1:A:2876:GLU:HG2	2.12	0.50
1:B:1997:GLU:HB2	1:B:2008:MET:HE1	1.94	0.50
1:B:3604:TYR:O	1:B:3607:GLU:HG3	2.12	0.50
1:B:3751:VAL:HG13	1:B:3755:GLU:HG2	1.93	0.50
1:D:906:CYS:SG	1:D:913:LEU:HD22	2.51	0.50
1:C:302:VAL:HB	1:C:306:LYS:HE3	1.92	0.50
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.46	0.50
1:C:4138:ASP:O	1:C:4142:ASN:ND2	2.35	0.50
1:A:2225:PHE:N	1:A:2226:PRO:HD3	2.26	0.50
1:A:2226:PRO:HB3	1:A:2267:MET:SD	2.51	0.50
2:E:4:VAL:HG22	2:E:74:LEU:HD22	1.93	0.50
1:B:653:ALA:HB3	1:B:656:SER:HB2	1.94	0.50
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.41	0.50
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.84	0.50
1:D:2538:THR:HG23	1:D:2541:PHE:H	1.77	0.50
1:D:3132:THR:HA	1:D:3136:LEU:HB3	1.93	0.50
1:C:2218:GLY:HA3	1:C:2224:ARG:HH12	1.76	0.50
1:B:2858:GLN:HB2	1:B:2859:PRO:HD3	1.93	0.50
1:B:3021:PRO:HD3	1:B:3030:HIS:CE1	2.46	0.50
1:B:3543:LYS:NZ	1:B:3604:TYR:OH	2.44	0.50
1:D:3799:LYS:NZ	1:D:3879:GLU:OE1	2.45	0.50
1:C:1737:PRO:HB2	1:C:1739:THR:HG23	1.92	0.50
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.45	0.50
1:C:3093:ARG:NH1	1:C:3160:ASP:OD2	2.43	0.50
1:A:1997:GLU:HB2	1:A:2008:MET:HE1	1.94	0.50
1:A:2871:LEU:HD11	1:A:2937:VAL:HG13	1.93	0.50
1:B:2102:VAL:HG13	1:B:2120:MET:HB2	1.93	0.50
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.29	0.50
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.38	0.50
1:A:302:VAL:HB	1:A:306:LYS:HE3	1.94	0.50
2:G:85:THR:OG1	2:G:86:GLY:N	2.45	0.50
1:B:1289:LEU:HD12	1:B:1562:ILE:HD11	1.93	0.50
1:B:2630:VAL:HG23	1:B:2637:ALA:HB1	1.92	0.50
1:B:2929:PHE:HA	1:B:2932:MET:SD	2.52	0.50
1:B:4902:GLU:O	1:B:4913:ARG:NH1	2.40	0.50
1:D:4821:LYS:HD3	1:D:4821:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:977:LEU:HD22	1:C:981:GLN:HB3	1.94	0.50
1:C:1993:ARG:O	1:C:1996:ARG:HD2	2.12	0.50
1:C:2531:ARG:HG2	1:C:2585:THR:HG21	1.94	0.50
1:A:3604:TYR:O	1:A:3607:GLU:HG3	2.12	0.50
1:A:3695:PRO:HB3	1:A:3699:HIS:HB3	1.94	0.50
1:D:1601:MET:HA	1:D:1601:MET:HE3	1.94	0.50
1:D:3540:TYR:HB3	1:D:3604:TYR:CD2	2.47	0.50
1:D:4924:VAL:HG12	1:D:4925:ILE:HD13	1.94	0.50
1:C:908:VAL:HG22	1:C:961:MET:HE1	1.93	0.50
1:C:950:LEU:HD13	1:C:970:LEU:HG	1.94	0.50
1:C:1559:GLN:H	1:C:1559:GLN:CD	2.18	0.50
1:C:1739:THR:HG22	1:C:2146:PRO:HB3	1.92	0.50
1:C:2323:TRP:CZ2	1:C:2422:ILE:HD12	2.47	0.50
1:C:2587:TYR:O	1:C:2590:SER:OG	2.30	0.50
1:C:3145:GLN:HG2	1:C:3196:ARG:HD2	1.94	0.50
2:G:4:VAL:HG22	2:G:74:LEU:HD22	1.92	0.49
1:B:56:GLN:HE21	1:B:57:ASN:ND2	2.09	0.49
1:D:923:GLN:O	1:D:927:GLU:HG2	2.12	0.49
1:D:3946:GLN:HE22	1:D:3949:ARG:HE	1.60	0.49
1:D:4769:MET:SD	1:D:4769:MET:N	2.68	0.49
1:C:2102:VAL:HG13	1:C:2120:MET:HB2	1.94	0.49
1:C:4904:PRO:HG3	1:C:4913:ARG:HG2	1.94	0.49
1:A:11:VAL:HG11	1:A:164:ARG:HD3	1.94	0.49
1:A:1024:TYR:CZ	1:A:1032:LYS:HG3	2.46	0.49
1:A:2660:GLY:HA3	1:A:2666:VAL:HG22	1.94	0.49
1:B:1986:MET:SD	1:B:1986:MET:N	2.85	0.49
1:A:69:LEU:HD13	1:A:101:LEU:HD11	1.95	0.49
1:A:2573:GLU:OE2	1:A:2615:ARG:NE	2.42	0.49
1:B:906:CYS:SG	1:B:913:LEU:HD22	2.52	0.49
1:B:1422:ASP:OD2	1:B:1568:LYS:NZ	2.34	0.49
1:B:3442:PHE:CD1	1:B:3514:LEU:HD22	2.47	0.49
1:B:3648:ARG:HH11	1:B:3648:ARG:HG3	1.77	0.49
1:D:2440:MET:HE2	1:D:2440:MET:HA	1.94	0.49
1:C:4853:VAL:HA	1:C:4879:MET:HE1	1.93	0.49
1:A:127:MET:N	1:A:127:MET:SD	2.75	0.49
1:A:2166:LEU:HD11	1:A:2206:THR:HG23	1.94	0.49
1:A:3366:ARG:NH1	1:A:3440:GLU:OE1	2.34	0.49
1:A:3629:ARG:HA	1:A:3632:VAL:HG22	1.95	0.49
1:B:1252:HIS:O	1:B:1275:ARG:NH1	2.45	0.49
1:B:1619:ARG:NH2	1:B:1622:GLU:OE1	2.46	0.49
1:B:2309:SER:OG	1:B:2321:ILE:O	2.17	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2812:SER:OG	1:B:2882:TYR:OH	2.13	0.49
1:D:3114:LYS:HD2	1:D:3125:VAL:HG11	1.94	0.49
1:D:3545:THR:HG23	1:D:3547:GLU:H	1.77	0.49
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.47	0.49
1:A:510:GLU:OE2	1:A:510:GLU:N	2.36	0.49
1:A:653:ALA:HB3	1:A:656:SER:HB2	1.95	0.49
1:A:1289:LEU:HD12	1:A:1562:ILE:HD11	1.94	0.49
1:A:2318:TYR:CZ	1:A:2395:PRO:HD3	2.48	0.49
1:A:3132:THR:HA	1:A:3136:LEU:HB3	1.94	0.49
1:A:3357:HIS:O	1:A:3361:THR:HG23	2.12	0.49
1:B:302:VAL:HB	1:B:306:LYS:HE3	1.93	0.49
1:B:2538:THR:HG23	1:B:2541:PHE:H	1.78	0.49
1:B:3269:VAL:HA	1:B:3273:THR:HB	1.95	0.49
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.46	0.49
1:B:3959:LYS:NZ	1:B:4022:ASP:OD2	2.39	0.49
1:D:81:MET:HE3	1:D:82:LEU:HG	1.94	0.49
1:D:2382:GLU:OE1	1:D:2385:ARG:NH1	2.38	0.49
1:C:1040:CYS:O	1:C:1044:ARG:HG2	2.12	0.49
1:C:3842:LEU:HB2	1:C:3929:SER:HB2	1.93	0.49
1:A:69:LEU:HD21	1:A:202:MET:HE1	1.94	0.49
1:A:758:ARG:HG2	1:A:763:PRO:HA	1.93	0.49
1:A:923:GLN:O	1:A:927:GLU:HG2	2.13	0.49
1:A:1040:CYS:O	1:A:1044:ARG:HG2	2.13	0.49
1:A:2967:MET:HE1	1:A:3049:LEU:HD22	1.95	0.49
1:A:3157:ILE:HA	1:A:3161:VAL:CG2	2.43	0.49
1:A:3240:CYS:HB3	1:A:3243:ILE:HG12	1.94	0.49
1:B:4000:MET:SD	1:B:4020:GLN:NE2	2.77	0.49
1:D:955:LEU:HD12	1:D:967:PRO:HD2	1.94	0.49
1:D:1289:LEU:HD12	1:D:1562:ILE:HD11	1.93	0.49
1:C:1867:GLU:OE2	1:C:1928:GLN:NE2	2.46	0.49
1:C:2680:TRP:CE3	1:C:2680:TRP:HA	2.47	0.49
1:C:2973:PHE:CE1	1:C:2995:ILE:HG12	2.46	0.49
1:C:3359:ILE:HD11	1:C:3434:LEU:HB2	1.94	0.49
1:C:3534:MET:N	1:C:3534:MET:SD	2.85	0.49
1:A:906:CYS:SG	1:A:913:LEU:HD22	2.51	0.49
1:A:3182:TYR:HA	1:A:3185:LYS:HG2	1.94	0.49
1:A:3719:ASP:O	1:A:3723:MET:HG3	2.13	0.49
1:A:3758:MET:HE3	1:A:4719:PHE:HE1	1.78	0.49
1:B:4818:MET:O	1:B:4824:ARG:NH1	2.45	0.49
1:D:26:ALA:HB2	1:D:182:LEU:HD21	1.95	0.49
1:D:653:ALA:HB3	1:D:656:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASP:OD1	1:C:228:ASP:N	2.45	0.49
1:C:830:ARG:NH2	1:C:832:GLU:OE2	2.43	0.49
1:C:881:LEU:HA	1:C:884:LEU:HB2	1.95	0.49
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.21	0.49
1:C:3788:GLY:HA3	1:C:3834:ALA:HB3	1.95	0.49
1:A:2174:GLU:HA	1:A:2177:LEU:HD12	1.94	0.49
2:G:35:LYS:HE3	1:C:636:ASN:HD21	1.78	0.49
1:B:1981:MET:HA	1:B:1981:MET:HE3	1.93	0.49
1:B:2001:PRO:HA	1:B:3638:MET:HE3	1.94	0.49
1:B:4569:LEU:HD21	1:B:4649:LEU:HD23	1.94	0.49
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.94	0.49
1:D:758:ARG:HG2	1:D:763:PRO:HA	1.94	0.49
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.46	0.49
1:D:2166:LEU:HD11	1:D:2206:THR:HG23	1.94	0.49
1:D:2185:ILE:HG21	1:D:2203:MET:HE1	1.95	0.49
1:C:475:GLN:NE2	1:C:528:SER:O	2.46	0.49
1:A:2537:ASP:OD2	1:A:2588:ARG:NH1	2.45	0.49
1:A:3201:MET:HE3	1:A:3203:VAL:HG22	1.94	0.49
2:E:3:GLN:OE1	2:E:5:GLU:HG3	2.12	0.49
1:B:2872:GLN:O	1:B:2876:GLU:HG2	2.12	0.49
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.45	0.49
1:D:2191:PHE:HD2	1:D:2198:MET:HG2	1.78	0.49
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.45	0.49
1:D:3343:GLN:O	1:D:3346:VAL:HG12	2.12	0.49
1:C:125:ARG:NH1	1:C:125:ARG:O	2.46	0.49
1:C:2308:GLN:NE2	1:C:2309:SER:O	2.46	0.49
1:C:4676:GLU:OE2	1:C:4698:LYS:NZ	2.46	0.49
1:B:2441:HIS:HA	1:B:2444:GLN:NE2	2.28	0.49
1:B:4555:LEU:HD21	1:B:4656:LEU:HD22	1.95	0.49
1:D:4205:TRP:CE3	1:D:4989:MET:HE2	2.48	0.49
1:C:2874:MET:HE1	1:C:2938:THR:HA	1.95	0.49
1:C:3334:TRP:HE3	1:C:3338:LEU:HD13	1.78	0.49
1:C:3691:GLU:HA	1:C:3693:LYS:HE3	1.94	0.49
1:A:4205:TRP:CE3	1:A:4989:MET:HE2	2.48	0.48
1:B:2218:GLY:HA3	1:B:2224:ARG:NH2	2.28	0.48
1:B:3553:LEU:HD13	1:B:3593:VAL:HA	1.95	0.48
1:B:3599:VAL:O	1:B:3603:LEU:HG	2.12	0.48
1:D:1168:VAL:HG11	1:D:1176:GLU:HG2	1.95	0.48
1:D:1277:TRP:CD1	1:D:1559:GLN:HE21	2.30	0.48
1:D:1759:ARG:HD3	1:D:1760:HIS:N	2.28	0.48
1:D:3157:ILE:HA	1:D:3161:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3377:GLU:HA	1:D:3380:ARG:HG2	1.95	0.48
1:C:2694:GLU:HA	1:C:2697:ARG:NH1	2.28	0.48
1:C:3718:GLU:HG3	1:C:3723:MET:HE1	1.95	0.48
1:C:3751:VAL:HG13	1:C:3755:GLU:HG2	1.94	0.48
1:A:54:ASN:OD1	1:A:56:GLN:NE2	2.46	0.48
1:A:2924:GLN:O	1:A:2928:LYS:HG2	2.13	0.48
1:D:69:LEU:HD13	1:D:101:LEU:HD11	1.95	0.48
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.94	0.48
1:D:1422:ASP:OD2	1:D:1568:LYS:NZ	2.34	0.48
1:D:3553:LEU:HB3	1:D:3593:VAL:HG12	1.95	0.48
1:C:3316:LEU:HD22	1:C:3346:VAL:HA	1.94	0.48
1:C:4158:PRO:HA	1:C:4161:ARG:CZ	2.42	0.48
1:A:613:ALA:HB2	1:A:1676:LEU:HD12	1.95	0.48
1:A:977:LEU:HG	1:A:1044:ARG:NH1	2.28	0.48
1:B:613:ALA:HB2	1:B:1676:LEU:HD12	1.95	0.48
1:B:758:ARG:HG2	1:B:763:PRO:HA	1.95	0.48
1:B:2108:GLU:O	1:B:3694:LYS:NZ	2.45	0.48
1:B:2185:ILE:HD13	1:B:2203:MET:SD	2.53	0.48
1:B:2661:TRP:HB3	1:B:2664:PHE:HB2	1.95	0.48
1:B:3449:HIS:O	1:B:3453:ARG:NE	2.39	0.48
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.46	0.48
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.46	0.48
1:C:2626:LEU:HD23	1:C:2644:LEU:HD21	1.96	0.48
1:A:869:ARG:HH22	1:A:941:MET:HE3	1.77	0.48
1:A:2765:LYS:NZ	1:A:2857:PRO:HB2	2.26	0.48
1:A:3130:THR:HA	1:A:3133:THR:HG22	1.95	0.48
1:B:2924:GLN:O	1:B:2928:LYS:HG2	2.12	0.48
1:B:3880:PHE:HA	1:B:3883:ASP:OD2	2.14	0.48
1:D:1252:HIS:O	1:D:1275:ARG:NH1	2.46	0.48
1:C:638:ILE:HD11	1:C:1636:MET:HE2	1.96	0.48
1:C:883:ALA:HB1	1:C:907:LEU:HD13	1.95	0.48
1:A:4091:LYS:HD2	1:A:4092:ASP:N	2.28	0.48
1:A:4719:PHE:O	1:A:4723:LYS:HG3	2.14	0.48
1:B:2383:ALA:HA	1:B:2386:ILE:HG12	1.96	0.48
1:B:4754:ASN:HB3	1:B:4756:ARG:HH21	1.78	0.48
1:D:70:GLU:OE2	1:D:110:ARG:NE	2.42	0.48
1:D:275:ARG:NH2	1:D:328:LYS:HZ2	2.12	0.48
1:D:2265:LEU:HA	1:D:2330:ARG:CZ	2.42	0.48
1:D:2917:ALA:HA	1:D:2920:ARG:HB3	1.95	0.48
1:D:3517:MET:HG3	1:D:3517:MET:O	2.13	0.48
1:C:3872:GLU:HG3	1:C:3874:VAL:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3208:PRO:HB2	1:B:3237:GLU:HG3	1.96	0.48
1:B:3514:LEU:HD21	1:B:3602:VAL:HG13	1.96	0.48
1:B:3705:PHE:HB2	1:B:3778:MET:HE2	1.95	0.48
1:D:475:GLN:NE2	1:D:528:SER:O	2.47	0.48
1:C:1690:ASP:OD2	1:C:1693:GLN:NE2	2.44	0.48
1:A:156:GLN:NE2	1:D:385:ASP:OD2	2.46	0.48
1:A:2108:GLU:O	1:A:3694:LYS:NZ	2.46	0.48
1:A:2173:GLN:O	1:A:2177:LEU:HG	2.13	0.48
1:B:1931:LEU:HB3	1:B:1935:VAL:HB	1.96	0.48
1:B:2265:LEU:O	1:B:2330:ARG:NH2	2.47	0.48
1:B:3629:ARG:HA	1:B:3632:VAL:HG22	1.95	0.48
1:D:3536:ALA:HB2	1:D:3553:LEU:HD21	1.95	0.48
1:D:3588:ASP:O	1:D:3592:ILE:HG12	2.13	0.48
1:D:3628:ARG:HG3	1:D:3631:ALA:HB3	1.96	0.48
1:D:3758:MET:HE3	1:D:4719:PHE:CE1	2.48	0.48
1:C:168:ASP:OD1	1:C:201:ASN:ND2	2.44	0.48
1:C:613:ALA:HB2	1:C:1676:LEU:HD12	1.94	0.48
1:C:1252:HIS:O	1:C:1275:ARG:NH1	2.47	0.48
1:A:3457:ASN:HA	1:A:3460:VAL:HG22	1.96	0.48
1:B:1929:MET:HE2	1:B:1929:MET:HB3	1.74	0.48
1:B:3235:SER:OG	1:B:3237:GLU:OE1	2.32	0.48
1:B:3695:PRO:HB3	1:B:3699:HIS:HB3	1.95	0.48
1:B:4627:MET:C	1:B:4627:MET:HE2	2.38	0.48
1:D:3157:ILE:HG23	1:D:3161:VAL:HG12	1.95	0.48
1:D:3235:SER:OG	1:D:3237:GLU:OE1	2.32	0.48
1:D:4676:GLU:OE2	1:D:4698:LYS:NZ	2.47	0.48
1:A:947:GLU:HA	1:A:1049:TYR:HD1	1.79	0.48
1:A:3862:ASP:OD1	1:A:3862:ASP:N	2.47	0.48
1:B:904:HIS:NE2	1:B:906:CYS:HB3	2.29	0.48
1:B:1168:VAL:HG11	1:B:1176:GLU:HG2	1.96	0.48
1:B:3545:THR:HG22	1:B:3548:GLU:HG3	1.95	0.48
1:D:302:VAL:HB	1:D:306:LYS:HE3	1.96	0.48
1:D:2587:TYR:O	1:D:2590:SER:OG	2.32	0.48
1:D:3208:PRO:HB2	1:D:3237:GLU:HG3	1.96	0.48
1:D:4152:GLU:OE1	1:D:4194:TYR:OH	2.26	0.48
1:D:4815:ASP:O	1:D:4819:GLY:N	2.42	0.48
1:C:13:PHE:CE1	1:C:164:ARG:HG2	2.49	0.48
1:C:2527:LEU:HA	1:C:2530:MET:HE3	1.96	0.48
1:C:3400:VAL:HG23	1:C:3403:ARG:NH2	2.28	0.48
1:C:3715:LYS:NZ	1:C:3717:ASP:HB3	2.29	0.48
1:C:4821:LYS:H	1:C:4821:LYS:CD	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4627:MET:C	1:A:4627:MET:HE2	2.39	0.48
1:B:930:LYS:HA	1:B:933:LEU:HD12	1.96	0.48
1:B:1023:PRO:HB3	1:B:1025:ARG:NH2	2.29	0.48
1:B:1057:ASP:OD1	1:B:1057:ASP:N	2.36	0.48
1:B:1751:GLY:HA3	1:B:1759:ARG:NH1	2.29	0.48
1:B:2309:SER:OG	1:B:2320:ASP:OD1	2.32	0.48
1:C:1071:ARG:HD3	1:C:1196:PRO:HG3	1.96	0.48
1:C:1087:ARG:HB3	1:C:1223:PHE:CD2	2.49	0.48
1:C:2175:GLU:HG3	1:C:2228:MET:HB2	1.96	0.48
1:C:3162:GLN:O	1:C:3166:TYR:HB2	2.13	0.48
1:A:901:LYS:HG3	1:A:903:LEU:HG	1.96	0.47
1:A:1107:PRO:HD2	1:A:1186:ASP:OD2	2.14	0.47
1:D:613:ALA:HB2	1:D:1676:LEU:HD12	1.95	0.47
1:D:3842:LEU:HB2	1:D:3929:SER:HB2	1.94	0.47
1:D:4188:ARG:HG2	1:D:4188:ARG:HH11	1.79	0.47
1:C:907:LEU:O	1:C:961:MET:HE3	2.14	0.47
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.45	0.47
1:A:1422:ASP:OD2	1:A:1568:LYS:NZ	2.33	0.47
1:A:1970:GLN:HG2	1:A:3642:TYR:HA	1.96	0.47
1:B:2587:TYR:O	1:B:2590:SER:OG	2.21	0.47
1:B:3157:ILE:HG23	1:B:3161:VAL:HG12	1.95	0.47
1:D:887:ILE:HG12	1:D:907:LEU:HD11	1.96	0.47
1:D:2858:GLN:HB2	1:D:2859:PRO:HD3	1.96	0.47
1:D:4569:LEU:HD13	1:D:4650:HIS:HA	1.95	0.47
1:D:4932:ILE:O	1:D:4936:ILE:HG12	2.14	0.47
1:C:1277:TRP:CD1	1:C:1559:GLN:HE21	2.32	0.47
1:C:2998:PHE:CD1	1:C:3002:LEU:HD11	2.49	0.47
1:A:1168:VAL:HG11	1:A:1176:GLU:HG2	1.96	0.47
1:A:2929:PHE:HA	1:A:2932:MET:SD	2.54	0.47
1:A:3414:ARG:HB2	1:A:3414:ARG:HH11	1.78	0.47
1:A:3880:PHE:HA	1:A:3883:ASP:OD2	2.14	0.47
1:A:4754:ASN:HB3	1:A:4756:ARG:HH21	1.79	0.47
1:B:3755:GLU:HA	1:B:3758:MET:HB2	1.94	0.47
1:D:4798:MET:HA	1:D:4798:MET:HE3	1.95	0.47
1:C:1866:ILE:HG12	1:C:1939:MET:HE1	1.95	0.47
1:A:2102:VAL:HG13	1:A:2120:MET:HB2	1.96	0.47
1:A:3166:TYR:CG	1:A:3239:MET:HG2	2.49	0.47
1:A:3731:LYS:HA	1:A:3734:HIS:CE1	2.49	0.47
1:B:1207:ASP:O	1:B:1210:SER:OG	2.29	0.47
1:B:1759:ARG:H	1:B:1759:ARG:HD3	1.80	0.47
1:B:3270:ILE:HA	1:B:3274:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3731:LYS:HA	1:B:3734:HIS:CE1	2.49	0.47
1:D:2625:ARG:HB3	1:D:2625:ARG:CZ	2.45	0.47
1:D:3517:MET:HE2	1:D:3517:MET:HB2	1.76	0.47
1:D:4910:GLU:O	1:D:4914:VAL:HG13	2.15	0.47
1:A:2285:GLU:OE2	1:A:3856:LEU:HD12	2.15	0.47
1:A:3959:LYS:NZ	1:A:4022:ASP:OD2	2.42	0.47
1:A:4112:LEU:O	1:A:4115:SER:OG	2.28	0.47
1:B:2538:THR:O	1:B:2542:SER:HB2	2.14	0.47
1:B:2986:VAL:HG22	1:B:2988:LYS:H	1.79	0.47
1:D:3450:ASN:HA	1:D:3453:ARG:NE	2.30	0.47
1:C:1997:GLU:HB2	1:C:2008:MET:HE1	1.95	0.47
1:C:2412:GLU:C	1:C:2414:ASN:H	2.23	0.47
1:C:2736:ASP:O	1:C:2738:ARG:NH1	2.47	0.47
1:C:2967:MET:SD	1:C:2970:SER:OG	2.73	0.47
1:C:3392:LEU:HD13	1:C:3395:ARG:HD2	1.97	0.47
1:C:3623:LEU:HD22	1:C:3624:LEU:HD23	1.97	0.47
1:A:3545:THR:HG22	1:A:3548:GLU:HG3	1.96	0.47
1:A:4818:MET:O	1:A:4824:ARG:NH1	2.47	0.47
1:D:2420:HIS:HA	1:D:2423:MET:HE3	1.95	0.47
1:D:2912:THR:OG1	1:D:2913:ALA:N	2.47	0.47
1:D:3078:ARG:NE	1:D:3155:ASP:OD2	2.48	0.47
1:A:157:ARG:NE	1:A:164:ARG:HE	2.13	0.47
1:A:2194:HIS:O	1:A:2198:MET:HE2	2.15	0.47
1:A:2736:ASP:O	1:A:2738:ARG:NH1	2.48	0.47
1:A:3705:PHE:HB2	1:A:3778:MET:HE2	1.97	0.47
1:A:4172:GLU:OE1	1:A:4175:ARG:NH1	2.48	0.47
1:A:4640:GLU:HB3	1:A:4641:PRO:HD3	1.96	0.47
1:A:4818:MET:N	1:A:4818:MET:SD	2.87	0.47
2:H:3:GLN:OE1	2:H:5:GLU:HG3	2.15	0.47
1:B:796:ARG:NH1	1:B:1622:GLU:OE2	2.48	0.47
1:B:2608:MET:HE3	1:B:2608:MET:HB3	1.76	0.47
1:B:2815:ALA:HB1	1:B:2881:ASN:ND2	2.30	0.47
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.48	0.47
1:B:3240:CYS:HB3	1:B:3243:ILE:HG12	1.96	0.47
1:B:3539:ARG:NH1	1:B:3544:ASP:OD2	2.47	0.47
1:B:4015:GLU:HA	1:B:4018:ASP:OD2	2.14	0.47
1:D:35:LEU:HD11	1:D:189:LEU:HD13	1.96	0.47
1:D:2892:GLN:NE2	1:D:2895:GLU:OE2	2.47	0.47
1:D:3603:LEU:HA	1:D:3606:LEU:HD23	1.96	0.47
1:C:460:GLN:HB2	1:C:463:GLU:OE1	2.15	0.47
1:C:4205:TRP:CE3	1:C:4989:MET:HE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2191:PHE:HD1	1:A:2198:MET:HG2	1.80	0.47
1:A:3564:GLU:HA	1:A:3564:GLU:OE2	2.15	0.47
1:A:4813:LEU:O	1:A:4816:ILE:HG13	2.15	0.47
1:B:2386:ILE:HG22	1:B:2392:ARG:CZ	2.45	0.47
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	1.97	0.47
1:B:4205:TRP:CZ3	1:B:4989:MET:HE3	2.50	0.47
1:D:3535:LEU:O	1:D:3538:THR:OG1	2.28	0.47
1:D:3540:TYR:OH	1:D:3549:VAL:HG21	2.15	0.47
1:C:4849:TYR:HB2	1:C:4883:TYR:CE1	2.50	0.47
1:A:1465:ASP:OD1	1:A:1468:LYS:HG2	2.15	0.47
1:A:2608:MET:HE3	1:A:2608:MET:HB3	1.76	0.47
1:A:3628:ARG:HG3	1:A:3631:ALA:HB3	1.96	0.47
1:A:4039:MET:HE2	1:A:4043:GLN:HG3	1.96	0.47
1:B:4016:LEU:O	1:B:4020:GLN:HG3	2.14	0.47
1:D:1690:ASP:OD2	1:D:1693:GLN:NE2	2.45	0.47
1:C:3695:PRO:HB2	1:C:3700:GLN:HG2	1.97	0.47
1:C:4754:ASN:HB3	1:C:4756:ARG:HH21	1.80	0.47
1:A:144:GLU:HG3	1:A:175:SER:HB3	1.97	0.47
1:A:981:GLN:HA	1:A:984:LEU:HD12	1.96	0.47
1:A:2747:ILE:HD13	1:A:2814:LYS:HG2	1.97	0.47
1:A:3354:LEU:HD22	1:A:3423:TRP:CZ2	2.50	0.47
1:A:4016:LEU:O	1:A:4020:GLN:HG3	2.14	0.47
1:B:929:LEU:O	1:B:932:LEU:HD23	2.15	0.47
1:D:4088:ILE:O	1:D:4123:ILE:HB	2.15	0.47
1:D:4860:ARG:NH1	1:C:4630:TYR:OH	2.48	0.47
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.96	0.47
1:C:1733:GLU:HG2	1:C:2201:LEU:HD23	1.97	0.47
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.33	0.46
2:F:85:THR:OG1	2:F:86:GLY:N	2.48	0.46
1:B:1465:ASP:OD1	1:B:1468:LYS:HG2	2.15	0.46
1:B:3445:TRP:NE1	1:B:3455:GLU:OE1	2.43	0.46
1:D:2208:MET:HE1	1:D:2250:MET:HE1	1.97	0.46
1:D:3638:MET:SD	1:D:3639:THR:N	2.88	0.46
1:C:1962:ALA:O	1:C:1966:VAL:HG22	2.16	0.46
1:C:2020:ASP:OD1	1:C:2020:ASP:N	2.47	0.46
1:C:2758:PHE:HA	1:C:2761:TYR:HB2	1.95	0.46
1:C:3335:MET:HE3	1:C:3403:ARG:NH1	2.30	0.46
1:A:483:MET:HE2	1:A:483:MET:HA	1.97	0.46
1:A:2815:ALA:HB1	1:A:2881:ASN:ND2	2.30	0.46
1:A:3106:MET:HE2	1:A:3186:LEU:HD13	1.98	0.46
1:A:3449:HIS:HB2	1:A:3453:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLU:CD	1:B:66:CYS:HB3	2.41	0.46
1:D:2522:LEU:HB3	1:D:2527:LEU:HD23	1.97	0.46
1:D:3269:VAL:HA	1:D:3273:THR:HB	1.97	0.46
1:C:758:ARG:HG2	1:C:763:PRO:HA	1.98	0.46
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.96	0.46
1:C:3588:ASP:O	1:C:3592:ILE:HG12	2.15	0.46
1:A:2747:ILE:HD12	1:A:2748:PRO:HD2	1.97	0.46
1:A:3532:LEU:HB3	1:A:3553:LEU:HD21	1.97	0.46
2:F:105:LYS:HB3	2:F:105:LYS:HE2	1.75	0.46
1:B:168:ASP:OD1	1:B:201:ASN:ND2	2.47	0.46
1:B:950:LEU:HD13	1:B:970:LEU:HD22	1.96	0.46
1:B:3343:GLN:O	1:B:3346:VAL:HG12	2.14	0.46
1:B:4177:TYR:CE1	1:B:4199:GLU:HG3	2.50	0.46
1:D:2694:GLU:HA	1:D:2697:ARG:NH1	2.26	0.46
1:C:2626:LEU:O	1:C:2630:VAL:HG12	2.15	0.46
1:C:2963:LEU:HD21	1:C:3006:ILE:HG12	1.97	0.46
1:C:3312:LEU:HD12	1:C:3345:ILE:HB	1.97	0.46
1:C:3719:ASP:HB3	1:C:3793:MET:HE1	1.97	0.46
1:C:3844:LEU:HD23	1:C:3844:LEU:HA	1.78	0.46
1:A:1479:GLU:OE1	1:A:1479:GLU:N	2.30	0.46
1:A:2211:MET:HA	1:A:2214:VAL:HG22	1.98	0.46
1:A:3078:ARG:NE	1:A:3155:ASP:OD2	2.49	0.46
1:A:3553:LEU:HD13	1:A:3593:VAL:HA	1.96	0.46
1:A:3638:MET:HE2	1:A:3638:MET:HB2	1.55	0.46
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.96	0.46
1:B:2123:LEU:O	1:B:2127:GLN:HG2	2.16	0.46
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.98	0.46
1:C:929:LEU:O	1:C:933:LEU:HD12	2.16	0.46
1:C:2604:GLU:HB3	1:C:2639:MET:HE3	1.96	0.46
1:C:4932:ILE:O	1:C:4936:ILE:HG12	2.15	0.46
1:B:1024:TYR:CZ	1:B:1032:LYS:HG3	2.51	0.46
1:B:1037:ASP:O	1:B:1041:GLN:HG2	2.16	0.46
1:B:2768:PHE:O	1:B:2771:ILE:HG22	2.16	0.46
1:B:4640:GLU:HB3	1:B:4641:PRO:HD3	1.97	0.46
1:C:1465:ASP:OD1	1:C:1468:LYS:HG2	2.16	0.46
1:C:2991:HIS:O	1:C:2995:ILE:N	2.42	0.46
1:C:3159:ASP:OD1	1:C:3159:ASP:N	2.44	0.46
1:A:924:MET:O	1:A:928:THR:HG23	2.15	0.46
1:A:1207:ASP:O	1:A:1210:SER:OG	2.30	0.46
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	1.98	0.46
1:B:35:LEU:HD11	1:B:189:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:HG21	1:B:252:VAL:HG21	1.98	0.46
1:B:893:TYR:CB	1:B:961:MET:HE1	2.41	0.46
1:B:2974:ILE:HG13	1:B:2975:ALA:N	2.30	0.46
1:B:3400:VAL:HG23	1:B:3403:ARG:NH2	2.30	0.46
1:D:4186:ALA:C	1:D:4188:ARG:HH12	2.16	0.46
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.41	0.46
1:C:3324:VAL:HA	1:C:3327:LEU:HB2	1.98	0.46
1:C:3349:ALA:HB1	1:C:3353:LEU:HD23	1.98	0.46
1:A:26:ALA:HB2	1:A:182:LEU:HD21	1.97	0.46
1:A:4245:MET:HE1	1:A:4989:MET:HE1	1.98	0.46
1:A:4555:LEU:HD21	1:A:4656:LEU:HD22	1.97	0.46
1:B:2490:MET:CE	1:B:2546:MET:HE2	2.46	0.46
1:D:683:ARG:HG2	1:D:717:ASP:HB3	1.97	0.46
1:D:1465:ASP:OD1	1:D:1468:LYS:HG2	2.15	0.46
1:D:2586:VAL:HG13	1:D:2607:LEU:HD13	1.97	0.46
1:D:3715:LYS:HD2	1:D:3715:LYS:C	2.41	0.46
1:D:3962:PHE:CZ	1:D:4023:MET:HG3	2.50	0.46
1:D:4632:LEU:HD13	1:D:4639:MET:HG2	1.98	0.46
1:C:3663:LEU:HD23	1:C:3663:LEU:HA	1.81	0.46
1:C:4954:MET:HE1	1:C:4959:PHE:HB2	1.96	0.46
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.48	0.46
1:A:4000:MET:SD	1:A:4020:GLN:NE2	2.84	0.46
1:B:3212:GLU:HG2	1:B:3213:TYR:CD2	2.51	0.46
1:B:4983:HIS:O	3:B:5301:ATP:N6	2.48	0.46
1:D:2765:LYS:NZ	1:D:2857:PRO:HB2	2.31	0.46
1:D:3449:HIS:O	1:D:3453:ARG:NE	2.41	0.46
1:D:4047:MET:HE3	1:D:4047:MET:HB3	1.80	0.46
1:C:2669:GLU:OE1	1:C:2669:GLU:O	2.34	0.46
1:A:232:THR:HG21	1:A:252:VAL:HG21	1.98	0.46
1:A:919:ASN:HA	1:A:922:LEU:HD23	1.98	0.46
1:A:1272:LEU:HD22	1:A:1289:LEU:HD11	1.98	0.46
1:A:2123:LEU:O	1:A:2127:GLN:HG2	2.16	0.46
1:B:462:GLU:OE2	1:B:462:GLU:N	2.43	0.46
1:B:893:TYR:HB3	1:B:962:SER:OG	2.16	0.46
1:B:3705:PHE:HA	1:B:3708:THR:HG22	1.98	0.46
1:D:3137:LEU:HD12	1:D:3137:LEU:HA	1.84	0.46
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.98	0.46
1:C:4885:PHE:O	1:C:4889:VAL:HG22	2.16	0.46
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.98	0.46
1:A:1931:LEU:HB3	1:A:1935:VAL:HB	1.98	0.46
1:A:2029:GLN:NE2	1:A:2033:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2856:ASN:ND2	1:A:2858:GLN:OE1	2.44	0.46
1:A:3316:LEU:HD21	1:A:3346:VAL:HG23	1.98	0.46
1:A:4092:ASP:HA	1:A:4095:LYS:HG2	1.97	0.46
1:B:330:ASP:OD1	1:B:330:ASP:N	2.49	0.46
1:B:913:LEU:HD11	1:B:918:ARG:HE	1.81	0.46
1:B:1601:MET:HA	1:B:1601:MET:HE3	1.98	0.46
1:B:2757:LYS:O	1:B:2761:TYR:HB2	2.16	0.46
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.30	0.46
1:D:4678:ALA:HB1	1:D:4720:VAL:HG21	1.98	0.46
1:D:4695:ASP:OD1	1:D:4695:ASP:N	2.45	0.46
1:C:3529:ASP:O	1:C:3533:ILE:HD13	2.16	0.46
1:C:4654:ALA:C	1:C:4796:MET:HE1	2.40	0.46
1:A:365:LYS:HE3	1:A:365:LYS:HB3	1.81	0.45
1:B:796:ARG:O	1:B:1619:ARG:NH2	2.44	0.45
1:B:1277:TRP:CD1	1:B:1559:GLN:HE21	2.34	0.45
1:B:2419:GLY:C	1:B:2423:MET:HE3	2.41	0.45
1:B:2628:PHE:HD1	1:B:2628:PHE:O	1.99	0.45
1:B:3312:LEU:HD22	1:B:3348:ARG:HG3	1.98	0.45
1:D:13:PHE:CE1	1:D:164:ARG:HG2	2.51	0.45
1:D:3758:MET:HE3	1:D:4719:PHE:CZ	2.51	0.45
1:D:4813:LEU:O	1:D:4816:ILE:HG13	2.16	0.45
1:C:499:THR:HG23	1:C:502:HIS:H	1.81	0.45
1:C:893:TYR:O	1:C:903:LEU:HD22	2.16	0.45
1:C:1163:THR:HG22	1:C:1168:VAL:HG22	1.98	0.45
1:C:3343:GLN:O	1:C:3346:VAL:HG12	2.16	0.45
1:C:3628:ARG:HG3	1:C:3631:ALA:HB3	1.99	0.45
2:H:85:THR:OG1	2:H:86:GLY:N	2.48	0.45
1:B:1805:GLU:H	1:B:1805:GLU:CD	2.24	0.45
1:B:2911:LEU:HB2	1:B:2915:GLU:HG3	1.98	0.45
1:B:3003:LEU:HB2	1:B:3004:PRO:HD3	1.98	0.45
1:D:336:PRO:HA	1:D:337:PRO:HD3	1.89	0.45
1:C:2858:GLN:HB2	1:C:2859:PRO:HD3	1.97	0.45
1:A:683:ARG:HG2	1:A:717:ASP:HB3	1.97	0.45
1:A:1931:LEU:HG	1:A:1935:VAL:HG11	1.99	0.45
1:A:2587:TYR:O	1:A:2590:SER:OG	2.22	0.45
1:A:3240:CYS:HB3	1:A:3243:ILE:CG1	2.47	0.45
1:A:3535:LEU:O	1:A:3538:THR:OG1	2.22	0.45
1:A:3788:GLY:HA3	1:A:3834:ALA:HB3	1.99	0.45
1:A:4177:TYR:CE1	1:A:4199:GLU:HG3	2.50	0.45
2:G:105:LYS:HE2	2:G:105:LYS:HB3	1.75	0.45
1:D:2608:MET:HE3	1:D:2608:MET:HB3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2668:SER:C	1:D:2670:GLU:H	2.24	0.45
1:D:3579:LEU:HD12	1:D:3582:ARG:HE	1.81	0.45
1:D:3949:ARG:HG3	1:D:3949:ARG:HH11	1.81	0.45
1:C:1168:VAL:HG11	1:C:1176:GLU:HG2	1.98	0.45
1:C:4902:GLU:O	1:C:4913:ARG:NH1	2.42	0.45
1:A:995:VAL:O	1:A:998:ARG:HG3	2.16	0.45
1:A:1115:LEU:HD13	1:A:1123:VAL:HG11	1.99	0.45
1:A:1532:ASN:HB2	1:A:1534:LYS:NZ	2.31	0.45
1:A:2441:HIS:O	1:A:2444:GLN:NE2	2.49	0.45
1:A:2538:THR:O	1:A:2542:SER:HB2	2.16	0.45
1:A:2611:CYS:HB2	1:A:2643:LEU:HD11	1.98	0.45
1:B:947:GLU:HA	1:B:1049:TYR:HD1	1.81	0.45
1:B:4571:PHE:HE2	1:B:4816:ILE:HD13	1.81	0.45
1:D:266:ARG:NH2	1:D:272:SER:OG	2.49	0.45
1:D:938:HIS:HB3	1:D:1054:GLU:HB3	1.98	0.45
1:D:2101:MET:HE2	1:D:2101:MET:HB3	1.65	0.45
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.97	0.45
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.49	0.45
1:D:3359:ILE:HG23	1:D:3437:MET:HE1	1.98	0.45
1:D:4177:TYR:CE1	1:D:4199:GLU:HG3	2.51	0.45
1:C:2630:VAL:HG13	1:C:2631:PRO:HD3	1.99	0.45
1:C:2765:LYS:HA	1:C:2765:LYS:HD3	1.81	0.45
1:C:4569:LEU:HD13	1:C:4650:HIS:HA	1.99	0.45
1:A:788:LYS:HE3	1:A:788:LYS:HB2	1.80	0.45
1:A:1601:MET:HA	1:A:1601:MET:HE3	1.99	0.45
1:A:2700:MET:HE3	1:A:2700:MET:HB3	1.77	0.45
1:A:3841:VAL:HA	1:A:3875:MET:HE3	1.99	0.45
1:B:1115:LEU:HD13	1:B:1123:VAL:HG11	1.99	0.45
1:B:1272:LEU:HD22	1:B:1289:LEU:HD11	1.99	0.45
1:B:3105:LYS:O	1:B:3108:GLU:HG3	2.17	0.45
1:D:1759:ARG:HA	1:D:1759:ARG:HH11	1.81	0.45
1:D:1861:GLN:O	1:D:1865:MET:HE3	2.17	0.45
1:D:2218:GLY:HA3	1:D:2224:ARG:NH2	2.31	0.45
1:D:2970:SER:O	1:D:2974:ILE:HG12	2.17	0.45
1:D:4968:PHE:O	1:D:4974:GLY:HA3	2.17	0.45
1:C:1000:ARG:HB3	1:C:1005:TRP:HB2	1.97	0.45
1:C:1815:LEU:O	1:C:1819:VAL:HG12	2.16	0.45
1:C:3104:GLU:OE2	1:C:3167:ARG:HB3	2.16	0.45
1:C:3940:LYS:O	1:C:4002:LYS:NZ	2.45	0.45
1:C:4544:LEU:HD12	1:C:4545:GLU:N	2.31	0.45
1:C:4627:MET:HE3	1:C:4627:MET:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:CD	1:A:66:CYS:HB3	2.41	0.45
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.49	0.45
1:A:636:ASN:HD21	2:E:35:LYS:HE3	1.80	0.45
1:A:2986:VAL:HG22	1:A:2988:LYS:H	1.81	0.45
1:B:877:ASN:O	1:B:881:LEU:HD22	2.17	0.45
1:B:907:LEU:O	1:B:961:MET:HE3	2.17	0.45
1:D:2614:ILE:HG23	1:D:2618:MET:HE3	1.98	0.45
1:C:3542:LEU:HD23	1:C:3542:LEU:O	2.17	0.45
1:A:2858:GLN:HB2	1:A:2859:PRO:HD3	1.98	0.45
1:A:3296:LEU:HB3	1:A:3297:PRO:HD3	1.99	0.45
1:A:3543:LYS:N	1:A:3543:LYS:HD2	2.32	0.45
1:A:4944:ARG:NH1	1:B:4942:GLU:OE1	2.48	0.45
1:B:1427:ILE:HG23	1:B:1428:LEU:HD23	1.97	0.45
1:B:2531:ARG:HG2	1:B:2585:THR:HG21	1.99	0.45
1:B:3110:LEU:C	1:B:3112:LEU:H	2.24	0.45
1:D:3999:MET:HE3	1:D:3999:MET:HB3	1.79	0.45
1:D:4868:ASP:OD1	1:D:4870:ASP:N	2.49	0.45
1:C:3038:MET:HB2	1:C:3038:MET:HE2	1.59	0.45
1:A:1037:ASP:O	1:A:1041:GLN:HG2	2.16	0.45
1:A:2498:HIS:O	1:A:2502:MET:HG2	2.17	0.45
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.81	0.45
1:A:3556:ASN:HB3	1:A:3559:LEU:HD23	1.99	0.45
2:E:85:THR:OG1	2:E:86:GLY:N	2.48	0.45
2:H:82:TYR:HD1	1:D:1786:LEU:HG	1.81	0.45
2:H:90:ILE:HD11	1:D:1684:ALA:HA	1.99	0.45
1:B:876:GLU:OE2	1:B:918:ARG:NH1	2.50	0.45
1:B:887:ILE:HG12	1:B:907:LEU:HD11	1.97	0.45
1:B:2970:SER:HA	1:B:2973:PHE:CE2	2.52	0.45
1:B:3532:LEU:HA	1:B:3535:LEU:HG	1.98	0.45
1:B:3844:LEU:HD23	1:B:3844:LEU:HA	1.78	0.45
1:B:4678:ALA:HB1	1:B:4720:VAL:HG21	1.97	0.45
1:D:947:GLU:HA	1:D:1049:TYR:HD1	1.80	0.45
1:D:3459:VAL:HG11	1:D:3503:TYR:HD1	1.82	0.45
1:D:3751:VAL:HG13	1:D:3755:GLU:HG2	1.98	0.45
1:D:3755:GLU:HA	1:D:3758:MET:HB2	1.99	0.45
1:D:3788:GLY:HA3	1:D:3834:ALA:HB3	1.99	0.45
1:C:1272:LEU:HD22	1:C:1289:LEU:HD11	1.99	0.45
1:C:1847:THR:O	1:C:1851:MET:HG3	2.17	0.45
1:C:2965:ARG:O	1:C:2969:ILE:HD12	2.17	0.45
1:C:3362:ILE:HG13	1:C:3412:LEU:HD21	1.99	0.45
1:A:35:LEU:HD11	1:A:189:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.43	0.45
1:A:3705:PHE:HA	1:A:3708:THR:HG22	1.99	0.45
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.99	0.45
1:B:2225:PHE:N	1:B:2226:PRO:HD3	2.32	0.45
1:B:3213:TYR:CD1	1:B:3302:PRO:HB2	2.52	0.45
1:B:4885:PHE:O	1:B:4889:VAL:HG22	2.17	0.45
1:D:1023:PRO:HB3	1:D:1025:ARG:HH22	1.81	0.45
1:D:1272:LEU:HD22	1:D:1289:LEU:HD11	1.99	0.45
1:C:530:ILE:HG22	1:C:536:ASN:HB3	1.98	0.45
1:C:2765:LYS:NZ	1:C:2857:PRO:HB2	2.28	0.45
1:C:3673:MET:HE3	1:C:3728:ILE:HD13	1.98	0.45
1:C:3751:VAL:HG12	1:C:3756:LYS:HE2	1.98	0.45
1:A:451:TYR:CZ	1:A:474:ARG:HD2	2.52	0.45
1:A:3566:SER:HB3	1:A:3569:LEU:HB3	1.98	0.45
1:A:4927:ILE:O	1:A:4931:ILE:HG13	2.16	0.45
1:B:3114:LYS:HE3	1:B:3123:LYS:HD2	1.97	0.45
1:B:4627:MET:HE1	1:B:4629:TYR:CD1	2.52	0.45
1:D:19:GLU:CD	1:D:66:CYS:HB3	2.41	0.45
1:D:328:LYS:HE3	1:D:328:LYS:HB3	1.68	0.45
1:D:1847:THR:O	1:D:1851:MET:HG3	2.17	0.45
1:D:3466:ASN:ND2	1:D:3507:THR:O	2.50	0.45
1:D:3531:ASP:OD2	1:D:3532:LEU:N	2.50	0.45
1:C:19:GLU:CD	1:C:66:CYS:HB3	2.42	0.45
1:C:2881:ASN:HA	1:C:2884:ASN:ND2	2.32	0.45
1:C:3391:GLU:HG3	1:C:3395:ARG:HE	1.82	0.45
1:C:3759:GLU:HA	1:C:3759:GLU:OE2	2.16	0.45
1:C:4910:GLU:O	1:C:4914:VAL:HG13	2.17	0.45
1:C:5034:ASP:OD2	1:C:5035:GLN:NE2	2.50	0.45
1:A:2228:MET:HG3	1:A:2229:VAL:N	2.32	0.44
1:A:2977:LEU:HA	1:A:2980:VAL:HG22	1.98	0.44
1:A:4015:GLU:HA	1:A:4018:ASP:OD2	2.17	0.44
2:E:17:LYS:HZ3	2:E:17:LYS:HB2	1.83	0.44
1:B:41:GLY:HA2	1:B:137:LEU:HD12	1.99	0.44
1:B:384:MET:HE3	1:B:384:MET:N	2.30	0.44
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.99	0.44
1:B:4944:ARG:NH1	1:C:4942:GLU:OE1	2.50	0.44
1:D:1820:ARG:HB3	1:D:1820:ARG:HH11	1.82	0.44
1:D:2456:ILE:O	1:D:2459:SER:OG	2.30	0.44
1:D:3686:GLU:N	1:D:3686:GLU:OE2	2.50	0.44
1:C:1019:PRO:HD2	1:C:1020:ARG:HH21	1.82	0.44
1:C:1066:GLN:HB2	1:C:1071:ARG:NH2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2101:MET:HE3	1:C:2105:TRP:CE3	2.52	0.44
1:C:2640:PRO:O	1:C:2644:LEU:HG	2.16	0.44
1:C:3159:ASP:HA	1:C:3218:VAL:HG12	2.00	0.44
1:A:904:HIS:CE1	1:A:906:CYS:HB3	2.52	0.44
1:A:1805:GLU:CD	1:A:1805:GLU:H	2.25	0.44
1:A:2599:GLN:O	1:A:2603:ILE:HG13	2.18	0.44
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.99	0.44
1:A:3182:TYR:HA	1:A:3185:LYS:HE3	1.98	0.44
1:B:2417:HIS:CG	1:B:2492:ALA:HB2	2.52	0.44
1:B:4867:GLU:OE2	1:B:4867:GLU:N	2.38	0.44
1:C:2438:PRO:HB2	1:C:2443:ILE:HD11	1.99	0.44
1:C:2652:TRP:CD1	1:C:2652:TRP:H	2.35	0.44
1:C:3123:LYS:HG3	1:C:3125:VAL:H	1.82	0.44
1:C:3245:VAL:HG23	1:C:3248:ARG:H	1.82	0.44
1:C:3436:ARG:NH1	1:C:3598:GLU:OE1	2.51	0.44
1:C:4849:TYR:HB2	1:C:4883:TYR:HE1	1.82	0.44
1:A:2310:CYS:SG	1:A:2313:LEU:HB2	2.57	0.44
1:A:3201:MET:HE3	1:A:3203:VAL:CG2	2.47	0.44
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	1.98	0.44
1:B:14:LEU:HD13	1:B:202:MET:HE2	1.99	0.44
1:B:451:TYR:CZ	1:B:474:ARG:HD2	2.52	0.44
1:B:501:ALA:O	1:B:505:GLU:HG3	2.17	0.44
1:B:924:MET:O	1:B:928:THR:HG23	2.18	0.44
1:B:2189:LYS:HA	1:B:2192:TYR:CE1	2.51	0.44
1:B:2514:ASN:OD1	1:B:2514:ASN:N	2.51	0.44
1:B:2862:LEU:HD22	1:B:2863:SER:H	1.82	0.44
1:B:4719:PHE:O	1:B:4723:LYS:HG3	2.18	0.44
1:D:208:CYS:O	1:D:334:MET:HG3	2.17	0.44
1:D:2881:ASN:HA	1:D:2884:ASN:ND2	2.32	0.44
1:D:3959:LYS:NZ	1:D:4022:ASP:OD2	2.47	0.44
1:C:913:LEU:HD11	1:C:918:ARG:HE	1.83	0.44
1:C:931:THR:HG21	1:C:991:ASN:OD1	2.16	0.44
1:C:3296:LEU:HB2	1:C:3297:PRO:HD3	2.00	0.44
1:C:4161:ARG:H	1:C:4161:ARG:NE	2.08	0.44
1:C:4928:LEU:HD23	1:C:4931:ILE:HD12	1.98	0.44
1:A:297:GLN:OE1	1:A:297:GLN:N	2.48	0.44
1:A:648:ILE:HD13	1:A:811:CYS:HB3	2.00	0.44
1:A:2234:ARG:HB3	1:A:2234:ARG:CZ	2.47	0.44
1:A:3199:ALA:HB2	1:A:3279:SER:OG	2.17	0.44
2:H:2:VAL:HG22	2:H:58:GLY:HA2	1.99	0.44
1:B:2234:ARG:HB3	1:B:2234:ARG:CZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.98	0.44
1:B:4710:SER:O	1:B:4713:SER:OG	2.35	0.44
1:D:227:MET:H	1:D:227:MET:HE2	1.82	0.44
1:D:227:MET:HE2	1:D:227:MET:N	2.32	0.44
1:D:1808:ARG:HD3	1:D:1853:ILE:HG22	1.99	0.44
1:D:2884:ASN:OD1	1:D:2885:THR:N	2.50	0.44
1:D:3199:ALA:HB2	1:D:3279:SER:OG	2.17	0.44
1:D:3556:ASN:HB3	1:D:3559:LEU:HD23	2.00	0.44
1:D:4148:THR:HG21	1:D:4180:ARG:HH21	1.83	0.44
1:D:4209:GLN:H	1:D:4209:GLN:CD	2.21	0.44
1:C:208:CYS:O	1:C:334:MET:HG3	2.18	0.44
1:C:935:LEU:HG	1:C:987:ARG:HH12	1.82	0.44
1:C:2198:MET:N	1:C:2198:MET:HE2	2.32	0.44
1:A:41:GLY:HA2	1:A:137:LEU:HD12	2.00	0.44
1:A:345:LEU:HB3	1:A:387:ALA:HB1	2.00	0.44
1:A:892:THR:HB	1:A:962:SER:OG	2.17	0.44
1:A:2464:ASP:OD1	1:A:2465:ASP:N	2.51	0.44
1:A:2495:VAL:HG22	1:A:2498:HIS:CE1	2.51	0.44
1:A:3183:VAL:O	1:A:3187:ARG:HG3	2.18	0.44
1:A:4056:GLU:HG2	1:A:4166:LEU:HD13	1.99	0.44
2:F:58:GLY:HA3	2:F:76:ILE:HD12	1.99	0.44
1:B:2599:GLN:O	1:B:2603:ILE:HG13	2.16	0.44
1:B:2912:THR:HG23	1:B:2914:LYS:HG3	2.00	0.44
1:B:3296:LEU:HB2	1:B:3297:PRO:HD3	2.00	0.44
1:B:3577:ARG:NE	1:B:3577:ARG:HA	2.32	0.44
1:B:4927:ILE:O	1:B:4931:ILE:HG13	2.18	0.44
1:D:913:LEU:HD11	1:D:918:ARG:HB2	1.98	0.44
1:D:2986:VAL:HG22	1:D:2988:LYS:H	1.82	0.44
1:D:3234:ASN:ND2	1:D:3234:ASN:C	2.74	0.44
1:C:793:LEU:HD12	1:C:821:LEU:HD21	1.99	0.44
1:C:1716:ILE:O	1:C:1721:GLU:N	2.50	0.44
1:C:2644:LEU:HD13	1:C:2678:LEU:HD21	1.99	0.44
1:C:3390:GLY:HA2	1:C:3393:LEU:HB2	2.00	0.44
1:A:227:MET:HE1	1:A:389:PHE:CD2	2.52	0.44
1:A:2768:PHE:O	1:A:2771:ILE:HG22	2.18	0.44
1:A:3346:VAL:HG11	1:A:3414:ARG:HB3	2.00	0.44
1:A:3400:VAL:HG23	1:A:3403:ARG:NH2	2.33	0.44
2:F:32:ASP:OD2	2:F:32:ASP:N	2.42	0.44
1:B:176:SER:OG	1:B:178:ARG:NH1	2.46	0.44
1:B:483:MET:HE2	1:B:483:MET:HA	1.99	0.44
1:B:923:GLN:O	1:B:927:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.99	0.44
1:B:2973:PHE:CD1	1:B:2973:PHE:C	2.95	0.44
1:B:3240:CYS:HB3	1:B:3243:ILE:CG1	2.48	0.44
1:D:156:GLN:NE2	1:C:385:ASP:OD2	2.51	0.44
1:D:3514:LEU:O	1:D:3518:LEU:N	2.50	0.44
1:C:157:ARG:NH2	1:C:164:ARG:HD2	2.33	0.44
1:C:1115:LEU:HD13	1:C:1123:VAL:HG11	1.99	0.44
1:C:2031:LEU:HD11	1:C:3657:TYR:CE1	2.53	0.44
1:C:2912:THR:OG1	1:C:2913:ALA:N	2.51	0.44
1:C:2952:GLU:HA	1:C:2957:PHE:CD1	2.52	0.44
1:C:3021:PRO:HD3	1:C:3030:HIS:CD2	2.52	0.44
1:C:3183:VAL:O	1:C:3187:ARG:HG3	2.18	0.44
1:C:3590:GLU:CD	1:C:3590:GLU:H	2.26	0.44
1:C:4247:ILE:HD11	1:C:4667:PRO:HB2	1.99	0.44
1:A:1172:ASP:OD2	1:A:1172:ASP:N	2.41	0.44
1:A:2412:GLU:HG3	1:A:2415:ARG:HG2	1.99	0.44
1:A:3680:ALA:HB1	1:A:3683:GLN:NE2	2.32	0.44
1:A:4911:LEU:HA	1:A:4914:VAL:HG22	2.00	0.44
1:B:568:LEU:HD12	1:B:602:VAL:HG13	1.99	0.44
1:B:1263:THR:OG1	1:B:1266:THR:OG1	2.30	0.44
1:B:2912:THR:OG1	1:B:2913:ALA:N	2.51	0.44
1:B:3268:HIS:CD2	1:B:3272:ILE:HD12	2.53	0.44
1:B:4112:LEU:O	1:B:4115:SER:OG	2.29	0.44
1:D:530:ILE:HG22	1:D:536:ASN:HB3	1.98	0.44
1:D:1127:HIS:CE1	1:D:1128:ARG:HH21	2.35	0.44
1:D:2238:TYR:HB2	1:D:2241:ARG:HH21	1.81	0.44
1:D:2801:ASP:HA	1:D:2804:ILE:HG12	1.99	0.44
1:D:4154:VAL:HG12	1:D:4157:ASP:HB2	2.00	0.44
1:C:2974:ILE:HG13	1:C:2975:ALA:N	2.33	0.44
1:C:3420:ARG:HD3	1:C:3516:LYS:O	2.18	0.44
1:C:4827:LEU:HD23	1:C:4827:LEU:HA	1.85	0.44
1:A:921:ASN:HA	1:A:924:MET:SD	2.58	0.44
1:A:3250:MET:HE3	1:A:3250:MET:HB3	1.87	0.44
1:A:3270:ILE:HA	1:A:3274:LEU:HD12	2.00	0.44
1:A:3771:HIS:O	1:A:3815:LYS:NZ	2.43	0.44
1:B:872:GLU:O	1:B:876:GLU:HG3	2.18	0.44
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.50	0.44
1:B:2856:ASN:ND2	1:B:2858:GLN:OE1	2.47	0.44
1:B:3638:MET:SD	1:B:3638:MET:C	3.01	0.44
1:B:4837:LEU:HD22	1:B:4932:ILE:HG23	1.98	0.44
1:D:232:THR:HG21	1:D:252:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1115:LEU:HD13	1:D:1123:VAL:HG11	1.99	0.44
1:D:2023:LEU:HD22	1:D:2027:ILE:HG21	1.99	0.44
1:D:3812:VAL:O	1:D:3816:MET:HG3	2.17	0.44
1:C:35:LEU:HD11	1:C:189:LEU:HD13	1.98	0.44
1:C:127:MET:H	1:C:127:MET:CE	2.31	0.44
1:C:232:THR:HG21	1:C:252:VAL:HG21	2.00	0.44
1:C:901:LYS:HA	1:C:901:LYS:HD2	1.85	0.44
1:A:1087:ARG:HB3	1:A:1223:PHE:CD2	2.52	0.44
1:A:1229:ASN:HB2	1:A:1827:ARG:HG3	1.99	0.44
1:A:1992:ALA:HA	1:A:1995:THR:HG22	2.00	0.44
1:A:2308:GLN:OE1	1:A:2309:SER:N	2.50	0.44
1:A:3562:LYS:HE2	1:A:3562:LYS:HB2	1.89	0.44
1:A:4047:MET:HE3	1:A:4047:MET:HB3	1.89	0.44
1:B:1992:ALA:HA	1:B:1995:THR:HG22	1.99	0.44
1:B:4091:LYS:HD2	1:B:4092:ASP:H	1.83	0.44
1:B:4172:GLU:OE1	1:B:4175:ARG:NH1	2.51	0.44
1:B:4928:LEU:HD23	1:B:4931:ILE:HD12	1.99	0.44
1:D:803:LEU:HD12	1:D:803:LEU:HA	1.83	0.44
1:D:1716:ILE:O	1:D:1721:GLU:N	2.50	0.44
1:D:4885:PHE:O	1:D:4889:VAL:HG22	2.17	0.44
1:C:1986:MET:SD	1:C:1986:MET:N	2.91	0.44
1:A:501:ALA:O	1:A:505:GLU:HG3	2.18	0.43
1:A:1929:MET:HE3	1:A:1929:MET:HB3	1.84	0.43
1:A:3194:LEU:HD12	1:A:3194:LEU:HA	1.86	0.43
1:A:3248:ARG:NH1	1:A:3248:ARG:HB3	2.33	0.43
1:A:3734:HIS:O	1:A:3736:GLU:HG3	2.18	0.43
1:A:4091:LYS:HD2	1:A:4092:ASP:H	1.83	0.43
1:A:4983:HIS:O	3:A:5301:ATP:N6	2.49	0.43
1:B:4238:CYS:HA	1:B:4989:MET:HE1	1.99	0.43
1:D:499:THR:HG23	1:D:502:HIS:H	1.82	0.43
1:D:1981:MET:SD	1:D:1981:MET:N	2.91	0.43
1:D:3332:ALA:HB3	1:D:3403:ARG:NH1	2.33	0.43
1:D:4754:ASN:HB3	1:D:4756:ARG:HH21	1.82	0.43
1:C:1808:ARG:HD3	1:C:1853:ILE:HG22	2.00	0.43
1:C:3532:LEU:HA	1:C:3535:LEU:HB3	2.00	0.43
1:C:3727:ASP:OD1	1:C:3728:ILE:N	2.51	0.43
1:A:938:HIS:HB3	1:A:1054:GLU:HB3	1.99	0.43
1:A:2758:PHE:HA	1:A:2761:TYR:HB2	1.99	0.43
1:A:3203:VAL:HG12	1:A:3214:ASN:ND2	2.33	0.43
1:A:4668:LEU:HD13	1:A:4672:LYS:HD2	2.01	0.43
2:G:3:GLN:OE1	2:G:5:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLU:HG3	1:B:175:SER:HB3	1.99	0.43
1:B:2586:VAL:HG13	1:B:2607:LEU:HD13	2.00	0.43
1:B:2677:LYS:HE2	1:B:2677:LYS:HB3	1.82	0.43
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.41	0.43
1:B:3459:VAL:HG11	1:B:3503:TYR:HD1	1.82	0.43
1:D:2661:TRP:HB3	1:D:2664:PHE:HB2	2.00	0.43
1:C:1127:HIS:CE1	1:C:1128:ARG:HH21	2.36	0.43
1:C:2902:HIS:CE1	1:C:2904:LEU:HB2	2.53	0.43
1:C:3147:ILE:HB	1:C:3152:PHE:HB2	1.98	0.43
1:C:3206:LEU:HD12	1:C:3280:TYR:CD2	2.52	0.43
1:A:1773:PRO:HA	1:A:1774:PRO:HD3	1.89	0.43
1:A:1930:LYS:HE2	1:A:1930:LYS:HB2	1.88	0.43
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	2.00	0.43
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.47	0.43
1:B:1229:ASN:HB2	1:B:1827:ARG:HG3	2.01	0.43
1:B:3534:MET:HE2	1:B:3534:MET:N	2.34	0.43
1:D:3123:LYS:HG3	1:D:3125:VAL:H	1.83	0.43
1:C:614:VAL:HG22	1:C:2169:GLN:HG3	2.00	0.43
1:C:893:TYR:HB2	1:C:961:MET:CE	2.35	0.43
1:C:1044:ARG:CZ	1:C:1044:ARG:HA	2.47	0.43
1:C:4047:MET:HE3	1:C:4047:MET:HB3	1.88	0.43
1:A:1753:LYS:HB3	1:A:1758:ARG:HA	2.01	0.43
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.99	0.43
1:A:2520:HIS:O	1:A:2524:VAL:HG22	2.19	0.43
1:A:2569:PHE:CZ	1:A:2582:MET:HE1	2.54	0.43
1:A:3226:GLU:C	1:A:3228:ALA:H	2.25	0.43
1:A:3955:MET:HG2	1:A:4019:LEU:HD22	2.00	0.43
2:H:73:LYS:NZ	2:H:75:THR:OG1	2.51	0.43
1:B:19:GLU:HG2	1:B:68:THR:HG22	1.99	0.43
1:B:2520:HIS:O	1:B:2524:VAL:HG22	2.18	0.43
1:B:3332:ALA:HB3	1:B:3403:ARG:NH1	2.33	0.43
1:D:1992:ALA:HA	1:D:1995:THR:HG22	2.00	0.43
1:D:2513:GLU:OE1	1:D:2513:GLU:N	2.51	0.43
1:D:2590:SER:O	1:D:2600:ARG:NH1	2.52	0.43
1:D:3346:VAL:HG11	1:D:3414:ARG:HB2	2.01	0.43
1:D:4902:GLU:O	1:D:4913:ARG:NH1	2.47	0.43
1:D:4954:MET:HE1	1:D:4959:PHE:HB2	2.00	0.43
1:C:707:VAL:HG23	1:C:782:SER:HB3	2.00	0.43
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.48	0.43
1:C:1753:LYS:HB3	1:C:1758:ARG:HG2	1.99	0.43
1:C:4834:GLY:O	1:C:4838:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HD11	1:A:1055:PRO:HA	2.00	0.43
1:A:1668:ARG:HG3	1:A:1671:ARG:NH2	2.33	0.43
1:A:2514:ASN:N	1:A:2514:ASN:OD1	2.51	0.43
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.99	0.43
1:A:4639:MET:HE3	1:A:4639:MET:HB3	1.83	0.43
1:A:4942:GLU:OE1	1:D:4944:ARG:NH1	2.50	0.43
2:H:79:ASP:OD1	2:H:80:TYR:HD2	2.02	0.43
2:G:49:MET:HE3	2:G:49:MET:HB2	1.89	0.43
1:B:977:LEU:HD22	1:B:981:GLN:HB3	2.01	0.43
1:B:2679:PHE:HB2	1:B:2706:ILE:CG2	2.46	0.43
1:D:886:ARG:HB3	1:D:891:TRP:CG	2.52	0.43
1:D:1024:TYR:HB3	1:D:1025:ARG:HH11	1.83	0.43
1:C:2382:GLU:OE1	1:C:2385:ARG:NH1	2.51	0.43
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.33	0.43
1:B:975:VAL:HG12	1:B:1044:ARG:NH1	2.34	0.43
1:B:982:THR:HA	1:B:985:VAL:HG12	2.00	0.43
1:B:1127:HIS:CE1	1:B:1128:ARG:HH21	2.35	0.43
1:B:1427:ILE:HD13	1:B:1571:ASN:HA	1.99	0.43
1:B:1931:LEU:HG	1:B:1935:VAL:HG11	2.01	0.43
1:B:3628:ARG:HG3	1:B:3631:ALA:HB3	2.01	0.43
1:B:4749:GLU:O	1:B:4753:HIS:ND1	2.51	0.43
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.47	0.43
1:D:707:VAL:HG23	1:D:782:SER:HB3	2.01	0.43
1:D:1141:ARG:HD3	1:C:3477:LYS:HB3	1.99	0.43
1:D:1506:GLN:OE1	1:D:1507:GLY:N	2.51	0.43
1:D:2212:VAL:O	1:D:2216:GLY:N	2.49	0.43
1:D:2355:ARG:HG3	1:D:2355:ARG:NH1	2.33	0.43
1:D:2867:LEU:HD21	1:D:2871:LEU:HB3	2.01	0.43
1:D:3144:PHE:CE2	1:D:3197:LEU:HD12	2.53	0.43
1:C:3758:MET:HE3	1:C:4719:PHE:CE2	2.54	0.43
1:C:4816:ILE:H	1:C:4816:ILE:HG13	1.64	0.43
1:C:4924:VAL:HG12	1:C:4925:ILE:HD13	2.01	0.43
1:A:749:ASP:O	1:A:753:PRO:HA	2.19	0.43
1:A:820:ARG:HD3	1:A:820:ARG:HA	1.82	0.43
1:A:1995:THR:HG23	1:A:1999:ARG:CZ	2.49	0.43
1:A:3260:GLY:HA2	1:A:3325:ASN:ND2	2.33	0.43
1:A:3633:VAL:HG12	1:A:3637:ARG:HE	1.82	0.43
1:B:2012:PHE:CZ	1:B:2031:LEU:HD23	2.54	0.43
1:D:788:LYS:HB2	1:D:788:LYS:HE3	1.80	0.43
1:D:1820:ARG:HB3	1:D:1820:ARG:NH1	2.34	0.43
1:D:2531:ARG:HG2	1:D:2585:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2782:ASP:N	1:D:2782:ASP:OD1	2.51	0.43
1:D:3230:LEU:HD23	1:D:3230:LEU:H	1.84	0.43
1:C:910:PHE:HA	1:C:913:LEU:HD23	2.01	0.43
1:C:923:GLN:O	1:C:927:GLU:HG2	2.19	0.43
1:C:1022:VAL:CG1	1:C:1026:LEU:HB2	2.48	0.43
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.99	0.43
1:C:2212:VAL:HG21	1:C:2256:TYR:OH	2.19	0.43
1:C:2907:PRO:O	1:C:2910:THR:OG1	2.33	0.43
1:C:3226:GLU:C	1:C:3228:ALA:H	2.26	0.43
1:C:4122:MET:HA	1:C:4122:MET:HE3	2.00	0.43
1:C:4154:VAL:HG12	1:C:4157:ASP:HB2	1.99	0.43
1:A:803:LEU:HD12	1:A:803:LEU:HA	1.79	0.43
1:A:1127:HIS:CE1	1:A:1128:ARG:HH21	2.36	0.43
1:A:1820:ARG:O	1:A:1824:GLN:HG2	2.19	0.43
1:A:1992:ALA:O	1:A:1999:ARG:NH2	2.52	0.43
1:A:2175:GLU:OE2	1:A:2227:LYS:HB2	2.18	0.43
1:A:2198:MET:HG3	1:A:2203:MET:CE	2.49	0.43
1:B:320:LYS:HA	1:B:356:TRP:CH2	2.53	0.43
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	2.00	0.43
1:B:3067:CYS:O	1:B:3071:LEU:HG	2.19	0.43
1:B:3260:GLY:HA2	1:B:3325:ASN:ND2	2.33	0.43
1:B:3539:ARG:HA	1:B:3539:ARG:HH11	1.84	0.43
1:D:296:ASP:HB2	1:D:297:GLN:OE1	2.18	0.43
1:D:483:MET:HE2	1:D:483:MET:HA	2.00	0.43
1:D:3805:LEU:HB3	1:D:3890:LEU:HB3	2.00	0.43
1:D:4823:LEU:HD23	1:D:4823:LEU:HA	1.83	0.43
1:C:683:ARG:HG2	1:C:717:ASP:HB3	2.01	0.43
1:C:866:HIS:CG	1:C:941:MET:HG2	2.54	0.43
1:C:3717:ASP:N	1:C:3717:ASP:OD1	2.52	0.43
1:A:1424:PRO:HA	1:A:1427:ILE:HG22	2.00	0.43
1:A:1808:ARG:HB2	1:A:1854:PHE:CE1	2.53	0.43
1:A:2782:ASP:N	1:A:2782:ASP:OD1	2.51	0.43
1:A:2867:LEU:HD21	1:A:2871:LEU:HB3	2.00	0.43
1:A:3414:ARG:NH2	1:A:3469:PHE:O	2.51	0.43
1:B:664:PHE:HB3	1:B:811:CYS:SG	2.59	0.43
1:B:954:LYS:HB3	1:B:966:LYS:HE3	2.01	0.43
1:B:3316:LEU:HD21	1:B:3346:VAL:HG23	2.00	0.43
1:B:3359:ILE:HG23	1:B:3437:MET:HE1	2.01	0.43
1:D:274:LEU:HD23	1:D:274:LEU:HA	1.84	0.43
1:D:935:LEU:HG	1:D:987:ARG:HH12	1.83	0.43
1:D:2639:MET:HE3	1:D:2639:MET:HB3	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3137:LEU:HD21	1:D:3190:LEU:HD23	2.00	0.43
1:C:41:GLY:HA2	1:C:137:LEU:HD12	2.00	0.43
1:C:176:SER:OG	1:C:178:ARG:NH1	2.47	0.43
1:C:460:GLN:N	1:C:463:GLU:OE2	2.50	0.43
1:C:1036:ARG:HG2	1:C:1036:ARG:HH11	1.83	0.43
1:C:1206:GLN:HA	1:C:1227:ALA:O	2.19	0.43
1:C:1861:GLN:O	1:C:1865:MET:HE3	2.18	0.43
1:C:2312:MET:C	1:C:2312:MET:HE2	2.44	0.43
1:A:19:GLU:HG2	1:A:68:THR:HG22	2.01	0.43
1:A:985:VAL:HG22	1:A:1043:VAL:HG21	2.00	0.43
1:A:2309:SER:OG	1:A:2320:ASP:OD1	2.35	0.43
1:A:3471:THR:HG22	1:B:1170:MET:HE1	2.00	0.43
2:E:2:VAL:HG21	2:E:61:GLU:HB2	2.01	0.43
2:H:58:GLY:HA3	2:H:76:ILE:HD12	2.00	0.43
2:F:17:LYS:HB2	2:F:17:LYS:HZ3	1.84	0.43
1:D:41:GLY:HA2	1:D:137:LEU:HD12	2.00	0.43
1:D:451:TYR:CZ	1:D:474:ARG:HD2	2.54	0.43
1:D:2293:GLN:H	1:D:2293:GLN:CD	2.20	0.43
1:D:2815:ALA:HB1	1:D:2881:ASN:ND2	2.34	0.43
1:C:323:LEU:HB3	1:C:325:THR:HG23	2.01	0.43
1:C:986:ASP:OD2	1:C:986:ASP:N	2.51	0.43
1:C:2099:SER:O	1:C:2103:VAL:HG12	2.19	0.43
1:C:3256:LEU:HD23	1:C:3256:LEU:HA	1.79	0.43
1:C:3648:ARG:O	1:C:3652:MET:HG3	2.19	0.43
1:A:1575:LEU:HD23	1:A:1575:LEU:HA	1.87	0.42
1:A:2462:PRO:HB2	1:A:2464:ASP:OD1	2.19	0.42
1:A:2578:MET:HB3	1:A:2578:MET:HE2	1.89	0.42
1:A:2629:ASP:O	1:A:2632:ILE:HD12	2.19	0.42
1:A:3514:LEU:HD11	1:A:3602:VAL:HG13	2.00	0.42
1:A:3688:GLU:C	1:A:3690:VAL:H	2.27	0.42
1:A:3969:ILE:HG21	1:A:3980:LEU:HD12	2.01	0.42
1:A:4885:PHE:O	1:A:4889:VAL:HG22	2.18	0.42
2:E:49:MET:HE3	2:E:49:MET:HB2	1.89	0.42
1:B:749:ASP:O	1:B:753:PRO:HA	2.19	0.42
1:B:3250:MET:HE3	1:B:3250:MET:HB3	1.83	0.42
1:B:3734:HIS:O	1:B:3736:GLU:HG3	2.18	0.42
1:B:3836:MET:HE3	1:B:3836:MET:HB2	1.83	0.42
1:D:793:LEU:HD12	1:D:821:LEU:HD21	2.00	0.42
1:D:878:ILE:HA	1:D:881:LEU:HD23	2.00	0.42
1:D:893:TYR:CG	1:D:894:GLY:N	2.86	0.42
1:D:1023:PRO:HB3	1:D:1025:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2700:MET:HB3	1:D:2700:MET:HE3	1.82	0.42
1:D:3601:ALA:O	1:D:3605:HIS:HD2	2.01	0.42
1:D:3695:PRO:HB3	1:D:3699:HIS:HB3	2.01	0.42
1:D:3872:GLU:HG3	1:D:3874:VAL:H	1.84	0.42
1:C:275:ARG:HG2	1:C:275:ARG:HH11	1.84	0.42
1:C:451:TYR:CZ	1:C:474:ARG:HD2	2.54	0.42
1:C:1128:ARG:HG2	1:C:1130:GLN:HG3	2.01	0.42
1:C:3002:LEU:O	1:C:3006:ILE:N	2.37	0.42
1:C:3003:LEU:HB2	1:C:3004:PRO:HD3	2.01	0.42
1:C:3715:LYS:HD2	1:C:3715:LYS:C	2.44	0.42
1:C:4177:TYR:CE1	1:C:4199:GLU:HG3	2.54	0.42
1:C:4821:LYS:H	1:C:4821:LYS:HD3	1.84	0.42
1:A:568:LEU:HD12	1:A:602:VAL:HG13	2.01	0.42
1:A:883:ALA:HB1	1:A:907:LEU:HD12	2.01	0.42
1:A:897:ARG:NH2	1:A:899:ASP:OD1	2.52	0.42
1:A:2128:TYR:CG	1:A:3673:MET:HE3	2.54	0.42
1:A:2586:VAL:HG13	1:A:2607:LEU:HD13	2.00	0.42
1:A:3836:MET:HE2	1:A:3836:MET:HB2	1.94	0.42
1:A:4090:LYS:HG2	1:A:4123:ILE:HD11	2.02	0.42
2:E:73:LYS:NZ	2:E:75:THR:OG1	2.52	0.42
2:F:73:LYS:NZ	2:F:75:THR:OG1	2.53	0.42
1:B:81:MET:HE1	1:B:147:TRP:CZ2	2.55	0.42
1:B:321:GLU:OE2	1:B:323:LEU:HD22	2.19	0.42
1:B:491:ILE:O	1:B:495:ASN:HB2	2.19	0.42
1:B:1668:ARG:HE	1:B:1668:ARG:HB2	1.63	0.42
1:B:2211:MET:HE1	1:B:2236:LEU:HD12	2.00	0.42
1:B:2992:GLU:OE2	1:B:2996:LYS:NZ	2.41	0.42
1:D:1739:THR:HG22	1:D:2146:PRO:HB3	2.00	0.42
1:D:2191:PHE:HE1	1:D:2238:TYR:HE2	1.66	0.42
1:D:2912:THR:HG23	1:D:2914:LYS:HG3	2.00	0.42
1:C:227:MET:HE2	1:C:227:MET:N	2.33	0.42
1:C:233:ILE:HD12	1:C:242:ARG:HB3	2.01	0.42
1:C:1008:SER:HB3	1:C:1017:ARG:HB3	2.01	0.42
1:C:1451:GLY:CA	1:C:1494:MET:HG2	2.48	0.42
1:C:1965:TYR:HE2	1:C:2030:ASP:HB3	1.84	0.42
1:C:2224:ARG:H	1:C:2224:ARG:CD	2.31	0.42
1:C:3266:MET:HB2	1:C:3269:VAL:HB	1.99	0.42
1:C:3414:ARG:HB2	1:C:3414:ARG:HH11	1.84	0.42
1:C:3573:MET:O	1:C:3577:ARG:HG2	2.20	0.42
1:A:2101:MET:HE2	1:A:2101:MET:HB3	1.79	0.42
1:A:2801:ASP:HA	1:A:2804:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3011:THR:OG1	1:A:3070:ILE:HD13	2.20	0.42
1:A:3765:TYR:CD2	1:A:4753:HIS:HA	2.54	0.42
1:A:4546:VAL:HA	1:A:4549:VAL:HG22	2.01	0.42
1:B:722:TRP:CZ2	1:B:727:ALA:HB2	2.55	0.42
1:B:2189:LYS:HA	1:B:2192:TYR:CD1	2.54	0.42
1:B:3556:ASN:HB3	1:B:3559:LEU:HD23	2.01	0.42
1:B:3621:HIS:C	1:B:3622:LYS:HG3	2.45	0.42
1:B:4056:GLU:HG2	1:B:4166:LEU:HD13	2.01	0.42
1:B:4686:LEU:HD12	1:B:4690:GLU:HG3	2.01	0.42
1:D:877:ASN:O	1:D:881:LEU:HD22	2.20	0.42
1:D:1018:ASN:HB3	1:D:1021:LEU:HB2	2.01	0.42
1:D:1733:GLU:HG2	1:D:2201:LEU:HD23	2.01	0.42
1:D:3527:PRO:CA	1:D:3530:GLN:HE22	2.33	0.42
1:D:3695:PRO:HB2	1:D:3700:GLN:HG2	2.01	0.42
1:D:3823:LYS:HD3	1:D:3823:LYS:HA	1.86	0.42
1:D:4839:MET:HA	1:D:4839:MET:HE3	2.01	0.42
1:C:328:LYS:HB3	1:C:328:LYS:HE3	1.78	0.42
1:C:975:VAL:HG11	1:C:1047:LEU:HB3	2.01	0.42
1:C:2191:PHE:CD2	1:C:2198:MET:HG3	2.54	0.42
1:C:2668:SER:O	1:C:2669:GLU:HB3	2.19	0.42
1:C:3715:LYS:HD2	1:C:3715:LYS:O	2.20	0.42
1:C:3962:PHE:CZ	1:C:4023:MET:HG3	2.54	0.42
1:A:590:LEU:HG	1:A:599:VAL:HG11	2.01	0.42
1:A:664:PHE:HB3	1:A:811:CYS:SG	2.59	0.42
1:A:707:VAL:HG23	1:A:782:SER:HB3	2.02	0.42
1:A:3105:LYS:O	1:A:3108:GLU:HG3	2.19	0.42
1:A:4217:PHE:O	1:A:4221:VAL:HG22	2.20	0.42
2:F:2:VAL:HG22	2:F:58:GLY:HA2	2.00	0.42
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.51	0.42
1:B:1808:ARG:HB2	1:B:1854:PHE:CE1	2.55	0.42
1:B:2534:ALA:HA	1:B:2588:ARG:HH21	1.84	0.42
1:D:140:ASP:OD1	1:D:142:THR:HG22	2.19	0.42
1:D:3648:ARG:O	1:D:3652:MET:HG3	2.19	0.42
1:D:4918:ILE:HD12	1:D:4919:THR:HG23	2.02	0.42
1:C:856:VAL:HG12	1:C:991:ASN:ND2	2.35	0.42
1:C:1072:VAL:HG13	1:C:1193:SER:HB2	2.00	0.42
1:C:1805:GLU:CD	1:C:1805:GLU:H	2.27	0.42
1:C:2884:ASN:OD1	1:C:2885:THR:N	2.52	0.42
1:C:3501:ASP:OD1	1:C:3501:ASP:N	2.51	0.42
1:A:1851:MET:HE2	1:A:1853:ILE:HD11	2.00	0.42
1:A:2012:PHE:CZ	1:A:2031:LEU:HD23	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3230:LEU:HD23	1:A:3230:LEU:H	1.84	0.42
1:A:3391:GLU:HG3	1:A:3395:ARG:HE	1.84	0.42
1:A:4778:TRP:O	1:A:4782:VAL:HG23	2.19	0.42
2:H:84:ALA:O	2:H:93:PRO:HB3	2.20	0.42
1:B:618:GLN:OE1	1:B:1678:ASN:ND2	2.43	0.42
1:B:3689:GLU:C	1:B:3691:GLU:H	2.27	0.42
1:B:3780:LEU:HD11	1:B:3816:MET:HG2	2.00	0.42
1:D:3734:HIS:CG	1:D:3735:LEU:N	2.88	0.42
1:C:19:GLU:HG2	1:C:68:THR:HG22	2.01	0.42
1:C:2135:LEU:HD22	1:C:3658:LYS:HE3	2.01	0.42
1:C:2516:ASP:OD1	1:C:2516:ASP:N	2.52	0.42
1:C:2578:MET:HE3	1:C:2579:VAL:N	2.34	0.42
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	2.01	0.42
1:C:4090:LYS:HD3	1:C:4121:GLU:HG2	2.00	0.42
1:C:4732:PHE:CD1	1:C:4732:PHE:N	2.88	0.42
1:A:330:ASP:OD1	1:A:330:ASP:N	2.53	0.42
1:A:1694:LEU:O	1:A:1698:LEU:HG	2.20	0.42
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.83	0.42
1:A:2992:GLU:OE2	1:A:2996:LYS:NZ	2.41	0.42
1:A:3591:LYS:HA	1:A:3594:ARG:HH11	1.84	0.42
1:A:3751:VAL:HG13	1:A:3755:GLU:HG2	2.02	0.42
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.79	0.42
2:H:54:GLU:H	2:H:54:GLU:HG3	1.69	0.42
1:B:2584[B]:HIS:CE1	1:B:2625:ARG:HG3	2.55	0.42
1:B:3321:ARG:HA	1:B:3324:VAL:HG12	2.02	0.42
1:B:4047:MET:HE3	1:B:4047:MET:HB3	1.88	0.42
1:B:4953:ASP:OD1	1:B:4957:LYS:NZ	2.53	0.42
1:D:1981:MET:HA	1:D:1981:MET:HE3	2.01	0.42
1:D:2031:LEU:HD11	1:D:3657:TYR:CE1	2.55	0.42
1:D:2628:PHE:C	1:D:2628:PHE:CD1	2.98	0.42
1:D:3186:LEU:O	1:D:3190:LEU:HG	2.20	0.42
1:D:3689:GLU:C	1:D:3691:GLU:H	2.27	0.42
1:D:4827:LEU:HD23	1:D:4827:LEU:HA	1.83	0.42
1:C:892:THR:O	1:C:904:HIS:N	2.51	0.42
1:C:1623:ARG:NH1	1:C:1623:ARG:HB2	2.35	0.42
1:C:2962:GLN:HE22	1:C:2965:ARG:HH11	1.66	0.42
1:C:3291:ALA:O	1:C:3293:PRO:HD3	2.19	0.42
1:C:3959:LYS:NZ	1:C:4022:ASP:OD2	2.42	0.42
1:C:4779:LYS:O	1:C:4783:ILE:HG12	2.19	0.42
1:A:208:CYS:O	1:A:334:MET:HG3	2.19	0.42
1:A:1559:GLN:OE1	1:A:1559:GLN:N	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.52	0.42
1:A:3996:PHE:CD2	1:A:4020:GLN:HG2	2.55	0.42
2:E:18:ARG:HB2	2:E:18:ARG:HH11	1.85	0.42
1:B:590:LEU:HG	1:B:599:VAL:HG11	2.02	0.42
1:B:1943:LEU:HB2	1:B:2123:LEU:HD21	2.01	0.42
1:B:2423:MET:HG3	1:B:2498:HIS:CD2	2.55	0.42
1:B:2957:PHE:HE2	1:B:3034:LYS:HG3	1.85	0.42
1:B:2973:PHE:CD1	1:B:2995:ILE:HG12	2.54	0.42
1:B:3457:ASN:OD1	1:B:3457:ASN:C	2.62	0.42
1:B:3996:PHE:CD2	1:B:4020:GLN:HG2	2.55	0.42
1:D:664:PHE:HB3	1:D:811:CYS:SG	2.60	0.42
1:D:878:ILE:O	1:D:882:TRP:HD1	2.02	0.42
1:D:893:TYR:CD1	1:D:905:PRO:HA	2.55	0.42
1:D:2754:PHE:HE2	1:D:2813:LEU:HD11	1.83	0.42
1:D:3003:LEU:HB2	1:D:3004:PRO:HD3	2.02	0.42
1:D:3296:LEU:HB3	1:D:3297:PRO:HD3	2.01	0.42
1:C:867:LEU:HB3	1:C:929:LEU:HD12	2.02	0.42
1:C:879:HIS:CE1	1:C:918:ARG:HA	2.55	0.42
1:C:1286:MET:HE1	1:C:1553:PHE:HB3	2.01	0.42
1:C:2537:ASP:OD2	1:C:2588:ARG:NH1	2.52	0.42
1:C:3320:LEU:HD12	1:C:3320:LEU:HA	1.87	0.42
1:A:879:HIS:NE2	1:A:921:ASN:HB2	2.35	0.42
1:A:2203:MET:HE2	1:A:2203:MET:HB2	1.85	0.42
1:A:3570:ARG:HB2	1:A:3570:ARG:HH11	1.84	0.42
1:A:3577:ARG:HA	1:A:3577:ARG:NE	2.35	0.42
1:B:1753:LYS:HD3	1:B:1759:ARG:N	2.35	0.42
1:B:2498:HIS:O	1:B:2502:MET:HG2	2.19	0.42
1:B:2611:CYS:HA	1:B:2614:ILE:HG22	2.02	0.42
1:B:3346:VAL:HG11	1:B:3414:ARG:HB3	2.01	0.42
1:B:4092:ASP:HA	1:B:4095:LYS:HG2	2.02	0.42
1:B:4571:PHE:CE2	1:B:4816:ILE:HD13	2.55	0.42
1:B:4853:VAL:O	1:B:4857:ASN:ND2	2.52	0.42
1:D:1297:PHE:CE2	1:D:1525:GLY:HA2	2.55	0.42
1:D:2107:GLN:CD	1:D:3681:GLY:HA3	2.44	0.42
1:D:3416:VAL:O	1:D:3420:ARG:N	2.50	0.42
1:D:4158:PRO:HA	1:D:4161:ARG:CZ	2.49	0.42
1:D:4247:ILE:HD11	1:D:4667:PRO:HB2	2.01	0.42
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.42	0.42
1:C:947:GLU:HA	1:C:1049:TYR:HD1	1.85	0.42
1:C:976:ARG:N	1:C:976:ARG:HD2	2.34	0.42
1:C:2218:GLY:HA3	1:C:2224:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2588:ARG:NH2	1:C:2589:LEU:HD23	2.34	0.42
1:C:2615:ARG:HG2	1:C:2664:PHE:CE2	2.55	0.42
1:C:2785:LEU:C	1:C:2786:LYS:HG3	2.45	0.42
1:C:3044:CYS:SG	1:C:3092:LEU:HA	2.60	0.42
1:C:3532:LEU:HD23	1:C:3535:LEU:HD13	2.02	0.42
1:C:3805:LEU:HB3	1:C:3890:LEU:HB3	2.00	0.42
1:C:4686:LEU:O	1:C:4690:GLU:HG2	2.19	0.42
1:A:426:ARG:NH2	1:A:509:GLU:OE2	2.53	0.42
1:A:793:LEU:HD12	1:A:821:LEU:HD21	2.01	0.42
1:A:1838:PHE:CZ	1:A:1929:MET:HE1	2.54	0.42
1:A:1948:ASP:OD1	1:A:2126:ARG:NH2	2.47	0.42
1:A:2639:MET:HE3	1:A:2640:PRO:HD3	2.00	0.42
1:B:208:CYS:O	1:B:334:MET:HG3	2.19	0.42
1:B:707:VAL:HG23	1:B:782:SER:HB3	2.01	0.42
1:B:2386:ILE:O	1:B:2393:ASP:HB2	2.20	0.42
1:B:2518:LEU:O	1:B:2521:VAL:HG12	2.19	0.42
1:B:2991:HIS:O	1:B:2995:ILE:HG13	2.19	0.42
1:B:3391:GLU:HG3	1:B:3395:ARG:HE	1.85	0.42
1:B:3400:VAL:HG23	1:B:3403:ARG:HH21	1.85	0.42
1:B:3771:HIS:O	1:B:3815:LYS:NZ	2.44	0.42
1:B:4651:THR:HG23	1:B:4796:MET:HE1	2.01	0.42
1:D:3158:LEU:HD23	1:D:3158:LEU:HA	1.84	0.42
1:D:3226:GLU:O	1:D:3227:ARG:HB3	2.20	0.42
1:D:3529:ASP:O	1:D:3533:ILE:HG12	2.20	0.42
1:D:4067:LYS:NZ	1:D:4102:GLN:O	2.46	0.42
1:C:938:HIS:HB3	1:C:1054:GLU:HB3	2.02	0.42
1:C:1043:VAL:HG12	1:C:1044:ARG:HH12	1.84	0.42
1:C:1860:LYS:O	1:C:1864:LYS:HG2	2.20	0.42
1:A:2668:SER:C	1:A:2670:GLU:H	2.27	0.42
1:A:2912:THR:HG23	1:A:2914:LYS:HG3	2.02	0.42
1:A:3332:ALA:HB3	1:A:3403:ARG:NH1	2.35	0.42
1:B:2785:LEU:C	1:B:2786:LYS:HG3	2.45	0.42
1:B:3209:GLN:HG2	1:B:3210:LEU:HG	2.01	0.42
1:B:4820:VAL:HB	1:B:4823:LEU:HB2	2.02	0.42
1:D:2697:ARG:NH1	1:D:2697:ARG:HB3	2.34	0.42
1:D:3412:LEU:HD11	1:D:3434:LEU:HD21	2.02	0.42
1:D:4816:ILE:HD12	1:D:4817:ALA:N	2.35	0.42
1:C:365:LYS:HB3	1:C:365:LYS:HE3	1.85	0.42
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.47	0.42
1:C:2107:GLN:CD	1:C:3681:GLY:HA3	2.45	0.42
1:C:3695:PRO:HB3	1:C:3699:HIS:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4568:PHE:CD1	1:C:4568:PHE:C	2.98	0.42
1:A:2123:LEU:HD12	1:A:2123:LEU:HA	1.94	0.41
1:A:2177:LEU:HA	1:A:2180:GLN:HG2	2.02	0.41
1:B:1206:GLN:HA	1:B:1227:ALA:O	2.20	0.41
1:B:2198:MET:HE2	1:B:2198:MET:N	2.34	0.41
1:B:2355:ARG:NH2	1:B:2449:GLU:OE2	2.51	0.41
1:B:2600:ARG:O	1:B:2604:GLU:HG3	2.20	0.41
1:B:2754:PHE:HB2	1:B:2935:TYR:OH	2.20	0.41
1:B:3633:VAL:HG13	1:B:3637:ARG:HH21	1.85	0.41
1:B:3648:ARG:HG3	1:B:3648:ARG:NH1	2.35	0.41
1:B:3722:TYR:CE2	1:B:3782:MET:HE2	2.55	0.41
1:D:722:TRP:CZ2	1:D:727:ALA:HB2	2.55	0.41
1:D:1929:MET:HB3	1:D:1929:MET:HE2	1.72	0.41
1:D:2309:SER:OG	1:D:2320:ASP:OD1	2.38	0.41
1:D:2630:VAL:HG22	1:D:2640:PRO:HB2	2.02	0.41
1:D:2819:TRP:O	1:D:2820:GLU:HG3	2.20	0.41
1:D:3562:LYS:HE2	1:D:3562:LYS:HB2	1.87	0.41
1:D:3596:VAL:O	1:D:3600:SER:OG	2.31	0.41
1:D:3638:MET:SD	1:D:3638:MET:C	3.03	0.41
1:D:3715:LYS:HD2	1:D:3715:LYS:O	2.20	0.41
1:C:3270:ILE:HG23	1:C:3338:LEU:HD11	2.02	0.41
1:C:3557:LEU:HD22	1:C:3592:ILE:HD12	2.02	0.41
1:C:3689:GLU:C	1:C:3691:GLU:H	2.28	0.41
1:C:3734:HIS:CG	1:C:3735:LEU:N	2.88	0.41
1:C:4000:MET:SD	1:C:4020:GLN:NE2	2.76	0.41
1:C:4632:LEU:HD13	1:C:4639:MET:HG2	2.02	0.41
1:A:647:ASN:ND2	1:A:820:ARG:O	2.39	0.41
1:A:722:TRP:CZ2	1:A:727:ALA:HB2	2.55	0.41
1:A:887:ILE:HG13	1:A:955:LEU:HD11	2.02	0.41
1:A:2231:SER:HA	1:A:2234:ARG:NH2	2.35	0.41
1:A:4772:ASP:O	1:A:4776:GLN:HG2	2.20	0.41
2:E:79:ASP:OD1	2:E:80:TYR:HD2	2.02	0.41
2:G:79:ASP:OD1	2:G:80:TYR:HD1	2.02	0.41
2:F:3:GLN:OE1	2:F:5:GLU:HG3	2.19	0.41
1:B:3765:TYR:CD2	1:B:4753:HIS:HA	2.55	0.41
1:B:4675:LYS:O	1:B:4679:ARG:HG3	2.20	0.41
1:B:4791:TYR:CE1	1:B:4818:MET:HE2	2.56	0.41
1:D:1786:LEU:HD23	1:D:1786:LEU:HA	1.84	0.41
1:C:182:LEU:HB3	1:C:198:THR:HG21	2.03	0.41
1:C:889:GLN:HB3	1:C:902:ARG:HH21	1.86	0.41
1:C:1634:LEU:HD23	1:C:1634:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2312:MET:HE1	1:C:2313:LEU:HD12	2.01	0.41
1:C:2527:LEU:HA	1:C:2527:LEU:HD12	1.80	0.41
1:C:3604:TYR:O	1:C:3608:GLN:HG2	2.21	0.41
1:A:156:GLN:HE21	1:D:385:ASP:HB3	1.85	0.41
1:A:2588:ARG:HH21	1:A:2589:LEU:HD23	1.85	0.41
1:A:3734:HIS:CG	1:A:3735:LEU:N	2.89	0.41
2:E:57:ARG:HE	2:E:57:ARG:HB3	1.55	0.41
1:B:938:HIS:HB3	1:B:1054:GLU:HB3	2.01	0.41
1:B:945:LYS:HD2	1:B:946:ALA:N	2.36	0.41
1:B:1694:LEU:O	1:B:1698:LEU:HG	2.20	0.41
1:B:1867:GLU:OE2	1:B:1928:GLN:NE2	2.53	0.41
1:B:2490:MET:HE3	1:B:2545:GLU:CB	2.50	0.41
1:B:4567:LEU:HD21	1:B:4816:ILE:HD12	2.01	0.41
1:D:2208:MET:HE3	1:D:2208:MET:HB2	1.67	0.41
1:D:2677:LYS:HE2	1:D:2677:LYS:HB3	1.82	0.41
1:D:3147:ILE:HG23	1:D:3152:PHE:HB2	2.01	0.41
1:D:3717:ASP:OD1	1:D:3717:ASP:N	2.52	0.41
1:D:4568:PHE:CD1	1:D:4568:PHE:C	2.98	0.41
1:C:1231[B]:GLN:H	1:C:1231[B]:GLN:HG3	1.61	0.41
1:C:2475:GLN:HG3	1:C:2488:PRO:HG3	2.02	0.41
1:C:2700:MET:HE3	1:C:2700:MET:HB3	1.85	0.41
1:A:550:LYS:HB3	1:A:560:ILE:HD13	2.03	0.41
1:A:829:TYR:CE1	1:A:1608:MET:HG2	2.55	0.41
1:A:2534:ALA:HA	1:A:2588:ARG:NH2	2.31	0.41
1:A:2881:ASN:HA	1:A:2884:ASN:HD21	1.85	0.41
1:A:3445:TRP:NE1	1:A:3455:GLU:OE1	2.45	0.41
1:A:4749:GLU:O	1:A:4753:HIS:ND1	2.53	0.41
2:H:13:ARG:HB2	2:H:13:ARG:NH1	2.36	0.41
1:B:1996:ARG:NH2	1:B:1999:ARG:HE	2.10	0.41
1:B:2175:GLU:OE2	1:B:2227:LYS:HB2	2.19	0.41
1:B:2527:LEU:O	1:B:2531:ARG:HG3	2.20	0.41
1:B:2765:LYS:NZ	1:B:2860:PRO:HA	2.35	0.41
1:B:3688:GLU:C	1:B:3690:VAL:H	2.28	0.41
1:B:3858:MET:HE2	1:B:3859:VAL:O	2.19	0.41
1:D:1992:ALA:O	1:D:1996:ARG:HG2	2.20	0.41
1:D:2214:VAL:HG21	1:D:2228:MET:SD	2.61	0.41
1:D:3100:SER:OG	1:D:3164:SER:O	2.33	0.41
1:D:3508:SER:OG	1:D:3510:ILE:HG22	2.19	0.41
1:C:722:TRP:CZ2	1:C:727:ALA:HB2	2.55	0.41
1:C:1291:LEU:HD12	1:C:1550:PRO:HG2	2.02	0.41
1:C:3060:ASP:O	1:C:3064:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.02	0.41
1:C:3209:GLN:HG2	1:C:3210:LEU:HG	2.02	0.41
1:C:3780:LEU:HD11	1:C:3816:MET:HG2	2.01	0.41
1:C:3946:GLN:HE22	1:C:3949:ARG:NH1	2.18	0.41
1:A:157:ARG:CZ	1:A:164:ARG:HE	2.34	0.41
1:A:929:LEU:O	1:A:932:LEU:HD23	2.20	0.41
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	2.01	0.41
1:A:3266:MET:HG3	1:A:3266:MET:O	2.20	0.41
1:A:3362:ILE:HG22	1:A:3437:MET:HB3	2.03	0.41
1:A:4868:ASP:OD1	1:A:4871:GLU:HG3	2.19	0.41
2:E:84:ALA:O	2:E:93:PRO:HB3	2.21	0.41
2:G:18:ARG:HB2	2:G:18:ARG:HH11	1.85	0.41
1:B:788:LYS:HB2	1:B:788:LYS:HE3	1.80	0.41
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.52	0.41
1:B:1297:PHE:CE2	1:B:1525:GLY:HA2	2.55	0.41
1:B:2607:LEU:HD23	1:B:2639:MET:SD	2.60	0.41
1:B:3788:GLY:HA3	1:B:3834:ALA:HB3	2.02	0.41
1:B:4769:MET:SD	1:B:4769:MET:N	2.78	0.41
1:B:4772:ASP:O	1:B:4776:GLN:HG2	2.20	0.41
1:D:648:ILE:HD13	1:D:811:CYS:HB3	2.02	0.41
1:D:2785:LEU:C	1:D:2786:LYS:HG3	2.45	0.41
1:D:3240:CYS:HB3	1:D:3243:ILE:HG12	2.01	0.41
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	2.01	0.41
1:D:3554:GLN:O	1:D:3557:LEU:HD22	2.20	0.41
1:D:4821:LYS:H	1:D:4821:LYS:CD	2.29	0.41
1:C:3035:GLU:O	1:C:3039:ILE:HG22	2.21	0.41
1:C:3154:ASP:O	1:C:3158:LEU:HD21	2.19	0.41
1:C:3227:ARG:HB3	1:C:3232:LEU:HD12	2.02	0.41
1:C:3346:VAL:HG11	1:C:3414:ARG:HB3	2.02	0.41
1:C:4695:ASP:OD1	1:C:4695:ASP:N	2.47	0.41
1:A:70:GLU:OE2	1:A:110:ARG:NE	2.45	0.41
1:A:663:TYR:CD2	1:A:804:PRO:HB3	2.55	0.41
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	2.03	0.41
1:A:1867:GLU:OE2	1:A:1928:GLN:NE2	2.51	0.41
1:A:2413:GLU:N	1:A:2413:GLU:OE2	2.54	0.41
1:A:2637:ALA:C	1:A:2640:PRO:HD2	2.45	0.41
1:A:2785:LEU:C	1:A:2786:LYS:HG3	2.45	0.41
1:A:2974:ILE:HG13	1:A:2975:ALA:N	2.35	0.41
1:A:3823:LYS:HA	1:A:3823:LYS:HD3	1.82	0.41
1:B:33:LEU:HD12	1:B:53:SER:HB2	2.02	0.41
1:B:70:GLU:OE2	1:B:110:ARG:NE	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:ASN:CG	1:B:970:LEU:HD12	2.46	0.41
1:B:2212:VAL:HG21	1:B:2256:TYR:OH	2.21	0.41
1:B:2222:GLU:O	1:B:2224:ARG:NH2	2.54	0.41
1:B:2440:MET:HE2	1:B:2440:MET:HA	2.03	0.41
1:B:4205:TRP:HZ3	1:B:4989:MET:HE3	1.85	0.41
1:B:4911:LEU:HA	1:B:4914:VAL:HG22	2.03	0.41
1:D:365:LYS:HE3	1:D:365:LYS:HB3	1.80	0.41
1:D:3546:ASP:O	1:D:3550:ARG:HG3	2.21	0.41
1:C:955:LEU:HD12	1:C:967:PRO:HD2	2.02	0.41
1:C:1229:ASN:HB2	1:C:1827:ARG:HG3	2.02	0.41
1:C:3688:GLU:C	1:C:3690:VAL:H	2.28	0.41
1:A:99:ARG:H	1:A:99:ARG:NE	2.19	0.41
1:A:866:HIS:O	1:A:869:ARG:NH1	2.54	0.41
1:A:1206:GLN:HA	1:A:1227:ALA:O	2.21	0.41
1:A:1782:PHE:CD1	2:E:90:ILE:HD13	2.55	0.41
1:A:2516:ASP:N	1:A:2516:ASP:OD1	2.54	0.41
1:A:2633:LEU:O	1:A:2689:LYS:NZ	2.53	0.41
1:A:3529:ASP:O	1:A:3533:ILE:HG13	2.20	0.41
1:A:3621:HIS:C	1:A:3622:LYS:HG3	2.45	0.41
1:B:884:LEU:HG	1:B:955:LEU:HD21	2.03	0.41
1:B:2001:PRO:O	1:B:2005:GLN:HG3	2.21	0.41
1:B:2149:VAL:O	1:B:2153:MET:HG2	2.20	0.41
1:B:2371:GLU:OE1	1:C:128:THR:HB	2.20	0.41
1:B:2881:ASN:HA	1:B:2884:ASN:HD21	1.85	0.41
1:B:3183:VAL:O	1:B:3187:ARG:HG3	2.21	0.41
1:B:3277:LEU:HD23	1:B:3277:LEU:HA	1.90	0.41
1:B:3731:LYS:HA	1:B:3734:HIS:HE1	1.86	0.41
1:B:3969:ILE:HG21	1:B:3980:LEU:HD12	2.01	0.41
1:B:4217:PHE:O	1:B:4221:VAL:HG22	2.20	0.41
1:D:749:ASP:O	1:D:753:PRO:HA	2.20	0.41
1:D:1759:ARG:HD3	1:D:1760:HIS:H	1.85	0.41
1:D:2247:GLN:HE21	1:D:2279:SER:C	2.28	0.41
1:D:3527:PRO:HA	1:D:3530:GLN:HE22	1.84	0.41
1:D:4772:ASP:O	1:D:4776:GLN:HG2	2.21	0.41
1:C:957:LYS:HD3	1:C:957:LYS:H	1.86	0.41
1:C:2490:MET:HE3	1:C:2545:GLU:HB2	2.03	0.41
1:C:4207:MET:HG2	1:C:4209:GLN:HE22	1.85	0.41
1:C:4722:ARG:HH11	1:C:4722:ARG:HG2	1.85	0.41
1:C:4878:ASP:OD1	1:C:4879:MET:N	2.54	0.41
1:A:309:THR:O	1:A:313:SER:OG	2.31	0.41
1:A:1506:GLN:CG	1:A:1507:GLY:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4968:PHE:O	1:A:4974:GLY:HA3	2.21	0.41
2:G:13:ARG:NH1	2:G:13:ARG:HB2	2.36	0.41
2:F:79:ASP:OD1	2:F:80:TYR:HD2	2.02	0.41
1:B:13:PHE:CE1	1:B:164:ARG:HG2	2.55	0.41
1:B:273:HIS:O	1:B:275:ARG:NH1	2.53	0.41
1:B:1008:SER:HB3	1:B:1017:ARG:HB3	2.02	0.41
1:B:1107:PRO:HD2	1:B:1186:ASP:CG	2.45	0.41
1:B:1534:LYS:H	1:B:1534:LYS:HG2	1.70	0.41
1:B:1773:PRO:HA	1:B:2153:MET:HE1	2.03	0.41
1:B:2263:ILE:HD12	1:B:2263:ILE:HA	1.95	0.41
1:B:2431:ASP:O	1:B:2435:ARG:HG3	2.21	0.41
1:B:2697:ARG:NH1	1:B:2697:ARG:HB3	2.36	0.41
1:B:2801:ASP:HA	1:B:2804:ILE:HG12	2.01	0.41
1:B:3158:LEU:HD23	1:B:3158:LEU:HA	1.78	0.41
1:B:3539:ARG:HB2	1:B:3549:VAL:HG12	2.02	0.41
1:D:663:TYR:CD2	1:D:804:PRO:HB3	2.56	0.41
1:D:774:ASP:OD1	1:D:774:ASP:N	2.51	0.41
1:D:2020:ASP:OD1	1:D:2020:ASP:N	2.47	0.41
1:D:2277:ALA:O	1:D:2281:ILE:HG13	2.20	0.41
1:D:2538:THR:O	1:D:2542:SER:HB2	2.21	0.41
1:D:2580:ASP:OD1	1:D:2621:HIS:HB2	2.21	0.41
1:D:3263:TYR:HD1	1:D:3270:ILE:HD12	1.86	0.41
1:D:3621:HIS:C	1:D:3622:LYS:HG3	2.46	0.41
1:D:3688:GLU:C	1:D:3690:VAL:H	2.29	0.41
1:D:3971:GLY:N	1:D:3972:PRO:HA	2.36	0.41
1:D:4930:ALA:HB2	1:C:4933:GLN:HG3	2.03	0.41
1:C:887:ILE:HD12	1:C:887:ILE:HA	1.85	0.41
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.51	0.41
1:C:3106:MET:SD	1:C:3110:LEU:HD13	2.61	0.41
1:C:4060:LYS:HD2	1:C:4060:LYS:HA	1.93	0.41
1:C:4989:MET:HE3	1:C:4989:MET:HB3	1.84	0.41
1:A:293:LEU:HD13	1:A:378:LEU:HD12	2.02	0.41
1:A:977:LEU:HG	1:A:1044:ARG:HH11	1.85	0.41
1:A:1008:SER:HB3	1:A:1017:ARG:HB3	2.02	0.41
1:A:1049:TYR:HB3	1:A:1051:TYR:CZ	2.56	0.41
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	2.03	0.41
1:A:3277:LEU:HD23	1:A:3277:LEU:HA	1.92	0.41
1:A:3343:GLN:O	1:A:3346:VAL:HG12	2.21	0.41
1:A:3459:VAL:HG11	1:A:3503:TYR:HD1	1.86	0.41
1:A:3689:GLU:C	1:A:3691:GLU:H	2.27	0.41
1:A:4651:THR:HG23	1:A:4796:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:ARG:HH11	2:H:18:ARG:HB2	1.85	0.41
2:F:18:ARG:HB2	2:F:18:ARG:HH11	1.85	0.41
1:B:350:HIS:CE1	1:B:352:ALA:HB3	2.55	0.41
1:B:516:LYS:O	1:B:520:ASN:ND2	2.38	0.41
1:B:1447:CYS:HB3	1:B:1555:LEU:HB3	2.03	0.41
1:B:1860:LYS:O	1:B:1864:LYS:HG2	2.21	0.41
1:B:2499:LYS:O	1:B:2503:VAL:HG23	2.21	0.41
1:B:2633:LEU:O	1:B:2689:LYS:NZ	2.54	0.41
1:B:2773:ASN:OD1	1:B:2786:LYS:NZ	2.36	0.41
1:B:2782:ASP:OD1	1:B:2782:ASP:N	2.54	0.41
1:B:3962:PHE:CZ	1:B:4023:MET:HG3	2.55	0.41
1:B:4868:ASP:OD1	1:B:4871:GLU:HG3	2.20	0.41
1:D:871:ARG:HB2	1:D:929:LEU:HD12	2.03	0.41
1:D:884:LEU:HG	1:D:955:LEU:HD21	2.02	0.41
1:D:897:ARG:NH2	1:D:899:ASP:OD1	2.52	0.41
1:D:1087:ARG:HB3	1:D:1223:PHE:CD2	2.55	0.41
1:D:1805:GLU:H	1:D:1805:GLU:CD	2.29	0.41
1:D:3166:TYR:CG	1:D:3239:MET:HG2	2.56	0.41
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	2.03	0.41
1:D:3501:ASP:OD1	1:D:3501:ASP:N	2.54	0.41
1:D:3531:ASP:OD1	1:D:3561:GLY:N	2.54	0.41
1:D:3621:HIS:O	1:D:3622:LYS:HG3	2.20	0.41
1:D:4771:ILE:HD12	1:D:4771:ILE:C	2.46	0.41
1:C:275:ARG:HD2	1:C:328:LYS:NZ	2.36	0.41
1:C:345:LEU:HB3	1:C:387:ALA:HB1	2.01	0.41
1:C:664:PHE:HB3	1:C:811:CYS:SG	2.61	0.41
1:C:884:LEU:HG	1:C:955:LEU:HD21	2.03	0.41
1:C:1992:ALA:HA	1:C:1995:THR:HG22	2.02	0.41
1:C:2417:HIS:CG	1:C:2492:ALA:HB2	2.56	0.41
1:C:2815:ALA:HB1	1:C:2881:ASN:HD22	1.86	0.41
1:C:2881:ASN:HA	1:C:2884:ASN:HD21	1.85	0.41
1:C:2917:ALA:HA	1:C:2920:ARG:HB3	2.02	0.41
1:C:3440:GLU:O	1:C:3443:ILE:HG13	2.21	0.41
1:C:3971:GLY:N	1:C:3972:PRO:HA	2.36	0.41
1:A:510:GLU:H	1:A:510:GLU:CD	2.25	0.41
1:A:1163:THR:HG22	1:A:1168:VAL:HA	2.03	0.41
1:A:3453:ARG:HD2	1:A:3453:ARG:H	1.86	0.41
1:A:3944:GLU:H	1:A:3944:GLU:HG3	1.76	0.41
1:B:860:GLN:HE21	1:B:934:ALA:HB2	1.85	0.41
1:B:995:VAL:O	1:B:998:ARG:HG3	2.20	0.41
1:B:1087:ARG:HB3	1:B:1223:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2029:GLN:NE2	1:B:2033:ASP:OD1	2.54	0.41
1:B:2977:LEU:HA	1:B:2980:VAL:HG22	2.03	0.41
1:B:4778:TRP:O	1:B:4782:VAL:HG23	2.21	0.41
1:D:61:ASP:OD2	1:D:402:ARG:NH2	2.40	0.41
1:D:345:LEU:HB3	1:D:387:ALA:HB1	2.03	0.41
1:D:1206:GLN:HA	1:D:1227:ALA:O	2.20	0.41
1:D:1447:CYS:HB3	1:D:1555:LEU:HB3	2.02	0.41
1:D:1996:ARG:HH11	1:D:1996:ARG:HA	1.86	0.41
1:D:2490:MET:HE3	1:D:2545:GLU:HB2	2.02	0.41
1:D:2759:ALA:HB1	1:D:2806:ARG:HB2	2.03	0.41
1:C:906:CYS:SG	1:C:913:LEU:HD22	2.61	0.41
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.90	0.41
1:C:2625:ARG:O	1:C:2625:ARG:HD3	2.20	0.41
1:C:2963:LEU:HD12	1:C:2963:LEU:HA	1.85	0.41
1:C:3329:ILE:HG22	1:C:3330:ASP:H	1.85	0.41
1:C:3621:HIS:C	1:C:3622:LYS:HG3	2.45	0.41
1:C:4968:PHE:O	1:C:4974:GLY:HA3	2.21	0.41
1:A:872:GLU:O	1:A:876:GLU:HG3	2.21	0.40
1:A:1748:PHE:HB2	1:A:1758:ARG:NH2	2.36	0.40
1:A:3543:LYS:NZ	1:A:3604:TYR:OH	2.46	0.40
1:A:4675:LYS:O	1:A:4679:ARG:HG3	2.22	0.40
2:F:2:VAL:HG21	2:F:61:GLU:HB2	2.02	0.40
1:B:883:ALA:HB1	1:B:907:LEU:CD1	2.51	0.40
1:B:3039:ILE:CD1	1:B:3071:LEU:HD22	2.48	0.40
1:B:3442:PHE:CG	1:B:3514:LEU:HD22	2.55	0.40
1:D:2713:ASP:OD1	1:D:2713:ASP:N	2.47	0.40
1:D:2902:HIS:CE1	1:D:2904:LEU:HB2	2.56	0.40
1:C:1018:ASN:HB3	1:C:1021:LEU:HB2	2.03	0.40
1:C:1781:CYS:SG	1:C:1783:VAL:HG22	2.62	0.40
1:C:2135:LEU:HA	1:C:2135:LEU:HD23	1.80	0.40
1:C:2574:HIS:CD2	1:C:2574:HIS:H	2.39	0.40
1:C:2588:ARG:HH21	1:C:2589:LEU:HD23	1.86	0.40
1:C:2977:LEU:HG	1:C:3056:LEU:HD23	2.02	0.40
1:C:3059:THR:O	1:C:3062:PRO:HD2	2.21	0.40
1:A:869:ARG:NH2	1:A:941:MET:HE3	2.36	0.40
1:A:1078:GLU:OE2	1:A:1654:SER:OG	2.32	0.40
1:A:2037:ASP:OD2	1:A:2038:LEU:N	2.53	0.40
1:A:2912:THR:OG1	1:A:2913:ALA:N	2.54	0.40
1:B:157:ARG:NH2	1:B:164:ARG:HD2	2.36	0.40
1:B:937:CYS:N	1:B:1056:PRO:HG3	2.36	0.40
1:B:2534:ALA:HA	1:B:2588:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2628:PHE:C	1:B:2628:PHE:CD1	2.99	0.40
1:B:2765:LYS:HD3	1:B:2765:LYS:HA	1.77	0.40
1:B:3320:LEU:O	1:B:3324:VAL:HG12	2.21	0.40
1:B:3356:SER:OG	1:B:3357:HIS:ND1	2.46	0.40
1:B:3384:LYS:HD2	1:B:3386:GLU:HB3	2.04	0.40
1:D:882:TRP:O	1:D:886:ARG:HG2	2.22	0.40
1:D:1488:LYS:HE3	1:D:1488:LYS:HB2	1.87	0.40
1:D:1867:GLU:OE2	1:D:1928:GLN:NE2	2.54	0.40
1:D:2974:ILE:HG13	1:D:2975:ALA:N	2.37	0.40
1:D:3751:VAL:HG12	1:D:3756:LYS:HZ2	1.86	0.40
1:D:4069:LYS:NZ	1:D:4133:GLN:OE1	2.50	0.40
1:D:4244:GLU:OE2	1:D:4668:LEU:HB2	2.21	0.40
1:D:4686:LEU:O	1:D:4690:GLU:HG2	2.21	0.40
1:C:2185:ILE:HG21	1:C:2203:MET:HE1	2.04	0.40
1:C:2637:ALA:C	1:C:2640:PRO:HD2	2.47	0.40
1:C:2813:LEU:HD13	1:C:2813:LEU:HA	1.87	0.40
1:C:3169:LEU:HD21	1:C:3205:PHE:CE2	2.56	0.40
1:C:3536:ALA:HB2	1:C:3553:LEU:HD21	2.03	0.40
1:A:1447:CYS:HB3	1:A:1555:LEU:HB3	2.02	0.40
1:A:1943:LEU:HB2	1:A:2123:LEU:HD21	2.03	0.40
1:A:3263:TYR:HD1	1:A:3270:ILE:HD12	1.87	0.40
1:A:3623:LEU:HD12	1:A:3624:LEU:N	2.37	0.40
1:A:3762:ARG:NH1	1:A:4755:GLU:HB2	2.37	0.40
1:A:4586:PRO:HG3	1:A:4629:TYR:CZ	2.57	0.40
1:A:4897:ILE:O	1:A:4901:ILE:HG12	2.21	0.40
1:A:4929:LEU:O	1:A:4933:GLN:HG3	2.21	0.40
2:H:2:VAL:HG21	2:H:61:GLU:HB2	2.02	0.40
2:F:49:MET:HE3	2:F:49:MET:HB2	1.85	0.40
1:B:612:VAL:HG12	1:B:2169:GLN:HG2	2.04	0.40
1:B:1286:MET:HE1	1:B:1553:PHE:HB3	2.02	0.40
1:B:2107:GLN:CD	1:B:3681:GLY:HA3	2.47	0.40
1:B:2240:CYS:SG	1:B:2250:MET:HG3	2.61	0.40
1:B:2577:ILE:H	1:B:2577:ILE:CD1	2.32	0.40
1:B:2668:SER:C	1:B:2670:GLU:H	2.28	0.40
1:B:3535:LEU:HD12	1:B:3536:ALA:N	2.36	0.40
1:B:3753:PHE:O	1:B:3757:GLU:HG2	2.21	0.40
1:B:4090:LYS:HD3	1:B:4121:GLU:HG3	2.03	0.40
1:D:931:THR:O	1:D:935:LEU:N	2.35	0.40
1:D:2881:ASN:HA	1:D:2884:ASN:HD21	1.86	0.40
1:D:4844:LEU:HD21	1:D:4924:VAL:HG13	2.03	0.40
1:C:330:ASP:OD1	1:C:330:ASP:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:882:TRP:O	1:C:885:THR:OG1	2.34	0.40
1:C:1044:ARG:HG2	1:C:1044:ARG:HH11	1.86	0.40
1:C:1055:PRO:HA	1:C:1056:PRO:HD3	1.98	0.40
1:C:2819:TRP:C	1:C:2820:GLU:HG3	2.46	0.40
1:C:3354:LEU:HD22	1:C:3423:TRP:CZ2	2.56	0.40
1:C:3638:MET:SD	1:C:3638:MET:C	3.05	0.40
1:C:4092:ASP:HA	1:C:4095:LYS:HG2	2.03	0.40
1:A:484:LEU:O	1:A:488:LEU:HG	2.21	0.40
1:A:2527:LEU:HA	1:A:2527:LEU:HD12	1.82	0.40
1:A:3019:SER:HA	1:A:3025:LEU:HD12	2.04	0.40
1:A:3300:ALA:HB3	1:A:3301:PRO:HD3	2.04	0.40
1:A:3753:PHE:O	1:A:3757:GLU:HG2	2.21	0.40
1:A:4972:PRO:HB3	1:B:5024:ALA:HB3	2.01	0.40
1:B:2576:ALA:HA	1:B:2579:VAL:HG12	2.03	0.40
1:B:4148:THR:HG21	1:B:4180:ARG:HH21	1.87	0.40
1:B:4821:LYS:HD3	1:B:4821:LYS:N	2.28	0.40
1:D:950:LEU:HD13	1:D:970:LEU:HD22	2.02	0.40
1:D:1249:PRO:HA	1:D:1250:PRO:HD3	1.98	0.40
1:D:1773:PRO:HA	1:D:1774:PRO:HD3	1.89	0.40
1:D:2690:LYS:HG3	1:D:2691:TYR:N	2.36	0.40
1:D:2773:ASN:OD1	1:D:2786:LYS:NZ	2.35	0.40
1:D:3052:HIS:HA	1:D:3127:GLN:OE1	2.21	0.40
1:D:3232:LEU:HD23	1:D:3232:LEU:HA	1.91	0.40
1:D:3400:VAL:HG23	1:D:3403:ARG:HH21	1.86	0.40
1:D:3633:VAL:HG12	1:D:3637:ARG:HE	1.87	0.40
1:D:4115:SER:HB2	1:D:4123:ILE:HG13	2.03	0.40
1:C:2186:MET:HE3	1:C:2235:PHE:HA	2.04	0.40
1:C:2534:ALA:HA	1:C:2588:ARG:NH2	2.33	0.40
1:C:2719:TYR:CD2	1:C:2953:LYS:HE2	2.56	0.40
1:C:2977:LEU:HA	1:C:2980:VAL:HG22	2.03	0.40
1:C:3163:VAL:O	1:C:3167:ARG:HG3	2.21	0.40
1:C:3868:ARG:NH1	1:C:3870:ASN:HB3	2.37	0.40
1:C:4134:GLU:HB3	1:C:4135:PRO:HD3	2.02	0.40
1:A:2420:HIS:HA	1:A:2423:MET:CE	2.51	0.40
1:A:2628:PHE:C	1:A:2628:PHE:CD1	2.99	0.40
1:A:2695:LEU:O	1:A:2698:MET:HE3	2.22	0.40
1:A:3528:THR:HG23	1:A:3573:MET:CE	2.50	0.40
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.33	0.40
2:F:84:ALA:O	2:F:93:PRO:HB3	2.20	0.40
1:B:866:HIS:HA	1:B:869:ARG:HG3	2.04	0.40
1:B:893:TYR:O	1:B:903:LEU:HD22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1739:THR:O	1:B:1743[B]:ARG:HG3	2.21	0.40
1:B:2680:TRP:CE3	1:B:2680:TRP:HA	2.57	0.40
1:B:4823:LEU:HD11	1:C:4843:LEU:HB2	2.03	0.40
1:B:4897:ILE:HD12	1:B:4897:ILE:HA	1.96	0.40
1:D:56:GLN:O	1:D:309:THR:OG1	2.28	0.40
1:D:3566:SER:HB3	1:D:3569:LEU:HB3	2.02	0.40
1:D:3924:LEU:HD23	1:D:3924:LEU:HA	1.96	0.40
1:C:416:LYS:HE3	1:C:416:LYS:HB2	1.91	0.40
1:C:2538:THR:OG1	1:C:2539:ALA:N	2.55	0.40
1:C:3131:TYR:O	1:C:3136:LEU:N	2.54	0.40
1:C:3582:ARG:HD3	1:C:3582:ARG:HA	1.90	0.40
1:C:4836:GLN:O	1:C:4840:THR:HG22	2.21	0.40
1:C:4861:LYS:H	1:C:4861:LYS:HG3	1.65	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%)	4260 (97%)	125 (3%)	0	100	100
1	B	4385/5037 (87%)	4251 (97%)	134 (3%)	0	100	100
1	C	4385/5037 (87%)	4264 (97%)	121 (3%)	0	100	100
1	D	4385/5037 (87%)	4272 (97%)	113 (3%)	0	100	100
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	17960/20580 (87%)	17447 (97%)	513 (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%)	3812 (99%)	24 (1%)	84	94
1	B	3836/4276 (90%)	3812 (99%)	24 (1%)	84	94
1	C	3836/4276 (90%)	3817 (100%)	19 (0%)	86	95
1	D	3836/4276 (90%)	3812 (99%)	24 (1%)	84	94
2	E	89/90 (99%)	83 (93%)	6 (7%)	13	37
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	65
2	G	89/90 (99%)	87 (98%)	2 (2%)	47	76
2	H	89/90 (99%)	85 (96%)	4 (4%)	23	54
All	All	15700/17464 (90%)	15594 (99%)	106 (1%)	80	93

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	VAL
1	A	898	ASP
1	A	911	HIS
1	A	957	LYS
1	A	1021	LEU
1	A	1057	ASP
1	A	1538	THR
1	A	1966	VAL
1	A	2290	LEU
1	A	2666	VAL
1	A	2803	GLU
1	A	2932	MET
1	A	2937	VAL
1	A	3002	LEU
1	A	3534	MET
1	A	3619	VAL

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Mol	Chain	Res	Type
1	A	3639	THR
1	A	3758	MET
1	A	3899	PHE
1	A	4026	MET
1	A	4122	MET
1	A	4871	GLU
1	A	4880	MET
1	A	5034	ASP
2	E	25	HIS
2	E	29	MET
2	E	32	ASP
2	E	38	SER
2	E	50	LEU
2	E	85	THR
2	H	2	VAL
2	H	25	HIS
2	H	59	TRP
2	H	85	THR
2	G	2	VAL
2	G	25	HIS
2	F	2	VAL
2	F	25	HIS
2	F	59	TRP
1	B	191	VAL
1	B	351	VAL
1	B	911	HIS
1	B	957	LYS
1	B	959	TYR
1	B	1021	LEU
1	B	1057	ASP
1	B	1506	GLN
1	B	1538	THR
1	B	1786	LEU
1	B	1872	THR
1	B	2192	TYR
1	B	2290	LEU
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2932	MET
1	B	3059	THR
1	B	3166	TYR
1	B	3899	PHE

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Mol	Chain	Res	Type
1	B	4122	MET
1	B	4722	ARG
1	B	4773	VAL
1	B	4871	GLU
1	B	4880	MET
1	D	32	GLN
1	D	81	MET
1	D	191	VAL
1	D	208	CYS
1	D	884	LEU
1	D	898	ASP
1	D	911	HIS
1	D	959	TYR
1	D	1021	LEU
1	D	1057	ASP
1	D	1170	MET
1	D	1538	THR
1	D	2008	MET
1	D	2009	LEU
1	D	2803	GLU
1	D	2862	LEU
1	D	2965	ARG
1	D	3030	HIS
1	D	3234	ASN
1	D	3639	THR
1	D	3693	LYS
1	D	3899	PHE
1	D	4652	LEU
1	D	4768	LEU
1	C	81	MET
1	C	191	VAL
1	C	275	ARG
1	C	898	ASP
1	C	945	LYS
1	C	1021	LEU
1	C	1538	THR
1	C	1872	THR
1	C	2290	LEU
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2747	ILE
1	C	3103	ILE

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Mol	Chain	Res	Type
1	C	3112	LEU
1	C	3558	HIS
1	C	3639	THR
1	C	3899	PHE
1	C	4107	GLU
1	C	4816	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	56	GLN
1	A	113	HIS
1	A	255	HIS
1	A	461	HIS
1	A	465	GLN
1	A	495	ASN
1	A	636	ASN
1	A	963	ASN
1	A	981	GLN
1	A	1206	GLN
1	A	1220	GLN
1	A	1229	ASN
1	A	1280	GLN
1	A	1938	GLN
1	A	2003	GLN
1	A	2161	GLN
1	A	2260	ASN
1	A	2444	GLN
1	A	2487	GLN
1	A	2498	HIS
1	A	2933	ASN
1	A	2962	GLN
1	A	3180	ASN
1	A	3766	GLN
1	A	3814	GLN
1	A	3860	ASN
1	A	3914	ASN
1	A	4120	ASN
1	A	4558	ASN
1	A	4700	GLN
1	A	4728	HIS

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Mol	Chain	Res	Type
1	A	4836	GLN
1	A	4864	ASN
2	H	94	HIS
2	G	94	HIS
2	F	94	HIS
1	B	56	GLN
1	B	113	HIS
1	B	461	HIS
1	B	465	GLN
1	B	495	ASN
1	B	838	HIS
1	B	860	GLN
1	B	938	HIS
1	B	981	GLN
1	B	1052	ASN
1	B	1066	GLN
1	B	1229	ASN
1	B	1280	GLN
1	B	2003	GLN
1	B	2245	GLN
1	B	2260	ASN
1	B	2342	ASN
1	B	2515	GLN
1	B	2933	ASN
1	B	2976	HIS
1	B	3211	ASN
1	B	3766	GLN
1	B	3914	ASN
1	B	4034	ASN
1	B	4558	ASN
1	B	4728	HIS
1	B	4836	GLN
1	D	57	ASN
1	D	79	GLN
1	D	255	HIS
1	D	461	HIS
1	D	495	ASN
1	D	581	ASN
1	D	919	ASN
1	D	949	ASN
1	D	963	ASN
1	D	1066	GLN

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Mol	Chain	Res	Type
1	D	1084	GLN
1	D	1220	GLN
1	D	1229	ASN
1	D	1558	HIS
1	D	1660	GLN
1	D	2003	GLN
1	D	2007	ASN
1	D	2260	ASN
1	D	2772	GLN
1	D	2883	HIS
1	D	2933	ASN
1	D	2962	GLN
1	D	3109	ASN
1	D	3180	ASN
1	D	3667	HIS
1	D	3860	ASN
1	D	4034	ASN
1	D	4094	GLN
1	D	4120	ASN
1	D	4156	HIS
1	D	4558	ASN
1	D	4836	GLN
1	D	4997	ASN
1	C	32	GLN
1	C	56	GLN
1	C	495	ASN
1	C	581	ASN
1	C	636	ASN
1	C	639	ASN
1	C	921	ASN
1	C	1229	ASN
1	C	1420	ASN
1	C	1631	GLN
1	C	1660	GLN
1	C	1938	GLN
1	C	2194	HIS
1	C	2260	ASN
1	C	2772	GLN
1	C	2883	HIS
1	C	2933	ASN
1	C	2962	GLN
1	C	3180	ASN

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Mol	Chain	Res	Type
1	C	3268	HIS
1	C	3355	HIS
1	C	3734	HIS
1	C	3914	ASN
1	C	4120	ASN
1	C	4558	ASN
1	C	4836	GLN
1	C	4864	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	URA	A	5304	-	8,8,8	0.59	0	10,10,10	1.08	1 (10%)
6	URA	D	5304	-	8,8,8	0.61	0	10,10,10	1.05	1 (10%)
3	ATP	B	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
3	ATP	C	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
6	URA	B	5304	-	8,8,8	0.60	0	10,10,10	1.12	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	D	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)
6	URA	C	5304	-	8,8,8	0.62	0	10,10,10	1.06	1 (10%)
3	ATP	A	5301	-	28,33,33	0.63	0	34,52,52	0.94	2 (5%)

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	URA	A	5304	-	-	-	0/1/1/1
6	URA	D	5304	-	-	-	0/1/1/1
3	ATP	B	5301	-	-	8/18/38/38	0/3/3/3
3	ATP	C	5301	-	-	6/18/38/38	0/3/3/3
6	URA	B	5304	-	-	-	0/1/1/1
3	ATP	D	5301	-	-	6/18/38/38	0/3/3/3
6	URA	C	5304	-	-	-	0/1/1/1
3	ATP	A	5301	-	-	6/18/38/38	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5301	ATP	C4'-O4'-C1'	-4.28	106.00	109.92
3	D	5301	ATP	C4'-O4'-C1'	-4.27	106.02	109.92
3	C	5301	ATP	C4'-O4'-C1'	-4.27	106.02	109.92
3	A	5301	ATP	C4'-O4'-C1'	-4.23	106.05	109.92
6	B	5304	URA	C4-N3-C2	2.41	127.88	125.55
3	D	5301	ATP	C5-C6-N6	2.32	123.84	120.31
6	A	5304	URA	C4-N3-C2	2.32	127.79	125.55
3	C	5301	ATP	C5-C6-N6	2.31	123.83	120.31
3	B	5301	ATP	C5-C6-N6	2.30	123.82	120.31
3	A	5301	ATP	C5-C6-N6	2.30	123.82	120.31
6	C	5304	URA	C4-N3-C2	2.24	127.72	125.55
6	D	5304	URA	C4-N3-C2	2.21	127.69	125.55

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O1A
3	A	5301	ATP	C5'-O5'-PA-O3A
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	C5'-O5'-PA-O1A
3	D	5301	ATP	C5'-O5'-PA-O3A
3	C	5301	ATP	C5'-O5'-PA-O1A
3	C	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	C5'-O5'-PA-O2A
3	D	5301	ATP	C5'-O5'-PA-O2A
3	C	5301	ATP	C5'-O5'-PA-O2A
3	B	5301	ATP	C4'-C5'-O5'-PA
3	A	5301	ATP	C4'-C5'-O5'-PA
3	A	5301	ATP	PG-O3B-PB-O1B
3	D	5301	ATP	C4'-C5'-O5'-PA
3	C	5301	ATP	C4'-C5'-O5'-PA
3	B	5301	ATP	O4'-C4'-C5'-O5'
3	B	5301	ATP	C3'-C4'-C5'-O5'
3	B	5301	ATP	PG-O3B-PB-O3A
3	D	5301	ATP	PG-O3B-PB-O3A
3	C	5301	ATP	PG-O3B-PB-O3A
3	D	5301	ATP	PG-O3B-PB-O1B
3	A	5301	ATP	PG-O3B-PB-O3A
3	B	5301	ATP	PG-O3B-PB-O1B
3	C	5301	ATP	PG-O3B-PB-O1B

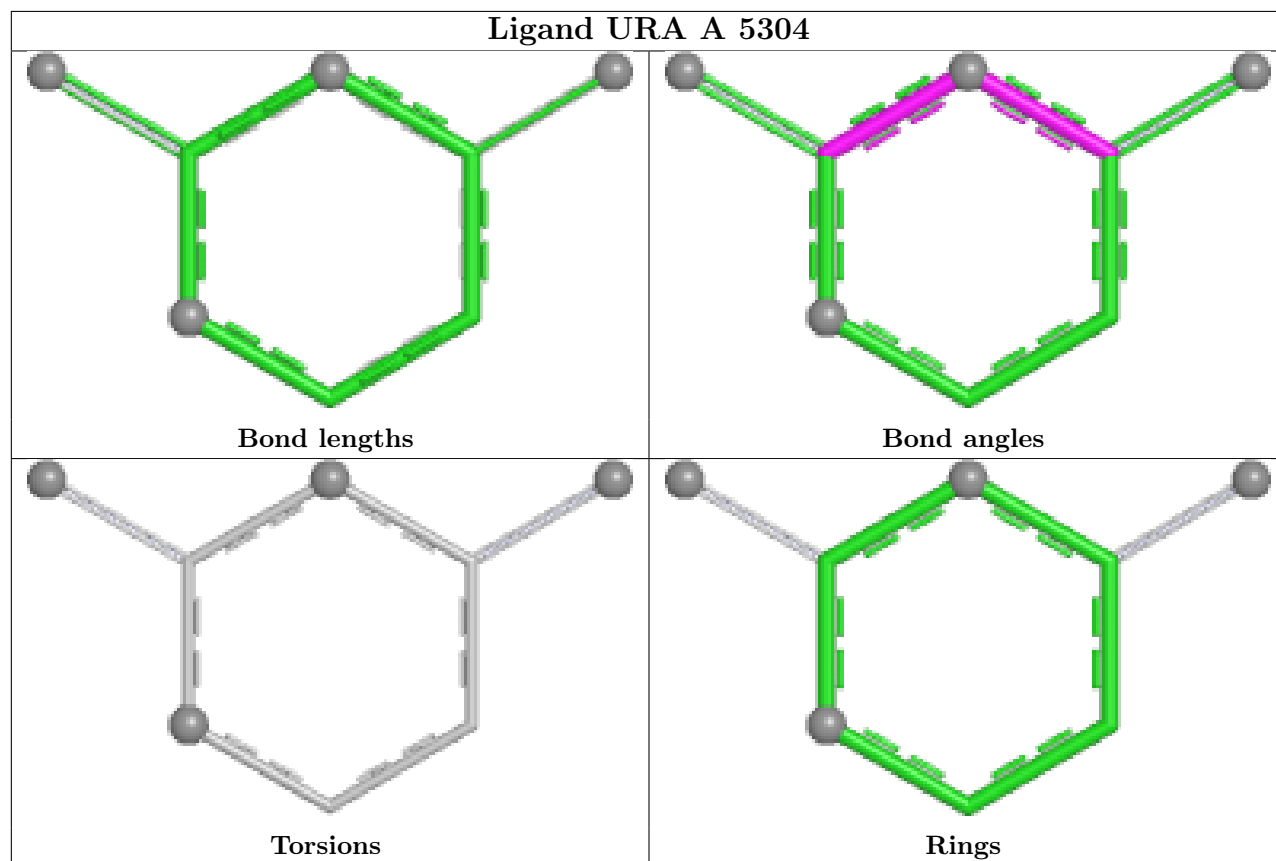
There are no ring outliers.

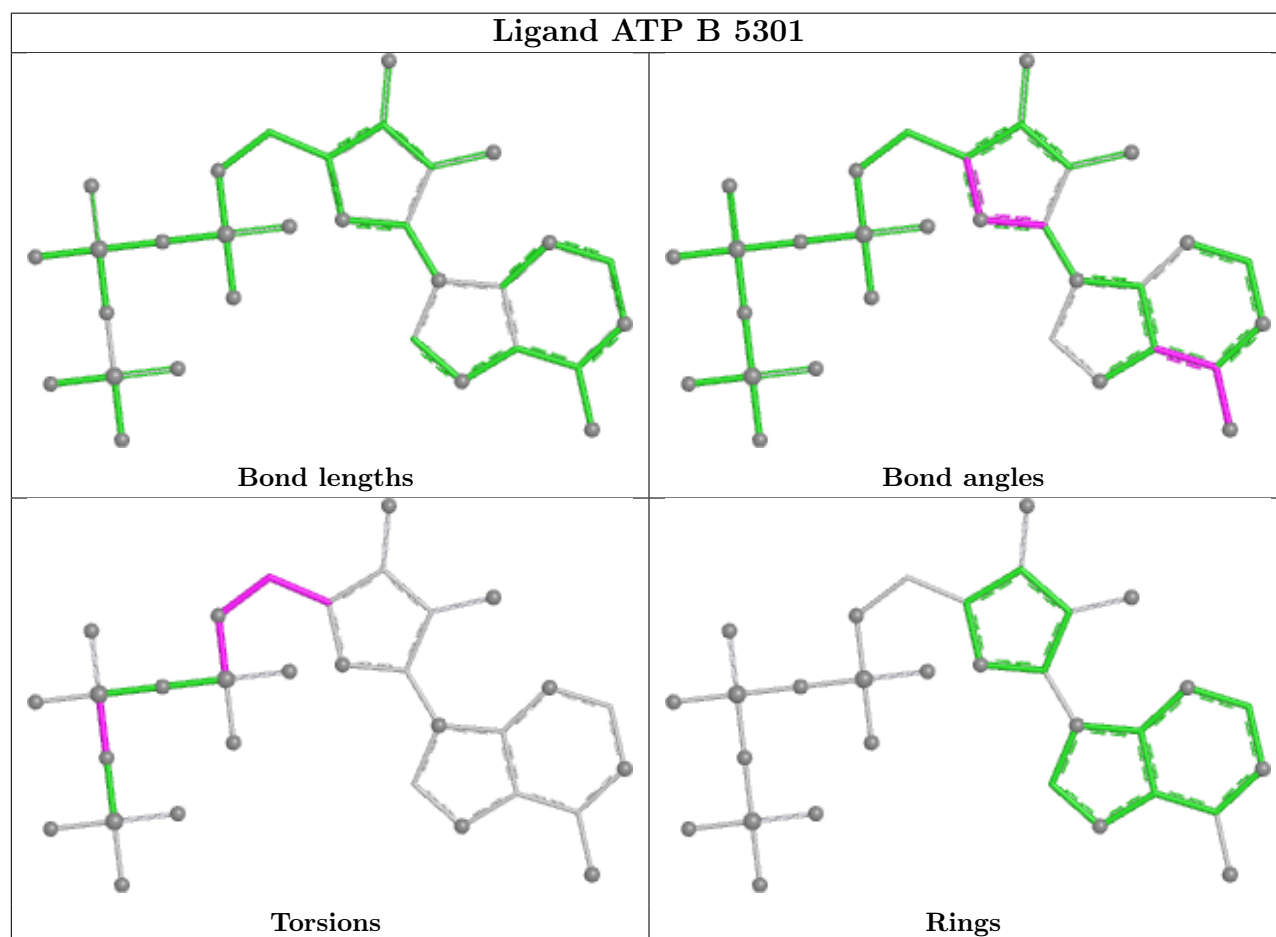
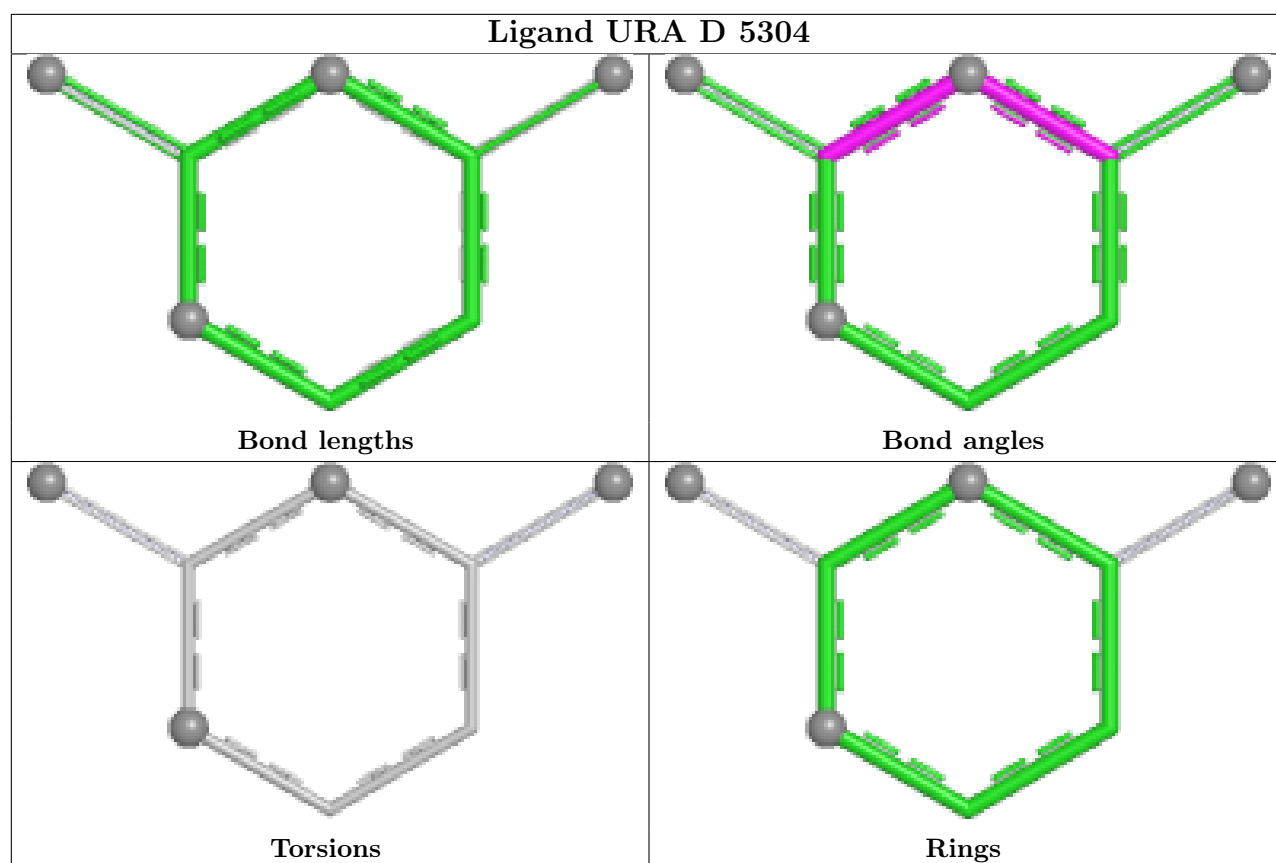
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5301	ATP	1	0
3	A	5301	ATP	1	0

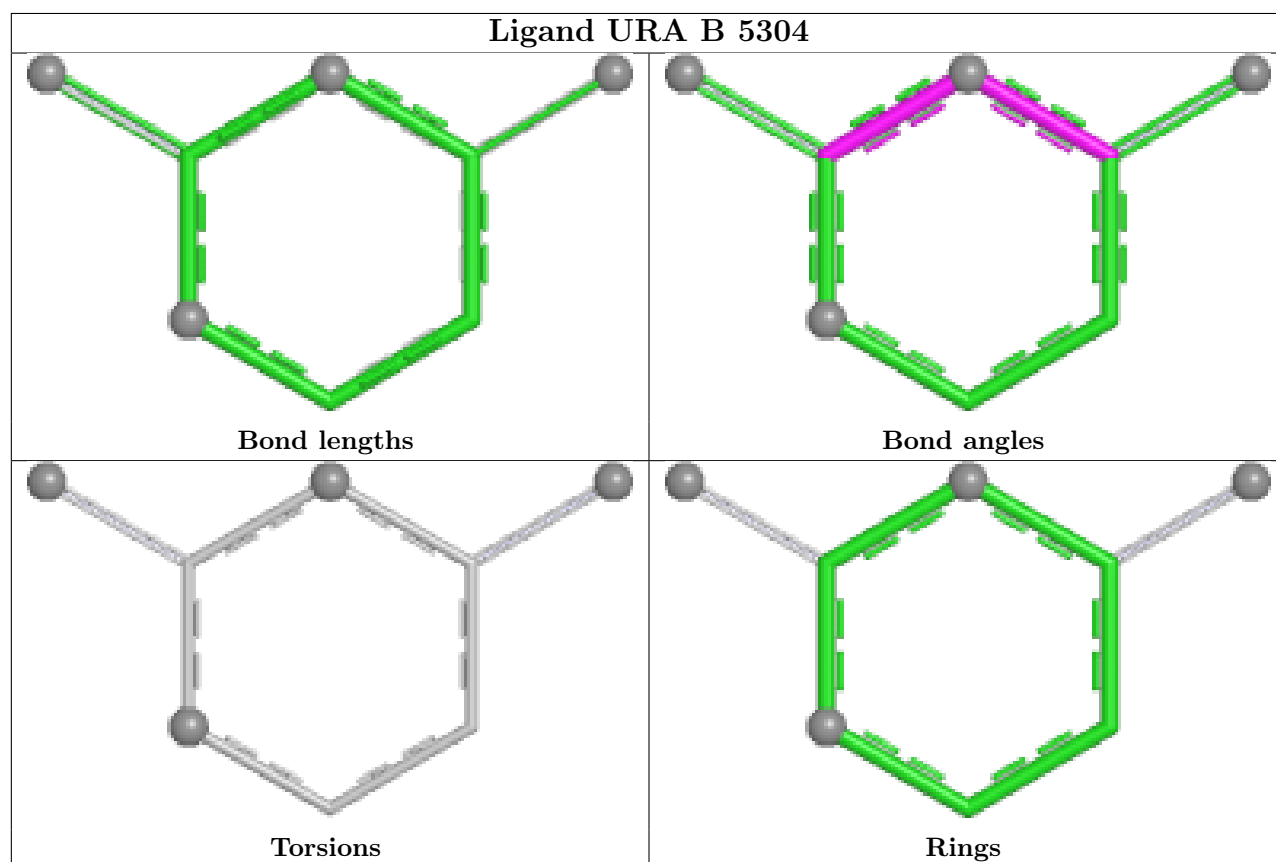
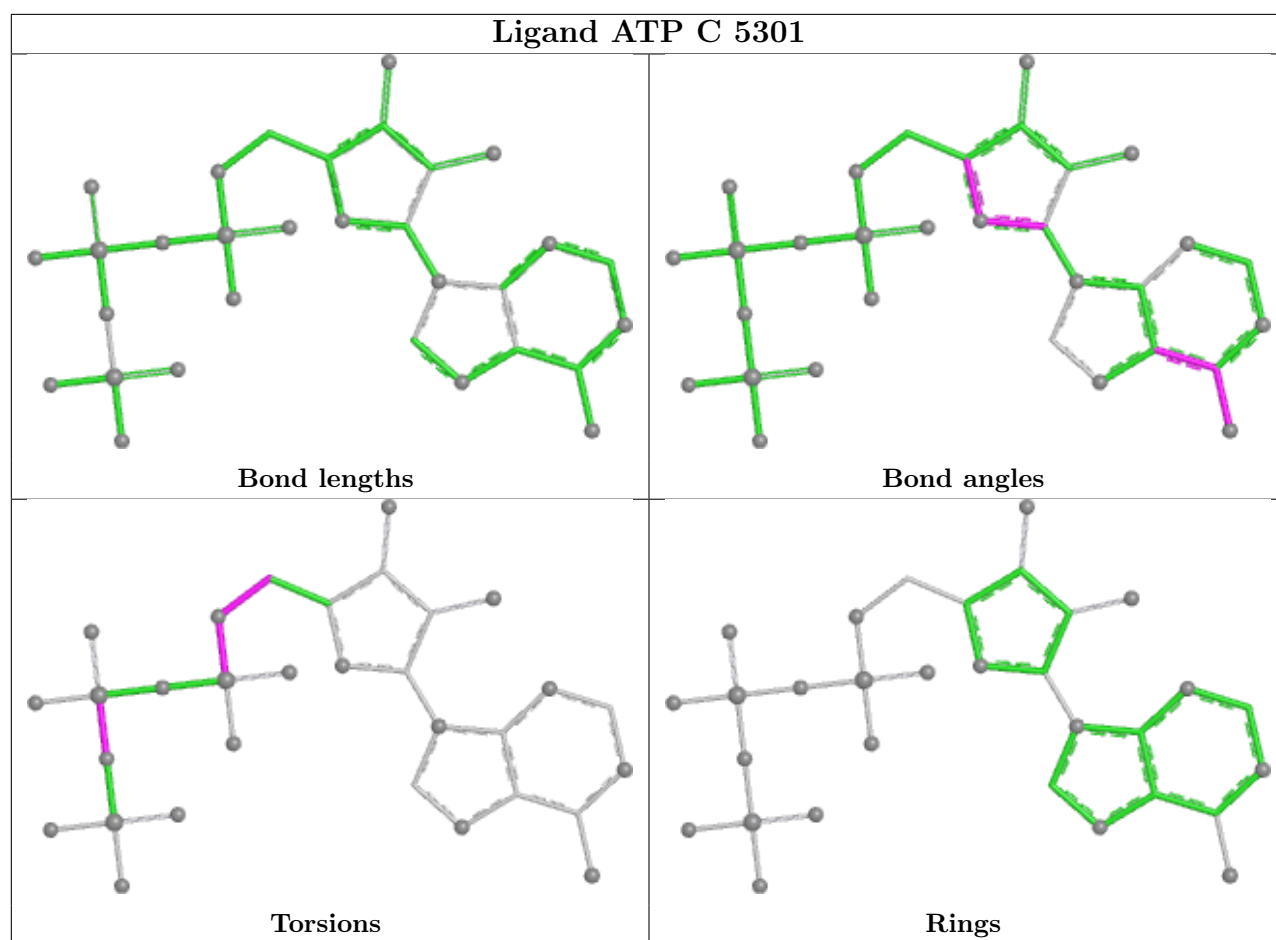
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

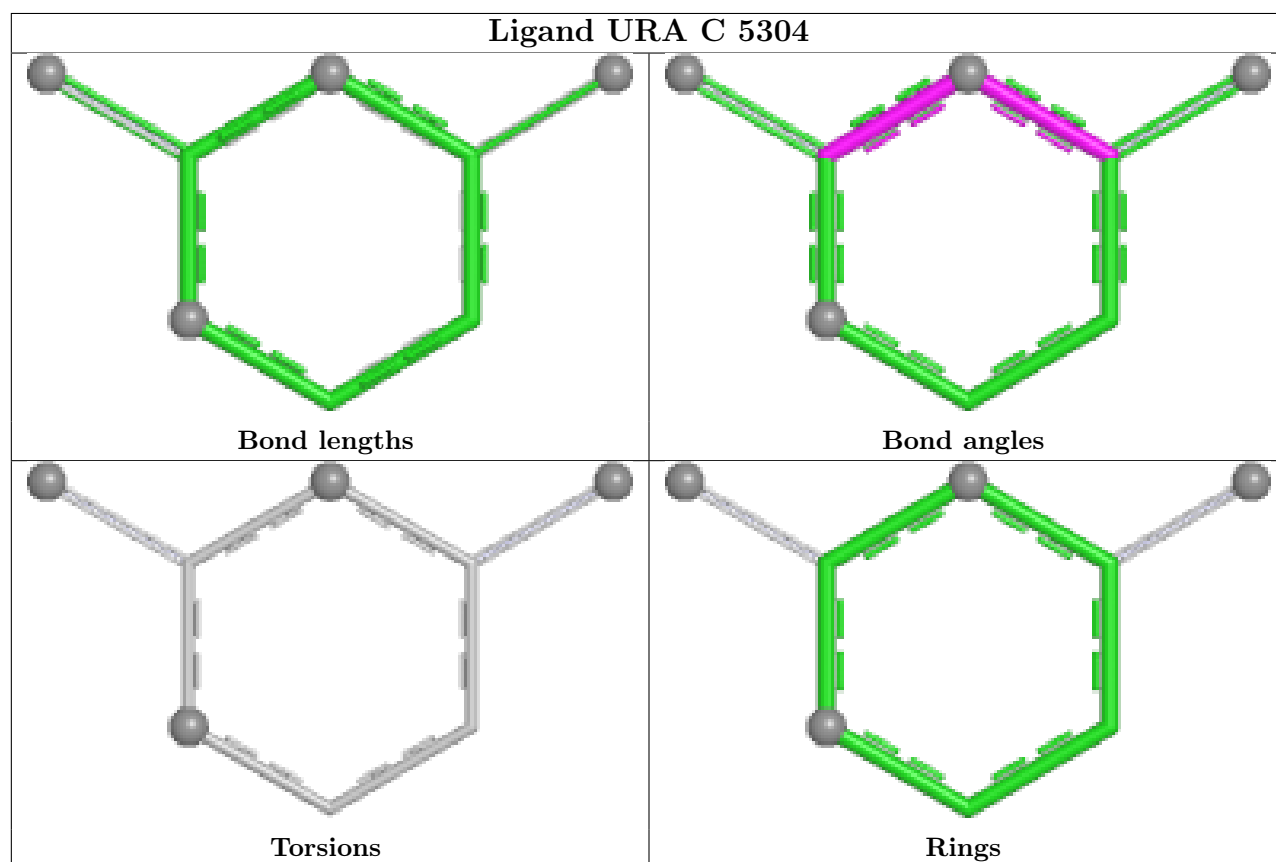
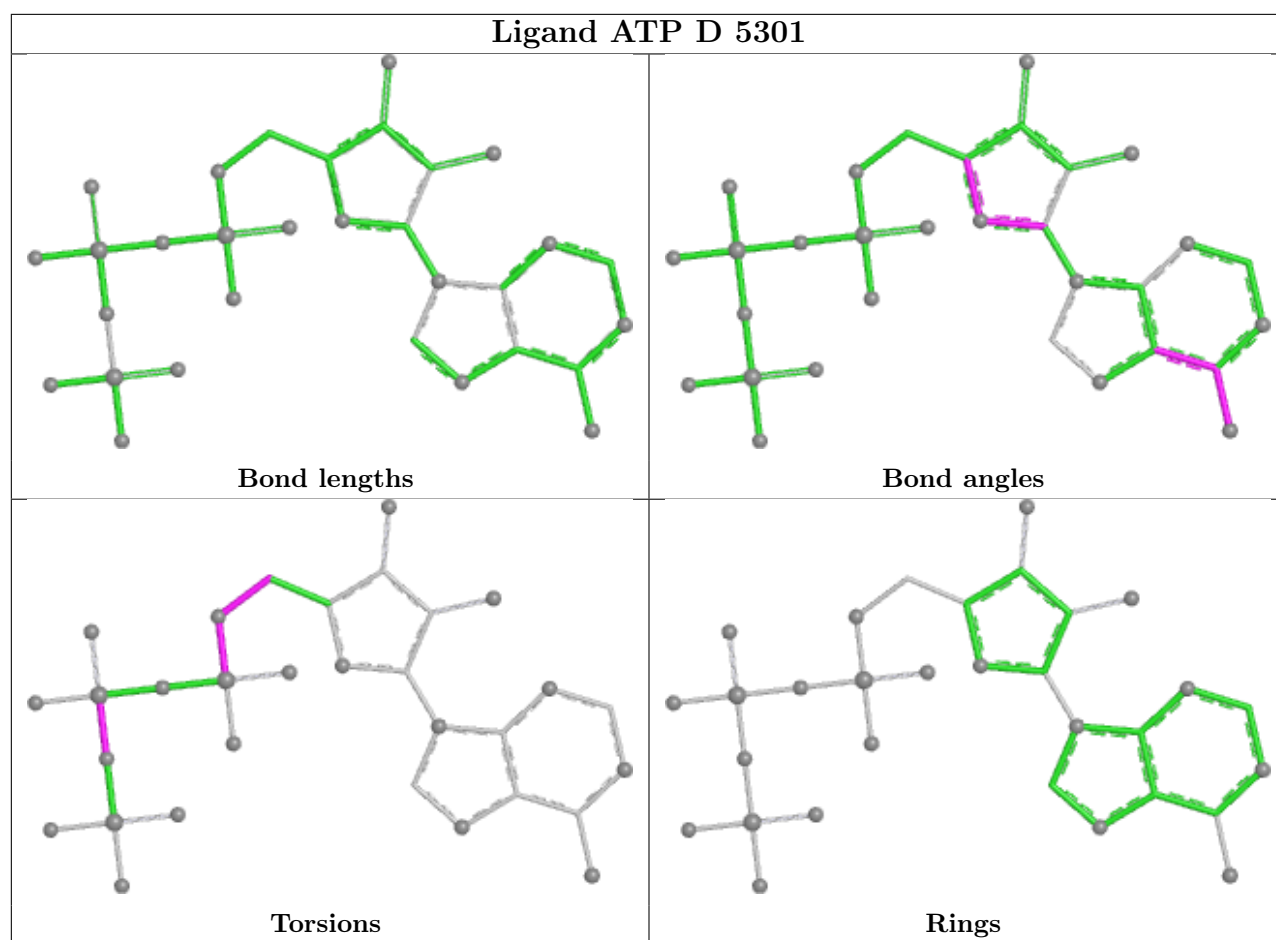
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

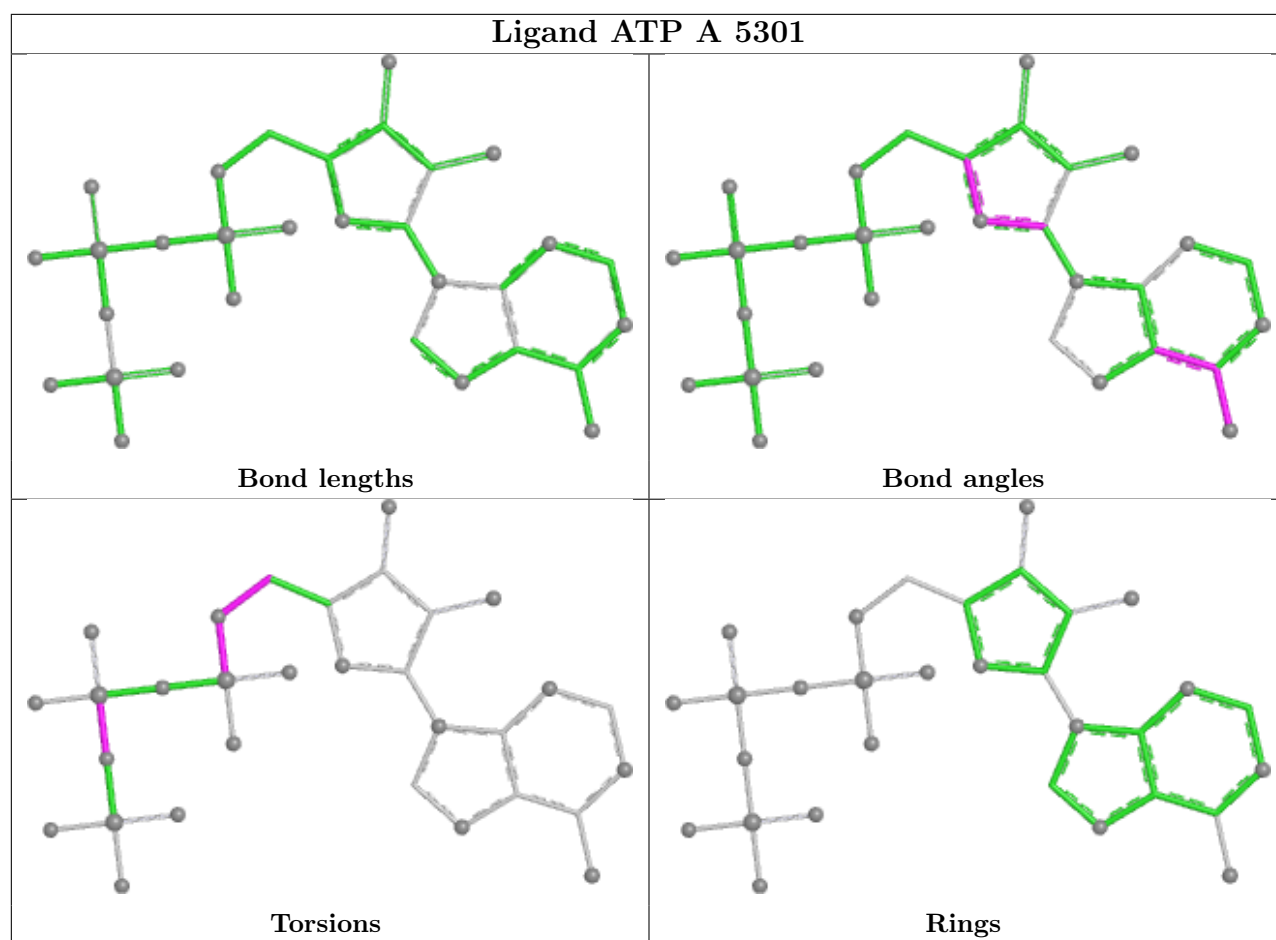












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

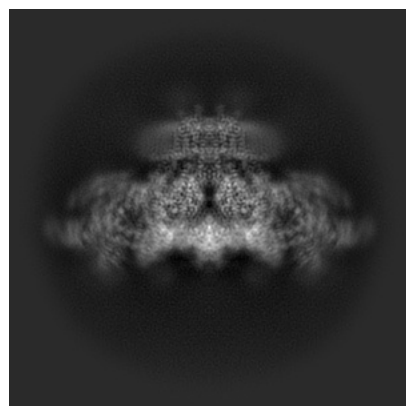
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47391. These allow visual inspection of the internal detail of the map and identification of artifacts.

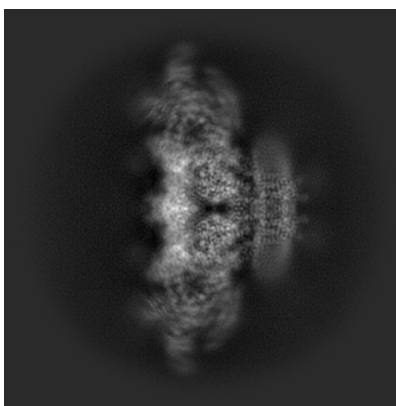
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

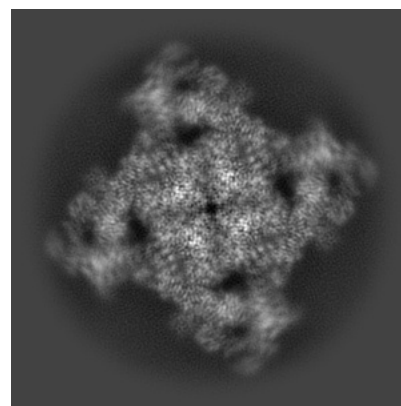
#### 6.1.1 Primary map



X

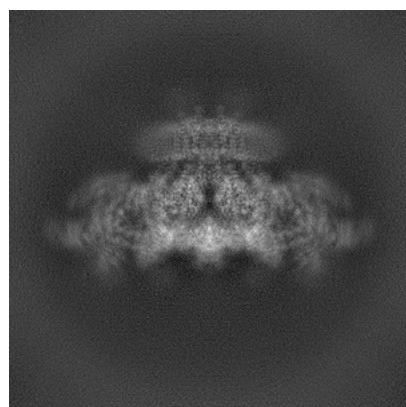


Y

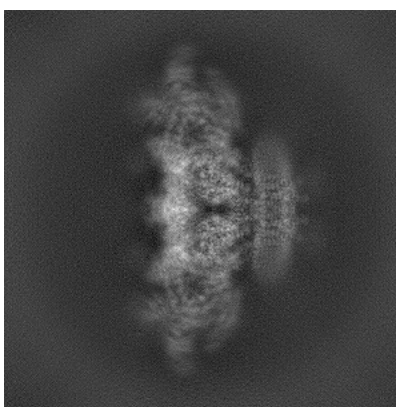


Z

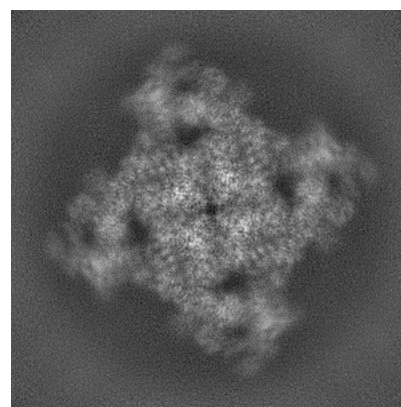
#### 6.1.2 Raw map



X



Y

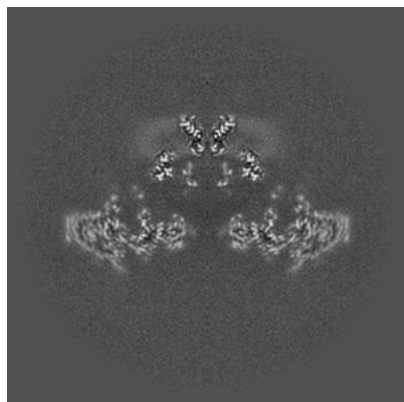


Z

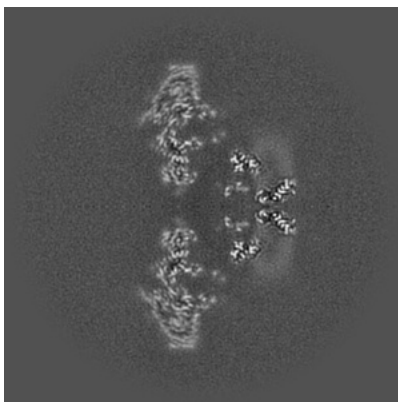
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

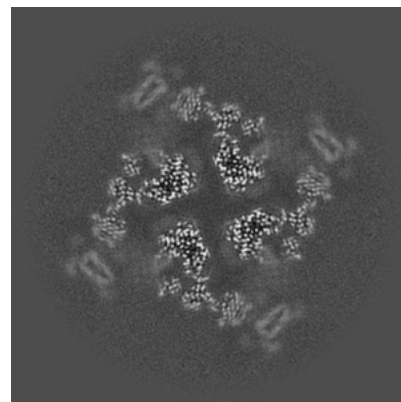
### 6.2.1 Primary map



X Index: 256

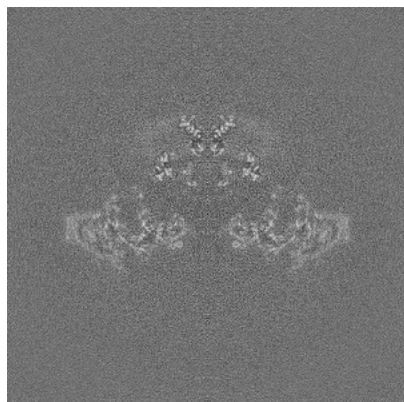


Y Index: 256

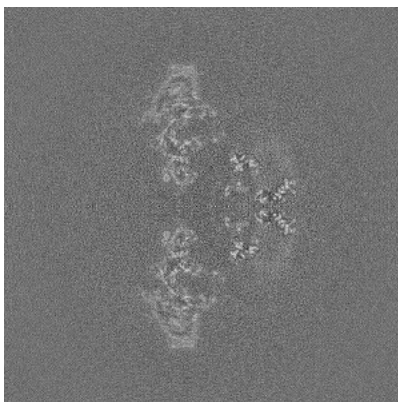


Z Index: 256

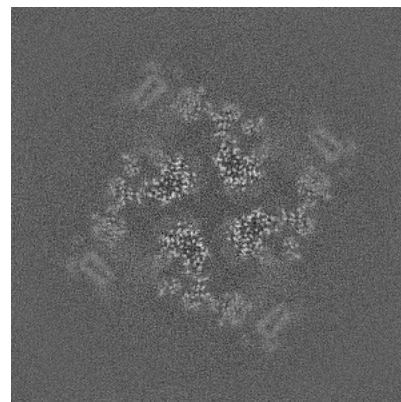
### 6.2.2 Raw map



X Index: 256



Y Index: 256



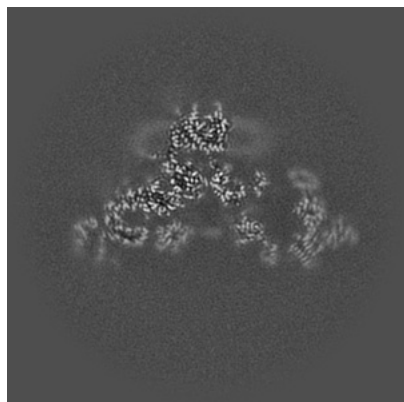
Z Index: 256

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

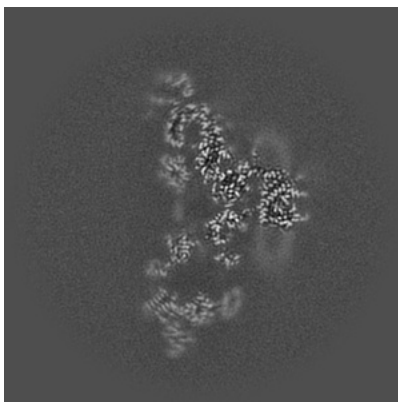


## 6.3 Largest variance slices [i](#)

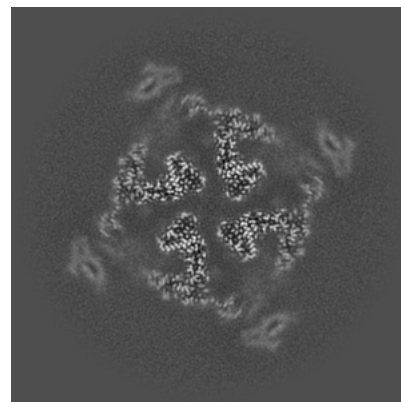
### 6.3.1 Primary map



X Index: 239

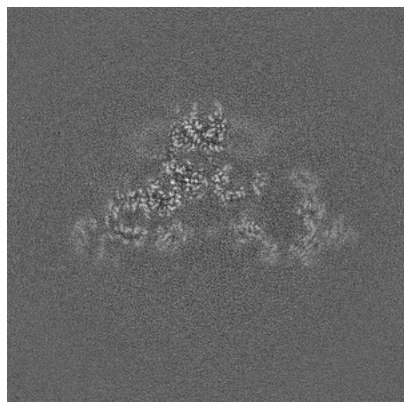


Y Index: 239

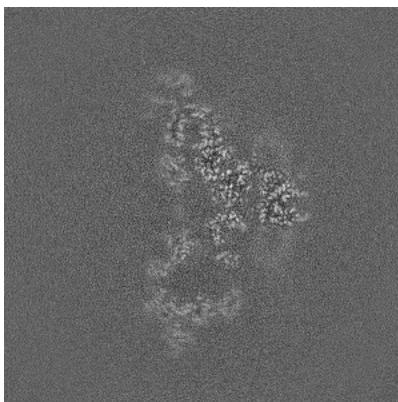


Z Index: 265

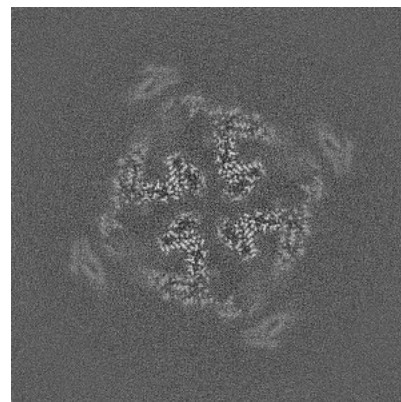
### 6.3.2 Raw map



X Index: 240



Y Index: 240

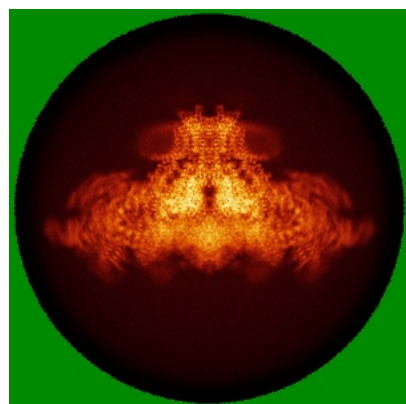


Z Index: 266

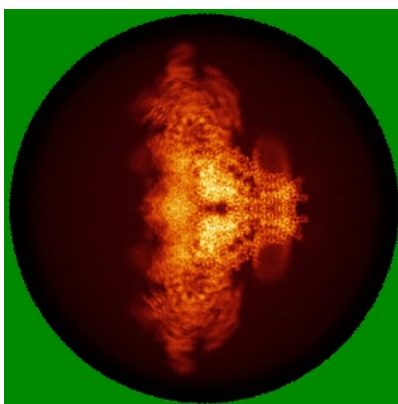
The images above show the largest variance slices of the map in three orthogonal directions.

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

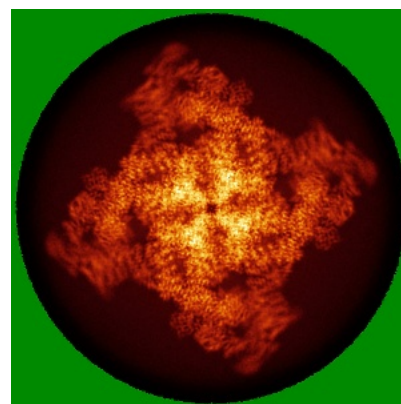
### 6.4.1 Primary map



X

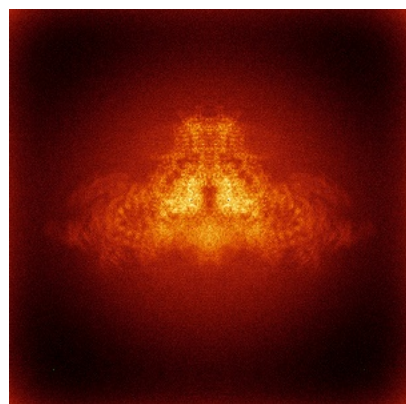


Y

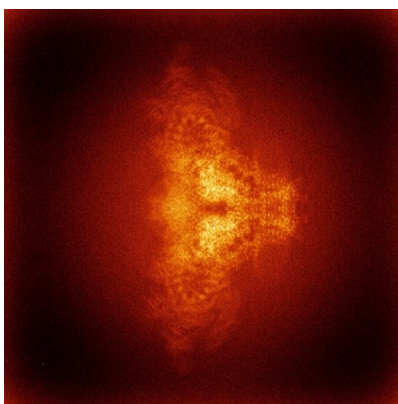


Z

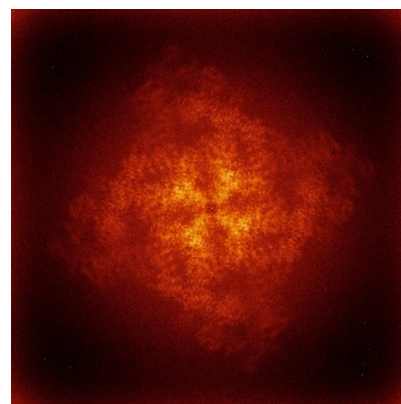
### 6.4.2 Raw map



X



Y

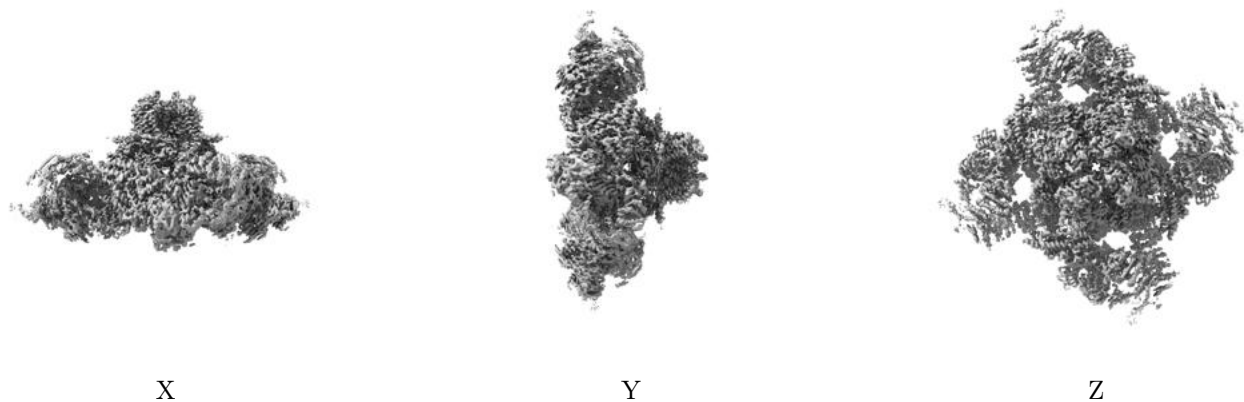


Z

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.

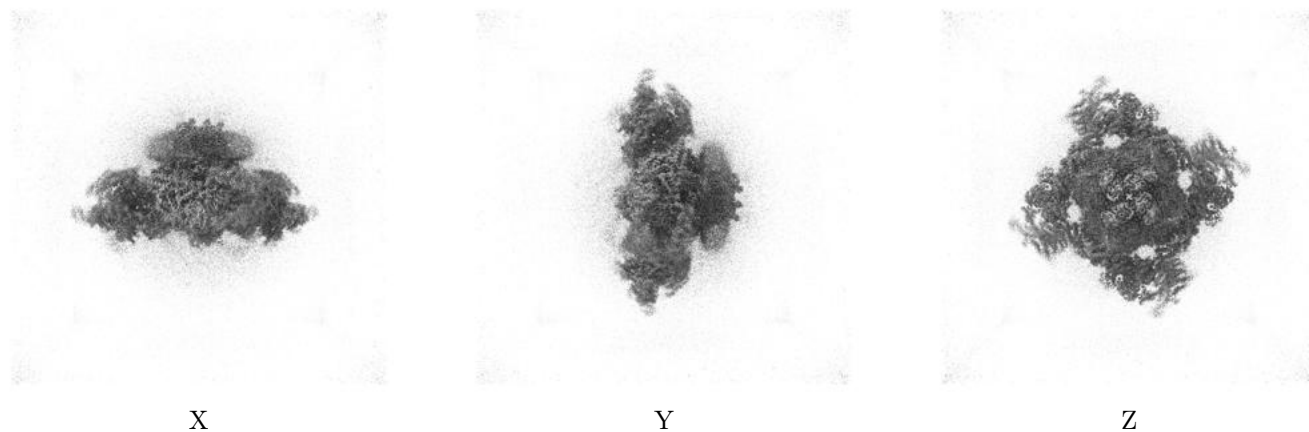
## 6.5 Orthogonal surface views [i](#)

### 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](#)

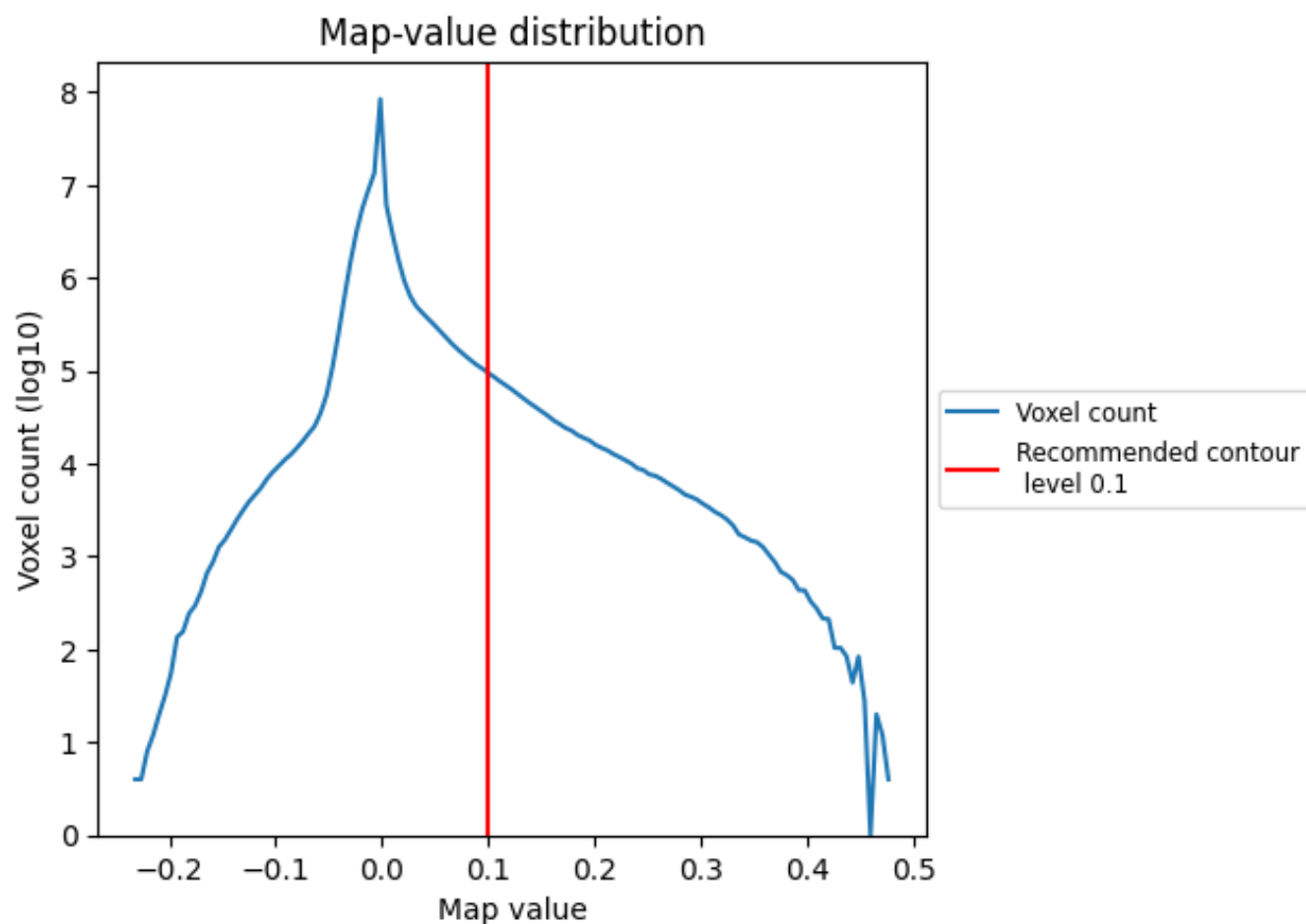
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

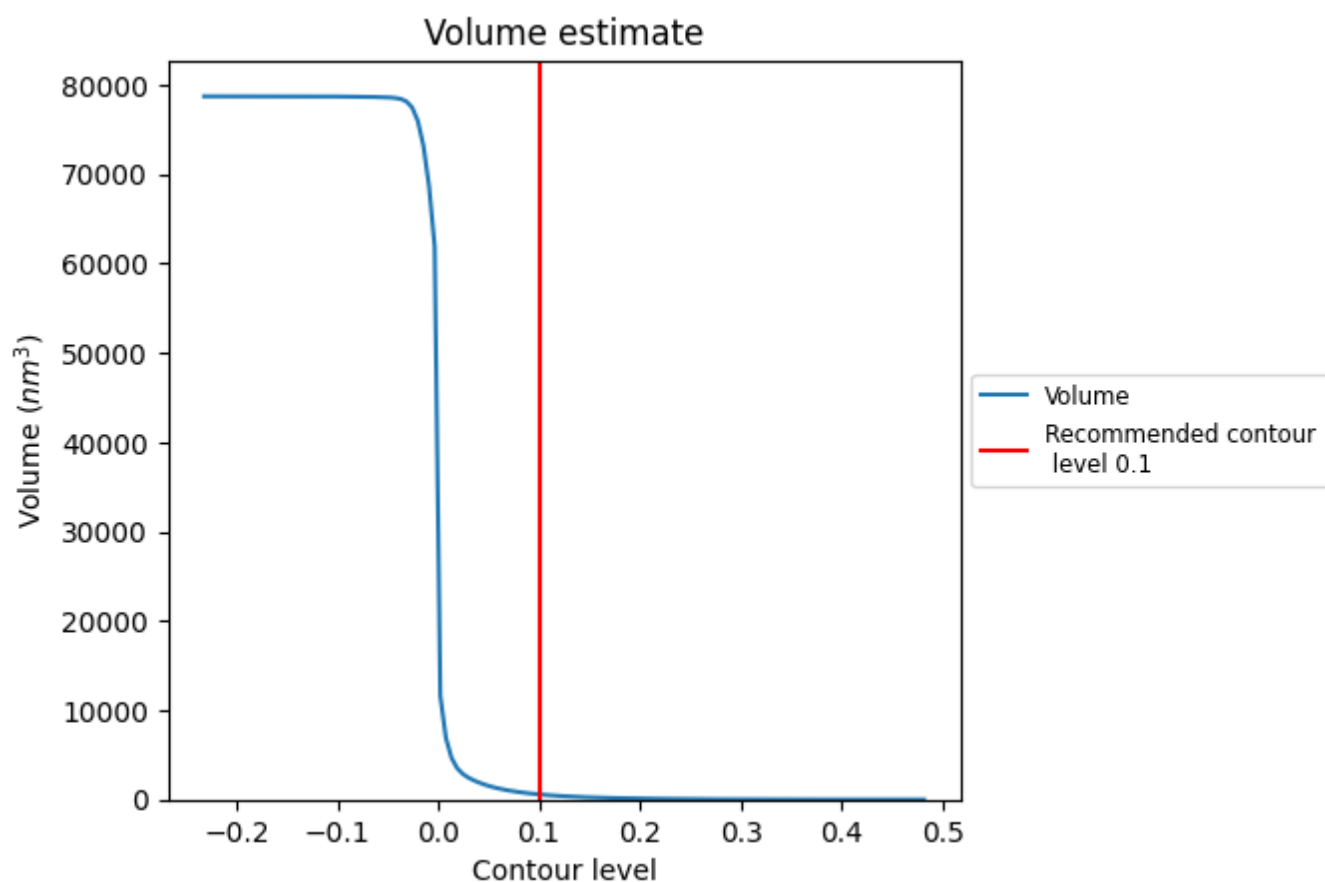
This section contains the results of statistical analysis of the map.

### 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.

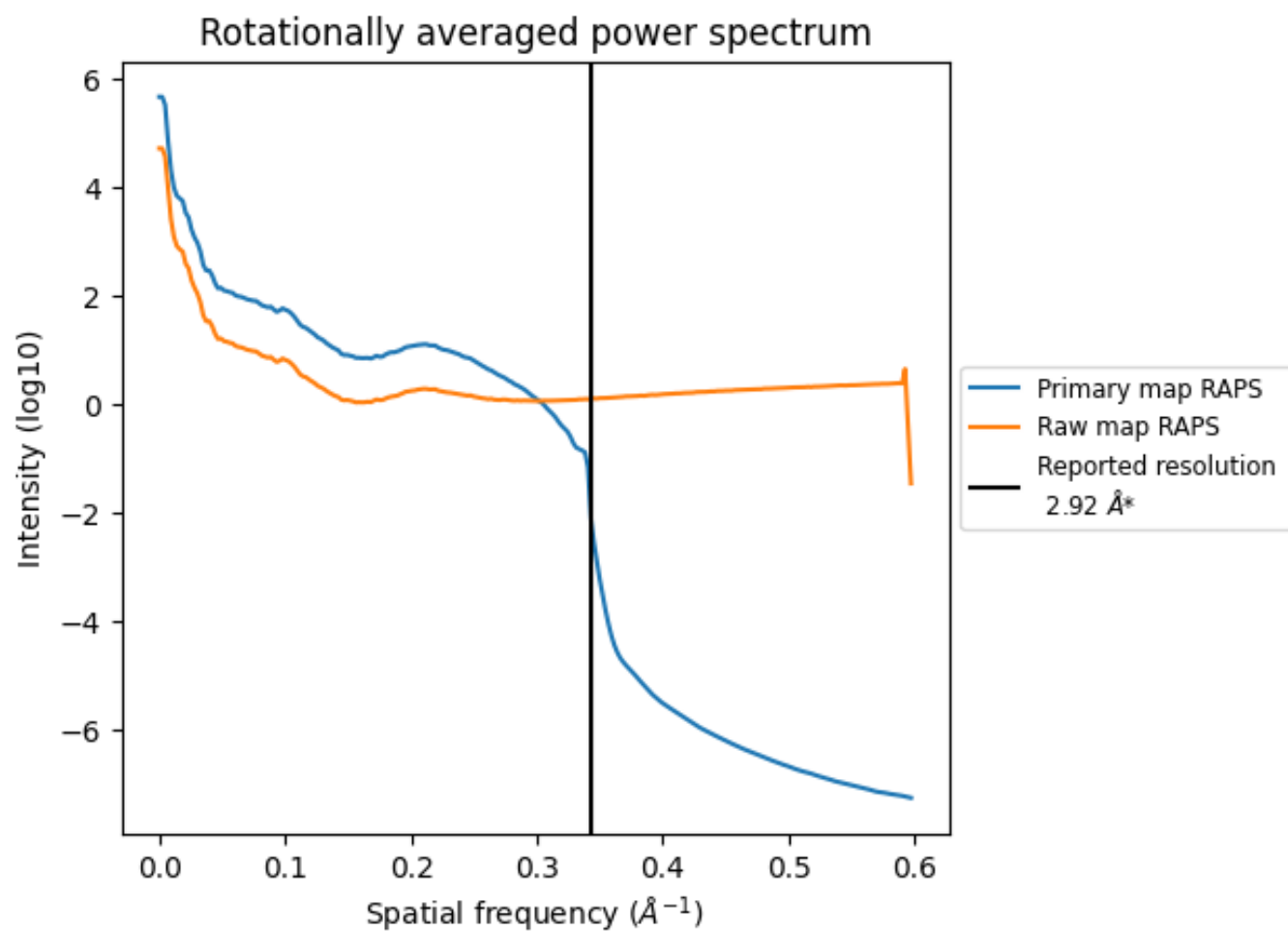
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 584 nm<sup>3</sup>; this corresponds to an approximate mass of 528 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 ⓘ

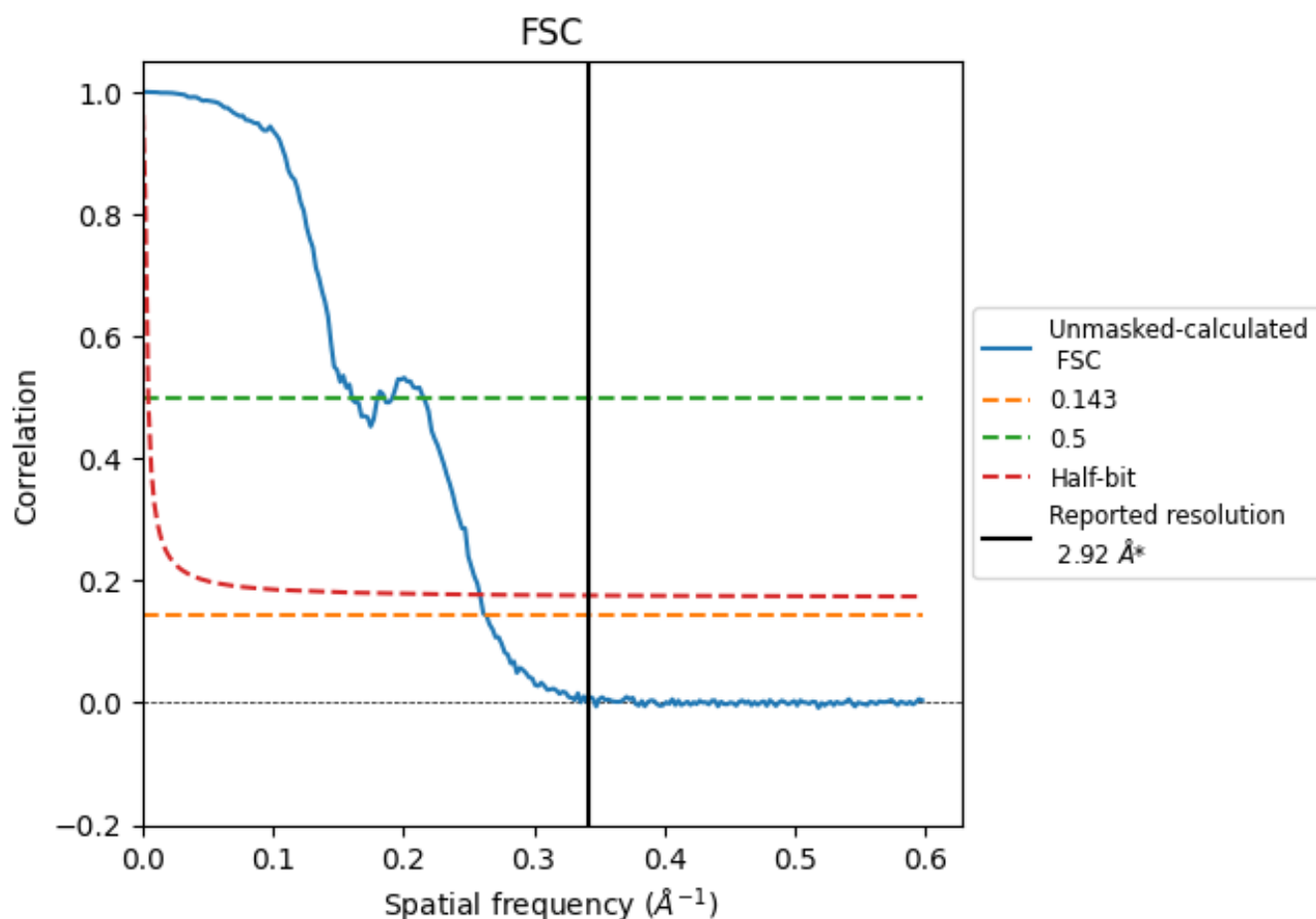


\*Reported resolution corresponds to spatial frequency of 0.342  $\text{\AA}^{-1}$

## 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  $0.342 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

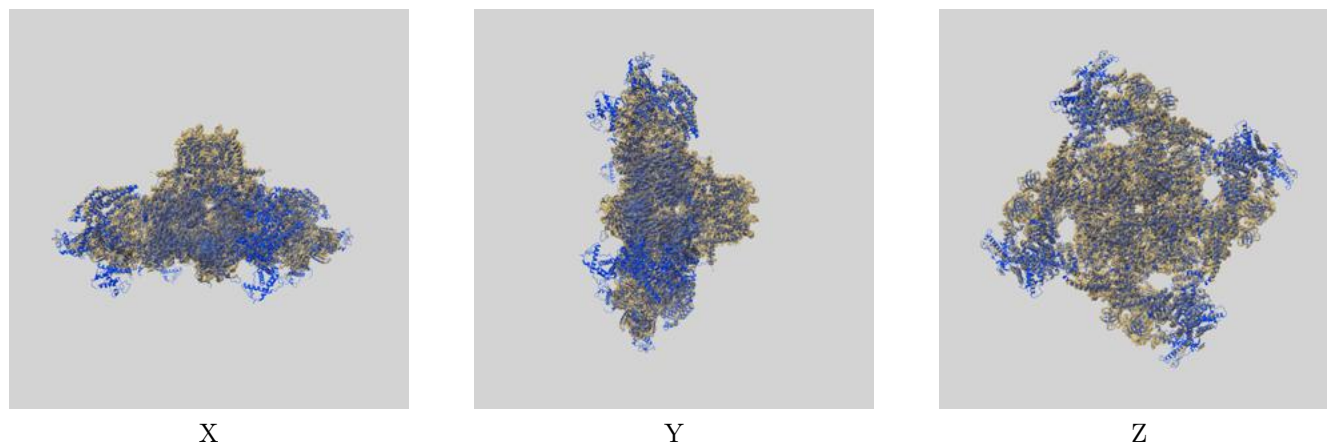
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.23	3.87

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.92 by more than 10 %

## 9 Map-model fit [i](#)

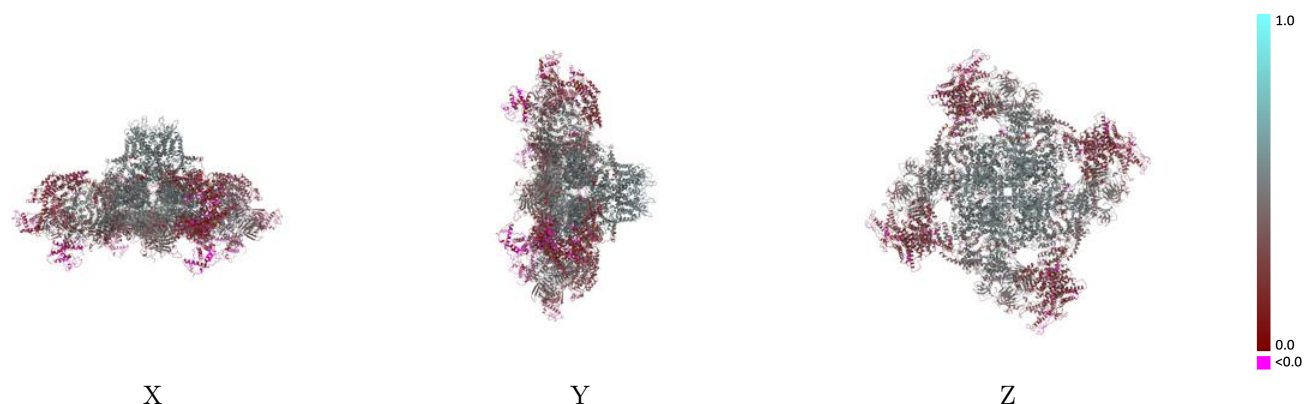
This section contains information regarding the fit between EMDB map EMD-47391 and PDB model 9E1E. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



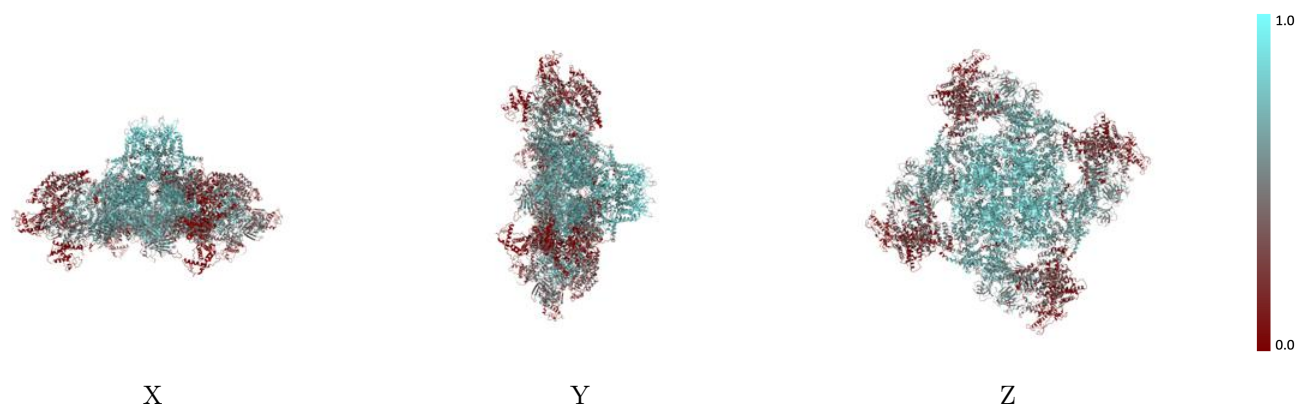
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



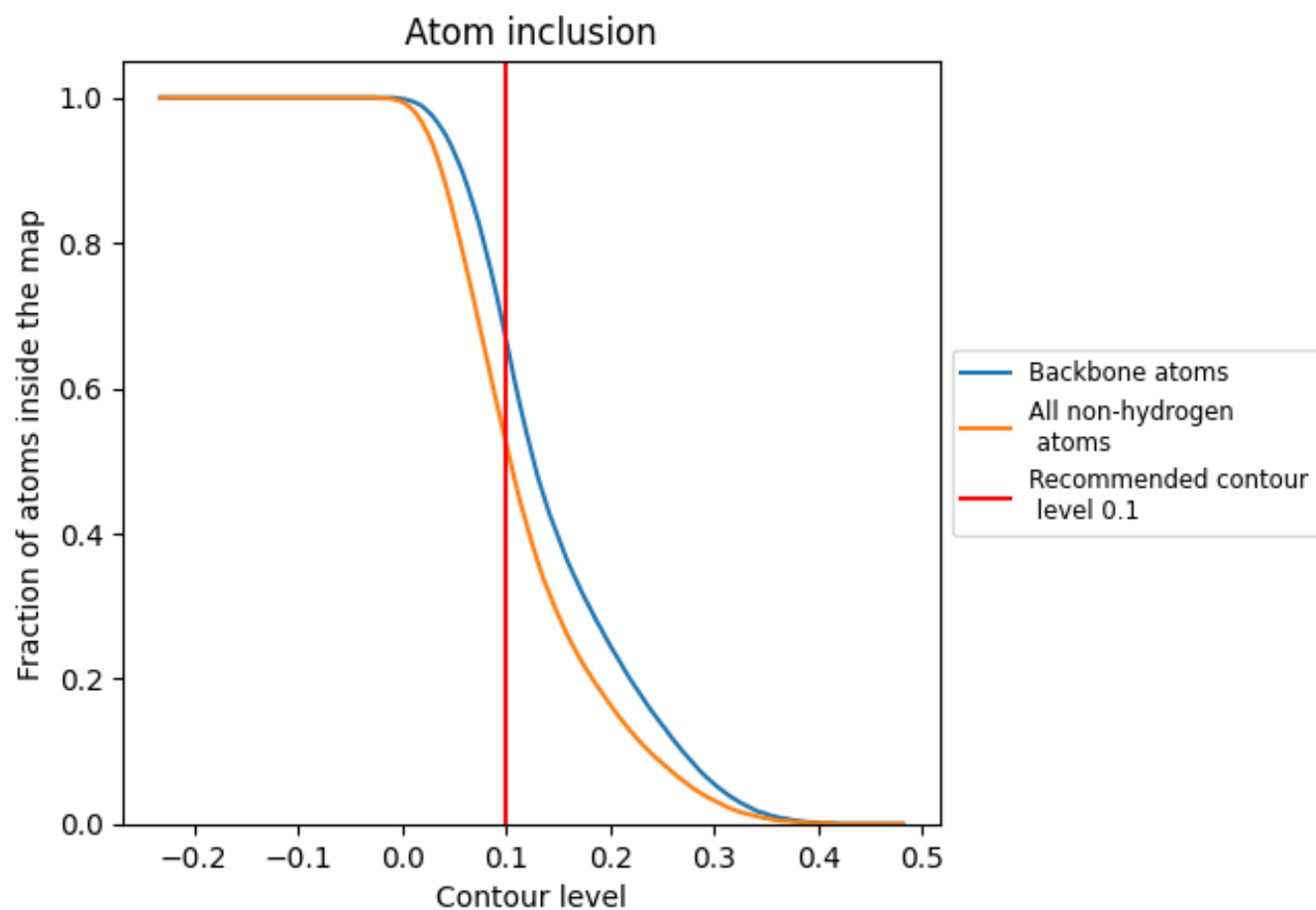
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 52% 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	<div><div></div></div> 0.5250	<div><div></div></div> 0.3760
A	<div><div></div></div> 0.5260	<div><div></div></div> 0.3740
B	<div><div></div></div> 0.5260	<div><div></div></div> 0.3740
C	<div><div></div></div> 0.5240	<div><div></div></div> 0.3730
D	<div><div></div></div> 0.5270	<div><div></div></div> 0.3750
E	<div><div></div></div> 0.4910	<div><div></div></div> 0.4340
F	<div><div></div></div> 0.4930	<div><div></div></div> 0.4290
G	<div><div></div></div> 0.4920	<div><div></div></div> 0.4280
H	<div><div></div></div> 0.4930	<div><div></div></div> 0.4300

1.0

0.0

<0.0