



## Full wwPDB EM Validation Report ⓘ

Jan 1, 2025 – 08:33 AM EST

PDB ID : 8RS0  
EMDB ID : EMD-19472  
Title : Structure of RyR1 in detergent in primed state in complex with nanobody and FKBP  
Authors : Li, C.; Efremov, R.G.  
Deposited on : 2024-01-24  
Resolution : 3.30 Å(reported)

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.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
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) : 2.40

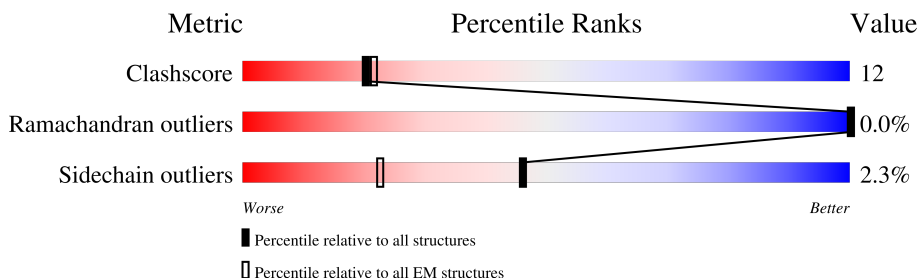
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	107	<div> <div>17%</div> <div>67%</div> <div>31%</div> <div>•</div> </div>
1	D	107	<div> <div>18%</div> <div>73%</div> <div>25%</div> <div>•</div> </div>
1	H	107	<div> <div>19%</div> <div>70%</div> <div>28%</div> <div>•</div> </div>
1	I	107	<div> <div>18%</div> <div>74%</div> <div>24%</div> <div>•</div> </div>
2	B	5027	<div> <div>•</div> <div>62%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
2	E	5027	<div> <div>•</div> <div>62%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
2	G	5027	<div> <div>•</div> <div>63%</div> <div>23%</div> <div>•</div> <div>14%</div> </div>
2	J	5027	<div> <div>•</div> <div>62%</div> <div>22%</div> <div>•</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	137	<div><div>23%</div><div><div></div><div>56%</div><div>34%</div><div>8%</div></div></div>
3	F	137	<div><div>23%</div><div><div></div><div>56%</div><div>34%</div><div>8%</div></div></div>
3	K	137	<div><div>23%</div><div><div></div><div>56%</div><div>34%</div><div>8%</div></div></div>
3	M	137	<div><div>22%</div><div><div></div><div>57%</div><div>33%</div><div>8%</div></div></div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 143570 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	D	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
1	I	107	Total	C	N	O	S	0	0
			816	514	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		
2	E	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		
2	G	4319	Total	C	N	O	S	1	0
			34149	21751	5887	6284	227		
2	J	4305	Total	C	N	O	S	1	0
			34043	21690	5866	6261	226		

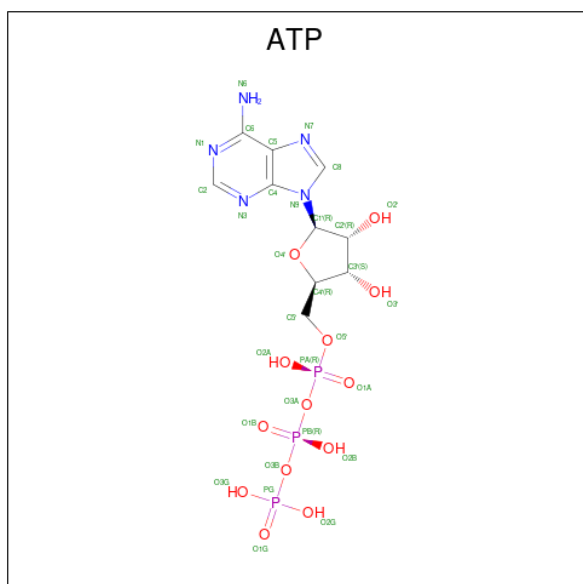
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	F	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	K	126	Total	C	N	O	S	0	0
			960	591	170	194	5		
3	M	126	Total	C	N	O	S	0	0
			960	591	170	194	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	
4	J	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



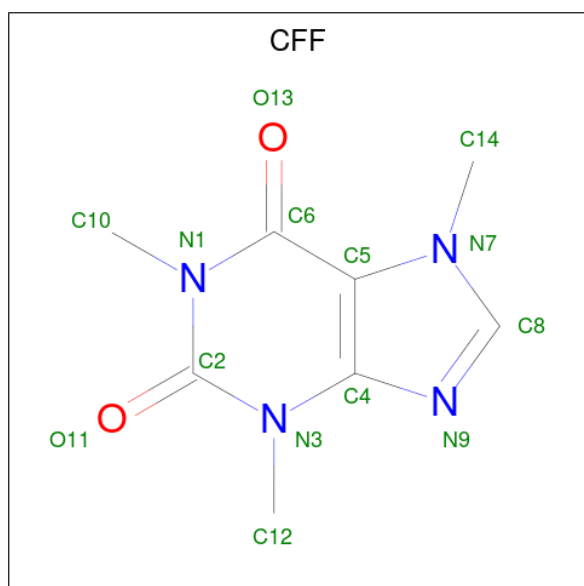
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula:  $C_8H_{10}N_4O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Ca	0
			1	1	

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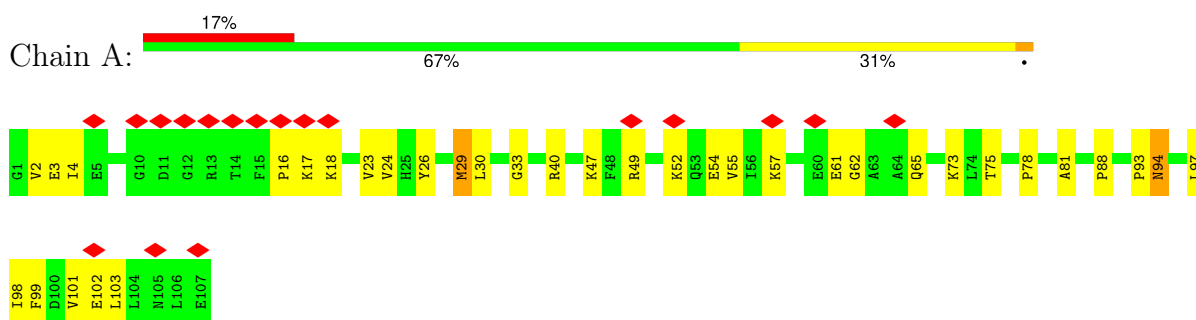
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Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total 1	Ca 1	0
7	G	1	Total 1	Ca 1	0
7	J	1	Total 1	Ca 1	0

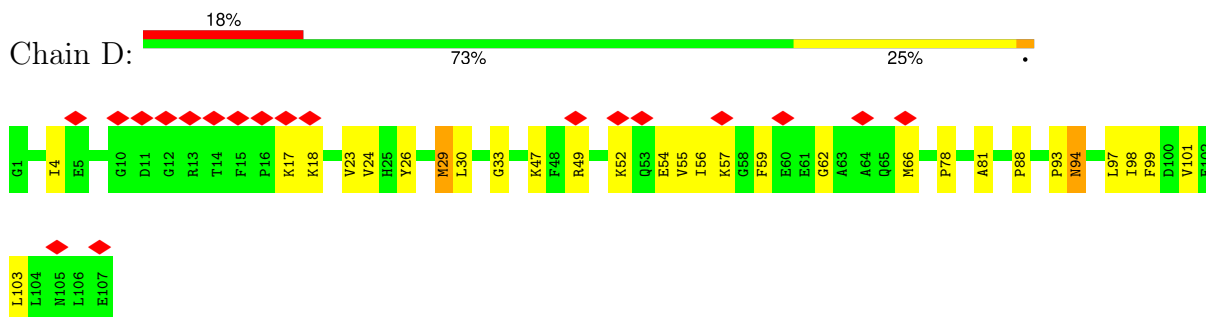
### 3 Residue-property plots [i](#)

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.

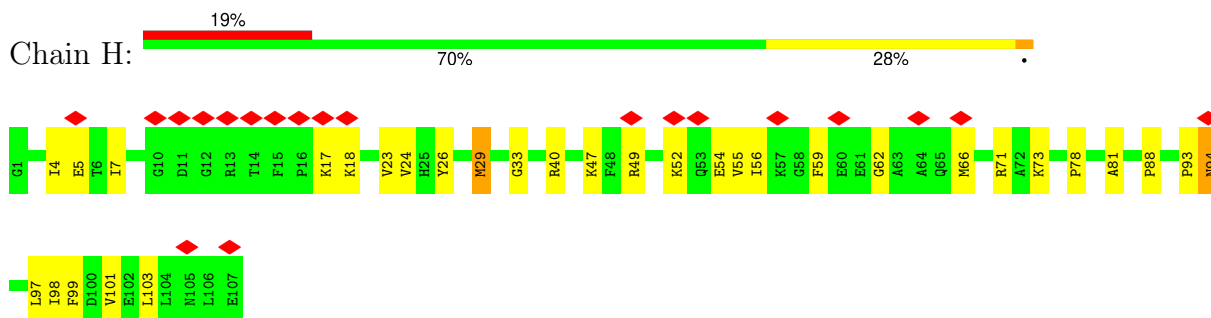
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



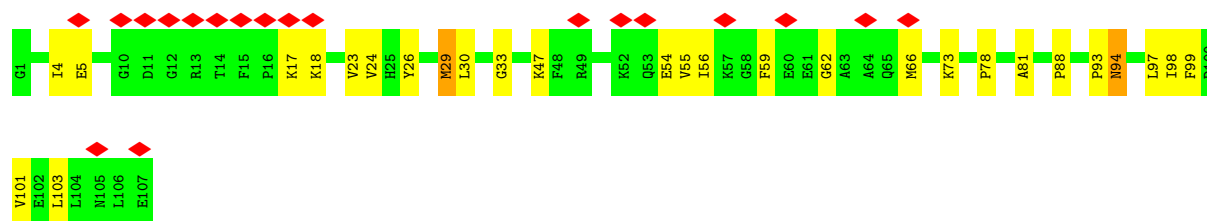
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

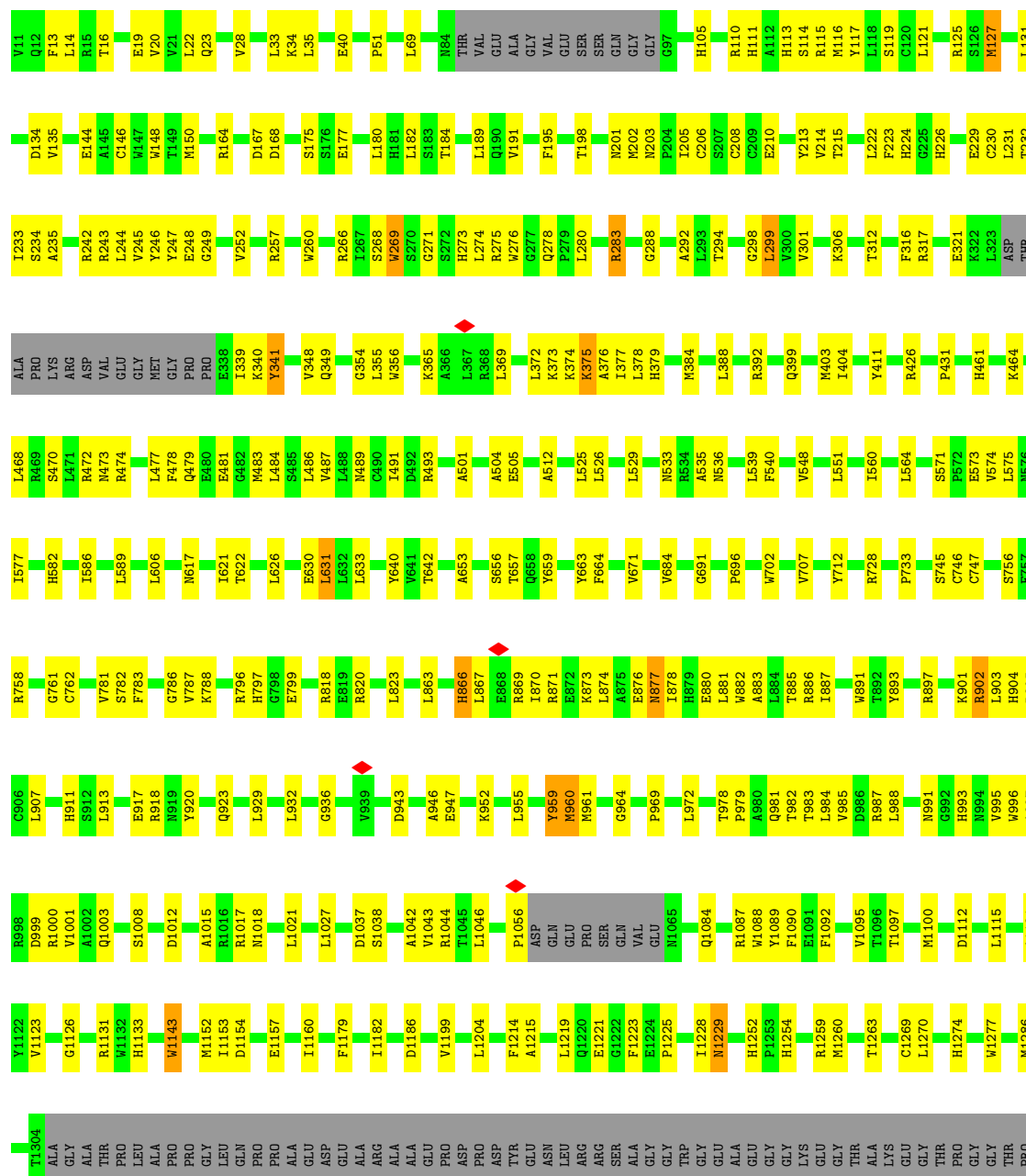






• Molecule 2: Ryanodine receptor 1

Chain B: 62% 23% 14%



E2820	E2821	T2822	E2823	E2824	K2825	A2826	E2827	E2828	E2829	E2830	GLU	GLU	GLU	ARG	THR	GLU	GLU	LYS	LYS	THR	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	THR	ASP	PRO	ARG	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	G2864	V2865	T2866	L2867	S2868	E2869	E2870	L2871	Q2872	A2875	L2878	A2879	E2880	N2881	Y2882	H2883																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
W2754	L2755	K2756	K2757	F2758	A2759	T2762	K2765	K2766	K2767	F2768	D2769	K2770	L2771	Q2772	Q2773	L2774	W2775	W2776	Y2777	E2778	E2779	N2780	D2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	F2789	N2790	L2791	R2792	F2793	V2794	K2795	T2796	F2797	S2798	E2799	D2800	L2801	E2802	E2803	L2804	Y2805	R2806	L2809	K2810	K2814	L2817	A2818	W2819																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
W2852	K2853	Y2854	W2857	F2858	T2859	F2864	L2867	H2867	L2868	L2869	I2869	F2869	L2870	S2871	H2872	Y2873	Y2874	Y2875	Y2876	Y2877	Y2878	Y2879	Y2880	Y2881	Y2882	Y2883	Y2884	Y2885	Y2886	Y2887	Y2888	Y2889	Y2890	Y2891	Y2892	Y2893	Y2894	Y2895	Y2896	Y2897	Y2898	Y2899	Y2900	Y2901	Y2902	Y2903	Y2904	Y2905	Y2906	Y2907	Y2908	Y2909	Y2910	Y2911	Y2912	Y2913	Y2914	Y2915	Y2916	Y2917	Y2918	Y2919	Y2920	Y2921	Y2922	Y2923	Y2924	Y2925	Y2926	Y2927	Y2928	Y2929	Y2930	Y2931	Y2932	Y2933	Y2934	Y2935	Y2936	Y2937	Y2938	Y2939	Y2940	Y2941	Y2942	Y2943	Y2944	Y2945	Y2946	Y2947	Y2948	Y2949	Y2950	Y2951	Y2952	Y2953	Y2954	Y2955	Y2956	Y2957	Y2958	Y2959	Y2960	Y2961	Y2962	Y2963	Y2964	Y2965	Y2966	Y2967	Y2968	Y2969	Y2970	Y2971	Y2972	Y2973	Y2974	Y2975	Y2976	Y2977	Y2978	Y2979	Y2980	Y2981	Y2982	Y2983	Y2984	Y2985	Y2986	Y2987	Y2988	Y2989	Y2990	Y2991	Y2992	Y2993	Y2994	Y2995	Y2996	Y2997	Y2998	Y2999	Y3000	Y3001	Y3002	Y3003	Y3004	Y3005	Y3006	Y3007	Y3008	Y3009	Y3010	Y3011	Y3012	Y3013	Y3014	Y3015	Y3016	Y3017	Y3018	Y3019	Y3020	Y3021	Y3022	Y3023	Y3024	Y3025	Y3026	Y3027	Y3028	Y3029	Y3030	Y3031	Y3032	Y3033	Y3034	Y3035	Y3036	Y3037	Y3038	Y3039	Y3040	Y3041	Y3042	Y3043	Y3044	Y3045	Y3046	Y3047	Y3048	Y3049	Y3050	Y3051	Y3052	Y3053	Y3054	Y3055	Y3056	Y3057	Y3058	Y3059	Y3060	Y3061	Y3062	Y3063	Y3064	Y3065	Y3066	Y3067	Y3068	Y3069	Y3070	Y3071	Y3072	Y3073	Y3074	Y3075	Y3076	Y3077	Y3078	Y3079	Y3080	Y3081	Y3082	Y3083	Y3084	Y3085	Y3086	Y3087	Y3088	Y3089	Y3090	Y3091	Y3092	Y3093	Y3094	Y3095	Y3096	Y3097	Y3098	Y3099	Y3100	Y3101	Y3102	Y3103	Y3104	Y3105	Y3106	Y3107	Y3108	Y3109	Y3110	Y3111	Y3112	Y3113	Y3114	Y3115	Y3116	Y3117	Y3118	Y3119	Y3120	Y3121	Y3122	Y3123	Y3124	Y3125	Y3126	Y3127	Y3128	Y3129	Y3130	Y3131	Y3132	Y3133	Y3134	Y3135	Y3136	Y3137	Y3138	Y3139	Y3140	Y3141	Y3142	Y3143	Y3144	Y3145	Y3146	Y3147	Y3148	Y3149	Y3150	Y3151	Y3152	Y3153	Y3154	Y3155	Y3156	Y3157	Y3158	Y3159	Y3160	Y3161	Y3162	Y3163	Y3164	Y3165	Y3166	Y3167	Y3168	Y3169	Y3170	Y3171	Y3172	Y3173	Y3174	Y3175	Y3176	Y3177	Y3178	Y3179	Y3180	Y3181	Y3182	Y3183	Y3184	Y3185	Y3186	Y3187	Y3188	Y3189	Y3190	Y3191	Y3192	Y3193	Y3194	Y3195	Y3196	Y3197	Y3198	Y3199	Y3200	Y3201	Y3202	Y3203	Y3204	Y3205	Y3206	Y3207	Y3208	Y3209	Y3210	Y3211	Y3212	Y3213	Y3214	Y3215	Y3216	Y3217	Y3218	Y3219	Y3220	Y3221	Y3222	Y3223	Y3224	Y3225	Y3226	Y3227	Y3228	Y3229	Y3230	Y3231	Y3232	Y3233	Y3234	Y3235	Y3236	Y3237	Y3238	Y3239	Y3240	Y3241	Y3242	Y3243	Y3244	Y3245	Y3246	Y3247	Y3248	Y3249	Y3250	Y3251	Y3252	Y3253	Y3254	Y3255	Y3256	Y3257	Y3258	Y3259	Y3260	Y3261	Y3262	Y3263	Y3264	Y3265	Y3266	Y3267	Y3268	Y3269	Y3270	Y3271	Y3272	Y3273	Y3274	Y3275	Y3276	Y3277	Y3278	Y3279	Y3280	Y3281	Y3282	Y3283	Y3284	Y3285	Y3286	Y3287	Y3288	Y3289	Y3290	Y3291	Y3292	Y3293	Y3294	Y3295	Y3296	Y3297	Y3298	Y3299	Y3300	Y3301	Y3302	Y3303	Y3304	Y3305	Y3306	Y3307	Y3308	Y3309	Y3310	Y3311	Y3312	Y3313	Y3314	Y3315	Y3316	Y3317	Y3318	Y3319	Y3320	Y3321	Y3322	Y3323	Y3324	Y3325	Y3326	Y3327	Y3328	Y3329	Y3330	Y3331	Y3332	Y3333	Y3334	Y3335	Y3336	Y3337	Y3338	Y3339	Y3340	Y3341	Y3342	Y3343	Y3344	Y3345	Y3346	Y3347	Y3348	Y3349	Y3350	Y3351	Y3352	Y3353	Y3354	Y3355	Y3356	Y3357	Y3358	Y3359	Y3360	Y3361	Y3362	Y3363	Y3364	Y3365	Y3366	Y3367	Y3368	Y3369	Y3370	Y3371	Y3372	Y3373	Y3374	Y3375	Y3376	Y3377	Y3378	Y3379	Y3380	Y3381	Y3382	Y3383	Y3384	Y3385	Y3386	Y3387	Y3388	Y3389	Y3390	Y3391	Y3392	Y3393	Y3394	Y3395	Y3396	Y3397	Y3398	Y3399	Y3400	Y3401	Y3402	Y3403	Y3404	Y3405	Y3406	Y3407	Y3408	Y3409	Y3410	Y3411	Y3412	Y3413	Y3414	Y3415	Y3416	Y3417	Y3418	Y3419	Y3420	Y3421	Y3422	Y3423	Y3424	Y3425	Y3426	Y3427	Y3428	Y3429	Y3430	Y3431	Y3432	Y3433	Y3434	Y3435	Y3436	Y3437	Y3438	Y3439	Y3440	Y3441	Y3442	Y3443	Y3444	Y3445	Y3446	Y3447	Y3448	Y3449	Y3450	Y3451	Y3452	Y3453	Y3454	Y3455	Y3456	Y3457	Y3458	Y3459	Y3460	Y3461	Y3462	Y3463	Y3464	Y3465	Y3466	Y3467	Y3468	Y3469	Y3470	Y3471	Y3472	Y3473	Y3474	Y3475	Y3476	Y3477	Y3478	Y3479	Y3480	Y3481	Y3482	Y3483	Y3484	Y3485	Y3486	Y3487	Y3488	Y3489	Y3490	Y3491	Y3492	Y3493	Y3494	Y3495	Y3496	Y3497	Y3498	Y3499	Y3500	Y3501	Y3502	Y3503	Y3504	Y3505	Y3506	Y3507	Y3508	Y3509	Y3510	Y3511	Y3512	Y3513	Y3514	Y3515	Y3516	Y3517	Y3518	Y3519	Y3520	Y3521	Y3522	Y3523	Y3524	Y3525	Y3526	Y3527	Y3528	Y3529	Y3530	Y3531	Y3532	Y3533	Y3534	Y3535	Y3536	Y3537	Y3538	Y3539	Y3540	Y3541	Y3542	Y3543	Y3544	Y3545	Y3546	Y3547	Y3548	Y3549	Y3550	Y3551	Y3552	Y3553	Y3554	Y3555	Y3556	Y3557	Y3558	Y3559	Y3560	Y3561	Y3562	Y3563	Y3564	Y3565	Y3566	Y3567	Y3568	Y3569	Y3570	Y3571	Y3572	Y3573	Y3574	Y3575	Y3576	Y3577	Y3578	Y3579	Y3580	Y3581	Y3582	Y3583	Y3584	Y3585	Y3586	Y3587	Y3588	Y3589	Y3590	Y3591	Y3592	Y3593	Y3594	Y3595	Y3596	Y3597	Y3598	Y3599	Y3600	Y3601	Y3602	Y3603	Y3604	Y3605	Y3606	Y3607	Y3608	Y3609	Y3610	Y3611	Y3612	Y3613	Y3614	Y3615	Y3616	Y3617	Y3618	Y3619	Y3620	Y3621	Y3622	Y3623	Y3624	Y3625	Y3626	Y3627	Y3628	Y3629	Y3630	Y3631	Y3632	Y3633	Y3634	Y3635	Y3636	Y3637	Y3638	Y3639	Y3640	Y3641	Y3642	Y3643	Y3644	Y3645	Y3646	Y3647	Y3648	Y3649	Y3650	Y3651	Y3652	Y3653	Y3654	Y3655	Y3656	Y3657	Y3658	Y3659	Y3660	Y3661	Y3662	Y3663	Y3664	Y3665	Y3666	Y3667	Y3668	Y3669	Y3670	Y3671	Y3672	Y3673	Y3674	Y3675	Y3676	Y3677	Y3678	Y3679	Y3680	Y3681	Y3682	Y3683	Y3684	Y3685	Y3686	Y3687	Y3688	Y3689	Y3690	Y3691	Y3692	Y3693	Y3694	Y3695	Y3696	Y3697	Y3698	Y3699	Y3700	Y3701	Y3702	Y3703	Y3704	Y3705	Y3706	Y3707	Y3708	Y3709	Y3710	Y3711	Y3712	Y3713	Y3714	Y3715	Y3716	Y3717	Y3718	Y3719	Y3720	Y3721	Y3722	Y3723	Y3724	Y3725	Y3726	Y3727	Y3728	Y3729	Y3730	Y3731	Y3732	Y3733	Y3734	Y3735	Y3736	Y3737	Y3738	Y3739	Y3740	Y3741	Y3742	Y3743	Y3744	Y3745	Y3746	Y3747	Y3748	Y3749	Y3750	Y3751	Y3752	Y3753	Y3754	Y3755	Y3756	Y3757	Y3758	Y3759	Y3760	Y3761	Y3762	Y3763	Y3764	Y3765	Y3766	Y3767	Y3768	Y3769	Y3770	Y3771	Y3772	Y3773	Y3774	Y3775	Y3776	Y3777	Y3778	Y3779	Y3780	Y3781	Y3782	Y3783	Y3784	Y3785	Y3786	Y3787	Y3788	Y3789	Y3790	Y3791	Y3792	Y3793	Y3794	Y3795	Y3796	Y3797	Y3798	Y3799	Y3800	Y3801	Y3802	Y3803	Y3804	Y3805	Y3806	Y3807	Y3808	Y3809	Y3810	Y3811	Y3812	Y3813	Y3814	Y3815	Y3816	Y3817	Y3818	Y3819	Y3820	Y3821	Y3822	Y3823	Y3824	Y3825	Y3826	Y3827	Y3828	Y3829	Y3830	Y3831	Y3832	Y3833	Y3834	Y3835	Y3836	Y3837	Y3838	Y3839	Y3840	Y3841	Y3842	Y3843	Y3844	Y3845	Y3846	Y3847	Y3848	Y3849	Y3850	Y3851	Y3852	Y3853	Y3854	Y3855	Y3856	Y3857	Y3858	Y3859	Y3860	Y3861	Y3862	Y3863	Y3864	Y3865	Y3866	Y3867	Y3868	Y3869	Y3870	Y3871	Y3872	Y3873	Y3874	Y3875	Y3876	Y3877	Y3878	Y3879	Y3880	Y3881	Y3882	Y3883	Y3884	Y3885	Y3886	Y3887	Y3888	Y3889	Y3890	Y3891	Y3892	Y3893	Y3894	Y3895	Y3896	Y3897	Y3898	Y3899	Y3900	Y3901	Y3902	Y3903	Y3904	Y3905	Y3906	Y3907	Y3908	Y3909	Y3910	Y3911	Y3912	Y3913	Y3914	Y3915	Y3916	Y3917	Y3918	Y3919	Y3920	Y3921	Y3922	Y3923	Y3924	Y3925	Y3926	Y3927	Y3928	Y3929	Y3930	Y3931	Y3932	Y3933	Y3934	Y3935	Y3936	Y3937	Y3938	Y3939	Y3940	Y3941	Y3942	Y3943	Y3944	Y3945	Y3946	Y3947	Y3948	Y3949	Y3950	Y3951	Y3952	Y3953	Y3954	Y3955	Y3956	Y3957	Y3958	Y3959	Y3960	Y3961	Y3962	Y3963	Y3964	Y3965	Y3966	Y3967	Y3968	Y3969	Y3970	Y3971	Y3972	Y3973	Y3974	Y3975	Y3976	Y3977	Y3978	Y3979	Y3980	Y3981	Y3982	Y3983	Y398

ALA	THR	L4181	Q4043	D3878	L3735	LYS	I3533	L3354	P3244	L3158	R3078	E2987	H2884
GLY	VAL	R4189	M4044	E3879	E3740	LEU	M3534	H3385	V3245	Q3162	T3079	E2987	K2897
ALA	ALA		V4045	F3880	ASN	LEU	L3535	S3356	L3246		X3080	H2991	G2898
ALA	GLY		L4048	F3887	GLY	LYS	A3536	H3357	D3247	C3165	M3081	E2992	G2899
ALA	THR		V4055	F3891	GLU	GLN	K3537	F3358	R3248	Y3166	K3082		
LEU	ALA		V4055	F3891	ALA	ARG	T3538	I3359		R3167	L3092	I2995	H2902
ARG	ALA		K4060	C3892	GLU	ARG	S3472	G3363			S3094	K2996	F2903
LEU	LEU		D4063	E3993	ALA	ARG	S3474	R3366		I3172	F3095	F2997	L2903
TRP	ALA		M4064	F3899	VAL	ALA	LYS	R3368		Y3173	F3096	F2998	L2905
ALA	ALA		I3315	L3542	VAL	ALA	ALA			L3175	K3097	A2989	
SER	ALA		K4067	E3754	ALA	LYS	LYS	K3371		N3180	S3098	K3000	Y2908
LEU	ALA		L4068	E3757	CYS	ALA	ALA	V3372		T3181	S3101	I3001	I3001
GLY	ALA		K4068	M3758	PHE	ALA	ALA			Y3182	L3110	L3002	D2909
GLY	ALA		F4077	Q3761	ARG	GLY	GLY	E3376		F3183	P3004	L2911	T2910
GLY	LEU		F4241	S3768	MET	ASP	ASP	E3377		L3103	D3102	L3005	A2913
GLY	ARG		Y4080	H3771	T3639	GLN	ALA	E3377		E3104	K3185	I3006	T2912
VAL	GLY		L4087	Q3781	P3640	GLN	GLN	R3380		K3105	N3007	N3007	K2914
GLY	TRP		S3938	L3780	L3643	SER	SER	L3384		K3106	Q3008	Q3008	
ALA	ALA		K4090	Q3781	L3644	GLY	GLY	K3384		V3107	N3012	H3013	Q2924
ALA	SER		K4091	P3645	ASP	ASP	ASP	A3387		L3110	L2927	C3014	L2927
LYS	LEU		N3950	R3648	GLN	GLN	GLU	E3397		R3111	K2928		
VAL	ARG		V3961	N3809	GLU	ARG	GLU			LEU	Q2931		
THR	ARG		L3965	N3651	ARG	ARG	ARG			GLY	M2932		
THR	VAL		T3966	V3812	THR	THR	THR	V3400		LYS	W2933		
GLY	VAL		E3967	E3655	LYS	LYS	LYS	L3405		VAL	G3029		
LEU	ARG		Q4105	K3658	LYS	LYS	LYS	Y3406		SER	H3030		
LEU	LEU		T4108	L3820	ARG	ARG	ARG			GLN	A3031		
ALA	ALA		Q4109	E3825	GLY	GLY	GLY	Y3409		ALA	P2934		
MET	LEU		F4110	Q3683	ASP	TYR	TYR	R3414		ALA	W2935		
ASP	THR		S4115	E3684	ARG	ARG	ARG			ARG	K3034		
ASP	ALA		D4118	E3687	ARG	ARG	ARG	P3410		THR	A2936		
PRO	ARG		E4119	E3687	GLY	GLY	GLY	L3411		GLN	K3036		
SER	ALA		M4120	E3691	ASP	ASP	ASP	L3412		VAL	V2937		
GLY	ALA		E4121	E3691	GLY	GLY	GLY	L3413		LYS	T2938		
ALA	THR		M4122	E3691	GLY	GLY	GLY	R3414		GLY	T2939		
ALA	ALA		I4123	E3691	GLY	GLY	GLY	Y3415		VAL	L2946		
GLY	ALA		N4130	E3691	GLY	GLY	GLY	V3416		GLY	L3040		
GLY	ALA		P4135	E3691	GLY	GLY	GLY	D3417		GLY	S3041		
ALA	ALA		D4138	E3691	GLY	GLY	GLY			GLY	F3043		
PRO	VAL		R4159	E3691	GLY	GLY	GLY	N3428		VAL	C3044		
GLY	VAL		M4023	E3691	GLY	GLY	GLY	E3432		L3136	L3049		
ASP	ALA		R4161	E3691	GLY	GLY	GLY	E3433		L3137	V3050		
ASP	ALA		L4184	E3691	GLY	GLY	GLY	L3434		F3138	R3051		
GLY	ALA		P4176	E3691	GLY	GLY	GLY	F3435		V3139	L2960		
ALA	ALA			E3691	GLY	GLY	GLY	R3436		L3140	Q2961		
GLY	GLY			E3691	GLY	GLY	GLY	M3437		T3141	G2962		
ALA	ALA			E3691	GLY	GLY	GLY	V3438		F3144	R3063		
ALA	ALA			E3691	GLY	GLY	GLY	G3439		L2964	L2963		
GLY	GLY			E3691	GLY	GLY	GLY			L3147	R2965		
GLY	GLY			E3691	GLY	GLY	GLY	T3443		I3070	W2966		
GLY	GLY			E3691	GLY	GLY	GLY	Y3444		F3152	M2967		
GLY	GLY			E3691	GLY	GLY	GLY	W3445		G3153	S2970		
GLY	GLY			E3691	GLY	GLY	GLY	F3451		D3154	Q2971		
GLY	GLY			E3691	GLY	GLY	GLY			I3157	E2972		
GLY	GLY			E3691	GLY	GLY	GLY	F3458			T2973		
GLY	GLY			E3691	GLY	GLY	GLY				T2974		
GLY	GLY			E3691	GLY	GLY	GLY				L2977		



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V4024	D3878	L3735	HIS	L3532	F3451	H3555	I3253	Y3166	L3092	I2995	P2903	R2827	T2762
V4025	E3879	E3740	LYS	L3533	F3458	S3556	I3257	R3167	R3093	L2996	L2904	E2828	K2765
G4038	F3880	ASN	LEU	L3535	F3459	H3557	A3257	F3173	R3094	F2997	L2905	G2829	W2766
A4041	F3887	GLY	SER	A3536	I3464	I3559	R3262	L3175	F3095	A2999	D2908	E2830	A2767
R4042	L3891	GLU	LYS	K3537	A3472	G3563	Y3263	N3180	F3096	K3000	T2910	F2768	F2768
Q4043	C3892	ALA	ARG	R3538	S3473	R3566	T3264	T3181	E3097	I3001	L2911	W2769	W2769
M4044	E3893	GLU	ARG	R3539	K3475	K3666	E3265	Y3182	A3099	L3002	T2912	W2770	K2770
V4045	E3893	GLU	ARG	L3542	K3475	K3666	E3265	Y3182	A3099	L3002	T2912	W2770	K2770
L4048	F3899	E3747	ALA	L3542	SER	R3368	I3272	E3184	A3101	P3004	K2914	L2772	Q2772
V4055	L3903	D3546	VAL	D3546	LYS	K3371	I3273	K3185	T3103	L3005	L2773	L2773	W2773
K4060	I3915	E3547	VAL	E3547	MET	K3372	P3275	K3185	E3104	N3007	W2774	W2774	W2774
K4067	E3757	E3548	ALA	E3548	ALA	V3372	M3276	L3186	K3105	Q3008	W2775	W2775	W2775
M4064	M3758	R3549	CYS	R3550	ALA	E3376	L3277	L3190	M3106	L2924	S2776	S2776	S2776
L4068	I3923	E3551	ARG	E3551	GLY	E3377	M3277	L3190	V3107	Q2924	W2777	W2777	W2777
F4077	L3923	F3552	MET	F3552	ASP	R3380	Y3280	C3193	L3110	L2927	W2778	W2778	W2778
Y4080	Q3927	L3553	GLN	L3553	ALA	R3380	L3281	L3194	R3111	K2928	E2779	E2779	E2779
L4087	F3933	Q3554	SER	Q3554	GLN	K3384	W3284	A3195	L3111	W2932	W2780	W2780	W2780
K4089	F3933	W3562	GLY	W3562	GLY	K3384	W3284	A3195	L3111	W2932	W2780	W2780	W2780
F4077	Y3936	L3557	GLY	L3557	GLY	A3387	E3286	L3197	LYS	G3029	W2781	W2781	W2781
Y4080	Y3937	Q3560	SER	Q3560	SER	E3391	R3287	M3201	VAL	H3030	E2782	E2782	E2782
L4087	S3933	Q3560	ASP	Q3560	ASP	E3391	L3296	P3203	GLN	A3031	E2783	E2783	E2783
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K4090	V3961	S3568	THR	S3568	THR	E3397	C3304	L3206	ALA	K3034	E2784	E2784	E2784
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A4096	L3965	W3571	LYS	W3571	LYS	V3400	T3308	Q3209	VAL	M3038	E2786	E2786	E2786
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G4105	Y3967	Y3576	GLY	Y3576	GLY	Y3406	L3315	A3215	GLY	S3041	E2788	E2788	E2788
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Q4109	Q3970	E3577	ARG	E3577	ARG	L3411	L3316	T3220	GLY	K3045	E2790	E2790	E2790
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L4112	V3985	E3577	ARG	E3577	ARG	L3411	L3316	T3220	GLY	K3045	E2790	E2790	E2790
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E4119	M4001	L3844	ASP	L3844	ASP	R3410	S3314	V3218	GLY	F3043	E2790	E2790	E2790
M4120	K4002	G3857	THR	G3857	THR	Y3415	L3320	E3226	VAL	H3052	E2791	E2791	E2791
K4014	K4014	MET	VAL	MET	VAL	V3416	R3321	R3227	L3140	R3053	E2792	E2792	E2792
L4017	L4017	VAL	THR	VAL	THR	D3417	N3325	A3228	T3141	V3054	E2793	E2793	E2793
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L4021	L4021	ASN	ASN	ASN	ASN	N3428	N3325	A3228	T3141	V3054	E2793	E2793	E2793
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L4024	L4024	ASN	ASN	ASN	ASN	N3428	N3325	A3228	T3141	V3054	E2793	E2793	E2793
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L4042	L4042	ASN	ASN	ASN	ASN	N3428	N3325	A3228	T3141	V3054	E2793	E2793	E2793
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R2359	R2360	P2361	F2364	L2376	T2380	E2381	E2382	A2383	T2384	R2385	R2392	P2395	GLY	VAL	ARG	ASP	ARG	ARG	ARG	C2305	C2310	P2311	M2312	L2313	L2314	GLU	GLU	PRO	PRO	GLU	N2414	R2415	H2416	L2418	G2419	T2422	H2423	L2429	L2430	D2431	R2435	E2449	R2452	T2453	L2457	L2460
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THR	SER	LEU	SER	ARG	LEU	ARG	SER	LEU	GLU	THR	VAL	ARG	LEU	VAL	LYS	LYS	GLU	GLU	PRO	GLU	GLU	PRO	ALA	GLU	GLU	K2089	V2102	V2103	R2104	E2108	D2109	L2116	M2120	F2121	S2122	L2123	R2126	Q2127	L2134	L2138	Y2142	P2146	L2357	T2152		
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PRO	GLY	LEU	PRO	PRO	ALA	GLY	ASP	GLY	ALA	ALA	GLY	PRO	ASP	PRO	ASP	TYR	GLY	ASN	ARG	SER	ALA	GLY	GLY	TRP	GLY	GLY	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
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D1012	A1015	M1016	R1017	M1018	L1021	L1027	D1037	S1038	A1042	V1043	R1044	T1046	T1053	P1056	ASP	GLN	GLU	PRO	SER	GLN	VAL	GLU	M1065	Q1084	R1087	W1088	T983	L984	E1091	F1092	C1093	L1095	T1096	T1097	M1100	D1112	Y995	W996	A997	R998	D999	R1000	V1001	A1002	Q1003	
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I586	L589	L606	T622	L626	E630	L631	L632	L633	H866	V641	T642	A653	S656	T657	Q658	Y659	Y663	F664	H879	E880	L881	W882	A883	L884	T885	R886	I887	W891	T892	Y893	R897	L988	N991	G992	H993	H994	Y995	W996	A997	R998	D999	R1000	V1001	A1002	Q1003	



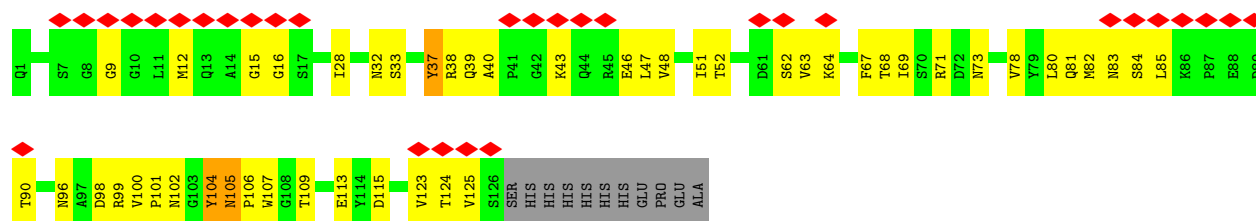
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CYS	L3642	V3549	ALA	E3376	L3274	E3184	I3007	A2917	THR	N2774	G2592	Q2475
PHE	N3643	R3550	GLY	E3377	L3275	K3185	N3007	Q2924	ARG	W2775	A2598	L2476
ARG	L3644	E3551	ASP	R3380	M3276	L3186	Q3008	Q2924	LYS	S2776	Q2599	L2479
MET	L3645	F3552	ALA	K3384	L3277	L3190	N3012	L2927	ILE	Y2777	D2600	P2496
		L3553	GLN	A3387	Y3280	C3193	H3013	K2928	SER	G2778	L2601	L2496
		N3554	SER	E3387	L3281	L3194	C3014	L2928	THR	E2779	V2602	L2496
		N3555	GLY	E3391	E3284	A3195	V3024	Q2931	ALA	N2780	L2603	P2496
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		P3567	ARG	L3286	P3202	F3202	K3034	A2936	PRO	E2784	L2614	S2501
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		L3569	LYS	L3312	L3206	L3206	K3036	V2937	GLY	K2786	L2615	L2506
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		W3571	ARG	E3314	N3214	N3214	M3038	T2939	VAL	H2788	S2617	E2513
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		R3577	ARG	G3317	G3222	G3222	S3041	LYS	GLY	R2792	L2623	L2519
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		S3592	GLY	L3320	T3221	T3221	K3045	GLU	THR	T2796	L2527	L2527
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		R3594	GLY	L3322	G3222	G3222	L3049	G2968	THR	S2798	N2634	L2527
		S3595	GLY	L3323	R3225	R3225	V3050	P2969	THR	T2741	R2635	R2530
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		V3602	GLY	E3334	R3227	R3227	H3052	Q2961	THR	L2743	A2637	R2531
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		H3607	GLY	I3345	P3233	P3233	H3069	R2965	THR	L2747	L2644	R2551
		W3608	GLY	V3346	N3234	N3234	I3070	M2966	THR	P2748	R2552	R2552
		L3612	GLY	S3347	G3234	G3234	L3074	M2967	THR	E2749	Y2648	L2559
		T3708	GLY	R3348	H3239	H3239	L3075	S2970	THR	K2750	R2649	L2559
		Y3720	GLY	A3349	R3350	R3350	L3076	Q2971	THR	L2751	R2650	T2563
		Y3725	GLY	E3344	I3243	I3243	A3077	E2972	THR	D2752	C2651	T2563
		M3729	GLY	V3245	V3245	V3245	R3078	F2973	THR	L2753	R2652	A2566
		A3730	GLY	L3246	L3246	L3246	T3079	L2974	THR	S2753	K2653	P2567
		K3731	GLY	H3355	H3247	H3247	V3080	L2977	THR	F2754	Y2654	L2568
		L3735	GLY	S3356	R3248	R3248	M3081	E2987	THR	L2755	W2661	F2569
		L3735	GLY	F3357	L3249	L3249	K3082	A2987	THR	N2756	F2664	T2572
		L3735	GLY	I3359	I3253	I3253	L3092	H2991	THR	K2757	L2672	R2573
		L3735	GLY	G3363	A3257	A3257	R3093	E2992	THR	A2759	H2673	L2576
		L3735	GLY	R3366	R3262	R3262	F3095	L2995	THR	T2762	L2678	L2576
		L3735	GLY	K3367	Y3263	Y3263	F3096	F2997	THR	L2766	L2678	L2576
		L3735	GLY	R3368	T3264	T3264	F3097	F2998	THR	K2765	L2678	L2576
		L3735	GLY	SER	SER	SER	S3098	F2998	THR	A2767	I2682	L2576
		L3735	GLY	ASN	ASN	ASN	L3099	A2999	THR	E2828	L2682	L2576
		L3735	GLY	GLN	GLN	GLN	D2909	K3000	THR	F2768	L2682	L2576
		L3735	GLY	GLU	GLU	GLU	T2910	L3001	THR	L2769	L2682	L2576
		L3735	GLY	ALA	ALA	ALA	L2911	L3001	THR	L2770	L2682	L2576
		L3735	GLY	GLU	GLU	GLU	L2911	L3001	THR	L2770	L2682	L2576



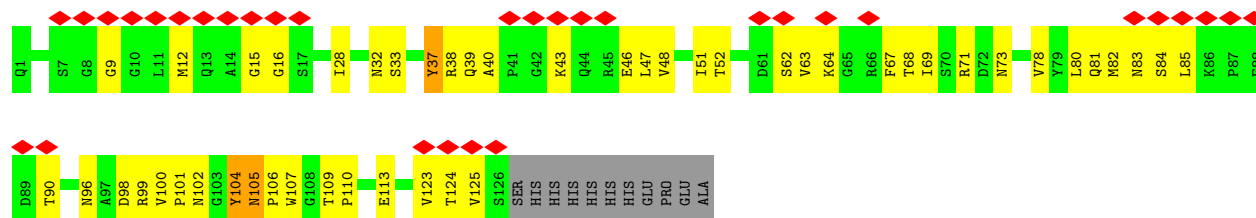
WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



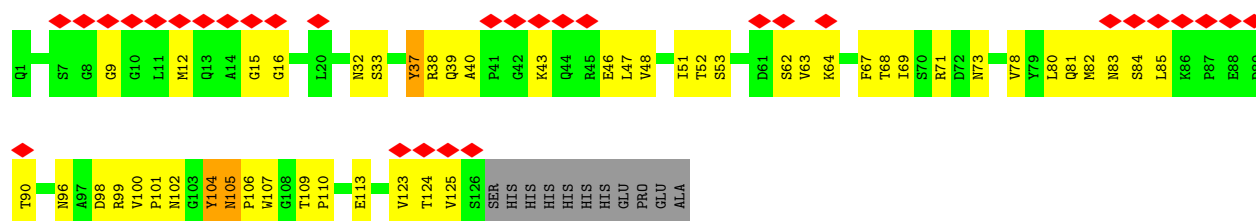




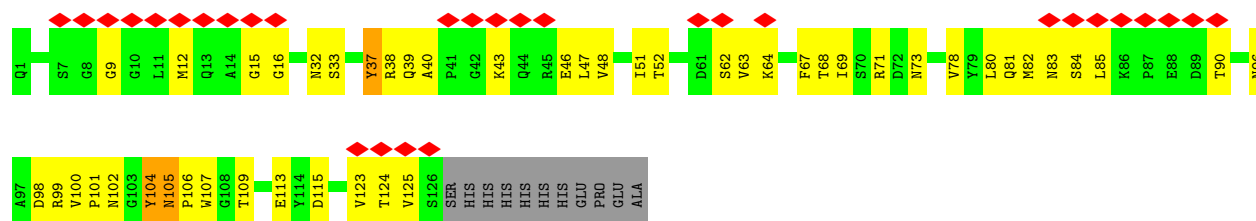
• Molecule 3: Nanobody 9657



• Molecule 3: Nanobody 9657



• Molecule 3: Nanobody 9657



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.519	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.057	Depositor
Map value standard deviation	0.125	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	500.64, 500.64, 500.64	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.49, 1.49, 1.49	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.27	0/831	0.55	0/1118
1	D	0.27	0/831	0.56	0/1118
1	H	0.27	0/831	0.56	0/1118
1	I	0.27	0/831	0.56	0/1118
2	B	0.25	0/34814	0.50	1/47183 (0.0%)
2	E	0.25	0/34814	0.50	1/47183 (0.0%)
2	G	0.25	0/34921	0.50	1/47329 (0.0%)
2	J	0.25	0/34814	0.50	1/47183 (0.0%)
3	C	0.28	0/979	0.58	0/1329
3	F	0.28	0/979	0.58	0/1329
3	K	0.28	0/979	0.58	0/1329
3	M	0.28	0/979	0.58	0/1329
All	All	0.25	0/146603	0.50	4/198666 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1503	PRO	N-CA-CB	5.74	110.19	103.30
2	J	1503	PRO	N-CA-CB	5.71	110.15	103.30
2	B	1503	PRO	N-CA-CB	5.68	110.11	103.30
2	G	1503	PRO	N-CA-CB	5.66	110.09	103.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	816	0	818	28	0
1	D	816	0	818	23	0
1	H	816	0	818	25	0
1	I	816	0	818	24	0
2	B	34043	0	33446	799	0
2	E	34043	0	33446	803	0
2	G	34149	0	33547	812	0
2	J	34043	0	33446	792	0
3	C	960	0	909	36	0
3	F	960	0	909	41	0
3	K	960	0	909	41	0
3	M	960	0	909	40	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	0	0
5	E	31	0	12	0	0
5	G	31	0	12	0	0
5	J	31	0	12	0	0
6	B	14	0	10	0	0
6	E	14	0	10	0	0
6	G	14	0	10	0	0
6	J	14	0	10	0	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	143570	0	140881	3411	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 12.

All (3411) 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)
2:B:4961:CYS:SG	2:B:4983:HIS:CE1	2.61	0.94
2:G:4961:CYS:SG	2:G:4983:HIS:CE1	2.60	0.93
2:E:4961:CYS:SG	2:E:4983:HIS:CE1	2.60	0.93
3:K:100:VAL:HG22	3:K:105:ASN:HD22	1.34	0.92
2:J:4961:CYS:SG	2:J:4983:HIS:CE1	2.60	0.92
3:M:100:VAL:HG22	3:M:105:ASN:HD22	1.33	0.92
2:B:3207:GLU:HB2	2:B:3246:LEU:HD22	1.51	0.92
2:B:2515:GLN:HA	2:B:2568:LEU:HD21	1.54	0.89
3:C:100:VAL:HG22	3:C:105:ASN:HD22	1.33	0.89
3:F:100:VAL:HG22	3:F:105:ASN:HD22	1.34	0.89
3:K:38:ARG:HH22	3:K:64:LYS:HG2	1.43	0.84
3:M:38:ARG:HH22	3:M:64:LYS:HG2	1.43	0.83
3:C:38:ARG:HH22	3:C:64:LYS:HG2	1.43	0.82
3:F:38:ARG:HH22	3:F:64:LYS:HG2	1.43	0.81
2:B:248:GLU:HB3	2:B:373:LYS:HD3	1.60	0.80
2:E:248:GLU:HA	2:E:372:LEU:HB3	1.65	0.78
2:G:248:GLU:HA	2:G:372:LEU:HB2	1.64	0.77
2:E:247:TYR:HD2	2:E:374:LYS:HB2	1.50	0.76
2:B:3277:LEU:HD13	2:B:3315:LEU:HD22	1.67	0.76
2:G:2974:ILE:HD12	2:G:3053:ARG:HG2	1.68	0.76
2:G:229:GLU:HA	2:G:249:GLY:HA3	1.68	0.76
2:J:2974:ILE:HD12	2:J:3053:ARG:HG2	1.68	0.76
2:E:1422:ASP:HB2	2:E:1427:ILE:HD11	1.68	0.76
2:B:229:GLU:HA	2:B:249:GLY:HA3	1.68	0.75
2:B:1422:ASP:HB2	2:B:1427:ILE:HD11	1.68	0.75
2:B:2974:ILE:HD12	2:B:3053:ARG:HG2	1.68	0.75
2:J:229:GLU:HA	2:J:249:GLY:HA3	1.68	0.75
2:G:1422:ASP:HB2	2:G:1427:ILE:HD11	1.68	0.75
2:E:2974:ILE:HD12	2:E:3053:ARG:HG2	1.68	0.74
2:B:3366:ARG:NH1	2:B:3437:MET:SD	2.60	0.74
2:B:891:TRP:HA	2:B:902:ARG:HB3	1.69	0.74
2:J:404:ILE:HD13	2:J:481:GLU:HG3	1.70	0.74
2:J:959:TYR:HB2	2:J:964:GLY:HA2	1.69	0.74
2:J:891:TRP:HA	2:J:902:ARG:HB3	1.69	0.74
2:J:248:GLU:HB3	2:J:373:LYS:HD3	1.69	0.74
2:G:3366:ARG:NH1	2:G:3437:MET:SD	2.60	0.74
2:E:229:GLU:HA	2:E:249:GLY:HA3	1.68	0.74
2:E:404:ILE:HD13	2:E:481:GLU:HG3	1.70	0.74
2:J:1422:ASP:HB2	2:J:1427:ILE:HD11	1.68	0.74
2:E:3366:ARG:NH1	2:E:3437:MET:SD	2.60	0.73
2:B:959:TYR:HB2	2:B:964:GLY:HA2	1.69	0.73
2:G:959:TYR:HB2	2:G:964:GLY:HA2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:891:TRP:HA	2:G:902:ARG:HB3	1.69	0.73
2:J:3366:ARG:HE	2:J:3367:LYS:HD2	1.54	0.73
2:B:3366:ARG:HE	2:B:3367:LYS:HD2	1.54	0.73
2:G:404:ILE:HD13	2:G:481:GLU:HG3	1.70	0.73
2:E:4852:THR:HG21	2:E:4883:TYR:HA	1.71	0.72
2:G:4715:TYR:HE2	2:G:4717:ASP:HB3	1.53	0.72
2:J:3366:ARG:NH1	2:J:3437:MET:SD	2.60	0.72
2:B:4852:THR:HG21	2:B:4883:TYR:HA	1.71	0.72
2:E:959:TYR:HB2	2:E:964:GLY:HA2	1.69	0.72
2:J:913:LEU:HB3	2:J:917:GLU:HB2	1.72	0.72
2:E:913:LEU:HB3	2:E:917:GLU:HB2	1.72	0.72
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.71	0.72
2:B:247:TYR:HD2	2:B:374:LYS:HB2	1.55	0.72
2:E:891:TRP:HA	2:E:902:ARG:HB3	1.69	0.72
2:B:404:ILE:HD13	2:B:481:GLU:HG3	1.70	0.72
2:G:3320:LEU:HD12	2:G:3357:HIS:CD2	2.25	0.72
2:E:4715:TYR:HE2	2:E:4717:ASP:HB3	1.54	0.72
2:B:3273:THR:HA	2:B:3276:MET:HG2	1.72	0.72
2:J:3277:LEU:HD13	2:J:3315:LEU:HD22	1.71	0.72
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.71	0.71
2:G:4852:THR:HG21	2:G:4883:TYR:HA	1.71	0.71
2:E:3366:ARG:HE	2:E:3367:LYS:HD2	1.54	0.71
2:G:3273:THR:HA	2:G:3276:MET:HG2	1.72	0.71
2:J:3809:ASN:HB3	2:J:3812:VAL:HG22	1.71	0.71
2:J:4715:TYR:HE2	2:J:4717:ASP:HB3	1.55	0.71
2:E:4546:VAL:HG22	2:E:4550:LYS:HE3	1.72	0.70
2:G:2244:ARG:HD3	2:G:3860:ASN:HA	1.73	0.70
2:J:3273:THR:HA	2:J:3276:MET:HG2	1.72	0.70
2:B:913:LEU:HB3	2:B:917:GLU:HB2	1.72	0.70
2:B:3144:PHE:HB2	2:B:3196:ARG:HB3	1.73	0.70
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.71	0.70
2:G:913:LEU:HB3	2:G:917:GLU:HB2	1.72	0.70
2:G:3366:ARG:HE	2:G:3367:LYS:HD2	1.54	0.70
2:E:3144:PHE:HB2	2:E:3196:ARG:HB3	1.73	0.70
2:E:3344:PRO:O	2:E:3348:ARG:NH2	2.25	0.70
2:J:3344:PRO:O	2:J:3348:ARG:NH2	2.25	0.70
2:B:4546:VAL:HG22	2:B:4550:LYS:HE3	1.72	0.70
2:J:4852:THR:HG21	2:J:4883:TYR:HA	1.71	0.70
2:G:3344:PRO:O	2:G:3348:ARG:NH2	2.25	0.70
2:G:4546:VAL:HG22	2:G:4550:LYS:HE3	1.72	0.70
2:E:3273:THR:HA	2:E:3276:MET:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3344:PRO:O	2:B:3348:ARG:NH2	2.25	0.70
2:B:4762:PRO:HD2	2:B:4766:THR:HG21	1.73	0.70
2:J:4762:PRO:HD2	2:J:4766:THR:HG21	1.73	0.70
2:G:3144:PHE:HB2	2:G:3196:ARG:HB3	1.73	0.69
2:J:4546:VAL:HG22	2:J:4550:LYS:HE3	1.72	0.69
2:B:399:GLN:O	2:B:403:MET:HG3	1.92	0.69
2:B:640:TYR:HB3	2:B:1613:LEU:HD11	1.75	0.69
2:B:2321:ILE:HD11	2:B:2418:LEU:HB2	1.74	0.69
2:E:3308:THR:H	2:E:3311:HIS:CD2	2.09	0.69
2:E:4762:PRO:HD2	2:E:4766:THR:HG21	1.73	0.69
2:G:399:GLN:O	2:G:403:MET:HG3	1.92	0.69
2:G:640:TYR:HB3	2:G:1613:LEU:HD11	1.75	0.69
2:G:3870:ASN:HD21	2:G:3873:LYS:HB3	1.57	0.69
2:J:2871:LEU:HG	2:J:2927:LEU:HD21	1.74	0.69
2:E:2321:ILE:HD11	2:E:2418:LEU:HB2	1.74	0.69
2:E:2871:LEU:HG	2:E:2927:LEU:HD21	1.74	0.69
2:J:2788:HIS:HB3	2:J:2791:LEU:HB2	1.75	0.69
2:G:4897:ILE:HG13	2:G:4901:ILE:HD11	1.75	0.69
2:E:4897:ILE:HG13	2:E:4901:ILE:HD11	1.75	0.69
2:J:3144:PHE:HB2	2:J:3196:ARG:HB3	1.73	0.69
2:B:3812:VAL:O	2:B:3816:MET:HG3	1.93	0.68
2:B:4176:PRO:O	2:B:4202:ARG:NH2	2.26	0.68
2:E:3812:VAL:O	2:E:3816:MET:HG3	1.93	0.68
2:G:2871:LEU:HG	2:G:2927:LEU:HD21	1.74	0.68
2:J:640:TYR:HB3	2:J:1613:LEU:HD11	1.75	0.68
2:B:2116:LEU:O	2:B:2120:MET:HG2	1.94	0.68
2:B:2871:LEU:HG	2:B:2927:LEU:HD21	1.74	0.68
2:G:4176:PRO:O	2:G:4202:ARG:NH2	2.26	0.68
2:E:399:GLN:O	2:E:403:MET:HG3	1.92	0.68
2:J:399:GLN:O	2:J:403:MET:HG3	1.92	0.68
2:B:4897:ILE:HG13	2:B:4901:ILE:HD11	1.75	0.68
2:E:640:TYR:HB3	2:E:1613:LEU:HD11	1.75	0.68
2:J:897:ARG:HD3	2:J:905:PRO:HD3	1.76	0.68
2:J:4897:ILE:HG13	2:J:4901:ILE:HD11	1.75	0.68
2:B:3077:ALA:O	2:B:3081:MET:HG2	1.94	0.68
3:F:71:ARG:NH1	3:F:73:ASN:OD1	2.26	0.68
2:E:3077:ALA:O	2:E:3081:MET:HG2	1.94	0.68
2:J:2116:LEU:O	2:J:2120:MET:HG2	1.94	0.68
2:B:1089:TYR:HD1	2:B:1152:MET:HG2	1.60	0.68
2:G:2321:ILE:HD11	2:G:2418:LEU:HB2	1.74	0.68
2:B:2788:HIS:HB3	2:B:2791:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:MET:HE1	1:H:101:VAL:HG23	1.77	0.67
2:E:2515:GLN:HA	2:E:2568:LEU:HD21	1.75	0.67
2:E:2788:HIS:HB3	2:E:2791:LEU:HB2	1.75	0.67
2:J:2321:ILE:HD11	2:J:2418:LEU:HB2	1.74	0.67
3:K:51:ILE:HG23	3:K:71:ARG:HD2	1.76	0.67
2:G:2116:LEU:O	2:G:2120:MET:HG2	1.94	0.67
2:G:4762:PRO:HD2	2:G:4766:THR:HG21	1.73	0.67
2:J:246:TYR:CG	2:J:373:LYS:HD2	2.30	0.67
2:J:2515:GLN:HA	2:J:2568:LEU:HD21	1.76	0.67
2:J:3262:ARG:HB2	2:J:3265:GLU:HG2	1.76	0.67
2:B:4679:ARG:HE	2:B:5017:ARG:NH2	1.92	0.67
2:E:4176:PRO:O	2:E:4202:ARG:NH2	2.26	0.67
2:G:897:ARG:HD3	2:G:905:PRO:HD3	1.76	0.67
2:G:3812:VAL:O	2:G:3816:MET:HG3	1.93	0.67
2:J:3812:VAL:O	2:J:3816:MET:HG3	1.93	0.67
2:J:4176:PRO:O	2:J:4202:ARG:NH2	2.26	0.67
2:E:897:ARG:HD3	2:E:905:PRO:HD3	1.76	0.67
2:G:3262:ARG:HB2	2:G:3265:GLU:HG2	1.76	0.67
2:E:2116:LEU:O	2:E:2120:MET:HG2	1.94	0.67
3:M:51:ILE:HG23	3:M:71:ARG:HD2	1.76	0.67
2:G:1089:TYR:HD1	2:G:1152:MET:HG2	1.60	0.67
2:G:3077:ALA:O	2:G:3081:MET:HG2	1.94	0.67
3:M:71:ARG:NH1	3:M:73:ASN:OD1	2.26	0.67
2:E:1089:TYR:HD1	2:E:1152:MET:HG2	1.60	0.67
2:E:3253:ILE:HG23	2:E:3318:ASN:HD22	1.60	0.67
2:G:2788:HIS:HB3	2:G:2791:LEU:HB2	1.75	0.67
2:J:2513:GLU:N	2:J:2513:GLU:OE2	2.28	0.67
2:J:3077:ALA:O	2:J:3081:MET:HG2	1.94	0.67
2:G:2513:GLU:N	2:G:2513:GLU:OE2	2.29	0.66
3:K:71:ARG:NH1	3:K:73:ASN:OD1	2.26	0.66
3:C:51:ILE:HG23	3:C:71:ARG:HD2	1.76	0.66
2:E:110:ARG:HD3	2:E:115:ARG:HE	1.60	0.66
2:G:248:GLU:HB3	2:G:373:LYS:HD3	1.77	0.66
2:E:3768:SER:HA	2:E:3771:HIS:CD2	2.31	0.66
2:J:110:ARG:HD3	2:J:115:ARG:HE	1.60	0.66
2:J:3433:GLU:HA	2:J:3436:ARG:HD2	1.78	0.66
2:B:3262:ARG:HB2	2:B:3265:GLU:HG2	1.76	0.66
2:G:3433:GLU:HA	2:G:3436:ARG:HD2	1.78	0.66
2:J:3768:SER:HA	2:J:3771:HIS:CD2	2.31	0.66
2:B:3768:SER:HA	2:B:3771:HIS:CD2	2.31	0.66
2:G:3768:SER:HA	2:G:3771:HIS:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2513:GLU:N	2:B:2513:GLU:OE2	2.29	0.66
2:G:1519:LEU:HD11	2:G:1572:ILE:HD13	1.78	0.66
2:B:897:ARG:HD3	2:B:905:PRO:HD3	1.76	0.66
2:J:247:TYR:HD2	2:J:374:LYS:HB2	1.60	0.66
2:E:2513:GLU:N	2:E:2513:GLU:OE2	2.29	0.65
2:E:2566:ALA:HA	2:E:2569:PHE:HD2	1.59	0.65
2:G:246:TYR:CG	2:G:373:LYS:HD2	2.31	0.65
2:J:1519:LEU:HD11	2:J:1572:ILE:HD13	1.78	0.65
2:B:3031:ALA:O	2:B:3036:LYS:NZ	2.30	0.65
2:E:3262:ARG:HB2	2:E:3265:GLU:HG2	1.76	0.65
2:B:1519:LEU:HD11	2:B:1572:ILE:HD13	1.78	0.65
2:B:3194:LEU:HD13	2:B:3276:MET:SD	2.36	0.65
2:J:3194:LEU:HD13	2:J:3276:MET:SD	2.36	0.65
2:J:1089:TYR:HD1	2:J:1152:MET:HG2	1.60	0.65
2:G:110:ARG:HD3	2:G:115:ARG:HE	1.60	0.65
2:G:3194:LEU:HD13	2:G:3276:MET:SD	2.36	0.65
2:B:3435:PHE:HE2	2:B:3518:LEU:HA	1.62	0.65
2:E:3031:ALA:O	2:E:3036:LYS:NZ	2.30	0.65
2:E:3245:VAL:HG23	2:E:3248:ARG:H	1.61	0.65
2:E:3433:GLU:HA	2:E:3436:ARG:HD2	1.78	0.65
2:J:2263:ILE:HA	2:J:2330:ARG:HH22	1.62	0.65
3:F:51:ILE:HG23	3:F:71:ARG:HD2	1.76	0.65
2:E:3194:LEU:HD13	2:E:3276:MET:SD	2.36	0.65
2:E:3435:PHE:HE2	2:E:3518:LEU:HA	1.62	0.65
2:J:622:THR:HA	2:J:626:LEU:HD13	1.79	0.65
3:M:52:THR:HG21	3:M:102:ASN:HA	1.79	0.65
2:B:110:ARG:HD3	2:B:115:ARG:HE	1.60	0.65
2:G:3031:ALA:O	2:G:3036:LYS:NZ	2.30	0.65
2:J:3594:ARG:NH1	2:J:3594:ARG:HA	2.12	0.65
2:B:2347:GLU:OE1	2:B:2347:GLU:N	2.27	0.64
2:E:1519:LEU:HD11	2:E:1572:ILE:HD13	1.78	0.64
2:E:3594:ARG:NH1	2:E:3594:ARG:HA	2.12	0.64
2:B:3281:LEU:HD12	2:B:3312:LEU:HG	1.79	0.64
2:E:622:THR:HA	2:E:626:LEU:HD13	1.79	0.64
2:G:247:TYR:HD2	2:G:374:LYS:HB2	1.62	0.64
2:B:2902:HIS:HB3	2:B:2905:LEU:HG	1.79	0.64
2:B:3433:GLU:HA	2:B:3436:ARG:HD2	1.78	0.64
2:E:246:TYR:CG	2:E:373:LYS:HG3	2.33	0.64
2:E:2902:HIS:HB3	2:E:2905:LEU:HG	1.79	0.64
2:G:2263:ILE:HA	2:G:2330:ARG:HH22	1.62	0.64
2:B:3567:PRO:HB2	2:B:3570:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3281:LEU:HD12	2:G:3312:LEU:HG	1.79	0.64
3:C:71:ARG:NH1	3:C:73:ASN:OD1	2.26	0.64
3:F:52:THR:HG21	3:F:102:ASN:HA	1.79	0.64
3:K:52:THR:HG21	3:K:102:ASN:HA	1.79	0.64
2:E:2347:GLU:OE1	2:E:2347:GLU:N	2.27	0.64
2:J:3263:TYR:HE2	2:J:3334:TRP:HD1	1.46	0.64
2:B:3253:ILE:HG23	2:B:3318:ASN:HD22	1.61	0.64
2:J:3031:ALA:O	2:J:3036:LYS:NZ	2.30	0.64
2:B:2518:LEU:HD23	2:B:2568:LEU:HD22	1.78	0.64
2:E:901:LYS:HD3	2:E:903:LEU:HD11	1.79	0.64
2:G:3435:PHE:HE2	2:G:3518:LEU:HA	1.62	0.64
2:B:3594:ARG:NH1	2:B:3594:ARG:HA	2.12	0.64
2:E:3263:TYR:HE2	2:E:3334:TRP:HD1	1.46	0.64
2:G:622:THR:HA	2:G:626:LEU:HD13	1.79	0.64
2:J:3567:PRO:HB2	2:J:3570:ARG:HH21	1.62	0.64
2:B:901:LYS:HD3	2:B:903:LEU:HD11	1.80	0.64
2:E:2575:ARG:HG3	2:E:2578:MET:HG3	1.80	0.64
2:E:2977:LEU:HD11	2:E:2995:ILE:HD13	1.80	0.64
2:G:2566:ALA:HA	2:G:2569:PHE:HD2	1.63	0.64
2:G:3548:GLU:HG2	2:G:3552:PHE:CZ	2.33	0.64
2:B:2263:ILE:HA	2:B:2330:ARG:HH22	1.62	0.63
2:G:3472:ALA:HA	2:G:3475:LYS:HE2	1.80	0.63
2:B:622:THR:HA	2:B:626:LEU:HD13	1.79	0.63
2:G:23:GLN:HE21	2:G:34:LYS:HB3	1.63	0.63
2:G:1087:ARG:NH1	2:G:1221:GLU:O	2.31	0.63
2:G:3594:ARG:NH1	2:G:3594:ARG:HA	2.12	0.63
2:J:985:VAL:HG22	2:J:1043:VAL:HG21	1.80	0.63
2:J:3245:VAL:HG23	2:J:3248:ARG:H	1.63	0.63
2:E:205:ILE:H	2:E:205:ILE:HD12	1.64	0.63
2:E:3548:GLU:HG2	2:E:3552:PHE:CZ	2.33	0.63
2:G:1229:ASN:HB3	2:G:1827:ARG:HG3	1.81	0.63
2:G:2630:VAL:HG12	2:G:2682:ILE:HD11	1.81	0.63
2:J:573:GLU:OE1	2:J:573:GLU:N	2.21	0.63
2:B:1087:ARG:NH1	2:B:1221:GLU:O	2.31	0.63
2:B:3263:TYR:HE2	2:B:3334:TRP:HD1	1.46	0.63
2:E:2630:VAL:HG12	2:E:2682:ILE:HD11	1.81	0.63
2:J:2630:VAL:HG12	2:J:2682:ILE:HD11	1.81	0.63
2:J:3253:ILE:HG23	2:J:3318:ASN:HD22	1.61	0.63
2:J:3435:PHE:HE2	2:J:3518:LEU:HA	1.62	0.63
2:J:3472:ALA:HA	2:J:3475:LYS:HE2	1.80	0.63
2:J:4087:LEU:HB3	2:J:4122:MET:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.63	0.63
2:B:1229:ASN:HB3	2:B:1827:ARG:HG3	1.81	0.63
2:B:2977:LEU:HD11	2:B:2995:ILE:HD13	1.80	0.63
2:B:3548:GLU:HG2	2:B:3552:PHE:CZ	2.33	0.63
2:E:985:VAL:HG22	2:E:1043:VAL:HG21	1.80	0.63
2:G:3567:PRO:HB2	2:G:3570:ARG:HH21	1.62	0.63
2:B:985:VAL:HG22	2:B:1043:VAL:HG21	1.80	0.63
2:E:1087:ARG:NH1	2:E:1221:GLU:O	2.32	0.63
2:J:205:ILE:H	2:J:205:ILE:HD12	1.64	0.63
2:J:365:LYS:HE2	2:J:369:LEU:HD21	1.80	0.63
1:D:24:VAL:HG12	1:D:103:LEU:HA	1.81	0.63
2:B:205:ILE:H	2:B:205:ILE:HD12	1.64	0.63
2:B:4087:LEU:HB3	2:B:4122:MET:HB3	1.80	0.63
2:E:981:GLN:O	2:E:985:VAL:HG23	1.99	0.63
2:E:3472:ALA:HA	2:E:3475:LYS:HE2	1.80	0.63
2:E:3567:PRO:HB2	2:E:3570:ARG:HH21	1.62	0.63
2:J:3281:LEU:HD12	2:J:3312:LEU:HG	1.80	0.63
2:G:3590:GLU:O	2:G:3594:ARG:HG2	1.99	0.63
2:B:246:TYR:CG	2:B:373:LYS:HD2	2.34	0.63
2:B:981:GLN:O	2:B:985:VAL:HG23	1.99	0.63
2:B:2630:VAL:HG12	2:B:2682:ILE:HD11	1.81	0.63
2:E:2263:ILE:HA	2:E:2330:ARG:HH22	1.62	0.63
2:J:1087:ARG:NH1	2:J:1221:GLU:O	2.32	0.63
3:C:52:THR:HG21	3:C:102:ASN:HA	1.79	0.63
2:E:23:GLN:HE21	2:E:34:LYS:HB3	1.63	0.62
2:G:901:LYS:HD3	2:G:903:LEU:HD11	1.80	0.62
2:G:3245:VAL:HG23	2:G:3248:ARG:H	1.63	0.62
2:J:1229:ASN:HB3	2:J:1827:ARG:HG3	1.81	0.62
2:J:3590:GLU:O	2:J:3594:ARG:HG2	1.99	0.62
2:E:3590:GLU:O	2:E:3594:ARG:HG2	1.99	0.62
2:G:2902:HIS:HB3	2:G:2905:LEU:HG	1.79	0.62
2:E:4087:LEU:HB3	2:E:4122:MET:HB3	1.81	0.62
2:G:3263:TYR:HE2	2:G:3334:TRP:HD1	1.46	0.62
2:J:2902:HIS:HB3	2:J:2905:LEU:HG	1.79	0.62
2:B:2283:ASN:HB3	2:B:2286:LEU:HB2	1.82	0.62
2:G:2977:LEU:HD11	2:G:2995:ILE:HD13	1.80	0.62
2:J:2977:LEU:HD11	2:J:2995:ILE:HD13	1.80	0.62
2:J:3548:GLU:HG2	2:J:3552:PHE:CZ	2.33	0.62
2:B:573:GLU:OE1	2:B:573:GLU:N	2.21	0.62
2:B:1447:CYS:HB3	2:B:1555:LEU:HB3	1.82	0.62
2:J:3359:ILE:H	2:J:3359:ILE:HD12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3590:GLU:O	2:B:3594:ARG:HG2	1.99	0.62
2:E:2283:ASN:HB3	2:E:2286:LEU:HB2	1.82	0.62
2:G:985:VAL:HG22	2:G:1043:VAL:HG21	1.80	0.62
2:J:901:LYS:HD3	2:J:903:LEU:HD11	1.80	0.62
2:B:3472:ALA:HA	2:B:3475:LYS:HE2	1.80	0.62
2:E:1229:ASN:HB3	2:E:1827:ARG:HG3	1.81	0.62
2:E:3568:SER:HA	2:E:3571:TRP:NE1	2.15	0.62
2:E:4090:LYS:HG2	2:E:4123:ILE:HD11	1.82	0.62
2:G:205:ILE:H	2:G:205:ILE:HD12	1.64	0.62
2:G:4091:LYS:HD3	2:G:4091:LYS:N	2.15	0.62
2:J:23:GLN:HE21	2:J:34:LYS:HB3	1.63	0.62
2:G:4087:LEU:HB3	2:G:4122:MET:HB3	1.80	0.62
2:J:4090:LYS:HG2	2:J:4123:ILE:HD11	1.82	0.62
1:H:93:PRO:O	1:H:94:ASN:ND2	2.33	0.62
2:E:3359:ILE:H	2:E:3359:ILE:HD12	1.65	0.62
2:J:952:LYS:H	2:J:969:PRO:HA	1.64	0.62
2:J:3511:VAL:HA	2:J:3515:LYS:HB2	1.81	0.62
1:I:66:MET:HE1	1:I:101:VAL:HG23	1.82	0.61
2:B:3054:VAL:HG11	2:B:3131:TYR:HB2	1.82	0.61
2:B:3511:VAL:HA	2:B:3515:LYS:HB2	1.81	0.61
2:E:3054:VAL:HG11	2:E:3131:TYR:HB2	1.82	0.61
2:B:3350:ARG:HB2	2:B:3353:LEU:HD13	1.81	0.61
2:E:3190:LEU:O	2:E:3194:LEU:HG	2.00	0.61
2:G:3359:ILE:H	2:G:3359:ILE:HD12	1.65	0.61
2:G:3511:VAL:HA	2:G:3515:LYS:HB2	1.81	0.61
2:J:981:GLN:O	2:J:985:VAL:HG23	1.99	0.61
2:J:3568:SER:HA	2:J:3571:TRP:NE1	2.15	0.61
2:B:799:GLU:N	2:B:799:GLU:OE1	2.33	0.61
2:B:4848:VAL:O	2:B:4852:THR:HG23	2.00	0.61
2:G:2515:GLN:HA	2:G:2568:LEU:HD11	1.82	0.61
2:E:1447:CYS:HB3	2:E:1555:LEU:HB3	1.82	0.61
2:E:4091:LYS:HD3	2:E:4091:LYS:N	2.15	0.61
2:G:551:LEU:HD13	2:G:589:LEU:HD11	1.83	0.61
2:G:3190:LEU:O	2:G:3194:LEU:HG	2.01	0.61
2:B:2570:ALA:HB2	2:B:2613:TYR:HB3	1.81	0.61
2:G:2283:ASN:HB3	2:G:2286:LEU:HB2	1.82	0.61
2:G:3384:LYS:HG3	2:G:3387:ALA:H	1.66	0.61
2:G:3568:SER:HA	2:G:3571:TRP:NE1	2.15	0.61
2:J:799:GLU:N	2:J:799:GLU:OE1	2.33	0.61
2:J:3054:VAL:HG11	2:J:3131:TYR:HB2	1.82	0.61
2:E:3384:LYS:HG3	2:E:3387:ALA:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2347:GLU:OE1	2:G:2347:GLU:N	2.27	0.61
2:J:3190:LEU:O	2:J:3194:LEU:HG	2.00	0.61
2:J:3384:LYS:HG3	2:J:3387:ALA:H	1.66	0.61
2:B:551:LEU:HD13	2:B:589:LEU:HD11	1.83	0.61
2:B:2512:ILE:HD13	2:B:2517:PHE:CE2	2.35	0.61
2:B:3359:ILE:H	2:B:3359:ILE:HD12	1.65	0.61
2:B:3568:SER:HA	2:B:3571:TRP:NE1	2.15	0.61
2:E:799:GLU:OE1	2:E:799:GLU:N	2.33	0.61
1:A:17:LYS:HZ2	1:A:18:LYS:HG2	1.66	0.61
2:B:548:VAL:HG21	2:B:582:HIS:HD2	1.66	0.61
2:E:2710:LEU:HD12	2:E:2711:PRO:HD2	1.83	0.61
2:G:799:GLU:N	2:G:799:GLU:OE1	2.33	0.61
2:G:981:GLN:O	2:G:985:VAL:HG23	1.99	0.61
2:G:4090:LYS:HG2	2:G:4123:ILE:HD11	1.82	0.61
2:J:4848:VAL:O	2:J:4852:THR:HG23	2.00	0.61
2:E:2678:LEU:O	2:E:2682:ILE:HG12	2.01	0.61
2:E:3996:PHE:O	2:E:4000:MET:HG2	2.01	0.61
2:G:3350:ARG:HB2	2:G:3353:LEU:HD13	1.81	0.61
1:H:24:VAL:HG12	1:H:103:LEU:HA	1.82	0.60
1:I:24:VAL:HG12	1:I:103:LEU:HA	1.81	0.60
2:E:3350:ARG:HB2	2:E:3353:LEU:HD13	1.82	0.60
2:G:952:LYS:H	2:G:969:PRO:HA	1.64	0.60
2:G:3536:ALA:HB2	2:G:3553:LEU:HD11	1.83	0.60
2:G:4848:VAL:O	2:G:4852:THR:HG23	2.00	0.60
1:A:26:TYR:HB2	1:A:101:VAL:HG12	1.84	0.60
2:B:4849:TYR:O	2:B:4853:VAL:HG23	2.01	0.60
2:E:984:LEU:O	2:E:988:LEU:HD22	2.01	0.60
2:E:3511:VAL:HA	2:E:3515:LYS:HB2	1.81	0.60
2:G:365:LYS:HE2	2:G:369:LEU:HD21	1.83	0.60
2:G:2678:LEU:O	2:G:2682:ILE:HG12	2.01	0.60
2:J:233:ILE:O	2:J:257:ARG:NH1	2.34	0.60
2:J:4867:GLU:OE1	2:J:4867:GLU:N	2.31	0.60
2:B:952:LYS:H	2:B:969:PRO:HA	1.64	0.60
2:B:3190:LEU:O	2:B:3194:LEU:HG	2.00	0.60
2:E:548:VAL:HG21	2:E:582:HIS:HD2	1.66	0.60
2:E:952:LYS:H	2:E:969:PRO:HA	1.64	0.60
2:G:993:HIS:CE1	2:G:1027:LEU:HD11	2.37	0.60
2:J:3350:ARG:HB2	2:J:3353:LEU:HD13	1.81	0.60
1:A:61:GLU:O	1:A:65:GLN:HG3	2.01	0.60
2:B:2710:LEU:HD12	2:B:2711:PRO:HD2	1.83	0.60
2:B:3536:ALA:HB2	2:B:3553:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4090:LYS:HG2	2:B:4123:ILE:HD11	1.82	0.60
2:E:4848:VAL:O	2:E:4852:THR:HG23	2.00	0.60
2:G:3054:VAL:HG11	2:G:3131:TYR:HB2	1.82	0.60
2:J:548:VAL:HG21	2:J:582:HIS:HD2	1.66	0.60
2:J:2283:ASN:HB3	2:J:2286:LEU:HB2	1.82	0.60
2:J:2678:LEU:O	2:J:2682:ILE:HG12	2.01	0.60
2:B:2678:LEU:O	2:B:2682:ILE:HG12	2.01	0.60
2:B:4091:LYS:HD3	2:B:4091:LYS:N	2.15	0.60
2:E:551:LEU:HD13	2:E:589:LEU:HD11	1.83	0.60
2:E:2333:ASP:HA	2:E:2336:ARG:HH11	1.65	0.60
2:G:3368:ARG:O	2:G:3372:VAL:HG23	2.01	0.60
2:J:1447:CYS:HB3	2:J:1555:LEU:HB3	1.82	0.60
2:J:3536:ALA:HB2	2:J:3553:LEU:HD11	1.84	0.60
2:J:4091:LYS:HD3	2:J:4091:LYS:N	2.15	0.60
2:B:993:HIS:CE1	2:B:1027:LEU:HD11	2.36	0.60
2:B:1944:GLU:HG2	2:B:2123:LEU:HD13	1.83	0.60
2:G:984:LEU:O	2:G:988:LEU:HD22	2.01	0.60
2:G:1735:ILE:HD11	2:G:2156:LEU:HD11	1.84	0.60
2:J:2710:LEU:HD12	2:J:2711:PRO:HD2	1.83	0.60
1:A:23:VAL:HG12	1:A:47:LYS:HG2	1.84	0.60
1:H:23:VAL:HG12	1:H:47:LYS:HG2	1.84	0.60
2:B:233:ILE:O	2:B:257:ARG:NH1	2.34	0.60
2:B:2959:PHE:O	2:B:2963:LEU:HG	2.02	0.60
2:G:233:ILE:O	2:G:257:ARG:NH1	2.34	0.60
2:G:3996:PHE:O	2:G:4000:MET:HG2	2.01	0.60
2:J:993:HIS:CE1	2:J:1027:LEU:HD11	2.37	0.60
3:F:38:ARG:NH2	3:F:64:LYS:HG2	2.16	0.60
1:H:17:LYS:HZ2	1:H:18:LYS:HG2	1.66	0.60
1:I:23:VAL:HG12	1:I:47:LYS:HG2	1.84	0.60
2:B:991:ASN:O	2:B:995:VAL:HG23	2.02	0.60
2:E:233:ILE:O	2:E:257:ARG:NH1	2.34	0.60
2:B:3384:LYS:HG3	2:B:3387:ALA:H	1.66	0.60
2:B:4715:TYR:HE2	2:B:4717:ASP:HB3	1.67	0.60
2:E:993:HIS:CE1	2:E:1027:LEU:HD11	2.36	0.60
2:G:2333:ASP:HA	2:G:2336:ARG:HH11	1.65	0.60
2:G:3102:ASP:HA	2:G:3105:LYS:HE2	1.84	0.60
2:J:1115:LEU:HB3	2:J:1123:VAL:HG11	1.84	0.60
2:J:4849:TYR:O	2:J:4853:VAL:HG23	2.01	0.60
2:E:1979:LEU:HD23	2:E:1982:ARG:HH12	1.67	0.60
2:J:551:LEU:HD13	2:J:589:LEU:HD11	1.83	0.60
2:J:1008:SER:HB2	2:J:1017:ARG:HE	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3536:ALA:HB2	2:E:3553:LEU:HD11	1.84	0.59
2:G:2575:ARG:HG3	2:G:2578:MET:HG3	1.83	0.59
2:J:248:GLU:HA	2:J:372:LEU:HB2	1.82	0.59
2:J:991:ASN:O	2:J:995:VAL:HG23	2.02	0.59
2:J:2002:PRO:O	2:J:2006:ILE:HG12	2.02	0.59
2:J:2333:ASP:HA	2:J:2336:ARG:HH11	1.65	0.59
2:J:2959:PHE:O	2:J:2963:LEU:HG	2.02	0.59
2:J:3368:ARG:O	2:J:3372:VAL:HG23	2.01	0.59
2:J:3996:PHE:O	2:J:4000:MET:HG2	2.01	0.59
2:B:984:LEU:O	2:B:988:LEU:HD22	2.01	0.59
2:E:3368:ARG:O	2:E:3372:VAL:HG23	2.01	0.59
2:G:1008:SER:HB2	2:G:1017:ARG:HE	1.67	0.59
2:G:2002:PRO:O	2:G:2006:ILE:HG12	2.02	0.59
2:J:984:LEU:O	2:J:988:LEU:HD22	2.02	0.59
1:D:23:VAL:HG12	1:D:47:LYS:HG2	1.84	0.59
2:B:1860:LYS:HG2	2:B:1864:LYS:HE3	1.84	0.59
2:B:3368:ARG:O	2:B:3372:VAL:HG23	2.02	0.59
2:E:246:TYR:CD1	2:E:373:LYS:HG3	2.37	0.59
2:E:2002:PRO:O	2:E:2006:ILE:HG12	2.02	0.59
2:E:2175:GLU:O	2:E:2179:ILE:HG12	2.02	0.59
2:E:3549:VAL:O	2:E:3553:LEU:HD13	2.02	0.59
2:G:4715:TYR:CE2	2:G:4717:ASP:HB3	2.36	0.59
2:J:2212:VAL:HG22	2:J:2256:TYR:HE1	1.68	0.59
1:H:97:LEU:HB3	1:H:99:PHE:HE2	1.67	0.59
2:B:2962:GLN:OE1	2:B:2965:ARG:NH1	2.36	0.59
2:B:3996:PHE:O	2:B:4000:MET:HG2	2.01	0.59
2:B:4681:LEU:HD12	2:B:4724:VAL:HG21	1.84	0.59
2:B:5017:ARG:HH11	2:B:5019:TRP:HZ2	1.49	0.59
2:E:2212:VAL:HG22	2:E:2256:TYR:HE1	1.68	0.59
2:E:3312:LEU:H	2:E:3312:LEU:HD12	1.67	0.59
2:J:2591:ARG:HA	2:J:2591:ARG:CZ	2.32	0.59
2:J:3549:VAL:O	2:J:3553:LEU:HD13	2.02	0.59
2:E:1008:SER:HB2	2:E:1017:ARG:HE	1.67	0.59
2:E:1944:GLU:HG2	2:E:2123:LEU:HD13	1.83	0.59
2:E:2591:ARG:HA	2:E:2591:ARG:CZ	2.33	0.59
2:J:2175:GLU:O	2:J:2179:ILE:HG12	2.02	0.59
2:B:235:ALA:O	2:B:242:ARG:NH2	2.36	0.59
2:B:1115:LEU:HB3	2:B:1123:VAL:HG11	1.84	0.59
2:B:1979:LEU:HD23	2:B:1982:ARG:HH12	1.67	0.59
2:B:2333:ASP:HA	2:B:2336:ARG:HH11	1.65	0.59
2:G:991:ASN:O	2:G:995:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1619:ARG:HA	2:G:1626:TRP:HA	1.85	0.59
2:G:4849:TYR:O	2:G:4853:VAL:HG23	2.01	0.59
2:J:3102:ASP:HA	2:J:3105:LYS:HE2	1.84	0.59
1:D:93:PRO:O	1:D:94:ASN:ND2	2.33	0.59
1:I:17:LYS:HZ2	1:I:18:LYS:HG2	1.66	0.59
2:B:3246:LEU:HG	2:B:3247:ASP:H	1.66	0.59
2:E:3281:LEU:HD12	2:E:3312:LEU:HG	1.84	0.59
2:G:2710:LEU:HD12	2:G:2711:PRO:HD2	1.83	0.59
2:G:2962:GLN:OE1	2:G:2965:ARG:NH1	2.35	0.59
2:J:1735:ILE:HD11	2:J:2156:LEU:HD11	1.84	0.59
2:J:1979:LEU:HD23	2:J:1982:ARG:HH12	1.67	0.59
2:B:783:PHE:HB2	2:B:787:VAL:HG11	1.85	0.59
2:B:2002:PRO:O	2:B:2006:ILE:HG12	2.02	0.59
2:B:2175:GLU:O	2:B:2179:ILE:HG12	2.02	0.59
2:B:2591:ARG:HA	2:B:2591:ARG:CZ	2.32	0.59
2:B:3050:VAL:HG11	2:B:3068:LEU:HD11	1.85	0.59
2:E:783:PHE:HB2	2:E:787:VAL:HG11	1.85	0.59
2:E:991:ASN:O	2:E:995:VAL:HG23	2.02	0.59
2:G:1447:CYS:HB3	2:G:1555:LEU:HB3	1.82	0.59
2:G:2591:ARG:HA	2:G:2591:ARG:CZ	2.32	0.59
3:K:38:ARG:NH2	3:K:64:LYS:HG2	2.16	0.59
2:B:1497:GLY:HA2	2:B:1500:PHE:HD2	1.68	0.59
2:B:2212:VAL:HG22	2:B:2256:TYR:HE1	1.68	0.59
2:B:2518:LEU:CD2	2:B:2568:LEU:HD22	2.33	0.59
2:B:3102:ASP:HA	2:B:3105:LYS:HE2	1.84	0.59
2:G:548:VAL:HG21	2:G:582:HIS:HD2	1.66	0.59
2:J:1860:LYS:HG2	2:J:1864:LYS:HE3	1.84	0.59
2:J:1944:GLU:HG2	2:J:2123:LEU:HD13	1.83	0.59
2:J:2962:GLN:OE1	2:J:2965:ARG:NH1	2.36	0.59
2:B:3549:VAL:O	2:B:3553:LEU:HD13	2.02	0.59
2:E:1860:LYS:HG2	2:E:1864:LYS:HE3	1.84	0.59
2:E:2959:PHE:O	2:E:2963:LEU:HG	2.02	0.59
2:E:4849:TYR:O	2:E:4853:VAL:HG23	2.01	0.59
2:G:573:GLU:OE1	2:G:573:GLU:N	2.21	0.59
2:J:2347:GLU:OE1	2:J:2347:GLU:N	2.27	0.59
2:E:3050:VAL:HG11	2:E:3068:LEU:HD11	1.85	0.58
2:J:235:ALA:O	2:J:242:ARG:NH2	2.36	0.58
2:E:1115:LEU:HB3	2:E:1123:VAL:HG11	1.84	0.58
2:G:1444:GLU:HG2	2:G:1557:THR:HG21	1.86	0.58
2:G:2175:GLU:O	2:G:2179:ILE:HG12	2.02	0.58
2:G:2212:VAL:HG22	2:G:2256:TYR:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1619:ARG:HA	2:J:1626:TRP:HA	1.85	0.58
3:M:109:THR:O	3:M:113:GLU:HG2	2.03	0.58
2:B:2519:LEU:HD21	2:B:2572:THR:HG21	1.85	0.58
2:B:2563:THR:HG22	2:B:2606:CYS:HA	1.85	0.58
2:B:3312:LEU:H	2:B:3312:LEU:HD12	1.68	0.58
2:E:1735:ILE:HD11	2:E:2156:LEU:HD11	1.84	0.58
2:E:2703:LEU:HD12	2:E:3001:ILE:HD11	1.86	0.58
2:E:2962:GLN:OE1	2:E:2965:ARG:NH1	2.36	0.58
2:G:2959:PHE:O	2:G:2963:LEU:HG	2.02	0.58
2:E:1497:GLY:HA2	2:E:1500:PHE:HD2	1.68	0.58
2:E:4681:LEU:HD12	2:E:4724:VAL:HG21	1.84	0.58
2:G:1115:LEU:HB3	2:G:1123:VAL:HG11	1.84	0.58
2:G:3050:VAL:HG11	2:G:3068:LEU:HD11	1.85	0.58
2:J:3312:LEU:H	2:J:3312:LEU:HD12	1.68	0.58
2:B:1619:ARG:HA	2:B:1626:TRP:HA	1.85	0.58
2:E:1424:PRO:O	2:E:1428:LEU:HG	2.04	0.58
2:G:1944:GLU:HG2	2:G:2123:LEU:HD13	1.83	0.58
2:G:1979:LEU:HD23	2:G:1982:ARG:HH12	1.68	0.58
2:G:3253:ILE:HG23	2:G:3318:ASN:HD22	1.68	0.58
2:G:3549:VAL:O	2:G:3553:LEU:HD13	2.02	0.58
2:J:881:LEU:O	2:J:885:THR:HG23	2.04	0.58
2:J:2575:ARG:HG3	2:J:2578:MET:HG3	1.84	0.58
2:J:3050:VAL:HG11	2:J:3068:LEU:HD11	1.85	0.58
3:K:109:THR:O	3:K:113:GLU:HG2	2.03	0.58
2:B:1735:ILE:HD11	2:B:2156:LEU:HD11	1.84	0.58
2:B:2519:LEU:HA	2:B:2522:LEU:HD12	1.84	0.58
2:J:4681:LEU:HD12	2:J:4724:VAL:HG21	1.84	0.58
2:B:341:TYR:CZ	2:B:392:ARG:HB2	2.38	0.58
2:B:653:ALA:HB3	2:B:656:SER:HB3	1.86	0.58
2:B:2703:LEU:HD12	2:B:3001:ILE:HD11	1.86	0.58
2:E:881:LEU:O	2:E:885:THR:HG23	2.04	0.58
2:G:235:ALA:O	2:G:242:ARG:NH2	2.36	0.58
2:J:341:TYR:CZ	2:J:392:ARG:HB2	2.38	0.58
3:C:109:THR:O	3:C:113:GLU:HG2	2.03	0.58
1:D:17:LYS:HZ2	1:D:18:LYS:HG2	1.67	0.58
2:E:653:ALA:HB3	2:E:656:SER:HB3	1.86	0.58
2:G:3349:ALA:HB1	2:G:3353:LEU:HD22	1.86	0.58
2:J:1497:GLY:HA2	2:J:1500:PHE:HD2	1.68	0.58
2:B:881:LEU:O	2:B:885:THR:HG23	2.04	0.58
2:E:1786:LEU:HD12	2:E:1787:PRO:HD2	1.86	0.58
2:G:783:PHE:HB2	2:G:787:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1860:LYS:HG2	2:G:1864:LYS:HE3	1.84	0.58
2:G:3257:ALA:O	2:G:3325:ASN:ND2	2.37	0.58
2:J:2703:LEU:HD12	2:J:3001:ILE:HD11	1.86	0.58
2:J:3257:ALA:O	2:J:3325:ASN:ND2	2.37	0.58
3:F:109:THR:O	3:F:113:GLU:HG2	2.03	0.58
1:H:17:LYS:NZ	1:H:18:LYS:HG2	2.19	0.58
2:B:1008:SER:HB2	2:B:1017:ARG:HE	1.67	0.58
2:B:1444:GLU:HG2	2:B:1557:THR:HG21	1.86	0.58
2:B:1786:LEU:HD12	2:B:1787:PRO:HD2	1.86	0.58
2:E:110:ARG:NH2	2:E:117:TYR:OH	2.37	0.58
2:E:235:ALA:O	2:E:242:ARG:NH2	2.36	0.58
2:J:110:ARG:NH2	2:J:117:TYR:OH	2.37	0.58
2:J:783:PHE:HB2	2:J:787:VAL:HG11	1.85	0.58
2:B:3349:ALA:HB1	2:B:3353:LEU:HD22	1.86	0.57
2:E:1444:GLU:HG2	2:E:1557:THR:HG21	1.86	0.57
2:E:1619:ARG:HA	2:E:1626:TRP:HA	1.85	0.57
2:E:3102:ASP:HA	2:E:3105:LYS:HE2	1.84	0.57
2:G:341:TYR:CZ	2:G:392:ARG:HB2	2.38	0.57
2:J:3347:SER:HB3	2:J:3348:ARG:NH2	2.19	0.57
3:C:38:ARG:NH2	3:C:64:LYS:HG2	2.16	0.57
2:B:13:PHE:HA	2:B:164:ARG:HA	1.86	0.57
2:B:2518:LEU:O	2:B:2522:LEU:HG	2.04	0.57
2:B:2566:ALA:HA	2:B:2569:PHE:HD2	1.69	0.57
2:E:341:TYR:CZ	2:E:392:ARG:HB2	2.38	0.57
2:G:13:PHE:HA	2:G:164:ARG:HA	1.86	0.57
2:G:881:LEU:O	2:G:885:THR:HG23	2.04	0.57
2:G:1424:PRO:O	2:G:1428:LEU:HG	2.04	0.57
2:J:653:ALA:HB3	2:J:656:SER:HB3	1.86	0.57
2:J:1424:PRO:O	2:J:1428:LEU:HG	2.04	0.57
2:E:882:TRP:CD1	3:F:106:PRO:HB3	2.40	0.57
2:E:3443:ILE:HG12	2:E:3605:HIS:HD2	1.70	0.57
2:G:2779:GLU:HG3	2:G:2792:ARG:HG2	1.86	0.57
2:G:3443:ILE:HG12	2:G:3605:HIS:HD2	1.70	0.57
2:J:1444:GLU:HG2	2:J:1557:THR:HG21	1.86	0.57
2:J:3110:LEU:HD13	2:J:3183:VAL:HG12	1.86	0.57
1:A:17:LYS:NZ	1:A:18:LYS:HG2	2.19	0.57
1:I:93:PRO:O	1:I:94:ASN:ND2	2.33	0.57
2:E:878:ILE:HG21	3:F:107:TRP:NE1	2.20	0.57
2:E:3347:SER:HB3	2:E:3348:ARG:NH2	2.19	0.57
2:G:1497:GLY:HA2	2:G:1500:PHE:HD2	1.68	0.57
2:G:1786:LEU:HD12	2:G:1787:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3347:SER:HB3	2:G:3348:ARG:NH2	2.19	0.57
2:G:4681:LEU:HD12	2:G:4724:VAL:HG21	1.84	0.57
2:J:2779:GLU:HG3	2:J:2792:ARG:HG2	1.86	0.57
3:K:39:GLN:NE2	3:K:40:ALA:O	2.38	0.57
3:M:39:GLN:NE2	3:M:40:ALA:O	2.37	0.57
2:B:1424:PRO:O	2:B:1428:LEU:HG	2.04	0.57
2:B:2779:GLU:HG3	2:B:2792:ARG:HG2	1.86	0.57
2:B:3443:ILE:HG12	2:B:3605:HIS:HD2	1.70	0.57
2:E:13:PHE:HA	2:E:164:ARG:HA	1.86	0.57
2:G:224:HIS:HB3	2:G:229:GLU:HG3	1.86	0.57
2:B:248:GLU:HA	2:B:372:LEU:HB2	1.86	0.57
2:B:3257:ALA:O	2:B:3325:ASN:ND2	2.37	0.57
2:G:355:LEU:HD23	2:G:378:LEU:HB3	1.87	0.57
2:G:2703:LEU:HD12	2:G:3001:ILE:HD11	1.86	0.57
2:J:3443:ILE:HG12	2:J:3605:HIS:HD2	1.70	0.57
3:C:39:GLN:NE2	3:C:40:ALA:O	2.38	0.57
2:B:2766:TRP:O	2:B:2770:LYS:HG2	2.05	0.57
2:E:224:HIS:HB3	2:E:229:GLU:HG3	1.86	0.57
2:G:110:ARG:NH2	2:G:117:TYR:OH	2.37	0.57
2:G:653:ALA:HB3	2:G:656:SER:HB3	1.86	0.57
2:J:684:VAL:HG22	2:J:781:VAL:HG12	1.86	0.57
2:J:2572:THR:HG22	2:J:2575:ARG:HB3	1.87	0.57
2:J:3227:ARG:HB3	2:J:3232:LEU:HB2	1.87	0.57
2:J:3349:ALA:HB1	2:J:3353:LEU:HD22	1.86	0.57
2:B:3347:SER:HB3	2:B:3348:ARG:NH2	2.19	0.57
2:B:4999:ASP:HB2	2:B:5002:GLU:HG2	1.87	0.57
2:E:3227:ARG:HB3	2:E:3232:LEU:HB2	1.87	0.57
2:G:2634:ASN:OD1	2:G:2636:PHE:N	2.37	0.57
2:B:210:GLU:HG3	2:B:213:TYR:HB2	1.87	0.57
2:B:244:LEU:HD13	2:B:375:LYS:HZ1	1.69	0.57
2:B:355:LEU:HD23	2:B:378:LEU:HB3	1.87	0.57
2:E:3257:ALA:O	2:E:3325:ASN:ND2	2.37	0.57
2:E:3349:ALA:HB1	2:E:3353:LEU:HD22	1.86	0.57
2:J:2766:TRP:O	2:J:2770:LYS:HG2	2.05	0.57
3:F:39:GLN:NE2	3:F:40:ALA:O	2.38	0.57
2:B:2991:HIS:O	2:B:2995:ILE:HG13	2.06	0.56
2:B:3110:LEU:HD13	2:B:3183:VAL:HG12	1.86	0.56
2:E:2626:LEU:O	2:E:2630:VAL:HG23	2.05	0.56
2:E:4688:ILE:HG22	2:E:4689:THR:HG23	1.87	0.56
2:G:2766:TRP:O	2:G:2770:LYS:HG2	2.05	0.56
2:G:4999:ASP:HB2	2:G:5002:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:210:GLU:HG3	2:J:213:TYR:HB2	1.87	0.56
3:M:38:ARG:NH2	3:M:64:LYS:HG2	2.16	0.56
2:G:633:LEU:HB3	2:G:1639:LEU:HD11	1.87	0.56
2:G:1947:CYS:SG	2:G:2127:GLN:NE2	2.77	0.56
2:J:224:HIS:HB3	2:J:229:GLU:HG3	1.86	0.56
1:D:97:LEU:HB3	1:D:99:PHE:HE2	1.70	0.56
1:I:17:LYS:NZ	1:I:18:LYS:HG2	2.19	0.56
2:B:633:LEU:HB3	2:B:1639:LEU:HD11	1.87	0.56
2:E:684:VAL:HG22	2:E:781:VAL:HG12	1.87	0.56
2:E:1225:PRO:HG2	2:E:1228:ILE:HD12	1.88	0.56
2:E:2766:TRP:O	2:E:2770:LYS:HG2	2.05	0.56
2:E:2779:GLU:HG3	2:E:2792:ARG:HG2	1.86	0.56
2:E:2991:HIS:O	2:E:2995:ILE:HG13	2.06	0.56
2:G:2575:ARG:HG3	2:G:2578:MET:CG	2.35	0.56
2:G:2626:LEU:O	2:G:2630:VAL:HG23	2.05	0.56
2:J:355:LEU:HD23	2:J:378:LEU:HB3	1.87	0.56
2:J:758:ARG:HH11	2:J:761:GLY:HA2	1.71	0.56
2:B:929:LEU:HA	2:B:932:LEU:HD12	1.87	0.56
2:B:4688:ILE:HG22	2:B:4689:THR:HG23	1.87	0.56
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.39	0.56
2:E:365:LYS:HE2	2:E:369:LEU:HD21	1.87	0.56
2:E:758:ARG:HH11	2:E:761:GLY:HA2	1.71	0.56
2:E:929:LEU:HA	2:E:932:LEU:HD12	1.87	0.56
2:G:210:GLU:HG3	2:G:213:TYR:HB2	1.87	0.56
2:G:878:ILE:HG21	3:M:107:TRP:NE1	2.21	0.56
2:G:2991:HIS:O	2:G:2995:ILE:HG13	2.06	0.56
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.39	0.56
2:J:13:PHE:HA	2:J:164:ARG:HA	1.86	0.56
2:J:1947:CYS:SG	2:J:2127:GLN:NE2	2.77	0.56
1:A:54:GLU:OE2	1:A:54:GLU:N	2.27	0.56
2:B:1225:PRO:HG2	2:B:1228:ILE:HD12	1.87	0.56
2:E:4999:ASP:HB2	2:E:5002:GLU:HG2	1.87	0.56
2:G:758:ARG:HH11	2:G:761:GLY:HA2	1.71	0.56
2:G:3110:LEU:HD13	2:G:3183:VAL:HG12	1.86	0.56
2:J:1786:LEU:HD12	2:J:1787:PRO:HD2	1.86	0.56
2:J:3439:GLY:O	2:J:3443:ILE:HG13	2.06	0.56
2:B:224:HIS:HB3	2:B:229:GLU:HG3	1.86	0.56
2:B:684:VAL:HG22	2:B:781:VAL:HG12	1.87	0.56
2:B:1947:CYS:SG	2:B:2127:GLN:NE2	2.77	0.56
2:B:2626:LEU:O	2:B:2630:VAL:HG23	2.05	0.56
2:E:210:GLU:HG3	2:E:213:TYR:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:633:LEU:HB3	2:E:1639:LEU:HD11	1.87	0.56
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.39	0.56
2:J:3547:GLU:O	2:J:3551:GLU:HG2	2.05	0.56
1:A:93:PRO:O	1:A:94:ASN:ND2	2.33	0.56
2:B:2875:ALA:HB2	2:B:2927:LEU:HD22	1.88	0.56
2:B:4715:TYR:CE2	2:B:4717:ASP:HB3	2.39	0.56
2:G:4943:LEU:O	2:G:4947:GLN:HG2	2.06	0.56
2:J:1225:PRO:HG2	2:J:1228:ILE:HD12	1.88	0.56
2:J:4999:ASP:HB2	2:J:5002:GLU:HG2	1.87	0.56
1:D:17:LYS:NZ	1:D:18:LYS:HG2	2.19	0.56
2:B:365:LYS:HE2	2:B:369:LEU:HD21	1.88	0.56
2:E:2575:ARG:HG3	2:E:2578:MET:CG	2.36	0.56
2:G:2498:HIS:O	2:G:2502:MET:HG3	2.06	0.56
2:G:4553:ASN:O	2:G:4557:ARG:HG3	2.06	0.56
2:J:4943:LEU:O	2:J:4947:GLN:HG2	2.06	0.56
2:E:355:LEU:HD23	2:E:378:LEU:HB3	1.87	0.56
2:E:3439:GLY:O	2:E:3443:ILE:HG13	2.06	0.56
2:E:3547:GLU:O	2:E:3551:GLU:HG2	2.05	0.56
2:G:684:VAL:HG22	2:G:781:VAL:HG12	1.87	0.56
2:G:3040:THR:HG21	2:G:3080:VAL:HG11	1.88	0.56
2:G:3547:GLU:O	2:G:3551:GLU:HG2	2.05	0.56
2:J:2575:ARG:HG3	2:J:2578:MET:CG	2.36	0.56
2:B:110:ARG:NH2	2:B:117:TYR:OH	2.37	0.56
2:B:127:MET:SD	2:B:127:MET:N	2.73	0.56
2:B:3040:THR:HG21	2:B:3080:VAL:HG11	1.88	0.56
2:G:2875:ALA:HB2	2:G:2927:LEU:HD22	1.88	0.56
2:G:3227:ARG:HB3	2:G:3232:LEU:HB2	1.87	0.56
2:J:2626:LEU:O	2:J:2630:VAL:HG23	2.05	0.56
2:J:3079:THR:HA	2:J:3082:LYS:HG2	1.88	0.56
2:J:3725:TYR:O	2:J:3729:MET:HG3	2.06	0.56
2:J:4688:ILE:HG22	2:J:4689:THR:HG23	1.87	0.56
2:B:758:ARG:HH11	2:B:761:GLY:HA2	1.71	0.55
2:B:3245:VAL:HG23	2:B:3248:ARG:H	1.71	0.55
2:B:3355:HIS:ND1	2:B:3355:HIS:O	2.40	0.55
2:B:3547:GLU:O	2:B:3551:GLU:HG2	2.05	0.55
2:E:3040:THR:HG21	2:E:3080:VAL:HG11	1.88	0.55
2:E:3110:LEU:HD13	2:E:3183:VAL:HG12	1.86	0.55
2:E:3206:LEU:HB2	2:E:3280:TYR:CE2	2.41	0.55
2:E:5009:TYR:HA	2:E:5012:LYS:HE3	1.87	0.55
2:J:2991:HIS:O	2:J:2995:ILE:HG13	2.06	0.55
2:B:3227:ARG:HB3	2:B:3232:LEU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4553:ASN:O	2:B:4557:ARG:HG3	2.06	0.55
2:E:2572:THR:HA	2:E:2574:HIS:CE1	2.41	0.55
2:G:3206:LEU:HB2	2:G:3280:TYR:HE2	1.72	0.55
2:G:3439:GLY:O	2:G:3443:ILE:HG13	2.06	0.55
2:J:633:LEU:HB3	2:J:1639:LEU:HD11	1.87	0.55
2:J:3040:THR:HG21	2:J:3080:VAL:HG11	1.88	0.55
2:E:920:TYR:HE1	3:F:99:ARG:HE	1.55	0.55
2:E:3592:ILE:HG12	2:E:3595:ARG:HH21	1.72	0.55
2:G:4688:ILE:HG22	2:G:4689:THR:HG23	1.87	0.55
2:J:4749:GLU:HG3	2:J:4753:HIS:CE1	2.42	0.55
2:B:384:MET:N	2:B:384:MET:SD	2.79	0.55
2:B:3206:LEU:HB2	2:B:3280:TYR:CE2	2.41	0.55
2:B:3532:LEU:HD11	2:B:3560:GLN:HB3	1.89	0.55
2:E:2992:GLU:HB2	2:E:2996:LYS:HZ1	1.71	0.55
2:G:2418:LEU:O	2:G:2422:ILE:HG12	2.07	0.55
2:G:3312:LEU:H	2:G:3312:LEU:HD12	1.70	0.55
2:G:3532:LEU:HD11	2:G:3560:GLN:HB3	1.89	0.55
2:G:3725:TYR:O	2:G:3729:MET:HG3	2.06	0.55
2:J:878:ILE:HG21	3:K:107:TRP:NE1	2.20	0.55
2:J:2827:ARG:NH2	2:J:2935:TYR:OH	2.40	0.55
2:J:3355:HIS:ND1	2:J:3355:HIS:O	2.39	0.55
2:J:3532:LEU:HD11	2:J:3560:GLN:HB3	1.89	0.55
2:J:3534:MET:O	2:J:3538:THR:HG23	2.07	0.55
3:K:40:ALA:HB3	3:K:43:LYS:HB2	1.88	0.55
2:B:886:ARG:HH12	2:B:904:HIS:CE1	2.25	0.55
2:B:2498:HIS:O	2:B:2502:MET:HG3	2.06	0.55
2:B:4749:GLU:HG3	2:B:4753:HIS:CE1	2.42	0.55
2:B:5013:MET:HE1	2:B:5021:PHE:HB3	1.88	0.55
2:E:384:MET:N	2:E:384:MET:SD	2.79	0.55
2:E:3532:LEU:HD11	2:E:3560:GLN:HB3	1.89	0.55
2:E:3725:TYR:O	2:E:3729:MET:HG3	2.06	0.55
2:G:1225:PRO:HG2	2:G:1228:ILE:HD12	1.88	0.55
2:G:3507:THR:O	2:G:3511:VAL:HG13	2.07	0.55
2:J:929:LEU:HA	2:J:932:LEU:HD12	1.87	0.55
2:J:2623:LEU:O	2:J:2627:VAL:HG23	2.07	0.55
2:E:2566:ALA:HA	2:E:2569:PHE:CD2	2.39	0.55
2:E:4943:LEU:O	2:E:4947:GLN:HG2	2.06	0.55
2:G:960:MET:SD	2:G:960:MET:N	2.75	0.55
2:G:1084:GLN:NE2	2:G:1186:ASP:O	2.40	0.55
2:J:4553:ASN:O	2:J:4557:ARG:HG3	2.06	0.55
3:M:62:SER:O	3:M:62:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:127:MET:SD	2:E:127:MET:N	2.73	0.55
2:E:3079:THR:HA	2:E:3082:LYS:HG2	1.88	0.55
2:E:3355:HIS:ND1	2:E:3355:HIS:O	2.39	0.55
2:G:384:MET:N	2:G:384:MET:SD	2.79	0.55
2:G:929:LEU:HA	2:G:932:LEU:HD12	1.87	0.55
2:G:2827:ARG:NH2	2:G:2935:TYR:OH	2.40	0.55
2:G:3206:LEU:HB2	2:G:3280:TYR:CE2	2.41	0.55
2:J:2875:ALA:HB2	2:J:2927:LEU:HD22	1.88	0.55
2:J:4978:HIS:ND1	2:J:4982:GLU:OE1	2.39	0.55
2:B:1087:ARG:HG2	2:B:1154:ASP:OD1	2.07	0.55
2:B:2178:MET:HB2	2:B:2228:MET:HE1	1.89	0.55
2:B:3507:THR:O	2:B:3511:VAL:HG13	2.06	0.55
2:B:4943:LEU:O	2:B:4947:GLN:HG2	2.06	0.55
2:E:1087:ARG:HG2	2:E:1154:ASP:OD1	2.07	0.55
2:G:1087:ARG:HG2	2:G:1154:ASP:OD1	2.07	0.55
2:G:1259:ARG:NH1	2:G:1591:CYS:SG	2.80	0.55
2:G:2623:LEU:O	2:G:2627:VAL:HG23	2.07	0.55
2:J:384:MET:N	2:J:384:MET:SD	2.79	0.55
2:J:2498:HIS:O	2:J:2502:MET:HG3	2.06	0.55
2:J:3592:ILE:HG12	2:J:3595:ARG:HH21	1.72	0.55
1:A:97:LEU:HB3	1:A:99:PHE:HE2	1.72	0.55
2:B:4572:ALA:O	2:B:4576:ILE:HG13	2.07	0.55
2:E:573:GLU:OE1	2:E:573:GLU:N	2.21	0.55
2:E:3207:GLU:HB2	2:E:3246:LEU:CD2	2.37	0.55
2:E:4715:TYR:CE2	2:E:4717:ASP:HB3	2.40	0.55
2:E:4749:GLU:HG3	2:E:4753:HIS:CE1	2.42	0.55
2:G:1940:CYS:O	2:G:1944:GLU:HG3	2.07	0.55
2:G:3079:THR:HA	2:G:3082:LYS:HG2	1.89	0.55
2:G:3355:HIS:ND1	2:G:3355:HIS:O	2.40	0.55
2:G:4867:GLU:OE1	2:G:4867:GLU:N	2.31	0.55
2:J:3206:LEU:HB2	2:J:3280:TYR:CE2	2.42	0.55
2:B:960:MET:HG2	2:B:961:MET:SD	2.47	0.55
2:B:2418:LEU:O	2:B:2422:ILE:HG12	2.07	0.55
2:B:3246:LEU:HG	2:B:3247:ASP:N	2.21	0.55
2:E:248:GLU:OE1	2:E:373:LYS:HE2	2.07	0.55
2:E:886:ARG:HH12	2:E:904:HIS:CE1	2.25	0.55
2:E:1084:GLN:NE2	2:E:1186:ASP:O	2.40	0.55
2:E:2498:HIS:O	2:E:2502:MET:HG3	2.06	0.55
2:E:3534:MET:O	2:E:3538:THR:HG23	2.07	0.55
2:E:3538:THR:O	2:E:3542:LEU:HG	2.07	0.55
2:E:4553:ASN:O	2:E:4557:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3534:MET:O	2:G:3538:THR:HG23	2.07	0.55
2:G:3538:THR:O	2:G:3542:LEU:HG	2.07	0.55
2:J:3206:LEU:HB2	2:J:3280:TYR:HE2	1.72	0.55
2:B:1259:ARG:NH1	2:B:1591:CYS:SG	2.80	0.54
2:B:2827:ARG:NH2	2:B:2935:TYR:OH	2.40	0.54
2:B:3592:ILE:HG12	2:B:3595:ARG:HH21	1.72	0.54
2:B:3725:TYR:O	2:B:3729:MET:HG3	2.06	0.54
2:E:504:ALA:HB2	2:E:512:ALA:HB2	1.89	0.54
2:E:2212:VAL:HG22	2:E:2256:TYR:CE1	2.43	0.54
2:E:3594:ARG:NH1	2:E:3597:GLN:OE1	2.34	0.54
2:G:886:ARG:HH12	2:G:904:HIS:CE1	2.25	0.54
2:G:4572:ALA:O	2:G:4576:ILE:HG13	2.07	0.54
2:J:1087:ARG:HG2	2:J:1154:ASP:OD1	2.07	0.54
2:J:2178:MET:HB2	2:J:2228:MET:HE1	1.88	0.54
2:J:2212:VAL:HG22	2:J:2256:TYR:CE1	2.43	0.54
2:J:3507:THR:O	2:J:3511:VAL:HG13	2.07	0.54
1:I:97:LEU:HB3	1:I:99:PHE:HE2	1.72	0.54
2:B:2518:LEU:HD22	2:B:2565:CYS:HB3	1.89	0.54
2:B:3538:THR:O	2:B:3542:LEU:HG	2.07	0.54
2:E:2875:ALA:HB2	2:E:2927:LEU:HD22	1.88	0.54
2:E:3194:LEU:HA	2:E:3197:LEU:HG	1.90	0.54
2:G:893:TYR:HA	2:G:904:HIS:HB3	1.89	0.54
2:J:1259:ARG:NH1	2:J:1591:CYS:SG	2.80	0.54
2:B:1940:CYS:O	2:B:1944:GLU:HG3	2.07	0.54
2:B:2992:GLU:HB2	2:B:2996:LYS:HZ1	1.71	0.54
2:B:3206:LEU:HB2	2:B:3280:TYR:HE2	1.72	0.54
2:B:3439:GLY:O	2:B:3443:ILE:HG13	2.06	0.54
2:E:2418:LEU:O	2:E:2422:ILE:HG12	2.07	0.54
2:E:2452:ARG:NH2	2:J:177:GLU:OE2	2.41	0.54
2:G:876:GLU:O	2:G:880:GLU:HG3	2.07	0.54
2:G:3277:LEU:HD13	2:G:3315:LEU:HD23	1.89	0.54
3:F:40:ALA:HB3	3:F:43:LYS:HB2	1.88	0.54
2:B:504:ALA:HB2	2:B:512:ALA:HB2	1.89	0.54
2:B:2610:LEU:O	2:B:2614:ILE:HG12	2.08	0.54
2:B:2998:PHE:HA	2:B:3002:LEU:HB2	1.90	0.54
2:B:3106:MET:N	2:B:3106:MET:SD	2.80	0.54
2:E:876:GLU:O	2:E:880:GLU:HG3	2.07	0.54
2:E:1699:GLU:HA	2:E:1814:MET:HE1	1.90	0.54
2:E:2827:ARG:NH2	2:E:2935:TYR:OH	2.40	0.54
2:E:2998:PHE:HA	2:E:3002:LEU:HB2	1.90	0.54
2:G:3592:ILE:HG12	2:G:3595:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4749:GLU:HG3	2:G:4753:HIS:CE1	2.42	0.54
2:J:1084:GLN:NE2	2:J:1186:ASP:O	2.40	0.54
2:J:3965:LEU:HA	2:J:3968:TYR:CD2	2.43	0.54
2:J:4572:ALA:O	2:J:4576:ILE:HG13	2.07	0.54
2:B:234:SER:HB2	2:B:242:ARG:HG2	1.89	0.54
2:B:2212:VAL:HG22	2:B:2256:TYR:CE1	2.43	0.54
2:E:3507:THR:O	2:E:3511:VAL:HG13	2.06	0.54
2:G:1970:GLN:NE2	2:G:3641:LEU:O	2.37	0.54
2:G:2749:GLU:HG3	2:G:2752:ASP:HB2	1.90	0.54
2:J:426:ARG:HG3	2:J:431:PRO:HD3	1.90	0.54
2:J:920:TYR:HE1	3:K:99:ARG:HE	1.56	0.54
2:J:2992:GLU:HB2	2:J:2996:LYS:HZ1	1.73	0.54
2:J:2998:PHE:HA	2:J:3002:LEU:HB2	1.90	0.54
2:J:3538:THR:O	2:J:3542:LEU:HG	2.07	0.54
2:B:2623:LEU:O	2:B:2627:VAL:HG23	2.07	0.54
2:B:4867:GLU:OE1	2:B:4867:GLU:N	2.31	0.54
2:E:960:MET:HG2	2:E:961:MET:SD	2.48	0.54
2:J:960:MET:HG2	2:J:961:MET:SD	2.48	0.54
2:J:1699:GLU:HA	2:J:1814:MET:HE1	1.90	0.54
2:B:3079:THR:HA	2:B:3082:LYS:HG2	1.89	0.54
2:E:1259:ARG:NH1	2:E:1591:CYS:SG	2.80	0.54
2:E:3445:TRP:CD1	2:E:3509:LEU:HG	2.43	0.54
2:G:177:GLU:OE2	2:J:2452:ARG:NH2	2.41	0.54
2:G:426:ARG:HG3	2:G:431:PRO:HD3	1.90	0.54
2:G:2123:LEU:O	2:G:2127:GLN:HG2	2.08	0.54
2:G:2238:TYR:O	2:G:2242:ILE:HG12	2.08	0.54
2:J:886:ARG:HH12	2:J:904:HIS:CE1	2.25	0.54
2:J:3445:TRP:CD1	2:J:3509:LEU:HG	2.43	0.54
2:G:960:MET:HG2	2:G:961:MET:SD	2.47	0.54
2:J:877:ASN:O	2:J:881:LEU:HD22	2.08	0.54
2:J:2123:LEU:O	2:J:2127:GLN:HG2	2.08	0.54
2:J:3194:LEU:HA	2:J:3197:LEU:HG	1.90	0.54
2:B:470:SER:HA	2:B:473:ASN:HD21	1.73	0.54
2:B:2749:GLU:HG3	2:B:2752:ASP:HB2	1.90	0.54
2:E:2178:MET:HB2	2:E:2228:MET:HE1	1.89	0.54
2:E:2238:TYR:O	2:E:2242:ILE:HG12	2.08	0.54
2:E:2312:MET:SD	2:E:2312:MET:N	2.79	0.54
2:E:3938:SER:O	2:E:4002:LYS:NZ	2.41	0.54
2:G:470:SER:HA	2:G:473:ASN:HD21	1.73	0.54
2:G:2312:MET:SD	2:G:2312:MET:N	2.79	0.54
2:G:3938:SER:O	2:G:4002:LYS:NZ	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2634:ASN:OD1	2:J:2636:PHE:N	2.37	0.54
3:C:40:ALA:HB3	3:C:43:LYS:HB2	1.88	0.54
3:M:40:ALA:HB3	3:M:43:LYS:HB2	1.89	0.54
2:B:1084:GLN:NE2	2:B:1186:ASP:O	2.40	0.54
2:B:2479:LEU:HD23	2:B:2479:LEU:H	1.73	0.54
2:E:877:ASN:O	2:E:881:LEU:HD22	2.08	0.54
2:E:2623:LEU:O	2:E:2627:VAL:HG23	2.07	0.54
2:E:4573:ILE:HG23	2:E:4643:LEU:HD11	1.91	0.54
2:J:3106:MET:N	2:J:3106:MET:SD	2.80	0.54
2:J:4063:ASP:HB2	2:J:4067:LYS:HE3	1.90	0.54
2:B:876:GLU:O	2:B:880:GLU:HG3	2.07	0.53
2:B:877:ASN:O	2:B:881:LEU:HD22	2.08	0.53
2:B:893:TYR:HA	2:B:904:HIS:HB3	1.89	0.53
2:B:1699:GLU:HA	2:B:1814:MET:HE1	1.90	0.53
2:B:2238:TYR:O	2:B:2242:ILE:HG12	2.08	0.53
2:B:3194:LEU:HA	2:B:3197:LEU:HG	1.90	0.53
2:E:2527:LEU:HA	2:E:2530:MET:HG2	1.90	0.53
2:G:2992:GLU:HB2	2:G:2996:LYS:HZ1	1.73	0.53
2:J:2238:TYR:O	2:J:2242:ILE:HG12	2.08	0.53
2:J:3280:TYR:HE1	2:J:3284:TRP:HD1	1.56	0.53
2:B:3280:TYR:CE1	2:B:3284:TRP:HD1	2.27	0.53
2:E:3201:MET:SD	2:E:3203:VAL:HG12	2.48	0.53
2:G:234:SER:HB2	2:G:242:ARG:HG2	1.90	0.53
2:G:877:ASN:O	2:G:881:LEU:HD22	2.08	0.53
2:G:1699:GLU:HA	2:G:1814:MET:HE1	1.90	0.53
2:G:2138:LEU:HD11	2:G:3662:ILE:HD12	1.90	0.53
2:G:3106:MET:N	2:G:3106:MET:SD	2.80	0.53
2:J:2418:LEU:O	2:J:2422:ILE:HG12	2.07	0.53
2:J:2749:GLU:HG3	2:J:2752:ASP:HB2	1.90	0.53
2:B:3201:MET:SD	2:B:3203:VAL:HG12	2.48	0.53
2:E:2123:LEU:O	2:E:2127:GLN:HG2	2.08	0.53
2:E:3093:ARG:O	2:E:3097:GLU:HG2	2.09	0.53
2:E:3106:MET:N	2:E:3106:MET:SD	2.80	0.53
2:E:3376:GLU:OE2	2:E:3380:ARG:NH2	2.39	0.53
2:E:3514:LEU:HD13	2:E:3602:VAL:HG13	1.91	0.53
2:E:4572:ALA:O	2:E:4576:ILE:HG13	2.07	0.53
2:G:2285:GLU:CD	2:G:3860:ASN:HD21	2.12	0.53
2:G:3201:MET:SD	2:G:3203:VAL:HG12	2.48	0.53
2:J:234:SER:HB2	2:J:242:ARG:HG2	1.90	0.53
2:B:206:CYS:HB2	2:B:271:GLY:HA3	1.90	0.53
2:B:426:ARG:HG3	2:B:431:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:ASP:O	2:B:1003:GLN:HG2	2.09	0.53
2:B:2518:LEU:HD21	2:B:2569:PHE:CE2	2.43	0.53
2:E:893:TYR:HA	2:E:904:HIS:HB3	1.89	0.53
2:E:999:ASP:O	2:E:1003:GLN:HG2	2.09	0.53
2:E:4063:ASP:HB2	2:E:4067:LYS:HE3	1.90	0.53
2:E:4867:GLU:OE1	2:E:4867:GLU:N	2.31	0.53
2:G:2178:MET:HB2	2:G:2228:MET:HE1	1.90	0.53
2:G:2527:LEU:HA	2:G:2530:MET:HG2	1.90	0.53
2:G:2736:ASP:OD1	2:G:2736:ASP:N	2.42	0.53
2:G:4573:ILE:HG23	2:G:4643:LEU:HD11	1.91	0.53
2:J:876:GLU:O	2:J:880:GLU:HG3	2.07	0.53
2:J:999:ASP:O	2:J:1003:GLN:HG2	2.09	0.53
2:J:3093:ARG:O	2:J:3097:GLU:HG2	2.09	0.53
2:B:2452:ARG:NH2	2:E:177:GLU:OE2	2.41	0.53
2:E:206:CYS:HB2	2:E:271:GLY:HA3	1.91	0.53
2:E:1947:CYS:SG	2:E:2127:GLN:NE2	2.77	0.53
2:E:2531:ARG:NH1	2:E:2585:THR:HB	2.24	0.53
2:E:2749:GLU:HG3	2:E:2752:ASP:HB2	1.90	0.53
2:G:3376:GLU:OE2	2:G:3380:ARG:NH2	2.39	0.53
2:G:3445:TRP:CD1	2:G:3509:LEU:HG	2.43	0.53
2:J:206:CYS:HB2	2:J:271:GLY:HA3	1.91	0.53
2:J:504:ALA:HB2	2:J:512:ALA:HB2	1.89	0.53
2:J:2792:ARG:NH2	2:J:2798:SER:OG	2.41	0.53
2:E:1569:GLN:HB2	2:E:1572:ILE:HD12	1.91	0.53
2:E:3147:ILE:HG23	2:E:3152:PHE:HB2	1.91	0.53
2:G:206:CYS:HB2	2:G:271:GLY:HA3	1.90	0.53
2:G:2531:ARG:NH1	2:G:2585:THR:HB	2.24	0.53
2:G:3194:LEU:HA	2:G:3197:LEU:HG	1.90	0.53
2:J:470:SER:HA	2:J:473:ASN:HD21	1.73	0.53
2:J:1940:CYS:O	2:J:1944:GLU:HG3	2.07	0.53
2:J:2527:LEU:HA	2:J:2530:MET:HG2	1.90	0.53
2:J:3162:GLN:HG2	2:J:3218:VAL:HG13	1.90	0.53
1:I:54:GLU:OE2	1:I:54:GLU:N	2.27	0.53
2:B:960:MET:SD	2:B:960:MET:N	2.75	0.53
2:B:1569:GLN:HB2	2:B:1572:ILE:HD12	1.91	0.53
2:B:3376:GLU:OE2	2:B:3380:ARG:NH2	2.39	0.53
2:E:3206:LEU:HB2	2:E:3280:TYR:HE2	1.72	0.53
2:E:3835:LEU:HD22	2:E:3880:PHE:HZ	1.74	0.53
2:E:3844:LEU:HD21	2:E:3936:TYR:HB2	1.90	0.53
2:E:4677:LEU:HD23	2:E:4711:PHE:HE1	1.72	0.53
2:G:999:ASP:O	2:G:1003:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2998:PHE:HA	2:G:3002:LEU:HB2	1.90	0.53
2:J:3938:SER:O	2:J:4002:LYS:NZ	2.41	0.53
2:B:1623:ARG:HH11	2:B:1623:ARG:HA	1.74	0.53
2:B:2123:LEU:O	2:B:2127:GLN:HG2	2.08	0.53
2:B:3445:TRP:CD1	2:B:3509:LEU:HG	2.43	0.53
2:B:3534:MET:O	2:B:3538:THR:HG23	2.07	0.53
2:E:234:SER:HB2	2:E:242:ARG:HG2	1.89	0.53
2:E:1940:CYS:O	2:E:1944:GLU:HG3	2.07	0.53
2:E:2616:PRO:HA	2:E:2619:LEU:HD12	1.90	0.53
2:G:1569:GLN:HB2	2:G:1572:ILE:HD12	1.91	0.53
2:G:1708:ARG:NH1	2:G:1836:PHE:O	2.42	0.53
2:G:2479:LEU:HD23	2:G:2479:LEU:H	1.73	0.53
2:G:2566:ALA:HA	2:G:2569:PHE:CD2	2.42	0.53
2:G:3280:TYR:CE1	2:G:3284:TRP:HD1	2.27	0.53
2:B:3008:GLN:O	2:B:3012:ASN:ND2	2.42	0.53
2:B:3938:SER:O	2:B:4002:LYS:NZ	2.41	0.53
2:E:426:ARG:HG3	2:E:431:PRO:HD3	1.90	0.53
2:E:470:SER:HA	2:E:473:ASN:HD21	1.73	0.53
2:E:3008:GLN:O	2:E:3012:ASN:ND2	2.42	0.53
2:G:504:ALA:HB2	2:G:512:ALA:HB2	1.89	0.53
2:J:671:VAL:HG22	2:J:787:VAL:HG23	1.91	0.53
2:J:1708:ARG:NH1	2:J:1836:PHE:O	2.42	0.53
2:J:1970:GLN:NE2	2:J:3641:LEU:O	2.37	0.53
2:J:3201:MET:SD	2:J:3203:VAL:HG12	2.48	0.53
2:B:3835:LEU:HD22	2:B:3880:PHE:HZ	1.74	0.53
2:E:2479:LEU:HD23	2:E:2479:LEU:H	1.73	0.53
2:E:3280:TYR:CE1	2:E:3284:TRP:HD1	2.27	0.53
2:G:2212:VAL:HG22	2:G:2256:TYR:CE1	2.43	0.53
2:J:1569:GLN:HB2	2:J:1572:ILE:HD12	1.91	0.53
2:J:2531:ARG:NH1	2:J:2585:THR:HB	2.24	0.53
2:J:3008:GLN:O	2:J:3012:ASN:ND2	2.42	0.53
2:B:2138:LEU:HD11	2:B:3662:ILE:HD12	1.90	0.52
2:B:3162:GLN:HG2	2:B:3218:VAL:HG13	1.90	0.52
2:B:3844:LEU:HD21	2:B:3936:TYR:HB2	1.90	0.52
2:E:3182:TYR:HA	2:E:3185:LYS:HE3	1.91	0.52
2:G:3008:GLN:O	2:G:3012:ASN:ND2	2.42	0.52
2:G:3076:ASP:O	2:G:3080:VAL:HG23	2.08	0.52
2:G:4104:THR:O	2:G:4108:ILE:HG12	2.09	0.52
2:J:3182:TYR:HA	2:J:3185:LYS:HE3	1.91	0.52
2:J:3280:TYR:CE1	2:J:3284:TRP:HD1	2.27	0.52
2:B:2531:ARG:NH1	2:B:2585:THR:HB	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3147:ILE:HG23	2:B:3152:PHE:HB2	1.91	0.52
2:B:4104:THR:O	2:B:4108:ILE:HG12	2.09	0.52
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.74	0.52
2:G:3093:ARG:O	2:G:3097:GLU:HG2	2.09	0.52
2:G:3891:LEU:HB3	2:G:3899:PHE:CE1	2.45	0.52
3:K:85:LEU:HD13	3:K:125:VAL:HG13	1.91	0.52
2:B:2245:GLN:HG2	2:B:2248:ARG:HH12	1.74	0.52
2:B:3891:LEU:HB3	2:B:3899:PHE:CE1	2.45	0.52
2:E:728:ARG:NH2	2:E:1489:CYS:SG	2.83	0.52
2:E:1623:ARG:HH11	2:E:1623:ARG:HA	1.74	0.52
2:E:3532:LEU:HD12	2:E:3532:LEU:H	1.74	0.52
2:E:4104:THR:O	2:E:4108:ILE:HG12	2.09	0.52
2:G:3835:LEU:HD22	2:G:3880:PHE:HZ	1.74	0.52
2:J:874:LEU:O	2:J:878:ILE:HG12	2.09	0.52
2:J:1727:ARG:NH2	2:J:1773:PRO:O	2.43	0.52
2:J:2265:LEU:HD12	2:J:2265:LEU:H	1.74	0.52
2:J:3076:ASP:O	2:J:3080:VAL:HG23	2.09	0.52
2:B:671:VAL:HG22	2:B:787:VAL:HG23	1.91	0.52
2:B:2312:MET:SD	2:B:2312:MET:N	2.79	0.52
2:B:3076:ASP:O	2:B:3080:VAL:HG23	2.09	0.52
2:B:3215:ALA:HA	2:B:3220:THR:HG21	1.91	0.52
2:E:2245:GLN:HG2	2:E:2248:ARG:HH12	1.73	0.52
2:E:3475:LYS:HD3	2:E:3516:LYS:NZ	2.25	0.52
3:C:85:LEU:HD13	3:C:125:VAL:HG13	1.91	0.52
2:B:40:GLU:O	2:B:114:SER:OG	2.28	0.52
2:B:3093:ARG:O	2:B:3097:GLU:HG2	2.09	0.52
2:E:2619:LEU:O	2:E:2623:LEU:HG	2.09	0.52
2:E:2634:ASN:OD1	2:E:2636:PHE:N	2.37	0.52
2:E:3923:LEU:HB2	2:E:3961:VAL:HG11	1.92	0.52
2:G:2245:GLN:HG2	2:G:2248:ARG:HH12	1.74	0.52
2:J:728:ARG:NH2	2:J:1489:CYS:SG	2.83	0.52
2:J:1854:PHE:HD1	2:J:1858:ASP:HB3	1.74	0.52
2:J:2479:LEU:HD23	2:J:2479:LEU:H	1.74	0.52
2:J:2759:ALA:HB2	2:J:2810:LYS:HZ1	1.74	0.52
2:J:3514:LEU:HD13	2:J:3602:VAL:HG13	1.91	0.52
2:J:4573:ILE:HG23	2:J:4643:LEU:HD11	1.91	0.52
2:B:874:LEU:O	2:B:878:ILE:HG12	2.09	0.52
2:B:2336:ARG:HG2	2:B:2435:ARG:HD3	1.92	0.52
2:B:2960:LEU:HD23	2:B:2963:LEU:HD12	1.92	0.52
2:B:3049:LEU:HA	2:B:3053:ARG:HH21	1.75	0.52
2:B:3280:TYR:HE1	2:B:3284:TRP:HD1	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4063:ASP:HB2	2:B:4067:LYS:HE3	1.90	0.52
2:B:4069:LYS:NZ	2:B:4130:ASN:OD1	2.37	0.52
2:B:4573:ILE:HG23	2:B:4643:LEU:HD11	1.91	0.52
2:E:3162:GLN:HG2	2:E:3218:VAL:HG13	1.90	0.52
2:E:3891:LEU:HB3	2:E:3899:PHE:CE1	2.45	0.52
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.52
2:J:3532:LEU:H	2:J:3532:LEU:HD12	1.74	0.52
2:J:3844:LEU:HD21	2:J:3936:TYR:HB2	1.90	0.52
2:B:1708:ARG:NH1	2:B:1836:PHE:O	2.42	0.52
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.75	0.52
2:B:2527:LEU:HA	2:B:2530:MET:HG2	1.90	0.52
2:B:2634:ASN:OD1	2:B:2636:PHE:N	2.37	0.52
2:E:3207:GLU:HB2	2:E:3246:LEU:HD22	1.91	0.52
2:E:3363:GLY:O	2:E:3367:LYS:HG2	2.10	0.52
2:G:40:GLU:O	2:G:114:SER:OG	2.28	0.52
2:G:2189:LYS:HA	2:G:2192:TYR:CZ	2.45	0.52
2:G:2336:ARG:HG2	2:G:2435:ARG:HD3	1.92	0.52
2:G:3049:LEU:HA	2:G:3053:ARG:HH21	1.75	0.52
2:G:3162:GLN:HG2	2:G:3218:VAL:HG13	1.90	0.52
2:G:4063:ASP:HB2	2:G:4067:LYS:HE3	1.90	0.52
2:J:246:TYR:CB	2:J:373:LYS:HD2	2.40	0.52
2:J:882:TRP:CD1	3:K:106:PRO:HB3	2.45	0.52
2:J:893:TYR:HA	2:J:904:HIS:HB3	1.90	0.52
2:J:2245:GLN:HG2	2:J:2248:ARG:HH12	1.74	0.52
2:J:3475:LYS:HD3	2:J:3516:LYS:NZ	2.25	0.52
2:B:3195:ALA:HB2	2:B:3275:PRO:HB3	1.92	0.52
2:E:2792:ARG:NH2	2:E:2798:SER:OG	2.41	0.52
2:E:3076:ASP:O	2:E:3080:VAL:HG23	2.09	0.52
2:G:671:VAL:HG22	2:G:787:VAL:HG23	1.91	0.52
2:G:3514:LEU:HD13	2:G:3602:VAL:HG13	1.91	0.52
2:G:3844:LEU:HD21	2:G:3936:TYR:HB2	1.90	0.52
2:J:1623:ARG:HA	2:J:1623:ARG:HH11	1.74	0.52
2:J:3835:LEU:HD22	2:J:3880:PHE:HZ	1.74	0.52
2:J:3891:LEU:HB3	2:J:3899:PHE:CE1	2.45	0.52
2:E:571:SER:HB2	2:E:574:VAL:HG22	1.92	0.52
2:G:874:LEU:O	2:G:878:ILE:HG12	2.09	0.52
2:G:3754:GLU:O	2:G:3758:MET:HG3	2.10	0.52
2:J:878:ILE:HG13	3:K:107:TRP:HZ2	1.75	0.52
2:J:3147:ILE:HG23	2:J:3152:PHE:HB2	1.91	0.52
1:I:26:TYR:HB2	1:I:101:VAL:HG12	1.92	0.52
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2970:SER:HA	2:B:2973:PHE:CZ	2.45	0.52
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.74	0.52
2:E:2336:ARG:HG2	2:E:2435:ARG:HD3	1.92	0.52
2:E:3962:PHE:O	2:E:3966:THR:HG23	2.09	0.52
2:G:2960:LEU:HD23	2:G:2963:LEU:HD12	1.92	0.52
2:J:4104:THR:O	2:J:4108:ILE:HG12	2.09	0.52
2:J:4715:TYR:CE2	2:J:4717:ASP:HB3	2.40	0.52
2:B:177:GLU:OE2	2:G:2452:ARG:NH2	2.41	0.51
2:B:1970:GLN:NE2	2:B:3641:LEU:O	2.37	0.51
2:B:3363:GLY:O	2:B:3367:LYS:HG2	2.10	0.51
2:E:671:VAL:HG22	2:E:787:VAL:HG23	1.91	0.51
2:E:2138:LEU:HD11	2:E:3662:ILE:HD12	1.90	0.51
2:E:2265:LEU:HD12	2:E:2265:LEU:H	1.74	0.51
2:E:2559:LEU:O	2:E:2563:THR:HG23	2.10	0.51
2:E:2736:ASP:OD1	2:E:2736:ASP:N	2.42	0.51
2:E:3215:ALA:HA	2:E:3220:THR:HG21	1.91	0.51
2:G:728:ARG:NH2	2:G:1489:CYS:SG	2.83	0.51
2:G:2265:LEU:H	2:G:2265:LEU:HD12	1.74	0.51
2:G:2992:GLU:HB2	2:G:2996:LYS:NZ	2.25	0.51
2:G:3147:ILE:HG23	2:G:3152:PHE:HB2	1.91	0.51
2:G:3195:ALA:HB2	2:G:3275:PRO:HB3	1.92	0.51
2:G:3280:TYR:HE1	2:G:3284:TRP:HD1	1.56	0.51
2:J:2138:LEU:HD11	2:J:3662:ILE:HD12	1.90	0.51
2:B:246:TYR:CB	2:B:373:LYS:HD2	2.40	0.51
2:B:3754:GLU:O	2:B:3758:MET:HG3	2.10	0.51
2:E:874:LEU:O	2:E:878:ILE:HG12	2.09	0.51
2:G:1623:ARG:HA	2:G:1623:ARG:HH11	1.74	0.51
2:G:2970:SER:HA	2:G:2973:PHE:CZ	2.45	0.51
2:G:3594:ARG:NH1	2:G:3597:GLN:OE1	2.34	0.51
2:J:210:GLU:HG2	2:J:273:HIS:CE1	2.46	0.51
2:J:4856:PHE:O	2:J:4860:ARG:NH2	2.39	0.51
2:B:728:ARG:NH2	2:B:1489:CYS:SG	2.83	0.51
2:B:3475:LYS:HD3	2:B:3516:LYS:NZ	2.25	0.51
2:B:3532:LEU:H	2:B:3532:LEU:HD12	1.74	0.51
2:E:210:GLU:HG2	2:E:273:HIS:CE1	2.46	0.51
2:E:3535:LEU:HD12	2:E:3539:ARG:HH12	1.76	0.51
2:G:3182:TYR:HA	2:G:3185:LYS:HE3	1.91	0.51
2:J:2336:ARG:HG2	2:J:2435:ARG:HD3	1.92	0.51
2:J:3225:ARG:O	2:J:3229:ILE:HG23	2.11	0.51
3:K:12:MET:HG2	3:K:16:GLY:HA3	1.93	0.51
2:B:231:LEU:O	2:B:260:TRP:NE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2792:ARG:NH2	2:B:2798:SER:OG	2.41	0.51
2:B:4630:TYR:HE1	2:E:4860:ARG:HH22	1.58	0.51
2:E:470:SER:HA	2:E:473:ASN:ND2	2.26	0.51
2:E:1708:ARG:NH1	2:E:1836:PHE:O	2.42	0.51
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.51
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.75	0.51
2:G:210:GLU:HG2	2:G:273:HIS:CE1	2.46	0.51
2:G:2619:LEU:O	2:G:2623:LEU:HG	2.09	0.51
2:G:3532:LEU:H	2:G:3532:LEU:HD12	1.75	0.51
2:G:3535:LEU:O	2:G:3539:ARG:HG2	2.11	0.51
2:J:470:SER:HA	2:J:473:ASN:ND2	2.26	0.51
2:J:2559:LEU:O	2:J:2563:THR:HG23	2.11	0.51
2:J:2992:GLU:HB2	2:J:2996:LYS:NZ	2.25	0.51
2:J:3049:LEU:HA	2:J:3053:ARG:HH21	1.75	0.51
2:J:3535:LEU:O	2:J:3539:ARG:HG2	2.11	0.51
3:F:85:LEU:HD13	3:F:125:VAL:HG13	1.91	0.51
2:B:2644:LEU:HD12	2:B:2648:TYR:HE2	1.76	0.51
2:E:3042:LEU:O	2:E:3046:LEU:HG	2.11	0.51
2:E:3049:LEU:HA	2:E:3053:ARG:HH21	1.75	0.51
2:E:3529:ASP:O	2:E:3533:ILE:HG13	2.11	0.51
2:G:2616:PRO:HA	2:G:2619:LEU:HD12	1.91	0.51
2:G:2644:LEU:HD12	2:G:2648:TYR:HE2	1.76	0.51
2:G:3219:TYR:HE1	2:G:3234:ASN:HA	1.76	0.51
2:J:3363:GLY:O	2:J:3367:LYS:HG2	2.10	0.51
2:J:3754:GLU:O	2:J:3758:MET:HG3	2.10	0.51
3:C:12:MET:HG2	3:C:16:GLY:HA3	1.93	0.51
3:F:12:MET:HG2	3:F:16:GLY:HA3	1.93	0.51
2:B:2189:LYS:HA	2:B:2192:TYR:CZ	2.45	0.51
2:B:3225:ARG:O	2:B:3229:ILE:HG23	2.11	0.51
2:E:878:ILE:HG13	3:F:107:TRP:HZ2	1.74	0.51
2:E:2970:SER:HA	2:E:2973:PHE:CZ	2.45	0.51
2:G:365:LYS:O	2:G:369:LEU:HG	2.10	0.51
2:G:920:TYR:O	2:G:923:GLN:HG2	2.11	0.51
2:G:920:TYR:HE1	3:M:99:ARG:HE	1.59	0.51
2:G:2559:LEU:O	2:G:2563:THR:HG23	2.11	0.51
2:G:4860:ARG:HH22	2:J:4630:TYR:HE1	1.58	0.51
2:J:3529:ASP:O	2:J:3533:ILE:HG13	2.11	0.51
2:J:4569:LEU:HD21	2:J:4649:LEU:HD23	1.93	0.51
2:E:3093:ARG:HA	2:E:3096:PHE:CD1	2.46	0.51
2:G:470:SER:HA	2:G:473:ASN:ND2	2.26	0.51
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:15:GLY:H	3:F:85:LEU:HB2	1.74	0.51
2:B:1000:ARG:HH12	3:C:115:ASP:H	1.59	0.51
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.74	0.51
2:B:3042:LEU:O	2:B:3046:LEU:HG	2.11	0.51
2:B:3182:TYR:HA	2:B:3185:LYS:HE3	1.91	0.51
2:E:3535:LEU:O	2:E:3539:ARG:HG2	2.11	0.51
2:G:878:ILE:HG13	3:M:107:TRP:HZ2	1.75	0.51
2:G:2682:ILE:HB	2:G:2703:LEU:HD21	1.93	0.51
2:G:3215:ALA:HA	2:G:3220:THR:HG21	1.91	0.51
2:G:3475:LYS:HD3	2:G:3516:LYS:NZ	2.25	0.51
2:J:243:ARG:HA	2:J:301:VAL:HG22	1.93	0.51
2:J:920:TYR:O	2:J:923:GLN:HG2	2.11	0.51
2:J:2189:LYS:HA	2:J:2192:TYR:CZ	2.45	0.51
2:J:2960:LEU:HD23	2:J:2963:LEU:HD12	1.92	0.51
2:J:3215:ALA:HA	2:J:3220:THR:HG21	1.91	0.51
2:J:3535:LEU:HD12	2:J:3539:ARG:HH12	1.76	0.51
3:C:90:THR:HG23	3:C:124:THR:HA	1.93	0.51
3:M:90:THR:HG23	3:M:124:THR:HA	1.93	0.51
1:D:97:LEU:HB3	1:D:99:PHE:CE2	2.46	0.51
1:H:54:GLU:OE2	1:H:54:GLU:N	2.27	0.51
1:I:26:TYR:CB	1:I:101:VAL:HG12	2.41	0.51
2:B:3644:LEU:HD11	2:B:3648:ARG:HD2	1.93	0.51
2:B:4856:PHE:O	2:B:4860:ARG:NH2	2.39	0.51
2:E:2572:THR:HG22	2:E:2575:ARG:HB3	1.93	0.51
2:E:3280:TYR:HE1	2:E:3284:TRP:HD1	1.56	0.51
2:G:3042:LEU:O	2:G:3046:LEU:HG	2.11	0.51
2:J:246:TYR:HE1	2:J:375:LYS:HG2	1.76	0.51
3:M:12:MET:HG2	3:M:16:GLY:HA3	1.93	0.51
3:M:15:GLY:H	3:M:85:LEU:HB2	1.74	0.51
2:B:243:ARG:HA	2:B:301:VAL:HG22	1.93	0.51
2:B:2265:LEU:HD12	2:B:2265:LEU:H	1.74	0.51
2:B:3514:LEU:HD13	2:B:3602:VAL:HG13	1.91	0.51
2:B:3535:LEU:O	2:B:3539:ARG:HG2	2.11	0.51
2:E:3225:ARG:O	2:E:3229:ILE:HG23	2.11	0.51
2:G:233:ILE:HG12	2:G:234:SER:H	1.76	0.51
2:G:571:SER:HB2	2:G:574:VAL:HG22	1.92	0.51
2:G:882:TRP:CD1	3:M:106:PRO:HB3	2.46	0.51
2:G:3698:LEU:O	2:G:3702:VAL:HG12	2.11	0.51
2:J:40:GLU:O	2:J:114:SER:OG	2.28	0.51
2:J:4671:PHE:HD1	2:J:4714:ASN:O	1.94	0.51
3:K:90:THR:HG23	3:K:124:THR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:571:SER:HB2	2:B:574:VAL:HG22	1.92	0.50
2:B:3535:LEU:HD12	2:B:3539:ARG:HH12	1.76	0.50
2:B:3594:ARG:NH1	2:B:3597:GLN:OE1	2.34	0.50
2:E:40:GLU:O	2:E:114:SER:OG	2.28	0.50
2:E:243:ARG:HA	2:E:301:VAL:HG22	1.93	0.50
2:E:246:TYR:HE1	2:E:375:LYS:HG2	1.76	0.50
2:E:479:GLN:HE21	2:E:539:LEU:HD11	1.77	0.50
2:E:4189:ARG:HB3	2:E:5031:GLN:HE22	1.76	0.50
2:G:2614:ILE:O	2:G:2650:ARG:NH1	2.41	0.50
2:G:3225:ARG:O	2:G:3229:ILE:HG23	2.11	0.50
2:G:3363:GLY:O	2:G:3367:LYS:HG2	2.10	0.50
2:G:3644:LEU:HD11	2:G:3648:ARG:HD2	1.93	0.50
2:J:2582:MET:HA	2:J:2585:THR:HG22	1.93	0.50
2:J:3195:ALA:HB2	2:J:3275:PRO:HB3	1.92	0.50
2:B:210:GLU:HG2	2:B:273:HIS:CE1	2.46	0.50
2:B:2736:ASP:OD1	2:B:2736:ASP:N	2.42	0.50
2:B:3246:LEU:CG	2:B:3247:ASP:H	2.24	0.50
2:B:3698:LEU:O	2:B:3702:VAL:HG12	2.11	0.50
2:E:2208:MET:O	2:E:2212:VAL:HG23	2.12	0.50
2:E:2582:MET:HA	2:E:2585:THR:HG22	1.93	0.50
2:E:2960:LEU:HD23	2:E:2963:LEU:HD12	1.92	0.50
2:E:4720:VAL:HG13	2:E:4721:LYS:H	1.76	0.50
2:G:3002:LEU:O	2:G:3006:ILE:HG22	2.12	0.50
2:J:233:ILE:HG12	2:J:234:SER:H	1.76	0.50
2:J:365:LYS:O	2:J:369:LEU:HG	2.10	0.50
2:J:2566:ALA:HA	2:J:2569:PHE:HD2	1.76	0.50
3:K:15:GLY:H	3:K:85:LEU:HB2	1.74	0.50
3:M:85:LEU:HD13	3:M:125:VAL:HG13	1.91	0.50
2:B:920:TYR:O	2:B:923:GLN:HG2	2.11	0.50
2:B:2759:ALA:HB2	2:B:2810:LYS:HZ1	1.75	0.50
2:B:4860:ARG:HH22	2:G:4630:TYR:HE1	1.58	0.50
2:E:2644:LEU:HD12	2:E:2648:TYR:HE2	1.76	0.50
2:E:2759:ALA:HB2	2:E:2810:LYS:HZ1	1.75	0.50
2:E:3002:LEU:O	2:E:3006:ILE:HG22	2.12	0.50
2:E:3195:ALA:HB2	2:E:3275:PRO:HB3	1.92	0.50
2:E:3698:LEU:O	2:E:3702:VAL:HG12	2.11	0.50
2:G:243:ARG:HA	2:G:301:VAL:HG22	1.93	0.50
2:G:3535:LEU:HD12	2:G:3539:ARG:HH12	1.76	0.50
2:G:3923:LEU:HB2	2:G:3961:VAL:HG11	1.92	0.50
2:G:4569:LEU:HD21	2:G:4649:LEU:HD23	1.93	0.50
2:J:3042:LEU:O	2:J:3046:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4189:ARG:HB3	2:J:5031:GLN:HE22	1.77	0.50
3:K:62:SER:O	3:K:62:SER:OG	2.24	0.50
2:B:2992:GLU:HB2	2:B:2996:LYS:NZ	2.25	0.50
2:B:3034:LYS:O	2:B:3037:GLU:HG3	2.12	0.50
2:B:3219:TYR:HE1	2:B:3234:ASN:HA	1.76	0.50
2:B:3923:LEU:HB2	2:B:3961:VAL:HG11	1.93	0.50
2:B:4189:ARG:HB3	2:B:5031:GLN:HE22	1.76	0.50
2:E:878:ILE:HG13	3:F:107:TRP:CZ2	2.45	0.50
2:E:2189:LYS:HA	2:E:2192:TYR:CZ	2.45	0.50
2:E:2992:GLU:HB2	2:E:2996:LYS:NZ	2.25	0.50
2:E:3141:THR:HA	2:E:3144:PHE:CD2	2.47	0.50
2:E:3219:TYR:HE1	2:E:3234:ASN:HA	1.76	0.50
2:G:479:GLN:HE21	2:G:539:LEU:HD11	1.76	0.50
2:G:1423:ASP:O	2:G:1427:ILE:HG12	2.12	0.50
2:G:2759:ALA:HB2	2:G:2810:LYS:HZ1	1.76	0.50
2:G:3529:ASP:O	2:G:3533:ILE:HG13	2.11	0.50
2:G:3965:LEU:HA	2:G:3968:TYR:CD2	2.46	0.50
2:G:4545:GLU:O	2:G:4549:VAL:HG13	2.11	0.50
2:J:1423:ASP:O	2:J:1427:ILE:HG12	2.12	0.50
2:J:2109:ASP:HA	2:J:3694:LYS:HD2	1.93	0.50
2:J:2970:SER:HA	2:J:2973:PHE:CZ	2.45	0.50
2:J:3227:ARG:HG2	2:J:3232:LEU:HD12	1.93	0.50
2:J:4545:GLU:O	2:J:4549:VAL:HG13	2.12	0.50
3:F:90:THR:HG23	3:F:124:THR:HA	1.93	0.50
1:D:54:GLU:OE2	1:D:54:GLU:N	2.27	0.50
2:B:470:SER:HA	2:B:473:ASN:ND2	2.26	0.50
2:B:479:GLN:HE21	2:B:539:LEU:HD11	1.76	0.50
2:B:1423:ASP:O	2:B:1427:ILE:HG12	2.12	0.50
2:B:3093:ARG:HA	2:B:3096:PHE:CD1	2.46	0.50
2:E:233:ILE:HG12	2:E:234:SER:H	1.76	0.50
2:E:3644:LEU:HD11	2:E:3648:ARG:HD2	1.93	0.50
2:E:4545:GLU:O	2:E:4549:VAL:HG13	2.12	0.50
2:G:2109:ASP:HA	2:G:3694:LYS:HD2	1.93	0.50
2:G:3227:ARG:HG2	2:G:3232:LEU:HD12	1.93	0.50
2:J:479:GLN:HE21	2:J:539:LEU:HD11	1.76	0.50
2:J:571:SER:HB2	2:J:574:VAL:HG22	1.92	0.50
2:J:2165:LEU:HD13	2:J:2178:MET:HG2	1.94	0.50
2:J:3698:LEU:O	2:J:3702:VAL:HG12	2.11	0.50
2:B:2208:MET:O	2:B:2212:VAL:HG23	2.12	0.50
2:B:2635:GLU:HG3	2:B:2636:PHE:CD2	2.47	0.50
2:B:2682:ILE:HB	2:B:2703:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3966:THR:HG23	2:B:4026:MET:HA	1.92	0.50
2:E:920:TYR:O	2:E:923:GLN:HG2	2.11	0.50
2:E:1970:GLN:NE2	2:E:3641:LEU:O	2.37	0.50
2:G:866:HIS:HE1	2:G:870:ILE:HD12	1.77	0.50
2:G:2635:GLU:HG3	2:G:2636:PHE:CD2	2.47	0.50
2:G:3093:ARG:HA	2:G:3096:PHE:CD1	2.46	0.50
2:G:3141:THR:HA	2:G:3144:PHE:CD2	2.47	0.50
2:J:2380:ILE:O	2:J:2384:ILE:HG13	2.12	0.50
2:J:2457:LEU:HA	2:J:2460:LEU:HD12	1.94	0.50
2:J:3376:GLU:OE2	2:J:3380:ARG:NH2	2.39	0.50
2:B:2576:ALA:HA	2:B:2579:VAL:HB	1.93	0.50
2:B:2879:ALA:HA	2:B:2882:TYR:CD2	2.47	0.50
2:B:3180:ASN:O	2:B:3184:GLU:HG2	2.12	0.50
2:B:4096:ALA:O	2:B:4100:GLN:HG2	2.12	0.50
2:E:1087:ARG:HB3	2:E:1223:PHE:HA	1.94	0.50
2:E:3180:ASN:O	2:E:3184:GLU:HG2	2.12	0.50
2:E:3754:GLU:O	2:E:3758:MET:HG3	2.10	0.50
2:G:246:TYR:HE1	2:G:375:LYS:HG2	1.76	0.50
2:G:2165:LEU:HD13	2:G:2178:MET:HG2	1.93	0.50
2:G:4189:ARG:HB3	2:G:5031:GLN:HE22	1.77	0.50
2:J:127:MET:SD	2:J:127:MET:N	2.73	0.50
2:J:2208:MET:O	2:J:2212:VAL:HG23	2.12	0.50
2:J:2572:THR:HA	2:J:2574:HIS:CE1	2.46	0.50
2:J:2644:LEU:HD12	2:J:2648:TYR:HE2	1.76	0.50
2:J:4105:GLY:O	2:J:4109:GLN:HG2	2.12	0.50
1:D:26:TYR:CB	1:D:101:VAL:HG12	2.42	0.50
2:B:526:LEU:HD11	2:B:540:PHE:HZ	1.77	0.50
2:B:866:HIS:HE1	2:B:870:ILE:HD12	1.76	0.50
2:B:3651:ASN:O	2:B:3655:GLU:HG2	2.12	0.50
2:E:121:LEU:N	2:E:134:ASP:O	2.45	0.50
2:E:365:LYS:O	2:E:369:LEU:HG	2.12	0.50
2:E:501:ALA:O	2:E:505:GLU:HG2	2.12	0.50
2:E:823:LEU:HD11	2:E:1626:TRP:HB3	1.94	0.50
2:E:2635:GLU:HG3	2:E:2636:PHE:CD2	2.47	0.50
2:E:3246:LEU:HD23	2:E:3247:ASP:H	1.77	0.50
2:G:2211:MET:HA	2:G:2214:VAL:HG12	1.94	0.50
2:G:2573:GLU:HB2	2:G:2615:ARG:NH2	2.27	0.50
2:G:2788:HIS:NE2	2:G:2805:TYR:OH	2.38	0.50
2:G:5013:MET:CE	2:G:5020:ASP:HB2	2.42	0.50
2:G:5013:MET:HE3	2:G:5020:ASP:HB2	1.93	0.50
2:J:526:LEU:HD11	2:J:540:PHE:HZ	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2635:GLU:HG3	2:J:2636:PHE:CD2	2.47	0.50
2:J:3093:ARG:HA	2:J:3096:PHE:CD1	2.46	0.50
2:J:3093:ARG:HA	2:J:3096:PHE:HD1	1.77	0.50
2:B:3093:ARG:HA	2:B:3096:PHE:HD1	1.77	0.50
2:B:3529:ASP:O	2:B:3533:ILE:HG13	2.11	0.50
2:G:2582:MET:HA	2:G:2585:THR:HG22	1.94	0.50
2:G:3180:ASN:O	2:G:3184:GLU:HG2	2.12	0.50
2:J:231:LEU:O	2:J:260:TRP:NE1	2.40	0.50
2:J:1619:ARG:HB3	2:J:1626:TRP:CD2	2.47	0.50
2:J:2364:PHE:HD1	2:J:2429:LEU:HD21	1.75	0.50
2:J:3002:LEU:O	2:J:3006:ILE:HG22	2.12	0.50
2:B:233:ILE:HG12	2:B:234:SER:H	1.76	0.49
2:B:2165:LEU:HD13	2:B:2178:MET:HG2	1.94	0.49
2:B:2211:MET:HA	2:B:2214:VAL:HG12	1.94	0.49
2:B:2415:ARG:HA	2:B:2415:ARG:HH11	1.77	0.49
2:B:2457:LEU:HA	2:B:2460:LEU:HD12	1.94	0.49
2:B:3002:LEU:O	2:B:3006:ILE:HG22	2.12	0.49
2:E:2165:LEU:HD13	2:E:2178:MET:HG2	1.94	0.49
2:E:2879:ALA:HA	2:E:2882:TYR:CD2	2.47	0.49
2:E:3034:LYS:O	2:E:3037:GLU:HG3	2.12	0.49
2:E:3227:ARG:HG2	2:E:3232:LEU:HD12	1.93	0.49
2:E:3406:TYR:HD2	2:E:3464:ILE:HG21	1.77	0.49
2:G:2380:ILE:O	2:G:2384:ILE:HG13	2.12	0.49
2:G:4105:GLY:O	2:G:4109:GLN:HG2	2.12	0.49
2:J:3277:LEU:HB3	2:J:3315:LEU:HD13	1.94	0.49
1:H:97:LEU:HB3	1:H:99:PHE:CE2	2.46	0.49
2:B:3970:GLN:HE21	2:B:5004:THR:HA	1.77	0.49
2:G:501:ALA:O	2:G:505:GLU:HG2	2.12	0.49
2:G:1619:ARG:HB3	2:G:1626:TRP:CD2	2.47	0.49
2:G:2572:THR:HG22	2:G:2575:ARG:HB3	1.94	0.49
2:G:3034:LYS:O	2:G:3037:GLU:HG3	2.12	0.49
2:G:3780:LEU:HD22	2:G:3820:LEU:HD21	1.95	0.49
2:J:2230:THR:O	2:J:2234:ARG:HG3	2.12	0.49
2:J:3034:LYS:O	2:J:3037:GLU:HG3	2.12	0.49
2:J:3219:TYR:HE1	2:J:3234:ASN:HA	1.76	0.49
3:M:37:TYR:HE1	3:M:96:ASN:HB3	1.78	0.49
2:B:3227:ARG:HG2	2:B:3232:LEU:HD12	1.93	0.49
2:B:4569:LEU:HD21	2:B:4649:LEU:HD23	1.93	0.49
2:E:3438:VAL:HB	2:E:3513:THR:HG22	1.94	0.49
2:E:3651:ASN:O	2:E:3655:GLU:HG2	2.12	0.49
2:E:4843:LEU:O	2:E:4847:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:526:LEU:HD11	2:G:540:PHE:HZ	1.76	0.49
2:G:1215:ALA:HA	2:G:1219:LEU:HB3	1.94	0.49
2:G:1260:MET:O	2:G:1263:THR:OG1	2.31	0.49
2:G:2415:ARG:HA	2:G:2415:ARG:HH11	1.77	0.49
2:G:2751:LEU:O	2:G:2755:ILE:HG12	2.13	0.49
2:G:3093:ARG:HA	2:G:3096:PHE:HD1	1.77	0.49
2:G:3531:ASP:O	2:G:3535:LEU:HD23	2.12	0.49
2:J:148:TRP:CZ3	2:J:180:LEU:HG	2.48	0.49
2:J:501:ALA:O	2:J:505:GLU:HG2	2.11	0.49
2:J:823:LEU:HD11	2:J:1626:TRP:HB3	1.94	0.49
2:J:2415:ARG:HA	2:J:2415:ARG:HH11	1.77	0.49
2:J:3438:VAL:HB	2:J:3513:THR:HG22	1.94	0.49
3:C:15:GLY:H	3:C:85:LEU:HB2	1.74	0.49
3:M:63:VAL:O	3:M:63:VAL:HG12	2.13	0.49
2:B:223:PHE:HA	2:B:230:CYS:HA	1.95	0.49
2:B:823:LEU:HD11	2:B:1626:TRP:HB3	1.94	0.49
2:B:1087:ARG:HB3	2:B:1223:PHE:HA	1.94	0.49
2:B:2751:LEU:O	2:B:2755:ILE:HG12	2.13	0.49
2:E:1423:ASP:O	2:E:1427:ILE:HG12	2.12	0.49
2:E:2211:MET:HA	2:E:2214:VAL:HG12	1.94	0.49
2:E:2614:ILE:O	2:E:2650:ARG:NH1	2.41	0.49
2:E:3093:ARG:HA	2:E:3096:PHE:HD1	1.77	0.49
2:E:3531:ASP:O	2:E:3535:LEU:HD23	2.12	0.49
2:E:4569:LEU:HD21	2:E:4649:LEU:HD23	1.93	0.49
2:E:4630:TYR:HE1	2:J:4860:ARG:HH22	1.59	0.49
2:G:2691:TYR:HA	2:G:2696:TYR:CE1	2.47	0.49
2:G:4843:LEU:O	2:G:4847:VAL:HG22	2.13	0.49
2:J:866:HIS:HE1	2:J:870:ILE:HD12	1.77	0.49
2:J:2879:ALA:HA	2:J:2882:TYR:CD2	2.47	0.49
3:F:63:VAL:HG12	3:F:63:VAL:O	2.13	0.49
2:B:501:ALA:O	2:B:505:GLU:HG2	2.12	0.49
2:B:1215:ALA:HA	2:B:1219:LEU:HB3	1.94	0.49
2:B:2567:PRO:HA	2:B:2613:TYR:CD1	2.48	0.49
2:B:3141:THR:HA	2:B:3144:PHE:CD2	2.47	0.49
2:B:4545:GLU:O	2:B:4549:VAL:HG13	2.12	0.49
2:E:1619:ARG:HB3	2:E:1626:TRP:CD2	2.47	0.49
2:E:2380:ILE:O	2:E:2384:ILE:HG13	2.12	0.49
2:E:2475:GLN:NE2	2:E:2476:ILE:O	2.46	0.49
2:E:2682:ILE:HB	2:E:2703:LEU:HD21	1.93	0.49
2:E:2751:LEU:O	2:E:2755:ILE:HG12	2.13	0.49
2:E:3970:GLN:HE21	2:E:5004:THR:HA	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4096:ALA:O	2:E:4100:GLN:HG2	2.12	0.49
2:G:2208:MET:O	2:G:2212:VAL:HG23	2.12	0.49
2:G:2496:PRO:HG3	2:G:2550:LEU:HD23	1.94	0.49
2:G:3651:ASN:O	2:G:3655:GLU:HG2	2.12	0.49
2:J:2211:MET:HA	2:J:2214:VAL:HG12	1.94	0.49
2:J:2431:ASP:HB2	2:J:2501:SER:HB2	1.95	0.49
2:J:3180:ASN:O	2:J:3184:GLU:HG2	2.12	0.49
2:J:3780:LEU:HD22	2:J:3820:LEU:HD21	1.95	0.49
2:B:2496:PRO:HG3	2:B:2550:LEU:HD23	1.94	0.49
2:B:2725:LYS:HZ1	2:B:2737:PRO:HA	1.76	0.49
2:E:2109:ASP:HA	2:E:3694:LYS:HD2	1.93	0.49
2:E:2415:ARG:HA	2:E:2415:ARG:HH11	1.77	0.49
2:E:2869:ARG:HH22	2:E:2946:LEU:HA	1.78	0.49
2:E:2881:ASN:HA	2:E:2884:ASN:ND2	2.28	0.49
2:G:2869:ARG:HH22	2:G:2946:LEU:HA	1.78	0.49
2:G:2881:ASN:HA	2:G:2884:ASN:ND2	2.28	0.49
2:G:3406:TYR:HD2	2:G:3464:ILE:HG21	1.77	0.49
2:G:3438:VAL:HB	2:G:3513:THR:HG22	1.95	0.49
2:J:1087:ARG:HB3	2:J:1223:PHE:HA	1.94	0.49
2:J:3141:THR:HA	2:J:3144:PHE:CD2	2.47	0.49
2:J:3644:LEU:HD11	2:J:3648:ARG:HD2	1.93	0.49
2:J:3970:GLN:NE2	2:J:5004:THR:HA	2.28	0.49
3:K:82:MET:HG3	3:K:84:SER:O	2.13	0.49
1:A:24:VAL:HG12	1:A:103:LEU:HA	1.93	0.49
2:B:349:GLN:HE21	2:B:354:GLY:HA2	1.78	0.49
2:B:3438:VAL:HB	2:B:3513:THR:HG22	1.95	0.49
2:B:3531:ASP:O	2:B:3535:LEU:HD23	2.12	0.49
2:E:148:TRP:CZ3	2:E:180:LEU:HG	2.48	0.49
2:E:866:HIS:HE1	2:E:870:ILE:HD12	1.76	0.49
2:E:4105:GLY:O	2:E:4109:GLN:HG2	2.12	0.49
2:G:148:TRP:CZ3	2:G:180:LEU:HG	2.48	0.49
2:G:2376:LEU:O	2:G:2380:ILE:HG12	2.13	0.49
2:G:2475:GLN:NE2	2:G:2476:ILE:O	2.46	0.49
2:G:2792:ARG:NH2	2:G:2798:SER:OG	2.41	0.49
2:G:3970:GLN:HE21	2:G:5004:THR:HA	1.78	0.49
2:G:4118:ASP:OD1	2:G:4119:GLU:N	2.46	0.49
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	1.95	0.49
2:J:1260:MET:O	2:J:1263:THR:OG1	2.31	0.49
2:J:2376:LEU:O	2:J:2380:ILE:HG12	2.13	0.49
2:J:2881:ASN:HA	2:J:2884:ASN:ND2	2.28	0.49
2:J:2970:SER:O	2:J:2974:ILE:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3406:TYR:HD2	2:J:3464:ILE:HG21	1.77	0.49
2:J:3573:MET:HE2	2:J:3576:TYR:HB3	1.95	0.49
2:J:3651:ASN:O	2:J:3655:GLU:HG2	2.12	0.49
2:J:4096:ALA:O	2:J:4100:GLN:HG2	2.12	0.49
2:J:4677:LEU:HD23	2:J:4711:PHE:HE1	1.77	0.49
1:H:26:TYR:CB	1:H:101:VAL:HG12	2.43	0.49
2:B:2109:ASP:HA	2:B:3694:LYS:HD2	1.93	0.49
2:B:2747:ILE:HG21	2:B:2814:LYS:HE3	1.95	0.49
2:B:3406:TYR:HD2	2:B:3464:ILE:HG21	1.77	0.49
2:B:3573:MET:HE2	2:B:3576:TYR:HB3	1.94	0.49
2:E:2747:ILE:HG21	2:E:2814:LYS:HE3	1.95	0.49
2:E:3051:ARG:NH2	2:E:3098:SER:O	2.46	0.49
2:E:3573:MET:HE2	2:E:3576:TYR:HB3	1.94	0.49
2:G:2431:ASP:HB2	2:G:2501:SER:HB2	1.95	0.49
2:G:2457:LEU:HA	2:G:2460:LEU:HD12	1.94	0.49
2:G:2747:ILE:HG21	2:G:2814:LYS:HE3	1.95	0.49
2:G:2879:ALA:HA	2:G:2882:TYR:CD2	2.47	0.49
2:J:878:ILE:HG13	3:K:107:TRP:CZ2	2.47	0.49
2:J:1215:ALA:HA	2:J:1219:LEU:HB3	1.94	0.49
2:J:2619:LEU:O	2:J:2623:LEU:HG	2.13	0.49
2:J:2751:LEU:O	2:J:2755:ILE:HG12	2.13	0.49
2:J:3531:ASP:O	2:J:3535:LEU:HD23	2.12	0.49
2:J:4843:LEU:O	2:J:4847:VAL:HG22	2.13	0.49
2:J:5009:TYR:HA	2:J:5012:LYS:HE3	1.94	0.49
3:K:37:TYR:HE1	3:K:96:ASN:HB3	1.77	0.49
1:A:78:PRO:HA	1:A:81:ALA:HB3	1.94	0.49
2:B:121:LEU:N	2:B:134:ASP:O	2.45	0.49
2:B:2475:GLN:NE2	2:B:2476:ILE:O	2.46	0.49
2:B:2691:TYR:HA	2:B:2696:TYR:CE1	2.47	0.49
2:B:2881:ASN:HA	2:B:2884:ASN:ND2	2.28	0.49
2:B:3051:ARG:NH2	2:B:3098:SER:O	2.46	0.49
2:E:208:CYS:H	2:E:269:TRP:HH2	1.61	0.49
2:E:882:TRP:CD2	3:F:106:PRO:HG3	2.47	0.49
2:G:371:VAL:CG1	2:G:373:LYS:HG2	2.43	0.49
2:G:863:LEU:HD22	2:G:867:LEU:HD21	1.95	0.49
2:G:1530:THR:HG23	2:G:1535:GLU:H	1.78	0.49
2:G:2230:THR:O	2:G:2234:ARG:HG3	2.12	0.49
2:G:2637:ALA:C	2:G:2640:PRO:HD2	2.33	0.49
2:G:2973:PHE:CD1	2:G:2995:ILE:HG12	2.48	0.49
2:J:1095:VAL:HB	2:J:1199:VAL:HG23	1.95	0.49
2:J:2475:GLN:NE2	2:J:2476:ILE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:PRO:HA	1:H:81:ALA:HB3	1.94	0.49
2:B:148:TRP:CZ3	2:B:180:LEU:HG	2.48	0.49
2:B:1154:ASP:HB3	2:B:1157:GLU:HB2	1.95	0.49
2:B:1619:ARG:HB3	2:B:1626:TRP:CD2	2.47	0.49
2:B:2230:THR:O	2:B:2234:ARG:HG3	2.12	0.49
2:E:526:LEU:HD11	2:E:540:PHE:HZ	1.77	0.49
2:E:1260:MET:O	2:E:1263:THR:OG1	2.31	0.49
2:E:3078:ARG:O	2:E:3082:LYS:HG2	2.13	0.49
2:E:3307:VAL:HA	2:E:3311:HIS:CE1	2.47	0.49
2:E:3316:LEU:HD21	2:E:3345:ILE:HG13	1.95	0.49
2:G:3246:LEU:HD12	2:G:3249:LEU:HD12	1.95	0.49
2:G:3573:MET:SD	2:G:3577:ARG:NH2	2.86	0.49
2:J:349:GLN:HE21	2:J:354:GLY:HA2	1.78	0.49
2:J:2970:SER:HA	2:J:2973:PHE:CE2	2.48	0.49
2:B:208:CYS:H	2:B:269:TRP:HH2	1.61	0.48
2:B:863:LEU:HD22	2:B:867:LEU:HD21	1.95	0.48
2:B:1530:THR:HG23	2:B:1535:GLU:H	1.78	0.48
2:B:2376:LEU:O	2:B:2380:ILE:HG12	2.13	0.48
2:B:2558:VAL:O	2:B:2562:ILE:HG12	2.14	0.48
2:B:2970:SER:HA	2:B:2973:PHE:CE2	2.48	0.48
2:E:349:GLN:HE21	2:E:354:GLY:HA2	1.78	0.48
2:E:2230:THR:O	2:E:2234:ARG:HG3	2.12	0.48
2:E:2431:ASP:HB2	2:E:2501:SER:HB2	1.95	0.48
2:E:2457:LEU:HA	2:E:2460:LEU:HD12	1.94	0.48
2:E:3206:LEU:HD13	2:E:3246:LEU:N	2.28	0.48
2:E:4651:THR:HG21	2:E:4803:HIS:CD2	2.48	0.48
2:J:1530:THR:HG23	2:J:1535:GLU:H	1.78	0.48
2:J:2637:ALA:C	2:J:2640:PRO:HD2	2.33	0.48
2:J:2747:ILE:HG21	2:J:2814:LYS:HE3	1.95	0.48
2:J:3078:ARG:O	2:J:3082:LYS:HG2	2.13	0.48
2:J:4802:GLY:HA2	2:J:4808:PHE:HB2	1.95	0.48
1:D:78:PRO:HA	1:D:81:ALA:HB3	1.94	0.48
2:B:4105:GLY:O	2:B:4109:GLN:HG2	2.12	0.48
2:B:4651:THR:HG21	2:B:4803:HIS:CD2	2.48	0.48
2:E:3573:MET:SD	2:E:3577:ARG:NH2	2.86	0.48
2:E:3780:LEU:HD22	2:E:3820:LEU:HD21	1.95	0.48
2:G:823:LEU:HD11	2:G:1626:TRP:HB3	1.94	0.48
2:G:870:ILE:O	2:G:874:LEU:HG	2.13	0.48
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.95	0.48
2:J:2616:PRO:HA	2:J:2619:LEU:HD12	1.94	0.48
2:J:2691:TYR:HA	2:J:2696:TYR:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2973:PHE:CD1	2:J:2995:ILE:HG12	2.48	0.48
2:B:2869:ARG:HH22	2:B:2946:LEU:HA	1.78	0.48
2:B:3315:LEU:O	2:B:3319:ILE:HG13	2.14	0.48
2:E:223:PHE:HA	2:E:230:CYS:HA	1.95	0.48
2:E:2867:LEU:HB2	2:E:2928:LYS:NZ	2.29	0.48
2:E:4118:ASP:OD1	2:E:4119:GLU:N	2.46	0.48
2:J:870:ILE:O	2:J:874:LEU:HG	2.13	0.48
2:J:2682:ILE:HB	2:J:2703:LEU:HD21	1.93	0.48
2:J:2869:ARG:HH22	2:J:2946:LEU:HA	1.78	0.48
2:J:3051:ARG:NH2	2:J:3098:SER:O	2.46	0.48
2:J:3262:ARG:N	2:J:3262:ARG:HD2	2.28	0.48
3:C:63:VAL:O	3:C:63:VAL:HG12	2.13	0.48
3:K:63:VAL:O	3:K:63:VAL:HG12	2.13	0.48
3:M:82:MET:HG3	3:M:84:SER:O	2.13	0.48
1:A:4:ILE:HD11	1:A:62:GLY:HA2	1.96	0.48
1:I:78:PRO:HA	1:I:81:ALA:HB3	1.94	0.48
2:B:733:PRO:HG2	2:B:762:CYS:HB3	1.96	0.48
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.95	0.48
2:B:2973:PHE:CD1	2:B:2995:ILE:HG12	2.48	0.48
2:B:3573:MET:SD	2:B:3577:ARG:NH2	2.86	0.48
2:G:1087:ARG:HB3	2:G:1223:PHE:HA	1.94	0.48
2:G:2158:CYS:O	2:G:2162:ILE:HG13	2.14	0.48
2:G:2867:LEU:HB2	2:G:2928:LYS:NZ	2.29	0.48
2:J:2788:HIS:NE2	2:J:2805:TYR:OH	2.38	0.48
2:J:4651:THR:HG21	2:J:4803:HIS:CD2	2.48	0.48
2:J:5013:MET:HE1	2:J:5021:PHE:HB3	1.95	0.48
3:C:37:TYR:HE1	3:C:96:ASN:HB3	1.78	0.48
1:A:4:ILE:HG13	1:A:65:GLN:NE2	2.28	0.48
1:D:4:ILE:HD11	1:D:62:GLY:HA2	1.96	0.48
1:I:4:ILE:HD11	1:I:62:GLY:HA2	1.96	0.48
2:B:28:VAL:HG12	2:B:33:LEU:HD23	1.96	0.48
2:B:1735:ILE:HG22	2:B:2142:TYR:HB3	1.95	0.48
2:B:2637:ALA:C	2:B:2640:PRO:HD2	2.33	0.48
2:B:3078:ARG:O	2:B:3082:LYS:HG2	2.13	0.48
2:E:299:LEU:HD21	2:E:377:ILE:HA	1.96	0.48
2:E:1154:ASP:HB3	2:E:1157:GLU:HB2	1.95	0.48
2:E:1623:ARG:HA	2:E:1623:ARG:NH1	2.28	0.48
2:E:2970:SER:HA	2:E:2973:PHE:CE2	2.48	0.48
2:E:3262:ARG:N	2:E:3262:ARG:HD2	2.28	0.48
2:G:121:LEU:N	2:G:134:ASP:O	2.45	0.48
2:G:299:LEU:HD21	2:G:377:ILE:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3573:MET:HE2	2:G:3576:TYR:HB3	1.95	0.48
2:J:863:LEU:HD22	2:J:867:LEU:HD21	1.95	0.48
2:J:2158:CYS:O	2:J:2162:ILE:HG13	2.14	0.48
2:J:2496:PRO:HG3	2:J:2550:LEU:HD23	1.93	0.48
3:C:82:MET:HG3	3:C:84:SER:O	2.13	0.48
3:F:37:TYR:HE1	3:F:96:ASN:HB3	1.77	0.48
1:H:4:ILE:HD11	1:H:62:GLY:HA2	1.96	0.48
2:B:2799:GLU:O	2:B:2803:GLU:HG2	2.14	0.48
2:B:3475:LYS:HD3	2:B:3516:LYS:HZ1	1.79	0.48
2:B:3780:LEU:HD22	2:B:3820:LEU:HD21	1.95	0.48
2:E:1426:ILE:HA	2:E:1429:ASN:OD1	2.13	0.48
2:E:2158:CYS:O	2:E:2162:ILE:HG13	2.14	0.48
2:E:2496:PRO:HG3	2:E:2550:LEU:HD23	1.94	0.48
2:E:2637:ALA:C	2:E:2640:PRO:HD2	2.33	0.48
2:E:2691:TYR:HA	2:E:2696:TYR:CE1	2.47	0.48
2:E:2799:GLU:O	2:E:2803:GLU:HG2	2.14	0.48
2:E:2970:SER:O	2:E:2974:ILE:HG23	2.13	0.48
2:E:2973:PHE:CD1	2:E:2995:ILE:HG12	2.48	0.48
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	1.95	0.48
2:G:1154:ASP:HB3	2:G:1157:GLU:HB2	1.95	0.48
2:G:1623:ARG:HA	2:G:1623:ARG:NH1	2.28	0.48
2:G:2970:SER:HA	2:G:2973:PHE:CE2	2.48	0.48
2:G:3051:ARG:NH2	2:G:3098:SER:O	2.46	0.48
2:G:4096:ALA:O	2:G:4100:GLN:HG2	2.12	0.48
2:J:4118:ASP:OD1	2:J:4119:GLU:N	2.46	0.48
2:B:870:ILE:O	2:B:874:LEU:HG	2.14	0.48
2:B:1260:MET:O	2:B:1263:THR:OG1	2.31	0.48
2:B:2626:LEU:HD22	2:B:2640:PRO:HB3	1.95	0.48
2:B:3704:HIS:O	2:B:3708:THR:HG23	2.14	0.48
2:B:4118:ASP:OD1	2:B:4119:GLU:N	2.46	0.48
2:E:369:LEU:HB3	2:E:371:VAL:HG23	1.96	0.48
2:E:3704:HIS:O	2:E:3708:THR:HG23	2.14	0.48
2:E:3836:MET:CE	2:E:3915:ILE:HG23	2.44	0.48
2:G:28:VAL:HG12	2:G:33:LEU:HD23	1.96	0.48
2:G:1735:ILE:HG22	2:G:2142:TYR:HB3	1.95	0.48
2:G:3262:ARG:N	2:G:3262:ARG:HD2	2.28	0.48
2:J:208:CYS:H	2:J:269:TRP:HH2	1.61	0.48
2:B:2431:ASP:HB2	2:B:2501:SER:HB2	1.94	0.48
2:B:2562:ILE:HG23	2:B:2569:PHE:CE2	2.48	0.48
2:B:2970:SER:O	2:B:2974:ILE:HG23	2.13	0.48
2:B:3836:MET:CE	2:B:3915:ILE:HG23	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3991:GLY:O	2:B:3995:VAL:HG23	2.13	0.48
2:B:4780:PHE:HA	2:B:4783:ILE:HG22	1.94	0.48
2:B:4843:LEU:O	2:B:4847:VAL:HG22	2.13	0.48
2:E:3354:LEU:HG	2:E:3359:ILE:HD11	1.96	0.48
2:E:3366:ARG:NE	2:E:3367:LYS:HD2	2.26	0.48
2:G:223:PHE:HA	2:G:230:CYS:HA	1.95	0.48
2:G:2626:LEU:HD22	2:G:2640:PRO:HB3	1.96	0.48
2:G:3078:ARG:O	2:G:3082:LYS:HG2	2.13	0.48
2:G:3836:MET:CE	2:G:3915:ILE:HG23	2.44	0.48
2:G:4780:PHE:HA	2:G:4783:ILE:HG22	1.94	0.48
2:J:2376:LEU:HD12	2:J:2376:LEU:H	1.79	0.48
2:J:2566:ALA:HA	2:J:2569:PHE:CD2	2.49	0.48
2:J:3320:LEU:HD23	2:J:3320:LEU:HA	1.74	0.48
3:F:82:MET:HG3	3:F:84:SER:O	2.13	0.48
2:B:2380:ILE:O	2:B:2384:ILE:HG13	2.12	0.48
2:B:3166:TYR:CE1	2:B:3239:MET:HG3	2.49	0.48
2:E:215:THR:HG22	2:E:273:HIS:HA	1.96	0.48
2:E:1215:ALA:HA	2:E:1219:LEU:HB3	1.94	0.48
2:E:3281:LEU:O	2:E:3285:TRP:HB2	2.14	0.48
2:G:1426:ILE:HA	2:G:1429:ASN:OD1	2.13	0.48
2:G:2531:ARG:HH12	2:G:2585:THR:HB	1.79	0.48
2:G:2970:SER:O	2:G:2974:ILE:HG23	2.13	0.48
2:G:3704:HIS:O	2:G:3708:THR:HG23	2.14	0.48
2:G:4064:MET:HE1	2:G:4110:PHE:HD2	1.79	0.48
2:J:1426:ILE:HA	2:J:1429:ASN:OD1	2.13	0.48
2:J:2736:ASP:OD1	2:J:2736:ASP:N	2.42	0.48
2:J:3353:LEU:HG	2:J:3357:HIS:CE1	2.49	0.48
2:J:3573:MET:SD	2:J:3577:ARG:NH2	2.86	0.48
2:J:3991:GLY:O	2:J:3995:VAL:HG23	2.13	0.48
2:B:299:LEU:HD21	2:B:377:ILE:HA	1.96	0.48
2:B:582:HIS:O	2:B:586:ILE:HG13	2.14	0.48
2:B:1089:TYR:CD1	2:B:1152:MET:HG2	2.45	0.48
2:B:1420:ASN:OD1	2:B:1421:ARG:N	2.47	0.48
2:B:2158:CYS:O	2:B:2162:ILE:HG13	2.14	0.48
2:B:3353:LEU:HG	2:B:3357:HIS:CE1	2.49	0.48
2:E:2376:LEU:O	2:E:2380:ILE:HG12	2.13	0.48
2:G:2134:LEU:O	2:G:2138:LEU:HG	2.14	0.48
2:G:2725:LYS:HZ1	2:G:2737:PRO:HA	1.77	0.48
2:G:4651:THR:HG21	2:G:4803:HIS:CD2	2.48	0.48
2:G:4679:ARG:HH21	2:G:5017:ARG:CZ	2.26	0.48
2:J:215:THR:HG22	2:J:273:HIS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1623:ARG:HA	2:J:1623:ARG:NH1	2.28	0.48
2:J:2867:LEU:HB2	2:J:2928:LYS:NZ	2.29	0.48
2:J:3281:LEU:O	2:J:3285:TRP:HB2	2.14	0.48
2:B:215:THR:HG22	2:B:273:HIS:HA	1.96	0.47
2:B:1426:ILE:HA	2:B:1429:ASN:OD1	2.13	0.47
2:B:3044:CYS:SG	2:B:3092:LEU:HB2	2.54	0.47
2:B:3514:LEU:HD12	2:B:3606:LEU:HB2	1.96	0.47
2:B:4679:ARG:NH1	2:B:4715:TYR:OH	2.46	0.47
2:E:630:GLU:HG3	2:E:631:LEU:HD23	1.96	0.47
2:E:3166:TYR:CE1	2:E:3239:MET:HG3	2.49	0.47
2:E:3313:ASN:OD1	2:E:3353:LEU:HD11	2.14	0.47
2:E:4069:LYS:NZ	2:E:4130:ASN:OD1	2.37	0.47
2:G:208:CYS:H	2:G:269:TRP:HH2	1.61	0.47
2:G:582:HIS:O	2:G:586:ILE:HG13	2.14	0.47
2:G:659:TYR:HB2	2:G:1017:ARG:HH22	1.79	0.47
2:G:2869:ARG:NH2	2:G:2947:ASP:H	2.12	0.47
2:J:121:LEU:N	2:J:134:ASP:O	2.45	0.47
2:J:1089:TYR:CD1	2:J:1152:MET:HG2	2.45	0.47
2:J:1154:ASP:HB3	2:J:1157:GLU:HB2	1.95	0.47
2:J:3166:TYR:CE1	2:J:3239:MET:HG3	2.49	0.47
1:I:17:LYS:HG3	1:I:18:LYS:H	1.79	0.47
2:B:630:GLU:HG3	2:B:631:LEU:HD23	1.96	0.47
2:B:2867:LEU:HB2	2:B:2928:LYS:NZ	2.28	0.47
2:B:3051:ARG:NH2	2:B:3102:ASP:HB2	2.30	0.47
2:B:3443:ILE:HG12	2:B:3605:HIS:CD2	2.49	0.47
2:E:404:ILE:HG23	2:E:483:MET:SD	2.54	0.47
2:E:659:TYR:HB2	2:E:1017:ARG:HH22	1.80	0.47
2:E:3044:CYS:SG	2:E:3092:LEU:HB2	2.54	0.47
2:E:3514:LEU:HD12	2:E:3606:LEU:HB2	1.96	0.47
2:E:4749:GLU:HG3	2:E:4753:HIS:NE2	2.29	0.47
2:E:4780:PHE:HA	2:E:4783:ILE:HG22	1.94	0.47
2:G:349:GLN:HE21	2:G:354:GLY:HA2	1.78	0.47
2:G:3044:CYS:SG	2:G:3092:LEU:HB2	2.54	0.47
2:G:4069:LYS:NZ	2:G:4130:ASN:OD1	2.37	0.47
2:J:111:HIS:CE1	2:J:113:HIS:HB3	2.49	0.47
2:J:4780:PHE:HA	2:J:4783:ILE:HG22	1.94	0.47
1:A:17:LYS:HG3	1:A:18:LYS:H	1.79	0.47
2:B:3354:LEU:HG	2:B:3359:ILE:HD11	1.96	0.47
2:B:3970:GLN:NE2	2:B:5004:THR:HA	2.30	0.47
2:E:283:ARG:HE	2:E:288:GLY:HA2	1.80	0.47
2:E:2376:LEU:HD12	2:E:2376:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3970:GLN:NE2	2:E:5004:THR:HA	2.29	0.47
2:G:1274:HIS:HB3	2:G:1277:TRP:HB2	1.97	0.47
2:G:3166:TYR:CE1	2:G:3239:MET:HG3	2.49	0.47
2:G:3991:GLY:O	2:G:3995:VAL:HG23	2.13	0.47
2:J:299:LEU:HD21	2:J:377:ILE:HA	1.96	0.47
2:J:747:CYS:SG	2:J:756:SER:HB2	2.55	0.47
1:D:17:LYS:HG3	1:D:18:LYS:H	1.79	0.47
1:H:17:LYS:HG3	1:H:18:LYS:H	1.79	0.47
2:B:2134:LEU:O	2:B:2138:LEU:HG	2.14	0.47
2:B:2673:HIS:CE1	2:B:2910:THR:HA	2.50	0.47
2:B:2869:ARG:NH2	2:B:2947:ASP:H	2.12	0.47
2:B:3262:ARG:N	2:B:3262:ARG:HD2	2.28	0.47
2:B:3313:ASN:OD1	2:B:3353:LEU:HD11	2.15	0.47
2:E:2788:HIS:NE2	2:E:2805:TYR:OH	2.38	0.47
2:E:3640:PRO:HG2	2:E:3643:ASN:HB2	1.96	0.47
2:G:747:CYS:SG	2:G:756:SER:HB2	2.55	0.47
2:G:818:ARG:NH1	2:G:1027:LEU:O	2.44	0.47
2:G:3970:GLN:NE2	2:G:5004:THR:HA	2.29	0.47
2:J:1735:ILE:HG22	2:J:2142:TYR:HB3	1.95	0.47
2:J:2134:LEU:O	2:J:2138:LEU:HG	2.14	0.47
2:J:3044:CYS:SG	2:J:3092:LEU:HB2	2.54	0.47
2:J:3825:GLU:H	2:J:3825:GLU:CD	2.17	0.47
3:K:71:ARG:HB3	3:K:78:VAL:HG22	1.97	0.47
1:D:26:TYR:HB2	1:D:101:VAL:HG12	1.96	0.47
2:B:4749:GLU:HG3	2:B:4753:HIS:NE2	2.29	0.47
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	1.95	0.47
2:E:582:HIS:O	2:E:586:ILE:HG13	2.14	0.47
2:E:863:LEU:HD22	2:E:867:LEU:HD21	1.95	0.47
2:E:1530:THR:HG23	2:E:1535:GLU:H	1.78	0.47
2:E:2806:ARG:O	2:E:2810:LYS:HG2	2.14	0.47
2:G:111:HIS:CE1	2:G:113:HIS:HB3	2.50	0.47
2:G:1089:TYR:CD1	2:G:1152:MET:HG2	2.45	0.47
2:G:3353:LEU:HG	2:G:3357:HIS:CE1	2.49	0.47
2:G:3475:LYS:HZ1	2:G:3511:VAL:HG21	1.79	0.47
2:J:223:PHE:HA	2:J:230:CYS:HA	1.95	0.47
2:J:2614:ILE:O	2:J:2650:ARG:NH1	2.41	0.47
2:J:2626:LEU:HD22	2:J:2640:PRO:HB3	1.95	0.47
2:E:747:CYS:SG	2:E:756:SER:HB2	2.55	0.47
2:E:870:ILE:O	2:E:874:LEU:HG	2.13	0.47
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.95	0.47
2:E:1274:HIS:HB3	2:E:1277:TRP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1813:ARG:O	2:E:1817:GLU:HG2	2.15	0.47
2:E:2134:LEU:O	2:E:2138:LEU:HG	2.14	0.47
2:E:2515:GLN:CA	2:E:2568:LEU:HD21	2.44	0.47
2:E:2531:ARG:HH12	2:E:2585:THR:HB	1.79	0.47
2:E:3209:GLN:CD	2:E:3209:GLN:H	2.18	0.47
2:G:2673:HIS:CE1	2:G:2910:THR:HA	2.50	0.47
2:G:2799:GLU:O	2:G:2803:GLU:HG2	2.14	0.47
2:G:2806:ARG:O	2:G:2810:LYS:HG2	2.14	0.47
2:J:404:ILE:HG23	2:J:483:MET:SD	2.54	0.47
2:J:487:VAL:O	2:J:491:ILE:HG13	2.15	0.47
2:J:582:HIS:O	2:J:586:ILE:HG13	2.14	0.47
2:J:863:LEU:HD13	2:J:867:LEU:HD21	1.97	0.47
2:J:3051:ARG:NH2	2:J:3102:ASP:HB2	2.30	0.47
2:J:3704:HIS:O	2:J:3708:THR:HG23	2.14	0.47
2:J:4181:ILE:HG22	2:J:4987:ASN:HB3	1.97	0.47
3:F:71:ARG:HB3	3:F:78:VAL:HG22	1.96	0.47
2:B:365:LYS:O	2:B:369:LEU:HG	2.14	0.47
2:B:404:ILE:HG23	2:B:483:MET:SD	2.54	0.47
2:B:1274:HIS:HB3	2:B:1277:TRP:HB2	1.97	0.47
2:B:1623:ARG:HA	2:B:1623:ARG:NH1	2.28	0.47
2:B:2353:VAL:O	2:B:2357:LEU:HG	2.15	0.47
2:B:2782:ASP:N	2:B:2782:ASP:OD1	2.47	0.47
2:B:3209:GLN:CD	2:B:3209:GLN:H	2.18	0.47
2:B:3280:TYR:HE1	2:B:3284:TRP:CD1	2.33	0.47
2:E:111:HIS:CE1	2:E:113:HIS:HB3	2.50	0.47
2:E:2673:HIS:CE1	2:E:2910:THR:HA	2.50	0.47
2:E:2869:ARG:NH2	2:E:2947:ASP:H	2.12	0.47
2:E:3316:LEU:HD11	2:E:3345:ILE:HG23	1.95	0.47
2:E:3353:LEU:HG	2:E:3357:HIS:CE1	2.49	0.47
2:E:3991:GLY:O	2:E:3995:VAL:HG23	2.14	0.47
2:G:283:ARG:HE	2:G:288:GLY:HA2	1.79	0.47
2:G:733:PRO:HG2	2:G:762:CYS:HB3	1.96	0.47
2:G:3354:LEU:HG	2:G:3359:ILE:HD11	1.96	0.47
2:G:3640:PRO:HG2	2:G:3643:ASN:HB2	1.96	0.47
2:G:4211:LYS:O	2:G:4215:ARG:HG3	2.15	0.47
2:J:28:VAL:HG12	2:J:33:LEU:HD23	1.96	0.47
2:J:246:TYR:CD1	2:J:373:LYS:HB3	2.50	0.47
2:J:799:GLU:OE1	2:J:1623:ARG:NH1	2.48	0.47
2:J:1420:ASN:OD1	2:J:1421:ARG:N	2.47	0.47
2:J:2806:ARG:O	2:J:2810:LYS:HG2	2.14	0.47
2:J:2869:ARG:NH2	2:J:2947:ASP:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3280:TYR:HE1	2:J:3284:TRP:CD1	2.33	0.47
2:J:4211:LYS:O	2:J:4215:ARG:HG3	2.15	0.47
2:B:283:ARG:HE	2:B:288:GLY:HA2	1.79	0.47
2:B:2518:LEU:HD21	2:B:2569:PHE:CZ	2.49	0.47
2:B:3965:LEU:HA	2:B:3968:TYR:CD2	2.50	0.47
2:E:20:VAL:HG12	2:E:22:LEU:H	1.80	0.47
2:E:733:PRO:HG2	2:E:762:CYS:HB3	1.96	0.47
2:E:1420:ASN:OD1	2:E:1421:ARG:N	2.47	0.47
2:E:1735:ILE:HG22	2:E:2142:TYR:HB3	1.95	0.47
2:E:2626:LEU:HD22	2:E:2640:PRO:HB3	1.95	0.47
2:E:2718:SER:OG	2:E:2909:ASP:O	2.25	0.47
2:E:3412:LEU:O	2:E:3416:VAL:HG12	2.15	0.47
2:G:20:VAL:HG12	2:G:22:LEU:H	1.80	0.47
2:G:1420:ASN:OD1	2:G:1421:ARG:N	2.47	0.47
2:G:2225:PHE:O	2:G:2229:VAL:HG23	2.15	0.47
2:G:2592:GLY:O	2:G:2600:ARG:NH1	2.48	0.47
2:G:3209:GLN:CD	2:G:3209:GLN:H	2.18	0.47
2:J:733:PRO:HG2	2:J:762:CYS:HB3	1.96	0.47
2:J:3313:ASN:OD1	2:J:3353:LEU:HD11	2.14	0.47
2:J:4749:GLU:HG3	2:J:4753:HIS:NE2	2.29	0.47
2:B:878:ILE:HG21	3:C:107:TRP:NE1	2.30	0.47
2:B:3197:LEU:O	2:B:3201:MET:HB3	2.15	0.47
2:B:3281:LEU:O	2:B:3285:TRP:HB2	2.14	0.47
2:B:3825:GLU:H	2:B:3825:GLU:CD	2.17	0.47
2:E:3825:GLU:H	2:E:3825:GLU:CD	2.17	0.47
2:G:3281:LEU:O	2:G:3285:TRP:HB2	2.14	0.47
2:J:2469:ILE:HA	2:J:2472:LEU:HG	1.97	0.47
2:J:2531:ARG:HH12	2:J:2585:THR:HB	1.79	0.47
2:J:3412:LEU:O	2:J:3416:VAL:HG12	2.15	0.47
2:B:487:VAL:O	2:B:491:ILE:HG13	2.15	0.47
2:B:747:CYS:SG	2:B:756:SER:HB2	2.55	0.47
2:B:2806:ARG:O	2:B:2810:LYS:HG2	2.14	0.47
2:B:3003:LEU:HB2	2:B:3004:PRO:HD3	1.97	0.47
2:B:3366:ARG:NE	2:B:3367:LYS:HD2	2.26	0.47
2:B:4181:ILE:HG22	2:B:4987:ASN:HB3	1.97	0.47
2:E:317:ARG:NH2	2:E:321:GLU:O	2.48	0.47
2:E:863:LEU:HD13	2:E:867:LEU:HD21	1.97	0.47
2:E:3443:ILE:HG12	2:E:3605:HIS:CD2	2.50	0.47
2:G:215:THR:HG22	2:G:273:HIS:HA	1.96	0.47
2:G:1745:ILE:HD11	2:G:1769:THR:HG23	1.97	0.47
2:G:2809:ILE:H	2:G:2809:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2958:GLY:O	2:G:2962:GLN:HG2	2.15	0.47
2:G:3051:ARG:NH2	2:G:3102:ASP:HB2	2.30	0.47
2:G:3316:LEU:HD21	2:G:3345:ILE:HG13	1.97	0.47
2:G:3475:LYS:HD3	2:G:3516:LYS:HZ1	1.80	0.47
2:J:4064:MET:HE1	2:J:4110:PHE:HD2	1.80	0.47
2:B:2225:PHE:O	2:B:2229:VAL:HG23	2.15	0.46
2:E:2576:ALA:HA	2:E:2579:VAL:HB	1.96	0.46
2:G:317:ARG:NH2	2:G:321:GLU:O	2.48	0.46
2:G:487:VAL:O	2:G:491:ILE:HG13	2.15	0.46
2:G:2152:THR:O	2:G:2156:LEU:HG	2.16	0.46
2:G:3825:GLU:H	2:G:3825:GLU:CD	2.17	0.46
2:J:2152:THR:O	2:J:2156:LEU:HG	2.16	0.46
2:J:3246:LEU:HD13	2:J:3280:TYR:CD2	2.49	0.46
2:J:3246:LEU:HD12	2:J:3249:LEU:HD12	1.97	0.46
2:J:3346:VAL:HG21	2:J:3411:LEU:HB3	1.96	0.46
2:B:111:HIS:CE1	2:B:113:HIS:HB3	2.50	0.46
2:B:659:TYR:HB2	2:B:1017:ARG:HH22	1.79	0.46
2:B:2592:GLY:O	2:B:2600:ARG:NH1	2.48	0.46
2:E:28:VAL:HG12	2:E:33:LEU:HD23	1.96	0.46
2:E:642:THR:HG21	2:E:1615:VAL:HG21	1.98	0.46
2:E:799:GLU:OE1	2:E:1623:ARG:NH1	2.48	0.46
2:E:2867:LEU:HB2	2:E:2928:LYS:HZ3	1.80	0.46
2:G:2469:ILE:HA	2:G:2472:LEU:HG	1.97	0.46
2:G:3197:LEU:O	2:G:3201:MET:HB3	2.15	0.46
2:G:3412:LEU:O	2:G:3416:VAL:HG12	2.15	0.46
2:J:1813:ARG:O	2:J:1817:GLU:HG2	2.15	0.46
2:J:3443:ILE:HG12	2:J:3605:HIS:CD2	2.49	0.46
2:J:4675:LYS:HG3	2:J:4715:TYR:HE1	1.80	0.46
1:I:97:LEU:HB3	1:I:99:PHE:CE2	2.51	0.46
2:B:213:TYR:HA	2:B:340:LYS:HA	1.98	0.46
2:B:642:THR:HG21	2:B:1615:VAL:HG21	1.98	0.46
2:E:487:VAL:O	2:E:491:ILE:HG13	2.15	0.46
2:E:2782:ASP:N	2:E:2782:ASP:OD1	2.47	0.46
2:E:4675:LYS:HG3	2:E:4715:TYR:HE1	1.80	0.46
2:G:213:TYR:HA	2:G:340:LYS:HA	1.97	0.46
2:G:799:GLU:OE1	2:G:1623:ARG:NH1	2.48	0.46
2:G:2294:ASP:O	2:G:2298:VAL:HG12	2.16	0.46
2:G:2376:LEU:H	2:G:2376:LEU:HD12	1.79	0.46
2:G:4181:ILE:HG22	2:G:4987:ASN:HB3	1.97	0.46
2:J:1042:ALA:O	2:J:1046:LEU:HG	2.16	0.46
2:J:2294:ASP:O	2:J:2298:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2353:VAL:O	2:J:2357:LEU:HG	2.15	0.46
2:J:3003:LEU:HB2	2:J:3004:PRO:HD3	1.97	0.46
2:J:3354:LEU:HG	2:J:3359:ILE:HD11	1.96	0.46
2:B:4240:ASP:O	2:B:4244:GLU:HG3	2.16	0.46
2:E:2102:VAL:HG13	2:E:2120:MET:HB2	1.97	0.46
2:E:2104:ARG:O	2:E:2108:GLU:HG2	2.16	0.46
2:E:2152:THR:O	2:E:2156:LEU:HG	2.16	0.46
2:E:2765:LYS:HD3	2:E:2765:LYS:HA	1.67	0.46
2:E:3002:LEU:HD23	2:E:3002:LEU:HA	1.81	0.46
2:E:3346:VAL:HG21	2:E:3411:LEU:HB3	1.96	0.46
2:G:19:GLU:HB3	2:G:205:ILE:HD13	1.98	0.46
2:G:863:LEU:HD13	2:G:867:LEU:HD21	1.97	0.46
2:G:1042:ALA:O	2:G:1046:LEU:HG	2.16	0.46
2:G:1669:LEU:O	2:G:1673:VAL:HG22	2.16	0.46
2:G:1813:ARG:O	2:G:1817:GLU:HG2	2.15	0.46
2:G:1964:ARG:HB3	2:G:1968:LYS:NZ	2.30	0.46
2:G:2782:ASP:N	2:G:2782:ASP:OD1	2.47	0.46
2:G:4749:GLU:HG3	2:G:4753:HIS:NE2	2.29	0.46
2:J:283:ARG:HE	2:J:288:GLY:HA2	1.79	0.46
2:J:1153:ILE:HG13	2:J:1160:ILE:HG12	1.97	0.46
2:J:1669:LEU:O	2:J:1673:VAL:HG22	2.16	0.46
2:J:2225:PHE:O	2:J:2229:VAL:HG23	2.15	0.46
2:J:2328:GLY:HA2	2:J:2331:TYR:HD2	1.81	0.46
2:J:2673:HIS:CE1	2:J:2910:THR:HA	2.50	0.46
2:B:882:TRP:O	2:B:885:THR:OG1	2.28	0.46
2:B:1153:ILE:HG13	2:B:1160:ILE:HG12	1.97	0.46
2:B:2328:GLY:HA2	2:B:2331:TYR:HD2	1.81	0.46
2:B:3412:LEU:O	2:B:3416:VAL:HG12	2.15	0.46
2:B:3640:PRO:HG2	2:B:3643:ASN:HB2	1.96	0.46
2:B:4160:LEU:O	2:B:4164:LEU:HG	2.16	0.46
2:B:4211:LYS:O	2:B:4215:ARG:HG3	2.15	0.46
2:E:1669:LEU:O	2:E:1673:VAL:HG22	2.16	0.46
2:E:1745:ILE:HD11	2:E:1769:THR:HG23	1.97	0.46
2:E:2294:ASP:O	2:E:2298:VAL:HG12	2.16	0.46
2:E:2515:GLN:O	2:E:2519:LEU:HG	2.14	0.46
2:E:3051:ARG:NH2	2:E:3102:ASP:HB2	2.30	0.46
2:E:4160:LEU:O	2:E:4164:LEU:HG	2.16	0.46
2:E:4204:GLN:O	2:E:4207:MET:HB2	2.16	0.46
2:G:630:GLU:HG3	2:G:631:LEU:HD23	1.96	0.46
2:G:3514:LEU:HD12	2:G:3606:LEU:HB2	1.96	0.46
2:G:4160:LEU:O	2:G:4164:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4679:ARG:NH1	2:G:4715:TYR:OH	2.49	0.46
2:J:630:GLU:HG3	2:J:631:LEU:HD23	1.96	0.46
2:J:2312:MET:SD	2:J:2312:MET:N	2.79	0.46
2:J:2592:GLY:O	2:J:2600:ARG:NH1	2.48	0.46
2:J:3428:ASN:O	2:J:3432:GLU:HG2	2.16	0.46
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.97	0.46
2:B:247:TYR:CD2	2:B:374:LYS:HB2	2.44	0.46
2:B:317:ARG:NH2	2:B:321:GLU:O	2.48	0.46
2:B:2958:GLY:O	2:B:2962:GLN:HG2	2.15	0.46
2:E:1153:ILE:HG13	2:E:1160:ILE:HG12	1.97	0.46
2:E:1964:ARG:HB3	2:E:1968:LYS:NZ	2.30	0.46
2:E:3548:GLU:HG2	2:E:3552:PHE:CE2	2.51	0.46
2:G:246:TYR:CB	2:G:373:LYS:HD2	2.45	0.46
2:G:478:PHE:HD2	2:G:483:MET:HG3	1.81	0.46
2:G:2328:GLY:HA2	2:G:2331:TYR:HD2	1.81	0.46
2:G:2353:VAL:O	2:G:2357:LEU:HG	2.15	0.46
2:G:2599:GLN:O	2:G:2603:ILE:HG13	2.16	0.46
2:G:4240:ASP:O	2:G:4244:GLU:HG3	2.16	0.46
2:J:642:THR:HG21	2:J:1615:VAL:HG21	1.98	0.46
2:J:1274:HIS:HB3	2:J:1277:TRP:HB2	1.97	0.46
2:J:3197:LEU:O	2:J:3201:MET:HB3	2.15	0.46
2:J:3514:LEU:HD12	2:J:3606:LEU:HB2	1.96	0.46
2:J:4160:LEU:O	2:J:4164:LEU:HG	2.16	0.46
2:B:248:GLU:HA	2:B:372:LEU:CB	2.46	0.46
2:B:799:GLU:OE1	2:B:1623:ARG:NH1	2.48	0.46
2:B:996:TRP:HE1	2:B:1000:ARG:HD2	1.81	0.46
2:B:1745:ILE:HD11	2:B:1769:THR:HG23	1.97	0.46
2:B:1813:ARG:O	2:B:1817:GLU:HG2	2.15	0.46
2:B:1964:ARG:HB3	2:B:1968:LYS:NZ	2.30	0.46
2:B:2376:LEU:HD12	2:B:2376:LEU:H	1.79	0.46
2:B:2531:ARG:HH12	2:B:2585:THR:HB	1.79	0.46
2:B:2696:TYR:HE2	2:B:2997:PHE:HA	1.81	0.46
2:E:996:TRP:HE1	2:E:1000:ARG:HD2	1.81	0.46
2:E:2469:ILE:HA	2:E:2472:LEU:HG	1.97	0.46
2:G:863:LEU:HD13	2:G:867:LEU:HD11	1.98	0.46
2:G:3428:ASN:O	2:G:3432:GLU:HG2	2.16	0.46
2:G:3969:ILE:O	2:G:3970:GLN:C	2.54	0.46
2:J:20:VAL:HG12	2:J:22:LEU:H	1.80	0.46
2:J:659:TYR:HB2	2:J:1017:ARG:HH22	1.79	0.46
2:J:2799:GLU:O	2:J:2803:GLU:HG2	2.14	0.46
2:J:2881:ASN:HA	2:J:2884:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2958:GLY:O	2:J:2962:GLN:HG2	2.15	0.46
2:J:3366:ARG:NE	2:J:3367:LYS:HD2	2.26	0.46
2:J:3405:LEU:HD13	2:J:3451:PHE:HZ	1.81	0.46
3:K:38:ARG:HD3	3:K:48:VAL:HG22	1.98	0.46
2:B:19:GLU:HB3	2:B:205:ILE:HD13	1.98	0.46
2:B:20:VAL:HG12	2:B:22:LEU:H	1.80	0.46
2:B:316:PHE:HE2	2:B:348:VAL:HG22	1.81	0.46
2:B:478:PHE:HD2	2:B:483:MET:HG3	1.81	0.46
2:B:696:PRO:HG2	2:B:1612:PHE:HE2	1.81	0.46
2:B:820:ARG:HG2	2:B:820:ARG:HH11	1.81	0.46
2:B:1042:ALA:O	2:B:1046:LEU:HG	2.16	0.46
2:B:2152:THR:O	2:B:2156:LEU:HG	2.16	0.46
2:B:3346:VAL:HG21	2:B:3411:LEU:HB3	1.96	0.46
2:E:1260:MET:HB2	2:E:1269:CYS:SG	2.56	0.46
2:E:2599:GLN:O	2:E:2603:ILE:HG13	2.16	0.46
2:E:3277:LEU:HD13	2:E:3315:LEU:HD13	1.96	0.46
2:G:404:ILE:HG23	2:G:483:MET:SD	2.54	0.46
2:G:642:THR:HG21	2:G:1615:VAL:HG21	1.98	0.46
2:G:2104:ARG:O	2:G:2108:GLU:HG2	2.16	0.46
2:G:3757:GLU:O	2:G:3761:GLN:HG2	2.16	0.46
2:J:317:ARG:NH2	2:J:321:GLU:O	2.48	0.46
2:J:478:PHE:HD2	2:J:483:MET:HG3	1.81	0.46
2:J:1964:ARG:HB3	2:J:1968:LYS:NZ	2.30	0.46
2:J:3342:ALA:HA	2:J:3345:ILE:HG22	1.98	0.46
2:J:3548:GLU:HG2	2:J:3552:PHE:CE2	2.51	0.46
2:J:3757:GLU:O	2:J:3761:GLN:HG2	2.16	0.46
3:C:71:ARG:HB3	3:C:78:VAL:HG22	1.97	0.46
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.97	0.46
1:H:88:PRO:HB2	2:G:1680:ARG:HH12	1.81	0.46
2:B:863:LEU:HD13	2:B:867:LEU:HD11	1.98	0.46
2:B:1260:MET:HB2	2:B:1269:CYS:SG	2.56	0.46
2:E:2225:PHE:O	2:E:2229:VAL:HG23	2.15	0.46
2:E:2353:VAL:O	2:E:2357:LEU:HG	2.15	0.46
2:E:2696:TYR:HE2	2:E:2997:PHE:HA	1.81	0.46
2:E:2809:ILE:H	2:E:2809:ILE:HD12	1.80	0.46
2:E:2881:ASN:HA	2:E:2884:ASN:HD21	1.81	0.46
2:E:2958:GLY:O	2:E:2962:GLN:HG2	2.15	0.46
2:E:3405:LEU:HD13	2:E:3451:PHE:HZ	1.81	0.46
2:G:231:LEU:O	2:G:260:TRP:NE1	2.40	0.46
2:G:316:PHE:HE2	2:G:348:VAL:HG22	1.81	0.46
2:G:1498:GLY:HA2	2:G:1501:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3003:LEU:HB2	2:G:3004:PRO:HD3	1.97	0.46
2:G:3346:VAL:HG21	2:G:3411:LEU:HB3	1.96	0.46
2:J:960:MET:SD	2:J:960:MET:N	2.75	0.46
2:J:1745:ILE:HD11	2:J:1769:THR:HG23	1.97	0.46
2:J:1927:LEU:HD23	2:J:1939:MET:HE1	1.98	0.46
2:J:2809:ILE:H	2:J:2809:ILE:HD12	1.80	0.46
2:J:3173:TYR:CG	2:J:3243:ILE:HG12	2.51	0.46
2:J:3475:LYS:HZ1	2:J:3511:VAL:HG21	1.80	0.46
2:J:3639:THR:N	2:J:3640:PRO:HD2	2.31	0.46
2:B:3969:ILE:O	2:B:3970:GLN:C	2.55	0.46
2:B:4238:CYS:O	2:B:4242:ILE:HG13	2.16	0.46
2:E:231:LEU:O	2:E:260:TRP:NE1	2.40	0.46
2:E:3197:LEU:O	2:E:3201:MET:HB3	2.15	0.46
2:E:3342:ALA:HA	2:E:3345:ILE:HG22	1.98	0.46
2:E:4112:LEU:HD12	2:E:4112:LEU:HA	1.84	0.46
2:E:4181:ILE:HG22	2:E:4987:ASN:HB3	1.97	0.46
2:E:4856:PHE:O	2:E:4860:ARG:NH2	2.39	0.46
2:G:797:HIS:HA	2:G:1619:ARG:HH22	1.81	0.46
2:G:2607:LEU:HD23	2:G:2607:LEU:HA	1.83	0.46
2:G:3137:LEU:HB3	2:G:3138:PRO:HD3	1.98	0.46
2:G:3313:ASN:OD1	2:G:3353:LEU:HD11	2.14	0.46
2:G:3443:ILE:HG12	2:G:3605:HIS:CD2	2.49	0.46
2:J:2688:HIS:ND1	2:J:2688:HIS:N	2.63	0.46
2:J:3640:PRO:HG2	2:J:3643:ASN:HB2	1.96	0.46
2:J:4240:ASP:O	2:J:4244:GLU:HG3	2.16	0.46
3:M:71:ARG:HB3	3:M:78:VAL:HG22	1.96	0.46
2:B:1669:LEU:O	2:B:1673:VAL:HG22	2.16	0.45
2:B:2104:ARG:O	2:B:2108:GLU:HG2	2.16	0.45
2:B:3034:LYS:O	2:B:3038:MET:HG2	2.16	0.45
2:B:3342:ALA:HA	2:B:3345:ILE:HG22	1.98	0.45
2:B:3475:LYS:HZ1	2:B:3511:VAL:HG21	1.81	0.45
2:E:210:GLU:H	2:E:273:HIS:CE1	2.34	0.45
2:E:818:ARG:NH1	2:E:1027:LEU:O	2.44	0.45
2:E:863:LEU:HD13	2:E:867:LEU:HD11	1.98	0.45
2:E:1042:ALA:O	2:E:1046:LEU:HG	2.16	0.45
2:E:2592:GLY:O	2:E:2600:ARG:NH1	2.48	0.45
2:E:3003:LEU:HB2	2:E:3004:PRO:HD3	1.97	0.45
2:E:3969:ILE:O	2:E:3970:GLN:C	2.55	0.45
2:E:4240:ASP:O	2:E:4244:GLU:HG3	2.16	0.45
2:E:4735:GLU:O	2:E:4739:GLU:HG2	2.17	0.45
2:G:820:ARG:HG2	2:G:820:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:873:LYS:NZ	2:G:947:GLU:OE1	2.48	0.45
2:G:3276:MET:O	2:G:3280:TYR:HB2	2.16	0.45
2:G:3280:TYR:HE1	2:G:3284:TRP:CD1	2.33	0.45
2:G:3554:GLN:O	2:G:3557:LEU:HD23	2.16	0.45
2:G:3639:THR:N	2:G:3640:PRO:HD2	2.31	0.45
2:J:210:GLU:H	2:J:273:HIS:CE1	2.34	0.45
2:J:818:ARG:NH1	2:J:1027:LEU:O	2.44	0.45
2:J:1260:MET:HB2	2:J:1269:CYS:SG	2.56	0.45
2:J:3209:GLN:CD	2:J:3209:GLN:H	2.18	0.45
2:B:210:GLU:H	2:B:273:HIS:CE1	2.35	0.45
2:B:2240:CYS:SG	2:B:2250:MET:HG3	2.57	0.45
2:B:2294:ASP:O	2:B:2298:VAL:HG12	2.16	0.45
2:B:2463:LEU:HD11	2:B:2506:LEU:HD13	1.98	0.45
2:B:2469:ILE:HA	2:B:2472:LEU:HG	1.97	0.45
2:B:2502:MET:HB2	2:B:2502:MET:HE3	1.66	0.45
2:B:2809:ILE:H	2:B:2809:ILE:HD12	1.80	0.45
2:B:2881:ASN:HA	2:B:2884:ASN:HD21	1.81	0.45
2:B:4207:MET:CE	2:B:4208:PRO:HD2	2.46	0.45
2:B:4651:THR:HG21	2:B:4803:HIS:NE2	2.31	0.45
2:E:3157:ILE:HG22	2:E:3162:GLN:OE1	2.16	0.45
2:G:996:TRP:HE1	2:G:1000:ARG:HD2	1.81	0.45
2:G:1153:ILE:HG13	2:G:1160:ILE:HG12	1.97	0.45
2:G:2463:LEU:HD11	2:G:2506:LEU:HD13	1.98	0.45
2:G:2765:LYS:HA	2:G:2765:LYS:HD3	1.67	0.45
2:G:4064:MET:HE1	2:G:4110:PHE:CD2	2.51	0.45
2:G:4856:PHE:O	2:G:4860:ARG:NH2	2.39	0.45
2:J:863:LEU:HD13	2:J:867:LEU:HD11	1.98	0.45
2:J:2104:ARG:O	2:J:2108:GLU:HG2	2.16	0.45
2:J:2463:LEU:HD11	2:J:2506:LEU:HD13	1.98	0.45
2:J:3034:LYS:O	2:J:3038:MET:HG2	2.16	0.45
2:J:3157:ILE:HG22	2:J:3162:GLN:OE1	2.16	0.45
2:J:3244:PRO:HB2	2:J:3248:ARG:HB3	1.98	0.45
2:J:4090:LYS:HG3	2:J:4121:GLU:HB3	1.98	0.45
2:J:4204:GLN:O	2:J:4207:MET:HB2	2.16	0.45
1:H:29:MET:SD	1:H:33:GLY:HA2	2.57	0.45
2:B:292:ALA:HB2	2:B:312:THR:HG22	1.98	0.45
2:B:818:ARG:NH1	2:B:1027:LEU:O	2.44	0.45
2:B:4204:GLN:O	2:B:4207:MET:HB2	2.16	0.45
2:E:372:LEU:HG	2:E:374:LYS:NZ	2.32	0.45
2:E:1089:TYR:CD1	2:E:1152:MET:HG2	2.45	0.45
2:E:3475:LYS:HZ1	2:E:3511:VAL:HG21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3757:GLU:O	2:E:3761:GLN:HG2	2.16	0.45
2:G:878:ILE:HG13	3:M:107:TRP:CZ2	2.50	0.45
2:G:3405:LEU:HD13	2:G:3451:PHE:HZ	1.81	0.45
2:G:3887:PHE:O	2:G:3891:LEU:HG	2.17	0.45
2:G:4238:CYS:O	2:G:4242:ILE:HG13	2.16	0.45
2:J:213:TYR:HA	2:J:340:LYS:HA	1.97	0.45
2:J:3107:VAL:HG12	2:J:3175:LEU:HD11	1.98	0.45
2:J:3140:LEU:HD12	2:J:3140:LEU:O	2.16	0.45
2:J:3887:PHE:O	2:J:3891:LEU:HG	2.17	0.45
3:C:9:GLY:HA3	3:C:123:VAL:HG22	1.99	0.45
1:D:57:LYS:HE2	1:D:57:LYS:HB2	1.75	0.45
2:B:2566:ALA:HA	2:B:2569:PHE:CD2	2.49	0.45
2:B:2599:GLN:O	2:B:2603:ILE:HG13	2.16	0.45
2:B:3137:LEU:HB3	2:B:3138:PRO:HD3	1.98	0.45
2:B:3548:GLU:HG2	2:B:3552:PHE:CE2	2.51	0.45
2:B:3554:GLN:O	2:B:3557:LEU:HD23	2.16	0.45
2:B:4696:ASP:O	2:B:4700:GLN:HG2	2.17	0.45
2:E:213:TYR:HA	2:E:340:LYS:HA	1.97	0.45
2:E:820:ARG:HH11	2:E:820:ARG:HG2	1.81	0.45
2:E:2463:LEU:HD11	2:E:2506:LEU:HD13	1.99	0.45
2:E:3034:LYS:O	2:E:3038:MET:HG2	2.16	0.45
2:E:3140:LEU:HD12	2:E:3140:LEU:O	2.16	0.45
2:E:3475:LYS:HD3	2:E:3516:LYS:HZ1	1.80	0.45
2:E:4064:MET:HE1	2:E:4110:PHE:HD2	1.81	0.45
2:E:4211:LYS:O	2:E:4215:ARG:HG3	2.15	0.45
2:G:3342:ALA:HA	2:G:3345:ILE:HG22	1.98	0.45
2:G:4204:GLN:O	2:G:4207:MET:HB2	2.16	0.45
2:G:4675:LYS:HG3	2:G:4715:TYR:HE1	1.81	0.45
2:J:2240:CYS:SG	2:J:2250:MET:HG3	2.57	0.45
2:J:2696:TYR:HE2	2:J:2997:PHE:HA	1.81	0.45
2:J:2782:ASP:N	2:J:2782:ASP:OD1	2.47	0.45
2:J:3276:MET:O	2:J:3280:TYR:HB2	2.16	0.45
2:J:3927:GLN:HB2	2:J:3992:PHE:CE2	2.52	0.45
1:D:29:MET:SD	1:D:33:GLY:HA2	2.57	0.45
1:I:29:MET:SD	1:I:33:GLY:HA2	2.57	0.45
2:B:863:LEU:HD13	2:B:867:LEU:HD21	1.97	0.45
2:B:1455:PRO:HG3	2:B:1549:PHE:HE1	1.82	0.45
2:B:2568:LEU:C	2:B:2568:LEU:HD23	2.37	0.45
2:B:3140:LEU:HD12	2:B:3140:LEU:O	2.16	0.45
2:B:3276:MET:O	2:B:3280:TYR:HB2	2.16	0.45
2:B:3757:GLU:O	2:B:3761:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4048:LEU:HD22	2:B:4055:VAL:HG21	1.99	0.45
2:B:4064:MET:HE1	2:B:4110:PHE:CD2	2.52	0.45
2:B:4090:LYS:HG3	2:B:4121:GLU:HB3	1.98	0.45
2:B:4735:GLU:O	2:B:4739:GLU:HG2	2.17	0.45
2:B:4744:ASP:HB3	2:B:4747:SER:HB3	1.99	0.45
2:E:3194:LEU:HD21	2:E:3272:ILE:HG23	1.98	0.45
2:E:3887:PHE:O	2:E:3891:LEU:HG	2.17	0.45
2:E:3927:GLN:HB2	2:E:3992:PHE:CE2	2.52	0.45
2:G:226:HIS:CD2	2:G:226:HIS:N	2.85	0.45
2:G:1260:MET:HB2	2:G:1269:CYS:SG	2.56	0.45
2:G:2515:GLN:CA	2:G:2568:LEU:HD11	2.46	0.45
2:J:292:ALA:HB2	2:J:312:THR:HG22	1.98	0.45
2:J:3104:GLU:HA	2:J:3107:VAL:HG22	1.98	0.45
2:J:4207:MET:CE	2:J:4208:PRO:HD2	2.46	0.45
2:J:4651:THR:HG21	2:J:4803:HIS:NE2	2.31	0.45
3:C:38:ARG:HD3	3:C:48:VAL:HG22	1.98	0.45
2:B:1179:PHE:HB2	2:B:1182:ILE:HD11	1.98	0.45
2:B:2102:VAL:HG13	2:B:2120:MET:HB2	1.97	0.45
2:B:3405:LEU:HG	2:B:3409:TYR:CE1	2.51	0.45
2:B:4232:GLU:HG2	2:B:5019:TRP:NE1	2.32	0.45
2:E:226:HIS:CD2	2:E:226:HIS:N	2.85	0.45
2:E:573:GLU:O	2:E:577:ILE:HG22	2.17	0.45
2:E:2240:CYS:SG	2:E:2250:MET:HG3	2.57	0.45
2:E:2688:HIS:ND1	2:E:2688:HIS:N	2.63	0.45
2:E:4207:MET:CE	2:E:4208:PRO:HD2	2.46	0.45
2:E:4720:VAL:O	2:E:4723:LYS:N	2.50	0.45
2:G:2102:VAL:HG13	2:G:2120:MET:HB2	1.97	0.45
2:G:2236:LEU:HD22	2:G:2250:MET:SD	2.57	0.45
2:G:2240:CYS:SG	2:G:2250:MET:HG3	2.57	0.45
2:G:2299:VAL:HG12	2:G:2360:LYS:HD2	1.99	0.45
2:G:2881:ASN:HA	2:G:2884:ASN:HD21	1.81	0.45
2:G:4207:MET:CE	2:G:4208:PRO:HD2	2.46	0.45
2:J:696:PRO:HG2	2:J:1612:PHE:HE2	1.81	0.45
2:J:2262:GLY:O	2:J:2266:GLY:N	2.47	0.45
2:J:4115:SER:HB2	2:J:4123:ILE:HG21	1.98	0.45
2:J:4238:CYS:O	2:J:4242:ILE:HG13	2.16	0.45
1:D:55:VAL:HA	2:E:1784:ALA:HA	1.99	0.45
2:B:873:LYS:NZ	2:B:947:GLU:OE1	2.49	0.45
2:B:1694:LEU:HD11	2:B:1718:ILE:HD11	1.99	0.45
2:B:3428:ASN:O	2:B:3432:GLU:HG2	2.16	0.45
2:B:3639:THR:N	2:B:3640:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4064:MET:HE1	2:B:4110:PHE:HD2	1.81	0.45
2:E:276:TRP:CE2	2:E:339:ILE:HG12	2.52	0.45
2:E:1455:PRO:HG3	2:E:1549:PHE:HE1	1.82	0.45
2:E:4048:LEU:HD22	2:E:4055:VAL:HG21	1.99	0.45
2:E:4064:MET:HE1	2:E:4110:PHE:CD2	2.52	0.45
2:E:4232:GLU:HG2	2:E:5019:TRP:NE1	2.32	0.45
2:E:4238:CYS:O	2:E:4242:ILE:HG13	2.16	0.45
2:G:993:HIS:HE1	2:G:1027:LEU:HD11	1.78	0.45
2:G:1455:PRO:HG3	2:G:1549:PHE:HE1	1.82	0.45
2:G:2503:VAL:HG21	2:G:2526:PHE:HZ	1.82	0.45
2:G:2867:LEU:HB2	2:G:2928:LYS:HZ3	1.82	0.45
2:G:3034:LYS:O	2:G:3038:MET:HG2	2.16	0.45
2:G:3107:VAL:HG12	2:G:3175:LEU:HD11	1.98	0.45
2:G:3316:LEU:HD11	2:G:3345:ILE:HG23	1.99	0.45
2:J:276:TRP:CE2	2:J:339:ILE:HG12	2.52	0.45
2:J:316:PHE:HE2	2:J:348:VAL:HG22	1.81	0.45
2:J:797:HIS:HA	2:J:1619:ARG:HH22	1.81	0.45
2:J:3405:LEU:HG	2:J:3409:TYR:CE1	2.51	0.45
2:J:4064:MET:HE1	2:J:4110:PHE:CD2	2.52	0.45
3:C:68:THR:OG1	3:C:81:GLN:HB3	2.17	0.45
2:B:1214:PHE:CZ	2:B:1225:PRO:HD3	2.52	0.45
2:B:1498:GLY:HA2	2:B:1501:VAL:HG12	1.98	0.45
2:B:2619:LEU:O	2:B:2623:LEU:HG	2.17	0.45
2:B:2725:LYS:NZ	2:B:2736:ASP:O	2.50	0.45
2:E:2012:PHE:CZ	2:E:2031:LEU:HD23	2.52	0.45
2:E:2691:TYR:CD2	2:E:2996:LYS:HD2	2.52	0.45
2:E:3104:GLU:HA	2:E:3107:VAL:HG22	1.98	0.45
2:E:3137:LEU:HB3	2:E:3138:PRO:HD3	1.98	0.45
2:E:3280:TYR:HE1	2:E:3284:TRP:CD1	2.33	0.45
2:E:3639:THR:N	2:E:3640:PRO:HD2	2.31	0.45
2:E:4696:ASP:O	2:E:4700:GLN:HG2	2.17	0.45
2:G:210:GLU:H	2:G:273:HIS:CE1	2.35	0.45
2:G:246:TYR:CD1	2:G:373:LYS:HB3	2.51	0.45
2:G:484:LEU:HD11	2:G:540:PHE:HE1	1.82	0.45
2:G:551:LEU:HD23	2:G:560:ILE:HG13	1.99	0.45
2:G:1179:PHE:HB2	2:G:1182:ILE:HD11	1.99	0.45
2:G:2575:ARG:HH11	2:G:2577:ILE:HG23	1.82	0.45
2:G:4696:ASP:O	2:G:4700:GLN:HG2	2.17	0.45
2:J:484:LEU:HD11	2:J:540:PHE:HE1	1.82	0.45
2:J:551:LEU:HD23	2:J:560:ILE:HG13	1.99	0.45
2:J:1435:TYR:CZ	2:J:1550:PRO:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1575:LEU:HD23	2:J:1575:LEU:HA	1.82	0.45
2:J:2157:GLU:O	2:J:2161:GLN:HG3	2.17	0.45
2:J:2299:VAL:HG12	2:J:2360:LYS:HD2	1.98	0.45
2:J:2599:GLN:O	2:J:2603:ILE:HG13	2.16	0.45
2:J:3377:GLU:HA	2:J:3380:ARG:HG2	1.99	0.45
3:K:68:THR:OG1	3:K:81:GLN:HB3	2.17	0.45
1:A:29:MET:SD	1:A:33:GLY:HA2	2.57	0.45
2:B:35:LEU:HG	2:B:51:PRO:HA	1.98	0.45
2:B:1930:LYS:HD2	2:B:1931:LEU:N	2.32	0.45
2:B:2654:TYR:HB2	2:B:2661:TRP:HE3	1.82	0.45
2:B:2691:TYR:CD2	2:B:2996:LYS:HD2	2.52	0.45
2:E:478:PHE:HD2	2:E:483:MET:HG3	1.81	0.45
2:E:2236:LEU:HD22	2:E:2250:MET:SD	2.57	0.45
2:E:3276:MET:O	2:E:3280:TYR:HB2	2.16	0.45
2:E:3428:ASN:O	2:E:3432:GLU:HG2	2.16	0.45
2:E:4090:LYS:HG3	2:E:4121:GLU:HB3	1.98	0.45
2:E:4115:SER:HB2	2:E:4123:ILE:HG21	1.98	0.45
2:E:4651:THR:HG21	2:E:4803:HIS:NE2	2.31	0.45
2:E:4671:PHE:HD1	2:E:4714:ASN:O	2.00	0.45
2:E:4744:ASP:HB3	2:E:4747:SER:HB3	1.99	0.45
2:E:4959:PHE:CD1	2:E:4985:LEU:HD11	2.52	0.45
2:G:374:LYS:O	2:G:375:LYS:C	2.53	0.45
2:G:489:ASN:OD1	2:G:493:ARG:NH1	2.50	0.45
2:G:2157:GLU:O	2:G:2161:GLN:HG3	2.17	0.45
2:G:3024:VAL:HG13	2:G:3029:GLY:HA2	1.99	0.45
2:G:3377:GLU:HA	2:G:3380:ARG:HG2	1.99	0.45
2:G:3405:LEU:HG	2:G:3409:TYR:CE1	2.52	0.45
2:G:3754:GLU:HG3	2:G:4719:PHE:CZ	2.52	0.45
2:J:35:LEU:HG	2:J:51:PRO:HA	1.98	0.45
2:J:993:HIS:HE1	2:J:1027:LEU:HD11	1.79	0.45
2:J:996:TRP:HE1	2:J:1000:ARG:HD2	1.81	0.45
2:J:1455:PRO:HG3	2:J:1549:PHE:HE1	1.82	0.45
2:J:2102:VAL:HG13	2:J:2120:MET:HB2	1.97	0.45
2:J:3137:LEU:HB3	2:J:3138:PRO:HD3	1.98	0.45
2:J:3194:LEU:HD21	2:J:3272:ILE:HG23	1.98	0.45
3:M:38:ARG:HD3	3:M:48:VAL:HG22	1.98	0.45
2:B:184:THR:HG22	2:B:189:LEU:HD13	1.99	0.45
2:B:797:HIS:HA	2:B:1619:ARG:HH22	1.82	0.45
2:B:876:GLU:HA	2:B:876:GLU:OE1	2.17	0.45
2:B:2688:HIS:ND1	2:B:2688:HIS:N	2.63	0.45
2:B:2960:LEU:HD13	2:B:3038:MET:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:GLU:HB3	2:E:205:ILE:HD13	1.98	0.45
2:E:1694:LEU:HD11	2:E:1718:ILE:HD11	1.99	0.45
2:E:2328:GLY:HA2	2:E:2331:TYR:HD2	1.81	0.45
2:E:3965:LEU:HA	2:E:3968:TYR:CD2	2.52	0.45
2:G:276:TRP:CE2	2:G:339:ILE:HG12	2.51	0.45
2:G:2691:TYR:CD2	2:G:2996:LYS:HD2	2.52	0.45
2:G:2696:TYR:HE2	2:G:2997:PHE:HA	1.81	0.45
2:G:4090:LYS:HG3	2:G:4121:GLU:HB3	1.98	0.45
2:G:4651:THR:HG21	2:G:4803:HIS:NE2	2.31	0.45
2:J:573:GLU:O	2:J:577:ILE:HG22	2.17	0.45
2:J:820:ARG:HG2	2:J:820:ARG:HH11	1.81	0.45
2:J:1214:PHE:CZ	2:J:1225:PRO:HD3	2.52	0.45
2:J:2549:ALA:HA	2:J:2552:ARG:NH1	2.32	0.45
2:J:2672:LEU:HD12	2:J:2672:LEU:HA	1.81	0.45
2:J:2725:LYS:NZ	2:J:2736:ASP:O	2.50	0.45
2:J:2924:GLN:O	2:J:2928:LYS:HG2	2.17	0.45
2:J:3024:VAL:HG13	2:J:3029:GLY:HA2	1.99	0.45
2:J:3316:LEU:HD11	2:J:3345:ILE:HG23	1.99	0.45
2:J:3554:GLN:O	2:J:3557:LEU:HD23	2.16	0.45
3:C:69:ILE:HB	3:C:80:LEU:HD13	1.99	0.45
3:F:38:ARG:HD3	3:F:48:VAL:HG22	1.98	0.45
1:H:5:GLU:HB2	1:H:73:LYS:HE2	1.99	0.44
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.99	0.44
2:E:489:ASN:OD1	2:E:493:ARG:NH1	2.50	0.44
2:E:797:HIS:HA	2:E:1619:ARG:HH22	1.81	0.44
2:E:876:GLU:OE1	2:E:876:GLU:HA	2.17	0.44
2:E:2570:ALA:HA	2:E:2613:TYR:O	2.17	0.44
2:E:2725:LYS:NZ	2:E:2736:ASP:O	2.50	0.44
2:E:3377:GLU:HA	2:E:3380:ARG:HG2	1.99	0.44
2:E:4021:LYS:O	2:E:4025:VAL:HG23	2.17	0.44
2:E:4679:ARG:NH1	2:E:4715:TYR:OH	2.50	0.44
2:G:127:MET:SD	2:G:127:MET:N	2.73	0.44
2:G:292:ALA:HB2	2:G:312:THR:HG22	1.98	0.44
2:G:1214:PHE:CZ	2:G:1225:PRO:HD3	2.52	0.44
2:G:3104:GLU:HA	2:G:3107:VAL:HG22	1.98	0.44
2:G:3140:LEU:HD12	2:G:3140:LEU:O	2.16	0.44
2:G:3865:VAL:HG22	2:G:3867:ASN:H	1.81	0.44
2:G:4048:LEU:HD22	2:G:4055:VAL:HG21	1.99	0.44
2:J:1498:GLY:HA2	2:J:1501:VAL:HG12	1.98	0.44
2:J:2880:GLU:HB2	2:J:2908:TYR:CD2	2.52	0.44
3:F:68:THR:OG1	3:F:81:GLN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:9:GLY:HA3	3:M:123:VAL:HG22	1.99	0.44
1:A:24:VAL:HG12	1:A:102:GLU:O	2.17	0.44
2:B:489:ASN:OD1	2:B:493:ARG:NH1	2.50	0.44
2:B:2012:PHE:CZ	2:B:2031:LEU:HD23	2.52	0.44
2:B:2604:GLU:HG2	2:B:2639:MET:HG3	2.00	0.44
2:B:3107:VAL:HG12	2:B:3175:LEU:HD11	1.98	0.44
2:B:3194:LEU:HD21	2:B:3272:ILE:HG23	1.98	0.44
2:E:525:LEU:O	2:E:529:LEU:HG	2.17	0.44
2:E:1018:ASN:OD1	2:E:1021:LEU:N	2.51	0.44
2:E:1435:TYR:CZ	2:E:1550:PRO:HB3	2.52	0.44
2:E:1930:LYS:HD2	2:E:1931:LEU:N	2.32	0.44
2:E:2549:ALA:HA	2:E:2552:ARG:NH1	2.32	0.44
2:E:2654:TYR:HB2	2:E:2661:TRP:HE3	1.82	0.44
2:E:2924:GLN:O	2:E:2928:LYS:HG2	2.17	0.44
2:E:3397:GLU:O	2:E:3400:VAL:HG12	2.18	0.44
2:E:3405:LEU:HG	2:E:3409:TYR:CE1	2.51	0.44
2:G:35:LEU:HG	2:G:51:PRO:HA	1.98	0.44
2:G:2262:GLY:O	2:G:2266:GLY:N	2.47	0.44
2:G:2858:GLN:HB2	2:G:2859:PRO:HD3	2.00	0.44
2:G:3157:ILE:HG22	2:G:3162:GLN:OE1	2.17	0.44
2:G:3548:GLU:HG2	2:G:3552:PHE:CE2	2.51	0.44
2:G:5017:ARG:NH1	2:G:5019:TRP:HZ2	2.15	0.44
2:J:1694:LEU:HD11	2:J:1718:ILE:HD11	1.99	0.44
2:J:4232:GLU:HG2	2:J:5019:TRP:NE1	2.32	0.44
3:K:69:ILE:HB	3:K:80:LEU:HD13	1.99	0.44
2:B:276:TRP:CE2	2:B:339:ILE:HG12	2.52	0.44
2:B:551:LEU:HD23	2:B:560:ILE:HG13	1.99	0.44
2:B:3887:PHE:O	2:B:3891:LEU:HG	2.17	0.44
2:E:2880:GLU:HB2	2:E:2908:TYR:CD2	2.53	0.44
2:G:696:PRO:HG2	2:G:1612:PHE:HE2	1.81	0.44
2:G:1694:LEU:HD11	2:G:1718:ILE:HD11	1.99	0.44
2:G:1930:LYS:HD2	2:G:1931:LEU:N	2.32	0.44
2:G:2138:LEU:HD12	2:G:3658:LYS:HG3	1.99	0.44
2:G:3567:PRO:O	2:G:3570:ARG:HB3	2.17	0.44
2:G:3731:LYS:NZ	2:G:3735:LEU:HD21	2.32	0.44
2:G:4115:SER:HB2	2:G:4123:ILE:HG21	1.98	0.44
2:J:3051:ARG:HH22	2:J:3102:ASP:HB2	1.83	0.44
3:M:68:THR:OG1	3:M:81:GLN:HB3	2.17	0.44
2:B:3024:VAL:HG13	2:B:3029:GLY:HA2	1.99	0.44
2:B:3377:GLU:HA	2:B:3380:ARG:HG2	1.99	0.44
2:B:3405:LEU:HD13	2:B:3451:PHE:HZ	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3836:MET:HE1	2:B:3915:ILE:HG23	1.99	0.44
2:B:3927:GLN:HB2	2:B:3992:PHE:CE2	2.52	0.44
2:B:4115:SER:HB2	2:B:4123:ILE:HG21	1.98	0.44
2:B:4652:LEU:O	2:B:4656:LEU:HG	2.18	0.44
2:E:696:PRO:HG2	2:E:1612:PHE:HE2	1.81	0.44
2:E:2157:GLU:O	2:E:2161:GLN:HG3	2.17	0.44
2:E:2960:LEU:HD13	2:E:3038:MET:HG3	2.00	0.44
2:G:184:THR:HG22	2:G:189:LEU:HD13	1.99	0.44
2:G:3194:LEU:HD21	2:G:3272:ILE:HG23	1.98	0.44
2:G:3366:ARG:NE	2:G:3367:LYS:HD2	2.26	0.44
2:G:3927:GLN:HB2	2:G:3992:PHE:CE2	2.52	0.44
2:G:5012:LYS:HE2	2:G:5016:GLU:OE2	2.16	0.44
2:J:525:LEU:O	2:J:529:LEU:HG	2.17	0.44
2:J:3971:GLY:O	2:J:3972:PRO:C	2.56	0.44
2:J:4696:ASP:O	2:J:4700:GLN:HG2	2.16	0.44
1:H:98:ILE:HD12	1:H:98:ILE:N	2.33	0.44
2:B:573:GLU:O	2:B:577:ILE:HG22	2.17	0.44
2:B:2503:VAL:HG21	2:B:2526:PHE:HZ	1.82	0.44
2:B:2718:SER:OG	2:B:2909:ASP:O	2.25	0.44
2:B:3157:ILE:HG22	2:B:3162:GLN:OE1	2.17	0.44
2:B:4021:LYS:O	2:B:4025:VAL:HG23	2.18	0.44
2:B:4959:PHE:CD1	2:B:4985:LEU:HD11	2.52	0.44
2:E:292:ALA:HB2	2:E:312:THR:HG22	1.98	0.44
2:E:316:PHE:HE2	2:E:348:VAL:HG22	1.81	0.44
2:E:2672:LEU:HD12	2:E:2672:LEU:HA	1.81	0.44
2:E:3107:VAL:HG12	2:E:3175:LEU:HD11	1.98	0.44
2:E:3874:VAL:HG21	2:E:3950:ASN:ND2	2.33	0.44
2:E:4021:LYS:HD3	2:E:4138:ASP:HB3	2.00	0.44
2:E:4911:LEU:HD23	2:E:4911:LEU:HA	1.85	0.44
2:G:573:GLU:O	2:G:577:ILE:HG22	2.17	0.44
2:G:876:GLU:OE1	2:G:876:GLU:HA	2.17	0.44
2:G:972:LEU:HB2	2:G:1044:ARG:HE	1.83	0.44
2:G:2012:PHE:CZ	2:G:2031:LEU:HD23	2.52	0.44
2:G:4021:LYS:O	2:G:4025:VAL:HG23	2.18	0.44
2:J:2330:ARG:HE	2:J:2330:ARG:HB2	1.68	0.44
2:J:2503:VAL:HG21	2:J:2526:PHE:HZ	1.82	0.44
2:J:3014:CYS:SG	2:J:3074:SER:HB3	2.58	0.44
2:J:3537:LYS:HE2	2:J:3537:LYS:HB3	1.85	0.44
2:J:3731:LYS:NZ	2:J:3735:LEU:HD21	2.32	0.44
2:J:3754:GLU:HG3	2:J:4719:PHE:CZ	2.53	0.44
2:J:4735:GLU:O	2:J:4739:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4959:PHE:CD1	2:J:4985:LEU:HD11	2.52	0.44
1:A:26:TYR:CB	1:A:101:VAL:HG12	2.46	0.44
1:I:98:ILE:N	1:I:98:ILE:HD12	2.32	0.44
2:B:2236:LEU:HD22	2:B:2250:MET:SD	2.57	0.44
2:B:2768:PHE:O	2:B:2772:GLN:HG2	2.18	0.44
2:B:3397:GLU:O	2:B:3400:VAL:HG12	2.18	0.44
2:E:1214:PHE:CZ	2:E:1225:PRO:HD3	2.52	0.44
2:E:2138:LEU:HD12	2:E:3658:LYS:HG3	1.99	0.44
2:E:2449:GLU:O	2:E:2453:ILE:HG12	2.17	0.44
2:G:525:LEU:O	2:G:529:LEU:HG	2.17	0.44
2:G:887:ILE:HD13	2:G:959:TYR:HB3	2.00	0.44
2:G:2359:ARG:HD3	2:G:2359:ARG:HA	1.82	0.44
2:G:2967:MET:CE	2:G:3045:LYS:HB3	2.48	0.44
2:G:3051:ARG:HH22	2:G:3102:ASP:HB2	1.83	0.44
2:J:135:VAL:HG21	2:J:191:VAL:HG22	2.00	0.44
2:J:371:VAL:HG12	2:J:373:LYS:HG2	1.98	0.44
2:J:371:VAL:CG1	2:J:373:LYS:HG2	2.47	0.44
2:J:882:TRP:CD2	3:K:106:PRO:HG3	2.52	0.44
2:J:2012:PHE:CZ	2:J:2031:LEU:HD23	2.52	0.44
2:J:2236:LEU:HD22	2:J:2250:MET:SD	2.57	0.44
2:J:2967:MET:CE	2:J:3045:LYS:HB3	2.48	0.44
2:J:3244:PRO:HG2	2:J:3249:LEU:HD23	1.98	0.44
2:J:3644:LEU:HD12	2:J:3645:PRO:HD2	1.99	0.44
2:J:4048:LEU:HD22	2:J:4055:VAL:HG21	1.99	0.44
2:J:4698:LYS:HE3	2:J:4698:LYS:HB2	1.84	0.44
2:J:4744:ASP:HB3	2:J:4747:SER:HB3	1.99	0.44
1:D:66:MET:HE2	1:D:66:MET:HB3	1.71	0.44
2:B:474:ARG:O	2:B:478:PHE:HD1	2.01	0.44
2:B:920:TYR:HE1	3:C:99:ARG:HE	1.65	0.44
2:B:2575:ARG:O	2:B:2579:VAL:HG23	2.17	0.44
2:B:2880:GLU:HB2	2:B:2908:TYR:CD2	2.53	0.44
2:B:3092:LEU:O	2:B:3095:PHE:HB3	2.18	0.44
2:B:3731:LYS:NZ	2:B:3735:LEU:HD21	2.32	0.44
2:E:35:LEU:HG	2:E:51:PRO:HA	1.98	0.44
2:E:2563:THR:HG22	2:E:2606:CYS:HA	2.00	0.44
2:E:3014:CYS:SG	2:E:3074:SER:HB3	2.58	0.44
2:G:2880:GLU:HB2	2:G:2908:TYR:CD2	2.53	0.44
2:G:3014:CYS:SG	2:G:3074:SER:HB3	2.58	0.44
2:G:3246:LEU:HD13	2:G:3280:TYR:CD2	2.53	0.44
2:J:882:TRP:CZ2	3:K:104:TYR:HB2	2.53	0.44
2:J:3284:TRP:CZ3	2:J:3287:ARG:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3874:VAL:HG21	2:J:3950:ASN:ND2	2.33	0.44
3:F:9:GLY:HA3	3:F:123:VAL:HG22	1.99	0.44
2:B:1018:ASN:OD1	2:B:1021:LEU:N	2.51	0.44
2:B:2157:GLU:O	2:B:2161:GLN:HG3	2.17	0.44
2:B:2788:HIS:NE2	2:B:2805:TYR:OH	2.38	0.44
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.99	0.44
2:E:2503:VAL:HG21	2:E:2526:PHE:HZ	1.82	0.44
2:E:2518:LEU:HD21	2:E:2569:PHE:CZ	2.52	0.44
2:E:2967:MET:CE	2:E:3045:LYS:HB3	2.48	0.44
2:G:2688:HIS:ND1	2:G:2688:HIS:N	2.63	0.44
2:G:2768:PHE:O	2:G:2772:GLN:HG2	2.18	0.44
2:G:2960:LEU:HD13	2:G:3038:MET:HG3	2.00	0.44
2:G:3284:TRP:CZ3	2:G:3287:ARG:HD3	2.53	0.44
2:G:4652:LEU:O	2:G:4656:LEU:HG	2.18	0.44
2:G:4735:GLU:O	2:G:4739:GLU:HG2	2.17	0.44
2:G:4817:ALA:HA	2:G:4823:LEU:HB3	2.00	0.44
2:J:19:GLU:HB3	2:J:205:ILE:HD13	1.98	0.44
2:J:489:ASN:OD1	2:J:493:ARG:NH1	2.50	0.44
2:J:873:LYS:NZ	2:J:947:GLU:OE1	2.48	0.44
2:J:2691:TYR:CD2	2:J:2996:LYS:HD2	2.52	0.44
2:J:3475:LYS:HD3	2:J:3516:LYS:HZ1	1.81	0.44
2:J:4652:LEU:O	2:J:4656:LEU:HG	2.18	0.44
1:H:56:ILE:HG13	1:H:59:PHE:HB2	2.00	0.44
1:I:56:ILE:HG13	1:I:59:PHE:HB2	2.00	0.44
2:B:226:HIS:CD2	2:B:226:HIS:N	2.85	0.44
2:B:2777:TYR:HB2	2:B:2791:LEU:O	2.18	0.44
2:B:2924:GLN:O	2:B:2928:LYS:HG2	2.17	0.44
2:B:3874:VAL:HG21	2:B:3950:ASN:ND2	2.33	0.44
2:B:3996:PHE:HZ	2:B:4019:LEU:HG	1.83	0.44
2:E:2607:LEU:HD23	2:E:2607:LEU:HA	1.83	0.44
2:E:2768:PHE:O	2:E:2772:GLN:HG2	2.18	0.44
2:E:3098:SER:O	2:E:3101:GLU:HG3	2.18	0.44
2:G:135:VAL:HG21	2:G:191:VAL:HG22	2.00	0.44
2:G:1435:TYR:CZ	2:G:1550:PRO:HB3	2.52	0.44
2:G:4671:PHE:HD1	2:G:4714:ASN:O	2.01	0.44
2:J:1433:TYR:CE1	2:J:1578:ALA:HB2	2.53	0.44
2:J:2960:LEU:HD13	2:J:3038:MET:HG3	1.99	0.44
2:J:4021:LYS:O	2:J:4025:VAL:HG23	2.18	0.44
2:J:4069:LYS:NZ	2:J:4130:ASN:OD1	2.37	0.44
2:B:2858:GLN:HB2	2:B:2859:PRO:HD3	2.00	0.43
2:B:3567:PRO:O	2:B:3570:ARG:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD23	2:E:560:ILE:HG13	1.99	0.43
2:E:1179:PHE:HB2	2:E:1182:ILE:HD11	1.99	0.43
2:E:1433:TYR:CE1	2:E:1578:ALA:HB2	2.53	0.43
2:E:1498:GLY:HA2	2:E:1501:VAL:HG12	1.98	0.43
2:G:1121:ALA:HB1	2:G:1123:VAL:HG13	2.01	0.43
2:G:3996:PHE:HZ	2:G:4019:LEU:HG	1.83	0.43
2:G:4744:ASP:HB3	2:G:4747:SER:HB3	1.98	0.43
2:G:4959:PHE:CD1	2:G:4985:LEU:HD11	2.52	0.43
2:J:1815:LEU:HD22	2:J:1845:VAL:HG21	1.99	0.43
2:J:1930:LYS:HD2	2:J:1931:LEU:N	2.32	0.43
2:J:2684:ASP:OD1	2:J:2685:SER:N	2.51	0.43
2:J:2858:GLN:HB2	2:J:2859:PRO:HD3	2.00	0.43
2:J:3567:PRO:O	2:J:3570:ARG:HB3	2.17	0.43
3:K:32:ASN:ND2	3:K:101:PRO:HB3	2.33	0.43
3:M:69:ILE:HB	3:M:80:LEU:HD13	1.99	0.43
1:D:56:ILE:HG13	1:D:59:PHE:HB2	2.00	0.43
2:B:887:ILE:HD13	2:B:959:TYR:HB3	2.00	0.43
2:B:2262:GLY:O	2:B:2266:GLY:N	2.47	0.43
2:B:2967:MET:CE	2:B:3045:LYS:HB3	2.48	0.43
2:B:3014:CYS:SG	2:B:3074:SER:HB3	2.58	0.43
2:B:3414:ARG:NH2	2:B:3474:SER:O	2.51	0.43
2:E:3458:PHE:CE2	2:E:3464:ILE:HG13	2.54	0.43
2:E:3554:GLN:O	2:E:3557:LEU:HD23	2.16	0.43
2:E:4642:ALA:O	2:E:4646:LEU:HD23	2.18	0.43
2:G:663:TYR:CE1	2:G:745:SER:HB3	2.53	0.43
2:G:1000:ARG:NH2	2:G:1003:GLN:HG3	2.34	0.43
2:G:2563:THR:HG22	2:G:2606:CYS:HA	2.00	0.43
2:G:2725:LYS:NZ	2:G:2736:ASP:O	2.50	0.43
2:G:2870[B]:GLU:CD	2:G:2870[B]:GLU:H	2.22	0.43
2:G:3092:LEU:O	2:G:3095:PHE:HB3	2.18	0.43
2:G:4698:LYS:HE3	2:G:4698:LYS:HB2	1.84	0.43
2:J:201:ASN:ND2	2:J:203:ASN:HD21	2.17	0.43
2:J:3594:ARG:NH1	2:J:3597:GLN:OE1	2.34	0.43
2:B:1426:ILE:O	2:B:1430:THR:HB	2.18	0.43
2:B:2138:LEU:HD12	2:B:3658:LYS:HG3	1.99	0.43
2:B:3458:PHE:CE2	2:B:3464:ILE:HG13	2.54	0.43
2:E:201:ASN:ND2	2:E:203:ASN:HD21	2.17	0.43
2:E:972:LEU:HB2	2:E:1044:ARG:HE	1.83	0.43
2:E:1738:LEU:HB2	2:E:2146:PRO:HD3	2.00	0.43
2:E:2604:GLU:HG2	2:E:2639:MET:HG3	2.00	0.43
2:E:2777:TYR:HB2	2:E:2791:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3024:VAL:HG13	2:E:3029:GLY:HA2	1.99	0.43
2:E:3284:TRP:CZ3	2:E:3287:ARG:HD3	2.53	0.43
2:E:3644:LEU:HD12	2:E:3645:PRO:HD2	1.99	0.43
2:E:3731:LYS:NZ	2:E:3735:LEU:HD21	2.32	0.43
2:G:882:TRP:CD2	3:M:106:PRO:HG3	2.53	0.43
2:G:882:TRP:O	2:G:885:THR:OG1	2.28	0.43
2:G:2654:TYR:HB2	2:G:2661:TRP:HE3	1.82	0.43
2:G:2768:PHE:HA	2:G:2771:ILE:HG22	2.00	0.43
2:G:3414:ARG:NH2	2:G:3474:SER:O	2.51	0.43
2:G:3874:VAL:HG21	2:G:3950:ASN:ND2	2.33	0.43
2:J:876:GLU:HA	2:J:876:GLU:OE1	2.17	0.43
2:J:1581:LEU:HD12	2:J:1584:ARG:HE	1.84	0.43
2:J:2449:GLU:O	2:J:2453:ILE:HG12	2.17	0.43
2:J:3996:PHE:HZ	2:J:4019:LEU:HG	1.83	0.43
3:C:32:ASN:OD1	3:C:33:SER:N	2.51	0.43
3:M:32:ASN:ND2	3:M:101:PRO:HB3	2.33	0.43
1:I:5:GLU:HB2	1:I:73:LYS:HE2	2.01	0.43
2:B:1000:ARG:NH2	2:B:1003:GLN:HG3	2.33	0.43
2:B:2449:GLU:O	2:B:2453:ILE:HG12	2.17	0.43
2:B:2878:LEU:HG	2:B:2882:TYR:CZ	2.53	0.43
2:B:3098:SER:O	2:B:3101:GLU:HG3	2.18	0.43
2:B:3284:TRP:CZ3	2:B:3287:ARG:HD3	2.53	0.43
2:B:3644:LEU:HD12	2:B:3645:PRO:HD2	1.99	0.43
2:B:4677:LEU:HD23	2:B:4711:PHE:HE1	1.84	0.43
2:E:2684:ASP:OD1	2:E:2685:SER:N	2.51	0.43
2:E:3567:PRO:O	2:E:3570:ARG:HB3	2.17	0.43
2:G:144:GLU:HG3	2:G:175:SER:HB2	2.01	0.43
2:G:1426:ILE:O	2:G:1430:THR:HB	2.18	0.43
2:G:2449:GLU:O	2:G:2453:ILE:HG12	2.17	0.43
2:G:2573:GLU:HB2	2:G:2615:ARG:HH21	1.82	0.43
2:G:2777:TYR:HB2	2:G:2791:LEU:O	2.18	0.43
2:G:2924:GLN:O	2:G:2928:LYS:HG2	2.17	0.43
2:G:2971:GLN:HA	2:G:2974:ILE:HG12	2.00	0.43
2:G:3644:LEU:HD12	2:G:3645:PRO:HD2	1.99	0.43
2:J:663:TYR:CE1	2:J:745:SER:HB3	2.53	0.43
2:J:1000:ARG:NH2	2:J:1003:GLN:HG3	2.33	0.43
2:J:3397:GLU:O	2:J:3400:VAL:HG12	2.18	0.43
2:J:3414:ARG:NH2	2:J:3474:SER:O	2.51	0.43
2:J:4021:LYS:HD3	2:J:4138:ASP:HB3	2.00	0.43
3:F:62:SER:O	3:F:62:SER:OG	2.24	0.43
3:F:69:ILE:HB	3:F:80:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:85:LEU:HD23	3:K:85:LEU:HA	1.92	0.43
2:B:135:VAL:HG21	2:B:191:VAL:HG22	2.00	0.43
2:B:484:LEU:HD11	2:B:540:PHE:HE1	1.82	0.43
2:B:1097:THR:HG23	2:B:1143:TRP:CD1	2.54	0.43
2:B:1435:TYR:CZ	2:B:1550:PRO:HB3	2.52	0.43
2:B:2299:VAL:HG12	2:B:2360:LYS:HD2	1.98	0.43
2:B:2318:TYR:HA	2:B:2395:PRO:HA	2.01	0.43
2:B:2549:ALA:HA	2:B:2552:ARG:NH1	2.33	0.43
2:B:2575:ARG:HG3	2:B:2578:MET:HG3	2.00	0.43
2:B:2870[B]:GLU:H	2:B:2870[B]:GLU:CD	2.22	0.43
2:B:3222:LYS:HB3	2:B:3226:GLU:HB3	2.00	0.43
2:B:4911:LEU:HD23	2:B:4911:LEU:HA	1.85	0.43
2:E:184:THR:HG22	2:E:189:LEU:HD13	1.99	0.43
2:E:663:TYR:CE1	2:E:745:SER:HB3	2.53	0.43
2:E:1012:ASP:HB3	2:E:1015:ALA:HB3	2.00	0.43
2:E:1575:LEU:HD23	2:E:1575:LEU:HA	1.82	0.43
2:E:2299:VAL:HG12	2:E:2360:LYS:HD2	1.99	0.43
2:E:3051:ARG:HH22	2:E:3102:ASP:HB2	1.83	0.43
2:G:232:THR:HG21	2:G:252:VAL:HG11	2.01	0.43
2:G:1433:TYR:CE1	2:G:1578:ALA:HB2	2.53	0.43
2:G:2604:GLU:HG2	2:G:2639:MET:HG3	2.00	0.43
2:G:2635:GLU:HG3	2:G:2636:PHE:HD2	1.83	0.43
2:G:4642:ALA:O	2:G:4646:LEU:HD23	2.18	0.43
2:J:232:THR:HG21	2:J:252:VAL:HG11	2.01	0.43
2:J:1012:ASP:HB3	2:J:1015:ALA:HB3	2.00	0.43
2:J:1179:PHE:HB2	2:J:1182:ILE:HD11	1.98	0.43
2:J:2318:TYR:HA	2:J:2395:PRO:HA	2.01	0.43
2:J:2768:PHE:O	2:J:2772:GLN:HG2	2.18	0.43
2:J:4112:LEU:HD12	2:J:4112:LEU:HA	1.84	0.43
3:C:64:LYS:N	3:C:64:LYS:HD2	2.33	0.43
3:K:9:GLY:HA3	3:K:123:VAL:HG22	1.99	0.43
3:M:46:GLU:HG3	3:M:62:SER:HB2	2.00	0.43
3:M:64:LYS:HD2	3:M:64:LYS:N	2.33	0.43
2:B:144:GLU:HG3	2:B:175:SER:HB2	2.00	0.43
2:B:972:LEU:HB2	2:B:1044:ARG:HE	1.83	0.43
2:B:1012:ASP:HB3	2:B:1015:ALA:HB3	2.00	0.43
2:B:1121:ALA:HB1	2:B:1123:VAL:HG13	2.00	0.43
2:B:1433:TYR:CE1	2:B:1578:ALA:HB2	2.53	0.43
2:B:1738:LEU:HB2	2:B:2146:PRO:HD3	2.00	0.43
2:B:2515:GLN:O	2:B:2519:LEU:HG	2.19	0.43
2:B:3104:GLU:HA	2:B:3107:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4720:VAL:O	2:B:4724:VAL:HG23	2.19	0.43
2:E:484:LEU:HD11	2:E:540:PHE:HE1	1.82	0.43
2:E:978:THR:O	2:E:982:THR:HG23	2.19	0.43
2:E:993:HIS:HE1	2:E:1027:LEU:HD11	1.78	0.43
2:E:2318:TYR:HA	2:E:2395:PRO:HA	2.01	0.43
2:E:2573:GLU:HA	2:E:2576:ALA:HB2	1.99	0.43
2:E:2870[B]:GLU:H	2:E:2870[B]:GLU:CD	2.22	0.43
2:E:3996:PHE:HZ	2:E:4019:LEU:HG	1.83	0.43
2:G:201:ASN:ND2	2:G:203:ASN:HD21	2.17	0.43
2:G:1496:TRP:CE2	2:G:1498:GLY:HA3	2.54	0.43
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.99	0.43
2:G:2223:ILE:HG21	2:G:2229:VAL:HG21	2.00	0.43
2:G:2867:LEU:HD23	2:G:2868:SER:O	2.18	0.43
2:J:245:VAL:HG13	2:J:376:ALA:HB3	2.01	0.43
2:J:2138:LEU:HD12	2:J:3658:LYS:HG3	1.99	0.43
2:J:2223:ILE:HG21	2:J:2229:VAL:HG21	2.01	0.43
3:F:64:LYS:N	3:F:64:LYS:HD2	2.33	0.43
2:B:119:SER:HA	2:B:146:CYS:HA	2.00	0.43
2:B:2684:ASP:OD1	2:B:2685:SER:N	2.51	0.43
2:B:2768:PHE:HA	2:B:2771:ILE:HG22	2.00	0.43
2:B:3417:ASP:OD1	2:B:3516:LYS:HG2	2.19	0.43
2:E:144:GLU:HG3	2:E:175:SER:HB2	2.01	0.43
2:E:2502:MET:HE3	2:E:2502:MET:HB2	1.66	0.43
2:E:2878:LEU:HG	2:E:2882:TYR:CZ	2.53	0.43
2:E:3836:MET:HE1	2:E:3915:ILE:HG23	2.00	0.43
2:E:4652:LEU:O	2:E:4656:LEU:HG	2.18	0.43
2:G:878:ILE:HG21	3:M:107:TRP:HE1	1.83	0.43
2:G:1097:THR:HG23	2:G:1143:TRP:CD1	2.54	0.43
2:G:2318:TYR:HA	2:G:2395:PRO:HA	2.01	0.43
2:G:2878:LEU:HG	2:G:2882:TYR:CZ	2.53	0.43
2:G:4021:LYS:HD3	2:G:4138:ASP:HB3	2.00	0.43
2:J:184:THR:HG22	2:J:189:LEU:HD13	1.99	0.43
2:J:1115:LEU:HD23	2:J:1123:VAL:HG11	2.01	0.43
2:J:2589:LEU:HD23	2:J:2589:LEU:HA	1.87	0.43
2:J:2635:GLU:HG3	2:J:2636:PHE:HD2	1.83	0.43
2:J:2654:TYR:HB2	2:J:2661:TRP:HE3	1.82	0.43
2:J:2768:PHE:HA	2:J:2771:ILE:HG22	2.00	0.43
2:J:2878:LEU:HG	2:J:2882:TYR:CZ	2.53	0.43
2:J:3206:LEU:HD13	2:J:3246:LEU:N	2.34	0.43
2:J:3458:PHE:CE2	2:J:3464:ILE:HG13	2.54	0.43
2:J:4888:TYR:O	2:J:4892:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LEU:O	3:C:62:SER:HB3	2.19	0.43
1:I:55:VAL:HA	2:J:1784:ALA:HA	2.00	0.43
2:B:525:LEU:O	2:B:529:LEU:HG	2.17	0.43
2:B:663:TYR:CE1	2:B:745:SER:HB3	2.53	0.43
2:B:867:LEU:O	2:B:871:ARG:HB3	2.19	0.43
2:B:2672:LEU:HD12	2:B:2672:LEU:HA	1.81	0.43
2:B:4642:ALA:O	2:B:4646:LEU:HD23	2.19	0.43
2:E:245:VAL:HG13	2:E:376:ALA:HB3	2.01	0.43
2:E:2858:GLN:HB2	2:E:2859:PRO:HD3	1.99	0.43
2:E:3354:LEU:HD11	2:E:3434:LEU:HD22	2.01	0.43
2:E:3414:ARG:NH2	2:E:3474:SER:O	2.51	0.43
2:G:882:TRP:CZ2	3:M:104:TYR:HB2	2.54	0.43
2:G:2003:GLN:NE2	2:G:3863:GLY:HA3	2.34	0.43
2:G:2549:ALA:HA	2:G:2552:ARG:NH1	2.32	0.43
2:G:2575:ARG:NH1	2:G:2577:ILE:HG23	2.34	0.43
2:G:3354:LEU:HD11	2:G:3434:LEU:HD22	2.01	0.43
2:G:3458:PHE:CE2	2:G:3464:ILE:HG13	2.54	0.43
2:J:867:LEU:O	2:J:871:ARG:HB3	2.19	0.43
2:J:1496:TRP:CE2	2:J:1498:GLY:HA3	2.54	0.43
2:J:2867:LEU:HD23	2:J:2868:SER:O	2.18	0.43
2:J:2971:GLN:HA	2:J:2974:ILE:HG12	2.00	0.43
2:J:3098:SER:O	2:J:3101:GLU:HG3	2.18	0.43
2:J:3222:LYS:HD2	2:J:3226:GLU:CD	2.39	0.43
2:J:3222:LYS:HB3	2:J:3226:GLU:HB3	2.00	0.43
2:J:4817:ALA:HA	2:J:4823:LEU:HB3	2.00	0.43
1:D:98:ILE:N	1:D:98:ILE:HD12	2.34	0.43
1:H:7:ILE:HD12	1:H:71:ARG:HG2	2.01	0.43
2:B:131:LEU:HD13	2:B:195:PHE:HD2	1.84	0.43
2:B:1092:PHE:HE2	2:B:1100:MET:HE3	1.84	0.43
2:B:1694:LEU:HD13	2:B:1715:LEU:HD12	2.01	0.43
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	2.00	0.43
2:B:2206:THR:O	2:B:2210:VAL:HG23	2.19	0.43
2:B:2765:LYS:NZ	2:B:2860:PRO:HA	2.34	0.43
2:B:2996:LYS:O	2:B:3000:LYS:HG2	2.19	0.43
2:B:4021:LYS:HD3	2:B:4138:ASP:HB3	2.00	0.43
2:B:4846:VAL:O	2:B:4850:LEU:HG	2.19	0.43
2:E:135:VAL:HG21	2:E:191:VAL:HG22	2.00	0.43
2:E:474:ARG:O	2:E:478:PHE:HD1	2.01	0.43
2:E:1121:ALA:HB1	2:E:1123:VAL:HG13	2.00	0.43
2:E:1426:ILE:O	2:E:1430:THR:HB	2.18	0.43
2:E:1581:LEU:HD12	2:E:1584:ARG:HE	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3367:LYS:O	2:E:3371:LYS:HG2	2.19	0.43
2:E:3754:GLU:HG3	2:E:4719:PHE:CZ	2.54	0.43
2:E:3989:VAL:HG13	2:E:4023:MET:HE2	2.01	0.43
2:G:796:ARG:HD3	2:G:1619:ARG:HH12	1.84	0.43
2:G:1012:ASP:HB3	2:G:1015:ALA:HB3	2.00	0.43
2:G:1115:LEU:HD23	2:G:1123:VAL:HG11	2.01	0.43
2:G:2765:LYS:NZ	2:G:2860:PRO:HA	2.34	0.43
2:G:3222:LYS:HD2	2:G:3226:GLU:CD	2.39	0.43
2:G:3346:VAL:HB	2:G:3411:LEU:HD22	2.01	0.43
2:G:3397:GLU:O	2:G:3400:VAL:HG12	2.18	0.43
2:J:2563:THR:HG22	2:J:2606:CYS:HA	2.00	0.43
2:J:2870[B]:GLU:H	2:J:2870[B]:GLU:CD	2.22	0.43
2:J:3511:VAL:HG12	2:J:3515:LYS:HD2	2.01	0.43
2:J:4679:ARG:NH1	2:J:4715:TYR:OH	2.51	0.43
3:C:32:ASN:ND2	3:C:101:PRO:HB3	2.33	0.43
3:M:32:ASN:OD1	3:M:33:SER:N	2.51	0.43
1:A:88:PRO:HB2	2:B:1680:ARG:HH12	1.84	0.43
2:B:294:THR:N	2:B:298:GLY:O	2.39	0.43
2:B:878:ILE:HG13	3:C:107:TRP:HZ2	1.84	0.43
2:B:3511:VAL:HG12	2:B:3515:LYS:HD2	2.01	0.43
2:E:232:THR:HG21	2:E:252:VAL:HG11	2.01	0.43
2:E:786:GLY:H	2:E:1631:GLN:HA	1.84	0.43
2:E:873:LYS:NZ	2:E:947:GLU:OE1	2.48	0.43
2:E:3222:LYS:HB3	2:E:3226:GLU:HB3	2.00	0.43
2:E:3878:ASP:OD1	2:E:3878:ASP:N	2.52	0.43
2:E:4817:ALA:HA	2:E:4823:LEU:HB3	2.00	0.43
2:G:474:ARG:O	2:G:478:PHE:HD1	2.01	0.43
2:G:1152:MET:HE2	2:G:1161:ILE:HB	2.01	0.43
2:G:2159:LEU:O	2:G:2163:ARG:HG3	2.19	0.43
2:G:2515:GLN:O	2:G:2519:LEU:HG	2.19	0.43
2:G:2684:ASP:OD1	2:G:2685:SER:N	2.51	0.43
2:G:3511:VAL:HG12	2:G:3515:LYS:HD2	2.01	0.43
2:G:4677:LEU:HD23	2:G:4711:PHE:HE1	1.84	0.43
2:G:4888:TYR:O	2:G:4892:ARG:HD3	2.18	0.43
2:J:707:VAL:HG23	2:J:782:SER:OG	2.19	0.43
2:J:887:ILE:HD13	2:J:959:TYR:HB3	2.00	0.43
2:J:979:PRO:O	2:J:983:THR:HG23	2.19	0.43
2:J:1018:ASN:OD1	2:J:1021:LEU:N	2.51	0.43
2:J:1738:LEU:HB2	2:J:2146:PRO:HD3	2.00	0.43
2:J:2604:GLU:HG2	2:J:2639:MET:HG3	2.00	0.43
2:J:3354:LEU:HD11	2:J:3434:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:32:ASN:OD1	3:F:33:SER:N	2.51	0.43
3:F:46:GLU:HG3	3:F:62:SER:HB2	2.00	0.43
3:F:47:LEU:O	3:F:62:SER:HB3	2.19	0.43
3:K:64:LYS:N	3:K:64:LYS:HD2	2.33	0.43
2:B:232:THR:HG21	2:B:252:VAL:HG11	2.01	0.42
2:B:993:HIS:HE1	2:B:1027:LEU:HD11	1.78	0.42
2:B:2618:MET:SD	2:B:2618:MET:N	2.91	0.42
2:B:3051:ARG:HH22	2:B:3102:ASP:HB2	1.83	0.42
2:B:3222:LYS:HD2	2:B:3226:GLU:CD	2.39	0.42
2:B:3346:VAL:HB	2:B:3411:LEU:HD22	2.01	0.42
2:B:3354:LEU:HD11	2:B:3434:LEU:HD22	2.01	0.42
2:E:887:ILE:HD13	2:E:959:TYR:HB3	2.00	0.42
2:E:1432:THR:HG23	2:E:1572:ILE:HG23	2.01	0.42
2:E:2867:LEU:HD23	2:E:2868:SER:O	2.18	0.42
2:E:4846:VAL:O	2:E:4850:LEU:HG	2.19	0.42
2:G:786:GLY:H	2:G:1631:GLN:HA	1.84	0.42
2:G:1018:ASN:OD1	2:G:1021:LEU:N	2.51	0.42
2:G:2206:THR:O	2:G:2210:VAL:HG23	2.19	0.42
2:G:2230:THR:HG22	2:G:2234:ARG:HH11	1.83	0.42
2:G:3367:LYS:O	2:G:3371:LYS:HG2	2.19	0.42
2:G:4232:GLU:HG2	2:G:5019:TRP:NE1	2.34	0.42
2:G:4818:MET:N	2:G:4818:MET:SD	2.92	0.42
2:J:978:THR:O	2:J:982:THR:HG23	2.19	0.42
2:J:1097:THR:HG23	2:J:1143:TRP:CD1	2.54	0.42
2:J:2515:GLN:O	2:J:2519:LEU:HG	2.19	0.42
2:J:2777:TYR:HB2	2:J:2791:LEU:O	2.18	0.42
2:J:3521:GLY:HA2	2:J:3524:MET:SD	2.59	0.42
2:J:4642:ALA:O	2:J:4646:LEU:HD23	2.19	0.42
3:K:47:LEU:O	3:K:62:SER:HB3	2.19	0.42
2:B:1432:THR:HG23	2:B:1572:ILE:HG23	2.01	0.42
2:B:4014:LYS:HG2	2:B:4135:PRO:HB3	2.01	0.42
2:B:4805:ASN:HB3	2:B:4808:PHE:CD2	2.54	0.42
2:E:248:GLU:O	2:E:372:LEU:HD23	2.19	0.42
2:E:424:LYS:HE2	2:E:424:LYS:HB2	1.92	0.42
2:E:468:LEU:O	2:E:472:ARG:HG2	2.19	0.42
2:E:979:PRO:O	2:E:983:THR:HG23	2.19	0.42
2:E:2768:PHE:HA	2:E:2771:ILE:HG22	2.00	0.42
2:E:3511:VAL:HG12	2:E:3515:LYS:HD2	2.01	0.42
2:G:1694:LEU:HD13	2:G:1715:LEU:HD12	2.01	0.42
2:G:3098:SER:O	2:G:3101:GLU:HG3	2.18	0.42
2:G:3157:ILE:HG23	2:G:3165:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:144:GLU:HG3	2:J:175:SER:HB2	2.01	0.42
2:J:275:ARG:HB3	2:J:278:GLN:HB2	2.01	0.42
2:J:3367:LYS:O	2:J:3371:LYS:HG2	2.19	0.42
2:J:4818:MET:N	2:J:4818:MET:SD	2.92	0.42
2:B:978:THR:O	2:B:982:THR:HG23	2.19	0.42
2:B:979:PRO:O	2:B:983:THR:HG23	2.19	0.42
2:B:2654:TYR:HB2	2:B:2661:TRP:CE3	2.55	0.42
2:B:2867:LEU:HD23	2:B:2868:SER:O	2.18	0.42
2:E:349:GLN:HB2	2:E:356:TRP:CZ3	2.54	0.42
2:E:2765:LYS:NZ	2:E:2860:PRO:HA	2.34	0.42
2:E:2971:GLN:HA	2:E:2974:ILE:HG12	2.00	0.42
2:E:3092:LEU:O	2:E:3095:PHE:HB3	2.18	0.42
2:E:4818:MET:N	2:E:4818:MET:SD	2.92	0.42
2:G:131:LEU:HD13	2:G:195:PHE:HD2	1.84	0.42
2:G:978:THR:O	2:G:982:THR:HG23	2.19	0.42
2:G:2312:MET:CE	2:G:2312:MET:H	2.32	0.42
2:G:2359:ARG:O	2:G:2361:PRO:HD3	2.19	0.42
2:G:2575:ARG:O	2:G:2578:MET:HG3	2.19	0.42
2:G:3521:GLY:HA2	2:G:3524:MET:SD	2.60	0.42
2:J:2159:LEU:O	2:J:2163:ARG:HG3	2.19	0.42
2:J:2765:LYS:NZ	2:J:2860:PRO:HA	2.34	0.42
3:K:53:SER:H	3:K:53:SER:HG	1.62	0.42
1:D:88:PRO:HB2	2:E:1680:ARG:HH12	1.84	0.42
2:B:182:LEU:HD13	2:B:198:THR:HG21	2.02	0.42
2:B:535:ALA:O	2:B:539:LEU:HG	2.19	0.42
2:B:707:VAL:HG23	2:B:782:SER:OG	2.19	0.42
2:B:1581:LEU:HD12	2:B:1584:ARG:HE	1.84	0.42
2:B:2312:MET:H	2:B:2312:MET:CE	2.32	0.42
2:B:2359:ARG:O	2:B:2361:PRO:HD3	2.19	0.42
2:E:371:VAL:HG12	2:E:373:LYS:H	1.85	0.42
2:E:372:LEU:HD12	2:E:372:LEU:HA	1.81	0.42
2:E:548:VAL:HA	2:E:551:LEU:HG	2.02	0.42
2:E:707:VAL:HG23	2:E:782:SER:OG	2.19	0.42
2:E:2654:TYR:HB2	2:E:2661:TRP:CE3	2.55	0.42
2:E:2790:MET:O	2:E:2792:ARG:NE	2.52	0.42
2:E:4888:TYR:O	2:E:4892:ARG:HD3	2.18	0.42
2:G:275:ARG:HB3	2:G:278:GLN:HB2	2.01	0.42
2:G:548:VAL:HA	2:G:551:LEU:HG	2.02	0.42
2:G:3222:LYS:HB3	2:G:3226:GLU:HB3	2.00	0.42
2:G:4232:GLU:HG2	2:G:5019:TRP:HE1	1.84	0.42
2:J:226:HIS:CD2	2:J:226:HIS:N	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:535:ALA:O	2:J:539:LEU:HG	2.19	0.42
2:J:1931:LEU:HD22	2:J:1935:VAL:HG11	2.00	0.42
2:J:2206:THR:O	2:J:2210:VAL:HG23	2.19	0.42
2:J:2351:ASN:O	2:J:2355:ARG:HG3	2.19	0.42
3:K:46:GLU:HG3	3:K:62:SER:HB2	2.00	0.42
3:M:63:VAL:HA	3:M:67:PHE:HE2	1.85	0.42
2:B:468:LEU:O	2:B:472:ARG:HG2	2.19	0.42
2:B:2159:LEU:O	2:B:2163:ARG:HG3	2.19	0.42
2:B:2971:GLN:HA	2:B:2974:ILE:HG12	2.00	0.42
2:B:3316:LEU:HD11	2:B:3345:ILE:HG23	2.01	0.42
2:B:3367:LYS:O	2:B:3371:LYS:HG2	2.19	0.42
2:B:4818:MET:N	2:B:4818:MET:SD	2.92	0.42
2:B:4888:TYR:O	2:B:4892:ARG:HD3	2.18	0.42
2:E:14:LEU:HD13	2:E:202:MET:HG2	2.02	0.42
2:E:943:ASP:HB2	2:E:946:ALA:HB3	2.02	0.42
2:E:1000:ARG:NH2	2:E:1003:GLN:HG3	2.33	0.42
2:E:1261:ASP:N	2:E:1261:ASP:OD1	2.53	0.42
2:E:1931:LEU:HD22	2:E:1935:VAL:HG11	2.00	0.42
2:E:2351:ASN:O	2:E:2355:ARG:HG3	2.20	0.42
2:G:707:VAL:HG23	2:G:782:SER:OG	2.19	0.42
2:G:867:LEU:O	2:G:871:ARG:HB3	2.19	0.42
2:G:1738:LEU:HB2	2:G:2146:PRO:HD3	2.00	0.42
2:G:1757:ALA:O	2:G:1759:ARG:HD2	2.20	0.42
2:G:2541:PHE:N	2:G:2541:PHE:CD1	2.87	0.42
2:G:2801:ASP:HA	2:G:2804:ILE:HG12	2.01	0.42
2:J:548:VAL:HG21	2:J:582:HIS:CD2	2.52	0.42
2:J:972:LEU:HB2	2:J:1044:ARG:HE	1.83	0.42
2:J:1757:ALA:O	2:J:1759:ARG:HD2	2.20	0.42
2:J:3007:ASN:OD1	2:J:3070:ILE:HG13	2.19	0.42
2:J:3092:LEU:O	2:J:3095:PHE:HB3	2.18	0.42
3:F:32:ASN:ND2	3:F:101:PRO:HB3	2.33	0.42
1:H:17:LYS:HG3	1:H:18:LYS:N	2.35	0.42
2:B:201:ASN:ND2	2:B:203:ASN:HD21	2.17	0.42
2:B:943:ASP:HB2	2:B:946:ALA:HB3	2.02	0.42
2:B:1496:TRP:CE2	2:B:1498:GLY:HA3	2.54	0.42
2:B:2725:LYS:HE3	2:B:2735:PHE:CE1	2.55	0.42
2:B:2902:HIS:CG	2:B:2903:PRO:HD2	2.55	0.42
2:B:3157:ILE:HG23	2:B:3165:CYS:SG	2.59	0.42
2:B:3343:GLN:HB3	2:B:3344:PRO:HD3	2.02	0.42
2:B:4817:ALA:HA	2:B:4823:LEU:HB3	2.00	0.42
2:E:131:LEU:HD13	2:E:195:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:182:LEU:HD13	2:E:198:THR:HG21	2.02	0.42
2:E:535:ALA:O	2:E:539:LEU:HG	2.19	0.42
2:E:657:THR:HB	2:E:1021:LEU:HG	2.02	0.42
2:E:1115:LEU:HD23	2:E:1123:VAL:HG11	2.01	0.42
2:E:2165:LEU:HD11	2:E:2177:LEU:HB3	2.02	0.42
2:E:2173:GLN:O	2:E:2177:LEU:HD23	2.20	0.42
2:E:2223:ILE:HG21	2:E:2229:VAL:HG21	2.00	0.42
2:E:2359:ARG:O	2:E:2361:PRO:HD3	2.19	0.42
2:E:2640:PRO:O	2:E:2644:LEU:HD23	2.20	0.42
2:E:3417:ASP:OD1	2:E:3516:LYS:HG2	2.19	0.42
2:E:4852:THR:HG22	2:E:4886:HIS:CG	2.55	0.42
2:G:1432:THR:HG23	2:G:1572:ILE:HG23	2.02	0.42
2:J:131:LEU:HD13	2:J:195:PHE:HD2	1.84	0.42
2:J:468:LEU:O	2:J:472:ARG:HG2	2.19	0.42
2:J:474:ARG:O	2:J:478:PHE:HD1	2.01	0.42
2:J:943:ASP:HB2	2:J:946:ALA:HB3	2.02	0.42
2:J:1426:ILE:O	2:J:1430:THR:HB	2.19	0.42
2:J:1432:THR:HG23	2:J:1572:ILE:HG23	2.01	0.42
2:J:2996:LYS:O	2:J:3000:LYS:HG2	2.19	0.42
2:J:4060:LYS:HA	2:J:4063:ASP:OD2	2.20	0.42
2:J:4805:ASN:HB3	2:J:4808:PHE:CD2	2.54	0.42
2:J:4852:THR:HG22	2:J:4886:HIS:CG	2.55	0.42
3:F:83:ASN:OD1	3:F:83:ASN:N	2.53	0.42
3:K:32:ASN:OD1	3:K:33:SER:N	2.51	0.42
1:I:17:LYS:HG3	1:I:18:LYS:N	2.35	0.42
2:B:14:LEU:HD13	2:B:202:MET:HG2	2.02	0.42
2:B:786:GLY:H	2:B:1631:GLN:HA	1.84	0.42
2:B:796:ARG:HD3	2:B:1619:ARG:HH12	1.84	0.42
2:B:2173:GLN:O	2:B:2177:LEU:HD23	2.20	0.42
2:B:2598:ALA:O	2:B:2602:VAL:HG23	2.20	0.42
2:B:2640:PRO:O	2:B:2644:LEU:HD23	2.20	0.42
2:B:3154:ASP:N	2:B:3154:ASP:OD1	2.53	0.42
2:E:867:LEU:O	2:E:871:ARG:HB3	2.19	0.42
2:E:1496:TRP:CE2	2:E:1498:GLY:HA3	2.54	0.42
2:E:2725:LYS:HE3	2:E:2735:PHE:CE1	2.55	0.42
2:E:2765:LYS:HZ2	2:E:2860:PRO:HA	1.85	0.42
2:E:3154:ASP:OD1	2:E:3154:ASP:N	2.53	0.42
2:G:245:VAL:HG13	2:G:376:ALA:HB3	2.01	0.42
2:G:2640:PRO:O	2:G:2644:LEU:HD23	2.20	0.42
2:G:2996:LYS:O	2:G:3000:LYS:HG2	2.19	0.42
2:J:119:SER:HA	2:J:146:CYS:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:461:HIS:HA	2:J:464:LYS:HE3	2.02	0.42
2:J:551:LEU:HD11	2:J:564:LEU:HD22	2.02	0.42
2:J:2312:MET:H	2:J:2312:MET:CE	2.31	0.42
2:J:2541:PHE:N	2:J:2541:PHE:CD1	2.87	0.42
2:J:3538:THR:OG1	2:J:3539:ARG:NH1	2.53	0.42
1:A:98:ILE:N	1:A:98:ILE:HD12	2.34	0.42
2:B:144:GLU:OE2	2:G:2452:ARG:HD2	2.20	0.42
2:B:245:VAL:HG13	2:B:376:ALA:HB3	2.01	0.42
2:B:883:ALA:O	2:B:887:ILE:HG13	2.20	0.42
2:B:2292:GLU:H	2:B:2292:GLU:CD	2.21	0.42
2:B:2664:PHE:CD1	2:B:2664:PHE:N	2.88	0.42
2:B:3002:LEU:HD23	2:B:3002:LEU:HA	1.81	0.42
2:B:3567:PRO:CB	2:B:3570:ARG:HH21	2.32	0.42
2:B:3735:LEU:O	2:B:3740:GLU:N	2.53	0.42
2:B:4677:LEU:HD12	2:B:4677:LEU:HA	1.91	0.42
2:E:1097:THR:HG23	2:E:1143:TRP:CD1	2.54	0.42
2:E:1694:LEU:HD13	2:E:1715:LEU:HD12	2.01	0.42
2:E:2122:SER:O	2:E:2126:ARG:HG3	2.20	0.42
2:E:2159:LEU:O	2:E:2163:ARG:HG3	2.19	0.42
2:E:2206:THR:O	2:E:2210:VAL:HG23	2.19	0.42
2:E:2312:MET:H	2:E:2312:MET:CE	2.32	0.42
2:E:2996:LYS:O	2:E:3000:LYS:HG2	2.19	0.42
2:E:3343:GLN:HB3	2:E:3344:PRO:HD3	2.02	0.42
2:E:3346:VAL:HB	2:E:3411:LEU:HD22	2.01	0.42
2:E:4655:PHE:O	2:E:4659:ILE:HG12	2.20	0.42
2:G:266:ARG:NE	2:G:268:SER:O	2.53	0.42
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	2.00	0.42
2:G:2330:ARG:HE	2:G:2330:ARG:HB2	1.68	0.42
2:G:2351:ASN:O	2:G:2355:ARG:HG3	2.19	0.42
2:G:3078:ARG:HG2	2:G:3152:PHE:CE1	2.55	0.42
2:J:349:GLN:HB2	2:J:356:TRP:CZ3	2.54	0.42
2:J:464:LYS:HE3	2:J:464:LYS:HB3	1.93	0.42
2:J:657:THR:HB	2:J:1021:LEU:HG	2.02	0.42
2:J:786:GLY:H	2:J:1631:GLN:HA	1.84	0.42
2:J:2359:ARG:O	2:J:2361:PRO:HD3	2.19	0.42
2:J:3250:MET:CE	2:J:3315:LEU:HD21	2.50	0.42
2:J:3771:HIS:CG	2:J:3812:VAL:HG12	2.55	0.42
2:J:3878:ASP:N	2:J:3878:ASP:OD1	2.52	0.42
3:C:46:GLU:HG3	3:C:62:SER:HB2	2.00	0.42
3:F:85:LEU:HD23	3:F:85:LEU:HA	1.92	0.42
2:B:266:ARG:NE	2:B:268:SER:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:GLN:HB2	2:B:356:TRP:CZ3	2.54	0.42
2:B:464:LYS:O	2:B:468:LEU:HG	2.20	0.42
2:B:911:HIS:HE1	2:B:918:ARG:NE	2.18	0.42
2:B:1115:LEU:HD23	2:B:1123:VAL:HG11	2.01	0.42
2:B:3136:LEU:O	2:B:3140:LEU:HB3	2.20	0.42
2:B:3521:GLY:HA2	2:B:3524:MET:SD	2.59	0.42
2:B:3771:HIS:CG	2:B:3812:VAL:HG12	2.55	0.42
2:B:3893:GLU:HA	2:B:3967:GLU:OE2	2.19	0.42
2:B:4852:THR:HG22	2:B:4886:HIS:CG	2.55	0.42
2:E:119:SER:HA	2:E:146:CYS:HA	2.00	0.42
2:E:551:LEU:HD11	2:E:564:LEU:HD22	2.02	0.42
2:E:1037:ASP:OD1	2:E:1038:SER:N	2.52	0.42
2:E:2230:THR:HG22	2:E:2234:ARG:HH11	1.83	0.42
2:E:2311:PRO:O	2:E:2314:LEU:HG	2.20	0.42
2:E:3007:ASN:OD1	2:E:3070:ILE:HG13	2.19	0.42
2:E:3157:ILE:HG23	2:E:3165:CYS:SG	2.59	0.42
2:E:3222:LYS:HD2	2:E:3226:GLU:CD	2.39	0.42
2:E:3320:LEU:HD23	2:E:3320:LEU:HA	1.74	0.42
2:E:4805:ASN:HB3	2:E:4808:PHE:CD2	2.54	0.42
2:E:4852:THR:HG21	2:E:4883:TYR:HD1	1.85	0.42
2:G:119:SER:HA	2:G:146:CYS:HA	2.00	0.42
2:G:883:ALA:O	2:G:887:ILE:HG13	2.20	0.42
2:G:3069:HIS:CD2	2:G:3139:VAL:HA	2.55	0.42
2:G:3546:ASP:O	2:G:3550:ARG:HG3	2.19	0.42
2:G:3878:ASP:N	2:G:3878:ASP:OD1	2.52	0.42
2:G:4928:LEU:HD23	2:G:4928:LEU:HA	1.89	0.42
2:J:411:TYR:HB2	2:J:486:LEU:HD21	2.02	0.42
2:J:2230:THR:HG22	2:J:2234:ARG:HH11	1.83	0.42
2:J:2725:LYS:HE3	2:J:2735:PHE:CE1	2.55	0.42
2:J:3257:ALA:HB1	2:J:3321:ARG:HB3	2.02	0.42
2:J:3316:LEU:HD21	2:J:3345:ILE:HG13	2.02	0.42
2:J:3546:ASP:O	2:J:3550:ARG:HG3	2.19	0.42
2:J:4846:VAL:O	2:J:4850:LEU:HG	2.19	0.42
3:K:83:ASN:OD1	3:K:83:ASN:N	2.53	0.42
3:K:104:TYR:HD1	3:K:106:PRO:HD3	1.85	0.42
3:M:47:LEU:O	3:M:62:SER:HB3	2.19	0.42
1:A:40:ARG:H	1:A:40:ARG:HG2	1.72	0.42
2:B:167:ASP:OD1	2:B:168:ASP:N	2.53	0.42
2:B:548:VAL:HA	2:B:551:LEU:HG	2.02	0.42
2:B:984:LEU:HA	2:B:987:ARG:NH1	2.35	0.42
2:B:2223:ILE:HG21	2:B:2229:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2351:ASN:O	2:B:2355:ARG:HG3	2.20	0.42
2:B:2559:LEU:O	2:B:2563:THR:HG23	2.20	0.42
2:B:2635:GLU:HG3	2:B:2636:PHE:HD2	1.84	0.42
2:B:2737:PRO:HB2	2:B:2884:ASN:HB2	2.02	0.42
2:B:3172:ILE:HD11	2:B:3190:LEU:HB3	2.02	0.42
2:B:3535:LEU:CD1	2:B:3539:ARG:HH12	2.33	0.42
2:B:4687:TYR:HE1	2:B:4692:PRO:HG3	1.85	0.42
2:E:167:ASP:OD1	2:E:168:ASP:N	2.53	0.42
2:E:266:ARG:NE	2:E:268:SER:O	2.53	0.42
2:E:788:LYS:HG2	2:E:1629:GLN:HB2	2.02	0.42
2:E:984:LEU:HA	2:E:987:ARG:NH1	2.35	0.42
2:E:1757:ALA:O	2:E:1759:ARG:HD2	2.20	0.42
2:E:2801:ASP:HA	2:E:2804:ILE:HG12	2.01	0.42
2:E:2905:LEU:HD23	2:E:2905:LEU:HA	1.93	0.42
2:E:3043:PHE:CD1	2:E:3043:PHE:C	2.93	0.42
2:E:3246:LEU:HA	2:E:3249:LEU:HG	2.02	0.42
2:E:3735:LEU:O	2:E:3740:GLU:N	2.53	0.42
2:E:4687:TYR:HE1	2:E:4692:PRO:HG3	1.85	0.42
2:G:461:HIS:HA	2:G:464:LYS:HE3	2.02	0.42
2:G:468:LEU:O	2:G:472:ARG:HG2	2.19	0.42
2:G:535:ALA:O	2:G:539:LEU:HG	2.20	0.42
2:G:3007:ASN:OD1	2:G:3070:ILE:HG13	2.19	0.42
2:G:3049:LEU:HA	2:G:3053:ARG:NH2	2.35	0.42
2:G:3206:LEU:HD13	2:G:3246:LEU:N	2.35	0.42
2:G:4014:LYS:HG2	2:G:4135:PRO:HB3	2.01	0.42
2:G:4852:THR:HG22	2:G:4886:HIS:CG	2.55	0.42
2:J:548:VAL:HA	2:J:551:LEU:HG	2.02	0.42
2:J:883:ALA:O	2:J:887:ILE:HG13	2.20	0.42
2:J:2598:ALA:O	2:J:2602:VAL:HG23	2.20	0.42
2:J:3069:HIS:CD2	2:J:3139:VAL:HA	2.55	0.42
2:J:4687:TYR:HE1	2:J:4692:PRO:HG3	1.85	0.42
2:J:4773:VAL:O	2:J:4777:ILE:HG13	2.20	0.42
1:I:73:LYS:HE2	1:I:73:LYS:HB3	1.92	0.41
2:B:214:VAL:HG13	2:B:274:LEU:HB2	2.02	0.41
2:B:664:PHE:CE1	2:B:746:CYS:HB2	2.55	0.41
2:B:1088:TRP:HB2	2:B:1153:ILE:HG22	2.02	0.41
2:B:2122:SER:O	2:B:2126:ARG:HG3	2.20	0.41
2:B:2652:TRP:CD1	2:B:2652:TRP:C	2.93	0.41
2:B:3186:LEU:HG	2:B:3190:LEU:HD21	2.02	0.41
2:B:3878:ASP:OD1	2:B:3878:ASP:N	2.52	0.41
2:B:4968:PHE:O	2:B:4974:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:461:HIS:HA	2:E:464:LYS:HE3	2.02	0.41
2:E:796:ARG:HD3	2:E:1619:ARG:HH12	1.84	0.41
2:E:2452:ARG:HD2	2:J:144:GLU:OE2	2.19	0.41
2:E:2652:TRP:CD1	2:E:2652:TRP:C	2.93	0.41
2:E:2902:HIS:CG	2:E:2903:PRO:HD2	2.55	0.41
2:E:3078:ARG:HG2	2:E:3152:PHE:CE1	2.55	0.41
2:E:3257:ALA:HB1	2:E:3321:ARG:HB3	2.02	0.41
2:E:3538:THR:OG1	2:E:3539:ARG:NH1	2.53	0.41
2:E:3546:ASP:O	2:E:3550:ARG:HG3	2.19	0.41
2:E:3771:HIS:CG	2:E:3812:VAL:HG12	2.55	0.41
2:E:4038:GLY:O	2:E:4042:ARG:NE	2.46	0.41
2:G:943:ASP:HB2	2:G:946:ALA:HB3	2.02	0.41
2:G:997:ALA:O	2:G:1001:VAL:HG23	2.20	0.41
2:G:1261:ASP:N	2:G:1261:ASP:OD1	2.53	0.41
2:G:2122:SER:O	2:G:2126:ARG:HG3	2.20	0.41
2:G:2654:TYR:HB2	2:G:2661:TRP:CE3	2.55	0.41
2:G:2725:LYS:HE3	2:G:2735:PHE:CE1	2.55	0.41
2:G:3172:ILE:HD11	2:G:3190:LEU:HB3	2.02	0.41
2:G:4041:ALA:O	2:G:4045:VAL:HG23	2.20	0.41
2:G:4060:LYS:HA	2:G:4063:ASP:OD2	2.20	0.41
2:J:464:LYS:O	2:J:468:LEU:HG	2.20	0.41
2:J:1090:PHE:HB2	2:J:1204:LEU:HA	2.02	0.41
2:J:3049:LEU:HA	2:J:3053:ARG:NH2	2.35	0.41
2:J:3078:ARG:HG2	2:J:3152:PHE:CE1	2.55	0.41
2:J:3157:ILE:HG23	2:J:3165:CYS:SG	2.59	0.41
2:J:3316:LEU:HD13	2:J:3316:LEU:HA	1.95	0.41
2:J:3346:VAL:HB	2:J:3411:LEU:HD22	2.01	0.41
2:J:4655:PHE:O	2:J:4659:ILE:HG12	2.20	0.41
1:A:2:VAL:HA	1:A:75:THR:O	2.20	0.41
2:B:1037:ASP:OD1	2:B:1038:SER:N	2.52	0.41
2:B:2230:THR:HG22	2:B:2234:ARG:HH11	1.83	0.41
2:B:3007:ASN:OD1	2:B:3070:ILE:HG13	2.19	0.41
2:B:3043:PHE:CD1	2:B:3043:PHE:C	2.93	0.41
2:B:3257:ALA:HB1	2:B:3321:ARG:HB3	2.02	0.41
2:E:688:LEU:HD12	2:E:688:LEU:HA	1.87	0.41
2:E:911:HIS:HB2	2:E:913:LEU:HG	2.02	0.41
2:E:2598:ALA:O	2:E:2602:VAL:HG23	2.20	0.41
2:G:979:PRO:O	2:G:983:THR:HG23	2.19	0.41
2:G:1581:LEU:HD12	2:G:1584:ARG:HE	1.83	0.41
2:G:3735:LEU:O	2:G:3740:GLU:N	2.53	0.41
2:G:4546:VAL:HA	2:G:4549:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4805:ASN:HB3	2:G:4808:PHE:CD2	2.54	0.41
2:J:266:ARG:NE	2:J:268:SER:O	2.53	0.41
2:J:796:ARG:HD3	2:J:1619:ARG:HH12	1.84	0.41
2:J:2522:LEU:HD11	2:J:2569:PHE:CE1	2.54	0.41
2:J:2652:TRP:CD1	2:J:2652:TRP:C	2.93	0.41
2:J:2801:ASP:HA	2:J:2804:ILE:HG12	2.01	0.41
3:C:104:TYR:HD1	3:C:106:PRO:HD3	1.85	0.41
3:K:63:VAL:HA	3:K:67:PHE:HE2	1.85	0.41
2:B:461:HIS:HA	2:B:464:LYS:HE3	2.02	0.41
2:B:911:HIS:HB2	2:B:913:LEU:HG	2.02	0.41
2:B:3069:HIS:CD2	2:B:3139:VAL:HA	2.55	0.41
2:B:4245:MET:HE3	2:B:4245:MET:HB3	1.91	0.41
2:E:214:VAL:HG13	2:E:274:LEU:HB2	2.02	0.41
2:E:575:LEU:HD13	2:E:606:LEU:HA	2.02	0.41
2:E:2123:LEU:HD12	2:E:2123:LEU:HA	1.91	0.41
2:E:3069:HIS:CD2	2:E:3139:VAL:HA	2.55	0.41
2:E:3683:GLN:O	2:E:3687:GLU:HB2	2.21	0.41
2:E:4014:LYS:HG2	2:E:4135:PRO:HB3	2.01	0.41
2:E:4041:ALA:O	2:E:4045:VAL:HG23	2.20	0.41
2:G:144:GLU:OE2	2:J:2452:ARG:HD2	2.19	0.41
2:G:182:LEU:HD13	2:G:198:THR:HG21	2.02	0.41
2:G:1037:ASP:OD1	2:G:1038:SER:N	2.52	0.41
2:G:2664:PHE:CD1	2:G:2664:PHE:N	2.88	0.41
2:G:2737:PRO:HB2	2:G:2884:ASN:HB2	2.02	0.41
2:G:3257:ALA:HB1	2:G:3321:ARG:HB3	2.02	0.41
2:G:3417:ASP:OD1	2:G:3516:LYS:HG2	2.19	0.41
2:G:4687:TYR:HE1	2:G:4692:PRO:HG3	1.85	0.41
2:J:167:ASP:OD1	2:J:168:ASP:N	2.53	0.41
2:J:182:LEU:HD13	2:J:198:THR:HG21	2.02	0.41
2:J:788:LYS:HG2	2:J:1629:GLN:HB2	2.02	0.41
2:J:1121:ALA:HB1	2:J:1123:VAL:HG13	2.00	0.41
2:J:1694:LEU:HD13	2:J:1715:LEU:HD12	2.01	0.41
2:J:2640:PRO:O	2:J:2644:LEU:HD23	2.20	0.41
2:J:2758:PHE:O	2:J:2762:THR:HG23	2.21	0.41
2:J:2902:HIS:CG	2:J:2903:PRO:HD2	2.55	0.41
2:J:3417:ASP:OD1	2:J:3516:LYS:HG2	2.19	0.41
2:J:3592:ILE:HG12	2:J:3595:ARG:NH2	2.35	0.41
2:J:4014:LYS:HG2	2:J:4135:PRO:HB3	2.01	0.41
2:J:4017:LEU:HD22	2:J:4139:ILE:HG21	2.03	0.41
2:J:4031:LEU:HD13	2:J:4044:MET:HE3	2.03	0.41
3:C:28:ILE:HD12	3:C:28:ILE:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:63:VAL:HA	3:F:67:PHE:HE2	1.85	0.41
1:I:88:PRO:HB2	2:J:1680:ARG:HH12	1.85	0.41
2:B:3078:ARG:HG2	2:B:3152:PHE:CE1	2.55	0.41
2:B:3546:ASP:O	2:B:3550:ARG:HG3	2.19	0.41
2:B:4060:LYS:HA	2:B:4063:ASP:OD2	2.20	0.41
2:B:4655:PHE:O	2:B:4659:ILE:HG12	2.20	0.41
2:B:4773:VAL:O	2:B:4777:ILE:HG13	2.20	0.41
2:B:4928:LEU:HD23	2:B:4928:LEU:HA	1.89	0.41
2:E:882:TRP:CZ2	3:F:104:TYR:HB2	2.55	0.41
2:E:911:HIS:HE1	2:E:918:ARG:NE	2.18	0.41
2:E:936:GLY:HA3	2:E:1056:PRO:HB3	2.01	0.41
2:E:937:CYS:HB3	2:E:1053:ILE:HB	2.02	0.41
2:E:1927:LEU:HD23	2:E:1939:MET:HE1	2.03	0.41
2:E:3521:GLY:HA2	2:E:3524:MET:SD	2.60	0.41
2:E:4060:LYS:HA	2:E:4063:ASP:OD2	2.20	0.41
2:E:4698:LYS:HE3	2:E:4698:LYS:HB2	1.84	0.41
2:G:14:LEU:HD13	2:G:202:MET:HG2	2.02	0.41
2:G:904:HIS:CD2	2:G:907:LEU:H	2.39	0.41
2:G:984:LEU:HA	2:G:987:ARG:NH1	2.35	0.41
2:G:2173:GLN:O	2:G:2177:LEU:HD23	2.20	0.41
2:G:2598:ALA:O	2:G:2602:VAL:HG23	2.20	0.41
2:G:2902:HIS:CG	2:G:2903:PRO:HD2	2.55	0.41
2:G:3836:MET:HE3	2:G:3915:ILE:HG23	2.02	0.41
2:G:4232:GLU:HG2	2:G:5019:TRP:CD1	2.56	0.41
2:G:4773:VAL:O	2:G:4777:ILE:HG13	2.20	0.41
2:G:4851:TYR:HD1	2:G:4916:PHE:CE1	2.39	0.41
2:G:4968:PHE:O	2:G:4974:GLY:HA3	2.20	0.41
2:J:984:LEU:HA	2:J:987:ARG:NH1	2.35	0.41
2:J:997:ALA:O	2:J:1001:VAL:HG23	2.20	0.41
2:J:2173:GLN:O	2:J:2177:LEU:HD23	2.20	0.41
2:J:2737:PRO:HB2	2:J:2884:ASN:HB2	2.02	0.41
2:J:4852:THR:HG21	2:J:4883:TYR:HD1	1.85	0.41
3:M:104:TYR:HD1	3:M:106:PRO:HD3	1.85	0.41
2:B:657:THR:HB	2:B:1021:LEU:HG	2.02	0.41
2:B:904:HIS:CD2	2:B:907:LEU:H	2.39	0.41
2:B:2452:ARG:HD2	2:E:144:GLU:OE2	2.19	0.41
2:B:2589:LEU:HD23	2:B:2589:LEU:HA	1.87	0.41
2:B:2615:ARG:HD2	2:B:2664:PHE:HA	2.01	0.41
2:B:3193:CYS:O	2:B:3197:LEU:HG	2.21	0.41
2:B:3683:GLN:O	2:B:3687:GLU:HB2	2.21	0.41
2:E:866:HIS:ND1	2:E:870:ILE:HB	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1088:TRP:HB2	2:E:1153:ILE:HG22	2.02	0.41
2:E:1092:PHE:HE2	2:E:1100:MET:HE3	1.86	0.41
2:E:1849:LEU:HG	2:E:1945:TYR:CE2	2.56	0.41
2:E:2737:PRO:HB2	2:E:2884:ASN:HB2	2.02	0.41
2:E:4968:PHE:O	2:E:4974:GLY:HA3	2.20	0.41
2:G:162:LYS:NZ	2:J:3987:ASP:OD2	2.49	0.41
2:G:167:ASP:OD1	2:G:168:ASP:N	2.53	0.41
2:G:349:GLN:HB2	2:G:356:TRP:CZ3	2.54	0.41
2:G:371:VAL:HG11	2:G:373:LYS:HG2	2.02	0.41
2:G:464:LYS:O	2:G:468:LEU:HG	2.20	0.41
2:G:657:THR:HB	2:G:1021:LEU:HG	2.02	0.41
2:G:911:HIS:HE1	2:G:918:ARG:NE	2.18	0.41
2:G:1088:TRP:HB2	2:G:1153:ILE:HG22	2.02	0.41
2:G:1090:PHE:HB2	2:G:1204:LEU:HA	2.02	0.41
2:G:2292:GLU:H	2:G:2292:GLU:CD	2.21	0.41
2:G:2340:PHE:HB2	2:G:2435:ARG:HE	1.86	0.41
2:G:2382:GLU:HA	2:G:2385:ARG:NE	2.36	0.41
2:G:2718:SER:OG	2:G:2909:ASP:O	2.25	0.41
2:G:2790:MET:O	2:G:2792:ARG:NE	2.52	0.41
2:G:2947:ASP:OD1	2:G:2947:ASP:N	2.54	0.41
2:G:3173:TYR:CG	2:G:3243:ILE:HG12	2.56	0.41
2:G:3193:CYS:O	2:G:3197:LEU:HG	2.21	0.41
2:G:3343:GLN:HB3	2:G:3344:PRO:HD3	2.02	0.41
2:G:3535:LEU:CD1	2:G:3539:ARG:HH12	2.33	0.41
2:G:3567:PRO:CB	2:G:3570:ARG:HH21	2.32	0.41
2:G:3771:HIS:CG	2:G:3812:VAL:HG12	2.55	0.41
2:J:102:LEU:HD21	2:J:105:HIS:CE1	2.56	0.41
2:J:214:VAL:HG13	2:J:274:LEU:HB2	2.02	0.41
2:J:3172:ILE:HD11	2:J:3190:LEU:HB3	2.02	0.41
2:J:3179:LYS:HE3	2:J:3179:LYS:HB3	1.95	0.41
2:J:3391:GLU:HA	2:J:3394:VAL:HG22	2.03	0.41
3:F:104:TYR:HD1	3:F:106:PRO:HD3	1.85	0.41
1:A:73:LYS:HB3	1:A:73:LYS:HE2	1.86	0.41
2:B:575:LEU:HD13	2:B:606:LEU:HA	2.02	0.41
2:B:997:ALA:O	2:B:1001:VAL:HG23	2.20	0.41
2:B:1637:MET:HG3	2:B:1696:HIS:ND1	2.36	0.41
2:B:2519:LEU:HD11	2:B:2572:THR:HG23	2.03	0.41
2:B:3049:LEU:HA	2:B:3053:ARG:NH2	2.35	0.41
2:E:705:ASN:N	2:E:705:ASN:HD22	2.19	0.41
2:E:997:ALA:O	2:E:1001:VAL:HG23	2.20	0.41
2:E:2479:LEU:HD22	2:E:2541:PHE:HZ	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:222:LEU:HB3	2:G:388:LEU:HD12	2.02	0.41
2:G:575:LEU:HD13	2:G:606:LEU:HA	2.02	0.41
2:G:1000:ARG:HH12	3:M:115:ASP:H	1.69	0.41
2:G:2311:PRO:O	2:G:2314:LEU:HG	2.20	0.41
2:G:3354:LEU:HD13	2:G:3415:TYR:HE2	1.86	0.41
2:J:473:ASN:O	2:J:477:LEU:HG	2.21	0.41
2:J:575:LEU:HD13	2:J:606:LEU:HA	2.02	0.41
2:J:904:HIS:CD2	2:J:907:LEU:H	2.39	0.41
2:J:2311:PRO:O	2:J:2314:LEU:HG	2.20	0.41
2:J:2368:LEU:HD23	2:J:2368:LEU:HA	1.88	0.41
2:J:4851:TYR:HD1	2:J:4916:PHE:CE1	2.39	0.41
2:B:222:LEU:HB3	2:B:388:LEU:HD12	2.02	0.41
2:B:473:ASN:O	2:B:477:LEU:HG	2.21	0.41
2:B:1757:ALA:O	2:B:1759:ARG:HD2	2.20	0.41
2:B:1849:LEU:HG	2:B:1945:TYR:CE2	2.56	0.41
2:B:2382:GLU:HA	2:B:2385:ARG:NE	2.35	0.41
2:B:4041:ALA:O	2:B:4045:VAL:HG23	2.20	0.41
2:E:102:LEU:HD21	2:E:105:HIS:CE1	2.56	0.41
2:E:275:ARG:HB3	2:E:278:GLN:HB2	2.01	0.41
2:E:898:ASP:O	2:E:902:ARG:N	2.54	0.41
2:E:1090:PHE:HB2	2:E:1204:LEU:HA	2.02	0.41
2:E:1658:ASP:N	2:E:1658:ASP:OD1	2.54	0.41
2:E:2262:GLY:O	2:E:2266:GLY:N	2.47	0.41
2:E:3186:LEU:HG	2:E:3190:LEU:HD21	2.02	0.41
2:E:3567:PRO:CB	2:E:3570:ARG:HH21	2.32	0.41
2:G:162:LYS:HG3	2:J:3984:ARG:HH22	1.86	0.41
2:G:788:LYS:HG2	2:G:1629:GLN:HB2	2.02	0.41
2:G:2165:LEU:HD11	2:G:2177:LEU:HB3	2.02	0.41
2:G:2575:ARG:NH1	2:G:2578:MET:HB3	2.36	0.41
2:G:3100:SER:HB3	2:G:3167:ARG:HE	1.85	0.41
2:G:3186:LEU:HG	2:G:3190:LEU:HD21	2.02	0.41
2:G:3316:LEU:O	2:G:3320:LEU:HG	2.20	0.41
2:G:4017:LEU:HD22	2:G:4139:ILE:HG21	2.03	0.41
2:G:4846:VAL:O	2:G:4850:LEU:HG	2.19	0.41
2:J:14:LEU:HD13	2:J:202:MET:HG2	2.02	0.41
2:J:222:LEU:HB3	2:J:388:LEU:HD12	2.02	0.41
2:J:878:ILE:HG21	3:K:107:TRP:HE1	1.85	0.41
2:J:936:GLY:HA3	2:J:1056:PRO:HB3	2.02	0.41
2:J:1126:GLY:HA3	2:J:1143:TRP:CE3	2.56	0.41
2:J:1658:ASP:N	2:J:1658:ASP:OD1	2.54	0.41
2:J:2292:GLU:H	2:J:2292:GLU:CD	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2414:ASN:HB2	2:J:2417:HIS:CE1	2.56	0.41
2:J:2672:LEU:HD11	2:J:2711:PRO:HD2	2.03	0.41
2:J:4546:VAL:HA	2:J:4549:VAL:HG22	2.03	0.41
3:C:83:ASN:OD1	3:C:83:ASN:N	2.53	0.41
1:H:88:PRO:HB2	2:G:1680:ARG:NH1	2.36	0.41
2:B:232:THR:OG1	2:B:248:GLU:HG2	2.21	0.41
2:B:2311:PRO:O	2:B:2314:LEU:HG	2.20	0.41
2:B:2758:PHE:O	2:B:2762:THR:HG23	2.21	0.41
2:B:2765:LYS:HD3	2:B:2765:LYS:HA	1.67	0.41
2:B:2871:LEU:HD11	2:B:2927:LEU:HD11	2.03	0.41
2:B:3552:PHE:HA	2:B:3555:ASN:OD1	2.21	0.41
2:E:411:TYR:HB2	2:E:486:LEU:HD21	2.02	0.41
2:E:664:PHE:CE1	2:E:746:CYS:HB2	2.56	0.41
2:E:883:ALA:O	2:E:887:ILE:HG13	2.20	0.41
2:E:2414:ASN:HB2	2:E:2417:HIS:CE1	2.56	0.41
2:E:2758:PHE:O	2:E:2762:THR:HG23	2.20	0.41
2:E:2871:LEU:HD11	2:E:2927:LEU:HD11	2.03	0.41
2:E:3347:SER:HB2	2:E:3414:ARG:HG3	2.03	0.41
2:G:473:ASN:O	2:G:477:LEU:HG	2.21	0.41
2:G:866:HIS:CD2	2:G:869:ARG:HH21	2.39	0.41
2:G:1126:GLY:HA3	2:G:1143:TRP:CE3	2.56	0.41
2:G:2285:GLU:H	2:G:2285:GLU:HG2	1.69	0.41
2:G:2522:LEU:HD11	2:G:2569:PHE:CE1	2.55	0.41
2:G:2672:LEU:HD12	2:G:2672:LEU:HA	1.81	0.41
2:G:3347:SER:HB2	2:G:3414:ARG:HG3	2.03	0.41
2:G:3545:THR:O	2:G:3549:VAL:HG13	2.21	0.41
2:G:3592:ILE:HG12	2:G:3595:ARG:NH2	2.35	0.41
2:G:3592:ILE:HA	2:G:3595:ARG:HE	1.86	0.41
2:G:3809:ASN:HB3	2:G:3812:VAL:CG2	2.48	0.41
2:J:1849:LEU:HG	2:J:1945:TYR:CE2	2.56	0.41
2:J:2359:ARG:HD3	2:J:2359:ARG:HA	1.82	0.41
2:J:2479:LEU:HD22	2:J:2541:PHE:HZ	1.86	0.41
2:J:2654:TYR:HB2	2:J:2661:TRP:CE3	2.55	0.41
1:A:17:LYS:HG3	1:A:18:LYS:N	2.35	0.41
2:B:275:ARG:HB3	2:B:278:GLN:HB2	2.02	0.41
2:B:551:LEU:HD11	2:B:564:LEU:HD22	2.02	0.41
2:B:866:HIS:CD2	2:B:869:ARG:HH21	2.39	0.41
2:B:1090:PHE:HB2	2:B:1204:LEU:HA	2.02	0.41
2:B:2165:LEU:HD11	2:B:2177:LEU:HB3	2.02	0.41
2:B:2419:GLY:O	2:B:2423:MET:HG2	2.21	0.41
2:B:2617:SER:OG	2:B:2618:MET:SD	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2790:MET:O	2:B:2792:ARG:NE	2.52	0.41
2:B:3354:LEU:HD13	2:B:3415:TYR:HE2	1.86	0.41
2:B:3835:LEU:HD22	2:B:3880:PHE:CZ	2.56	0.41
2:B:4852:THR:HG21	2:B:4883:TYR:HD1	1.85	0.41
2:E:1126:GLY:HA3	2:E:1143:TRP:CE3	2.56	0.41
2:E:1637:MET:HG3	2:E:1696:HIS:ND1	2.36	0.41
2:E:2382:GLU:HA	2:E:2385:ARG:NE	2.36	0.41
2:E:2664:PHE:N	2:E:2664:PHE:CD1	2.88	0.41
2:E:3214:ASN:HB2	2:E:3304:CYS:HB3	2.02	0.41
2:E:3391:GLU:HA	2:E:3394:VAL:HG22	2.03	0.41
2:E:4773:VAL:O	2:E:4777:ILE:HG13	2.20	0.41
2:E:4851:TYR:HD1	2:E:4916:PHE:CE1	2.39	0.41
2:E:4992:LEU:HD13	2:E:5014:TYR:CZ	2.56	0.41
2:G:214:VAL:HG13	2:G:274:LEU:HB2	2.02	0.41
2:G:548:VAL:HG21	2:G:582:HIS:CD2	2.52	0.41
2:G:551:LEU:HD11	2:G:564:LEU:HD22	2.02	0.41
2:G:1637:MET:HG3	2:G:1696:HIS:ND1	2.36	0.41
2:G:1849:LEU:HG	2:G:1945:TYR:CE2	2.56	0.41
2:G:1931:LEU:HD13	2:G:1935:VAL:HG12	2.03	0.41
2:G:2331:TYR:O	2:G:2335:LEU:HG	2.21	0.41
2:G:2414:ASN:HB2	2:G:2417:HIS:CE1	2.56	0.41
2:G:2652:TRP:CD1	2:G:2652:TRP:C	2.93	0.41
2:G:2672:LEU:HD11	2:G:2711:PRO:HD2	2.03	0.41
2:G:2912:THR:OG1	2:G:2913:ALA:N	2.54	0.41
2:G:3214:ASN:HB2	2:G:3304:CYS:HB3	2.02	0.41
2:G:3316:LEU:HD13	2:G:3316:LEU:HA	1.92	0.41
2:G:3391:GLU:HA	2:G:3394:VAL:HG22	2.03	0.41
2:G:3683:GLN:O	2:G:3687:GLU:HB2	2.21	0.41
2:G:4852:THR:HG21	2:G:4883:TYR:HD1	1.85	0.41
2:J:911:HIS:HE1	2:J:918:ARG:NE	2.18	0.41
2:J:911:HIS:HB2	2:J:913:LEU:HG	2.02	0.41
2:J:1252:HIS:CE1	2:J:1254:HIS:HB2	2.56	0.41
2:J:2122:SER:O	2:J:2126:ARG:HG3	2.20	0.41
2:J:2165:LEU:HD11	2:J:2177:LEU:HB3	2.02	0.41
2:J:2515:GLN:CA	2:J:2568:LEU:HD21	2.48	0.41
2:J:2566:ALA:O	2:J:2569:PHE:HB2	2.21	0.41
2:J:2664:PHE:CD1	2:J:2664:PHE:N	2.88	0.41
2:J:2947:ASP:OD1	2:J:2947:ASP:N	2.54	0.41
2:J:3343:GLN:HB3	2:J:3344:PRO:HD3	2.02	0.41
2:J:3354:LEU:HD13	2:J:3415:TYR:HE2	1.86	0.41
2:J:3552:PHE:HA	2:J:3555:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3683:GLN:O	2:J:3687:GLU:HB2	2.21	0.41
2:J:4041:ALA:O	2:J:4045:VAL:HG23	2.20	0.41
2:J:4968:PHE:O	2:J:4974:GLY:HA3	2.20	0.41
3:C:63:VAL:HA	3:C:67:PHE:HE2	1.85	0.41
3:C:85:LEU:HD23	3:C:85:LEU:HA	1.92	0.41
3:C:101:PRO:O	3:C:104:TYR:N	2.48	0.41
3:F:109:THR:OG1	3:F:110:PRO:HD3	2.21	0.41
3:M:101:PRO:O	3:M:104:TYR:N	2.48	0.41
1:D:17:LYS:HG3	1:D:18:LYS:N	2.35	0.41
1:D:49:ARG:HB2	1:D:52:LYS:HG2	2.03	0.41
1:I:88:PRO:HB2	2:J:1680:ARG:NH1	2.36	0.41
2:B:214:VAL:HA	2:B:341:TYR:CD2	2.56	0.41
2:B:411:TYR:HB2	2:B:486:LEU:HD21	2.02	0.41
2:B:866:HIS:ND1	2:B:870:ILE:HB	2.36	0.41
2:B:1126:GLY:HA3	2:B:1143:TRP:CE3	2.56	0.41
2:B:2562:ILE:HG23	2:B:2569:PHE:CZ	2.56	0.41
2:E:222:LEU:HB3	2:E:388:LEU:HD12	2.02	0.41
2:E:464:LYS:O	2:E:468:LEU:HG	2.20	0.41
2:E:691:GLY:HA3	2:E:712:TYR:CD1	2.56	0.41
2:E:866:HIS:CD2	2:E:869:ARG:HH21	2.39	0.41
2:E:878:ILE:HG21	3:F:107:TRP:CE2	2.55	0.41
2:E:1131:ARG:HB2	2:E:1179:PHE:CZ	2.56	0.41
2:E:3100:SER:HB3	2:E:3167:ARG:HE	1.85	0.41
2:E:3193:CYS:O	2:E:3197:LEU:HG	2.21	0.41
2:E:3893:GLU:HA	2:E:3967:GLU:OE2	2.21	0.41
2:E:4017:LEU:HD22	2:E:4139:ILE:HG21	2.03	0.41
2:G:102:LEU:HD21	2:G:105:HIS:CE1	2.56	0.41
2:G:424:LYS:HE2	2:G:424:LYS:HB2	1.92	0.41
2:G:911:HIS:HB2	2:G:913:LEU:HG	2.02	0.41
2:G:3552:PHE:HA	2:G:3555:ASN:OD1	2.21	0.41
2:J:575:LEU:HA	2:J:578:ILE:HG12	2.03	0.41
2:J:937:CYS:HB3	2:J:1053:ILE:HB	2.02	0.41
2:J:2340:PHE:HB2	2:J:2435:ARG:HE	1.86	0.41
2:J:3137:LEU:HD12	2:J:3137:LEU:HA	1.91	0.41
2:J:3535:LEU:CD1	2:J:3539:ARG:HH12	2.33	0.41
2:J:4666:VAL:O	2:J:4670:ILE:HG12	2.21	0.41
1:H:49:ARG:HB2	1:H:52:LYS:HG2	2.03	0.40
1:I:29:MET:HG3	1:I:30:LEU:O	2.21	0.40
2:B:533:ASN:HB3	2:B:536:ASN:HB2	2.04	0.40
2:B:691:GLY:HA3	2:B:712:TYR:CD1	2.56	0.40
2:B:788:LYS:HG2	2:B:1629:GLN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2479:LEU:HD22	2:B:2541:PHE:HZ	1.86	0.40
2:B:2801:ASP:HA	2:B:2804:ILE:HG12	2.01	0.40
2:B:2947:ASP:OD1	2:B:2947:ASP:N	2.54	0.40
2:B:3173:TYR:CG	2:B:3243:ILE:HG12	2.56	0.40
2:B:3277:LEU:HB3	2:B:3315:LEU:HD13	2.03	0.40
2:B:3354:LEU:HD13	2:B:3415:TYR:CE2	2.57	0.40
2:B:3592:ILE:HA	2:B:3595:ARG:HE	1.86	0.40
2:B:4851:TYR:HD1	2:B:4916:PHE:CE1	2.39	0.40
2:E:105:HIS:O	2:E:150:MET:HG2	2.22	0.40
2:E:232:THR:OG1	2:E:248:GLU:HG2	2.21	0.40
2:E:294:THR:N	2:E:298:GLY:O	2.39	0.40
2:E:473:ASN:O	2:E:477:LEU:HG	2.21	0.40
2:E:2575:ARG:NH1	2:E:2577:ILE:HG23	2.36	0.40
2:E:2947:ASP:OD1	2:E:2947:ASP:N	2.54	0.40
2:E:3535:LEU:CD1	2:E:3539:ARG:HH12	2.33	0.40
2:G:2419:GLY:O	2:G:2423:MET:HG2	2.21	0.40
2:G:2566:ALA:O	2:G:2569:PHE:HB2	2.21	0.40
2:G:3136:LEU:O	2:G:3140:LEU:HB3	2.20	0.40
2:G:3471:THR:O	2:G:3475:LYS:HG3	2.21	0.40
2:J:866:HIS:ND1	2:J:870:ILE:HB	2.36	0.40
2:J:1131:ARG:HB2	2:J:1179:PHE:CZ	2.56	0.40
2:J:1261:ASP:N	2:J:1261:ASP:OD1	2.53	0.40
2:J:2382:GLU:HA	2:J:2385:ARG:NE	2.35	0.40
2:J:2871:LEU:HD11	2:J:2927:LEU:HD11	2.03	0.40
2:J:3193:CYS:O	2:J:3197:LEU:HG	2.21	0.40
2:J:3592:ILE:HA	2:J:3595:ARG:HE	1.86	0.40
3:F:28:ILE:HD12	3:F:28:ILE:HA	1.93	0.40
1:A:49:ARG:HB2	1:A:52:LYS:HG2	2.03	0.40
1:A:57:LYS:HB2	1:A:57:LYS:HE2	1.75	0.40
1:H:26:TYR:HB2	1:H:101:VAL:HG12	2.03	0.40
2:B:936:GLY:HA3	2:B:1056:PRO:HB3	2.01	0.40
2:B:1252:HIS:CE1	2:B:1254:HIS:HB2	2.56	0.40
2:B:1733:GLU:HG2	2:B:2201:LEU:HD23	2.03	0.40
2:B:2359:ARG:HD3	2:B:2359:ARG:HA	1.82	0.40
2:B:3100:SER:HB3	2:B:3167:ARG:HE	1.85	0.40
2:B:3137:LEU:HD12	2:B:3137:LEU:HA	1.91	0.40
2:B:4546:VAL:HA	2:B:4549:VAL:HG22	2.03	0.40
2:B:4898:GLY:HA2	2:B:4901:ILE:HD12	2.03	0.40
2:E:664:PHE:HB3	2:E:811:CYS:SG	2.62	0.40
2:E:3173:TYR:CG	2:E:3243:ILE:HG12	2.56	0.40
2:E:3354:LEU:HD13	2:E:3415:TYR:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4666:VAL:O	2:E:4670:ILE:HG12	2.21	0.40
2:E:4928:LEU:HA	2:E:4928:LEU:HD23	1.89	0.40
2:G:16:THR:HA	2:G:69:LEU:HD22	2.04	0.40
2:G:664:PHE:CE1	2:G:746:CYS:HB2	2.55	0.40
2:G:4655:PHE:O	2:G:4659:ILE:HG12	2.20	0.40
2:G:4847:VAL:O	2:G:4851:TYR:HD2	2.04	0.40
2:G:4898:GLY:HA2	2:G:4901:ILE:HD12	2.03	0.40
2:J:1637:MET:HG3	2:J:1696:HIS:ND1	2.36	0.40
2:J:2912:THR:OG1	2:J:2913:ALA:N	2.54	0.40
2:J:3985:LEU:O	2:J:3989:VAL:HG23	2.21	0.40
3:K:109:THR:OG1	3:K:110:PRO:HD3	2.21	0.40
1:A:16:PRO:HG3	1:A:103:LEU:HD21	2.03	0.40
1:H:40:ARG:H	1:H:40:ARG:HG2	1.72	0.40
2:B:105:HIS:O	2:B:150:MET:HG2	2.22	0.40
2:B:617:ASN:O	2:B:621:ILE:HG13	2.22	0.40
2:B:2352:VAL:O	2:B:2356:LEU:HG	2.22	0.40
2:B:2414:ASN:HB2	2:B:2417:HIS:CE1	2.56	0.40
2:B:3214:ASN:HB2	2:B:3304:CYS:HB3	2.03	0.40
2:B:3347:SER:HB2	2:B:3414:ARG:HG3	2.03	0.40
2:B:3989:VAL:HG13	2:B:4023:MET:HE2	2.03	0.40
2:E:548:VAL:HG21	2:E:582:HIS:CD2	2.52	0.40
2:E:904:HIS:CD2	2:E:907:LEU:H	2.39	0.40
2:E:960:MET:SD	2:E:960:MET:N	2.75	0.40
2:E:2331:TYR:O	2:E:2335:LEU:HG	2.21	0.40
2:E:2575:ARG:O	2:E:2578:MET:HG3	2.21	0.40
2:E:3136:LEU:O	2:E:3140:LEU:HB3	2.20	0.40
2:E:3552:PHE:HA	2:E:3555:ASN:OD1	2.21	0.40
2:G:411:TYR:HB2	2:G:486:LEU:HD21	2.02	0.40
2:G:898:ASP:O	2:G:902:ARG:N	2.54	0.40
2:G:936:GLY:HA3	2:G:1056:PRO:HB3	2.01	0.40
2:G:937:CYS:HB3	2:G:1053:ILE:HB	2.02	0.40
2:G:1092:PHE:HE2	2:G:1100:MET:HE3	1.86	0.40
2:G:2310:CYS:SG	2:G:2313:LEU:HB2	2.62	0.40
2:G:2758:PHE:O	2:G:2762:THR:HG23	2.20	0.40
2:G:3246:LEU:HD22	2:G:3280:TYR:CE2	2.56	0.40
2:G:4020:GLN:O	2:G:4024:VAL:HG23	2.21	0.40
2:J:866:HIS:CD2	2:J:869:ARG:HH21	2.39	0.40
2:J:2575:ARG:NH1	2:J:2577:ILE:HG23	2.37	0.40
2:J:3186:LEU:HG	2:J:3190:LEU:HD21	2.02	0.40
2:J:3347:SER:HB2	2:J:3414:ARG:HG3	2.03	0.40
2:J:3545:THR:O	2:J:3549:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:3731:LYS:HZ2	2:J:3735:LEU:HD21	1.86	0.40
1:A:29:MET:HG3	1:A:30:LEU:O	2.21	0.40
2:B:1509:ILE:HG22	2:B:1511:HIS:H	1.86	0.40
2:B:2340:PHE:HB2	2:B:2435:ARG:HE	1.86	0.40
2:B:2867:LEU:HB2	2:B:2928:LYS:HZ3	1.84	0.40
2:B:2912:THR:OG1	2:B:2913:ALA:N	2.54	0.40
2:B:3462:ASN:HB2	2:B:3464:ILE:HG12	2.04	0.40
2:B:4020:GLN:O	2:B:4024:VAL:HG23	2.21	0.40
2:B:4666:VAL:O	2:B:4670:ILE:HG12	2.22	0.40
2:E:1252:HIS:CE1	2:E:1254:HIS:HB2	2.56	0.40
2:E:1981:MET:CE	2:E:1981:MET:HA	2.52	0.40
2:E:3285:TRP:CD1	2:E:3312:LEU:HD11	2.56	0.40
2:G:2479:LEU:HD22	2:G:2541:PHE:HZ	1.86	0.40
2:G:2578:MET:HE2	2:G:2578:MET:HB2	2.01	0.40
2:G:4048:LEU:HD23	2:G:4048:LEU:HA	1.88	0.40
2:J:2331:TYR:O	2:J:2335:LEU:HG	2.21	0.40
2:J:3462:ASN:HB2	2:J:3464:ILE:HG12	2.04	0.40
2:J:3471:THR:O	2:J:3475:LYS:HG3	2.21	0.40
2:J:3892:CYS:SG	2:J:3903:LEU:HD12	2.62	0.40
3:M:83:ASN:OD1	3:M:83:ASN:N	2.53	0.40
1:A:3:GLU:HB2	1:A:75:THR:HB	2.02	0.40
1:D:29:MET:HG3	1:D:30:LEU:O	2.21	0.40
2:B:16:THR:HA	2:B:69:LEU:HD22	2.04	0.40
2:B:1131:ARG:HB2	2:B:1179:PHE:CZ	2.56	0.40
2:B:1931:LEU:HD13	2:B:1935:VAL:HG12	2.03	0.40
2:B:2541:PHE:N	2:B:2541:PHE:CD1	2.87	0.40
2:E:2626:LEU:CD2	2:E:2640:PRO:HB3	2.51	0.40
2:E:2912:THR:OG1	2:E:2913:ALA:N	2.54	0.40
2:E:3835:LEU:HD22	2:E:3880:PHE:CZ	2.56	0.40
2:E:3892:CYS:SG	2:E:3903:LEU:HD12	2.62	0.40
2:E:4631:PHE:CE2	2:E:4633:GLU:HB2	2.57	0.40
2:G:866:HIS:ND1	2:G:870:ILE:HB	2.36	0.40
2:G:1436:SER:OG	2:G:1565:GLU:HB2	2.22	0.40
2:G:1815:LEU:O	2:G:1819:VAL:HG23	2.22	0.40
2:G:2871:LEU:HD11	2:G:2927:LEU:HD11	2.03	0.40
2:G:3154:ASP:OD1	2:G:3154:ASP:N	2.53	0.40
2:J:105:HIS:O	2:J:150:MET:HG2	2.22	0.40
2:J:424:LYS:HE2	2:J:424:LYS:HB2	1.92	0.40
2:J:1088:TRP:HB2	2:J:1153:ILE:HG22	2.03	0.40
2:J:1733:GLU:HG2	2:J:2201:LEU:HD23	2.03	0.40
2:J:2310:CYS:SG	2:J:2313:LEU:HB2	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:2419:GLY:O	2:J:2423:MET:HG2	2.21	0.40
2:J:2575:ARG:NH1	2:J:2578:MET:HB3	2.37	0.40
2:J:2575:ARG:O	2:J:2578:MET:HG3	2.21	0.40
2:J:3214:ASN:HB2	2:J:3304:CYS:HB3	2.02	0.40
2:J:3893:GLU:HA	2:J:3967:GLU:OE2	2.21	0.40
2:J:4631:PHE:CE2	2:J:4633:GLU:HB2	2.57	0.40
2:J:4847:VAL:O	2:J:4851:TYR:HD2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	D	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
1	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	I	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	B	4264/5027 (85%)	4160 (98%)	103 (2%)	1 (0%)	100	100
2	E	4264/5027 (85%)	4162 (98%)	102 (2%)	0	100	100
2	G	4280/5027 (85%)	4175 (98%)	105 (2%)	0	100	100
2	J	4264/5027 (85%)	4161 (98%)	103 (2%)	0	100	100
3	C	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	F	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	K	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	M	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
All	All	17988/21084 (85%)	17529 (97%)	458 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	375	LYS

### 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	87/88 (99%)	85 (98%)	2 (2%)	45	68
1	D	87/88 (99%)	85 (98%)	2 (2%)	45	68
1	H	87/88 (99%)	85 (98%)	2 (2%)	45	68
1	I	87/88 (99%)	85 (98%)	2 (2%)	45	68
2	B	3662/4270 (86%)	3580 (98%)	82 (2%)	47	69
2	E	3662/4270 (86%)	3581 (98%)	81 (2%)	47	69
2	G	3674/4270 (86%)	3594 (98%)	80 (2%)	47	69
2	J	3662/4270 (86%)	3580 (98%)	82 (2%)	47	69
3	C	103/114 (90%)	99 (96%)	4 (4%)	27	55
3	F	103/114 (90%)	99 (96%)	4 (4%)	27	55
3	K	103/114 (90%)	99 (96%)	4 (4%)	27	55
3	M	103/114 (90%)	99 (96%)	4 (4%)	27	55
All	All	15420/17888 (86%)	15071 (98%)	349 (2%)	46	68

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	94	ASN
1	D	29	MET
1	D	94	ASN
1	H	29	MET
1	H	94	ASN
1	I	29	MET
1	I	94	ASN
2	B	116	MET
2	B	125	ARG

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Mol	Chain	Res	Type
2	B	127	MET
2	B	269	TRP
2	B	280	LEU
2	B	283	ARG
2	B	299	LEU
2	B	306	LYS
2	B	341	TYR
2	B	379	HIS
2	B	631	LEU
2	B	702	TRP
2	B	866	HIS
2	B	877	ASN
2	B	902	ARG
2	B	955	LEU
2	B	959	TYR
2	B	960	MET
2	B	1112	ASP
2	B	1133	HIS
2	B	1143	TRP
2	B	1229	ASN
2	B	1270	LEU
2	B	1286	MET
2	B	1421	ARG
2	B	1435	TYR
2	B	1532	ASN
2	B	1647	CYS
2	B	1981	MET
2	B	2178	MET
2	B	2256	TYR
2	B	2305	CYS
2	B	2312	MET
2	B	2326	CYS
2	B	2340	PHE
2	B	2392	ARG
2	B	2475	GLN
2	B	2530	MET
2	B	2574	HIS
2	B	2591	ARG
2	B	2618	MET
2	B	2634	ASN
2	B	2664	PHE
2	B	2688	HIS

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Mol	Chain	Res	Type
2	B	2738	ARG
2	B	2797	PHE
2	B	2806	ARG
2	B	2827	ARG
2	B	2869	ARG
2	B	2872	GLN
2	B	2914	LYS
2	B	2947	ASP
2	B	2992	GLU
2	B	3034	LYS
2	B	3043	PHE
2	B	3053	ARG
2	B	3096	PHE
2	B	3144	PHE
2	B	3158	LEU
2	B	3239	MET
2	B	3334	TRP
2	B	3348	ARG
2	B	3355	HIS
2	B	3366	ARG
2	B	3451	PHE
2	B	3516	LYS
2	B	3720	TYR
2	B	3782	MET
2	B	3933	PHE
2	B	3966	THR
2	B	4000	MET
2	B	4042	ARG
2	B	4044	MET
2	B	4077	PHE
2	B	4080	TYR
2	B	4159	ARG
2	B	4161	ARG
2	B	4207	MET
2	B	4655	PHE
2	B	4767	TRP
2	B	4844	LEU
2	B	4933	GLN
2	E	116	MET
2	E	125	ARG
2	E	127	MET
2	E	269	TRP

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Mol	Chain	Res	Type
2	E	280	LEU
2	E	283	ARG
2	E	299	LEU
2	E	306	LYS
2	E	341	TYR
2	E	379	HIS
2	E	631	LEU
2	E	702	TRP
2	E	866	HIS
2	E	877	ASN
2	E	902	ARG
2	E	955	LEU
2	E	959	TYR
2	E	960	MET
2	E	1112	ASP
2	E	1133	HIS
2	E	1143	TRP
2	E	1170	MET
2	E	1229	ASN
2	E	1270	LEU
2	E	1286	MET
2	E	1421	ARG
2	E	1435	TYR
2	E	1532	ASN
2	E	1647	CYS
2	E	1981	MET
2	E	2178	MET
2	E	2256	TYR
2	E	2305	CYS
2	E	2312	MET
2	E	2326	CYS
2	E	2340	PHE
2	E	2392	ARG
2	E	2475	GLN
2	E	2530	MET
2	E	2591	ARG
2	E	2618	MET
2	E	2634	ASN
2	E	2664	PHE
2	E	2688	HIS
2	E	2738	ARG
2	E	2797	PHE

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Mol	Chain	Res	Type
2	E	2806	ARG
2	E	2827	ARG
2	E	2869	ARG
2	E	2872	GLN
2	E	2914	LYS
2	E	2947	ASP
2	E	2992	GLU
2	E	3034	LYS
2	E	3043	PHE
2	E	3053	ARG
2	E	3096	PHE
2	E	3144	PHE
2	E	3158	LEU
2	E	3239	MET
2	E	3334	TRP
2	E	3348	ARG
2	E	3355	HIS
2	E	3366	ARG
2	E	3451	PHE
2	E	3516	LYS
2	E	3720	TYR
2	E	3782	MET
2	E	3933	PHE
2	E	4000	MET
2	E	4042	ARG
2	E	4044	MET
2	E	4077	PHE
2	E	4080	TYR
2	E	4159	ARG
2	E	4161	ARG
2	E	4207	MET
2	E	4655	PHE
2	E	4767	TRP
2	E	4844	LEU
2	E	4933	GLN
2	G	116	MET
2	G	125	ARG
2	G	127	MET
2	G	269	TRP
2	G	280	LEU
2	G	283	ARG
2	G	299	LEU

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Mol	Chain	Res	Type
2	G	306	LYS
2	G	341	TYR
2	G	379	HIS
2	G	631	LEU
2	G	702	TRP
2	G	866	HIS
2	G	877	ASN
2	G	902	ARG
2	G	955	LEU
2	G	959	TYR
2	G	960	MET
2	G	1112	ASP
2	G	1133	HIS
2	G	1143	TRP
2	G	1229	ASN
2	G	1270	LEU
2	G	1286	MET
2	G	1421	ARG
2	G	1435	TYR
2	G	1532	ASN
2	G	1647	CYS
2	G	1981	MET
2	G	2178	MET
2	G	2256	TYR
2	G	2305	CYS
2	G	2312	MET
2	G	2326	CYS
2	G	2340	PHE
2	G	2392	ARG
2	G	2475	GLN
2	G	2530	MET
2	G	2591	ARG
2	G	2618	MET
2	G	2634	ASN
2	G	2664	PHE
2	G	2688	HIS
2	G	2738	ARG
2	G	2797	PHE
2	G	2806	ARG
2	G	2827	ARG
2	G	2869	ARG
2	G	2872	GLN

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Mol	Chain	Res	Type
2	G	2914	LYS
2	G	2947	ASP
2	G	2992	GLU
2	G	3034	LYS
2	G	3043	PHE
2	G	3053	ARG
2	G	3096	PHE
2	G	3144	PHE
2	G	3158	LEU
2	G	3239	MET
2	G	3334	TRP
2	G	3348	ARG
2	G	3355	HIS
2	G	3366	ARG
2	G	3451	PHE
2	G	3516	LYS
2	G	3720	TYR
2	G	3782	MET
2	G	3933	PHE
2	G	4000	MET
2	G	4042	ARG
2	G	4044	MET
2	G	4077	PHE
2	G	4080	TYR
2	G	4159	ARG
2	G	4161	ARG
2	G	4207	MET
2	G	4655	PHE
2	G	4767	TRP
2	G	4844	LEU
2	G	4933	GLN
2	J	116	MET
2	J	125	ARG
2	J	127	MET
2	J	269	TRP
2	J	280	LEU
2	J	283	ARG
2	J	299	LEU
2	J	306	LYS
2	J	341	TYR
2	J	379	HIS
2	J	631	LEU

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Mol	Chain	Res	Type
2	J	702	TRP
2	J	866	HIS
2	J	877	ASN
2	J	902	ARG
2	J	955	LEU
2	J	959	TYR
2	J	960	MET
2	J	1112	ASP
2	J	1133	HIS
2	J	1143	TRP
2	J	1229	ASN
2	J	1270	LEU
2	J	1286	MET
2	J	1421	ARG
2	J	1435	TYR
2	J	1532	ASN
2	J	1647	CYS
2	J	1981	MET
2	J	2178	MET
2	J	2256	TYR
2	J	2305	CYS
2	J	2312	MET
2	J	2326	CYS
2	J	2340	PHE
2	J	2392	ARG
2	J	2475	GLN
2	J	2530	MET
2	J	2591	ARG
2	J	2618	MET
2	J	2634	ASN
2	J	2664	PHE
2	J	2688	HIS
2	J	2738	ARG
2	J	2797	PHE
2	J	2806	ARG
2	J	2827	ARG
2	J	2869	ARG
2	J	2872	GLN
2	J	2914	LYS
2	J	2947	ASP
2	J	2992	GLU
2	J	3034	LYS

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Mol	Chain	Res	Type
2	J	3043	PHE
2	J	3053	ARG
2	J	3096	PHE
2	J	3144	PHE
2	J	3158	LEU
2	J	3239	MET
2	J	3250	MET
2	J	3334	TRP
2	J	3348	ARG
2	J	3355	HIS
2	J	3366	ARG
2	J	3451	PHE
2	J	3516	LYS
2	J	3720	TYR
2	J	3782	MET
2	J	3933	PHE
2	J	4000	MET
2	J	4042	ARG
2	J	4044	MET
2	J	4077	PHE
2	J	4080	TYR
2	J	4159	ARG
2	J	4161	ARG
2	J	4207	MET
2	J	4655	PHE
2	J	4767	TRP
2	J	4844	LEU
2	J	4933	GLN
2	J	5014	TYR
3	C	37	TYR
3	C	98	ASP
3	C	104	TYR
3	C	105	ASN
3	F	37	TYR
3	F	98	ASP
3	F	104	TYR
3	F	105	ASN
3	K	37	TYR
3	K	98	ASP
3	K	104	TYR
3	K	105	ASN
3	M	37	TYR

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Mol	Chain	Res	Type
3	M	98	ASP
3	M	104	TYR
3	M	105	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	65	GLN
1	H	25	HIS
1	I	25	HIS
2	B	23	GLN
2	B	203	ASN
2	B	273	HIS
2	B	879	HIS
2	B	904	HIS
2	B	1220	GLN
2	B	1300	HIS
2	B	3318	ASN
2	B	3605	HIS
2	B	3960	GLN
2	B	3970	GLN
2	E	23	GLN
2	E	203	ASN
2	E	273	HIS
2	E	879	HIS
2	E	904	HIS
2	E	1300	HIS
2	E	2574	HIS
2	E	3311	HIS
2	E	3318	ASN
2	E	3605	HIS
2	E	3960	GLN
2	E	3970	GLN
2	E	4714	ASN
2	G	23	GLN
2	G	203	ASN
2	G	273	HIS
2	G	879	HIS
2	G	1300	HIS
2	G	2574	HIS
2	G	3318	ASN

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Mol	Chain	Res	Type
2	G	3605	HIS
2	G	3860	ASN
2	G	3870	ASN
2	G	3960	GLN
2	G	3970	GLN
2	J	23	GLN
2	J	203	ASN
2	J	273	HIS
2	J	879	HIS
2	J	904	HIS
2	J	1220	GLN
2	J	1300	HIS
2	J	3318	ASN
2	J	3605	HIS
3	C	105	ASN
3	F	105	ASN
3	K	105	ASN
3	M	105	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	$\# Z  > 2$
5	ATP	E	5102	-	28,33,33	0.62	0	34,52,52	0.76	2 (5%)
5	ATP	G	5102	-	28,33,33	0.62	0	34,52,52	0.77	2 (5%)
6	CFF	J	5103	-	8,15,15	2.21	3 (37%)	8,23,23	1.23	1 (12%)
5	ATP	J	5102	-	28,33,33	0.63	0	34,52,52	0.76	2 (5%)
5	ATP	B	5102	-	28,33,33	0.62	0	34,52,52	0.77	2 (5%)
6	CFF	G	5103	-	8,15,15	2.21	3 (37%)	8,23,23	1.21	1 (12%)
6	CFF	B	5103	-	8,15,15	2.20	3 (37%)	8,23,23	1.21	1 (12%)
6	CFF	E	5103	-	8,15,15	2.20	3 (37%)	8,23,23	1.23	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	E	5102	-	-	7/18/38/38	0/3/3/3
5	ATP	G	5102	-	-	7/18/38/38	0/3/3/3
6	CFF	J	5103	-	-	-	0/2/2/2
5	ATP	J	5102	-	-	7/18/38/38	0/3/3/3
5	ATP	B	5102	-	-	7/18/38/38	0/3/3/3
6	CFF	G	5103	-	-	-	0/2/2/2
6	CFF	B	5103	-	-	-	0/2/2/2
6	CFF	E	5103	-	-	-	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5103	CFF	C5-C6	4.21	1.48	1.41
6	J	5103	CFF	C5-C6	4.20	1.48	1.41
6	E	5103	CFF	C5-C6	4.20	1.48	1.41
6	B	5103	CFF	C5-C6	4.16	1.48	1.41
6	B	5103	CFF	C5-C4	3.91	1.45	1.39
6	J	5103	CFF	C5-C4	3.85	1.45	1.39
6	G	5103	CFF	C5-C4	3.83	1.45	1.39
6	E	5103	CFF	C5-C4	3.82	1.45	1.39
6	E	5103	CFF	C6-N1	2.19	1.41	1.38
6	J	5103	CFF	C6-N1	2.18	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	5103	CFF	C6-N1	2.16	1.41	1.38
6	B	5103	CFF	C6-N1	2.03	1.41	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5102	ATP	C4'-O4'-C1'	-2.85	107.31	109.92
5	B	5102	ATP	C4'-O4'-C1'	-2.84	107.33	109.92
5	J	5102	ATP	C4'-O4'-C1'	-2.82	107.34	109.92
5	E	5102	ATP	C4'-O4'-C1'	-2.81	107.35	109.92
6	J	5103	CFF	C5-C6-N1	-2.39	115.77	118.20
6	B	5103	CFF	C5-C6-N1	-2.36	115.80	118.20
6	G	5103	CFF	C5-C6-N1	-2.35	115.81	118.20
6	E	5103	CFF	C5-C6-N1	-2.35	115.81	118.20
5	G	5102	ATP	C5-C6-N6	2.31	123.84	120.31
5	B	5102	ATP	C5-C6-N6	2.29	123.80	120.31
5	E	5102	ATP	C5-C6-N6	2.29	123.80	120.31
5	J	5102	ATP	C5-C6-N6	2.29	123.80	120.31

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	5102	ATP	PB-O3B-PG-O2G
5	B	5102	ATP	C5'-O5'-PA-O3A
5	E	5102	ATP	PB-O3B-PG-O2G
5	E	5102	ATP	C5'-O5'-PA-O3A
5	G	5102	ATP	PB-O3B-PG-O2G
5	G	5102	ATP	C5'-O5'-PA-O3A
5	J	5102	ATP	PB-O3B-PG-O2G
5	J	5102	ATP	C5'-O5'-PA-O3A
5	B	5102	ATP	O4'-C4'-C5'-O5'
5	E	5102	ATP	O4'-C4'-C5'-O5'
5	G	5102	ATP	O4'-C4'-C5'-O5'
5	J	5102	ATP	O4'-C4'-C5'-O5'
5	B	5102	ATP	C3'-C4'-C5'-O5'
5	E	5102	ATP	C3'-C4'-C5'-O5'
5	G	5102	ATP	C3'-C4'-C5'-O5'
5	J	5102	ATP	C3'-C4'-C5'-O5'
5	B	5102	ATP	C5'-O5'-PA-O1A
5	E	5102	ATP	C5'-O5'-PA-O1A
5	G	5102	ATP	C5'-O5'-PA-O1A

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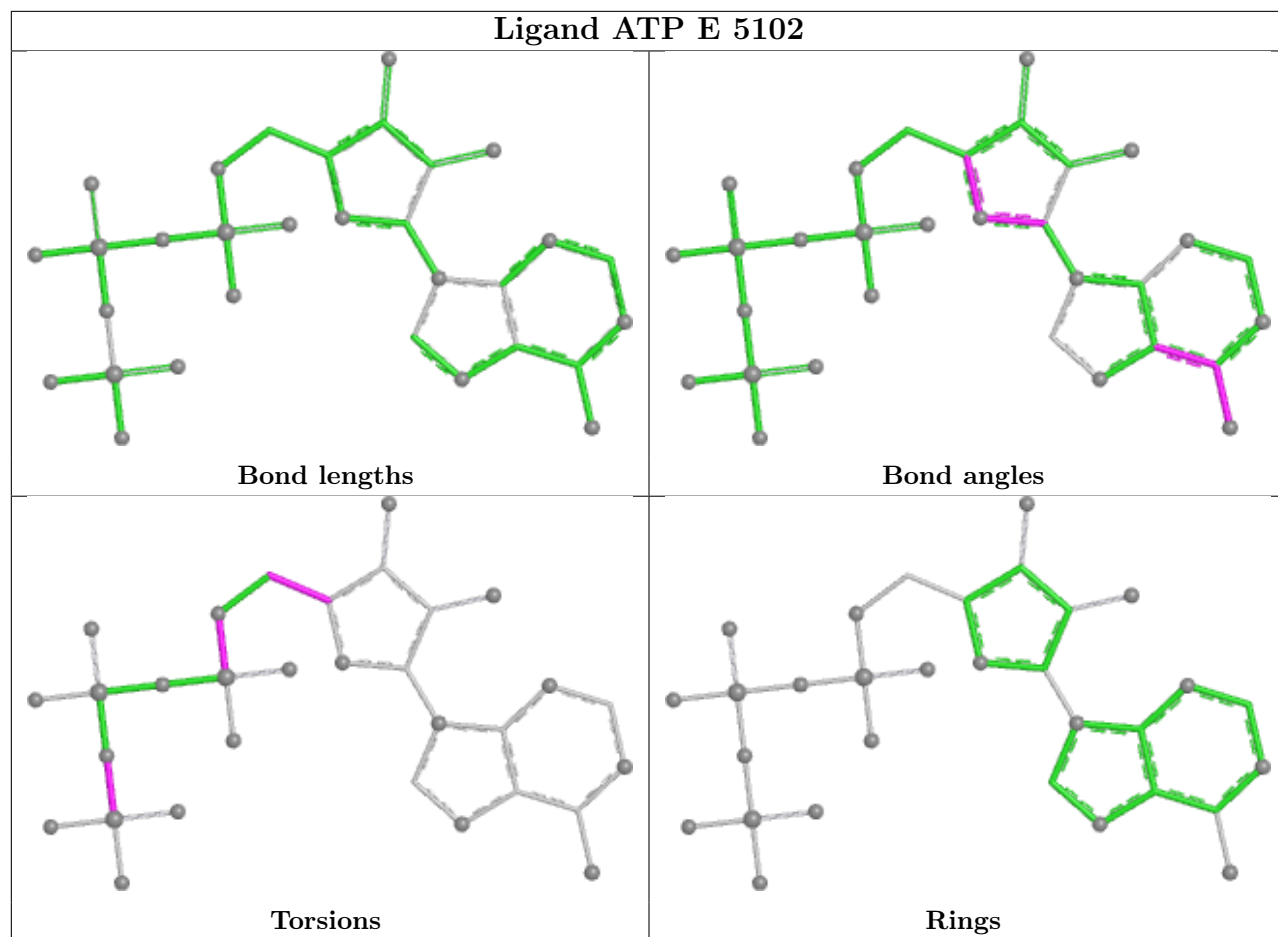
*Continued from previous page...*

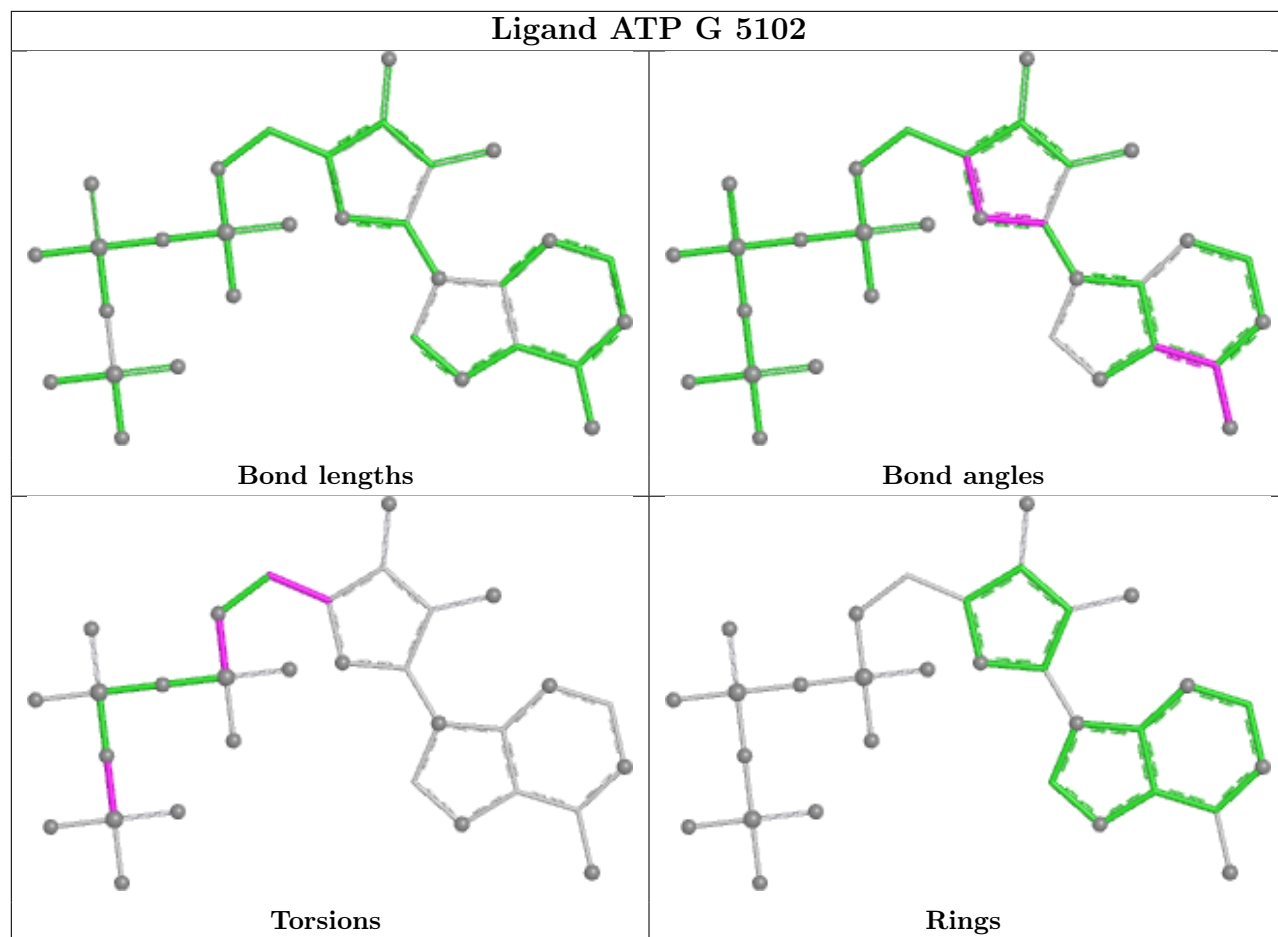
Mol	Chain	Res	Type	Atoms
5	J	5102	ATP	C5'-O5'-PA-O1A
5	B	5102	ATP	PB-O3B-PG-O1G
5	E	5102	ATP	PB-O3B-PG-O1G
5	G	5102	ATP	PB-O3B-PG-O1G
5	J	5102	ATP	PB-O3B-PG-O1G
5	B	5102	ATP	PB-O3B-PG-O3G
5	E	5102	ATP	PB-O3B-PG-O3G
5	G	5102	ATP	PB-O3B-PG-O3G
5	J	5102	ATP	PB-O3B-PG-O3G

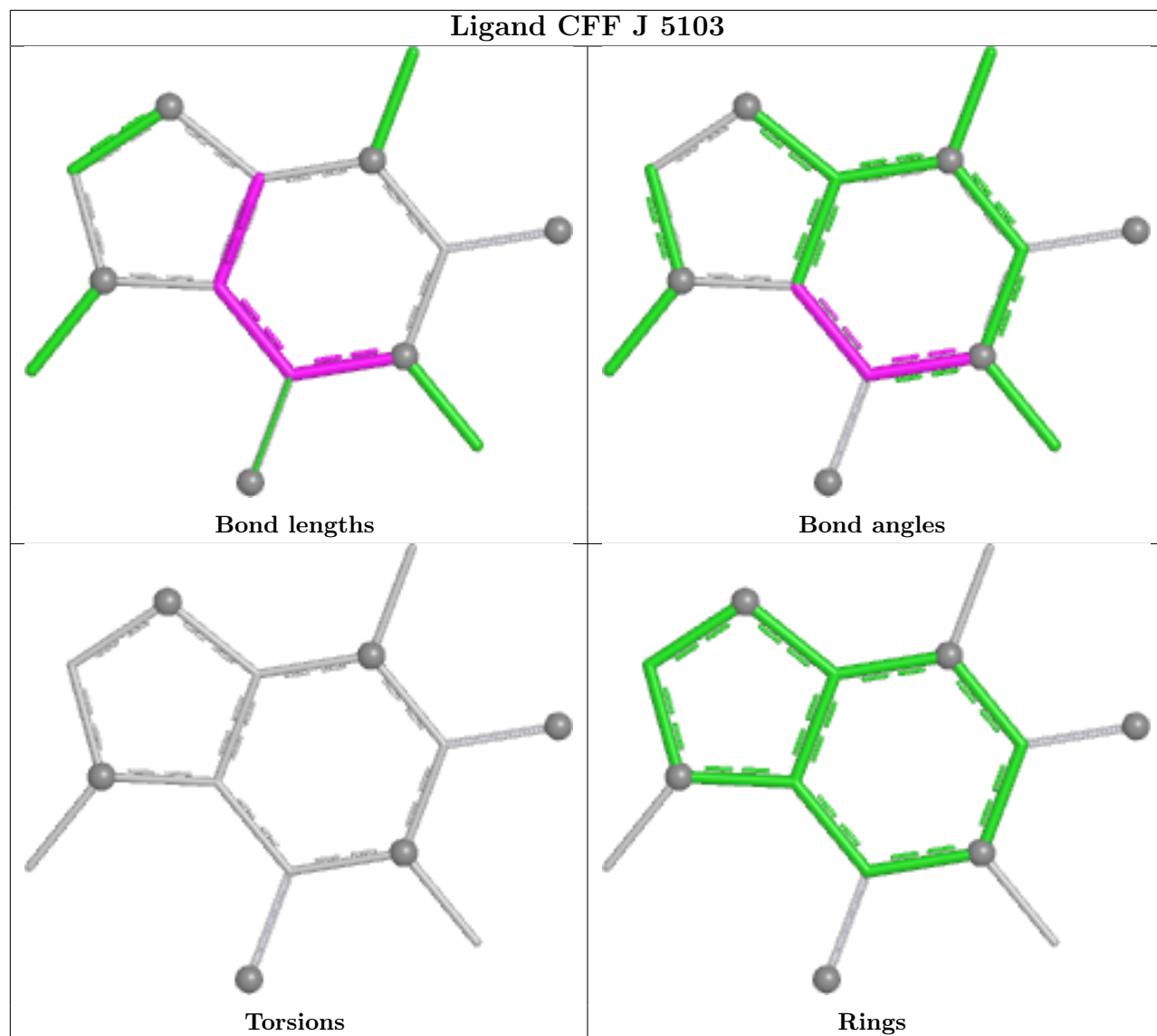
There are no ring outliers.

No monomer is involved in short contacts.

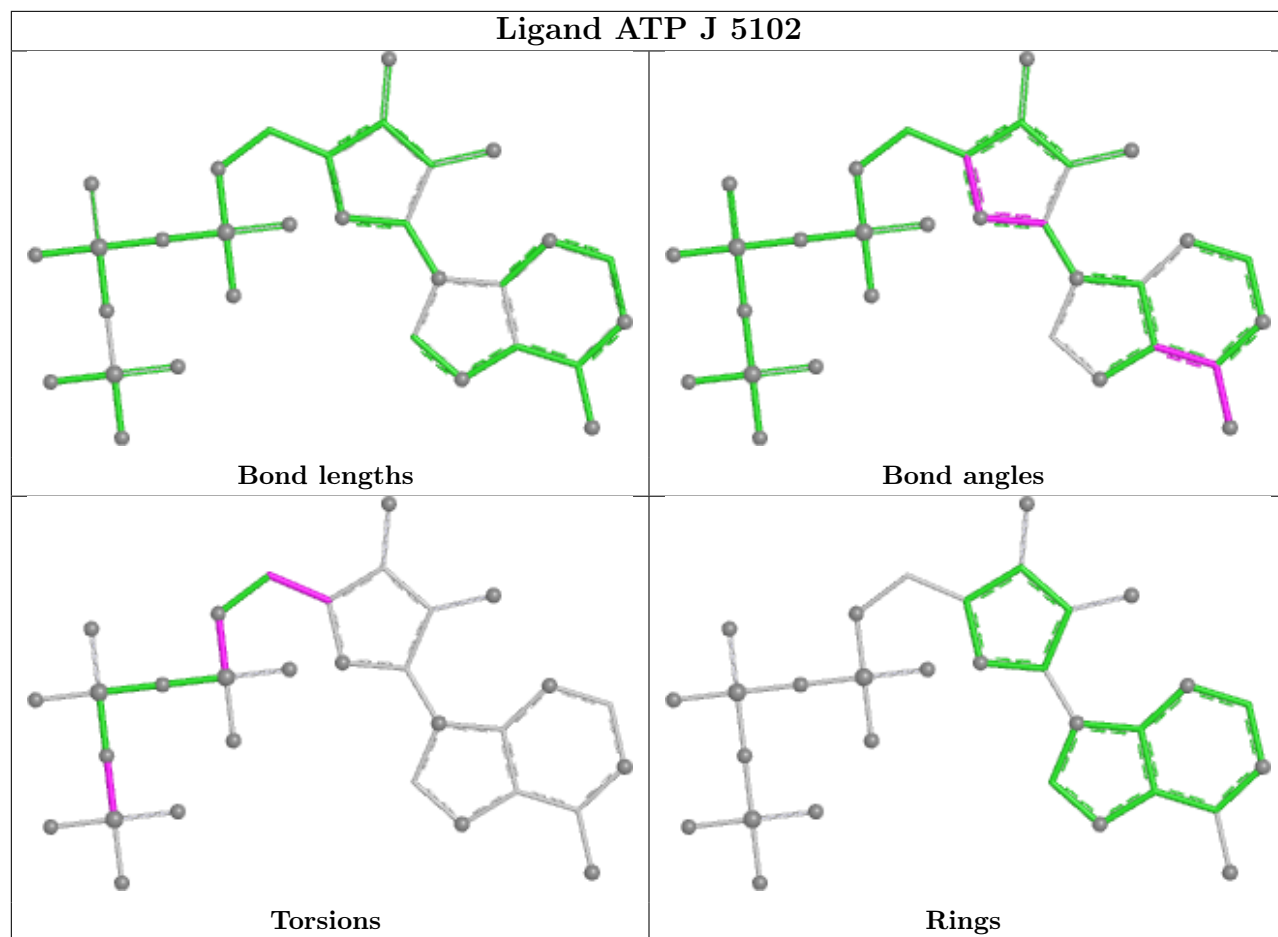
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

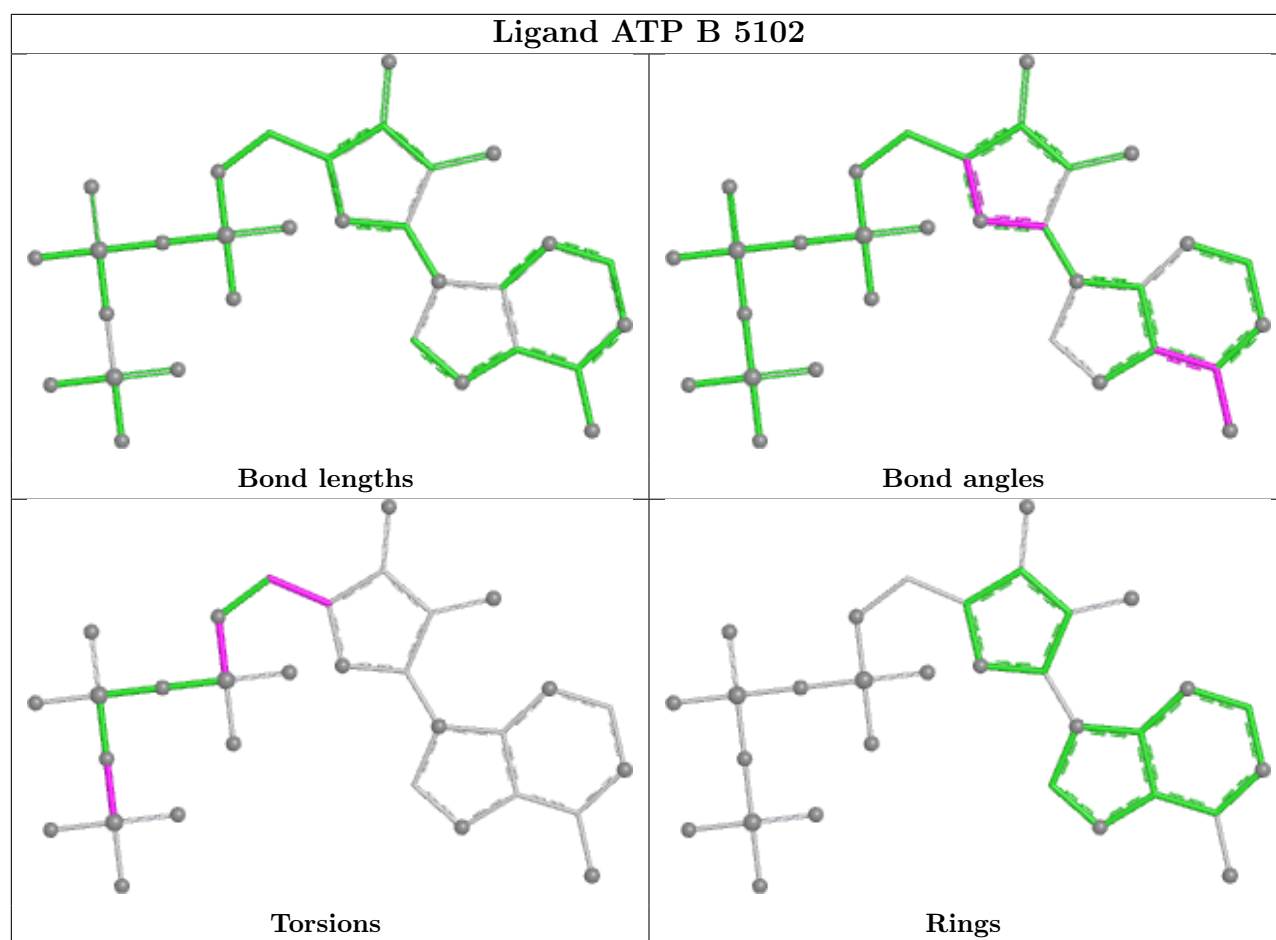


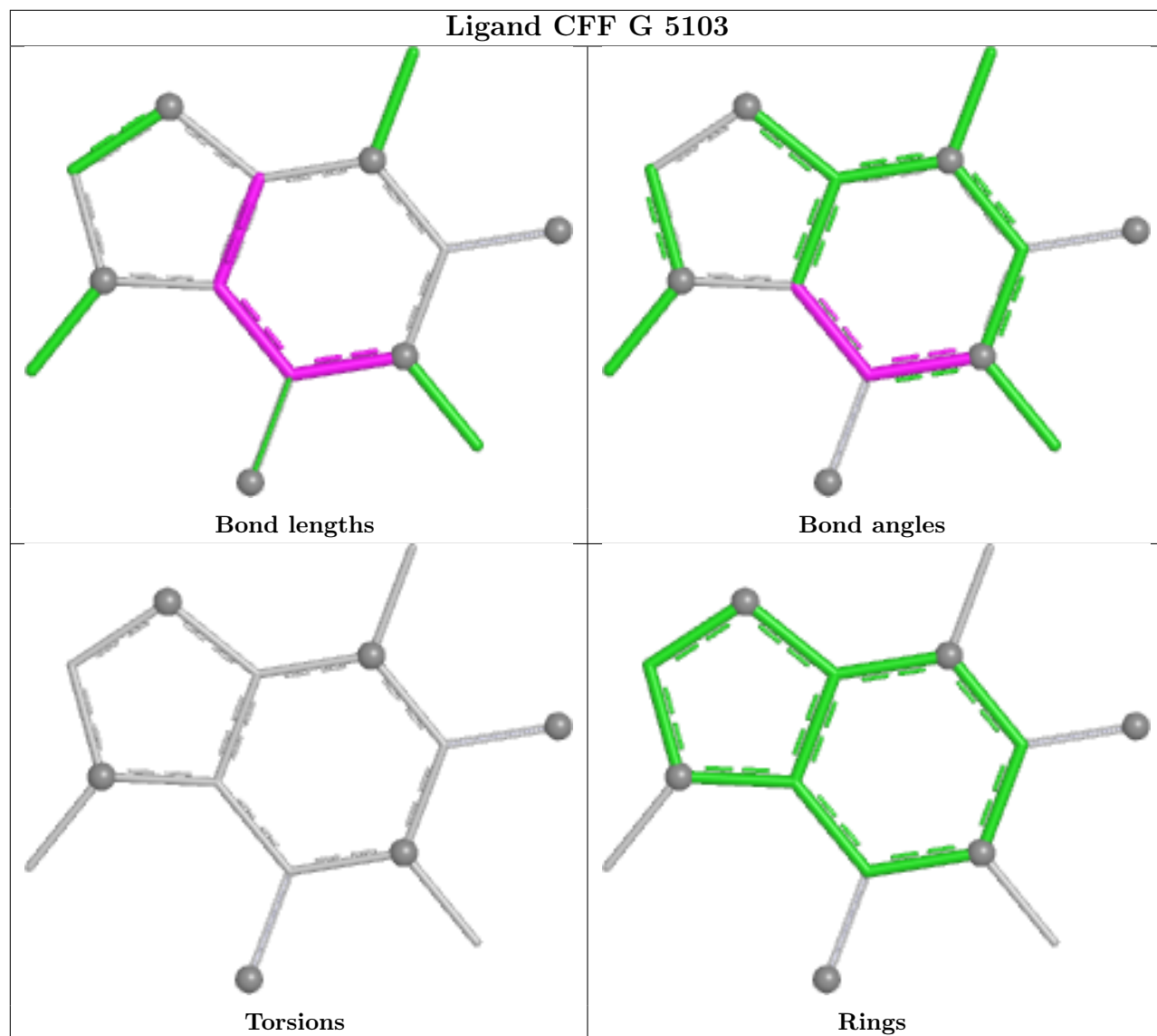


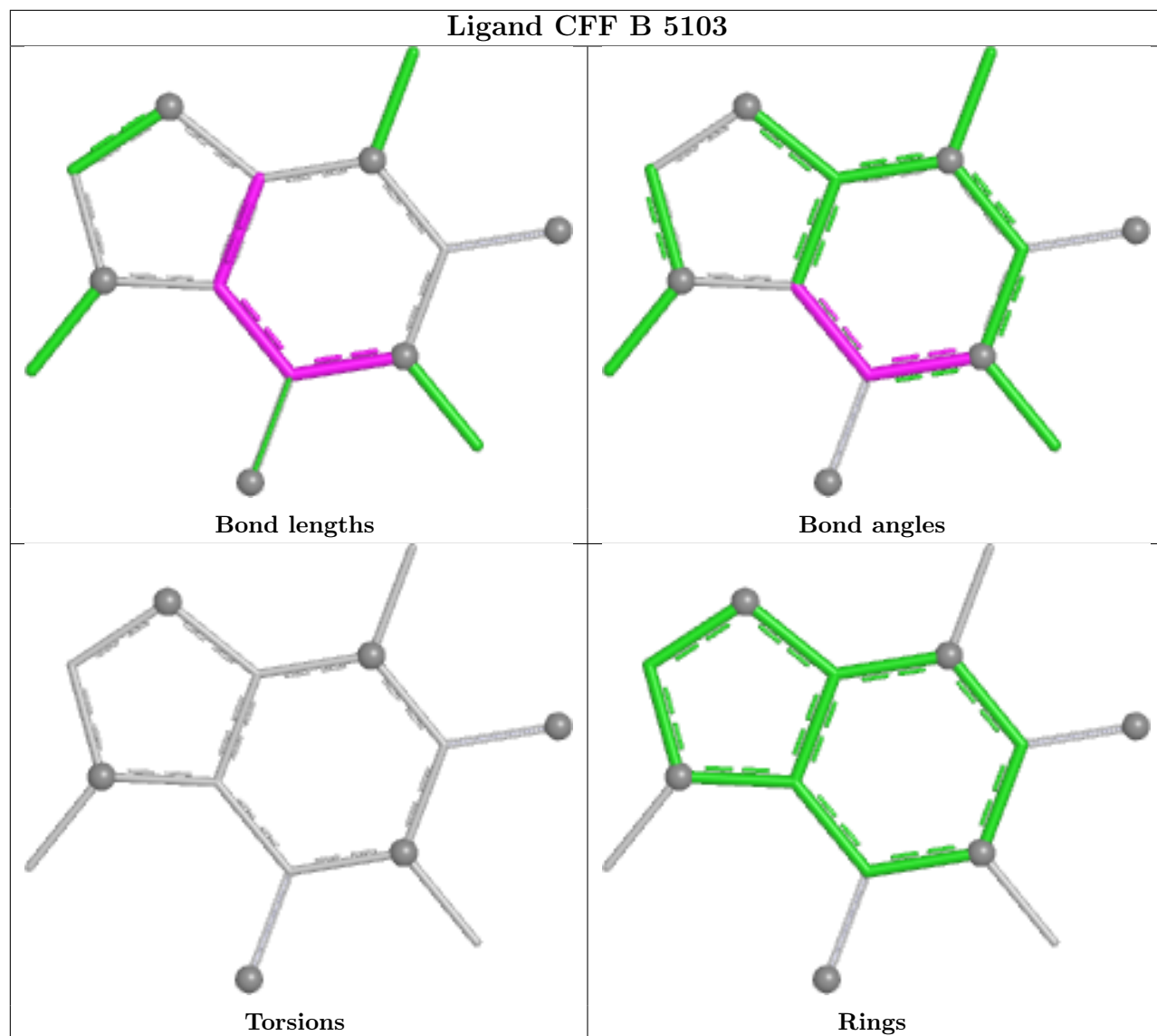


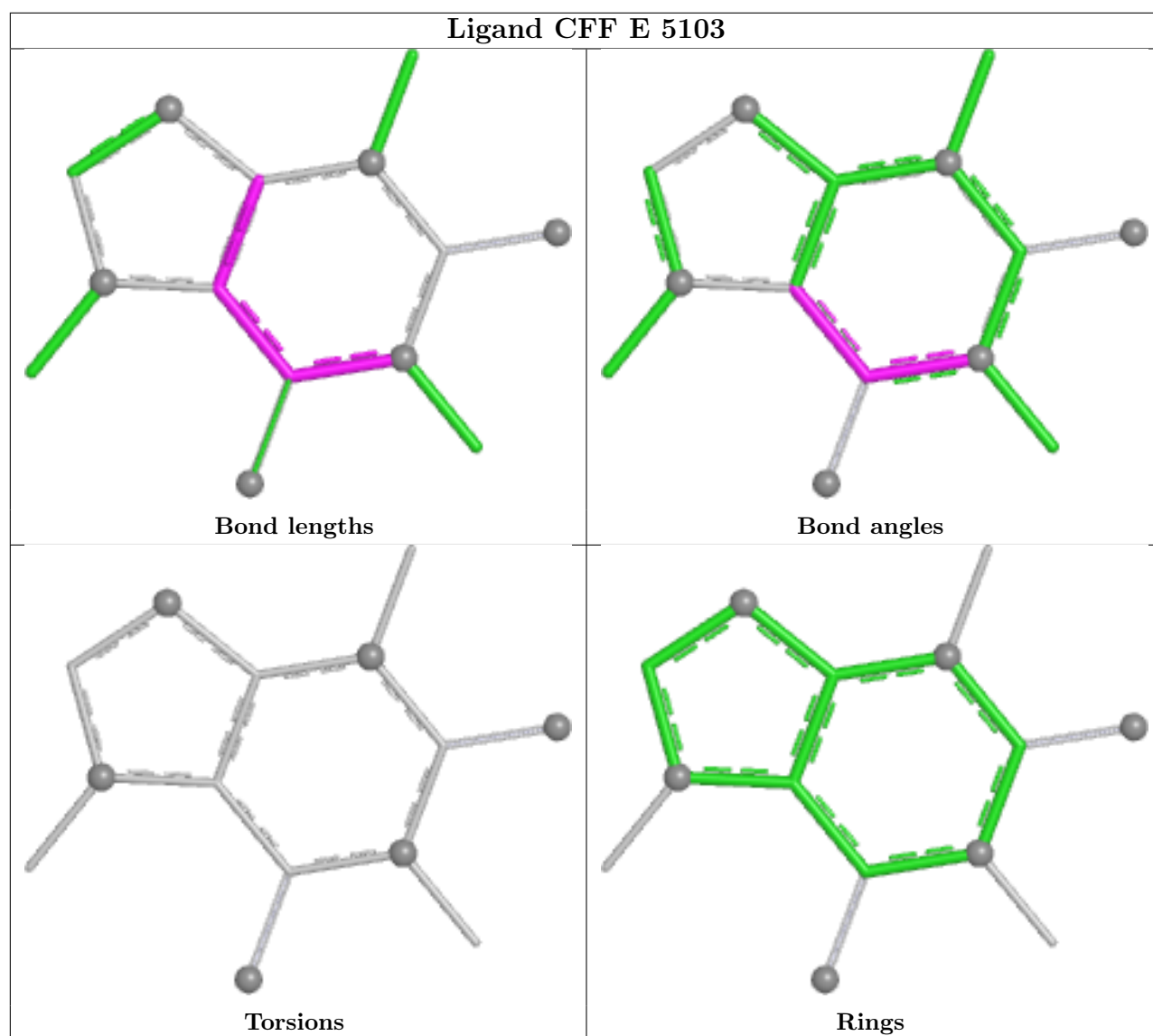












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

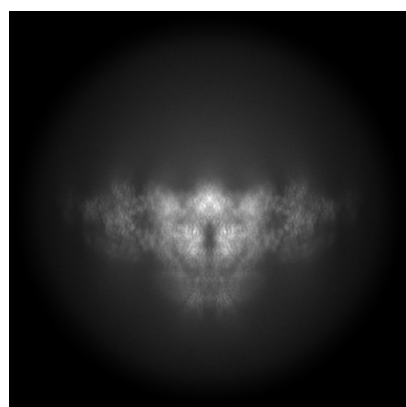
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19472. These allow visual inspection of the internal detail of the map and identification of artifacts.

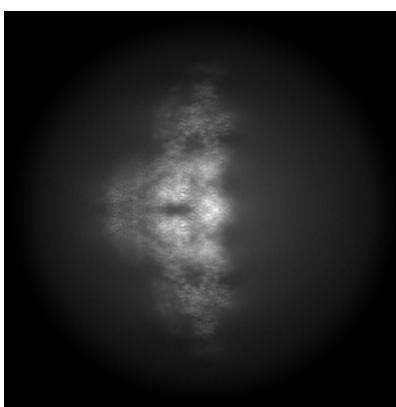
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

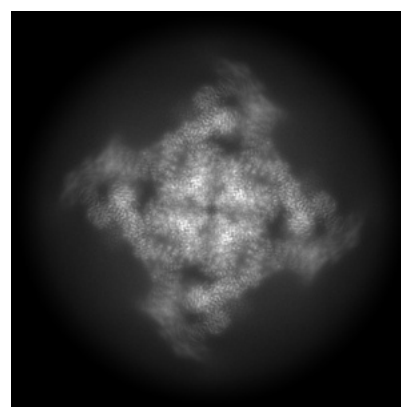
#### 6.1.1 Primary map



X



Y

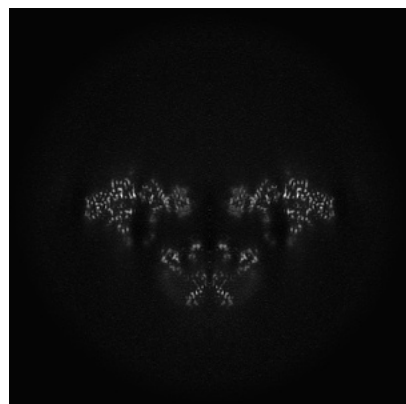


Z

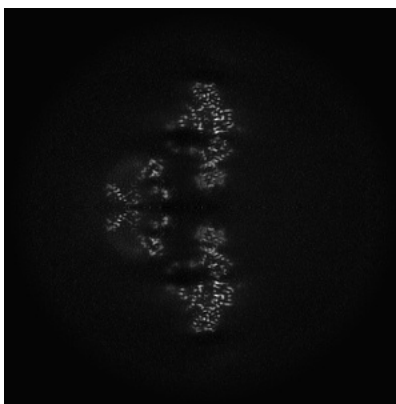
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

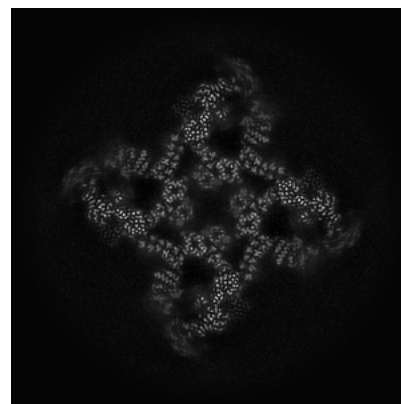
#### 6.2.1 Primary map



X Index: 168



Y Index: 168

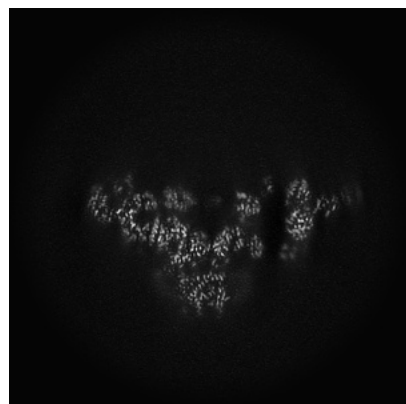


Z Index: 168

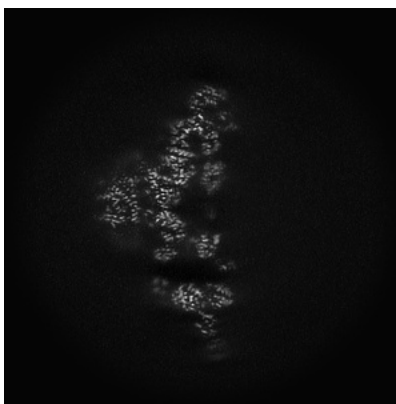
The images above show central slices of the map in three orthogonal directions.

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

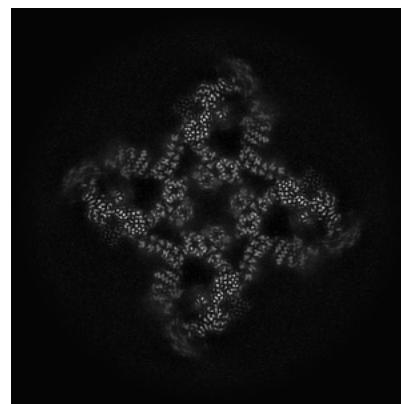
### 6.3.1 Primary map



X Index: 178



Y Index: 178

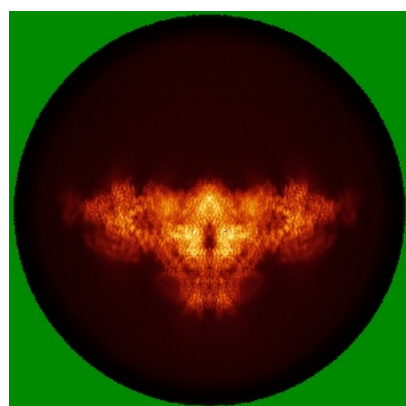


Z Index: 168

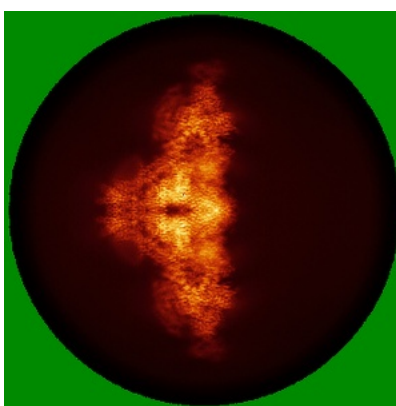
The images above show the largest variance slices of the map in three orthogonal directions.

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

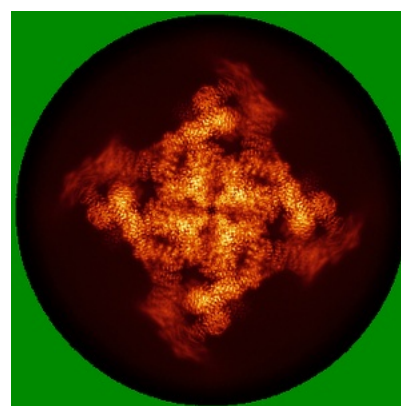
### 6.4.1 Primary map



X



Y

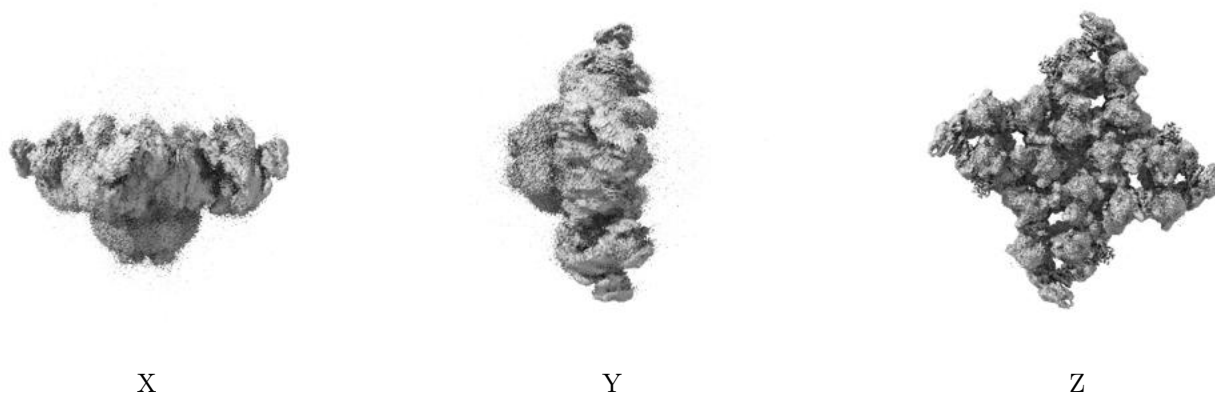


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

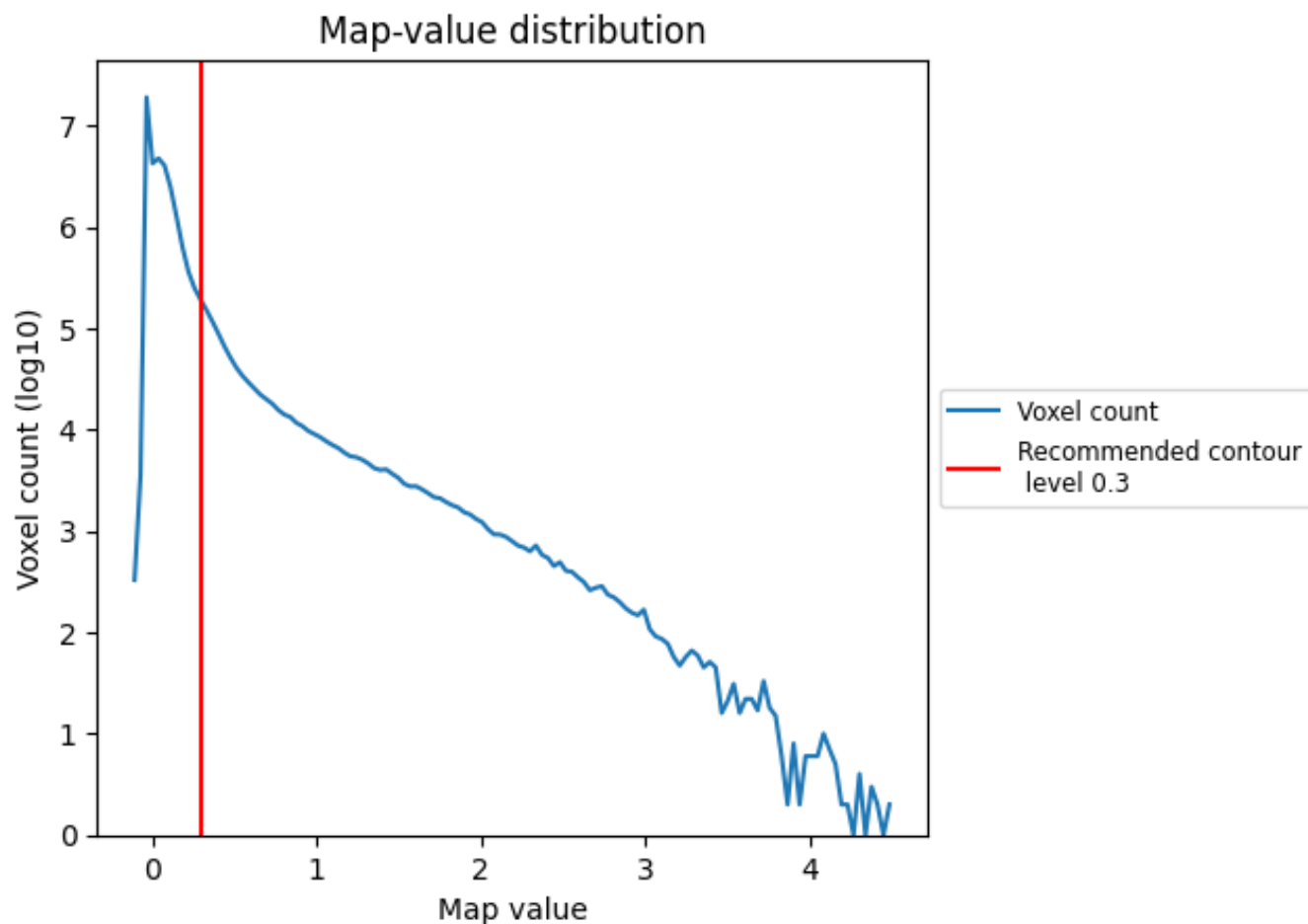
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

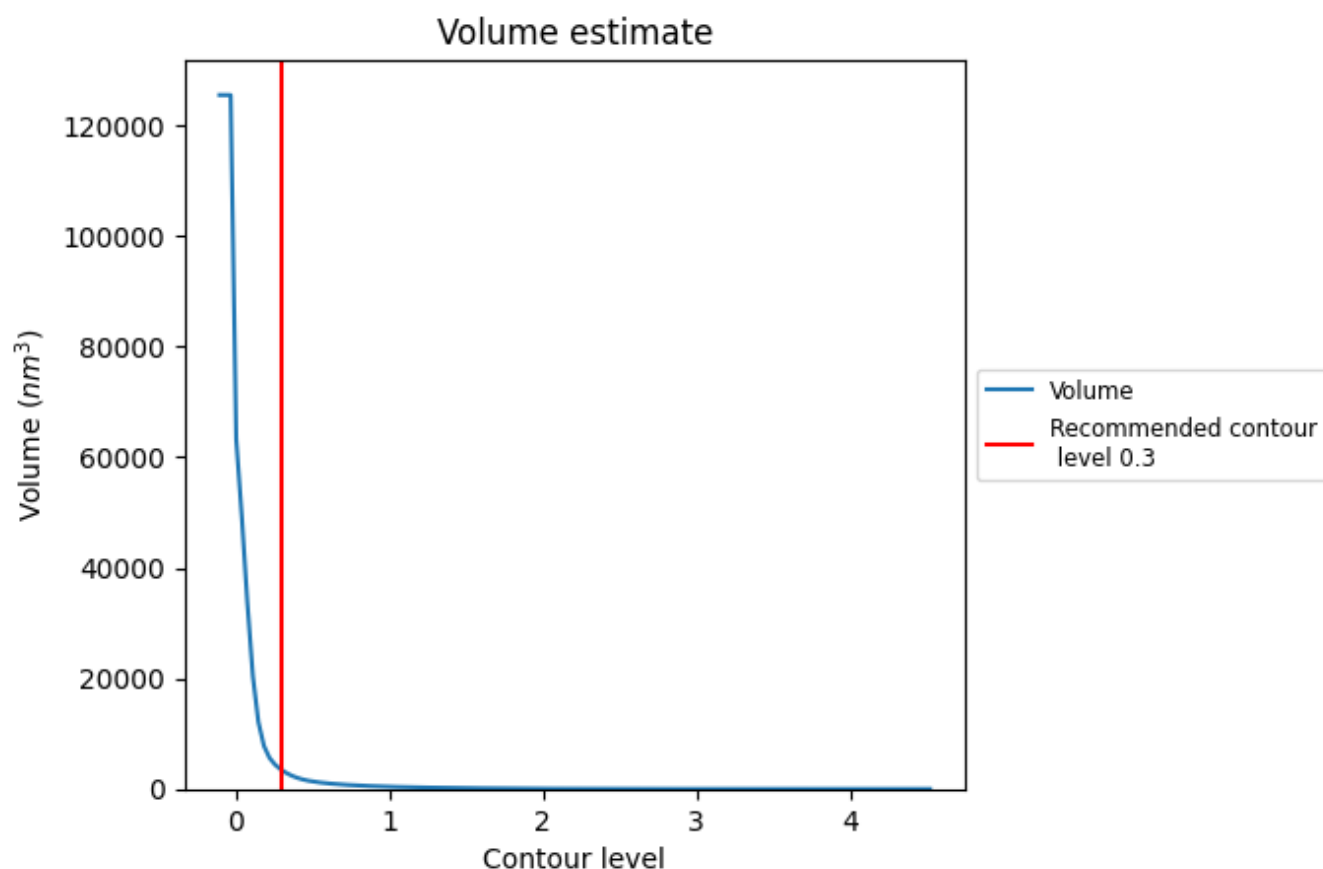
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

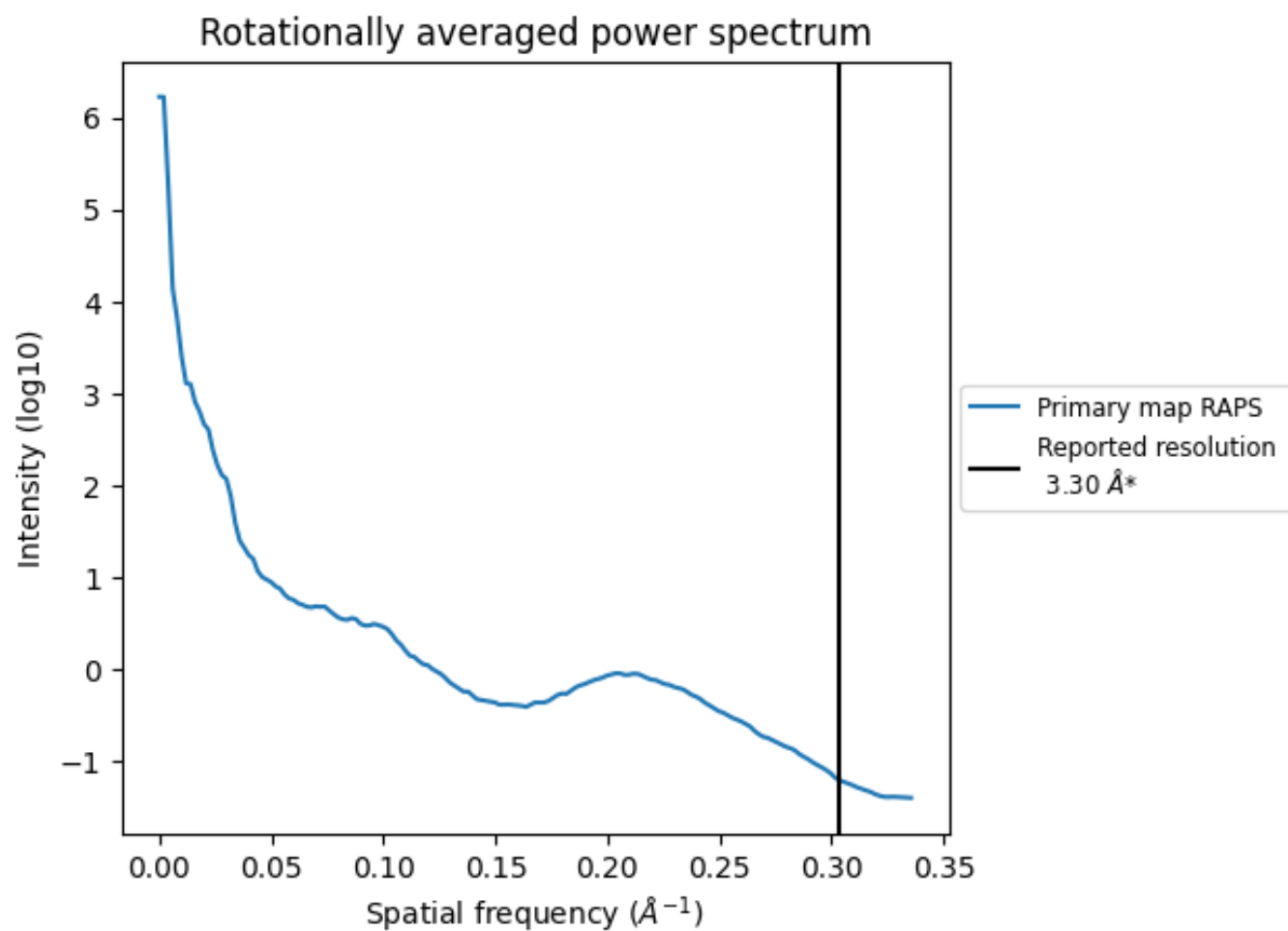
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $3395 \text{ nm}^3$ ; this corresponds to an approximate mass of 3067 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 ⓘ

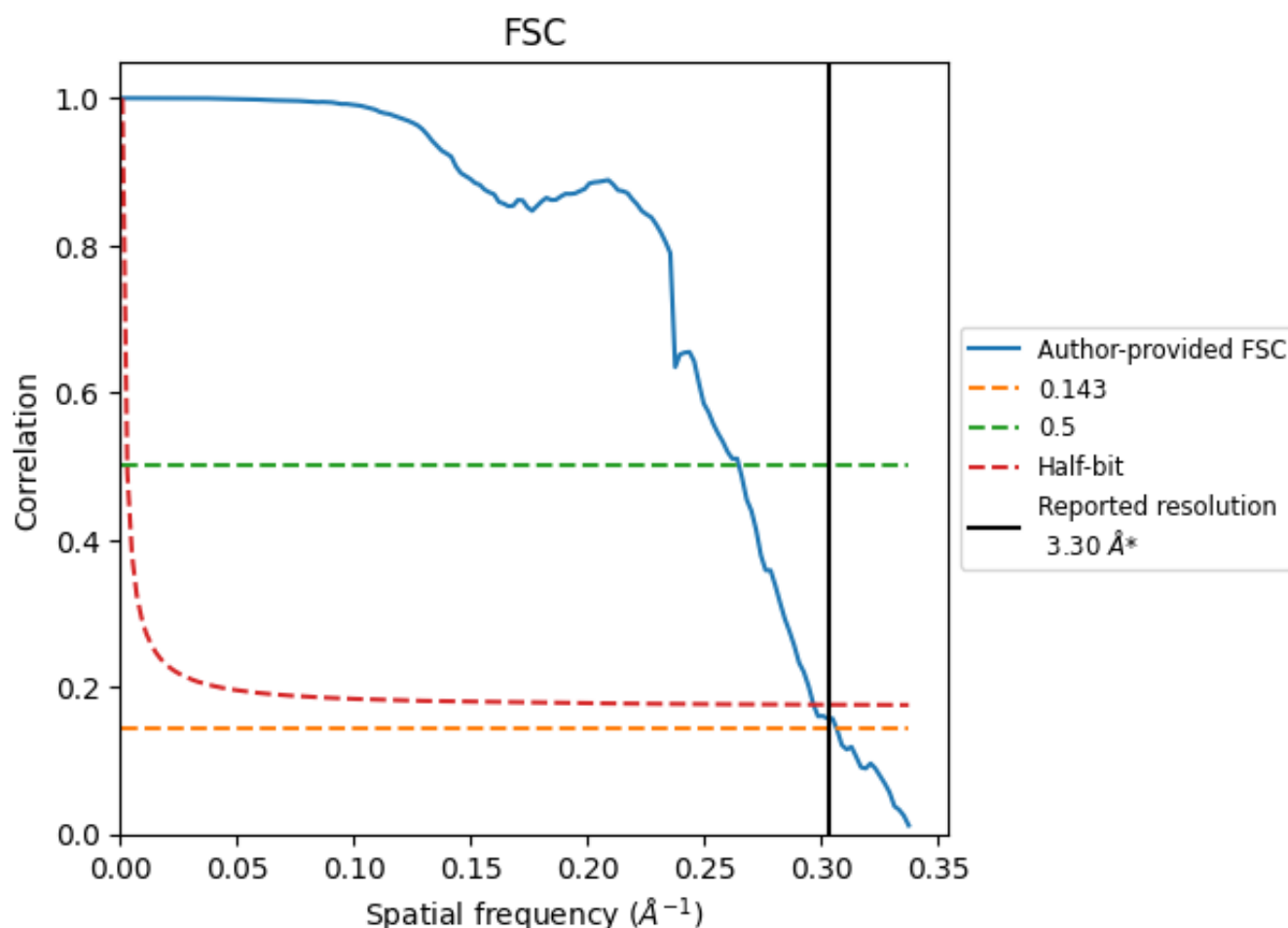


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

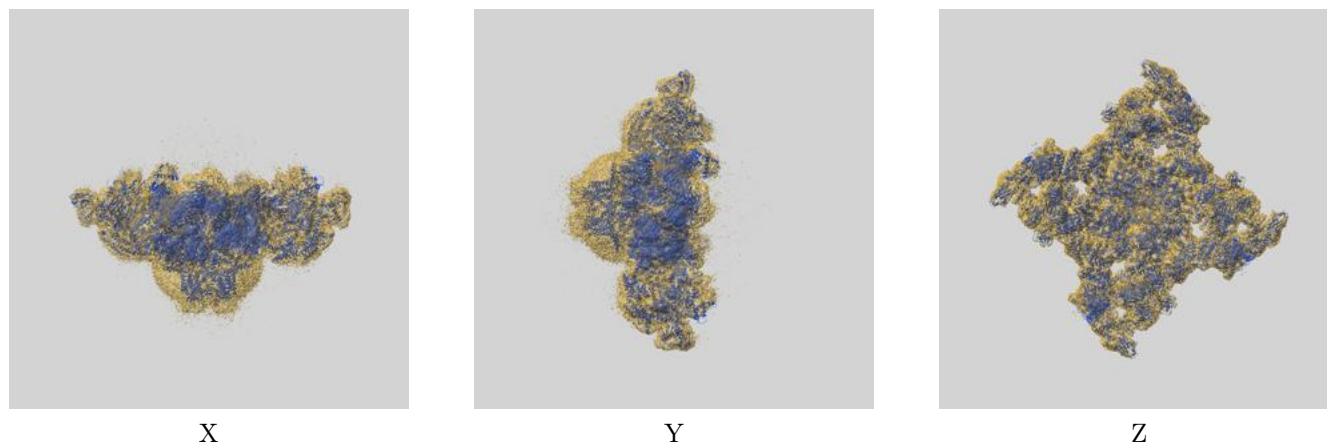
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.26	3.78	3.37
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

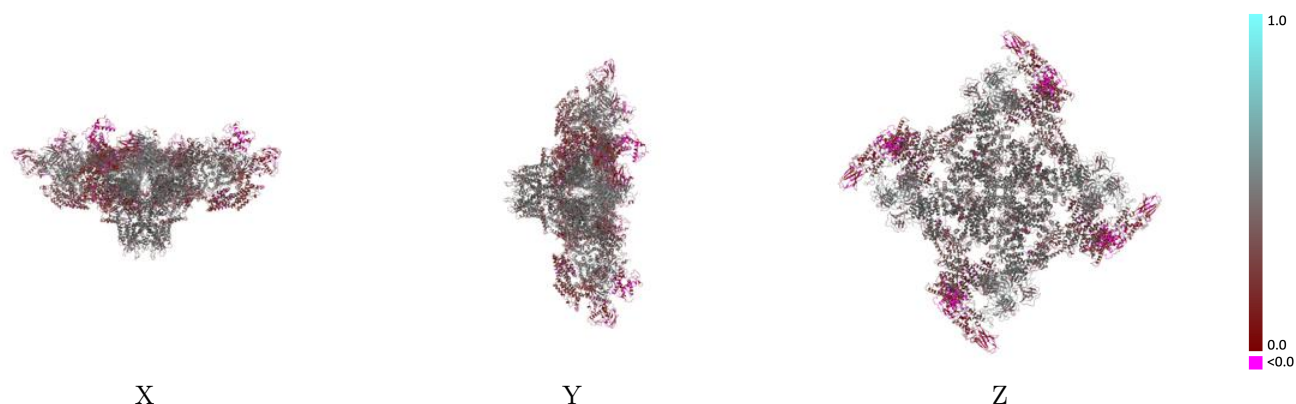
This section contains information regarding the fit between EMDB map EMD-19472 and PDB model 8RS0. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



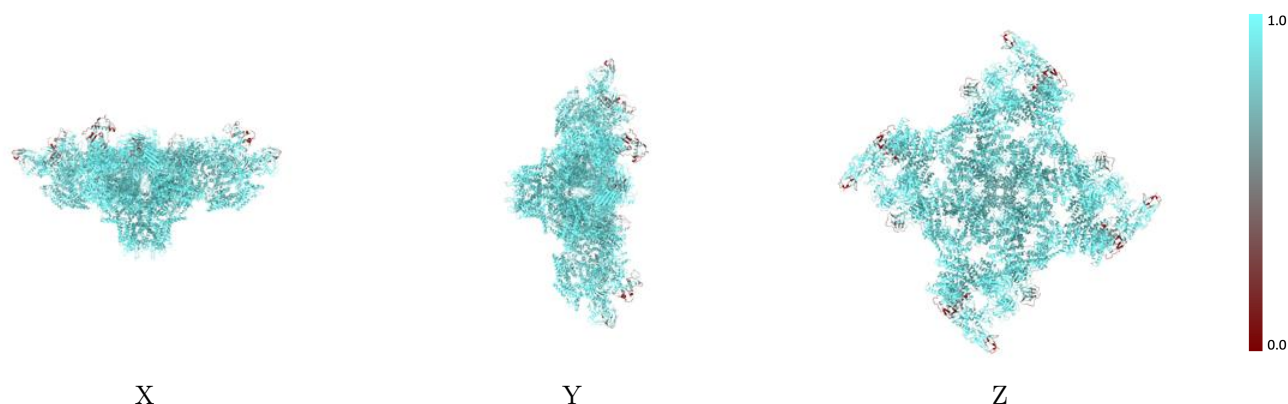
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



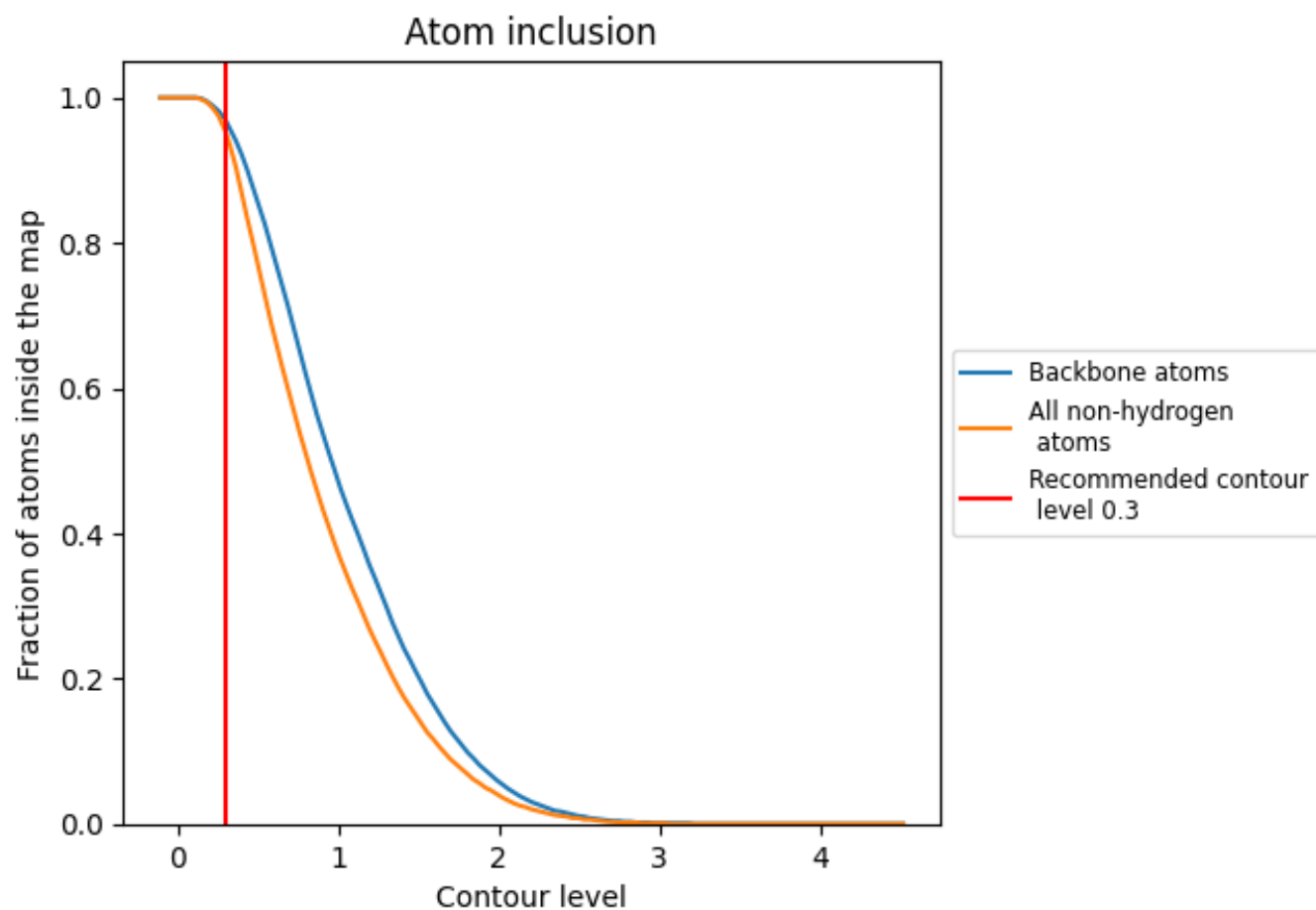
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9530	<div></div> 0.3560
A	<div></div> 0.6870	<div></div> 0.3860
B	<div></div> 0.9670	<div></div> 0.3620
C	<div></div> 0.6930	<div></div> 0.1320
D	<div></div> 0.6890	<div></div> 0.3950
E	<div></div> 0.9670	<div></div> 0.3620
F	<div></div> 0.6880	<div></div> 0.1320
G	<div></div> 0.9670	<div></div> 0.3610
H	<div></div> 0.6880	<div></div> 0.3920
I	<div></div> 0.6850	<div></div> 0.3940
J	<div></div> 0.9670	<div></div> 0.3620
K	<div></div> 0.6880	<div></div> 0.1340
M	<div></div> 0.6910	<div></div> 0.1310

