



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:06 AM UTC

PDB ID : 8UXC / pdb_00008uxc
EMDB ID : EMD-42759
Title : Structure of PKA phosphorylated human RyR2-R420Q in the primed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 2.86 Å(reported)
Based on initial model : 7UA5

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

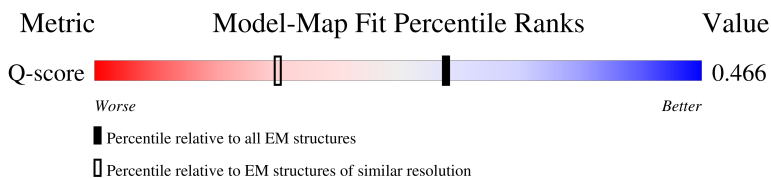
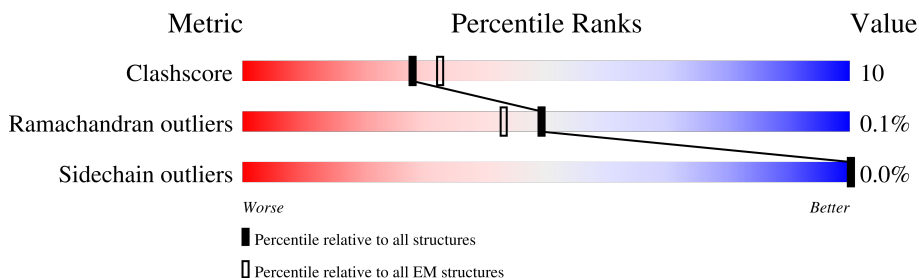
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12017 (2.36 - 3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4967	
1	B	4967	
1	C	4967	
1	D	4967	

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Mol	Chain	Length	Quality of chain
2	E	108	 82%17%
2	F	108	 83%16%
2	G	108	 84%15%
2	H	108	 82%17%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 138600 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
1	B	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
1	C	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		
1	D	4224	Total	C	N	O	S	2	0
			33769	21515	5743	6281	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	GLN	ARG	engineered mutation	UNP Q92736
B	420	GLN	ARG	engineered mutation	UNP Q92736
C	420	GLN	ARG	engineered mutation	UNP Q92736
D	420	GLN	ARG	engineered mutation	UNP Q92736

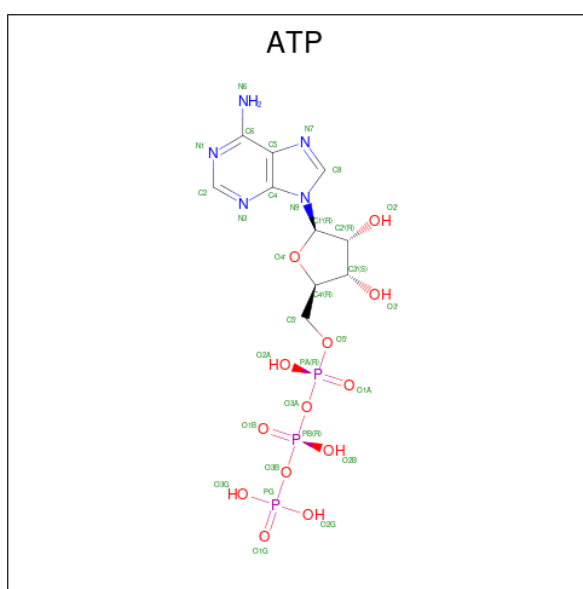
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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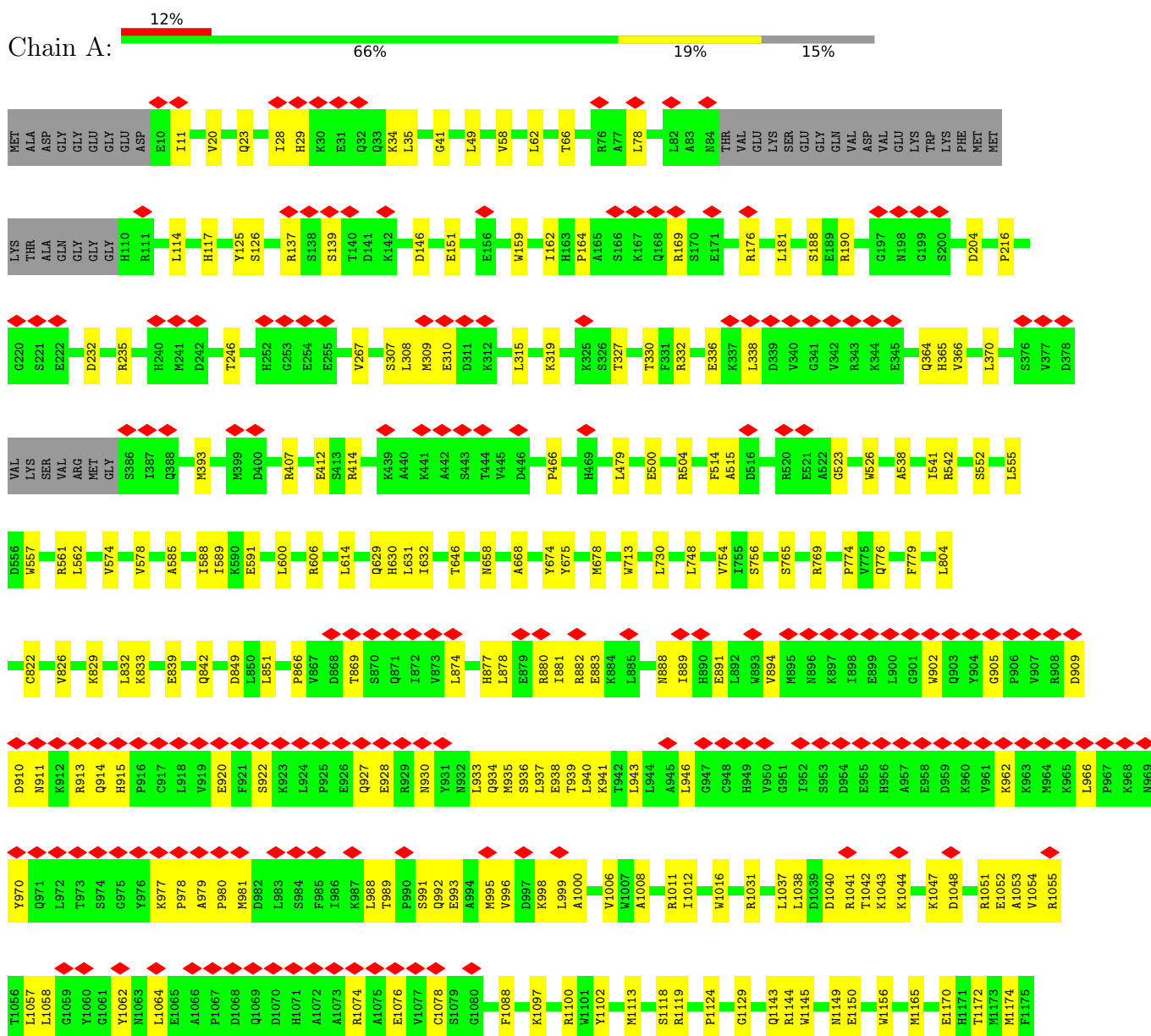
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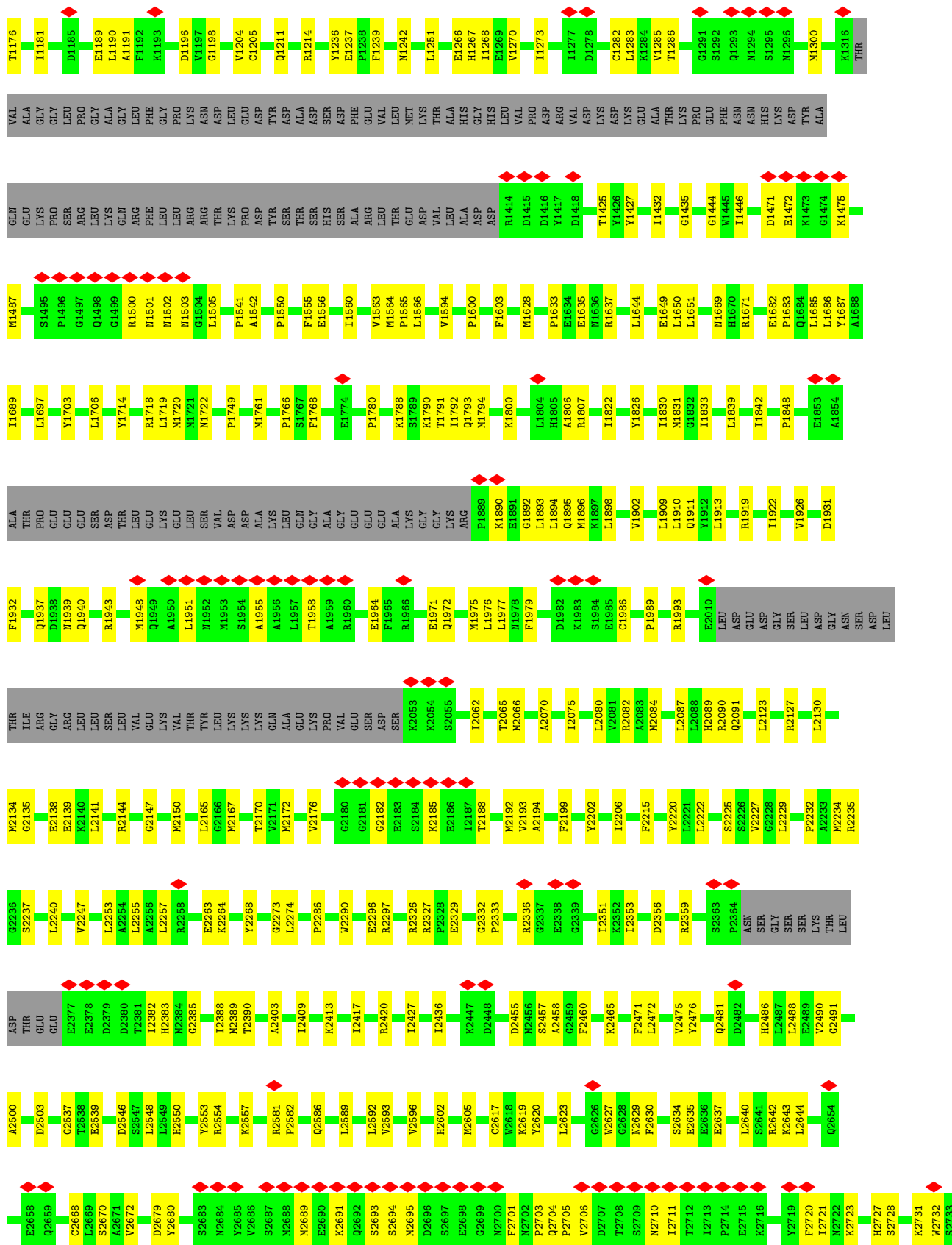
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	D	1	31	10	5	13	3	0

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: Ryanodine receptor 2



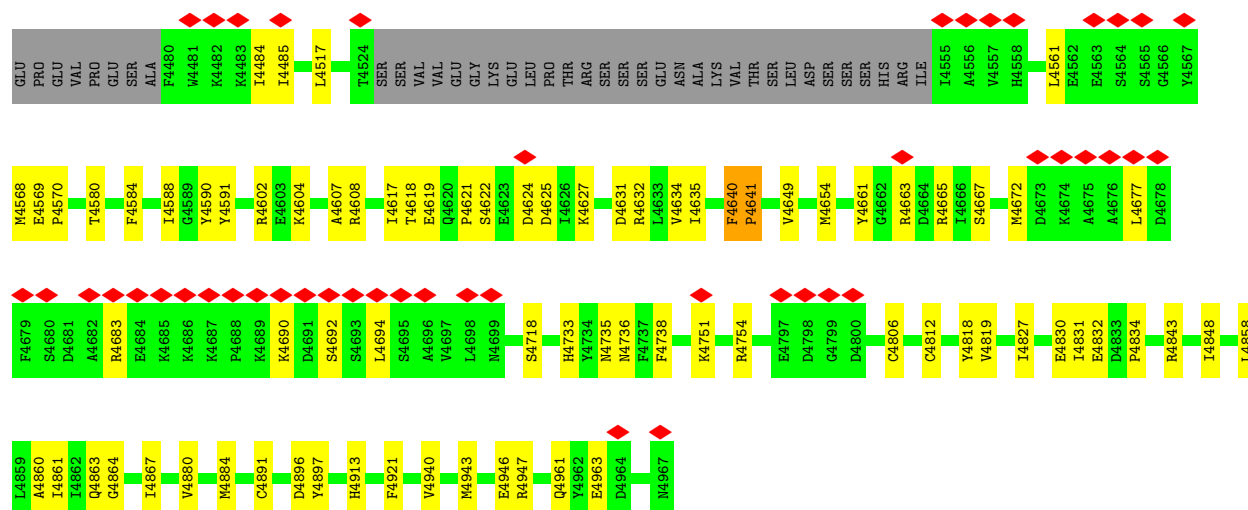


K3689	K3690	M3695	A3696	K3697	H3700	D3701	E3702	GLU	ASP	ASP	ASP	GLY	GLU	E3710	V3711	K3712	K3719	E3720	Q3728	A3729	R3730	L3731	H3732	A3737	N3770	K3777	L3793	L3796	K3797	L3803	D3804	L3805	R3810	K3813	G3816	L3817	G3818	K3819	V3820	T3821	E3822	E3823	G3824	S3825	G3826																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
SER	LYS	LYS	ALA	TRP	HIS	LYS	LEU	LEU	SER	LYS	GLN	LYS	GLN	V3899	V3900	A3901	F3903	R3904	M3905	A3906	P3907	L3908	Y3909	F3920	K3939	E3942	E3950	P3951	P3952	E3953	E3954	D3955	G3956	G3957	T3958	K3959	R3960	V3961	D3962	H3965	T3967	K3968	F3969	D3970	E3971	G3972	S3973	G3974	E3975	E3976	E3977	E3978	E3979	D3980	E3981	E3982	E3983	E3984	E3985	E3986	E3987	E3988	E3989	E3990	E3991	E3992	E3993	E3994	E3995	E3996	E3997	E3998	E3999	E3000	E3001	E3002	E3003	E3004	E3005	E3006	E3007	E3008	E3009	E3010	E3011	E3012	E3013	E3014	E3015	E3016	E3017	E3018	E3019	E3020	E3021	E3022	E3023	E3024	E3025	E3026	E3027	E3028	E3029	E3030	E3031	E3032	E3033	E3034	E3035	E3036	E3037	E3038	E3039	E3040	E3041	E3042	E3043	E3044	E3045	E3046	E3047	E3048	E3049	E3050	E3051	E3052	E3053	E3054	E3055	E3056	E3057	E3058	E3059	E3060	E3061	E3062	E3063	E3064	E3065	E3066	E3067	E3068	E3069	E3070	E3071	E3072	E3073	E3074	E3075	E3076	E3077	E3078	E3079	E3080	E3081	E3082	E3083	E3084	E3085	E3086	E3087	E3088	E3089	E3090	E3091	E3092	E3093	E3094	E3095	E3096	E3097	E3098	E3099	E3100	E3101	E3102	E3103	E3104	E3105	E3106	E3107	E3108	E3109	E3110	E3111	E3112	E3113	E3114	E3115	E3116	E3117	E3118	E3119	E3120	E3121	E3122	E3123	E3124	E3125	E3126	E3127	E3128	E3129	E3130	E3131	E3132	E3133	E3134	E3135	E3136	E3137	E3138	E3139	E3140	E3141	E3142	E3143	E3144	E3145	E3146	E3147	E3148	E3149	E3150	E3151	E3152	E3153	E3154	E3155	E3156	E3157	E3158	E3159	E3160	E3161	E3162	E3163	E3164	E3165	E3166	E3167	E3168	E3169	E3170	E3171	E3172	E3173	E3174	E3175	E3176	E3177	E3178	E3179	E3180	E3181	E3182	E3183	E3184	E3185	E3186	E3187	E3188	E3189	E3190	E3191	E3192	E3193	E3194	E3195	E3196	E3197	E3198	E3199	E3200	E3201	E3202	E3203	E3204	E3205	E3206	E3207	E3208	E3209	E3210	E3211	E3212	E3213	E3214	E3215	E3216	E3217	E3218	E3219	E3220	E3221	E3222	E3223	E3224	E3225	E3226	E3227	E3228	E3229	E3230	E3231	E3232	E3233	E3234	E3235	E3236	E3237	E3238	E3239	E3240	E3241	E3242	E3243	E3244	E3245	E3246	E3247	E3248	E3249	E3250	E3251	E3252	E3253	E3254	E3255	E3256	E3257	E3258	E3259	E3260	E3261	E3262	E3263	E3264	E3265	E3266	E3267	E3268	E3269	E3270	E3271	E3272	E3273	E3274	E3275	E3276	E3277	E3278	E3279	E3280	E3281	E3282	E3283	E3284	E3285	E3286	E3287	E3288	E3289	E3290	E3291	E3292	E3293	E3294	E3295	E3296	E3297	E3298	E3299	E3300	E3301	E3302	E3303	E3304	E3305	E3306	E3307	E3308	E3309	E3310	E3311	E3312	E3313	E3314	E3315	E3316	E3317	E3318	E3319	E3320	E3321	E3322	E3323	E3324	E3325	E3326	E3327	E3328	E3329	E3330	E3331	E3332	E3333	E3334	E3335	E3336	E3337	E3338	E3339	E3340	E3341	E3342	E3343	E3344	E3345	E3346	E3347	E3348	E3349	E3350	E3351	E3352	E3353	E3354	E3355	E3356	E3357	E3358	E3359	E3360	E3361	E3362	E3363	E3364	E3365	E3366	E3367	E3368	E3369	E3370	E3371	E3372	E3373	E3374	E3375	E3376	E3377	E3378	E3379	E3380	E3381	E3382	E3383	E3384	E3385	E3386	E3387	E3388	E3389	E3390	E3391	E3392	E3393	E3394	E3395	E3396	E3397	E3398	E3399	E3400	E3401	E3402	E3403	E3404	E3405	E3406	E3407	E3408	E3409	E3410	E3411	E3412	E3413	E3414	E3415	E3416	E3417	E3418	E3419	E3420	E3421	E3422	E3423	E3424	E3425	E3426	E3427	E3428	E3429	E3430	E3431	E3432	E3433	E3434	E3435	E3436	E3437	E3438	E3439	E3440	E3441	E3442	E3443	E3444	E3445	E3446	E3447	E3448	E3449	E3450	E3451	E3452	E3453	E3454	E3455	E3456	E3457	E3458	E3459	E3460	E3461	E3462	E3463	E3464	E3465	E3466	E3467	E3468	E3469	E3470	E3471	E3472	E3473	E3474	E3475	E3476	E3477	E3478	E3479	E3480	E3481	E3482	E3483	E3484	E3485	E3486	E3487	E3488	E3489	E3490	E3491	E3492	E3493	E3494	E3495	E3496	E3497	E3498	E3499	E3500	E3501	E3502	E3503	E3504	E3505	E3506	E3507	E3508	E3509	E3510	E3511	E3512	E3513	E3514	E3515	E3516	E3517	E3518	E3519	E3520	E3521	E3522	E3523	E3524	E3525	E3526	E3527	E3528	E3529	E3530	E3531	E3532	E3533	E3534	E3535	E3536	E3537	E3538	E3539	E3540	E3541	E3542	E3543	E3544	E3545	E3546	E3547	E3548	E3549	E3550	E3551	E3552	E3553	E3554	E3555	E3556	E3557	E3558	E3559	E3560	E3561	E3562	E3563	E3564	E3565	E3566	E3567	E3568	E3569	E3570	E3571	E3572	E3573	E3574	E3575	E3576	E3577	E3578	E3579	E3580	E3581	E3582	E3583	E3584	E3585	E3586	E3587	E3588	E3589	E3590	E3591	E3592	E3593	E3594	E3595	E3596	E3597	E3598	E3599	E3600	E3601	E3602	E3603	E3604	E3605	E3606	E3607	E3608	E3609	E3610	E3611	E3612	E3613	E3614	E3615	E3616	E3617	E3618	E3619	E3620	E3621	E3622	E3623	E3624	E3625	E3626	E3627	E3628	E3629	E3630	E3631	E3632	E3633	E3634	E3635	E3636	E3637	E3638	E3639	E3640	E3641	E3642	E3643	E3644	E3645	E3646	E3647	E3648	E3649	E3650	E3651	E3652	E3653	E3654	E3655	E3656	E3657	E3658	E3659	E3660	E3661	E3662	E3663	E3664	E3665	E3666	E3667	E3668	E3669	E3670	E3671	E3672	E3673	E3674	E3675	E3676	E3677	E3678	E3679	E3680	E3681	E3682	E3683	E3684	E3685	E3686	E3687	E3688	E3689	E3690	E3691	E3692	E3693	E3694	E3695	E3696	E3697	E3698	E3699	E3700	E3701	E3702	E3703	E3704	E3705	E3706	E3707	E3708	E3709	E3710	E3711	E3712	E3713	E3714	E3715	E3716	E3717	E3718	E3719	E3720	E3721	E3722	E3723	E3724	E3725	E3726	E3727	E3728	E3729	E3730	E3731	E3732	E3733	E3734	E3735	E3736	E3737	E3738	E3739	E3740	E3741	E3742	E3743	E3744	E3745	E3746	E3747	E3748	E3749	E3750	E3751	E3752	E3753	E3754	E3755	E3756	E3757	E3758	E3759	E3760	E3761	E3762	E3763	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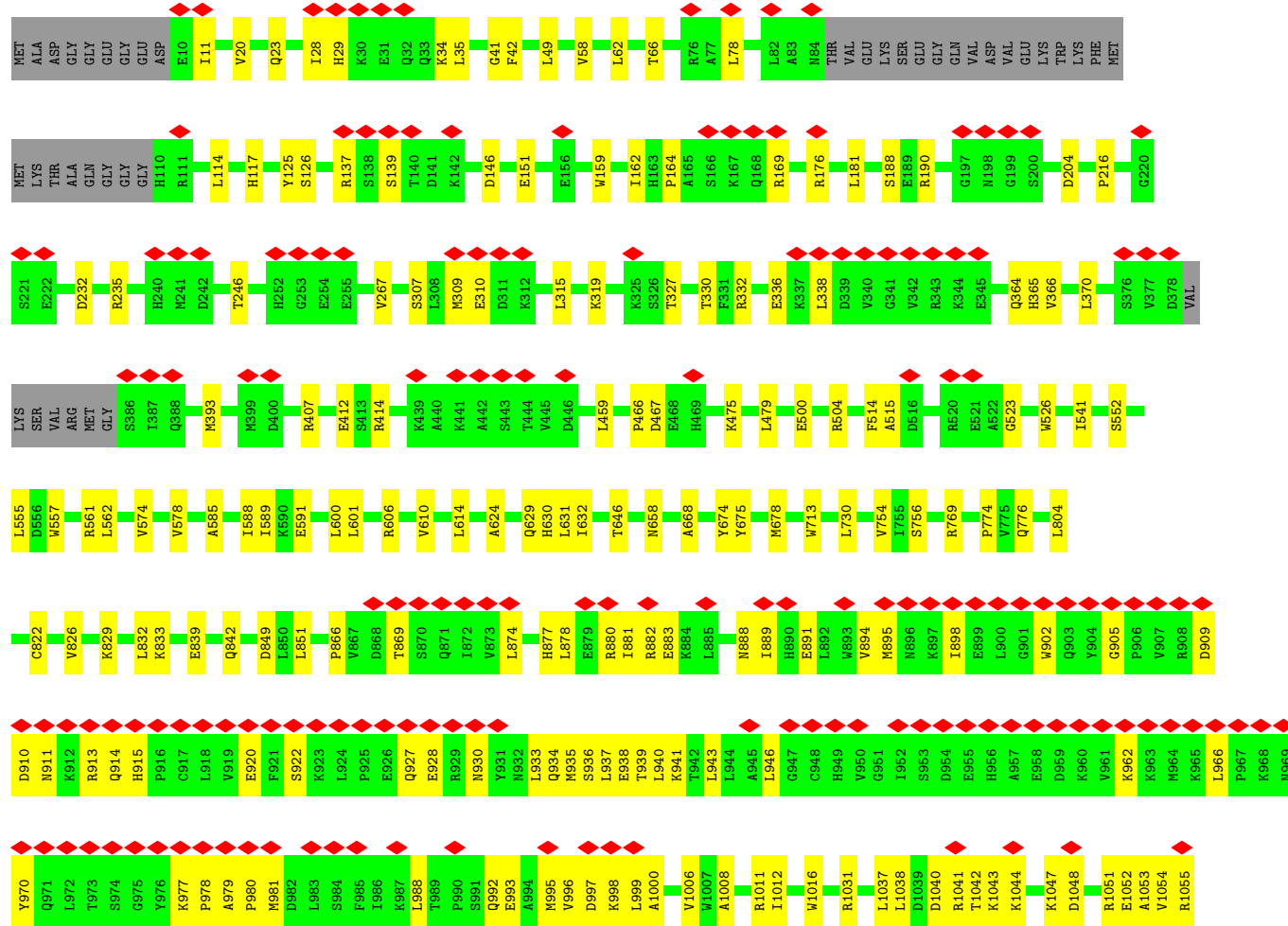








• Molecule 1: Ryanodine receptor 2



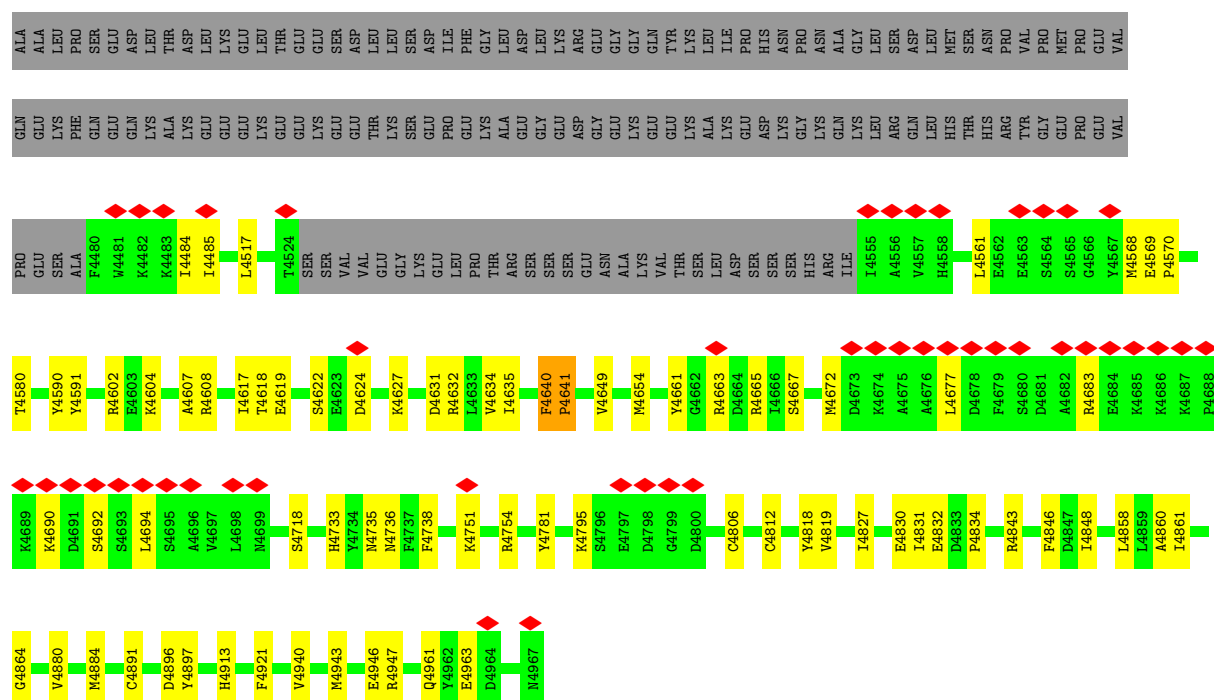


LYS	L3559	THR	PHE	L3276	Q3116	L3011	Y2939	M2867	L2800	K2736	E2658
LYS	V3600	SER	ILE	L3277	F3117	G3012	I2940	H2868	Y2801	L2737	C2668
VAL	A3601	LEU	TYR	L3281	G3118	R3016	L2941	P2869	M2802	A2738	L2669
TRP	V3599	VAL	ASP	K3282	E3119	S3019	F2943	L2870	ARG	N2739	S2670
HIS	V3600	ALA	LYS	I3283	I3122	S3020	D2944	L2871	THR	G2740	A2671
LEU	A3601	ALA	ASN	I3284	L3123	S3021	G2945	V2872	ARG	W2741	V2672
LEU	V3599	LEU	ASP	E3285	E3124	L3021	D2946	Y2874	ARG	I2742	D2679
SER	F3603	LEU	ASN	N3286	D3125	L3034	S2947	D2875	ILE	Y2743	Y2680
GLN	F3603	LEU	LYS	N3287	V3126	H3034	R2948	T2876	GLN	G2744	S2683
ARG	F3603	LEU	ARG	E3288	S3129	I3035	G2949	L2877	THR	E2745	M2684
LYS	F3603	LEU	ILE	G3289	Q3038	Q3038	K2950	E2881	SER	I2746	Y2685
ALA	F3603	LEU	GLU	I3290	T3039	T3039	G2951	K2882	GLN	Y2747	Y2686
ASP	F3603	LEU	GLN	D3291	L3133	L3040	G2952	A2883	VAL	S2748	S2687
ASP	F3603	LEU	ASN	E3292	L3134	L3041	H2953	K2884	ASP	D2749	M2688
THR	F3603	LEU	PHE	E3293	E3135	E3041	R2954	D2885	ALA	S2750	M2689
THR	F3603	LEU	THR	I3218	S3136	R3043	P2955	K2886	ALA	S2751	E2690
GLN	F3603	LEU	VAL	V3219	K3144	T3044	Y2956	E2887	HIS	K2752	K2691
ALA	F3603	LEU	GLN	E3220	S3145	V3045	E2957	Q2890	GLN	V2753	Q2692
ASP	F3603	LEU	ASP	E3223	I3146	K3046	Q2958	D2891	VAL	Q2754	S2693
PRO	F3603	LEU	ASP	I3226	V3147	L3050	E2959	I2892	VAL	P2755	S2694
GLY	F3603	LEU	ASN	R3227	E3148	S3051	I2960	L2893	ASP	L2756	M2695
LYS	F3603	LEU	TYR	I3228	I3149	V3053	A2964	K2894	ASP	M2757	D2696
VAL	F3603	LEU	ALA	Y3228	R3150	S3052	K2965	F2895	ASP	K2758	S2697
ASP	F3603	LEU	PHE	I3229	Q3151	V3053	V2966	L2896	ASP	P2759	E2698
GLU	F3603	LEU	THR	K3231	R3152	L3068	P2967	Q2897	ASP	Y2760	Q2699
LEU	F3603	LEU	LEU	P3232	R3153	L3068	L2968	I2898	ASP	K2761	M2700
LEU	F3603	LEU	LEU	H3233	L3155	T3071	P2969	M2899	ASP	L2762	F2701
ILE	F3603	LEU	ILE	V3234	L3156	E3072	L2970	R2905	ASP	L2763	N2702
ARG	F3603	LEU	ARG	M3235	L3159	E3073	D2972	Q2906	ASP	S2764	P2703
THR	F3603	LEU	THR	E3236	F3162	N3074	Q2973	K2907	ASP	E2765	Q2704
VAL	F3603	LEU	VAL	V3237	A3163	L3075	R2979	F2907	ASP	K2766	P2705
VAL	F3603	LEU	ASP	I3238	G3164	K3076	L2980	K2908	ASP	E2767	V2706
TYR	F3603	LEU	TYR	L3239	A3165	Q3077	L2981	D2909	ASP	I2770	D2707
ASN	F3603	LEU	ASN	P3240	F3166	G3078	F2982	L2910	ASP	Y2771	T2708
ARG	F3603	LEU	ARG	M3241	P3167	Q3079	L2983	E2911	ASP	S2772	S2709
ALA	F3603	LEU	ALA	H3318	R3167	F3080	S2984	L2912	ASP	N2773	N2710
LYS	F3603	LEU	LYS	K3246	V3168	T3081	A2985	D2913	ASP	P2774	I2711
LEU	F3603	LEU	LEU	S3247	F3169	HIS	R2988	T2914	ASP	I2775	T2712
LEU	F3603	LEU	LEU	R3248	L3171	THR	P2989	P2915	ASP	K2776	I2713
LEU	F3603	LEU	LEU	W3249	H3174	ARG	R2991	E2918	ASP	L2779	P2714
LYS	F3603	LEU	LYS	V3250	L3175	ASN	S2992	R2919	ASP	Y2782	E2715
GLU	F3603	LEU	GLU	M3256	H3176	PRO	H2995	K2920	ASP	W2785	F2720
PRO	F3603	LEU	PRO	R3260	N3179	K3088	K2999	Q2921	ASP	G2786	I2721
ALA	F3603	LEU	ALA	A3261	I3183	Q3089	E3000	Y2923	ASP	W2787	K2723
GLU	F3603	LEU	GLU	E3262	Y3184	Q3092	K3001	L2926	ASP	R2788	N2719
GLU	F3603	LEU	GLU	C3264	N3095	I3093	E3002	Q2927	ASP	I2789	F2720
ALA	F3603	LEU	ALA	C3265	Q3096	N3094	M3003	Q2928	ASP	E2790	I2721
ASP	F3603	LEU	ASP	C3266	T3097	V3097	V3004	L2929	ASP	R2791	K2723
ASP	F3603	LEU	ASP	L3268	A3193	T3098	T3005	I2930	ASP	S2792	H2727
VAL	F3603	LEU	VAL	M3269	A3194	T3098	S3006	E2935	ASP	T2793	S2728
VAL	F3603	LEU	VAL	S3270	A3194	T3098	K3010	K2936	ASP	E2794	K2731
VAL	F3603	LEU	VAL	M3273	A3194	T3098	K3010	H2937	ASP	G2795	S2733
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ASP	F3603	LEU	ASP	E3337	A3194	T3098	K3010	Q2938	ASP	S2797	N2735
HIS	F3603	LEU	HIS	E3337	A3194	T3098	K3010	Q2938	ASP	M2798	
LEU	F3603	LEU	LEU	E3337	A3194	T3098	K3010	Q2938	ASP		
LYS	F3603	LEU	LYS	E3337	A3194	T3098	K3010	Q2938	ASP		
ALA	F3603	LEU	ALA	E3337	A3194	T3098	K3010	Q2938	ASP		

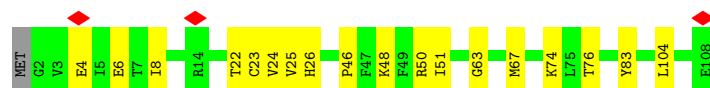
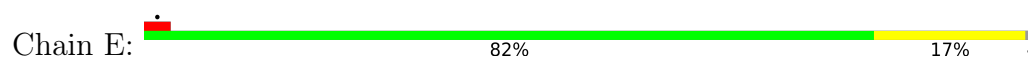
E1649	L1650	L1651	L1667	G1668	L1669	H1670	R1671	E1682	P1683	D1684	L1685	L1686	Y1687	I1688	Y1703	L1706	I1707	I1708	S1712	S1713	Y1714	R1718	L1719	G1504	M1721	M1722	P1749	M1761	P1766	S1767	F1768	E1774	P1780	K1788	S1789	T1791	L1792	Q1793	M1794	K1800	L1804	H1805	A1806															
Y1427	I1432	G1435	G1444	W1445	I1446	D1471	E1472	K1473	G1474	K1475	M1487	S1495	P1496	G1497	Q1498	G1499	R1500	N1501	N1502	N1503	G1504	L1505	P1541	A1542	P1550	F1555	I1560	V1563	M1564	P1565	L1566	V1594	P1600	F1603	M1628	P1633	E1634	E1635	N1636	R1637	L1644																	
GLU	ALA	THR	LYS	PRO	GLU	PHE	ASN	ASN	HIS	LYS	ASP	TYR	ALA	GLN	GLU	LYS	PRO	SER	ARG	LEU	ARG	GLY	THR	SER	THR	SER	ALA	ARG	LEU	THR	GLU	VAL	ASP	ALA	ASP	HIS	GLY	HIS	LEU	VAL	PRO	ASP	ARG	VAL	ASP	LYS												
TI286	FI290	G1291	S1292	Q1293	NI294	S1295	NI296	M1300	K1316	THR	VAL	ALA	GLY	GLY	LEU	PRO	GLY	ALA	GLY	LEU	PHE	GLY	ASP	TYR	THR	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	LYS														
NI1149	EI1150	W1156	M1165	EI1170	HI1171	TI1172	M1173	MI1174	FI1175	TI1176	II1181	D1185	EI1189	L11190	AI1191	FI1192	K11193	DI1196	VI1197	G11198	VI204	C1205	Q1211	R1214	Y1236	E1237	PI238	F1239	N1242	L1251	E1266	HI267	I1268	E1269	V1270	II273	II277	DI278	C1282	X1284	V1285																	
K963	H964	K965	L966	P967	K968	K969	Y970	Q971	L972	T973	S974	Y976	K977	P978	A979	P980	M981	D982	L983	S984	P985	I986	K987	L988	T989	P990	S991	Q992	E993	A994	H995	V996	D997	K998	L999	A1000	V1006	W1007	A1008	R1011	I1012	W1016	R1031	L1037	L1038	P1039	D1040	R1041	T1042	K1043	K1044	K1047						
DI048	RI051	EI052	AI053	VI054	RI055	TI056	LI058	GI059	YI060	GI061	YI062	NI063	LI064	EI065	AI066	PI067	DI068	QI069	HI071	AI072	AI073	RI074	AI075	EI076	YI077	CI078	SI079	GI080	TI081	GI082	FI088	KI097	RI100	W1101	Y1102	M1113	SI118	RI119	PI120	GI121	PI124	GI129	RI133	QI143	RI144	W1145												
Q903	Y904	G905	P906	V907	K908	D909	D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	A945	L946	G947	C948	H949	V950	G951	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962
Q776	L804	C922	V826	K929	L832	K833	E839	Q842	D849	L850	L851	L857	A860	P866	V867	D868	T869	S870	Q871	I872	V873	L874	H877	L878	E879	R880	I881	R882	E883	K884	L885	N888	I889	H890	E891	L892	M893	V894	M895	N896	K897	I898	E899	L900	G901	W902												
I541	S552	D555	W557	R561	L562	V574	V578	A585	I588	L589	K590	E591	L600	L601	R606	V610	L614	Q629	H630	L631	I632	T646	N658	A668	Q669	Y670	W673	Y674	Y675	M678	W713	V754	I755	S756	R769	P774	V775																					
LYS	SER	VAL	ARG	GLN	GLY	S386	I387	Q388	M393	M399	D400	R407	E412	S413	R414	T419	K439	A440	K441	A442	S443	T444	V445	D446	L459	P466	D467	E468	H469	K475	L479	E492	E500	R504	F514	A515	D516	R520	E521	A522	G523	W526																
MET	LYS	THR	ALA	GLN	GLY	GLY	HI10	RI11	LI14	HI17	Y125	SI26	RI37	SI38	SI39	TI40	DI41	KI42	DI46	EI51	EI56	WI59	TI62	HI63	PI64	AI65	S166	K167	Q168	RI69	RI76	LI81	SI88	EI89	RI90	G197	NI98	G199	S200	D204	P216	G220																
S221	E222	D232	R235	HI240	M241	D242	T246	HI252	G253	E254	E255	V267	S307	L308	M309	E310	D311	K312	L315	K319	K325	S326	T327	T330	F331	R332	E336	K337	L338	D339	V340	G341	V342	R343	K344	E345	Q364	H365	V366	L370	S376	V377	D378	VAL														



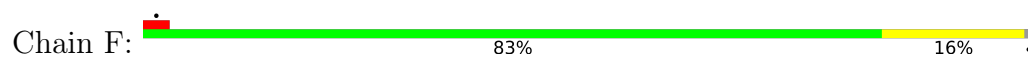




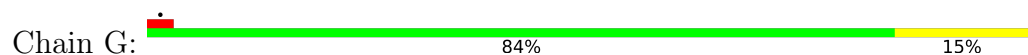
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



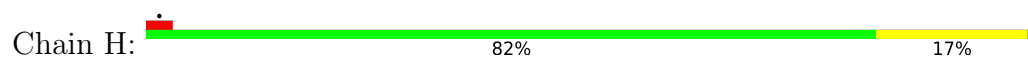
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143933	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.730	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	427.52, 427.52, 427.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.14	0/34509	0.41	2/46612 (0.0%)
1	B	0.14	0/34509	0.41	2/46612 (0.0%)
1	C	0.14	0/34509	0.41	2/46612 (0.0%)
1	D	0.14	0/34509	0.41	2/46612 (0.0%)
2	E	0.13	0/834	0.35	0/1123
2	F	0.14	0/834	0.35	0/1123
2	G	0.14	0/834	0.35	0/1123
2	H	0.13	0/834	0.35	0/1123
All	All	0.14	0/141372	0.41	8/190940 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3072	MET	CB-CG-SD	-6.03	94.61	112.70
1	B	3072	MET	CB-CG-SD	-6.03	94.62	112.70
1	C	3072	MET	CB-CG-SD	-6.03	94.62	112.70
1	D	3072	MET	CB-CG-SD	-6.03	94.62	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3235	MET	CB-CG-SD	-5.20	97.09	112.70
1	A	3235	MET	CB-CG-SD	-5.20	97.11	112.70
1	D	3235	MET	CB-CG-SD	-5.19	97.12	112.70
1	C	3235	MET	CB-CG-SD	-5.19	97.14	112.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4640	PHE	Peptide
1	B	4640	PHE	Peptide
1	C	4640	PHE	Peptide
1	D	4640	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33769	0	33450	655	0
1	B	33769	0	33450	659	0
1	C	33769	0	33450	659	0
1	D	33769	0	33450	650	0
2	E	818	0	821	13	0
2	F	818	0	821	12	0
2	G	818	0	821	11	0
2	H	818	0	821	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	1	0
4	C	62	0	24	1	0
4	D	62	0	24	1	0
All	All	138600	0	137180	2640	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 10.

All (2640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1940:GLN:HE22	1:C:1972:GLN:HE21	1.16	0.90
1:D:1940:GLN:HE22	1:D:1972:GLN:HE21	1.16	0.90
1:A:3293:GLY:H	1:A:3296:MET:HE1	1.37	0.89
1:A:1940:GLN:HE22	1:A:1972:GLN:HE21	1.16	0.89
1:B:1940:GLN:HE22	1:B:1972:GLN:HE21	1.16	0.89
1:A:4831:ILE:HG13	1:A:4843:ARG:HH21	1.38	0.89
1:D:4831:ILE:HG13	1:D:4843:ARG:HH21	1.38	0.88
1:D:3293:GLY:H	1:D:3296:MET:HE1	1.37	0.88
1:C:4831:ILE:HG13	1:C:4843:ARG:HH21	1.39	0.87
1:B:4831:ILE:HG13	1:B:4843:ARG:HH21	1.39	0.87
1:B:3293:GLY:H	1:B:3296:MET:HE1	1.37	0.87
1:C:3293:GLY:H	1:C:3296:MET:HE1	1.37	0.86
1:C:4640:PHE:CD2	1:C:4641:PRO:HD3	2.16	0.80
1:B:4640:PHE:CD2	1:B:4641:PRO:HD3	2.16	0.80
1:D:4640:PHE:CD2	1:D:4641:PRO:HD3	2.16	0.80
1:C:1790:LYS:HG2	1:C:1794:MET:HE2	1.64	0.79
1:A:4640:PHE:CD2	1:A:4641:PRO:HD3	2.16	0.79
1:A:2732:TRP:CD1	1:A:2736:LYS:HZ1	2.00	0.79
1:B:1790:LYS:HG2	1:B:1794:MET:HE2	1.64	0.78
1:D:2732:TRP:CD1	1:D:2736:LYS:HZ1	2.01	0.78
1:D:1790:LYS:HG2	1:D:1794:MET:HE2	1.64	0.78
1:A:1790:LYS:HG2	1:A:1794:MET:HE2	1.64	0.78
1:D:3197:LEU:HD23	1:D:3199:THR:H	1.49	0.78
1:C:2732:TRP:CD1	1:C:2736:LYS:HZ1	2.01	0.77
1:C:3227:ARG:NH2	1:C:3291:ASP:OD1	2.17	0.77
1:C:3197:LEU:HD23	1:C:3199:THR:H	1.49	0.77
1:A:2229:LEU:HD13	1:A:2297:ARG:HE	1.51	0.76
1:A:3197:LEU:HD23	1:A:3199:THR:H	1.49	0.76
1:B:3197:LEU:HD23	1:B:3199:THR:H	1.49	0.76
1:D:2229:LEU:HD13	1:D:2297:ARG:HE	1.51	0.76
1:B:1911:GLN:OE1	1:B:2090:ARG:NH1	2.19	0.76
1:C:2229:LEU:HD13	1:C:2297:ARG:HE	1.51	0.76
1:C:1911:GLN:OE1	1:C:2090:ARG:NH1	2.19	0.75
1:D:3227:ARG:NH2	1:D:3291:ASP:OD1	2.17	0.75
1:B:2706:VAL:HG21	1:B:2785:TRP:HE1	1.52	0.75
1:A:1911:GLN:OE1	1:A:2090:ARG:NH1	2.19	0.75
1:B:658:ASN:HD21	1:B:833:LYS:HG2	1.52	0.75
1:C:2706:VAL:HG21	1:C:2785:TRP:HE1	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:HD21	1:A:833:LYS:HG2	1.52	0.74
1:A:3227:ARG:NH2	1:A:3291:ASP:OD1	2.17	0.74
1:D:2500:ALA:O	1:D:2554:ARG:NH1	2.20	0.74
1:B:2229:LEU:HD13	1:B:2297:ARG:HE	1.51	0.74
1:C:3674:THR:O	1:C:3679:LYS:NZ	2.20	0.74
1:D:1911:GLN:OE1	1:D:2090:ARG:NH1	2.19	0.74
1:A:2706:VAL:HG21	1:A:2785:TRP:HE1	1.52	0.74
1:B:2500:ALA:O	1:B:2554:ARG:NH1	2.20	0.74
1:B:2732:TRP:CD1	1:B:2736:LYS:HZ1	2.04	0.74
1:A:2500:ALA:O	1:A:2554:ARG:NH1	2.20	0.74
1:D:658:ASN:HD21	1:D:833:LYS:HG2	1.52	0.74
1:D:365:HIS:HB2	1:D:393:MET:HE1	1.69	0.74
1:B:365:HIS:HB2	1:B:393:MET:HE1	1.69	0.74
1:C:658:ASN:HD21	1:C:833:LYS:HG2	1.52	0.74
1:A:365:HIS:HB2	1:A:393:MET:HE1	1.69	0.74
1:C:365:HIS:HB2	1:C:393:MET:HE1	1.69	0.73
1:A:3674:THR:O	1:A:3679:LYS:NZ	2.20	0.73
1:B:3227:ARG:NH2	1:B:3291:ASP:OD1	2.17	0.73
1:D:3674:THR:O	1:D:3679:LYS:NZ	2.20	0.73
1:B:3674:THR:O	1:B:3679:LYS:NZ	2.20	0.73
2:G:22:THR:HG22	2:G:50:ARG:HG2	1.70	0.73
1:C:2500:ALA:O	1:C:2554:ARG:NH1	2.20	0.73
2:H:22:THR:HG22	2:H:50:ARG:HG2	1.70	0.73
1:D:2706:VAL:HG21	1:D:2785:TRP:HE1	1.52	0.73
1:D:3695:MET:HB3	1:D:3731:LEU:HD11	1.71	0.72
1:A:2436:ILE:HA	1:A:2465:LYS:HE3	1.71	0.72
1:B:2436:ILE:HA	1:B:2465:LYS:HE3	1.71	0.72
1:D:2436:ILE:HA	1:D:2465:LYS:HE3	1.71	0.72
1:A:3695:MET:HB3	1:A:3731:LEU:HD11	1.71	0.72
1:C:2436:ILE:HA	1:C:2465:LYS:HE3	1.71	0.72
1:A:3285:TYR:CE1	1:A:3325:LYS:HG3	2.25	0.72
2:F:22:THR:HG22	2:F:50:ARG:HG2	1.70	0.72
1:D:3285:TYR:CE1	1:D:3325:LYS:HG3	2.25	0.72
1:B:3285:TYR:CE1	1:B:3325:LYS:HG3	2.25	0.72
1:C:3832:ASP:HB3	1:C:3835:PHE:HB3	1.72	0.72
1:B:3832:ASP:HB3	1:B:3835:PHE:HB3	1.72	0.72
1:C:3285:TYR:CE1	1:C:3325:LYS:HG3	2.25	0.72
1:A:3832:ASP:HB3	1:A:3835:PHE:HB3	1.72	0.72
1:B:930:ASN:O	1:B:934:GLN:NE2	2.23	0.72
1:C:930:ASN:O	1:C:934:GLN:NE2	2.23	0.72
2:E:22:THR:HG22	2:E:50:ARG:HG2	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3152:ARG:NH2	1:C:3232:PRO:O	2.23	0.71
1:C:1972:GLN:HA	1:C:1975:MET:HE2	1.73	0.71
1:D:930:ASN:O	1:D:934:GLN:NE2	2.23	0.71
1:D:1972:GLN:HA	1:D:1975:MET:HE2	1.72	0.71
1:D:3832:ASP:HB3	1:D:3835:PHE:HB3	1.72	0.71
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.71	0.71
1:C:3695:MET:HB3	1:C:3731:LEU:HD11	1.71	0.71
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.71	0.71
1:A:3285:TYR:HE1	1:A:3325:LYS:HG3	1.56	0.71
1:A:930:ASN:O	1:A:934:GLN:NE2	2.23	0.71
1:B:3152:ARG:NH2	1:B:3232:PRO:O	2.23	0.71
1:D:3285:TYR:HE1	1:D:3325:LYS:HG3	1.56	0.71
1:C:962:LYS:HE3	1:C:981:MET:HG2	1.73	0.70
1:C:1964:GLU:HA	1:C:1975:MET:HE1	1.73	0.70
1:A:3152:ARG:NH2	1:A:3232:PRO:O	2.23	0.70
1:B:1964:GLU:HA	1:B:1975:MET:HE1	1.73	0.70
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.71	0.70
1:A:1964:GLU:HA	1:A:1975:MET:HE1	1.73	0.70
1:B:3695:MET:HB3	1:B:3731:LEU:HD11	1.71	0.70
1:A:962:LYS:HE3	1:A:981:MET:HG2	1.73	0.70
1:C:2640:LEU:HD23	1:C:2643:LYS:HZ1	1.56	0.70
1:C:3285:TYR:HE1	1:C:3325:LYS:HG3	1.56	0.70
1:D:3955:GLN:NE2	1:D:3975:GLN:OE1	2.25	0.70
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.71	0.70
1:D:3152:ARG:NH2	1:D:3232:PRO:O	2.23	0.70
1:B:1972:GLN:HA	1:B:1975:MET:HE2	1.73	0.70
1:D:1964:GLU:HA	1:D:1975:MET:HE1	1.73	0.70
1:A:3955:GLN:NE2	1:A:3975:GLN:OE1	2.25	0.69
1:C:3246:MET:HG2	1:C:3268:LEU:HD11	1.73	0.69
1:A:1972:GLN:HA	1:A:1975:MET:HE2	1.73	0.69
1:C:3955:GLN:NE2	1:C:3975:GLN:OE1	2.25	0.69
1:D:962:LYS:HE3	1:D:981:MET:HG2	1.73	0.69
1:B:3285:TYR:HE1	1:B:3325:LYS:HG3	1.56	0.69
1:B:3297:LYS:NZ	1:B:3333:VAL:O	2.25	0.69
1:D:3246:MET:HG2	1:D:3268:LEU:HD11	1.73	0.69
1:D:2503:ASP:HB2	1:D:2554:ARG:HH12	1.58	0.69
1:D:3297:LYS:NZ	1:D:3333:VAL:O	2.25	0.69
1:A:2640:LEU:HD23	1:A:2643:LYS:HZ1	1.56	0.69
1:C:3297:LYS:NZ	1:C:3333:VAL:O	2.25	0.69
1:B:962:LYS:HE3	1:B:981:MET:HG2	1.73	0.69
1:A:3297:LYS:NZ	1:A:3333:VAL:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3246:MET:HG2	1:B:3268:LEU:HD11	1.73	0.69
1:D:2640:LEU:HD23	1:D:2643:LYS:HZ1	1.56	0.69
1:A:3325:LYS:HD2	1:A:3328:LYS:HE3	1.76	0.68
1:C:2503:ASP:HB2	1:C:2554:ARG:HH12	1.58	0.68
1:D:332:ARG:NH1	1:D:364:GLN:OE1	2.27	0.68
1:B:3955:GLN:NE2	1:B:3975:GLN:OE1	2.25	0.68
1:D:3325:LYS:HD2	1:D:3328:LYS:HE3	1.76	0.68
1:B:332:ARG:NH1	1:B:364:GLN:OE1	2.27	0.68
1:D:2999:LYS:HG3	1:D:3003:MET:HE2	1.76	0.68
1:A:891:GLU:HA	1:A:894:VAL:HG22	1.76	0.68
1:A:3246:MET:HG2	1:A:3268:LEU:HD11	1.73	0.68
1:A:2503:ASP:HB2	1:A:2554:ARG:HH12	1.58	0.68
1:C:3325:LYS:HD2	1:C:3328:LYS:HE3	1.76	0.68
1:A:332:ARG:NH1	1:A:364:GLN:OE1	2.27	0.68
1:D:891:GLU:HA	1:D:894:VAL:HG22	1.76	0.68
2:F:6:GLU:HG3	2:F:74:LYS:HE2	1.76	0.67
1:B:2640:LEU:HD23	1:B:2643:LYS:HZ1	1.58	0.67
2:H:6:GLU:HG3	2:H:74:LYS:HE2	1.76	0.67
1:B:939:THR:HG23	1:B:999:LEU:HD21	1.76	0.67
1:B:3325:LYS:HD2	1:B:3328:LYS:HE3	1.76	0.67
2:G:6:GLU:HG3	2:G:74:LYS:HE2	1.76	0.67
1:B:988:LEU:HB2	1:B:1055:ARG:HE	1.60	0.67
1:C:2999:LYS:HG3	1:C:3003:MET:HE2	1.76	0.67
1:A:3260:ARG:HH11	1:A:3264:CYS:HA	1.60	0.67
1:C:332:ARG:NH1	1:C:364:GLN:OE1	2.27	0.67
1:C:988:LEU:HB2	1:C:1055:ARG:HE	1.60	0.67
1:A:939:THR:HG23	1:A:999:LEU:HD21	1.76	0.67
1:B:3260:ARG:HH11	1:B:3264:CYS:HA	1.60	0.67
1:C:891:GLU:HA	1:C:894:VAL:HG22	1.76	0.67
1:A:2999:LYS:HG3	1:A:3003:MET:HE2	1.76	0.67
1:D:939:THR:HG23	1:D:999:LEU:HD21	1.76	0.67
1:D:988:LEU:HB2	1:D:1055:ARG:HE	1.60	0.67
1:A:2351:ILE:HD11	1:A:2460:PHE:HB2	1.77	0.66
2:E:6:GLU:HG3	2:E:74:LYS:HE2	1.76	0.66
1:B:2503:ASP:HB2	1:B:2554:ARG:HH12	1.58	0.66
1:B:2999:LYS:HG3	1:B:3003:MET:HE2	1.76	0.66
1:A:988:LEU:HB2	1:A:1055:ARG:HE	1.60	0.66
1:A:2840:MET:HE1	1:A:2905:ARG:HA	1.78	0.66
1:D:2232:PRO:HG3	1:D:2382:ILE:HD11	1.76	0.66
1:D:3260:ARG:HH11	1:D:3264:CYS:HA	1.60	0.66
1:B:891:GLU:HA	1:B:894:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2232:PRO:HG3	1:B:2382:ILE:HD11	1.76	0.66
1:C:2232:PRO:HG3	1:C:2382:ILE:HD11	1.77	0.66
1:C:2840:MET:HE1	1:C:2905:ARG:HA	1.78	0.66
1:B:2351:ILE:HD11	1:B:2460:PHE:HB2	1.77	0.66
1:B:2758:LYS:HE3	1:B:2763:LEU:HA	1.77	0.66
1:C:541:ILE:HD11	1:C:574:VAL:HG13	1.77	0.66
1:D:2840:MET:HE1	1:D:2905:ARG:HA	1.78	0.66
1:A:2758:LYS:HE3	1:A:2763:LEU:HA	1.77	0.66
1:A:4832:GLU:O	1:A:4843:ARG:NH2	2.29	0.66
1:D:4690:LYS:HG3	1:D:4692:SER:H	1.61	0.66
1:C:920:GLU:OE2	1:C:922:SER:OG	2.14	0.65
1:D:2263:GLU:OE2	1:D:2327:ARG:NH1	2.29	0.65
1:A:2232:PRO:HG3	1:A:2382:ILE:HD11	1.76	0.65
1:A:4690:LYS:HG3	1:A:4692:SER:H	1.61	0.65
1:C:939:THR:HG23	1:C:999:LEU:HD21	1.76	0.65
1:C:2263:GLU:OE2	1:C:2327:ARG:NH1	2.29	0.65
1:D:2351:ILE:HD11	1:D:2460:PHE:HB2	1.77	0.65
1:C:2758:LYS:HE3	1:C:2763:LEU:HA	1.77	0.65
1:C:4832:GLU:O	1:C:4843:ARG:NH2	2.29	0.65
1:D:541:ILE:HD11	1:D:574:VAL:HG13	1.77	0.65
1:A:541:ILE:HD11	1:A:574:VAL:HG13	1.77	0.65
1:A:1165:MET:HE1	1:A:1176:THR:HG23	1.79	0.65
1:B:1165:MET:HE1	1:B:1176:THR:HG23	1.79	0.65
1:C:3260:ARG:HH11	1:C:3264:CYS:HA	1.60	0.65
1:C:4690:LYS:HG3	1:C:4692:SER:H	1.61	0.65
1:A:3803:LEU:HB2	1:A:3884:SER:HB3	1.78	0.65
1:C:3803:LEU:HB2	1:C:3884:SER:HB3	1.78	0.65
1:A:920:GLU:OE2	1:A:922:SER:OG	2.14	0.65
1:B:2979:ARG:HG2	1:B:3039:THR:HG22	1.78	0.65
1:C:4834:PRO:HB3	1:C:4843:ARG:HD3	1.79	0.65
1:D:4561:LEU:HD11	1:D:4568:MET:HE3	1.79	0.65
2:G:4:GLU:HB3	2:G:76:THR:HB	1.79	0.65
1:B:2840:MET:HE1	1:B:2905:ARG:HA	1.78	0.65
1:C:2351:ILE:HD11	1:C:2460:PHE:HB2	1.77	0.65
1:B:3803:LEU:HB2	1:B:3884:SER:HB3	1.78	0.65
1:C:2979:ARG:HG2	1:C:3039:THR:HG22	1.78	0.65
1:B:2263:GLU:OE2	1:B:2327:ARG:NH1	2.29	0.65
1:C:4561:LEU:HD11	1:C:4568:MET:HE3	1.79	0.65
1:D:2979:ARG:HG2	1:D:3039:THR:HG22	1.78	0.65
1:D:3281:LEU:O	1:D:3284:ILE:HG22	1.97	0.65
1:A:3323:MET:HB3	1:A:3327:LYS:HZ3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:GLU:HB3	2:F:76:THR:HB	1.79	0.65
1:B:4690:LYS:HG3	1:B:4692:SER:H	1.61	0.65
1:C:977:LYS:NZ	1:C:979:ALA:O	2.29	0.65
1:D:2758:LYS:HE3	1:D:2763:LEU:HA	1.77	0.65
1:C:4897:TYR:OH	1:C:4963:GLU:OE2	2.14	0.64
1:A:2982:PHE:O	1:A:3001:LYS:NZ	2.31	0.64
1:A:4834:PRO:HB3	1:A:4843:ARG:HD3	1.79	0.64
1:D:1165:MET:HE1	1:D:1176:THR:HG23	1.79	0.64
1:A:4177:VAL:HG11	1:A:4880:VAL:HA	1.78	0.64
1:B:2982:PHE:O	1:B:3001:LYS:NZ	2.31	0.64
1:D:3803:LEU:HB2	1:D:3884:SER:HB3	1.78	0.64
1:C:1165:MET:HE1	1:C:1176:THR:HG23	1.79	0.64
1:A:2979:ARG:HG2	1:A:3039:THR:HG22	1.78	0.64
1:B:3281:LEU:O	1:B:3284:ILE:HG22	1.97	0.64
1:D:1788:LYS:HD2	1:D:1833:ILE:HG22	1.78	0.64
1:A:829:LYS:NZ	1:A:1037:LEU:O	2.31	0.64
1:B:541:ILE:HD11	1:B:574:VAL:HG13	1.78	0.64
1:C:3281:LEU:O	1:C:3284:ILE:HG22	1.97	0.64
1:D:3932:GLN:HA	1:D:3985:MET:HE1	1.79	0.64
1:A:3932:GLN:HA	1:A:3985:MET:HE1	1.79	0.64
1:C:1788:LYS:HD2	1:C:1833:ILE:HG22	1.78	0.64
2:H:4:GLU:HB3	2:H:76:THR:HB	1.79	0.64
1:C:2982:PHE:O	1:C:3001:LYS:NZ	2.30	0.64
1:D:4177:VAL:HG11	1:D:4880:VAL:HA	1.78	0.64
1:A:4561:LEU:HD11	1:A:4568:MET:HE3	1.79	0.64
1:B:4561:LEU:HD11	1:B:4568:MET:HE3	1.79	0.64
1:D:2982:PHE:O	1:D:3001:LYS:NZ	2.31	0.64
1:B:4834:PRO:HB3	1:B:4843:ARG:HD3	1.79	0.64
1:D:920:GLU:OE2	1:D:922:SER:OG	2.14	0.64
1:D:4834:PRO:HB3	1:D:4843:ARG:HD3	1.79	0.64
1:B:2939:TYR:HB3	1:B:2956:TYR:CE2	2.33	0.63
1:B:4177:VAL:HG11	1:B:4880:VAL:HA	1.79	0.63
1:D:829:LYS:NZ	1:D:1037:LEU:O	2.30	0.63
1:A:3924:ILE:HG21	1:A:3985:MET:HE3	1.80	0.63
2:E:4:GLU:HB3	2:E:76:THR:HB	1.79	0.63
1:B:4264:LEU:HD11	1:C:4694:LEU:HD11	1.80	0.63
1:B:1788:LYS:HD2	1:B:1833:ILE:HG22	1.78	0.63
1:B:3932:GLN:HA	1:B:3985:MET:HE1	1.79	0.63
1:A:1788:LYS:HD2	1:A:1833:ILE:HG22	1.78	0.63
1:A:2263:GLU:OE2	1:A:2327:ARG:NH1	2.29	0.63
1:A:2939:TYR:HB3	1:A:2956:TYR:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4264:LEU:HD11	1:B:4694:LEU:HD11	1.81	0.63
1:B:4832:GLU:O	1:B:4843:ARG:NH2	2.29	0.63
1:C:829:LYS:NZ	1:C:1037:LEU:O	2.31	0.63
1:C:3932:GLN:HA	1:C:3985:MET:HE1	1.79	0.63
1:C:4177:VAL:HG11	1:C:4880:VAL:HA	1.78	0.63
1:B:3924:ILE:HG21	1:B:3985:MET:HE3	1.80	0.63
1:B:4618:THR:OG1	1:B:4619:GLU:OE1	2.16	0.63
1:C:2080:LEU:HG	1:C:2084:MET:HE2	1.80	0.63
1:A:3145:SER:HB3	1:A:3148:VAL:HG12	1.81	0.63
1:A:3281:LEU:O	1:A:3284:ILE:HG22	1.97	0.63
1:D:4832:GLU:O	1:D:4843:ARG:NH2	2.29	0.63
1:B:2080:LEU:HG	1:B:2084:MET:HE2	1.80	0.63
1:D:2939:TYR:HB3	1:D:2956:TYR:CE2	2.33	0.63
1:C:2905:ARG:HE	1:C:2906:GLY:H	1.47	0.63
1:C:3145:SER:HB3	1:C:3148:VAL:HG12	1.80	0.63
1:C:3924:ILE:HG21	1:C:3985:MET:HE3	1.80	0.62
1:D:2127:ARG:NH2	1:D:2165:LEU:O	2.32	0.62
1:C:1053:ALA:O	1:C:1057:LEU:HD12	2.00	0.62
1:C:1266:GLU:HG2	1:C:1267:HIS:CD2	2.34	0.62
1:C:2539:GLU:OE2	1:C:2581:ARG:NE	2.32	0.62
1:D:1058:LEU:HD21	1:D:1064:LEU:HG	1.81	0.62
1:D:1266:GLU:HG2	1:D:1267:HIS:CD2	2.34	0.62
1:D:4618:THR:OG1	1:D:4619:GLU:OE1	2.16	0.62
1:A:2920:ARG:NH2	1:A:2981:TYR:OH	2.32	0.62
1:D:1053:ALA:O	1:D:1057:LEU:HD12	2.00	0.62
1:B:2920:ARG:NH2	1:B:2981:TYR:OH	2.32	0.62
1:D:2920:ARG:NH2	1:D:2981:TYR:OH	2.32	0.62
1:B:4897:TYR:OH	1:B:4963:GLU:OE2	2.14	0.62
1:D:2539:GLU:OE2	1:D:2581:ARG:NE	2.32	0.62
1:C:2127:ARG:NH2	1:C:2165:LEU:O	2.32	0.62
1:C:2920:ARG:NH2	1:C:2981:TYR:OH	2.32	0.62
1:C:4187:GLU:OE2	1:C:4947:ARG:NH2	2.33	0.62
1:D:3924:ILE:HG21	1:D:3985:MET:HE3	1.80	0.62
1:A:2758:LYS:HB2	1:A:2762:LEU:HD23	1.82	0.62
1:A:2080:LEU:HG	1:A:2084:MET:HE2	1.80	0.62
1:B:2539:GLU:OE2	1:B:2581:ARG:NE	2.32	0.62
1:C:4618:THR:OG1	1:C:4619:GLU:OE1	2.16	0.62
1:D:2080:LEU:HG	1:D:2084:MET:HE2	1.80	0.62
1:D:3145:SER:HB3	1:D:3148:VAL:HG12	1.80	0.62
1:B:1053:ALA:O	1:B:1057:LEU:HD12	2.00	0.62
1:B:3145:SER:HB3	1:B:3148:VAL:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3277:LEU:HD21	1:B:3307:ILE:HG22	1.81	0.62
1:C:2939:TYR:HB3	1:C:2956:TYR:CE2	2.33	0.62
1:A:1766:PRO:HG3	1:A:1780:PRO:HB3	1.82	0.62
1:A:4897:TYR:OH	1:A:4963:GLU:OE2	2.14	0.62
1:B:829:LYS:NZ	1:B:1037:LEU:O	2.30	0.62
1:B:2127:ARG:NH2	1:B:2165:LEU:O	2.32	0.62
1:B:2905:ARG:HE	1:B:2906:GLY:H	1.47	0.62
1:A:1053:ALA:O	1:A:1057:LEU:HD12	2.00	0.61
1:D:2905:ARG:HE	1:D:2906:GLY:H	1.48	0.61
1:B:977:LYS:NZ	1:B:979:ALA:O	2.29	0.61
1:B:2741:TRP:HA	1:B:2752:LYS:HB3	1.82	0.61
1:A:2741:TRP:HA	1:A:2752:LYS:HB3	1.82	0.61
1:A:3320:LEU:HA	1:A:3323:MET:HE2	1.82	0.61
1:C:1058:LEU:HD21	1:C:1064:LEU:HG	1.81	0.61
1:C:4264:LEU:HD11	1:D:4694:LEU:HD11	1.80	0.61
1:D:1766:PRO:HG3	1:D:1780:PRO:HB3	1.82	0.61
1:D:3277:LEU:HD21	1:D:3307:ILE:HG22	1.81	0.61
1:A:2539:GLU:OE2	1:A:2581:ARG:NE	2.32	0.61
1:B:1058:LEU:HD21	1:B:1064:LEU:HG	1.81	0.61
1:B:3320:LEU:HA	1:B:3323:MET:HE2	1.82	0.61
1:C:2557:LYS:NZ	1:C:2602:HIS:O	2.33	0.61
1:C:3602:CYS:HA	1:C:3605:MET:HE2	1.82	0.61
1:D:555:LEU:HD12	1:D:588:ILE:HD11	1.83	0.61
1:D:3250:TRP:O	1:D:3256:ASN:ND2	2.33	0.61
1:A:1058:LEU:HD21	1:A:1064:LEU:HG	1.81	0.61
1:D:977:LYS:NZ	1:D:979:ALA:O	2.29	0.61
1:D:4897:TYR:OH	1:D:4963:GLU:OE2	2.14	0.61
1:A:3119:GLU:OE2	1:A:3248:ARG:NH2	2.34	0.61
1:B:3321:PRO:HA	1:B:3324:GLU:HG3	1.83	0.61
1:A:1266:GLU:HG2	1:A:1267:HIS:CD2	2.34	0.61
1:A:2127:ARG:NH2	1:A:2165:LEU:O	2.32	0.61
1:A:2905:ARG:HE	1:A:2906:GLY:H	1.47	0.61
1:B:1266:GLU:HG2	1:B:1267:HIS:CD2	2.34	0.61
1:B:1766:PRO:HG3	1:B:1780:PRO:HB3	1.82	0.61
1:B:2758:LYS:HB2	1:B:2762:LEU:HD23	1.82	0.61
1:C:125:TYR:O	1:C:414:ARG:NH1	2.34	0.61
1:D:2557:LYS:NZ	1:D:2602:HIS:O	2.33	0.61
1:D:2758:LYS:HB2	1:D:2762:LEU:HD23	1.82	0.61
1:D:3187:LYS:HE3	1:D:3191:GLU:HB3	1.83	0.61
1:D:4187:GLU:OE2	1:D:4947:ARG:NH2	2.33	0.61
1:B:2972:ASP:HA	1:B:3035:ILE:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:PRO:HB3	1:A:169:ARG:HB2	1.83	0.61
1:A:3321:PRO:HA	1:A:3324:GLU:HG3	1.83	0.61
1:B:164:PRO:HB3	1:B:169:ARG:HB2	1.83	0.61
1:B:3602:CYS:HA	1:B:3605:MET:HE2	1.82	0.61
1:C:3277:LEU:HD21	1:C:3307:ILE:HG22	1.81	0.61
1:D:4661:TYR:HB3	1:D:4665:ARG:HH21	1.66	0.61
1:A:2557:LYS:NZ	1:A:2602:HIS:O	2.33	0.61
1:B:125:TYR:O	1:B:414:ARG:NH1	2.34	0.61
1:C:3119:GLU:OE2	1:C:3248:ARG:NH2	2.34	0.61
1:A:4694:LEU:HD11	1:D:4264:LEU:HD11	1.81	0.60
1:B:920:GLU:OE2	1:B:922:SER:OG	2.14	0.60
1:C:3321:PRO:HA	1:C:3324:GLU:HG3	1.83	0.60
1:C:4690:LYS:HZ2	1:C:4692:SER:HB3	1.67	0.60
1:B:3119:GLU:OE2	1:B:3248:ARG:NH2	2.34	0.60
1:C:2385:GLY:O	1:C:2389:MET:HG3	2.01	0.60
1:C:2981:TYR:HA	1:C:2990:LEU:HD21	1.83	0.60
1:C:3320:LEU:HA	1:C:3323:MET:HE2	1.82	0.60
1:D:164:PRO:HB3	1:D:169:ARG:HB2	1.83	0.60
1:D:2385:GLY:O	1:D:2389:MET:HG3	2.01	0.60
1:D:3320:LEU:HA	1:D:3323:MET:HE2	1.82	0.60
1:C:4661:TYR:HB3	1:C:4665:ARG:HH21	1.66	0.60
1:D:4690:LYS:HZ2	1:D:4692:SER:HB3	1.67	0.60
1:B:2557:LYS:NZ	1:B:2602:HIS:O	2.33	0.60
1:A:977:LYS:NZ	1:A:979:ALA:O	2.29	0.60
1:A:4661:TYR:HB3	1:A:4665:ARG:HH21	1.66	0.60
1:B:2385:GLY:O	1:B:2389:MET:HG3	2.01	0.60
1:A:125:TYR:O	1:A:414:ARG:NH1	2.34	0.60
1:A:2972:ASP:HA	1:A:3035:ILE:HD11	1.82	0.60
1:A:3250:TRP:O	1:A:3256:ASN:ND2	2.33	0.60
1:A:3602:CYS:HA	1:A:3605:MET:HE2	1.82	0.60
1:B:1502:ASN:OD1	1:B:1503:ASN:N	2.35	0.60
1:D:125:TYR:O	1:D:414:ARG:NH1	2.34	0.60
1:D:3602:CYS:HA	1:D:3605:MET:HE2	1.82	0.60
1:A:555:LEU:HD12	1:A:588:ILE:HD11	1.83	0.60
1:A:2593:VAL:HG12	1:A:2644:LEU:HB2	1.84	0.60
1:B:3250:TRP:O	1:B:3256:ASN:ND2	2.33	0.60
1:C:164:PRO:HB3	1:C:169:ARG:HB2	1.83	0.60
1:C:2758:LYS:HB2	1:C:2762:LEU:HD23	1.82	0.60
1:A:2964:ALA:HA	1:A:2968:LEU:HD12	1.84	0.60
1:A:3277:LEU:HD21	1:A:3307:ILE:HG22	1.81	0.60
1:C:1502:ASN:OD1	1:C:1503:ASN:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2741:TRP:HA	1:C:2752:LYS:HB3	1.82	0.60
1:C:2972:ASP:HA	1:C:3035:ILE:HD11	1.82	0.60
1:D:2981:TYR:HA	1:D:2990:LEU:HD21	1.83	0.60
1:A:1283:LEU:HB2	1:A:1555:PHE:HB2	1.84	0.60
1:A:2385:GLY:O	1:A:2389:MET:HG3	2.01	0.60
1:A:3159:LEU:HD11	1:A:3241:MET:HE3	1.84	0.60
1:A:4827:ILE:O	1:A:4831:ILE:HG12	2.02	0.60
1:B:3187:LYS:HE3	1:B:3191:GLU:HB3	1.83	0.60
1:B:4661:TYR:HB3	1:B:4665:ARG:HH21	1.66	0.60
1:D:1097:LYS:NZ	1:D:1198:GLY:O	2.35	0.60
1:D:2972:ASP:HA	1:D:3035:ILE:HD11	1.82	0.60
1:D:3129:SER:O	1:D:3133:ILE:HG13	2.02	0.60
1:A:3187:LYS:HE3	1:A:3191:GLU:HB3	1.83	0.60
1:B:1283:LEU:HB2	1:B:1555:PHE:HB2	1.84	0.60
1:B:2964:ALA:HA	1:B:2968:LEU:HD12	1.84	0.60
1:B:2981:TYR:HA	1:B:2990:LEU:HD21	1.83	0.60
1:C:3187:LYS:HE3	1:C:3191:GLU:HB3	1.83	0.60
1:D:3321:PRO:HA	1:D:3324:GLU:HG3	1.83	0.60
1:B:3844:GLN:HG3	1:B:3922:GLU:HG3	1.84	0.59
1:A:1097:LYS:NZ	1:A:1198:GLY:O	2.35	0.59
1:B:2593:VAL:HG12	1:B:2644:LEU:HB2	1.84	0.59
1:B:3159:LEU:HD11	1:B:3241:MET:HE3	1.84	0.59
1:C:2964:ALA:HA	1:C:2968:LEU:HD12	1.84	0.59
1:D:878:LEU:HA	1:D:881:ILE:HG22	1.84	0.59
1:D:4116:GLN:HA	1:D:4119:LEU:HD12	1.84	0.59
1:A:4019:MET:HE2	1:A:4062:GLU:HG2	1.84	0.59
1:B:1239:PHE:O	1:B:1807:ARG:NH2	2.35	0.59
1:B:1940:GLN:HE22	1:B:1972:GLN:NE2	1.96	0.59
1:B:3129:SER:O	1:B:3133:ILE:HG13	2.02	0.59
1:C:839:GLU:HB2	1:C:851:LEU:HD12	1.85	0.59
1:C:1766:PRO:HG3	1:C:1780:PRO:HB3	1.82	0.59
1:C:3844:GLN:HG3	1:C:3922:GLU:HG3	1.84	0.59
1:D:2964:ALA:HA	1:D:2968:LEU:HD12	1.84	0.59
1:A:839:GLU:HB2	1:A:851:LEU:HD12	1.85	0.59
1:B:555:LEU:HD12	1:B:588:ILE:HD11	1.83	0.59
1:B:913:ARG:O	1:B:914:GLN:NE2	2.34	0.59
1:C:555:LEU:HD12	1:C:588:ILE:HD11	1.83	0.59
1:C:2593:VAL:HG12	1:C:2644:LEU:HB2	1.84	0.59
1:C:4116:GLN:HA	1:C:4119:LEU:HD12	1.84	0.59
1:D:839:GLU:HB2	1:D:851:LEU:HD12	1.84	0.59
1:D:2134:MET:HE3	1:D:2192:MET:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2741:TRP:HA	1:D:2752:LYS:HB3	1.82	0.59
1:A:4187:GLU:OE2	1:A:4947:ARG:NH2	2.33	0.59
1:C:1097:LYS:NZ	1:C:1198:GLY:O	2.35	0.59
1:C:3250:TRP:O	1:C:3256:ASN:ND2	2.33	0.59
1:C:4019:MET:HE2	1:C:4062:GLU:HG2	1.84	0.59
1:D:1502:ASN:OD1	1:D:1503:ASN:N	2.35	0.59
1:A:878:LEU:HA	1:A:881:ILE:HG22	1.84	0.59
1:A:4690:LYS:HZ2	1:A:4692:SER:HB3	1.67	0.59
1:D:1283:LEU:HB2	1:D:1555:PHE:HB2	1.84	0.59
1:D:4827:ILE:O	1:D:4831:ILE:HG12	2.02	0.59
1:A:4116:GLN:HA	1:A:4119:LEU:HD12	1.84	0.59
1:B:2436:ILE:HG22	1:B:2491:GLY:HA3	1.85	0.59
1:B:2890:GLN:O	1:B:2894:LYS:HG2	2.03	0.59
1:C:2134:MET:HE3	1:C:2192:MET:HG2	1.85	0.59
1:C:4827:ILE:O	1:C:4831:ILE:HG12	2.02	0.59
1:D:2593:VAL:HG12	1:D:2644:LEU:HB2	1.84	0.59
1:A:3068:LEU:O	1:A:3071:THR:OG1	2.21	0.59
1:B:878:LEU:HA	1:B:881:ILE:HG22	1.84	0.59
1:B:1097:LYS:NZ	1:B:1198:GLY:O	2.35	0.59
1:C:3129:SER:O	1:C:3133:ILE:HG13	2.02	0.59
1:C:3159:LEU:HD11	1:C:3241:MET:HE3	1.83	0.59
1:B:4827:ILE:O	1:B:4831:ILE:HG12	2.02	0.59
1:C:2890:GLN:O	1:C:2894:LYS:HG2	2.03	0.59
1:A:3129:SER:O	1:A:3133:ILE:HG13	2.01	0.59
1:A:4618:THR:OG1	1:A:4619:GLU:OE1	2.16	0.59
1:B:4116:GLN:HA	1:B:4119:LEU:HD12	1.84	0.59
1:C:1283:LEU:HB2	1:C:1555:PHE:HB2	1.84	0.59
1:D:2890:GLN:O	1:D:2894:LYS:HG2	2.03	0.59
1:B:4019:MET:HE2	1:B:4062:GLU:HG2	1.84	0.58
1:C:878:LEU:HA	1:C:881:ILE:HG22	1.84	0.58
1:A:309:MET:HE3	1:A:315:LEU:HB3	1.85	0.58
1:A:1113:MET:HB2	1:A:1156:TRP:HZ2	1.69	0.58
1:A:2981:TYR:HA	1:A:2990:LEU:HD21	1.84	0.58
1:A:3284:ILE:HD11	1:A:3296:MET:HG3	1.85	0.58
1:B:839:GLU:HB2	1:B:851:LEU:HD12	1.85	0.58
1:C:3068:LEU:O	1:C:3071:THR:OG1	2.21	0.58
1:D:1471:ASP:OD1	1:D:1475:LYS:N	2.36	0.58
1:A:2202:TYR:O	1:A:2206:ILE:HG12	2.04	0.58
1:A:2890:GLN:O	1:A:2894:LYS:HG2	2.03	0.58
1:D:309:MET:HE3	1:D:315:LEU:HB3	1.86	0.58
1:C:3955:GLN:NE2	1:C:3972:MET:SD	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2202:TYR:O	1:D:2206:ILE:HG12	2.04	0.58
1:D:3284:ILE:HD11	1:D:3296:MET:HG3	1.85	0.58
1:B:309:MET:HE3	1:B:315:LEU:HB3	1.85	0.58
1:B:3284:ILE:HD11	1:B:3296:MET:HG3	1.85	0.58
1:D:769:ARG:HG2	1:D:774:PRO:HA	1.85	0.58
1:D:3844:GLN:HG3	1:D:3922:GLU:HG3	1.84	0.58
1:D:4019:MET:HE2	1:D:4062:GLU:HG2	1.84	0.58
1:A:2436:ILE:HG22	1:A:2491:GLY:HA3	1.85	0.58
1:A:3955:GLN:NE2	1:A:3972:MET:SD	2.77	0.58
1:B:4831:ILE:HG13	1:B:4843:ARG:NH2	2.15	0.58
1:D:2436:ILE:HG22	1:D:2491:GLY:HA3	1.85	0.58
1:D:3159:LEU:HD11	1:D:3241:MET:HE3	1.84	0.58
1:A:1239:PHE:O	1:A:1807:ARG:NH2	2.35	0.58
1:A:2134:MET:HE3	1:A:2192:MET:HG2	1.84	0.58
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.86	0.58
1:B:606:ARG:HH21	1:B:1633:PRO:HD2	1.68	0.58
1:B:1471:ASP:OD1	1:B:1475:LYS:N	2.37	0.58
1:B:2202:TYR:O	1:B:2206:ILE:HG12	2.04	0.58
1:B:2760:TYR:HA	1:B:2763:LEU:HD13	1.86	0.58
1:D:1113:MET:HB2	1:D:1156:TRP:HZ2	1.69	0.58
1:A:1502:ASN:OD1	1:A:1503:ASN:N	2.35	0.58
2:F:24:VAL:HG22	2:F:48:LYS:HG2	1.86	0.58
1:B:880:ARG:NH1	1:B:1062:TYR:OH	2.37	0.58
1:C:309:MET:HE3	1:C:315:LEU:HB3	1.86	0.58
1:C:1113:MET:HB2	1:C:1156:TRP:HZ2	1.69	0.58
1:C:2436:ILE:HG22	1:C:2491:GLY:HA3	1.85	0.58
1:C:2670:SER:HB2	1:C:2973:GLN:HG2	1.86	0.58
1:B:2134:MET:HE3	1:B:2192:MET:HG2	1.85	0.58
1:C:606:ARG:HH21	1:C:1633:PRO:HD2	1.68	0.58
1:A:3844:GLN:HG3	1:A:3922:GLU:HG3	1.84	0.58
1:B:188:SER:HB2	1:B:190:ARG:HH11	1.69	0.58
1:B:1113:MET:HB2	1:B:1156:TRP:HZ2	1.69	0.58
1:B:3034:HIS:CE1	1:B:3038:GLN:HE22	2.22	0.58
1:B:3955:GLN:NE2	1:B:3972:MET:SD	2.77	0.58
1:C:769:ARG:HG2	1:C:774:PRO:HA	1.85	0.58
1:C:2202:TYR:O	1:C:2206:ILE:HG12	2.04	0.58
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.86	0.57
1:B:849:ASP:OD1	1:B:1214:ARG:NE	2.36	0.57
1:B:3323:MET:HB3	1:B:3327:LYS:HZ3	1.69	0.57
1:B:4187:GLU:OE2	1:B:4947:ARG:NH2	2.33	0.57
1:D:1628:MET:HB2	1:D:1687:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1501:ASN:OD1	1:A:1502:ASN:N	2.37	0.57
1:B:943:LEU:HD21	1:B:999:LEU:HD22	1.86	0.57
1:C:943:LEU:HD21	1:C:999:LEU:HD22	1.87	0.57
1:C:3034:HIS:CE1	1:C:3038:GLN:HE22	2.22	0.57
1:D:2760:TYR:HA	1:D:2763:LEU:HD13	1.86	0.57
1:D:3119:GLU:OE2	1:D:3248:ARG:NH2	2.34	0.57
1:A:2979:ARG:HH11	1:A:2983:LEU:HD12	1.69	0.57
1:C:3284:ILE:HD11	1:C:3296:MET:HG3	1.85	0.57
1:D:2670:SER:HB2	1:D:2973:GLN:HG2	1.86	0.57
1:D:2754:GLN:HE22	1:D:2756:LEU:HB2	1.69	0.57
1:D:2979:ARG:HH11	1:D:2983:LEU:HD12	1.69	0.57
1:D:4040:LYS:HG3	1:D:4042:VAL:H	1.70	0.57
1:C:2754:GLN:HE22	1:C:2756:LEU:HB2	1.69	0.57
1:A:188:SER:HB2	1:A:190:ARG:HH11	1.69	0.57
1:A:880:ARG:NH1	1:A:1062:TYR:OH	2.37	0.57
1:B:2670:SER:HB2	1:B:2973:GLN:HG2	1.86	0.57
1:B:3050:LEU:HD23	1:B:3052:SER:H	1.70	0.57
1:B:4040:LYS:HG3	1:B:4042:VAL:H	1.70	0.57
1:C:188:SER:HB2	1:C:190:ARG:HH11	1.69	0.57
1:C:913:ARG:O	1:C:914:GLN:NE2	2.34	0.57
1:C:4040:LYS:HG3	1:C:4042:VAL:H	1.70	0.57
1:D:880:ARG:NH1	1:D:1062:TYR:OH	2.37	0.57
1:D:1446:ILE:HG12	1:D:1542:ALA:HB2	1.87	0.57
1:D:3034:HIS:CE1	1:D:3038:GLN:HE22	2.22	0.57
1:A:943:LEU:HD21	1:A:999:LEU:HD22	1.86	0.57
1:A:1446:ILE:HG12	1:A:1542:ALA:HB2	1.87	0.57
1:A:1471:ASP:OD1	1:A:1475:LYS:N	2.36	0.57
1:A:1940:GLN:HE22	1:A:1972:GLN:NE2	1.96	0.57
1:A:2760:TYR:HA	1:A:2763:LEU:HD13	1.86	0.57
1:A:3134:LEU:HB2	1:A:3162:PHE:CE2	2.40	0.57
1:A:3152:ARG:HA	1:A:3155:LEU:HD12	1.86	0.57
1:B:1628:MET:HB2	1:B:1687:TYR:CE2	2.39	0.57
1:B:2642:ARG:HH12	1:B:2921:PHE:HA	1.70	0.57
1:B:3314:LEU:O	1:B:3318:HIS:ND1	2.38	0.57
1:C:1471:ASP:OD1	1:C:1475:LYS:N	2.37	0.57
1:C:1501:ASN:OD1	1:C:1502:ASN:N	2.37	0.57
1:A:2642:ARG:HH12	1:A:2921:PHE:HA	1.70	0.57
1:B:1501:ASN:OD1	1:B:1502:ASN:N	2.37	0.57
1:C:3050:LEU:HD23	1:C:3052:SER:H	1.70	0.57
1:D:606:ARG:HH21	1:D:1633:PRO:HD2	1.68	0.57
1:D:943:LEU:HD21	1:D:999:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3955:GLN:NE2	1:D:3972:MET:SD	2.77	0.57
1:D:3965:ILE:HD12	1:D:4086:ARG:HD2	1.87	0.57
1:A:1628:MET:HB2	1:A:1687:TYR:CE2	2.39	0.57
1:A:3314:LEU:O	1:A:3318:HIS:ND1	2.38	0.57
1:C:3231:MET:HE3	1:C:3233:HIS:HB2	1.86	0.57
1:C:3323:MET:HB3	1:C:3327:LYS:HZ3	1.68	0.57
1:D:3000:GLU:HA	1:D:3003:MET:HE3	1.87	0.57
1:A:769:ARG:HG2	1:A:774:PRO:HA	1.85	0.57
1:A:2141:LEU:HD23	1:A:2144:ARG:HE	1.70	0.57
1:A:3034:HIS:CE1	1:A:3038:GLN:HE22	2.22	0.57
1:A:4040:LYS:HG3	1:A:4042:VAL:H	1.70	0.57
1:B:2979:ARG:HH11	1:B:2983:LEU:HD12	1.69	0.57
1:B:3000:GLU:HA	1:B:3003:MET:HE3	1.87	0.57
1:B:3965:ILE:HD12	1:B:4086:ARG:HD2	1.87	0.57
1:D:188:SER:HB2	1:D:190:ARG:HH11	1.69	0.57
1:D:2642:ARG:HH12	1:D:2921:PHE:HA	1.70	0.57
1:D:3050:LEU:HD23	1:D:3052:SER:H	1.70	0.57
1:D:3152:ARG:HA	1:D:3155:LEU:HD12	1.87	0.57
1:D:3650:GLU:HB2	1:D:3659:LYS:HE2	1.87	0.57
1:A:3965:ILE:HD12	1:A:4086:ARG:HD2	1.87	0.57
2:E:24:VAL:HG22	2:E:48:LYS:HG2	1.86	0.57
1:B:3650:GLU:HB2	1:B:3659:LYS:HE2	1.87	0.57
1:C:1628:MET:HB2	1:C:1687:TYR:CE2	2.39	0.57
1:C:3314:LEU:O	1:C:3318:HIS:ND1	2.38	0.57
1:D:2141:LEU:HD23	1:D:2144:ARG:HE	1.70	0.57
1:D:3134:LEU:HB2	1:D:3162:PHE:CE2	2.40	0.57
1:D:3231:MET:HE3	1:D:3233:HIS:HB2	1.86	0.57
1:A:2734:MET:SD	1:A:2823:PRO:HB2	2.45	0.56
1:B:4690:LYS:HZ2	1:B:4692:SER:HB3	1.70	0.56
1:C:946:LEU:HB2	1:C:995:MET:HE1	1.87	0.56
1:C:2141:LEU:HD23	1:C:2144:ARG:HE	1.70	0.56
1:D:3314:LEU:O	1:D:3318:HIS:ND1	2.38	0.56
1:A:606:ARG:HH21	1:A:1633:PRO:HD2	1.68	0.56
1:A:2758:LYS:HG3	1:A:2763:LEU:HD12	1.87	0.56
1:B:2679:ASP:HB3	1:B:2920:ARG:HH21	1.70	0.56
1:C:3650:GLU:HB2	1:C:3659:LYS:HE2	1.87	0.56
1:C:4831:ILE:HG13	1:C:4843:ARG:NH2	2.16	0.56
1:D:1501:ASN:OD1	1:D:1502:ASN:N	2.37	0.56
1:D:3323:MET:HB3	1:D:3327:LYS:NZ	2.21	0.56
1:A:2670:SER:HB2	1:A:2973:GLN:HG2	1.86	0.56
1:A:3231:MET:HE3	1:A:3233:HIS:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3134:LEU:HB2	1:B:3162:PHE:CE2	2.40	0.56
1:B:3231:MET:HE3	1:B:3233:HIS:HB2	1.86	0.56
1:C:2642:ARG:HH12	1:C:2921:PHE:HA	1.70	0.56
1:C:2758:LYS:HG3	1:C:2763:LEU:HD12	1.87	0.56
1:C:2760:TYR:HA	1:C:2763:LEU:HD13	1.86	0.56
1:C:2979:ARG:HH11	1:C:2983:LEU:HD12	1.69	0.56
1:C:3134:LEU:HB2	1:C:3162:PHE:CE2	2.40	0.56
1:C:3152:ARG:HA	1:C:3155:LEU:HD12	1.87	0.56
1:D:562:LEU:HG	1:D:600:LEU:HD13	1.88	0.56
1:D:946:LEU:HB2	1:D:995:MET:HE1	1.87	0.56
1:D:2758:LYS:HD2	1:D:2762:LEU:HG	1.87	0.56
1:A:614:LEU:HD22	1:A:632:ILE:HG12	1.88	0.56
1:B:2141:LEU:HD23	1:B:2144:ARG:HE	1.70	0.56
1:B:2734:MET:SD	1:B:2823:PRO:HB2	2.45	0.56
1:D:2734:MET:SD	1:D:2823:PRO:HB2	2.45	0.56
1:A:913:ARG:O	1:A:914:GLN:NE2	2.34	0.56
1:A:3650:GLU:HB2	1:A:3659:LYS:HE2	1.87	0.56
1:B:3903:GLN:HG2	1:B:3967:LEU:HD22	1.88	0.56
1:C:614:LEU:HD22	1:C:632:ILE:HG12	1.88	0.56
1:C:2679:ASP:HB3	1:C:2920:ARG:HH21	1.70	0.56
1:D:3903:GLN:HG2	1:D:3967:LEU:HD22	1.88	0.56
1:B:562:LEU:HG	1:B:600:LEU:HD13	1.88	0.56
1:B:769:ARG:HG2	1:B:774:PRO:HA	1.85	0.56
1:B:966:LEU:HB3	1:B:970:TYR:HD2	1.70	0.56
1:B:1446:ILE:HG12	1:B:1542:ALA:HB2	1.87	0.56
1:B:2754:GLN:HE22	1:B:2756:LEU:HB2	1.69	0.56
1:B:2758:LYS:HG3	1:B:2763:LEU:HD12	1.87	0.56
1:B:3295:TRP:HZ3	1:B:3299:LEU:HD22	1.71	0.56
1:C:562:LEU:HG	1:C:600:LEU:HD13	1.88	0.56
1:C:2296:GLU:HG3	1:C:2390:THR:HG22	1.88	0.56
1:C:2734:MET:SD	1:C:2823:PRO:HB2	2.45	0.56
1:D:2679:ASP:HB3	1:D:2920:ARG:HH21	1.70	0.56
1:D:4921:PHE:HE2	1:D:4940:VAL:HG11	1.71	0.56
1:A:2296:GLU:HG3	1:A:2390:THR:HG22	1.88	0.56
1:A:2754:GLN:HE22	1:A:2756:LEU:HB2	1.70	0.56
1:B:3152:ARG:HA	1:B:3155:LEU:HD12	1.87	0.56
1:C:880:ARG:NH1	1:C:1062:TYR:OH	2.37	0.56
1:C:3270:SER:HA	1:C:3273:MET:HG2	1.88	0.56
1:C:3965:ILE:HD12	1:C:4086:ARG:HD2	1.87	0.56
1:D:2758:LYS:HG3	1:D:2763:LEU:HD12	1.87	0.56
1:D:3292:GLU:HB2	1:D:3296:MET:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:946:LEU:HB2	1:B:995:MET:HE1	1.87	0.56
1:C:2758:LYS:HD2	1:C:2762:LEU:HG	1.87	0.56
1:C:2773:TRP:HB3	1:C:2774:PRO:HD3	1.88	0.56
1:A:3295:TRP:HZ3	1:A:3299:LEU:HD22	1.71	0.56
1:A:3903:GLN:HG2	1:A:3967:LEU:HD22	1.88	0.56
1:A:4831:ILE:HG13	1:A:4843:ARG:NH2	2.15	0.56
1:B:2773:TRP:HB3	1:B:2774:PRO:HD3	1.88	0.56
1:B:3068:LEU:O	1:B:3071:THR:OG1	2.21	0.56
1:C:3184:TYR:HA	1:C:3192:ARG:HD3	1.88	0.56
1:C:3903:GLN:HG2	1:C:3967:LEU:HD22	1.88	0.56
1:D:2296:GLU:HG3	1:D:2390:THR:HG22	1.88	0.56
1:A:2247:VAL:HG11	1:A:2257:LEU:HD21	1.88	0.56
1:B:614:LEU:HD22	1:B:632:ILE:HG12	1.88	0.56
1:B:2296:GLU:HG3	1:B:2390:THR:HG22	1.88	0.56
1:B:3323:MET:HB3	1:B:3327:LYS:NZ	2.21	0.56
1:D:614:LEU:HD22	1:D:632:ILE:HG12	1.88	0.56
1:D:3270:SER:HA	1:D:3273:MET:HG2	1.88	0.56
1:A:562:LEU:HG	1:A:600:LEU:HD13	1.88	0.55
1:A:966:LEU:HB3	1:A:970:TYR:HD2	1.71	0.55
1:A:2679:ASP:HB3	1:A:2920:ARG:HH21	1.70	0.55
1:A:3050:LEU:HD23	1:A:3052:SER:H	1.70	0.55
1:C:1446:ILE:HG12	1:C:1542:ALA:HB2	1.87	0.55
1:C:2956:TYR:HB2	1:C:2959:GLU:HB2	1.88	0.55
1:C:4921:PHE:HE2	1:C:4940:VAL:HG11	1.71	0.55
1:D:913:ARG:O	1:D:914:GLN:NE2	2.34	0.55
1:A:515:ALA:HB2	1:A:523:GLY:HA3	1.89	0.55
1:A:946:LEU:HB2	1:A:995:MET:HE1	1.87	0.55
1:A:3323:MET:HB3	1:A:3327:LYS:NZ	2.21	0.55
1:C:966:LEU:HB3	1:C:970:TYR:HD2	1.71	0.55
1:B:515:ALA:HB2	1:B:523:GLY:HA3	1.89	0.55
1:C:4622:SER:OG	1:C:4624:ASP:OD1	2.21	0.55
1:A:2758:LYS:HD2	1:A:2762:LEU:HG	1.87	0.55
1:A:3000:GLU:HA	1:A:3003:MET:HE3	1.87	0.55
1:A:3292:GLU:HB2	1:A:3296:MET:HE1	1.88	0.55
1:B:3184:TYR:HA	1:B:3192:ARG:HD3	1.89	0.55
1:D:4831:ILE:HG13	1:D:4843:ARG:NH2	2.15	0.55
1:B:2273:GLY:O	1:B:2336:ARG:NH2	2.40	0.55
1:C:3000:GLU:HA	1:C:3003:MET:HE3	1.87	0.55
1:C:3323:MET:HB3	1:C:3327:LYS:NZ	2.21	0.55
1:C:2629:ASN:OD1	1:C:2630:PHE:N	2.40	0.55
1:C:4144:ARG:HB3	1:C:4961:GLN:HE22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:ALA:HB2	1:D:523:GLY:HA3	1.89	0.55
1:A:869:THR:O	1:A:941:LYS:HE2	2.07	0.55
1:A:3270:SER:HA	1:A:3273:MET:HG2	1.88	0.55
1:A:3805:LEU:HD21	1:A:3888:PHE:HA	1.89	0.55
1:B:869:THR:O	1:B:941:LYS:HE2	2.07	0.55
1:B:2956:TYR:HB2	1:B:2959:GLU:HB2	1.89	0.55
1:C:515:ALA:HB2	1:C:523:GLY:HA3	1.89	0.55
1:C:1955:ALA:O	1:C:1958:THR:OG1	2.25	0.55
1:C:1986:CYS:O	1:C:1993:ARG:NH2	2.40	0.55
1:C:2772:ARG:HG2	1:C:2776:LYS:HE2	1.89	0.55
1:C:3295:TRP:HZ3	1:C:3299:LEU:HD22	1.71	0.55
1:D:2247:VAL:HG11	1:D:2257:LEU:HD21	1.88	0.55
1:D:2926:LEU:HD23	1:D:3003:MET:HB2	1.89	0.55
1:D:3295:TRP:HZ3	1:D:3299:LEU:HD22	1.71	0.55
1:A:3184:TYR:HA	1:A:3192:ARG:HD3	1.88	0.55
1:C:927:GLN:NE2	1:C:928:GLU:HG2	2.22	0.55
1:D:3184:TYR:HA	1:D:3192:ARG:HD3	1.88	0.55
1:C:3042:ALA:HB3	1:C:3117:PHE:HB3	1.89	0.55
1:D:2235:ARG:HG3	1:D:2297:ARG:HH12	1.72	0.55
1:D:3805:LEU:HD21	1:D:3888:PHE:HA	1.89	0.55
1:A:2926:LEU:HD23	1:A:3003:MET:HB2	1.89	0.55
1:B:2758:LYS:HD2	1:B:2762:LEU:HG	1.87	0.55
1:D:137:ARG:HH12	1:D:204:ASP:HB3	1.72	0.55
1:A:2235:ARG:HG3	1:A:2297:ARG:HH12	1.72	0.54
1:B:1031:ARG:HG3	1:B:1038:LEU:HD11	1.89	0.54
1:B:2235:ARG:HG3	1:B:2297:ARG:HH12	1.72	0.54
1:B:2727:HIS:CE1	1:B:2828:MET:HE3	2.42	0.54
1:C:658:ASN:ND2	1:C:833:LYS:HG2	2.22	0.54
1:C:1031:ARG:HG3	1:C:1038:LEU:HD11	1.89	0.54
1:C:2247:VAL:HG11	1:C:2257:LEU:HD21	1.88	0.54
1:C:2727:HIS:CE1	1:C:2828:MET:HE3	2.42	0.54
1:C:3043:ARG:NH2	1:C:3116:GLN:O	2.40	0.54
1:C:3639:LYS:HD2	1:C:4683:ARG:NH2	2.23	0.54
1:D:966:LEU:HB3	1:D:970:TYR:HD2	1.71	0.54
1:D:2273:GLY:O	1:D:2336:ARG:NH2	2.40	0.54
1:A:137:ARG:HH12	1:A:204:ASP:HB3	1.72	0.54
1:A:2273:GLY:O	1:A:2336:ARG:NH2	2.40	0.54
1:B:2629:ASN:OD1	1:B:2630:PHE:N	2.40	0.54
1:C:1074:ARG:HH11	1:C:1076:GLU:HA	1.73	0.54
1:C:2273:GLY:O	1:C:2336:ARG:NH2	2.40	0.54
1:C:3813:LYS:HE2	1:C:3817:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1986:CYS:O	1:D:1993:ARG:NH2	2.40	0.54
1:D:2930:ILE:HG23	1:D:3010:LYS:HE3	1.90	0.54
1:D:3068:LEU:O	1:D:3071:THR:OG1	2.21	0.54
1:B:927:GLN:NE2	1:B:928:GLU:HG2	2.22	0.54
1:B:2939:TYR:HB3	1:B:2956:TYR:CZ	2.43	0.54
1:B:3043:ARG:NH2	1:B:3116:GLN:O	2.40	0.54
1:B:3270:SER:HA	1:B:3273:MET:HG2	1.88	0.54
1:B:3639:LYS:HD2	1:B:4683:ARG:NH2	2.23	0.54
1:B:3813:LYS:HE2	1:B:3817:LEU:HD11	1.89	0.54
1:C:2926:LEU:HD23	1:C:3003:MET:HB2	1.89	0.54
1:C:3072:MET:CE	1:C:3136:SER:HA	2.38	0.54
1:D:869:THR:O	1:D:941:LYS:HE2	2.07	0.54
1:D:2773:TRP:HB3	1:D:2774:PRO:HD3	1.88	0.54
1:A:2629:ASN:OD1	1:A:2630:PHE:N	2.40	0.54
1:A:3043:ARG:NH2	1:A:3116:GLN:O	2.40	0.54
1:A:3072:MET:CE	1:A:3136:SER:HA	2.38	0.54
1:B:466:PRO:HG2	1:B:479:LEU:HG	1.90	0.54
1:B:905:GLY:HA3	1:B:914:GLN:HB3	1.90	0.54
1:B:2247:VAL:HG11	1:B:2257:LEU:HD21	1.88	0.54
1:B:3072:MET:CE	1:B:3136:SER:HA	2.38	0.54
1:B:3805:LEU:HD21	1:B:3888:PHE:HA	1.89	0.54
1:B:4144:ARG:HB3	1:B:4961:GLN:HE22	1.71	0.54
1:D:2727:HIS:CE1	1:D:2828:MET:HE3	2.42	0.54
1:D:2772:ARG:HG2	1:D:2776:LYS:HE2	1.89	0.54
1:D:2956:TYR:HB2	1:D:2959:GLU:HB2	1.89	0.54
1:D:3043:ARG:NH2	1:D:3116:GLN:O	2.40	0.54
1:A:905:GLY:HA3	1:A:914:GLN:HB3	1.90	0.54
1:A:992:GLN:O	1:A:996:VAL:HG23	2.07	0.54
1:A:2773:TRP:HB3	1:A:2774:PRO:HD3	1.88	0.54
1:A:3642:GLU:HB3	1:A:4683:ARG:HH22	1.73	0.54
1:B:4921:PHE:HE2	1:B:4940:VAL:HG11	1.71	0.54
1:C:869:THR:O	1:C:941:LYS:HE2	2.07	0.54
1:D:3642:GLU:HB3	1:D:4683:ARG:HH22	1.73	0.54
1:D:3813:LYS:HE2	1:D:3817:LEU:HD11	1.90	0.54
1:A:1986:CYS:O	1:A:1993:ARG:NH2	2.40	0.54
1:A:2939:TYR:HB3	1:A:2956:TYR:CZ	2.43	0.54
1:A:3042:ALA:HB3	1:A:3117:PHE:HB3	1.89	0.54
1:A:4921:PHE:HE2	1:A:4940:VAL:HG11	1.71	0.54
1:B:2772:ARG:HG2	1:B:2776:LYS:HE2	1.89	0.54
1:C:878:LEU:HD23	1:C:940:LEU:HD13	1.89	0.54
1:D:713:TRP:HH2	1:D:1251:LEU:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1955:ALA:O	1:D:1958:THR:OG1	2.25	0.54
1:D:3072:MET:CE	1:D:3136:SER:HA	2.38	0.54
1:A:2705:PRO:HB3	1:A:2851:ILE:HG12	1.90	0.54
1:A:3043:ARG:HG2	1:A:3047:LYS:NZ	2.23	0.54
1:B:3174:HIS:ND1	1:B:3175:LEU:HG	2.23	0.54
1:B:3292:GLU:HB2	1:B:3296:MET:HE1	1.88	0.54
1:B:4047:ASP:OD1	1:B:4050:LYS:NZ	2.41	0.54
1:C:992:GLN:O	1:C:996:VAL:HG23	2.07	0.54
1:C:4250:TYR:O	1:C:4254:THR:HG23	2.08	0.54
1:D:927:GLN:NE2	1:D:928:GLU:HG2	2.22	0.54
1:D:3246:MET:HE1	1:D:3276:LEU:HD22	1.90	0.54
1:D:4622:SER:OG	1:D:4624:ASP:OD1	2.21	0.54
1:A:2956:TYR:HB2	1:A:2959:GLU:HB2	1.89	0.54
1:B:878:LEU:HD23	1:B:940:LEU:HD13	1.89	0.54
1:B:992:GLN:O	1:B:996:VAL:HG23	2.07	0.54
1:B:4250:TYR:O	1:B:4254:THR:HG23	2.08	0.54
1:C:3805:LEU:HD21	1:C:3888:PHE:HA	1.89	0.54
1:D:804:LEU:HD13	1:D:832:LEU:HD21	1.90	0.54
1:D:849:ASP:OD1	1:D:1214:ARG:NE	2.36	0.54
1:D:1239:PHE:O	1:D:1807:ARG:NH2	2.35	0.54
1:D:3639:LYS:HD2	1:D:4683:ARG:NH2	2.23	0.54
1:D:4047:ASP:OD1	1:D:4050:LYS:NZ	2.41	0.54
1:A:713:TRP:HH2	1:A:1251:LEU:HD21	1.73	0.54
1:A:993:GLU:OE2	1:A:1051:ARG:NH2	2.40	0.54
1:A:4047:ASP:OD1	1:A:4050:LYS:NZ	2.41	0.54
1:A:4144:ARG:HB3	1:A:4961:GLN:HE22	1.71	0.54
1:B:1986:CYS:O	1:B:1993:ARG:NH2	2.40	0.54
1:C:2930:ILE:HG23	1:C:3010:LYS:HE3	1.90	0.54
1:C:4047:ASP:OD1	1:C:4050:LYS:NZ	2.41	0.54
1:D:1074:ARG:HH11	1:D:1076:GLU:HA	1.73	0.54
1:D:3043:ARG:HG2	1:D:3047:LYS:NZ	2.23	0.54
1:D:3986:LEU:HD12	1:D:4101:LEU:HD12	1.90	0.54
1:A:466:PRO:HG2	1:A:479:LEU:HG	1.90	0.54
1:A:804:LEU:HD13	1:A:832:LEU:HD21	1.90	0.54
1:A:2930:ILE:HG23	1:A:3010:LYS:HE3	1.90	0.54
1:A:4617:ILE:HG23	1:A:4665:ARG:HH22	1.73	0.54
1:B:804:LEU:HD13	1:B:832:LEU:HD21	1.90	0.54
1:C:137:ARG:HH12	1:C:204:ASP:HB3	1.72	0.54
1:C:804:LEU:HD13	1:C:832:LEU:HD21	1.90	0.54
1:C:2939:TYR:HB3	1:C:2956:TYR:CZ	2.43	0.54
1:C:3292:GLU:HB2	1:C:3296:MET:HE1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:992:GLN:O	1:D:996:VAL:HG23	2.07	0.54
1:D:2629:ASN:OD1	1:D:2630:PHE:N	2.40	0.54
1:D:2693:SER:OG	1:D:2704:GLN:NE2	2.41	0.54
1:A:2693:SER:OG	1:A:2704:GLN:NE2	2.41	0.53
1:A:3174:HIS:ND1	1:A:3175:LEU:HG	2.23	0.53
1:A:4113:THR:O	1:A:4117:THR:HG23	2.08	0.53
1:A:4250:TYR:O	1:A:4254:THR:HG23	2.08	0.53
1:B:1955:ALA:O	1:B:1958:THR:OG1	2.25	0.53
1:C:713:TRP:HH2	1:C:1251:LEU:HD21	1.73	0.53
1:C:3260:ARG:HD2	1:C:3260:ARG:O	2.08	0.53
1:C:4113:THR:O	1:C:4117:THR:HG23	2.08	0.53
1:D:4604:LYS:O	1:D:4608:ARG:HG2	2.08	0.53
1:A:878:LEU:HD23	1:A:940:LEU:HD13	1.89	0.53
1:A:2727:HIS:CE1	1:A:2828:MET:HE3	2.42	0.53
1:A:3260:ARG:HD2	1:A:3260:ARG:O	2.08	0.53
1:A:4622:SER:OG	1:A:4624:ASP:OD1	2.21	0.53
1:B:1635:GLU:OE1	1:B:1637:ARG:NH1	2.42	0.53
1:B:3012:GLY:O	1:B:3016:ARG:HG3	2.08	0.53
1:C:1635:GLU:OE1	1:C:1637:ARG:NH1	2.42	0.53
1:C:4617:ILE:HG23	1:C:4665:ARG:HH22	1.73	0.53
1:D:1685:LEU:O	1:D:1689:ILE:HG12	2.09	0.53
1:D:2705:PRO:HB3	1:D:2851:ILE:HG12	1.90	0.53
1:D:3042:ALA:HB3	1:D:3117:PHE:HB3	1.89	0.53
1:D:3174:HIS:ND1	1:D:3175:LEU:HG	2.23	0.53
1:B:2176:VAL:HG22	1:B:2220:TYR:CZ	2.44	0.53
1:B:2693:SER:OG	1:B:2704:GLN:NE2	2.42	0.53
1:B:2723:LYS:HG3	1:B:2895:PHE:HZ	1.74	0.53
1:B:3965:ILE:HG22	1:B:3969:LYS:HE2	1.91	0.53
1:B:4113:THR:O	1:B:4117:THR:HG23	2.08	0.53
1:B:4604:LYS:O	1:B:4608:ARG:HG2	2.08	0.53
1:C:905:GLY:HA3	1:C:914:GLN:HB3	1.90	0.53
1:C:1239:PHE:O	1:C:1807:ARG:NH2	2.35	0.53
1:C:2235:ARG:HG3	1:C:2297:ARG:HH12	1.72	0.53
1:C:3246:MET:HE1	1:C:3276:LEU:HD22	1.90	0.53
1:D:2723:LYS:HG3	1:D:2895:PHE:HZ	1.74	0.53
1:D:3012:GLY:O	1:D:3016:ARG:HG3	2.08	0.53
1:A:23:GLN:HB3	1:A:34:LYS:HD2	1.91	0.53
1:A:1685:LEU:O	1:A:1689:ILE:HG12	2.09	0.53
1:A:2176:VAL:HG22	1:A:2220:TYR:CZ	2.44	0.53
1:A:2772:ARG:HG2	1:A:2776:LYS:HE2	1.89	0.53
1:A:3639:LYS:HD2	1:A:4683:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1074:ARG:HH11	1:B:1076:GLU:HA	1.73	0.53
1:B:3042:ALA:HB3	1:B:3117:PHE:HB3	1.89	0.53
1:C:466:PRO:HG2	1:C:479:LEU:HG	1.90	0.53
1:C:2723:LYS:HG3	1:C:2895:PHE:HZ	1.74	0.53
1:C:3174:HIS:ND1	1:C:3175:LEU:HG	2.23	0.53
1:D:1031:ARG:HG3	1:D:1038:LEU:HD11	1.89	0.53
1:D:4617:ILE:HG23	1:D:4665:ARG:HH22	1.73	0.53
1:A:1722:ASN:O	1:A:1919:ARG:NH2	2.41	0.53
1:A:2723:LYS:HG3	1:A:2895:PHE:HZ	1.74	0.53
1:A:3986:LEU:HD12	1:A:4101:LEU:HD12	1.90	0.53
1:A:4604:LYS:O	1:A:4608:ARG:HG2	2.08	0.53
1:B:3260:ARG:O	1:B:3260:ARG:HD2	2.08	0.53
1:C:1685:LEU:O	1:C:1689:ILE:HG12	2.09	0.53
1:C:1893:LEU:HA	1:C:1896:MET:HE3	1.91	0.53
1:A:927:GLN:NE2	1:A:928:GLU:HG2	2.22	0.53
1:A:1768:PHE:O	2:E:83:TYR:OH	2.21	0.53
1:A:3813:LYS:HE2	1:A:3817:LEU:HD11	1.89	0.53
1:A:3965:ILE:HG22	1:A:3969:LYS:HE2	1.91	0.53
1:B:713:TRP:HH2	1:B:1251:LEU:HD21	1.73	0.53
1:D:993:GLU:OE2	1:D:1051:ARG:NH2	2.40	0.53
1:D:1040:ASP:HA	1:D:1043:LYS:HG2	1.91	0.53
1:D:2176:VAL:HG22	1:D:2220:TYR:CZ	2.44	0.53
1:D:4144:ARG:HB3	1:D:4961:GLN:HE22	1.72	0.53
1:D:4250:TYR:O	1:D:4254:THR:HG23	2.08	0.53
1:B:137:ARG:HH12	1:B:204:ASP:HB3	1.72	0.53
1:B:658:ASN:ND2	1:B:833:LYS:HG2	2.22	0.53
1:B:2868:HIS:CE1	1:B:2870:LEU:HB2	2.44	0.53
1:B:3043:ARG:HG2	1:B:3047:LYS:NZ	2.23	0.53
1:C:849:ASP:OD1	1:C:1214:ARG:NE	2.36	0.53
1:C:2176:VAL:HG22	1:C:2220:TYR:CZ	2.44	0.53
1:C:2693:SER:OG	1:C:2704:GLN:NE2	2.41	0.53
1:C:3012:GLY:O	1:C:3016:ARG:HG3	2.08	0.53
1:D:1722:ASN:O	1:D:1919:ARG:NH2	2.41	0.53
1:D:2868:HIS:CE1	1:D:2870:LEU:HB2	2.44	0.53
1:A:658:ASN:ND2	1:A:833:LYS:HG2	2.22	0.53
1:A:1031:ARG:HG3	1:A:1038:LEU:HD11	1.90	0.53
1:A:1893:LEU:HA	1:A:1896:MET:HE3	1.91	0.53
1:B:993:GLU:OE2	1:B:1051:ARG:NH2	2.40	0.53
1:B:1722:ASN:O	1:B:1919:ARG:NH2	2.41	0.53
1:B:2930:ILE:HG23	1:B:3010:LYS:HE3	1.90	0.53
1:C:23:GLN:HB3	1:C:34:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:GLU:HB3	1:C:504:ARG:NH1	2.24	0.53
1:C:3642:GLU:HB3	1:C:4683:ARG:HH22	1.73	0.53
1:D:878:LEU:HD23	1:D:940:LEU:HD13	1.89	0.53
1:D:888:ASN:HD21	1:D:980:PRO:HD3	1.74	0.53
1:D:905:GLY:HA3	1:D:914:GLN:HB3	1.90	0.53
1:D:1893:LEU:HA	1:D:1896:MET:HE3	1.91	0.53
1:D:2939:TYR:HB3	1:D:2956:TYR:CZ	2.43	0.53
1:D:3879:LEU:O	1:D:3882:GLN:HG3	2.09	0.53
1:A:1074:ARG:HH11	1:A:1076:GLU:HA	1.73	0.53
1:B:3642:GLU:HB3	1:B:4683:ARG:HH22	1.73	0.53
1:B:4617:ILE:HG23	1:B:4665:ARG:HH22	1.73	0.53
1:C:3043:ARG:HG2	1:C:3047:LYS:NZ	2.23	0.53
1:D:1635:GLU:OE1	1:D:1637:ARG:NH1	2.42	0.53
1:D:1682:GLU:HG2	1:D:1683:PRO:HD3	1.90	0.53
1:A:585:ALA:O	1:A:589:ILE:HG12	2.09	0.53
1:A:1682:GLU:HG2	1:A:1683:PRO:HD3	1.90	0.53
1:B:2926:LEU:HD23	1:B:3003:MET:HB2	1.89	0.53
1:C:3986:LEU:HD12	1:C:4101:LEU:HD12	1.90	0.53
1:A:849:ASP:OD1	1:A:1214:ARG:NE	2.36	0.52
1:A:888:ASN:HD21	1:A:980:PRO:HD3	1.74	0.52
1:B:1682:GLU:HG2	1:B:1683:PRO:HD3	1.90	0.52
1:B:1893:LEU:HA	1:B:1896:MET:HE3	1.91	0.52
1:B:2705:PRO:HB3	1:B:2851:ILE:HG12	1.90	0.52
1:C:585:ALA:O	1:C:589:ILE:HG12	2.09	0.52
1:C:1722:ASN:O	1:C:1919:ARG:NH2	2.41	0.52
1:D:500:GLU:HB3	1:D:504:ARG:NH1	2.24	0.52
1:A:1635:GLU:OE1	1:A:1637:ARG:NH1	2.42	0.52
1:B:1685:LEU:O	1:B:1689:ILE:HG12	2.09	0.52
1:D:23:GLN:HB3	1:D:34:LYS:HD2	1.91	0.52
1:D:3074:ASN:OD1	1:D:3075:LEU:N	2.43	0.52
1:A:3074:ASN:OD1	1:A:3075:LEU:N	2.43	0.52
1:A:3246:MET:HE1	1:A:3276:LEU:HD22	1.90	0.52
1:B:3879:LEU:O	1:B:3882:GLN:HG3	2.09	0.52
1:C:3965:ILE:HG22	1:C:3969:LYS:HE2	1.91	0.52
1:C:4604:LYS:O	1:C:4608:ARG:HG2	2.08	0.52
1:A:646:THR:HG21	1:A:1628:MET:HE2	1.92	0.52
1:A:3012:GLY:O	1:A:3016:ARG:HG3	2.08	0.52
1:A:3068:LEU:HD22	1:A:3136:SER:HB2	1.92	0.52
1:B:23:GLN:HB3	1:B:34:LYS:HD2	1.91	0.52
1:B:500:GLU:HB3	1:B:504:ARG:NH1	2.24	0.52
1:B:3246:MET:HE1	1:B:3276:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3986:LEU:HD12	1:B:4101:LEU:HD12	1.90	0.52
1:C:1040:ASP:HA	1:C:1043:LYS:HG2	1.91	0.52
1:C:1940:GLN:HE22	1:C:1972:GLN:NE2	1.96	0.52
1:C:4040:LYS:HE2	1:C:4042:VAL:HB	1.92	0.52
1:D:466:PRO:HG2	1:D:479:LEU:HG	1.90	0.52
1:D:646:THR:HG21	1:D:1628:MET:HE2	1.92	0.52
1:D:4040:LYS:HE2	1:D:4042:VAL:HB	1.92	0.52
1:D:4113:THR:O	1:D:4117:THR:HG23	2.08	0.52
1:A:935:MET:O	1:A:938:GLU:HG3	2.10	0.52
1:A:2593:VAL:HG12	1:A:2644:LEU:HD13	1.92	0.52
1:B:646:THR:HG21	1:B:1628:MET:HE2	1.92	0.52
1:C:646:THR:HG21	1:C:1628:MET:HE2	1.92	0.52
1:C:888:ASN:HD21	1:C:980:PRO:HD3	1.74	0.52
1:C:935:MET:O	1:C:938:GLU:HG3	2.10	0.52
1:C:1682:GLU:HG2	1:C:1683:PRO:HD3	1.90	0.52
1:C:2705:PRO:HB3	1:C:2851:ILE:HG12	1.90	0.52
1:C:2868:HIS:CE1	1:C:2870:LEU:HB2	2.44	0.52
1:C:3074:ASN:OD1	1:C:3075:LEU:N	2.43	0.52
1:D:151:GLU:OE2	1:D:151:GLU:N	2.41	0.52
1:D:3293:GLY:N	1:D:3296:MET:HE1	2.17	0.52
1:A:1791:THR:HA	1:A:1794:MET:HE3	1.92	0.52
1:B:3068:LEU:HD22	1:B:3136:SER:HB2	1.92	0.52
1:C:330:THR:HG23	1:C:366:VAL:HG22	1.92	0.52
1:C:993:GLU:OE2	1:C:1051:ARG:NH2	2.40	0.52
1:C:3068:LEU:HD22	1:C:3136:SER:HB2	1.92	0.52
1:D:2413:LYS:O	1:D:2417:ILE:HG12	2.10	0.52
1:D:3323:MET:HB3	1:D:3327:LYS:HZ3	1.73	0.52
1:A:3879:LEU:O	1:A:3882:GLN:HG3	2.09	0.52
1:B:585:ALA:O	1:B:589:ILE:HG12	2.10	0.52
1:B:2413:LYS:O	1:B:2417:ILE:HG12	2.10	0.52
1:B:2593:VAL:HG12	1:B:2644:LEU:HD13	1.92	0.52
1:B:3074:ASN:OD1	1:B:3075:LEU:N	2.43	0.52
1:D:3260:ARG:HD2	1:D:3260:ARG:O	2.08	0.52
1:B:2070:ALA:HA	1:B:2075:ILE:HD11	1.92	0.52
1:C:3879:LEU:O	1:C:3882:GLN:HG3	2.09	0.52
1:D:3965:ILE:HG22	1:D:3969:LYS:HE2	1.91	0.52
1:A:1040:ASP:HA	1:A:1043:LYS:HG2	1.91	0.52
1:A:2868:HIS:CE1	1:A:2870:LEU:HB2	2.44	0.52
1:A:2070:ALA:HA	1:A:2075:ILE:HD11	1.92	0.52
1:A:2123:LEU:HD13	1:A:2167:MET:HG2	1.92	0.52
1:A:4040:LYS:HE2	1:A:4042:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:MET:O	1:B:938:GLU:HG3	2.10	0.52
1:C:2874:TYR:CE1	1:C:2882:LYS:HG2	2.45	0.52
1:C:4031:THR:O	1:C:4034:GLU:HG3	2.11	0.52
1:D:2789:ILE:HD11	1:D:2896:LEU:HD11	1.92	0.52
1:A:2874:TYR:CE1	1:A:2882:LYS:HG2	2.45	0.51
1:A:3293:GLY:N	1:A:3296:MET:HE1	2.17	0.51
1:B:4023:LEU:HD12	1:B:4026:LEU:HD23	1.92	0.51
1:B:4031:THR:O	1:B:4034:GLU:HG3	2.11	0.51
1:B:4040:LYS:HE2	1:B:4042:VAL:HB	1.92	0.51
1:C:2488:LEU:HD21	1:C:2548:LEU:HD22	1.92	0.51
1:C:3072:MET:HE3	1:C:3136:SER:HA	1.92	0.51
1:D:2874:TYR:CE1	1:D:2882:LYS:HG2	2.45	0.51
1:A:500:GLU:HB3	1:A:504:ARG:NH1	2.24	0.51
1:A:1955:ALA:O	1:A:1958:THR:OG1	2.25	0.51
1:A:4023:LEU:HD12	1:A:4026:LEU:HD23	1.92	0.51
1:B:3072:MET:HE3	1:B:3136:SER:HA	1.92	0.51
1:B:4622:SER:OG	1:B:4624:ASP:OD1	2.21	0.51
1:C:882:ARG:HD3	1:C:937:LEU:HD21	1.93	0.51
1:C:2413:LYS:O	1:C:2417:ILE:HG12	2.10	0.51
1:D:585:ALA:O	1:D:589:ILE:HG12	2.09	0.51
1:D:2841:ALA:HA	1:D:2844:MET:HG2	1.93	0.51
1:D:3068:LEU:HD22	1:D:3136:SER:HB2	1.92	0.51
1:A:882:ARG:HD3	1:A:937:LEU:HD21	1.92	0.51
1:A:2789:ILE:HD11	1:A:2896:LEU:HD11	1.92	0.51
1:B:888:ASN:HD21	1:B:980:PRO:HD3	1.74	0.51
1:B:1791:THR:HA	1:B:1794:MET:HE3	1.92	0.51
1:B:2754:GLN:HB3	1:B:2757:MET:HE1	1.92	0.51
1:A:2413:LYS:O	1:A:2417:ILE:HG12	2.10	0.51
1:A:3072:MET:HE3	1:A:3136:SER:HA	1.92	0.51
1:B:1040:ASP:HA	1:B:1043:LYS:HG2	1.91	0.51
1:B:2488:LEU:HD21	1:B:2548:LEU:HD22	1.92	0.51
1:B:2841:ALA:HA	1:B:2844:MET:HG2	1.93	0.51
1:B:4667:SER:OG	1:B:4672:MET:O	2.29	0.51
1:C:3214:LEU:O	1:C:3218:ILE:HG12	2.11	0.51
1:D:330:THR:HG23	1:D:366:VAL:HG22	1.92	0.51
1:D:658:ASN:ND2	1:D:833:LYS:HG2	2.22	0.51
1:D:3072:MET:HE3	1:D:3136:SER:HA	1.92	0.51
1:D:3214:LEU:O	1:D:3218:ILE:HG12	2.11	0.51
1:A:2235:ARG:HG3	1:A:2297:ARG:NH1	2.26	0.51
1:A:2843:MET:HE1	1:A:2905:ARG:HH12	1.76	0.51
1:B:232:ASP:OD2	1:B:407:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ARG:NH2	1:B:412:GLU:OE2	2.25	0.51
1:B:330:THR:HG23	1:B:366:VAL:HG22	1.92	0.51
1:B:882:ARG:HD3	1:B:937:LEU:HD21	1.93	0.51
1:B:2123:LEU:HD13	1:B:2167:MET:HG2	1.92	0.51
1:B:2874:TYR:CE1	1:B:2882:LYS:HG2	2.45	0.51
1:D:882:ARG:HD3	1:D:937:LEU:HD21	1.93	0.51
1:C:1791:THR:HA	1:C:1794:MET:HE3	1.92	0.51
1:C:2593:VAL:HG12	1:C:2644:LEU:HD13	1.91	0.51
1:D:1791:THR:HA	1:D:1794:MET:HE3	1.92	0.51
1:D:1931:ASP:OD1	1:D:1932:PHE:N	2.44	0.51
1:D:2235:ARG:HG3	1:D:2297:ARG:NH1	2.26	0.51
1:A:232:ASP:OD2	1:A:407:ARG:NH1	2.44	0.51
1:A:1011:ARG:NE	4:A:5003:ATP:O1A	2.41	0.51
1:A:2481:GLN:NE2	1:A:2537:GLY:O	2.42	0.51
1:B:4028:SER:O	1:B:4033:LYS:NZ	2.44	0.51
1:C:2754:GLN:HB3	1:C:2757:MET:HE1	1.92	0.51
1:C:4667:SER:OG	1:C:4672:MET:O	2.29	0.51
1:D:935:MET:O	1:D:938:GLU:HG3	2.10	0.51
1:D:2754:GLN:HB3	1:D:2757:MET:HE1	1.92	0.51
1:D:4023:LEU:HD12	1:D:4026:LEU:HD23	1.92	0.51
1:D:4031:THR:O	1:D:4034:GLU:HG3	2.11	0.51
1:A:2841:ALA:HA	1:A:2844:MET:HG2	1.93	0.51
1:B:1894:LEU:HD22	1:B:2065:THR:HG21	1.93	0.51
1:C:882:ARG:HH11	1:C:933:LEU:HD11	1.76	0.51
1:C:2841:ALA:HA	1:C:2844:MET:HG2	1.93	0.51
1:A:35:LEU:HD23	1:A:49:LEU:HB3	1.93	0.51
1:A:151:GLU:N	1:A:151:GLU:OE2	2.41	0.51
1:A:235:ARG:NH2	1:A:412:GLU:OE2	2.25	0.51
1:A:4028:SER:O	1:A:4033:LYS:NZ	2.44	0.51
1:A:4031:THR:O	1:A:4034:GLU:HG3	2.10	0.51
1:B:3293:GLY:N	1:B:3296:MET:HE1	2.17	0.51
1:C:2123:LEU:HD13	1:C:2167:MET:HG2	1.92	0.51
1:D:2070:ALA:HA	1:D:2075:ILE:HD11	1.92	0.51
1:D:2123:LEU:HD13	1:D:2167:MET:HG2	1.92	0.51
1:D:2593:VAL:HG12	1:D:2644:LEU:HD13	1.92	0.51
1:D:3288:LEU:HD23	1:D:3332:THR:HG21	1.92	0.51
1:A:674:TYR:CE1	1:A:756:SER:HB2	2.46	0.51
1:A:1686:LEU:O	1:A:1790:LYS:NZ	2.44	0.51
1:A:2694:SER:N	1:A:2704:GLN:HE22	2.09	0.51
1:A:2754:GLN:HB3	1:A:2757:MET:HE1	1.92	0.51
1:A:4667:SER:OG	1:A:4672:MET:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:674:TYR:CE1	1:B:756:SER:HB2	2.46	0.51
1:B:3228:TYR:HA	1:B:3235:MET:SD	2.51	0.51
1:C:232:ASP:OD2	1:C:407:ARG:NH1	2.44	0.51
1:C:1894:LEU:HD22	1:C:2065:THR:HG21	1.93	0.51
1:C:2694:SER:N	1:C:2704:GLN:HE22	2.09	0.51
1:C:3219:VAL:O	1:C:3223:GLU:HG2	2.11	0.51
1:D:1686:LEU:O	1:D:1790:LYS:NZ	2.44	0.51
1:D:4028:SER:O	1:D:4033:LYS:NZ	2.44	0.51
1:D:4943:MET:HA	1:D:4946:GLU:HG2	1.93	0.51
1:A:2966:VAL:HG12	1:A:2970:LEU:HD23	1.94	0.50
1:B:1686:LEU:O	1:B:1790:LYS:NZ	2.44	0.50
1:C:3288:LEU:HD23	1:C:3332:THR:HG21	1.92	0.50
1:C:4818:TYR:HA	1:D:4848:ILE:HD11	1.93	0.50
1:D:1011:ARG:NE	4:D:5003:ATP:O1A	2.41	0.50
1:D:1894:LEU:HD22	1:D:2065:THR:HG21	1.93	0.50
1:A:882:ARG:HH11	1:A:933:LEU:HD11	1.76	0.50
1:A:3261:ALA:C	1:A:3263:MET:H	2.19	0.50
1:B:151:GLU:OE2	1:B:151:GLU:N	2.41	0.50
1:B:882:ARG:HH11	1:B:933:LEU:HD11	1.76	0.50
1:B:1931:ASP:OD1	1:B:1932:PHE:N	2.44	0.50
1:B:2640:LEU:HA	1:B:2643:LYS:HZ3	1.76	0.50
1:C:2070:ALA:HA	1:C:2075:ILE:HD11	1.92	0.50
1:C:2481:GLN:NE2	1:C:2537:GLY:O	2.42	0.50
1:C:2937:HIS:O	1:C:2940:ILE:HG22	2.11	0.50
1:C:4023:LEU:HD12	1:C:4026:LEU:HD23	1.92	0.50
1:D:2728:SER:HA	1:D:2731:LYS:HZ3	1.76	0.50
1:A:678:MET:SD	1:A:754:VAL:HG22	2.51	0.50
1:A:3219:VAL:O	1:A:3223:GLU:HG2	2.11	0.50
1:B:678:MET:SD	1:B:754:VAL:HG22	2.51	0.50
1:B:2843:MET:HE1	1:B:2905:ARG:HH12	1.76	0.50
1:B:3214:LEU:O	1:B:3218:ILE:HG12	2.11	0.50
1:B:3234:VAL:HG22	1:B:3238:ILE:HD12	1.94	0.50
1:C:3228:TYR:HA	1:C:3235:MET:SD	2.51	0.50
1:C:4943:MET:HA	1:C:4946:GLU:HG2	1.93	0.50
1:D:674:TYR:CE1	1:D:756:SER:HB2	2.46	0.50
1:A:330:THR:HG23	1:A:366:VAL:HG22	1.92	0.50
1:A:1931:ASP:OD1	1:A:1932:PHE:N	2.44	0.50
1:A:3305:PRO:HA	1:A:3308:ASN:HD22	1.77	0.50
1:B:2966:VAL:HG12	1:B:2970:LEU:HD23	1.93	0.50
1:C:1686:LEU:O	1:C:1790:LYS:NZ	2.44	0.50
1:C:2843:MET:HE1	1:C:2905:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4036:ASP:OD2	1:C:4080:TYR:OH	2.20	0.50
1:D:35:LEU:HD23	1:D:49:LEU:HB3	1.93	0.50
1:D:3305:PRO:HA	1:D:3308:ASN:HD22	1.77	0.50
1:A:3228:TYR:HA	1:A:3235:MET:SD	2.51	0.50
1:A:3246:MET:HA	1:A:3268:LEU:HD21	1.94	0.50
1:A:4858:LEU:HD23	1:A:4861:ILE:HD12	1.93	0.50
1:B:2135:GLY:H	1:B:2138:GLU:HB2	1.77	0.50
1:B:2235:ARG:HG3	1:B:2297:ARG:NH1	2.26	0.50
1:B:3187:LYS:O	1:B:3188:SER:OG	2.25	0.50
1:C:591:GLU:HG3	1:C:631:LEU:HD22	1.94	0.50
1:C:1931:ASP:OD1	1:C:1932:PHE:N	2.44	0.50
1:D:232:ASP:OD2	1:D:407:ARG:NH1	2.44	0.50
1:D:4858:LEU:HD23	1:D:4861:ILE:HD12	1.93	0.50
1:A:1100:ARG:HG3	1:A:1236:TYR:HA	1.94	0.50
1:A:1894:LEU:HD22	1:A:2065:THR:HG21	1.93	0.50
1:A:2937:HIS:O	1:A:2940:ILE:HG22	2.11	0.50
1:A:3071:THR:HA	1:A:3074:ASN:HD21	1.77	0.50
1:A:3304:GLN:O	1:A:3308:ASN:ND2	2.45	0.50
1:A:4654:MET:O	1:A:4663:ARG:NH1	2.45	0.50
1:B:1031:ARG:HE	1:B:1042:THR:HG21	1.77	0.50
1:B:2937:HIS:O	1:B:2940:ILE:HG22	2.11	0.50
1:B:3288:LEU:HD23	1:B:3332:THR:HG21	1.92	0.50
1:B:4654:MET:O	1:B:4663:ARG:NH1	2.45	0.50
1:C:3304:GLN:O	1:C:3308:ASN:ND2	2.45	0.50
1:D:678:MET:SD	1:D:754:VAL:HG22	2.51	0.50
1:D:1268:ILE:HD11	1:D:1300:MET:HE2	1.94	0.50
1:D:2937:HIS:O	1:D:2940:ILE:HG22	2.11	0.50
1:D:3219:VAL:O	1:D:3223:GLU:HG2	2.11	0.50
1:D:4667:SER:OG	1:D:4672:MET:O	2.29	0.50
1:A:514:PHE:CD2	1:A:526:TRP:HB2	2.47	0.50
1:A:1268:ILE:HD11	1:A:1300:MET:HE2	1.94	0.50
1:A:1685:LEU:HD22	1:A:1706:LEU:HB2	1.93	0.50
1:B:1268:ILE:HD11	1:B:1300:MET:HE2	1.94	0.50
1:B:2789:ILE:HD11	1:B:2896:LEU:HD11	1.92	0.50
1:B:3071:THR:HA	1:B:3074:ASN:HD21	1.77	0.50
1:B:3246:MET:HA	1:B:3268:LEU:HD21	1.93	0.50
1:C:3261:ALA:C	1:C:3263:MET:H	2.19	0.50
1:C:4654:MET:O	1:C:4663:ARG:NH1	2.45	0.50
1:C:4858:LEU:HD23	1:C:4861:ILE:HD12	1.93	0.50
1:D:514:PHE:CD2	1:D:526:TRP:HB2	2.47	0.50
1:D:1286:THR:OG1	1:D:1550:PRO:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2843:MET:HE1	1:D:2905:ARG:HH12	1.76	0.50
1:A:2135:GLY:H	1:A:2138:GLU:HB2	1.77	0.50
1:B:3219:VAL:O	1:B:3223:GLU:HG2	2.11	0.50
1:B:4858:LEU:HD23	1:B:4861:ILE:HD12	1.93	0.50
1:C:137:ARG:NE	1:C:139:SER:OG	2.45	0.50
1:C:2728:SER:HA	1:C:2731:LYS:HZ3	1.76	0.50
1:D:2694:SER:N	1:D:2704:GLN:HE22	2.09	0.50
1:D:2966:VAL:HG12	1:D:2970:LEU:HD23	1.93	0.50
1:D:3304:GLN:O	1:D:3308:ASN:ND2	2.45	0.50
1:A:1172:THR:HB	1:A:1190:LEU:HD22	1.94	0.50
1:A:2172:MET:O	1:A:2176:VAL:HG23	2.12	0.50
1:A:2488:LEU:HD21	1:A:2548:LEU:HD22	1.92	0.50
1:A:3234:VAL:HG22	1:A:3238:ILE:HD12	1.94	0.50
1:B:1172:THR:HB	1:B:1190:LEU:HD22	1.94	0.50
1:B:3712:LYS:NZ	1:B:3720:GLU:OE2	2.32	0.50
1:B:3846:LEU:HB3	1:B:3854:PHE:CE2	2.47	0.50
1:C:1008:ALA:O	1:C:1012:ILE:HG12	2.12	0.50
1:C:2135:GLY:H	1:C:2138:GLU:HB2	1.77	0.50
1:C:2789:ILE:HD11	1:C:2896:LEU:HD11	1.92	0.50
1:C:3843:LEU:HD23	1:C:3846:LEU:HD12	1.94	0.50
1:C:3846:LEU:HB3	1:C:3854:PHE:CE2	2.47	0.50
1:D:1124:PRO:HD2	1:D:1594:VAL:HG23	1.94	0.50
1:D:1790:LYS:HA	1:D:1793:GLN:HG2	1.94	0.50
1:D:2488:LEU:HD21	1:D:2548:LEU:HD22	1.92	0.50
1:D:3900:GLU:OE2	1:D:3904:ARG:NH2	2.45	0.50
1:D:4654:MET:O	1:D:4663:ARG:NH1	2.45	0.50
1:A:137:ARG:NE	1:A:139:SER:OG	2.45	0.49
1:A:1031:ARG:HE	1:A:1042:THR:HG21	1.77	0.49
1:A:3214:LEU:O	1:A:3218:ILE:HG12	2.10	0.49
1:A:3288:LEU:HD23	1:A:3332:THR:HG21	1.92	0.49
1:A:3846:LEU:HB3	1:A:3854:PHE:CE2	2.47	0.49
1:A:4818:TYR:HA	1:B:4848:ILE:HD11	1.94	0.49
1:B:1444:GLY:HA3	1:B:1487:MET:HA	1.94	0.49
1:C:246:THR:HG21	1:C:267:VAL:HG11	1.94	0.49
1:C:674:TYR:CE1	1:C:756:SER:HB2	2.46	0.49
1:C:678:MET:SD	1:C:754:VAL:HG22	2.51	0.49
1:C:1268:ILE:HD11	1:C:1300:MET:HE2	1.94	0.49
1:C:4028:SER:O	1:C:4033:LYS:NZ	2.44	0.49
1:D:137:ARG:NE	1:D:139:SER:OG	2.45	0.49
1:D:467:ASP:O	1:D:475:LYS:NZ	2.37	0.49
1:D:996:VAL:HG22	1:D:1054:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1940:GLN:HE22	1:D:1972:GLN:NE2	1.96	0.49
1:D:2172:MET:O	1:D:2176:VAL:HG23	2.12	0.49
1:D:3843:LEU:HD23	1:D:3846:LEU:HD12	1.94	0.49
1:A:591:GLU:HG3	1:A:631:LEU:HD22	1.94	0.49
1:A:1444:GLY:HA3	1:A:1487:MET:HA	1.94	0.49
1:B:514:PHE:CD2	1:B:526:TRP:HB2	2.47	0.49
1:B:1100:ARG:HG3	1:B:1236:TYR:HA	1.94	0.49
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.94	0.49
1:B:2062:ILE:O	1:B:2066:MET:HG2	2.12	0.49
1:B:2694:SER:N	1:B:2704:GLN:HE22	2.09	0.49
1:C:1685:LEU:HD22	1:C:1706:LEU:HB2	1.93	0.49
1:C:2235:ARG:HG3	1:C:2297:ARG:NH1	2.26	0.49
1:C:2710:ASN:OD1	1:C:2711:ILE:N	2.46	0.49
1:C:3845:LEU:HD23	1:C:3848:GLU:HG3	1.94	0.49
1:D:882:ARG:HH11	1:D:933:LEU:HD11	1.76	0.49
1:D:1800:LYS:HA	1:D:1890:LYS:HZ1	1.77	0.49
1:B:555:LEU:HD11	1:B:578:VAL:HG11	1.94	0.49
1:B:996:VAL:HG22	1:B:1054:VAL:HG21	1.94	0.49
1:B:2710:ASN:OD1	1:B:2711:ILE:N	2.46	0.49
1:B:3305:PRO:HA	1:B:3308:ASN:HD22	1.77	0.49
1:B:3900:GLU:OE2	1:B:3904:ARG:NH2	2.45	0.49
1:C:2966:VAL:HG12	1:C:2970:LEU:HD23	1.93	0.49
1:C:3305:PRO:HA	1:C:3308:ASN:HD22	1.77	0.49
1:D:3234:VAL:HG22	1:D:3238:ILE:HD12	1.94	0.49
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.94	0.49
1:A:2710:ASN:OD1	1:A:2711:ILE:N	2.46	0.49
1:A:3906:PHE:HB3	1:A:3967:LEU:HD11	1.94	0.49
1:B:2172:MET:O	1:B:2176:VAL:HG23	2.12	0.49
1:B:3845:LEU:HD23	1:B:3848:GLU:HG3	1.94	0.49
1:B:4818:TYR:HA	1:C:4848:ILE:HD11	1.93	0.49
1:C:35:LEU:HD23	1:C:49:LEU:HB3	1.93	0.49
1:C:1124:PRO:HD2	1:C:1594:VAL:HG23	1.94	0.49
1:C:1910:LEU:HD13	1:C:2062:ILE:HG12	1.95	0.49
1:D:500:GLU:HB3	1:D:504:ARG:HH12	1.78	0.49
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.94	0.49
1:D:1172:THR:HB	1:D:1190:LEU:HD22	1.94	0.49
1:D:1685:LEU:HD22	1:D:1706:LEU:HB2	1.93	0.49
1:D:2821:TYR:CE2	1:D:2823:PRO:HG3	2.48	0.49
1:D:3228:TYR:HA	1:D:3235:MET:SD	2.51	0.49
1:D:3846:LEU:HB3	1:D:3854:PHE:CE2	2.47	0.49
1:A:1790:LYS:HA	1:A:1793:GLN:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3171:LEU:HB3	1:A:3211:LEU:HB2	1.95	0.49
1:A:3729:ALA:HA	1:A:3732:HIS:CD2	2.48	0.49
1:A:4819:VAL:HG12	1:A:4830:GLU:HG3	1.94	0.49
1:A:4943:MET:HA	1:A:4946:GLU:HG2	1.93	0.49
1:B:137:ARG:NE	1:B:139:SER:OG	2.45	0.49
1:B:246:THR:HG21	1:B:267:VAL:HG11	1.94	0.49
1:B:3261:ALA:C	1:B:3263:MET:H	2.19	0.49
1:B:3729:ALA:HA	1:B:3732:HIS:CD2	2.48	0.49
1:B:4819:VAL:HG12	1:B:4830:GLU:HG3	1.94	0.49
1:C:151:GLU:OE2	1:C:151:GLU:N	2.41	0.49
1:C:1790:LYS:HA	1:C:1793:GLN:HG2	1.94	0.49
1:D:1008:ALA:O	1:D:1012:ILE:HG12	2.12	0.49
1:D:1444:GLY:HA3	1:D:1487:MET:HA	1.94	0.49
1:D:1910:LEU:HD13	1:D:2062:ILE:HG12	1.95	0.49
1:D:2710:ASN:OD1	1:D:2711:ILE:N	2.46	0.49
1:D:3729:ALA:HA	1:D:3732:HIS:CD2	2.48	0.49
1:A:1008:ALA:O	1:A:1012:ILE:HG12	2.12	0.49
1:A:1910:LEU:HD13	1:A:2062:ILE:HG12	1.94	0.49
1:A:2619:LYS:HA	1:A:2623:LEU:HD13	1.95	0.49
1:A:3712:LYS:NZ	1:A:3720:GLU:OE2	2.32	0.49
1:B:1008:ALA:O	1:B:1012:ILE:HG12	2.12	0.49
1:B:2619:LYS:HA	1:B:2623:LEU:HD13	1.95	0.49
1:C:514:PHE:CD2	1:C:526:TRP:HB2	2.47	0.49
1:C:1172:THR:HB	1:C:1190:LEU:HD22	1.94	0.49
1:C:3293:GLY:N	1:C:3296:MET:HE1	2.17	0.49
1:C:3900:GLU:OE2	1:C:3904:ARG:NH2	2.45	0.49
1:D:1031:ARG:HE	1:D:1042:THR:HG21	1.77	0.49
1:D:1100:ARG:HG3	1:D:1236:TYR:HA	1.94	0.49
1:D:2062:ILE:O	1:D:2066:MET:HG2	2.12	0.49
1:D:3326:LEU:HD22	1:D:3336:GLU:OE1	2.13	0.49
1:A:555:LEU:HD11	1:A:578:VAL:HG11	1.94	0.49
1:A:1124:PRO:HD2	1:A:1594:VAL:HG23	1.94	0.49
1:B:591:GLU:HG3	1:B:631:LEU:HD22	1.94	0.49
1:B:2274:LEU:HD21	1:B:2329:GLU:HG2	1.94	0.49
1:C:3071:THR:HA	1:C:3074:ASN:HD21	1.77	0.49
1:A:1800:LYS:HA	1:A:1890:LYS:NZ	2.28	0.49
2:G:25:VAL:HG12	2:G:104:LEU:HA	1.95	0.49
1:B:1685:LEU:HD22	1:B:1706:LEU:HB2	1.94	0.49
1:B:2383:HIS:CG	1:B:2458:ALA:HB2	2.48	0.49
1:B:2968:LEU:HB2	1:B:2969:PRO:HD3	1.94	0.49
1:B:3281:LEU:HB3	1:B:3285:TYR:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2383:HIS:CG	1:C:2458:ALA:HB2	2.48	0.49
1:D:1800:LYS:HA	1:D:1890:LYS:NZ	2.28	0.49
1:D:3071:THR:HA	1:D:3074:ASN:HD21	1.77	0.49
1:D:3906:PHE:HB3	1:D:3967:LEU:HD11	1.94	0.49
1:A:2383:HIS:CG	1:A:2458:ALA:HB2	2.48	0.49
1:A:2821:TYR:CE2	1:A:2823:PRO:HG3	2.48	0.49
1:A:3246:MET:CG	1:A:3268:LEU:HD11	2.43	0.49
1:B:35:LEU:HD23	1:B:49:LEU:HB3	1.93	0.49
1:B:1124:PRO:HD2	1:B:1594:VAL:HG23	1.94	0.49
1:B:3304:GLN:O	1:B:3308:ASN:ND2	2.45	0.49
1:B:4943:MET:HA	1:B:4946:GLU:HG2	1.94	0.49
1:C:1242:ASN:OD1	1:C:1806:ALA:HA	2.13	0.49
1:C:3246:MET:HA	1:C:3268:LEU:HD21	1.94	0.49
1:D:3166:PHE:CE2	1:D:3168:VAL:HB	2.48	0.49
1:D:3246:MET:HA	1:D:3268:LEU:HD21	1.93	0.49
1:D:3261:ALA:C	1:D:3263:MET:H	2.19	0.49
1:A:1041:ARG:O	1:A:1044:LYS:HG3	2.13	0.49
1:A:1242:ASN:OD1	1:A:1806:ALA:HA	2.13	0.49
1:B:1910:LEU:HD13	1:B:2062:ILE:HG12	1.95	0.49
1:B:2723:LYS:HG3	1:B:2895:PHE:CZ	2.48	0.49
1:C:555:LEU:HD11	1:C:578:VAL:HG11	1.94	0.49
1:C:1100:ARG:HG3	1:C:1236:TYR:HA	1.94	0.49
1:C:2062:ILE:O	1:C:2066:MET:HG2	2.12	0.49
1:D:2193:VAL:HG11	1:D:2227:VAL:HG11	1.95	0.49
1:D:2937:HIS:O	1:D:2941:LEU:HG	2.13	0.49
1:D:2968:LEU:HB2	1:D:2969:PRO:HD3	1.94	0.49
1:A:996:VAL:HG22	1:A:1054:VAL:HG21	1.94	0.48
1:C:2172:MET:O	1:C:2176:VAL:HG23	2.12	0.48
1:C:2821:TYR:CE2	1:C:2823:PRO:HG3	2.47	0.48
1:D:246:THR:HG21	1:D:267:VAL:HG11	1.94	0.48
1:D:555:LEU:HD11	1:D:578:VAL:HG11	1.94	0.48
1:D:3171:LEU:HB3	1:D:3211:LEU:HB2	1.95	0.48
1:D:4819:VAL:HG12	1:D:4830:GLU:HG3	1.94	0.48
1:A:2150:MET:SD	1:A:2199:PHE:HD1	2.37	0.48
1:A:3281:LEU:HB3	1:A:3285:TYR:CE2	2.48	0.48
1:A:3845:LEU:HD23	1:A:3848:GLU:HG3	1.94	0.48
1:B:137:ARG:NH1	1:B:146:ASP:OD1	2.34	0.48
1:B:2193:VAL:HG11	1:B:2227:VAL:HG11	1.95	0.48
1:B:3171:LEU:HB3	1:B:3211:LEU:HB2	1.95	0.48
1:C:996:VAL:HG22	1:C:1054:VAL:HG21	1.94	0.48
1:C:3230:GLN:OE1	1:C:3230:GLN:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2150:MET:SD	1:D:2199:PHE:HD1	2.37	0.48
1:D:2723:LYS:HG3	1:D:2895:PHE:CZ	2.48	0.48
1:D:4632:ARG:HA	1:D:4635:ILE:HD12	1.96	0.48
1:B:1041:ARG:O	1:B:1044:LYS:HG3	2.13	0.48
1:B:3230:GLN:OE1	1:B:3230:GLN:N	2.46	0.48
1:B:4035:TYR:CE1	1:B:4050:LYS:HE2	2.48	0.48
1:C:1031:ARG:HE	1:C:1042:THR:HG21	1.77	0.48
1:C:1041:ARG:O	1:C:1044:LYS:HG3	2.13	0.48
1:C:2150:MET:SD	1:C:2199:PHE:HD1	2.36	0.48
1:C:2872:VAL:HG23	1:C:2877:LEU:HD22	1.94	0.48
1:C:3234:VAL:HG22	1:C:3238:ILE:HD12	1.94	0.48
1:C:3326:LEU:HD22	1:C:3336:GLU:OE1	2.12	0.48
1:C:3729:ALA:HA	1:C:3732:HIS:CD2	2.48	0.48
1:C:3906:PHE:HB3	1:C:3967:LEU:HD11	1.94	0.48
1:D:1242:ASN:OD1	1:D:1806:ALA:HA	2.13	0.48
1:D:2215:PHE:CG	1:D:2253:LEU:HD22	2.49	0.48
1:D:2383:HIS:CG	1:D:2458:ALA:HB2	2.48	0.48
1:D:2872:VAL:HG23	1:D:2877:LEU:HD22	1.94	0.48
1:D:3845:LEU:HD23	1:D:3848:GLU:HG3	1.94	0.48
1:A:2062:ILE:O	1:A:2066:MET:HG2	2.12	0.48
1:A:2937:HIS:O	1:A:2941:LEU:HG	2.13	0.48
1:A:3166:PHE:CE2	1:A:3168:VAL:HB	2.48	0.48
1:B:2821:TYR:CE2	1:B:2823:PRO:HG3	2.48	0.48
1:B:3326:LEU:HD22	1:B:3336:GLU:OE1	2.13	0.48
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.95	0.48
1:D:1041:ARG:O	1:D:1044:LYS:HG3	2.13	0.48
1:D:2274:LEU:HD21	1:D:2329:GLU:HG2	1.94	0.48
1:D:2481:GLN:NE2	1:D:2537:GLY:O	2.42	0.48
1:A:137:ARG:NH1	1:A:146:ASP:OD1	2.34	0.48
1:A:2193:VAL:HG11	1:A:2227:VAL:HG11	1.95	0.48
1:A:3900:GLU:OE2	1:A:3904:ARG:NH2	2.45	0.48
1:B:1790:LYS:HA	1:B:1793:GLN:HG2	1.94	0.48
1:B:2872:VAL:HG23	1:B:2877:LEU:HD22	1.94	0.48
1:C:514:PHE:HD2	1:C:526:TRP:HB2	1.79	0.48
1:C:1444:GLY:HA3	1:C:1487:MET:HA	1.94	0.48
1:C:3166:PHE:CE2	1:C:3168:VAL:HB	2.48	0.48
1:D:2130:LEU:HD11	1:D:2170:THR:HG23	1.95	0.48
1:D:2135:GLY:H	1:D:2138:GLU:HB2	1.77	0.48
1:A:2274:LEU:HD21	1:A:2329:GLU:HG2	1.94	0.48
1:A:2695:MET:HE1	1:A:2873:PRO:HB3	1.96	0.48
1:B:500:GLU:HB3	1:B:504:ARG:HH12	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:PHE:HD2	1:B:526:TRP:HB2	1.79	0.48
1:C:500:GLU:HB3	1:C:504:ARG:HH12	1.77	0.48
1:C:2723:LYS:HG3	1:C:2895:PHE:CZ	2.48	0.48
1:D:514:PHE:HD2	1:D:526:TRP:HB2	1.79	0.48
1:D:591:GLU:HG3	1:D:631:LEU:HD22	1.94	0.48
1:A:4268:MET:HA	1:A:4271:VAL:HG12	1.96	0.48
2:G:8:ILE:HD11	2:G:74:LYS:HB2	1.96	0.48
1:B:1800:LYS:HA	1:B:1890:LYS:NZ	2.28	0.48
1:B:3843:LEU:HD23	1:B:3846:LEU:HD12	1.94	0.48
1:B:3906:PHE:HB3	1:B:3967:LEU:HD11	1.94	0.48
1:B:4632:ARG:HA	1:B:4635:ILE:HD12	1.96	0.48
1:C:2130:LEU:HD11	1:C:2170:THR:HG23	1.95	0.48
1:C:2193:VAL:HG11	1:C:2227:VAL:HG11	1.95	0.48
1:C:3281:LEU:HB3	1:C:3285:TYR:CE2	2.48	0.48
1:C:3830:LEU:HB3	1:C:3833:ASP:OD2	2.14	0.48
1:C:4819:VAL:HG12	1:C:4830:GLU:HG3	1.94	0.48
1:D:2619:LYS:HA	1:D:2623:LEU:HD13	1.95	0.48
1:D:2695:MET:HE1	1:D:2873:PRO:HB3	1.96	0.48
1:A:2968:LEU:HB2	1:A:2969:PRO:HD3	1.94	0.48
1:A:4632:ARG:HA	1:A:4635:ILE:HD12	1.96	0.48
2:E:25:VAL:HG12	2:E:104:LEU:HA	1.95	0.48
2:H:25:VAL:HG12	2:H:104:LEU:HA	1.95	0.48
1:B:1119:ARG:NH2	1:B:1196:ASP:OD1	2.47	0.48
1:B:3246:MET:CG	1:B:3268:LEU:HD11	2.43	0.48
1:C:4634:VAL:HG22	1:C:4640:PHE:HD1	1.79	0.48
1:D:2727:HIS:NE2	1:D:2825:ALA:HB1	2.29	0.48
1:D:3830:LEU:HB3	1:D:3833:ASP:OD2	2.14	0.48
1:D:4035:TYR:CE1	1:D:4050:LYS:HE2	2.48	0.48
1:A:500:GLU:HB3	1:A:504:ARG:HH12	1.78	0.48
1:A:2723:LYS:HG3	1:A:2895:PHE:CZ	2.48	0.48
1:A:3217:GLU:HA	1:A:3220:GLU:HG3	1.96	0.48
1:A:3326:LEU:HD22	1:A:3336:GLU:OE1	2.13	0.48
1:A:4634:VAL:HG22	1:A:4640:PHE:HD1	1.79	0.48
2:H:8:ILE:HD11	2:H:74:LYS:HB2	1.96	0.48
1:C:1800:LYS:HA	1:C:1890:LYS:NZ	2.28	0.48
1:C:2215:PHE:CG	1:C:2253:LEU:HD22	2.49	0.48
1:C:2619:LYS:HA	1:C:2623:LEU:HD13	1.95	0.48
1:C:2968:LEU:HB2	1:C:2969:PRO:HD3	1.94	0.48
1:C:3171:LEU:HB3	1:C:3211:LEU:HB2	1.95	0.48
1:C:3217:GLU:HA	1:C:3220:GLU:HG3	1.96	0.48
1:D:3281:LEU:HB3	1:D:3285:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2130:LEU:HD11	1:A:2170:THR:HG23	1.95	0.48
1:A:2727:HIS:NE2	1:A:2825:ALA:HB1	2.29	0.48
1:A:4035:TYR:CE1	1:A:4050:LYS:HE2	2.48	0.48
1:B:3042:ALA:HA	1:B:3045:VAL:HG12	1.96	0.48
1:B:4268:MET:HA	1:B:4271:VAL:HG12	1.96	0.48
1:C:3260:ARG:NH1	1:C:3264:CYS:HA	2.29	0.48
1:D:4079:ASP:O	1:D:4082:GLU:HG3	2.14	0.48
1:A:126:SER:HA	1:A:414:ARG:HH12	1.79	0.47
1:A:246:THR:HG21	1:A:267:VAL:HG11	1.94	0.47
1:A:730:LEU:HD11	2:E:8:ILE:HA	1.96	0.47
1:A:2872:VAL:HG23	1:A:2877:LEU:HD22	1.94	0.47
1:A:3230:GLN:N	1:A:3230:GLN:OE1	2.46	0.47
1:A:3843:LEU:HD23	1:A:3846:LEU:HD12	1.94	0.47
1:B:1242:ASN:OD1	1:B:1806:ALA:HA	2.13	0.47
1:B:2481:GLN:NE2	1:B:2537:GLY:O	2.42	0.47
1:B:3830:LEU:HB3	1:B:3833:ASP:OD2	2.14	0.47
1:C:2274:LEU:HD21	1:C:2329:GLU:HG2	1.94	0.47
1:C:2695:MET:HE1	1:C:2873:PRO:HB3	1.96	0.47
1:C:2937:HIS:O	1:C:2941:LEU:HG	2.13	0.47
1:D:1119:ARG:NH2	1:D:1196:ASP:OD1	2.47	0.47
1:D:4268:MET:HA	1:D:4271:VAL:HG12	1.96	0.47
1:A:675:TYR:HB3	1:A:822:CYS:SG	2.54	0.47
1:B:776:GLN:HG2	1:B:1472:GLU:HA	1.95	0.47
1:B:2215:PHE:CG	1:B:2253:LEU:HD22	2.48	0.47
1:B:2695:MET:HE1	1:B:2873:PRO:HB3	1.96	0.47
1:C:2727:HIS:NE2	1:C:2825:ALA:HB1	2.29	0.47
1:C:4632:ARG:HA	1:C:4635:ILE:HD12	1.96	0.47
1:D:675:TYR:HB3	1:D:822:CYS:SG	2.54	0.47
1:D:4634:VAL:HG22	1:D:4640:PHE:HD1	1.79	0.47
1:A:3042:ALA:HA	1:A:3045:VAL:HG12	1.96	0.47
1:A:3830:LEU:HB3	1:A:3833:ASP:OD2	2.14	0.47
2:F:8:ILE:HD11	2:F:74:LYS:HB2	1.96	0.47
2:F:25:VAL:HG12	2:F:104:LEU:HA	1.95	0.47
1:B:1011:ARG:NE	4:B:5003:ATP:O1A	2.41	0.47
1:B:1685:LEU:HB3	1:B:1706:LEU:HD12	1.96	0.47
1:B:4159:GLN:HA	1:B:4162:LYS:HG2	1.97	0.47
1:C:235:ARG:NH2	1:C:412:GLU:OE2	2.25	0.47
1:C:1685:LEU:HB3	1:C:1706:LEU:HD12	1.96	0.47
2:H:83:TYR:OH	1:D:1768:PHE:O	2.22	0.47
1:B:2582:PRO:HG3	1:B:2617:CYS:SG	2.55	0.47
1:B:2745:GLU:HA	1:B:2755:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2937:HIS:O	1:B:2941:LEU:HG	2.13	0.47
1:C:675:TYR:HB3	1:C:822:CYS:SG	2.54	0.47
1:C:1119:ARG:NH2	1:C:1196:ASP:OD1	2.47	0.47
1:C:3042:ALA:HA	1:C:3045:VAL:HG12	1.96	0.47
1:D:1685:LEU:HB3	1:D:1706:LEU:HD12	1.96	0.47
1:D:2745:GLU:HA	1:D:2755:PRO:HB3	1.97	0.47
1:A:2745:GLU:HA	1:A:2755:PRO:HB3	1.97	0.47
1:B:2150:MET:SD	1:B:2199:PHE:HD1	2.36	0.47
1:B:2727:HIS:NE2	1:B:2825:ALA:HB1	2.29	0.47
1:B:3304:GLN:HG3	1:B:3305:PRO:HD3	1.96	0.47
1:C:776:GLN:HG2	1:C:1472:GLU:HA	1.95	0.47
1:C:1074:ARG:NH1	1:C:1076:GLU:HA	2.30	0.47
1:C:4268:MET:HA	1:C:4271:VAL:HG12	1.96	0.47
1:D:2586:GLN:HG3	1:D:2637:GLU:HG3	1.97	0.47
1:D:3216:GLU:HA	1:D:3219:VAL:HG22	1.97	0.47
1:D:4089:GLU:HB2	1:D:4090:PRO:HD3	1.96	0.47
1:A:776:GLN:HG2	1:A:1472:GLU:HA	1.95	0.47
1:A:2215:PHE:CG	1:A:2253:LEU:HD22	2.49	0.47
1:A:4014:LEU:HD13	1:A:4122:ALA:HB2	1.96	0.47
1:B:713:TRP:CE2	1:B:1600:PRO:HD3	2.50	0.47
1:B:1074:ARG:NH1	1:B:1076:GLU:HA	2.30	0.47
1:B:3166:PHE:CE2	1:B:3168:VAL:HB	2.48	0.47
1:C:336:GLU:HB2	1:C:338:LEU:HD23	1.97	0.47
1:C:713:TRP:CE2	1:C:1600:PRO:HD3	2.50	0.47
1:C:1011:ARG:NE	4:C:5003:ATP:O1A	2.41	0.47
1:C:3282:LYS:HA	1:C:3285:TYR:HD2	1.79	0.47
1:C:4079:ASP:O	1:C:4082:GLU:HG3	2.14	0.47
1:D:126:SER:HA	1:D:414:ARG:HH12	1.79	0.47
1:D:1270:VAL:HG22	1:D:1285:VAL:HG22	1.97	0.47
1:D:2582:PRO:HG3	1:D:2617:CYS:SG	2.55	0.47
1:A:877:HIS:HA	1:A:880:ARG:CD	2.45	0.47
1:A:1119:ARG:NH2	1:A:1196:ASP:OD1	2.47	0.47
1:A:1685:LEU:HB3	1:A:1706:LEU:HD12	1.96	0.47
1:A:3239:LEU:HB2	1:A:3240:PRO:HD3	1.97	0.47
1:A:3260:ARG:NH1	1:A:3264:CYS:HA	2.29	0.47
1:A:4159:GLN:HA	1:A:4162:LYS:HG2	1.97	0.47
2:E:8:ILE:HD11	2:E:74:LYS:HB2	1.96	0.47
1:B:126:SER:HA	1:B:414:ARG:HH12	1.79	0.47
1:B:668:ALA:HB2	1:B:1012:ILE:HD11	1.97	0.47
1:B:1011:ARG:HB3	1:B:1016:TRP:HB2	1.97	0.47
1:B:1689:ILE:HG23	1:B:1703:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2130:LEU:HD11	1:B:2170:THR:HG23	1.95	0.47
1:B:2225:SER:HB2	1:B:2240:LEU:HD13	1.97	0.47
1:B:2286:PRO:HG3	1:B:2359:ARG:HA	1.97	0.47
1:B:2455:ASP:OD2	1:B:2457:SER:OG	2.23	0.47
1:B:3318:HIS:C	1:B:3321:PRO:HD2	2.40	0.47
1:B:4079:ASP:O	1:B:4082:GLU:HG3	2.14	0.47
1:C:126:SER:HA	1:C:414:ARG:HH12	1.79	0.47
1:C:2640:LEU:HA	1:C:2643:LYS:HZ3	1.79	0.47
1:C:2745:GLU:HA	1:C:2755:PRO:HB3	1.97	0.47
1:D:137:ARG:NH1	1:D:146:ASP:OD1	2.34	0.47
1:D:3005:THR:HG22	1:D:3040:LEU:HD22	1.97	0.47
1:D:3042:ALA:HA	1:D:3045:VAL:HG12	1.96	0.47
1:A:514:PHE:HD2	1:A:526:TRP:HB2	1.79	0.47
1:A:992:GLN:NE2	1:A:1064:LEU:O	2.47	0.47
1:A:1011:ARG:HB3	1:A:1016:TRP:HB2	1.97	0.47
1:A:1689:ILE:HG23	1:A:1703:TYR:CZ	2.50	0.47
1:A:2087:LEU:O	1:A:2091:GLN:HG2	2.15	0.47
1:A:2582:PRO:HG3	1:A:2617:CYS:SG	2.55	0.47
1:A:3200:ASN:HB2	1:A:3203:ASP:HB2	1.97	0.47
1:A:4848:ILE:HD11	1:D:4818:TYR:HA	1.97	0.47
1:B:336:GLU:HB2	1:B:338:LEU:HD23	1.97	0.47
1:B:877:HIS:HA	1:B:880:ARG:CD	2.45	0.47
1:B:3200:ASN:HB2	1:B:3203:ASP:HB2	1.97	0.47
1:C:1273:ILE:HB	1:C:1282:CYS:HB2	1.97	0.47
1:C:2586:GLN:HG3	1:C:2637:GLU:HG3	1.97	0.47
1:D:776:GLN:HG2	1:D:1472:GLU:HA	1.96	0.47
1:D:2884:LYS:O	1:D:2887:GLU:HG3	2.15	0.47
1:A:4079:ASP:O	1:A:4082:GLU:HG3	2.14	0.47
1:A:4254:THR:HG22	1:A:4257:ARG:HH21	1.80	0.47
1:B:3035:ILE:O	1:B:3039:THR:HG23	2.15	0.47
1:B:4014:LEU:HD13	1:B:4122:ALA:HB2	1.96	0.47
1:C:629:GLN:OE1	1:C:1669:ASN:ND2	2.47	0.47
1:C:3304:GLN:HG3	1:C:3305:PRO:HD3	1.96	0.47
1:C:4035:TYR:CE1	1:C:4050:LYS:HE2	2.48	0.47
1:C:4159:GLN:HA	1:C:4162:LYS:HG2	1.97	0.47
1:D:668:ALA:HB2	1:D:1012:ILE:HD11	1.97	0.47
1:D:4014:LEU:HD13	1:D:4122:ALA:HB2	1.96	0.47
1:A:668:ALA:HB2	1:A:1012:ILE:HD11	1.97	0.47
1:A:713:TRP:CE2	1:A:1600:PRO:HD3	2.50	0.47
1:A:2689:MET:HB3	1:A:2689:MET:HE2	1.73	0.47
1:A:2884:LYS:O	1:A:2887:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3035:ILE:O	1:A:3039:THR:HG23	2.15	0.47
1:A:3175:LEU:HD22	1:A:3178:HIS:CE1	2.50	0.47
1:A:3216:GLU:HA	1:A:3219:VAL:HG22	1.97	0.47
1:B:3217:GLU:HA	1:B:3220:GLU:HG3	1.96	0.47
1:B:3239:LEU:HB2	1:B:3240:PRO:HD3	1.97	0.47
1:B:3282:LYS:HA	1:B:3285:TYR:HD2	1.80	0.47
1:B:4254:THR:HG22	1:B:4257:ARG:HH21	1.80	0.47
1:C:1270:VAL:HG22	1:C:1285:VAL:HG22	1.97	0.47
1:C:1286:THR:OG1	1:C:1550:PRO:O	2.29	0.47
1:C:2954:PHE:HE2	1:C:2956:TYR:CE1	2.33	0.47
1:D:3239:LEU:HB2	1:D:3240:PRO:HD3	1.97	0.47
1:D:3304:GLN:HG3	1:D:3305:PRO:HD3	1.96	0.47
1:A:2225:SER:HB2	1:A:2240:LEU:HD13	1.97	0.46
1:A:3005:THR:HG22	1:A:3040:LEU:HD22	1.97	0.46
1:A:3304:GLN:HG3	1:A:3305:PRO:HD3	1.96	0.46
1:B:1000:ALA:HB3	1:B:1047:LYS:HZ3	1.79	0.46
1:B:3986:LEU:HD11	1:B:4105:LEU:HG	1.97	0.46
1:C:668:ALA:HB2	1:C:1012:ILE:HD11	1.97	0.46
1:C:1689:ILE:HG23	1:C:1703:TYR:CZ	2.50	0.46
1:C:2582:PRO:HG3	1:C:2617:CYS:SG	2.55	0.46
1:C:3005:THR:HG22	1:C:3040:LEU:HD22	1.97	0.46
1:C:3200:ASN:HB2	1:C:3203:ASP:HB2	1.97	0.46
1:D:877:HIS:HA	1:D:880:ARG:CD	2.45	0.46
1:D:992:GLN:NE2	1:D:1064:LEU:O	2.47	0.46
1:D:1689:ILE:HG23	1:D:1703:TYR:CZ	2.50	0.46
1:D:3200:ASN:HB2	1:D:3203:ASP:HB2	1.97	0.46
1:D:3217:GLU:HA	1:D:3220:GLU:HG3	1.96	0.46
1:D:3230:GLN:N	1:D:3230:GLN:OE1	2.46	0.46
1:A:1922:ILE:O	1:A:1926:VAL:HG23	2.16	0.46
1:A:2779:LEU:HA	1:A:2782:MET:HE2	1.97	0.46
1:A:3986:LEU:HD11	1:A:4105:LEU:HG	1.98	0.46
1:C:1011:ARG:HB3	1:C:1016:TRP:HB2	1.97	0.46
1:C:1720:MET:SD	1:C:2127:ARG:HB3	2.56	0.46
1:C:2472:LEU:HD12	1:C:2476:TYR:HB2	1.97	0.46
1:C:2980:LEU:HG	1:C:2990:LEU:HD23	1.98	0.46
1:C:3650:GLU:HB2	1:C:3651:PRO:HD3	1.98	0.46
1:C:4014:LEU:HD13	1:C:4122:ALA:HB2	1.96	0.46
1:C:4089:GLU:HB2	1:C:4090:PRO:HD3	1.96	0.46
1:D:319:LYS:HB3	1:D:319:LYS:HE2	1.70	0.46
1:D:1720:MET:SD	1:D:2127:ARG:HB3	2.56	0.46
1:D:1922:ILE:O	1:D:1926:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2779:LEU:HA	1:D:2782:MET:HE2	1.97	0.46
1:D:3043:ARG:HG2	1:D:3047:LYS:HZ2	1.79	0.46
1:D:4159:GLN:HA	1:D:4162:LYS:HG2	1.97	0.46
1:D:4735:ASN:HB3	1:D:4738:PHE:CD2	2.50	0.46
1:A:2954:PHE:HE2	1:A:2956:TYR:CE1	2.33	0.46
1:A:4089:GLU:HB2	1:A:4090:PRO:HD3	1.96	0.46
1:B:1273:ILE:HB	1:B:1282:CYS:HB2	1.97	0.46
1:B:2884:LYS:O	1:B:2887:GLU:HG3	2.15	0.46
1:B:2954:PHE:HE2	1:B:2956:TYR:CE1	2.33	0.46
1:C:3216:GLU:HA	1:C:3219:VAL:HG22	1.97	0.46
1:C:3935:LEU:HD23	1:C:3940:LEU:HD22	1.97	0.46
1:D:713:TRP:CE2	1:D:1600:PRO:HD3	2.50	0.46
1:D:2087:LEU:O	1:D:2091:GLN:HG2	2.15	0.46
1:D:3187:LYS:O	1:D:3188:SER:OG	2.25	0.46
1:A:1273:ILE:HB	1:A:1282:CYS:HB2	1.97	0.46
1:B:675:TYR:HB3	1:B:822:CYS:SG	2.54	0.46
1:B:1839:LEU:HA	1:B:1842:ILE:HD12	1.98	0.46
1:B:2472:LEU:HD12	1:B:2476:TYR:HB2	1.98	0.46
1:B:2736:LYS:HB3	1:B:2741:TRP:HB2	1.97	0.46
1:B:2980:LEU:HG	1:B:2990:LEU:HD23	1.98	0.46
1:C:3035:ILE:O	1:C:3039:THR:HG23	2.15	0.46
1:D:1074:ARG:NH1	1:D:1076:GLU:HA	2.30	0.46
1:D:2176:VAL:HG22	1:D:2220:TYR:CE2	2.51	0.46
1:D:2640:LEU:HA	1:D:2643:LYS:HZ3	1.79	0.46
1:D:3318:HIS:C	1:D:3321:PRO:HD2	2.40	0.46
1:D:3986:LEU:HD11	1:D:4105:LEU:HG	1.97	0.46
1:D:4254:THR:HG22	1:D:4257:ARG:HH21	1.80	0.46
1:A:3281:LEU:O	1:A:3285:TYR:CD2	2.69	0.46
1:B:58:VAL:HG13	1:B:319:LYS:HG2	1.97	0.46
1:B:1270:VAL:HG22	1:B:1285:VAL:HG22	1.97	0.46
1:B:3260:ARG:NH1	1:B:3264:CYS:HA	2.29	0.46
1:B:3650:GLU:HB2	1:B:3651:PRO:HD3	1.98	0.46
1:B:4634:VAL:HG22	1:B:4640:PHE:HD1	1.79	0.46
1:C:2176:VAL:HG22	1:C:2220:TYR:CE2	2.51	0.46
1:C:2736:LYS:HB3	1:C:2741:TRP:HB2	1.97	0.46
1:C:2884:LYS:O	1:C:2887:GLU:HG3	2.15	0.46
1:C:3318:HIS:C	1:C:3321:PRO:HD2	2.40	0.46
1:C:3986:LEU:HD11	1:C:4105:LEU:HG	1.97	0.46
1:C:4254:THR:HG22	1:C:4257:ARG:HH21	1.80	0.46
1:D:1898:LEU:HD22	1:D:1902:VAL:HG11	1.98	0.46
1:D:2886:ARG:O	1:D:2890:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3935:LEU:HD23	1:D:3940:LEU:HD22	1.97	0.46
1:A:1000:ALA:HB3	1:A:1047:LYS:HZ3	1.81	0.46
1:A:1074:ARG:NH1	1:A:1076:GLU:HA	2.30	0.46
1:A:2176:VAL:HG22	1:A:2220:TYR:CE2	2.51	0.46
1:A:2286:PRO:HG3	1:A:2359:ARG:HA	1.97	0.46
1:A:2640:LEU:HA	1:A:2643:LYS:HZ3	1.79	0.46
1:B:114:LEU:HB2	1:B:117:HIS:CE1	2.51	0.46
1:B:2586:GLN:HG3	1:B:2637:GLU:HG3	1.97	0.46
1:B:3005:THR:HG22	1:B:3040:LEU:HD22	1.97	0.46
1:B:3043:ARG:HG2	1:B:3047:LYS:HZ2	1.80	0.46
1:B:3175:LEU:HD22	1:B:3178:HIS:CE1	2.50	0.46
1:B:3216:GLU:HA	1:B:3219:VAL:HG22	1.97	0.46
1:B:4089:GLU:HB2	1:B:4090:PRO:HD3	1.96	0.46
1:B:4735:ASN:HB3	1:B:4738:PHE:CD2	2.50	0.46
1:C:842:GLN:HB2	1:C:1603:PHE:HB2	1.98	0.46
1:C:3124:GLU:C	1:C:3126:VAL:H	2.24	0.46
1:C:3246:MET:CG	1:C:3268:LEU:HD11	2.43	0.46
1:D:1011:ARG:HB3	1:D:1016:TRP:HB2	1.97	0.46
1:D:2139:GLU:HA	1:D:2192:MET:HE3	1.97	0.46
1:D:2286:PRO:HG3	1:D:2359:ARG:HA	1.97	0.46
1:D:3035:ILE:O	1:D:3039:THR:HG23	2.15	0.46
1:D:4602:ARG:NH1	1:D:4627:LYS:HG3	2.31	0.46
1:A:319:LYS:HB3	1:A:319:LYS:HE2	1.70	0.46
1:A:874:LEU:HD11	1:A:940:LEU:HD11	1.98	0.46
1:A:2980:LEU:HG	1:A:2990:LEU:HD23	1.98	0.46
1:A:3187:LYS:O	1:A:3188:SER:OG	2.25	0.46
1:A:3318:HIS:C	1:A:3321:PRO:HD2	2.40	0.46
1:A:4602:ARG:NH1	1:A:4627:LYS:HG3	2.31	0.46
1:C:114:LEU:HB2	1:C:117:HIS:CE1	2.51	0.46
1:C:1922:ILE:O	1:C:1926:VAL:HG23	2.16	0.46
1:C:2087:LEU:O	1:C:2091:GLN:HG2	2.15	0.46
1:C:3175:LEU:HD22	1:C:3178:HIS:CE1	2.50	0.46
1:D:2980:LEU:HG	1:D:2990:LEU:HD23	1.98	0.46
1:D:3124:GLU:C	1:D:3126:VAL:H	2.24	0.46
1:D:3175:LEU:HD22	1:D:3178:HIS:CE1	2.50	0.46
1:D:3282:LYS:HA	1:D:3285:TYR:HD2	1.79	0.46
1:A:336:GLU:HB2	1:A:338:LEU:HD23	1.97	0.46
1:A:2642:ARG:HD2	1:A:2680:TYR:HE2	1.81	0.46
1:A:2985:ALA:HA	1:A:2995:HIS:CE1	2.51	0.46
1:A:4735:ASN:HB3	1:A:4738:PHE:CD2	2.50	0.46
1:B:842:GLN:HB2	1:B:1603:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2176:VAL:HG22	1:B:2220:TYR:CE2	2.51	0.46
1:C:1898:LEU:HD22	1:C:1902:VAL:HG11	1.98	0.46
1:C:2286:PRO:HG3	1:C:2359:ARG:HA	1.97	0.46
1:C:3235:MET:HE3	1:C:3287:ASN:HD21	1.81	0.46
1:C:3239:LEU:HB2	1:C:3240:PRO:HD3	1.97	0.46
1:C:3921:THR:HA	1:C:3924:ILE:HG12	1.98	0.46
1:C:4602:ARG:NH1	1:C:4627:LYS:HG3	2.31	0.46
1:D:114:LEU:HB2	1:D:117:HIS:CE1	2.51	0.46
1:D:1273:ILE:HB	1:D:1282:CYS:HB2	1.97	0.46
1:D:2954:PHE:HE2	1:D:2956:TYR:CE1	2.33	0.46
1:D:3650:GLU:HB2	1:D:3651:PRO:HD3	1.98	0.46
1:D:3845:LEU:HA	1:D:3848:GLU:HG3	1.98	0.46
1:A:58:VAL:HG13	1:A:319:LYS:HG2	1.97	0.46
1:A:1720:MET:SD	1:A:2127:ARG:HB3	2.55	0.46
1:A:2586:GLN:HG3	1:A:2637:GLU:HG3	1.97	0.46
1:A:2736:LYS:HB3	1:A:2741:TRP:HB2	1.97	0.46
1:A:2886:ARG:O	1:A:2890:GLN:HG2	2.16	0.46
1:B:2087:LEU:O	1:B:2091:GLN:HG2	2.15	0.46
1:B:2290:TRP:CZ2	1:B:2388:ILE:HG12	2.51	0.46
1:B:4002:MET:HE3	1:B:4002:MET:HB3	1.87	0.46
1:C:20:VAL:HG12	1:C:216:PRO:HA	1.97	0.46
1:C:58:VAL:HG13	1:C:319:LYS:HG2	1.97	0.46
1:C:877:HIS:HA	1:C:880:ARG:CD	2.45	0.46
1:C:1839:LEU:HA	1:C:1842:ILE:HD12	1.98	0.46
1:C:2139:GLU:HA	1:C:2192:MET:HE3	1.97	0.46
1:D:3234:VAL:HA	1:D:3238:ILE:HD12	1.98	0.46
1:D:3604:ARG:NH2	1:D:3607:PRO:HG3	2.31	0.46
1:D:3642:GLU:HB3	1:D:4683:ARG:NH2	2.31	0.46
1:D:4196:THR:O	1:D:4200:MET:HG3	2.16	0.46
1:A:3650:GLU:HB2	1:A:3651:PRO:HD3	1.98	0.45
1:B:3921:THR:HA	1:B:3924:ILE:HG12	1.98	0.45
1:D:336:GLU:HB2	1:D:338:LEU:HD23	1.97	0.45
1:D:2225:SER:HB2	1:D:2240:LEU:HD13	1.97	0.45
1:D:2290:TRP:CZ2	1:D:2388:ILE:HG12	2.51	0.45
1:A:1839:LEU:HA	1:A:1842:ILE:HD12	1.98	0.45
1:A:2290:TRP:CZ2	1:A:2388:ILE:HG12	2.51	0.45
1:A:2990:LEU:HD12	1:A:2990:LEU:O	2.16	0.45
1:A:4179:GLU:HG2	1:A:4179:GLU:O	2.17	0.45
1:B:874:LEU:HD11	1:B:940:LEU:HD11	1.98	0.45
1:B:1749:PRO:HB2	1:B:1913:LEU:HD22	1.99	0.45
1:B:2990:LEU:HD12	1:B:2990:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:909:ASP:HB2	1:C:914:GLN:HB2	1.99	0.45
1:C:2225:SER:HB2	1:C:2240:LEU:HD13	1.97	0.45
1:C:3281:LEU:O	1:C:3285:TYR:CD2	2.69	0.45
1:D:2455:ASP:OD2	1:D:2457:SER:OG	2.23	0.45
1:D:2990:LEU:HD12	1:D:2990:LEU:O	2.16	0.45
1:A:2139:GLU:HA	1:A:2192:MET:HE3	1.97	0.45
1:A:4173:ILE:HD13	1:A:4884:MET:HE2	1.99	0.45
1:B:1720:MET:SD	1:B:2127:ARG:HB3	2.56	0.45
1:B:3234:VAL:HA	1:B:3238:ILE:HD12	1.98	0.45
1:C:2886:ARG:O	1:C:2890:GLN:HG2	2.16	0.45
1:C:2985:ALA:HA	1:C:2995:HIS:CE1	2.51	0.45
1:C:3043:ARG:HG2	1:C:3047:LYS:HZ2	1.80	0.45
1:C:3845:LEU:HA	1:C:3848:GLU:HG3	1.98	0.45
1:D:20:VAL:HG12	1:D:216:PRO:HA	1.97	0.45
1:D:909:ASP:HB2	1:D:914:GLN:HB2	1.99	0.45
1:D:3281:LEU:O	1:D:3285:TYR:CD2	2.69	0.45
1:D:3797:MET:HE1	1:D:3870:ILE:HG23	1.99	0.45
1:D:4179:GLU:HG2	1:D:4179:GLU:O	2.17	0.45
1:A:606:ARG:NH2	1:A:1633:PRO:HD2	2.31	0.45
1:A:842:GLN:HB2	1:A:1603:PHE:HB2	1.98	0.45
1:A:3282:LYS:HA	1:A:3285:TYR:HD2	1.80	0.45
1:A:3935:LEU:HD23	1:A:3940:LEU:HD22	1.97	0.45
1:B:20:VAL:HG12	1:B:216:PRO:HA	1.97	0.45
1:B:2886:ARG:O	1:B:2890:GLN:HG2	2.16	0.45
1:B:3235:MET:HE3	1:B:3287:ASN:HD21	1.81	0.45
1:B:3604:ARG:NH2	1:B:3607:PRO:HG3	2.32	0.45
1:B:4036:ASP:OD2	1:B:4080:TYR:OH	2.20	0.45
1:C:4173:ILE:HD13	1:C:4884:MET:HE2	1.99	0.45
1:D:2736:LYS:HB3	1:D:2741:TRP:HB2	1.97	0.45
1:A:20:VAL:HG12	1:A:216:PRO:HA	1.97	0.45
1:A:114:LEU:HB2	1:A:117:HIS:CE1	2.51	0.45
1:A:3234:VAL:HA	1:A:3238:ILE:HD12	1.98	0.45
1:A:3246:MET:CE	1:A:3276:LEU:HD22	2.47	0.45
1:A:3797:MET:HE1	1:A:3870:ILE:HG23	1.99	0.45
1:B:891:GLU:CG	1:B:978:PRO:HB3	2.47	0.45
1:B:1922:ILE:O	1:B:1926:VAL:HG23	2.16	0.45
1:B:2139:GLU:HA	1:B:2192:MET:HE3	1.97	0.45
1:C:2691:LYS:O	1:C:2695:MET:HB2	2.17	0.45
1:C:3234:VAL:HA	1:C:3238:ILE:HD12	1.98	0.45
1:C:3642:GLU:HB3	1:C:4683:ARG:NH2	2.31	0.45
1:C:3797:MET:HE1	1:C:3870:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4735:ASN:HB3	1:C:4738:PHE:CD2	2.50	0.45
1:D:310:GLU:H	1:D:310:GLU:CD	2.25	0.45
1:D:2642:ARG:HD2	1:D:2680:TYR:HE2	1.81	0.45
1:D:2691:LYS:O	1:D:2695:MET:HB2	2.16	0.45
1:A:891:GLU:CG	1:A:978:PRO:HB3	2.47	0.45
1:A:1270:VAL:HG22	1:A:1285:VAL:HG22	1.97	0.45
1:A:3277:LEU:HD22	1:A:3306:ILE:HG22	1.99	0.45
1:A:3642:GLU:HB3	1:A:4683:ARG:NH2	2.31	0.45
1:A:3796:LEU:HD22	1:A:3835:PHE:HZ	1.82	0.45
1:B:2841:ALA:HB2	1:B:2893:LEU:HD12	1.99	0.45
1:B:2985:ALA:HA	1:B:2995:HIS:CE1	2.51	0.45
1:B:3281:LEU:O	1:B:3285:TYR:CD2	2.69	0.45
1:B:3935:LEU:HD23	1:B:3940:LEU:HD22	1.97	0.45
1:B:4602:ARG:NH1	1:B:4627:LYS:HG3	2.31	0.45
1:C:310:GLU:CD	1:C:310:GLU:H	2.25	0.45
1:C:2353:ILE:HG23	1:C:2359:ARG:HB2	1.99	0.45
1:D:58:VAL:HG13	1:D:319:LYS:HG2	1.97	0.45
1:D:874:LEU:HD11	1:D:940:LEU:HD11	1.98	0.45
1:D:1174:MET:HE3	1:D:1189:GLU:HB3	1.99	0.45
1:D:4173:ILE:HD13	1:D:4884:MET:HE2	1.99	0.45
1:A:3604:ARG:NH2	1:A:3607:PRO:HG3	2.31	0.45
1:A:3921:THR:HA	1:A:3924:ILE:HG12	1.98	0.45
1:A:4196:THR:O	1:A:4200:MET:HG3	2.16	0.45
1:B:1898:LEU:HD22	1:B:1902:VAL:HG11	1.98	0.45
1:B:2779:LEU:HA	1:B:2782:MET:HE2	1.97	0.45
1:C:137:ARG:H	1:C:137:ARG:HD3	1.82	0.45
1:C:891:GLU:CG	1:C:978:PRO:HB3	2.47	0.45
1:C:2255:LEU:O	1:C:3810:ARG:NH1	2.46	0.45
1:C:3277:LEU:HD22	1:C:3306:ILE:HG22	1.99	0.45
1:C:3604:ARG:NH2	1:C:3607:PRO:HG3	2.31	0.45
1:D:2472:LEU:HD12	1:D:2476:TYR:HB2	1.98	0.45
1:D:3284:ILE:HD11	1:D:3296:MET:CG	2.46	0.45
1:D:3892:TYR:OH	1:D:3899:ASP:OD1	2.21	0.45
1:A:1749:PRO:HB2	1:A:1913:LEU:HD22	1.99	0.45
1:A:2727:HIS:CE1	1:A:2731:LYS:HZ2	2.34	0.45
1:A:3892:TYR:OH	1:A:3899:ASP:OD1	2.21	0.45
1:B:1714:TYR:CZ	1:B:1761:MET:HB2	2.52	0.45
1:B:3124:GLU:C	1:B:3126:VAL:H	2.24	0.45
1:B:4196:THR:O	1:B:4200:MET:HG3	2.16	0.45
1:C:874:LEU:HD11	1:C:940:LEU:HD11	1.98	0.45
1:C:2290:TRP:CZ2	1:C:2388:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4262:LYS:O	1:C:4265:LYS:NZ	2.32	0.45
1:D:370:LEU:HB2	1:D:393:MET:HE2	1.99	0.45
1:D:1714:TYR:CZ	1:D:1761:MET:HB2	2.52	0.45
1:D:2356:ASP:OD2	1:D:2359:ARG:HG3	2.17	0.45
1:D:3277:LEU:HD22	1:D:3306:ILE:HG22	1.99	0.45
1:D:3986:LEU:HG	1:D:3999:MET:HE1	1.99	0.45
1:A:2353:ILE:HG23	1:A:2359:ARG:HB2	1.99	0.45
1:A:2691:LYS:O	1:A:2695:MET:HB2	2.17	0.45
1:A:3604:ARG:NH2	1:A:3609:TYR:OH	2.39	0.45
1:A:3845:LEU:HA	1:A:3848:GLU:HG3	1.98	0.45
2:F:8:ILE:HA	1:B:730:LEU:HD11	1.99	0.45
1:B:1977:LEU:HD11	1:B:3620:PHE:CD1	2.52	0.45
1:B:2954:PHE:CD1	1:B:2955:PRO:HD2	2.52	0.45
1:B:3246:MET:CE	1:B:3276:LEU:HD22	2.47	0.45
1:B:3642:GLU:HB3	1:B:4683:ARG:NH2	2.31	0.45
1:C:370:LEU:HB2	1:C:393:MET:HE2	1.99	0.45
1:C:1174:MET:HE3	1:C:1189:GLU:HB3	1.99	0.45
1:C:1977:LEU:HD11	1:C:3620:PHE:CD1	2.52	0.45
1:C:2779:LEU:HA	1:C:2782:MET:HE2	1.97	0.45
1:C:2990:LEU:O	1:C:2990:LEU:HD12	2.16	0.45
1:D:11:ILE:HD13	1:D:176:ARG:HD2	1.99	0.45
1:D:842:GLN:HB2	1:D:1603:PHE:HB2	1.98	0.45
1:D:1113:MET:HE3	1:D:1211:GLN:HB3	1.99	0.45
1:D:2985:ALA:HA	1:D:2995:HIS:CE1	2.51	0.45
1:D:3152:ARG:NH2	1:D:3236:GLU:HG2	2.32	0.45
1:D:3921:THR:HA	1:D:3924:ILE:HG12	1.98	0.45
1:A:1174:MET:HE3	1:A:1189:GLU:HB3	1.99	0.45
1:A:1644:LEU:HD23	1:A:1651:LEU:HA	1.98	0.45
1:A:3152:ARG:NH2	1:A:3236:GLU:HG2	2.32	0.45
1:B:3697:LYS:HA	1:B:3700:HIS:NE2	2.32	0.45
1:B:3796:LEU:HD22	1:B:3835:PHE:HZ	1.82	0.45
1:C:467:ASP:O	1:C:475:LYS:NZ	2.37	0.45
1:C:1170:GLU:HG2	1:C:1172:THR:HG23	1.99	0.45
1:C:1644:LEU:HD23	1:C:1651:LEU:HA	1.99	0.45
1:C:3986:LEU:HG	1:C:3999:MET:HE1	1.99	0.45
1:C:4196:THR:O	1:C:4200:MET:HG3	2.16	0.45
1:D:2353:ILE:HG23	1:D:2359:ARG:HB2	1.99	0.45
1:D:2841:ALA:HB2	1:D:2893:LEU:HD12	1.99	0.45
1:D:3697:LYS:HA	1:D:3700:HIS:NE2	2.32	0.45
1:A:3284:ILE:HD11	1:A:3296:MET:CG	2.46	0.44
1:A:3329:LYS:O	1:A:3332:THR:OG1	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4090:PRO:HA	1:A:4093:ASP:OD1	2.17	0.44
1:A:4607:ALA:HB1	1:A:4649:VAL:HG21	1.99	0.44
1:B:370:LEU:HB2	1:B:393:MET:HE2	1.99	0.44
1:B:606:ARG:NH2	1:B:1633:PRO:HD2	2.31	0.44
1:B:909:ASP:HB2	1:B:914:GLN:HB2	1.99	0.44
1:B:992:GLN:NE2	1:B:1064:LEU:O	2.47	0.44
1:B:3845:LEU:HA	1:B:3848:GLU:HG3	1.98	0.44
1:B:3986:LEU:HG	1:B:3999:MET:HE1	1.99	0.44
1:B:4179:GLU:O	1:B:4179:GLU:HG2	2.17	0.44
1:B:4267:GLN:O	1:B:4270:LYS:HG3	2.17	0.44
1:C:11:ILE:HD13	1:C:176:ARG:HD2	1.99	0.44
1:C:2642:ARG:HD2	1:C:2680:TYR:HE2	1.81	0.44
1:C:3152:ARG:NH2	1:C:3236:GLU:HG2	2.32	0.44
1:C:3329:LYS:O	1:C:3332:THR:OG1	2.30	0.44
1:C:3712:LYS:NZ	1:C:3720:GLU:OE2	2.32	0.44
1:D:4569:GLU:HB3	1:D:4570:PRO:HD3	1.99	0.44
1:A:1898:LEU:HD22	1:A:1902:VAL:HG11	1.98	0.44
1:A:2938:GLN:O	1:A:2942:GLU:OE1	2.35	0.44
1:A:2999:LYS:O	1:A:3003:MET:HG3	2.17	0.44
1:A:3697:LYS:HA	1:A:3700:HIS:NE2	2.32	0.44
1:B:11:ILE:HD13	1:B:176:ARG:HD2	1.99	0.44
1:B:2691:LYS:O	1:B:2695:MET:HB2	2.17	0.44
1:B:2727:HIS:CE1	1:B:2731:LYS:HZ2	2.35	0.44
1:B:2954:PHE:O	1:B:2957:GLU:N	2.47	0.44
1:C:1714:TYR:CZ	1:C:1761:MET:HB2	2.52	0.44
1:D:606:ARG:NH2	1:D:1633:PRO:HD2	2.31	0.44
1:D:1839:LEU:HA	1:D:1842:ILE:HD12	1.97	0.44
1:A:909:ASP:HB2	1:A:914:GLN:HB2	1.99	0.44
1:A:1714:TYR:CZ	1:A:1761:MET:HB2	2.52	0.44
1:A:2356:ASP:OD2	1:A:2359:ARG:HG3	2.17	0.44
1:A:2472:LEU:HD12	1:A:2476:TYR:HB2	1.98	0.44
1:A:3124:GLU:C	1:A:3126:VAL:H	2.24	0.44
1:A:4640:PHE:CG	1:A:4641:PRO:HD3	2.52	0.44
1:B:1113:MET:HB2	1:B:1156:TRP:CZ2	2.52	0.44
1:B:3187:LYS:O	1:B:3191:GLU:HB2	2.18	0.44
1:B:4640:PHE:CG	1:B:4641:PRO:HD3	2.52	0.44
1:C:3796:LEU:HD22	1:C:3835:PHE:HZ	1.82	0.44
1:C:4090:PRO:HA	1:C:4093:ASP:OD1	2.17	0.44
1:D:1749:PRO:HB2	1:D:1913:LEU:HD22	1.99	0.44
1:D:3246:MET:CE	1:D:3276:LEU:HD22	2.47	0.44
1:A:370:LEU:HB2	1:A:393:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2841:ALA:HB2	1:A:2893:LEU:HD12	1.99	0.44
1:A:2954:PHE:CD1	1:A:2955:PRO:HD2	2.52	0.44
1:A:2954:PHE:O	1:A:2957:GLU:N	2.47	0.44
1:A:3187:LYS:O	1:A:3191:GLU:HB2	2.18	0.44
1:A:3986:LEU:HG	1:A:3999:MET:HE1	1.99	0.44
1:A:4287:TYR:HE1	1:B:4591:TYR:CD2	2.36	0.44
1:B:2353:ILE:HG23	1:B:2359:ARG:HB2	1.99	0.44
1:B:2642:ARG:HD2	1:B:2680:TYR:HE2	1.81	0.44
1:B:3284:ILE:HD11	1:B:3296:MET:CG	2.46	0.44
1:B:3797:MET:HE1	1:B:3870:ILE:HG23	1.99	0.44
1:C:2356:ASP:OD2	1:C:2359:ARG:HG3	2.17	0.44
1:C:2841:ALA:HB2	1:C:2893:LEU:HD12	1.99	0.44
1:C:2954:PHE:CD1	1:C:2955:PRO:HD2	2.52	0.44
1:C:2999:LYS:O	1:C:3003:MET:HG3	2.17	0.44
1:D:891:GLU:CG	1:D:978:PRO:HB3	2.47	0.44
1:D:1977:LEU:HD11	1:D:3620:PHE:CD1	2.52	0.44
1:D:2954:PHE:O	1:D:2957:GLU:N	2.47	0.44
1:A:137:ARG:HD3	1:A:137:ARG:H	1.82	0.44
1:A:4063:THR:O	1:A:4067:LEU:HD23	2.18	0.44
1:A:4070:ALA:HB1	1:A:4078:LEU:HD13	2.00	0.44
1:A:4569:GLU:HB3	1:A:4570:PRO:HD3	1.99	0.44
1:B:2728:SER:HA	1:B:2731:LYS:HZ3	1.82	0.44
1:B:4173:ILE:HD13	1:B:4884:MET:HE2	1.99	0.44
1:C:137:ARG:NH1	1:C:146:ASP:OD1	2.34	0.44
1:C:606:ARG:NH2	1:C:1633:PRO:HD2	2.31	0.44
1:C:1113:MET:HE3	1:C:1211:GLN:HB3	1.99	0.44
1:C:2938:GLN:O	1:C:2942:GLU:OE1	2.35	0.44
1:C:3697:LYS:HA	1:C:3700:HIS:NE2	2.32	0.44
1:C:4063:THR:O	1:C:4067:LEU:HD23	2.18	0.44
1:C:4751:LYS:HA	1:C:4754:ARG:HH11	1.83	0.44
1:D:629:GLN:OE1	1:D:1669:ASN:ND2	2.47	0.44
1:D:3823:GLU:OE1	1:D:3826:GLY:N	2.51	0.44
1:D:4267:GLN:O	1:D:4270:LYS:HG3	2.17	0.44
1:D:4751:LYS:HA	1:D:4754:ARG:HH11	1.83	0.44
1:A:11:ILE:HD13	1:A:176:ARG:HD2	1.99	0.44
1:A:310:GLU:CD	1:A:310:GLU:H	2.25	0.44
1:A:1977:LEU:HD11	1:A:3620:PHE:CD1	2.52	0.44
2:G:8:ILE:HA	1:C:730:LEU:HD11	2.00	0.44
1:B:1644:LEU:HD23	1:B:1651:LEU:HA	1.99	0.44
1:B:1800:LYS:HA	1:B:1890:LYS:HZ1	1.82	0.44
1:B:2356:ASP:OD2	1:B:2359:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2999:LYS:O	1:B:3003:MET:HG3	2.17	0.44
1:B:3006:SER:HB2	1:B:3053:VAL:HG22	2.00	0.44
1:B:3152:ARG:NH2	1:B:3236:GLU:HG2	2.32	0.44
1:B:3277:LEU:HD22	1:B:3306:ILE:HG22	1.99	0.44
1:C:4640:PHE:CG	1:C:4641:PRO:HD3	2.52	0.44
1:D:2999:LYS:O	1:D:3003:MET:HG3	2.17	0.44
1:D:3187:LYS:O	1:D:3191:GLU:HB2	2.18	0.44
1:D:3796:LEU:HD22	1:D:3835:PHE:HZ	1.82	0.44
1:D:4640:PHE:CG	1:D:4641:PRO:HD3	2.52	0.44
1:A:1979:PHE:CG	1:A:1993:ARG:HG2	2.53	0.44
1:B:137:ARG:HD3	1:B:137:ARG:H	1.82	0.44
1:B:1143:GLN:CD	1:B:1149:ASN:HB2	2.43	0.44
1:B:2938:GLN:O	1:B:2942:GLU:OE1	2.35	0.44
1:B:3152:ARG:HH22	1:B:3232:PRO:C	2.25	0.44
1:C:1800:LYS:HA	1:C:1890:LYS:HZ1	1.81	0.44
1:C:4179:GLU:O	1:C:4179:GLU:HG2	2.17	0.44
1:C:4607:ALA:HB1	1:C:4649:VAL:HG21	1.99	0.44
1:D:552:SER:HB2	1:D:588:ILE:HD13	2.00	0.44
1:D:3712:LYS:NZ	1:D:3720:GLU:OE2	2.32	0.44
1:A:552:SER:HB2	1:A:588:ILE:HD13	2.00	0.44
1:A:902:TRP:HH2	1:A:910:ASP:HA	1.83	0.44
1:A:1170:GLU:HG2	1:A:1172:THR:HG23	1.99	0.44
1:A:3075:LEU:HD12	1:A:3076:LYS:HD2	2.00	0.44
1:A:4267:GLN:O	1:A:4270:LYS:HG3	2.17	0.44
1:A:4591:TYR:CD2	1:D:4287:TYR:HE1	2.36	0.44
1:B:310:GLU:H	1:B:310:GLU:CD	2.25	0.44
1:B:902:TRP:HH2	1:B:910:ASP:HA	1.83	0.44
1:B:1170:GLU:HG2	1:B:1172:THR:HG23	1.99	0.44
1:B:1174:MET:HE3	1:B:1189:GLU:HB3	1.99	0.44
1:B:2689:MET:HE2	1:B:2689:MET:HB3	1.73	0.44
1:B:3044:THR:HA	1:B:3047:LYS:HG2	2.00	0.44
1:B:4090:PRO:HA	1:B:4093:ASP:OD1	2.17	0.44
1:B:4607:ALA:HB1	1:B:4649:VAL:HG21	1.99	0.44
1:C:319:LYS:HB3	1:C:319:LYS:HE2	1.70	0.44
1:C:1749:PRO:HB2	1:C:1913:LEU:HD22	1.99	0.44
1:C:2954:PHE:CG	1:C:2955:PRO:HD2	2.53	0.44
1:C:3246:MET:CE	1:C:3276:LEU:HD22	2.47	0.44
1:D:137:ARG:HD3	1:D:137:ARG:H	1.82	0.44
1:D:902:TRP:HH2	1:D:910:ASP:HA	1.83	0.44
1:D:1939:ASN:ND2	1:D:1989:PRO:HD3	2.33	0.44
1:D:3152:ARG:HH22	1:D:3232:PRO:C	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3235:MET:HE3	1:D:3287:ASN:HD21	1.81	0.44
1:D:4063:THR:O	1:D:4067:LEU:HD23	2.18	0.44
1:D:4090:PRO:HA	1:D:4093:ASP:OD1	2.17	0.44
1:A:1113:MET:HE3	1:A:1211:GLN:HB3	1.99	0.44
1:A:1939:ASN:ND2	1:A:1989:PRO:HD3	2.33	0.44
1:A:2182:GLY:HA2	1:A:2185:LYS:HG2	2.00	0.44
1:A:4834:PRO:HB3	1:A:4843:ARG:HH11	1.83	0.44
1:B:4751:LYS:HA	1:B:4754:ARG:HH11	1.83	0.44
1:C:62:LEU:O	1:C:66:THR:HG23	2.18	0.44
1:D:1564:MET:SD	1:D:1565:PRO:HD2	2.58	0.44
1:D:4607:ALA:HB1	1:D:4649:VAL:HG21	1.99	0.44
1:A:630:HIS:CE1	1:A:1671:ARG:HE	2.36	0.43
1:A:2455:ASP:OD2	1:A:2457:SER:OG	2.23	0.43
1:A:3044:THR:HA	1:A:3047:LYS:HG2	2.00	0.43
1:A:3823:GLU:OE1	1:A:3826:GLY:N	2.51	0.43
1:B:552:SER:HB2	1:B:588:ILE:HD13	2.00	0.43
1:B:1564:MET:SD	1:B:1565:PRO:HD2	2.58	0.43
1:B:3075:LEU:HD12	1:B:3076:LYS:HD2	2.00	0.43
1:B:3227:ARG:HD3	1:B:3228:TYR:N	2.33	0.43
1:B:3823:GLU:OE1	1:B:3826:GLY:N	2.51	0.43
1:B:4569:GLU:HB3	1:B:4570:PRO:HD3	1.99	0.43
1:C:1979:PHE:CG	1:C:1993:ARG:HG2	2.53	0.43
1:C:2147:GLY:HA2	1:C:2150:MET:HE2	2.00	0.43
1:C:2326:ARG:HD3	1:C:2326:ARG:HA	1.77	0.43
1:C:2689:MET:HE2	1:C:2689:MET:HB3	1.73	0.43
1:D:235:ARG:NH2	1:D:412:GLU:OE2	2.25	0.43
1:D:1000:ALA:HB3	1:D:1047:LYS:HZ3	1.83	0.43
1:D:1170:GLU:HG2	1:D:1172:THR:HG23	1.99	0.43
1:D:1979:PHE:CG	1:D:1993:ARG:HG2	2.53	0.43
1:D:2089:HIS:CE1	1:D:3690:ALA:HB1	2.53	0.43
1:D:3006:SER:HB2	1:D:3053:VAL:HG22	2.00	0.43
1:D:3019:ILE:HG13	1:D:3020:SER:N	2.33	0.43
1:D:3094:ILE:O	1:D:3098:THR:HG23	2.19	0.43
1:D:4834:PRO:HB3	1:D:4843:ARG:HH11	1.83	0.43
1:A:2939:TYR:O	1:A:2956:TYR:OH	2.36	0.43
1:B:1939:ASN:ND2	1:B:1989:PRO:HD3	2.33	0.43
1:B:2089:HIS:CE1	1:B:3690:ALA:HB1	2.53	0.43
1:B:2553:TYR:HD1	1:B:2605:MET:HE1	1.83	0.43
1:B:3019:ILE:HG13	1:B:3020:SER:N	2.33	0.43
1:C:2553:TYR:HD1	1:C:2605:MET:HE1	1.83	0.43
1:C:2913:ASP:HB3	1:C:2919:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4896:ASP:OD1	1:C:4897:TYR:N	2.52	0.43
1:D:1143:GLN:CD	1:D:1149:ASN:HB2	2.43	0.43
1:D:3019:ILE:HD13	1:D:3096:TYR:HA	2.00	0.43
1:D:3910:ILE:HG23	1:D:3974:LEU:HD22	2.00	0.43
1:D:4590:TYR:OH	1:D:4718:SER:HB2	2.18	0.43
1:A:62:LEU:O	1:A:66:THR:HG23	2.18	0.43
1:A:995:MET:HA	1:A:998:LYS:HE2	1.99	0.43
1:A:1649:GLU:HG2	1:A:1650:LEU:N	2.34	0.43
1:A:2232:PRO:C	1:A:2234:MET:H	2.26	0.43
1:A:2721:ILE:CG2	1:A:2772:ARG:HG3	2.48	0.43
1:A:2728:SER:HA	1:A:2731:LYS:HZ3	1.83	0.43
1:B:2409:ILE:HG21	1:B:2420:ARG:NH1	2.33	0.43
1:B:3861:GLN:H	1:B:3867:THR:HG23	1.84	0.43
1:C:1939:ASN:ND2	1:C:1989:PRO:HD3	2.33	0.43
1:C:2182:GLY:HA2	1:C:2185:LYS:HG2	2.00	0.43
1:C:2232:PRO:C	1:C:2234:MET:H	2.26	0.43
1:C:3019:ILE:HD13	1:C:3096:TYR:HA	2.00	0.43
1:C:3044:THR:HA	1:C:3047:LYS:HG2	2.00	0.43
1:C:3075:LEU:HD12	1:C:3076:LYS:HD2	2.00	0.43
1:C:3823:GLU:OE1	1:C:3826:GLY:N	2.51	0.43
1:C:3918:ASN:HA	1:C:3921:THR:HG22	2.01	0.43
1:C:4569:GLU:HB3	1:C:4570:PRO:HD3	1.99	0.43
1:D:1644:LEU:HD23	1:D:1651:LEU:HA	1.99	0.43
1:D:2954:PHE:CD1	1:D:2955:PRO:HD2	2.52	0.43
1:D:3260:ARG:NH1	1:D:3264:CYS:HA	2.29	0.43
1:A:2705:PRO:HD2	1:A:2854:LYS:HD2	2.00	0.43
1:A:2927:GLN:NE2	1:A:3003:MET:SD	2.92	0.43
1:A:3642:GLU:OE1	1:A:3730:ARG:NH1	2.51	0.43
1:B:630:HIS:CE1	1:B:1671:ARG:HE	2.36	0.43
1:B:2147:GLY:HA2	1:B:2150:MET:HE2	2.00	0.43
1:B:2705:PRO:HD2	1:B:2854:LYS:HD2	2.00	0.43
1:B:3642:GLU:OE1	1:B:3730:ARG:NH1	2.51	0.43
1:B:4070:ALA:HB1	1:B:4078:LEU:HD13	2.00	0.43
1:C:1649:GLU:HG2	1:C:1650:LEU:N	2.34	0.43
1:C:2832:THR:HG21	1:D:1290:PHE:HE2	1.84	0.43
1:C:3019:ILE:HG13	1:C:3020:SER:N	2.33	0.43
1:D:995:MET:HA	1:D:998:LYS:HE2	1.99	0.43
1:D:2147:GLY:HA2	1:D:2150:MET:HE2	2.00	0.43
1:D:2194:ALA:HA	1:D:2237:SER:HB3	2.00	0.43
1:D:2546:ASP:O	1:D:2550:HIS:ND1	2.52	0.43
1:D:2705:PRO:HB3	1:D:2851:ILE:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2721:ILE:CG2	1:D:2772:ARG:HG3	2.48	0.43
1:D:2913:ASP:HB3	1:D:2919:LYS:HD2	2.01	0.43
1:D:2918:GLU:HG3	1:D:2923:TYR:CE1	2.53	0.43
1:D:2938:GLN:O	1:D:2942:GLU:OE1	2.35	0.43
1:A:1564:MET:SD	1:A:1565:PRO:HD2	2.58	0.43
1:A:2771:TYR:O	1:A:2774:PRO:HD2	2.19	0.43
1:A:3006:SER:HB2	1:A:3053:VAL:HG22	2.00	0.43
1:A:3227:ARG:HD3	1:A:3228:TYR:N	2.33	0.43
1:A:3235:MET:HE3	1:A:3287:ASN:HD21	1.81	0.43
1:B:1113:MET:HE3	1:B:1211:GLN:HB3	1.99	0.43
1:B:3006:SER:OG	1:B:3010:LYS:NZ	2.52	0.43
1:B:3094:ILE:O	1:B:3098:THR:HG23	2.18	0.43
1:B:3213:LYS:HA	1:B:3216:GLU:OE1	2.19	0.43
1:B:4287:TYR:HE1	1:C:4591:TYR:CD2	2.37	0.43
1:C:1940:GLN:OE1	1:C:1976:LEU:HD11	2.19	0.43
1:C:2957:GLU:HA	1:C:2960:ILE:HG12	2.01	0.43
1:C:3187:LYS:O	1:C:3191:GLU:HB2	2.18	0.43
1:C:3213:LYS:HA	1:C:3216:GLU:OE1	2.19	0.43
1:C:4267:GLN:O	1:C:4270:LYS:HG3	2.17	0.43
1:D:2232:PRO:C	1:D:2234:MET:H	2.26	0.43
1:D:4896:ASP:OD1	1:D:4897:TYR:N	2.52	0.43
1:A:826:VAL:HG21	1:A:832:LEU:HB2	2.00	0.43
1:A:1143:GLN:CD	1:A:1149:ASN:HB2	2.43	0.43
1:A:1940:GLN:OE1	1:A:1976:LEU:HD11	2.19	0.43
1:A:2913:ASP:HB3	1:A:2919:LYS:HD2	2.01	0.43
1:A:3019:ILE:HD13	1:A:3096:TYR:HA	2.00	0.43
1:A:3304:GLN:O	1:A:3307:ILE:HG12	2.19	0.43
1:A:3910:ILE:HG23	1:A:3974:LEU:HD22	2.00	0.43
1:A:4896:ASP:OD1	1:A:4897:TYR:N	2.52	0.43
2:F:63:GLY:O	2:F:67:MET:HG3	2.18	0.43
1:B:1940:GLN:OE1	1:B:1976:LEU:HD11	2.19	0.43
1:B:1979:PHE:CG	1:B:1993:ARG:HG2	2.53	0.43
1:B:2771:TYR:O	1:B:2774:PRO:HD2	2.19	0.43
1:B:3910:ILE:HG23	1:B:3974:LEU:HD22	2.00	0.43
1:B:3918:ASN:HA	1:B:3921:THR:HG22	2.01	0.43
1:B:3967:LEU:HD12	1:B:3967:LEU:HA	1.90	0.43
1:B:4896:ASP:OD1	1:B:4897:TYR:N	2.52	0.43
1:C:41:GLY:HA3	1:C:126:SER:HB3	2.01	0.43
1:C:902:TRP:HH2	1:C:910:ASP:HA	1.83	0.43
1:C:1113:MET:HB2	1:C:1156:TRP:CZ2	2.52	0.43
1:C:2089:HIS:CE1	1:C:3690:ALA:HB1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2546:ASP:O	1:C:2550:HIS:ND1	2.52	0.43
1:C:2721:ILE:CG2	1:C:2772:ARG:HG3	2.48	0.43
1:C:3304:GLN:O	1:C:3307:ILE:HG12	2.19	0.43
1:C:3737:ALA:HB1	1:C:3777:MET:HG3	2.01	0.43
1:C:4863:GLN:NE2	1:D:4860:ALA:HB2	2.34	0.43
1:D:41:GLY:HA3	1:D:126:SER:HB3	2.01	0.43
1:D:2182:GLY:HA2	1:D:2185:LYS:HG2	2.00	0.43
1:D:3044:THR:HA	1:D:3047:LYS:HG2	2.00	0.43
1:D:3306:ILE:O	1:D:3310:VAL:HG23	2.19	0.43
1:A:882:ARG:HD2	1:A:883:GLU:N	2.33	0.43
1:A:1144:ARG:HG2	1:A:1150:GLU:O	2.19	0.43
1:A:2089:HIS:CE1	1:A:3690:ALA:HB1	2.53	0.43
1:A:2954:PHE:CG	1:A:2955:PRO:HD2	2.53	0.43
1:A:4751:LYS:HA	1:A:4754:ARG:HH11	1.83	0.43
1:B:62:LEU:O	1:B:66:THR:HG23	2.18	0.43
1:C:1144:ARG:HG2	1:C:1150:GLU:O	2.19	0.43
1:C:2918:GLU:HG3	1:C:2923:TYR:CE1	2.53	0.43
1:C:3094:ILE:O	1:C:3098:THR:HG23	2.18	0.43
1:C:3284:ILE:HD11	1:C:3296:MET:CG	2.46	0.43
1:D:557:TRP:NE1	1:D:561:ARG:HH12	2.17	0.43
1:D:902:TRP:CZ2	1:D:915:HIS:HB2	2.54	0.43
1:D:1649:GLU:HG2	1:D:1650:LEU:N	2.34	0.43
1:D:2403:ALA:HB2	1:D:2475:VAL:HG22	2.00	0.43
1:D:2409:ILE:HG21	1:D:2420:ARG:NH1	2.33	0.43
1:D:2786:GLY:O	1:D:2788:ARG:HD3	2.19	0.43
1:D:2927:GLN:NE2	1:D:3003:MET:SD	2.92	0.43
1:D:3642:GLU:OE1	1:D:3730:ARG:NH1	2.51	0.43
1:A:1000:ALA:HB3	1:A:1047:LYS:NZ	2.34	0.43
1:A:1113:MET:HB2	1:A:1156:TRP:CZ2	2.51	0.43
1:A:2786:GLY:O	1:A:2788:ARG:HD3	2.19	0.43
1:A:3315:LEU:HA	1:A:3319:PHE:CD1	2.54	0.43
1:B:995:MET:HA	1:B:998:LYS:HE2	2.00	0.43
1:B:2927:GLN:NE2	1:B:3003:MET:SD	2.92	0.43
1:B:2954:PHE:CG	1:B:2955:PRO:HD2	2.53	0.43
1:B:3304:GLN:O	1:B:3307:ILE:HG12	2.19	0.43
1:B:3719:MET:HE1	1:B:4677:LEU:HD12	2.01	0.43
1:B:3737:ALA:HB1	1:B:3777:MET:HG3	2.01	0.43
1:B:4590:TYR:OH	1:B:4718:SER:HB2	2.19	0.43
1:C:552:SER:HB2	1:C:588:ILE:HD13	2.00	0.43
1:C:630:HIS:CE1	1:C:1671:ARG:HE	2.36	0.43
1:C:977:LYS:HA	1:C:978:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1564:MET:SD	1:C:1565:PRO:HD2	2.58	0.43
1:C:3227:ARG:HD3	1:C:3228:TYR:N	2.33	0.43
1:D:1113:MET:HB2	1:D:1156:TRP:CZ2	2.52	0.43
1:D:2326:ARG:HD3	1:D:2326:ARG:HA	1.77	0.43
1:D:2705:PRO:CD	1:D:2854:LYS:HD2	2.49	0.43
1:D:3246:MET:CG	1:D:3268:LEU:HD11	2.43	0.43
1:D:3737:ALA:HB1	1:D:3777:MET:HG3	2.01	0.43
1:A:888:ASN:HD22	1:A:888:ASN:C	2.26	0.43
1:A:3306:ILE:O	1:A:3310:VAL:HG23	2.19	0.43
1:A:3653:GLU:OE1	1:A:3660:ARG:NH2	2.52	0.43
2:E:63:GLY:O	2:E:67:MET:HG3	2.19	0.43
2:H:26:HIS:CE1	2:H:46:PRO:HA	2.54	0.43
1:B:2232:PRO:C	1:B:2234:MET:H	2.26	0.43
1:B:2786:GLY:O	1:B:2788:ARG:HD3	2.19	0.43
1:C:2409:ILE:HG21	1:C:2420:ARG:NH1	2.33	0.43
1:C:2705:PRO:HB3	1:C:2851:ILE:CG1	2.49	0.43
1:C:3006:SER:HB2	1:C:3053:VAL:HG22	2.00	0.43
1:C:3653:GLU:OE1	1:C:3660:ARG:NH2	2.52	0.43
1:C:3910:ILE:HG23	1:C:3974:LEU:HD22	2.00	0.43
1:D:62:LEU:O	1:D:66:THR:HG23	2.18	0.43
1:D:630:HIS:CE1	1:D:1671:ARG:HE	2.36	0.43
1:D:1000:ALA:HB3	1:D:1047:LYS:NZ	2.34	0.43
1:D:1144:ARG:HG2	1:D:1150:GLU:O	2.19	0.43
1:D:2939:TYR:O	1:D:2956:TYR:OH	2.36	0.43
1:D:2954:PHE:CG	1:D:2955:PRO:HD2	2.53	0.43
1:D:3861:GLN:H	1:D:3867:THR:HG23	1.84	0.43
1:A:2409:ILE:HG21	1:A:2420:ARG:NH1	2.33	0.43
1:A:2620:TYR:HB2	1:A:2627:TRP:HD1	1.84	0.43
1:A:2705:PRO:HB3	1:A:2851:ILE:CG1	2.49	0.43
1:A:3861:GLN:H	1:A:3867:THR:HG23	1.84	0.43
2:G:63:GLY:O	2:G:67:MET:HG3	2.19	0.43
1:B:557:TRP:NE1	1:B:561:ARG:HH12	2.17	0.43
1:B:1649:GLU:HG2	1:B:1650:LEU:N	2.34	0.43
1:B:2403:ALA:HB2	1:B:2475:VAL:HG22	2.00	0.43
1:B:2546:ASP:O	1:B:2550:HIS:ND1	2.52	0.43
1:B:2913:ASP:HB3	1:B:2919:LYS:HD2	2.01	0.43
1:B:3164:GLY:O	1:B:3248:ARG:HG3	2.19	0.43
1:C:557:TRP:NE1	1:C:561:ARG:HH12	2.17	0.43
1:C:882:ARG:HD2	1:C:883:GLU:N	2.33	0.43
1:C:1143:GLN:CD	1:C:1149:ASN:HB2	2.43	0.43
1:C:3719:MET:HE1	1:C:4677:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4070:ALA:HB1	1:C:4078:LEU:HD13	2.00	0.43
1:C:4834:PRO:HB3	1:C:4843:ARG:HH11	1.83	0.43
1:C:4867:ILE:HG12	1:D:4864:GLY:HA2	2.01	0.43
1:D:2771:TYR:O	1:D:2774:PRO:HD2	2.19	0.43
1:D:2957:GLU:HA	1:D:2960:ILE:HG12	2.01	0.43
1:D:3075:LEU:HD12	1:D:3076:LYS:HD2	2.00	0.43
1:A:2918:GLU:HG3	1:A:2923:TYR:CE1	2.53	0.42
1:A:3006:SER:OG	1:A:3010:LYS:NZ	2.52	0.42
1:A:3213:LYS:HA	1:A:3216:GLU:OE1	2.19	0.42
1:A:3269:ASN:OD1	1:A:3270:SER:N	2.52	0.42
1:B:2194:ALA:HA	1:B:2237:SER:HB3	2.00	0.42
1:B:2264:LYS:HG2	1:B:2268:TYR:CE2	2.54	0.42
1:B:3326:LEU:HB2	1:B:3336:GLU:OE2	2.19	0.42
1:B:3653:GLU:OE1	1:B:3660:ARG:NH2	2.52	0.42
1:C:995:MET:HA	1:C:998:LYS:HE2	1.99	0.42
1:C:1000:ALA:HB3	1:C:1047:LYS:NZ	2.34	0.42
1:C:2264:LYS:HG2	1:C:2268:TYR:CE2	2.54	0.42
1:C:2705:PRO:CD	1:C:2854:LYS:HD2	2.49	0.42
1:C:3072:MET:O	1:C:3073:GLU:C	2.62	0.42
1:C:3187:LYS:O	1:C:3188:SER:OG	2.25	0.42
1:C:3306:ILE:O	1:C:3310:VAL:HG23	2.19	0.42
1:D:1940:GLN:OE1	1:D:1976:LEU:HD11	2.19	0.42
1:D:2255:LEU:O	1:D:3810:ARG:NH1	2.46	0.42
1:D:3213:LYS:HA	1:D:3216:GLU:OE1	2.19	0.42
1:D:3269:ASN:OD1	1:D:3270:SER:N	2.52	0.42
1:D:3304:GLN:O	1:D:3307:ILE:HG12	2.19	0.42
1:D:4070:ALA:HB1	1:D:4078:LEU:HD13	2.00	0.42
1:A:1102:TYR:N	1:A:1237:GLU:O	2.52	0.42
1:A:2147:GLY:HA2	1:A:2150:MET:HE2	2.00	0.42
1:A:2553:TYR:HD1	1:A:2605:MET:HE1	1.83	0.42
1:A:3918:ASN:HA	1:A:3921:THR:HG22	2.01	0.42
1:A:4590:TYR:OH	1:A:4718:SER:HB2	2.19	0.42
2:H:63:GLY:O	2:H:67:MET:HG3	2.19	0.42
1:B:1000:ALA:HB3	1:B:1047:LYS:NZ	2.34	0.42
1:B:1144:ARG:HG2	1:B:1150:GLU:O	2.19	0.42
1:B:1286:THR:OG1	1:B:1550:PRO:O	2.29	0.42
1:B:2721:ILE:HG21	1:B:2772:ARG:HG3	2.00	0.42
1:B:3306:ILE:O	1:B:3310:VAL:HG23	2.19	0.42
1:B:4834:PRO:HB3	1:B:4843:ARG:HH11	1.83	0.42
1:B:4863:GLN:NE2	1:C:4860:ALA:HB2	2.34	0.42
1:C:992:GLN:NE2	1:C:1064:LEU:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1074:ARG:NH2	1:C:1078:CYS:O	2.52	0.42
1:C:1088:PHE:HB2	1:C:1205:CYS:SG	2.59	0.42
1:C:2927:GLN:NE2	1:C:3003:MET:SD	2.92	0.42
1:C:3152:ARG:HH22	1:C:3232:PRO:C	2.25	0.42
1:C:3269:ASN:OD1	1:C:3270:SER:N	2.52	0.42
1:C:3315:LEU:HA	1:C:3319:PHE:CD1	2.54	0.42
1:C:3321:PRO:HA	1:C:3324:GLU:CG	2.50	0.42
1:C:4590:TYR:OH	1:C:4718:SER:HB2	2.19	0.42
1:D:3604:ARG:NH2	1:D:3609:TYR:OH	2.39	0.42
1:D:3653:GLU:OE1	1:D:3660:ARG:NH2	2.52	0.42
1:A:2546:ASP:O	1:A:2550:HIS:ND1	2.52	0.42
1:B:882:ARG:HD2	1:B:883:GLU:N	2.33	0.42
1:B:902:TRP:CZ2	1:B:915:HIS:HB2	2.54	0.42
1:B:2182:GLY:HA2	1:B:2185:LYS:HG2	2.00	0.42
1:B:3269:ASN:OD1	1:B:3270:SER:N	2.52	0.42
1:B:4063:THR:O	1:B:4067:LEU:HD23	2.18	0.42
1:B:4867:ILE:HG12	1:C:4864:GLY:HA2	2.01	0.42
1:C:307:SER:OG	1:C:315:LEU:O	2.34	0.42
1:C:2620:TYR:HB2	1:C:2627:TRP:HD1	1.84	0.42
1:C:3861:GLN:H	1:C:3867:THR:HG23	1.84	0.42
1:C:4287:TYR:HE1	1:D:4591:TYR:CD2	2.37	0.42
1:D:1822:ILE:HD12	1:D:1902:VAL:HG13	2.01	0.42
1:D:2082:ARG:HH12	1:D:3685:ASP:CG	2.28	0.42
1:D:2553:TYR:HD1	1:D:2605:MET:HE1	1.83	0.42
1:A:1088:PHE:HB2	1:A:1205:CYS:SG	2.59	0.42
1:A:2264:LYS:HG2	1:A:2268:TYR:CE2	2.54	0.42
1:A:3019:ILE:HG13	1:A:3020:SER:N	2.33	0.42
2:G:26:HIS:CE1	2:G:46:PRO:HA	2.54	0.42
1:B:2326:ARG:HD3	1:B:2326:ARG:HA	1.77	0.42
1:B:2620:TYR:HB2	1:B:2627:TRP:HD1	1.84	0.42
1:B:2721:ILE:CG2	1:B:2772:ARG:HG3	2.48	0.42
1:B:3019:ILE:HD13	1:B:3096:TYR:HA	2.00	0.42
1:B:3315:LEU:HA	1:B:3319:PHE:CD1	2.54	0.42
1:C:902:TRP:CZ2	1:C:915:HIS:HB2	2.54	0.42
1:C:2705:PRO:HD2	1:C:2854:LYS:HD2	2.00	0.42
1:C:2771:TYR:O	1:C:2774:PRO:HD2	2.19	0.42
1:C:3122:ILE:HA	1:C:3126:VAL:CG2	2.50	0.42
1:D:2264:LYS:HG2	1:D:2268:TYR:CE2	2.55	0.42
1:D:3006:SER:OG	1:D:3010:LYS:NZ	2.52	0.42
1:D:3227:ARG:HD3	1:D:3228:TYR:N	2.33	0.42
1:A:557:TRP:NE1	1:A:561:ARG:HH12	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2255:LEU:O	1:A:3810:ARG:NH1	2.46	0.42
1:A:2403:ALA:HB2	1:A:2475:VAL:HG22	2.00	0.42
1:A:3094:ILE:O	1:A:3098:THR:HG23	2.19	0.42
1:A:3164:GLY:O	1:A:3248:ARG:HG3	2.19	0.42
1:A:3719:MET:HE1	1:A:4677:LEU:HD12	2.01	0.42
1:A:3737:ALA:HB1	1:A:3777:MET:HG3	2.01	0.42
1:B:41:GLY:HA3	1:B:126:SER:HB3	2.01	0.42
1:B:1088:PHE:HB2	1:B:1205:CYS:SG	2.59	0.42
1:B:2705:PRO:HB3	1:B:2851:ILE:CG1	2.49	0.42
1:B:2918:GLU:HG3	1:B:2923:TYR:CE1	2.53	0.42
1:B:3072:MET:O	1:B:3073:GLU:C	2.62	0.42
1:C:826:VAL:HG21	1:C:832:LEU:HB2	2.00	0.42
1:C:997:ASP:HA	1:C:1047:LYS:HZ3	1.85	0.42
1:C:1541:PRO:HG2	1:C:1566:LEU:HD21	2.01	0.42
1:C:1719:LEU:HD21	1:C:1830:ILE:HD12	2.01	0.42
1:C:2194:ALA:HA	1:C:2237:SER:HB3	2.00	0.42
1:C:2786:GLY:O	1:C:2788:ARG:HD3	2.19	0.42
1:D:1074:ARG:NH2	1:D:1078:CYS:O	2.52	0.42
1:D:1088:PHE:HB2	1:D:1205:CYS:SG	2.59	0.42
1:D:1102:TYR:N	1:D:1237:GLU:O	2.52	0.42
1:D:2620:TYR:HB2	1:D:2627:TRP:HD1	1.84	0.42
1:D:3183:ILE:HD11	1:D:3187:LYS:HD3	2.01	0.42
1:D:3213:LYS:O	1:D:3217:GLU:OE1	2.38	0.42
1:D:3321:PRO:HA	1:D:3324:GLU:CG	2.49	0.42
1:D:4580:THR:OG1	1:D:4733:HIS:NE2	2.43	0.42
1:A:889:ILE:HD11	1:A:936:SER:OG	2.19	0.42
1:A:1822:ILE:HD12	1:A:1902:VAL:HG13	2.01	0.42
1:A:2333:PRO:HA	1:A:2336:ARG:HG3	2.02	0.42
1:A:2721:ILE:HG21	1:A:2772:ARG:HG3	2.00	0.42
1:B:1102:TYR:N	1:B:1237:GLU:O	2.52	0.42
1:B:1718:ARG:HD3	1:B:1831:MET:HA	2.01	0.42
1:B:2957:GLU:HA	1:B:2960:ILE:HG12	2.01	0.42
1:B:3122:ILE:HA	1:B:3126:VAL:CG2	2.50	0.42
1:B:3604:ARG:NH2	1:B:3609:TYR:OH	2.39	0.42
1:C:1943:ARG:HH12	1:C:1964:GLU:CD	2.28	0.42
1:C:2721:ILE:HG21	1:C:2772:ARG:HG3	2.01	0.42
1:C:3164:GLY:O	1:C:3248:ARG:HG3	2.19	0.42
1:D:28:ILE:HG22	1:D:29:HIS:CD2	2.55	0.42
1:D:882:ARG:HD2	1:D:883:GLU:N	2.33	0.42
1:D:2333:PRO:HA	1:D:2336:ARG:HG3	2.02	0.42
1:D:2705:PRO:HD2	1:D:2854:LYS:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3326:LEU:HB2	1:D:3336:GLU:OE2	2.19	0.42
1:A:28:ILE:HG22	1:A:29:HIS:CD2	2.55	0.42
1:A:1074:ARG:NH2	1:A:1078:CYS:O	2.52	0.42
1:A:2194:ALA:HA	1:A:2237:SER:HB3	2.00	0.42
1:A:4002:MET:HE3	1:A:4002:MET:HB3	1.87	0.42
1:B:889:ILE:HD11	1:B:936:SER:OG	2.20	0.42
1:B:1719:LEU:HD21	1:B:1830:ILE:HD12	2.01	0.42
1:B:1943:ARG:HH12	1:B:1964:GLU:CD	2.28	0.42
1:C:1102:TYR:N	1:C:1237:GLU:O	2.52	0.42
1:C:3213:LYS:O	1:C:3217:GLU:OE1	2.38	0.42
1:C:3892:TYR:OH	1:C:3899:ASP:OD1	2.21	0.42
1:D:3918:ASN:HA	1:D:3921:THR:HG22	2.01	0.42
1:A:3326:LEU:HB2	1:A:3336:GLU:OE2	2.19	0.42
1:B:826:VAL:HG21	1:B:832:LEU:HB2	2.00	0.42
1:B:1074:ARG:NH2	1:B:1078:CYS:O	2.52	0.42
1:B:2634:SER:O	1:B:2635:GLU:HB3	2.20	0.42
1:B:2705:PRO:CD	1:B:2854:LYS:HD2	2.49	0.42
1:B:3152:ARG:NH2	1:B:3237:VAL:HG23	2.35	0.42
1:B:3983:LEU:HD23	1:B:3983:LEU:HA	1.91	0.42
1:B:4625:ASP:OD1	1:B:4625:ASP:N	2.49	0.42
1:C:28:ILE:HG22	1:C:29:HIS:CD2	2.55	0.42
1:C:2403:ALA:HB2	1:C:2475:VAL:HG22	2.00	0.42
1:C:2929:LEU:HD13	1:C:2971:ILE:HG12	2.02	0.42
1:C:3006:SER:OG	1:C:3010:LYS:NZ	2.52	0.42
1:C:3326:LEU:HB2	1:C:3336:GLU:OE2	2.19	0.42
1:D:1718:ARG:HD3	1:D:1831:MET:HA	2.01	0.42
1:A:902:TRP:CZ2	1:A:915:HIS:HB2	2.54	0.42
1:A:1718:ARG:HD3	1:A:1831:MET:HA	2.01	0.42
1:A:2182:GLY:HA3	1:A:2188:THR:HG22	2.01	0.42
1:A:2701:PHE:CE2	1:A:2703:PRO:HG3	2.55	0.42
1:A:2705:PRO:CD	1:A:2854:LYS:HD2	2.49	0.42
1:A:2957:GLU:HA	1:A:2960:ILE:HG12	2.01	0.42
1:A:3072:MET:O	1:A:3073:GLU:C	2.62	0.42
1:B:2486:HIS:O	1:B:2490:VAL:HG22	2.20	0.42
1:B:3213:LYS:O	1:B:3217:GLU:OE1	2.38	0.42
1:B:4806:CYS:HA	1:B:4812:CYS:HB2	2.02	0.42
1:C:3744:ILE:O	1:C:3747:SER:OG	2.34	0.42
1:D:1541:PRO:HG2	1:D:1566:LEU:HD21	2.02	0.42
1:D:1937:GLN:HG2	1:D:3609:TYR:HA	2.02	0.42
1:D:3164:GLY:O	1:D:3248:ARG:HG3	2.19	0.42
1:A:2486:HIS:O	1:A:2490:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3281:LEU:HB3	1:A:3285:TYR:HE2	1.85	0.42
2:G:6:GLU:HB2	2:G:74:LYS:HB3	2.02	0.42
1:B:888:ASN:C	1:B:888:ASN:HD22	2.26	0.42
1:B:1144:ARG:NH1	1:B:1191:ALA:O	2.53	0.42
1:B:4832:GLU:O	1:B:4843:ARG:NH1	2.53	0.42
1:C:2486:HIS:O	1:C:2490:VAL:HG22	2.20	0.42
1:C:3152:ARG:NH2	1:C:3237:VAL:HG23	2.35	0.42
1:C:4002:MET:HE3	1:C:4002:MET:HB3	1.87	0.42
1:D:826:VAL:HG21	1:D:832:LEU:HB2	2.00	0.42
1:D:3152:ARG:NH2	1:D:3237:VAL:HG23	2.35	0.42
1:D:3719:MET:HE1	1:D:4677:LEU:HD12	2.01	0.42
1:A:3122:ILE:HA	1:A:3126:VAL:HG21	2.02	0.41
1:A:4036:ASP:OD2	1:A:4080:TYR:OH	2.20	0.41
1:A:4863:GLN:NE2	1:B:4860:ALA:HB2	2.34	0.41
2:F:6:GLU:HB2	2:F:74:LYS:HB3	2.02	0.41
1:B:307:SER:HB3	1:B:327:THR:HG22	2.02	0.41
1:B:2082:ARG:HH12	1:B:3685:ASP:CG	2.28	0.41
1:B:3183:ILE:HD11	1:B:3187:LYS:HD3	2.01	0.41
1:C:866:PRO:HB3	1:C:1006:VAL:HG22	2.02	0.41
1:C:1971:GLU:O	1:C:1975:MET:HG2	2.20	0.41
1:C:3935:LEU:HD22	1:C:3985:MET:HE3	2.02	0.41
1:D:1420:LEU:HD23	1:D:1420:LEU:HA	1.88	0.41
1:D:2720:PHE:CE1	1:D:2896:LEU:HA	2.55	0.41
1:D:3315:LEU:HA	1:D:3319:PHE:CD1	2.54	0.41
1:A:41:GLY:HA3	1:A:126:SER:HB3	2.01	0.41
1:A:1435:GLY:H	1:A:1500:ARG:HH11	1.68	0.41
1:A:2929:LEU:HD13	1:A:2971:ILE:HG12	2.02	0.41
1:A:4832:GLU:O	1:A:4843:ARG:NH1	2.53	0.41
2:E:26:HIS:CE1	2:E:46:PRO:HA	2.54	0.41
1:B:1822:ILE:HD12	1:B:1902:VAL:HG13	2.01	0.41
1:B:2832:THR:HG21	1:C:1290:PHE:HE2	1.84	0.41
1:B:4580:THR:OG1	1:B:4733:HIS:NE2	2.43	0.41
1:C:889:ILE:HD11	1:C:936:SER:OG	2.20	0.41
1:C:962:LYS:HG3	1:C:981:MET:HB2	2.02	0.41
1:C:1560:ILE:HG13	1:C:1563:VAL:HB	2.03	0.41
1:C:1718:ARG:HD3	1:C:1831:MET:HA	2.01	0.41
1:C:3292:GLU:HB2	1:C:3296:MET:CE	2.50	0.41
1:C:3891:TYR:HA	1:D:76:ARG:NH2	2.35	0.41
1:C:3926:GLY:O	1:C:3927:PRO:C	2.63	0.41
1:D:1144:ARG:NH1	1:D:1191:ALA:O	2.53	0.41
1:D:1560:ILE:HG13	1:D:1563:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2938:GLN:HA	1:D:2941:LEU:HD12	2.03	0.41
1:D:3677:THR:HB	1:D:3679:LYS:NZ	2.35	0.41
1:A:748:LEU:HB2	2:E:8:ILE:HG23	2.03	0.41
1:A:1848:PRO:HG3	1:A:1890:LYS:O	2.21	0.41
1:A:1937:GLN:HG2	1:A:3609:TYR:HA	2.02	0.41
1:A:3122:ILE:HA	1:A:3126:VAL:CG2	2.50	0.41
1:A:3983:LEU:HD23	1:A:3983:LEU:HA	1.91	0.41
1:B:28:ILE:HG22	1:B:29:HIS:CD2	2.55	0.41
1:B:866:PRO:HB3	1:B:1006:VAL:HG22	2.03	0.41
1:B:1971:GLU:O	1:B:1975:MET:HG2	2.20	0.41
1:B:3179:ASN:HB2	1:B:3265:CYS:SG	2.61	0.41
1:C:42:PHE:HZ	1:C:459:LEU:HG	1.85	0.41
1:C:888:ASN:C	1:C:888:ASN:HD22	2.26	0.41
1:C:940:LEU:O	1:C:943:LEU:HB2	2.20	0.41
1:C:2332:GLY:O	1:C:2336:ARG:HG3	2.21	0.41
1:C:3183:ILE:HD11	1:C:3187:LYS:HD3	2.01	0.41
1:D:866:PRO:HB3	1:D:1006:VAL:HG22	2.02	0.41
1:D:2332:GLY:O	1:D:2336:ARG:HG3	2.21	0.41
1:D:2833:LEU:HD22	1:D:2837:LEU:HD13	2.01	0.41
1:D:3122:ILE:HA	1:D:3126:VAL:HG21	2.02	0.41
1:A:2332:GLY:O	1:A:2336:ARG:HG3	2.21	0.41
1:A:3183:ILE:HD11	1:A:3187:LYS:HD3	2.01	0.41
1:A:3213:LYS:O	1:A:3217:GLU:OE1	2.38	0.41
1:A:3292:GLU:HB2	1:A:3296:MET:CE	2.50	0.41
1:A:4806:CYS:HA	1:A:4812:CYS:HB2	2.02	0.41
2:H:6:GLU:HB2	2:H:74:LYS:HB3	2.02	0.41
1:B:162:ILE:HB	1:B:181:LEU:HD23	2.03	0.41
1:B:1427:TYR:HB2	1:B:1563:VAL:HG11	2.02	0.41
1:B:1826:TYR:HD1	1:B:1909:LEU:HD23	1.86	0.41
1:B:1848:PRO:HG3	1:B:1890:LYS:O	2.21	0.41
1:B:2332:GLY:O	1:B:2336:ARG:HG3	2.21	0.41
1:B:2333:PRO:HA	1:B:2336:ARG:HG3	2.02	0.41
1:B:3920:LEU:O	1:B:3924:ILE:HG12	2.21	0.41
1:B:4048:PHE:CD2	1:B:4052:MET:HE2	2.56	0.41
1:C:307:SER:HB3	1:C:327:THR:HG22	2.02	0.41
1:C:1826:TYR:HD1	1:C:1909:LEU:HD23	1.86	0.41
1:C:1848:PRO:HG3	1:C:1890:LYS:O	2.21	0.41
1:C:2954:PHE:O	1:C:2957:GLU:N	2.47	0.41
1:D:962:LYS:HG3	1:D:981:MET:HB2	2.02	0.41
1:D:1719:LEU:HD21	1:D:1830:ILE:HD12	2.01	0.41
1:D:2182:GLY:HA3	1:D:2188:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2486:HIS:O	1:D:2490:VAL:HG22	2.20	0.41
1:D:2592:LEU:O	1:D:2596:VAL:HG12	2.21	0.41
1:D:2701:PHE:CE2	1:D:2703:PRO:HG3	2.55	0.41
1:A:162:ILE:HB	1:A:181:LEU:HD23	2.03	0.41
1:A:877:HIS:CE1	1:A:878:LEU:HD12	2.56	0.41
1:A:1176:THR:HG22	1:A:1181:ILE:HA	2.03	0.41
1:A:1425:THR:HG22	1:A:1563:VAL:HG13	2.03	0.41
1:A:1541:PRO:HG2	1:A:1566:LEU:HD21	2.02	0.41
1:A:1560:ILE:HG13	1:A:1563:VAL:HB	2.02	0.41
1:A:2720:PHE:CE1	1:A:2896:LEU:HA	2.55	0.41
1:A:2894:LYS:O	1:A:2898:ILE:HG12	2.21	0.41
1:A:2938:GLN:HA	1:A:2941:LEU:HD12	2.03	0.41
1:A:3277:LEU:O	1:A:3281:LEU:HG	2.20	0.41
1:A:3677:THR:HB	1:A:3679:LYS:NZ	2.35	0.41
1:B:42:PHE:HZ	1:B:459:LEU:HG	1.85	0.41
1:B:1176:THR:HG22	1:B:1181:ILE:HA	2.03	0.41
1:B:1594:VAL:O	1:B:1594:VAL:HG13	2.20	0.41
1:B:2592:LEU:O	1:B:2596:VAL:HG12	2.21	0.41
1:B:2701:PHE:CE2	1:B:2703:PRO:HG3	2.55	0.41
1:B:3787:VAL:HG22	1:B:3864:ASN:HB3	2.03	0.41
1:C:1937:GLN:HG2	1:C:3609:TYR:HA	2.02	0.41
1:C:2634:SER:O	1:C:2635:GLU:HB3	2.20	0.41
1:C:2877:LEU:HB3	1:C:2882:LYS:HG3	2.03	0.41
1:C:3179:ASN:HB2	1:C:3265:CYS:SG	2.61	0.41
1:C:3677:THR:HB	1:C:3679:LYS:NZ	2.35	0.41
1:C:3787:VAL:HG22	1:C:3864:ASN:HB3	2.03	0.41
1:C:3871:ILE:O	1:C:3875:VAL:HG23	2.21	0.41
1:D:307:SER:HB3	1:D:327:THR:HG22	2.02	0.41
1:D:889:ILE:HD11	1:D:936:SER:OG	2.20	0.41
1:D:1176:THR:HG22	1:D:1181:ILE:HA	2.03	0.41
1:D:1425:THR:HG22	1:D:1563:VAL:HG13	2.03	0.41
1:D:1427:TYR:HB2	1:D:1563:VAL:HG11	2.02	0.41
1:D:3179:ASN:HB2	1:D:3265:CYS:SG	2.61	0.41
1:D:3871:ILE:O	1:D:3875:VAL:HG23	2.21	0.41
1:A:78:LEU:HD11	1:A:159:TRP:CG	2.56	0.41
1:A:940:LEU:O	1:A:943:LEU:HB2	2.20	0.41
1:A:2589:LEU:O	1:A:2593:VAL:HG13	2.21	0.41
1:A:2668:CYS:O	1:A:2672:VAL:HG23	2.21	0.41
1:A:3152:ARG:NH2	1:A:3237:VAL:HG23	2.35	0.41
1:A:3662:ASP:OD1	1:A:3665:HIS:HB2	2.21	0.41
1:A:3920:LEU:O	1:A:3924:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ASP:O	1:B:475:LYS:NZ	2.37	0.41
1:B:2589:LEU:O	1:B:2593:VAL:HG13	2.21	0.41
1:B:2833:LEU:HD22	1:B:2837:LEU:HD13	2.01	0.41
1:B:2935:GLU:O	1:B:2938:GLN:HG3	2.21	0.41
1:B:3817:LEU:HB2	1:B:3819:MET:HE1	2.03	0.41
1:B:3871:ILE:O	1:B:3875:VAL:HG23	2.21	0.41
1:C:601:LEU:HG	1:C:610:VAL:HG11	2.03	0.41
1:C:910:ASP:OD1	1:C:911:ASN:N	2.54	0.41
1:C:2082:ARG:HH12	1:C:3685:ASP:CG	2.28	0.41
1:C:4602:ARG:NH1	1:C:4631:ASP:OD1	2.52	0.41
1:D:1971:GLU:O	1:D:1975:MET:HG2	2.20	0.41
1:D:2721:ILE:HG21	1:D:2772:ARG:HG3	2.01	0.41
1:D:2929:LEU:HD13	1:D:2971:ILE:HG12	2.02	0.41
1:A:910:ASP:OD1	1:A:911:ASN:N	2.54	0.41
1:A:2222:LEU:HD23	1:A:2222:LEU:HA	1.93	0.41
1:A:2634:SER:O	1:A:2635:GLU:HB3	2.20	0.41
1:A:3871:ILE:O	1:A:3875:VAL:HG23	2.21	0.41
1:A:3935:LEU:HD22	1:A:3985:MET:HE3	2.02	0.41
1:A:4621:PRO:HD2	1:A:4632:ARG:NH2	2.36	0.41
2:E:6:GLU:HB2	2:E:74:LYS:HB3	2.02	0.41
1:B:78:LEU:HD11	1:B:159:TRP:CG	2.56	0.41
1:B:1435:GLY:H	1:B:1500:ARG:HH11	1.68	0.41
1:B:1560:ILE:HG13	1:B:1563:VAL:HB	2.02	0.41
1:B:3277:LEU:O	1:B:3281:LEU:HG	2.20	0.41
1:C:78:LEU:HD11	1:C:159:TRP:CG	2.56	0.41
1:C:1144:ARG:NH1	1:C:1191:ALA:O	2.53	0.41
1:C:1176:THR:HG22	1:C:1181:ILE:HA	2.03	0.41
1:C:2592:LEU:O	1:C:2596:VAL:HG12	2.21	0.41
1:C:2935:GLU:O	1:C:2938:GLN:HG3	2.21	0.41
1:C:3662:ASP:OD1	1:C:3665:HIS:HB2	2.21	0.41
1:C:3728:GLN:OE1	1:C:3770:ASN:ND2	2.48	0.41
1:C:4048:PHE:CD2	1:C:4052:MET:HE2	2.56	0.41
1:D:162:ILE:HB	1:D:181:LEU:HD23	2.03	0.41
1:D:877:HIS:CE1	1:D:878:LEU:HD12	2.56	0.41
1:D:1432:ILE:HD13	1:D:1505:LEU:HD22	2.03	0.41
1:D:2760:TYR:O	1:D:2763:LEU:HB2	2.21	0.41
1:D:3072:MET:O	1:D:3073:GLU:C	2.62	0.41
1:D:3122:ILE:HA	1:D:3126:VAL:CG2	2.50	0.41
1:D:3889:TYR:OH	1:D:3953:HIS:HB3	2.21	0.41
1:A:308:LEU:HD21	1:A:370:LEU:HD12	2.03	0.41
1:A:2592:LEU:O	1:A:2596:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2935:GLU:O	1:A:2938:GLN:HG3	2.21	0.41
1:A:3926:GLY:O	1:A:3927:PRO:C	2.63	0.41
2:F:8:ILE:HG23	1:B:748:LEU:HB2	2.03	0.41
2:F:26:HIS:CD2	2:F:46:PRO:HA	2.55	0.41
1:B:601:LEU:HG	1:B:610:VAL:HG11	2.03	0.41
1:B:910:ASP:OD1	1:B:911:ASN:N	2.54	0.41
1:B:989:THR:HG22	1:B:991:SER:H	1.86	0.41
1:B:2668:CYS:O	1:B:2672:VAL:HG23	2.21	0.41
1:B:4517:LEU:HD21	1:B:4736:ASN:HB3	2.03	0.41
1:C:1822:ILE:HD12	1:C:1902:VAL:HG13	2.01	0.41
1:C:2668:CYS:O	1:C:2672:VAL:HG23	2.21	0.41
1:C:2760:TYR:O	1:C:2763:LEU:HB2	2.21	0.41
1:C:2914:THR:N	1:C:2915:PRO:HD2	2.36	0.41
1:C:2938:GLN:HA	1:C:2941:LEU:HD12	2.03	0.41
1:C:3122:ILE:HA	1:C:3126:VAL:HG21	2.02	0.41
1:D:601:LEU:HG	1:D:610:VAL:HG11	2.03	0.41
1:D:2877:LEU:HB3	1:D:2882:LYS:HG3	2.03	0.41
1:D:2935:GLU:O	1:D:2938:GLN:HG3	2.21	0.41
1:D:3281:LEU:HB3	1:D:3285:TYR:HE2	1.85	0.41
1:A:866:PRO:HB3	1:A:1006:VAL:HG22	2.02	0.41
1:A:989:THR:HG22	1:A:991:SER:H	1.86	0.41
1:A:1144:ARG:NH1	1:A:1191:ALA:O	2.53	0.41
1:A:1286:THR:OG1	1:A:1550:PRO:O	2.29	0.41
1:A:1594:VAL:HG13	1:A:1594:VAL:O	2.20	0.41
1:A:1719:LEU:HD21	1:A:1830:ILE:HD12	2.01	0.41
1:A:1943:ARG:HH12	1:A:1964:GLU:CD	2.28	0.41
1:A:1948:MET:O	1:A:1951:LEU:HD22	2.21	0.41
1:A:2832:THR:HG21	1:B:1290:PHE:HE2	1.85	0.41
1:A:3152:ARG:HH22	1:A:3232:PRO:C	2.25	0.41
1:A:3179:ASN:HB2	1:A:3265:CYS:SG	2.61	0.41
1:A:3728:GLN:OE1	1:A:3770:ASN:ND2	2.48	0.41
1:A:3817:LEU:HB2	1:A:3819:MET:HE1	2.03	0.41
1:A:3889:TYR:OH	1:A:3953:HIS:HB3	2.21	0.41
2:F:78:THR:OG1	2:F:80:ASP:OD2	2.37	0.41
1:B:765:SER:HA	1:B:779:PHE:O	2.21	0.41
1:B:877:HIS:CE1	1:B:878:LEU:HD12	2.56	0.41
1:B:895:MET:HA	1:B:898:ILE:HG22	2.03	0.41
1:B:1282:CYS:SG	1:B:1556:GLU:HG2	2.61	0.41
1:B:1541:PRO:HG2	1:B:1566:LEU:HD21	2.01	0.41
1:B:1929:SER:OG	1:B:3617:VAL:HG13	2.21	0.41
1:B:2182:GLY:HA3	1:B:2188:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2427:ILE:HD13	1:B:2471:PHE:CZ	2.56	0.41
1:B:2959:GLU:OE1	1:B:2959:GLU:N	2.54	0.41
1:B:3889:TYR:OH	1:B:3953:HIS:HB3	2.20	0.41
1:B:4621:PRO:HD2	1:B:4632:ARG:NH2	2.36	0.41
1:C:162:ILE:HB	1:C:181:LEU:HD23	2.03	0.41
1:C:895:MET:HA	1:C:898:ILE:HG22	2.03	0.41
1:C:2182:GLY:HA3	1:C:2188:THR:HG22	2.01	0.41
1:C:2333:PRO:HA	1:C:2336:ARG:HG3	2.02	0.41
1:C:2727:HIS:CE1	1:C:2731:LYS:HZ2	2.39	0.41
1:C:2894:LYS:O	1:C:2898:ILE:HG12	2.21	0.41
1:C:2939:TYR:O	1:C:2956:TYR:OH	2.36	0.41
1:C:3889:TYR:OH	1:C:3953:HIS:HB3	2.21	0.41
1:C:4484:ILE:HG13	1:C:4485:ILE:N	2.36	0.41
1:C:4621:PRO:HD2	1:C:4632:ARG:NH2	2.36	0.41
1:D:910:ASP:OD1	1:D:911:ASN:N	2.54	0.41
1:D:940:LEU:O	1:D:943:LEU:HB2	2.20	0.41
1:D:1435:GLY:H	1:D:1500:ARG:HH11	1.68	0.41
1:D:1667:LEU:HD13	1:D:2131:SER:HB3	2.03	0.41
1:D:2427:ILE:HD13	1:D:2471:PHE:CZ	2.56	0.41
1:D:2589:LEU:O	1:D:2593:VAL:HG13	2.21	0.41
1:D:2914:THR:N	1:D:2915:PRO:HD2	2.36	0.41
1:D:3038:GLN:NE2	1:D:3107:SER:HB2	2.36	0.41
1:D:4048:PHE:CD2	1:D:4052:MET:HE2	2.56	0.41
1:D:4517:LEU:HD21	1:D:4736:ASN:HB3	2.03	0.41
1:A:2833:LEU:HD22	1:A:2837:LEU:HD13	2.01	0.41
1:A:3011:LEU:HD23	1:A:3011:LEU:HA	1.89	0.41
1:A:3038:GLN:NE2	1:A:3107:SER:HB2	2.36	0.41
1:B:308:LEU:HD21	1:B:370:LEU:HD12	2.03	0.41
1:B:2938:GLN:HA	1:B:2941:LEU:HD12	2.03	0.41
1:B:2939:TYR:O	1:B:2956:TYR:OH	2.36	0.41
1:B:3197:LEU:HA	1:B:3198:PRO:HD3	1.94	0.41
1:B:3281:LEU:HB3	1:B:3285:TYR:HE2	1.85	0.41
1:B:3662:ASP:OD1	1:B:3665:HIS:HB2	2.21	0.41
1:B:3935:LEU:HD22	1:B:3985:MET:HE3	2.02	0.41
1:B:4484:ILE:HG13	1:B:4485:ILE:N	2.36	0.41
1:C:891:GLU:HB3	1:C:978:PRO:HB3	2.03	0.41
1:C:997:ASP:OD1	1:C:1047:LYS:HD2	2.21	0.41
1:C:1048:ASP:O	1:C:1052:GLU:HG2	2.21	0.41
1:C:1594:VAL:HG13	1:C:1594:VAL:O	2.20	0.41
1:C:1667:LEU:HD13	1:C:2131:SER:HB3	2.03	0.41
1:C:2356:ASP:OD2	1:C:2358:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2701:PHE:CE2	1:C:2703:PRO:HG3	2.55	0.41
1:C:2959:GLU:OE1	1:C:2959:GLU:N	2.54	0.41
1:C:4806:CYS:HA	1:C:4812:CYS:HB2	2.02	0.41
1:D:1048:ASP:O	1:D:1052:GLU:HG2	2.21	0.41
1:D:1826:TYR:HD1	1:D:1909:LEU:HD23	1.86	0.41
1:D:2894:LYS:O	1:D:2898:ILE:HG12	2.21	0.41
1:D:2959:GLU:OE1	1:D:2959:GLU:N	2.54	0.41
1:D:3920:LEU:O	1:D:3924:ILE:HG12	2.21	0.41
1:D:4036:ASP:OD2	1:D:4080:TYR:OH	2.20	0.41
1:D:4891:CYS:HB3	1:D:4913:HIS:CE1	2.56	0.41
1:A:1282:CYS:SG	1:A:1556:GLU:HG2	2.61	0.40
1:A:1826:TYR:HD1	1:A:1909:LEU:HD23	1.86	0.40
1:A:1892:GLY:H	1:A:1895:GLN:NE2	2.19	0.40
1:A:2082:ARG:HH12	1:A:3685:ASP:CG	2.28	0.40
1:A:4048:PHE:CD2	1:A:4052:MET:HE2	2.56	0.40
1:A:4484:ILE:HG13	1:A:4485:ILE:N	2.36	0.40
2:G:83:TYR:OH	1:C:1768:PHE:O	2.25	0.40
1:B:940:LEU:O	1:B:943:LEU:HB2	2.20	0.40
1:B:988:LEU:HB2	1:B:1055:ARG:NE	2.33	0.40
1:B:1048:ASP:O	1:B:1052:GLU:HG2	2.21	0.40
1:B:1425:THR:HG22	1:B:1563:VAL:HG13	2.03	0.40
1:B:1947:VAL:HG12	1:B:1948:MET:HE2	2.04	0.40
1:B:2787:TRP:HE1	1:B:2905:ARG:HH21	1.69	0.40
1:B:3213:LYS:HA	1:B:3216:GLU:CD	2.47	0.40
1:B:4584:PHE:O	1:B:4588:ILE:HG13	2.21	0.40
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	2.03	0.40
1:C:1929:SER:OG	1:C:3617:VAL:HG13	2.21	0.40
1:C:1947:VAL:HG12	1:C:1948:MET:HE2	2.03	0.40
1:C:2720:PHE:CE1	1:C:2896:LEU:HA	2.55	0.40
1:C:3277:LEU:O	1:C:3281:LEU:HG	2.20	0.40
1:D:857:LEU:HG	1:D:860:ALA:HB2	2.03	0.40
1:D:2727:HIS:CE1	1:D:2731:LYS:HZ2	2.39	0.40
1:D:4484:ILE:HG13	1:D:4485:ILE:N	2.36	0.40
1:D:4806:CYS:HA	1:D:4812:CYS:HB2	2.02	0.40
1:A:307:SER:HB3	1:A:327:THR:HG22	2.02	0.40
1:A:538:ALA:O	1:A:542:ARG:HB2	2.21	0.40
1:A:1427:TYR:HB2	1:A:1563:VAL:HG11	2.02	0.40
1:A:1971:GLU:O	1:A:1975:MET:HG2	2.20	0.40
1:A:2326:ARG:HA	1:A:2326:ARG:HD3	1.77	0.40
1:A:2427:ILE:HD13	1:A:2471:PHE:CZ	2.56	0.40
1:A:2788:ARG:NH2	1:A:2908:LYS:HG2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2959:GLU:OE1	1:A:2959:GLU:N	2.54	0.40
1:A:3227:ARG:NH1	1:A:3228:TYR:HB3	2.36	0.40
1:B:1892:GLY:H	1:B:1895:GLN:NE2	2.19	0.40
1:B:1937:GLN:HG2	1:B:3609:TYR:HA	2.02	0.40
1:B:2914:THR:N	1:B:2915:PRO:HD2	2.36	0.40
1:C:1708:ASP:HA	1:C:1712:SER:HB3	2.03	0.40
1:C:2833:LEU:HD22	1:C:2837:LEU:HD13	2.01	0.40
1:C:2835:ARG:NH2	1:C:2838[B]:HIS:HB3	2.37	0.40
1:C:3235:MET:O	1:C:3239:LEU:HD12	2.22	0.40
1:C:3817:LEU:HB2	1:C:3819:MET:HE1	2.03	0.40
1:D:78:LEU:HD11	1:D:159:TRP:CG	2.56	0.40
1:D:1594:VAL:O	1:D:1594:VAL:HG13	2.20	0.40
1:D:2668:CYS:O	1:D:2672:VAL:HG23	2.21	0.40
1:D:2689:MET:HE2	1:D:2689:MET:HB3	1.73	0.40
1:D:3277:LEU:O	1:D:3281:LEU:HG	2.20	0.40
1:D:3292:GLU:HB2	1:D:3296:MET:CE	2.50	0.40
1:D:3728:GLN:OE1	1:D:3770:ASN:ND2	2.48	0.40
1:D:3926:GLY:O	1:D:3927:PRO:C	2.63	0.40
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.47	0.40
1:A:891:GLU:HB3	1:A:978:PRO:HB3	2.03	0.40
1:A:962:LYS:HG3	1:A:981:MET:HB2	2.02	0.40
1:A:1048:ASP:O	1:A:1052:GLU:HG2	2.21	0.40
1:A:3793:LEU:HD23	1:A:3793:LEU:HA	1.94	0.40
1:A:4306:PHE:HA	1:A:4309:ILE:HG12	2.03	0.40
1:B:1086:ARG:NH2	1:B:1254:ARG:HG3	2.37	0.40
1:B:1432:ILE:HD13	1:B:1505:LEU:HD22	2.03	0.40
1:B:2720:PHE:CE1	1:B:2896:LEU:HA	2.55	0.40
1:B:2929:LEU:HD13	1:B:2971:ILE:HG12	2.02	0.40
1:B:3122:ILE:HA	1:B:3126:VAL:HG21	2.02	0.40
1:C:137:ARG:HH22	1:C:204:ASP:HB3	1.86	0.40
1:C:2319:VAL:O	1:C:2323:LEU:HG	2.22	0.40
1:C:3920:LEU:O	1:C:3924:ILE:HG12	2.21	0.40
1:C:4891:CYS:HB3	1:C:4913:HIS:CE1	2.56	0.40
1:D:42:PHE:HZ	1:D:459:LEU:HG	1.85	0.40
1:D:891:GLU:HB3	1:D:978:PRO:HB3	2.03	0.40
1:D:2634:SER:O	1:D:2635:GLU:HB3	2.20	0.40
1:D:3213:LYS:HA	1:D:3216:GLU:CD	2.47	0.40
1:D:3235:MET:O	1:D:3239:LEU:HD12	2.22	0.40
1:D:3935:LEU:HD22	1:D:3985:MET:HE3	2.02	0.40
1:D:4306:PHE:HA	1:D:4309:ILE:HG12	2.03	0.40
1:A:765:SER:HA	1:A:779:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1432:ILE:HD13	1:A:1505:LEU:HD22	2.03	0.40
1:A:1697:LEU:HD23	1:A:1697:LEU:HA	1.95	0.40
1:A:2914:THR:N	1:A:2915:PRO:HD2	2.36	0.40
1:A:3214:LEU:HA	1:A:3217:GLU:CD	2.47	0.40
1:A:3840:PHE:CE1	1:A:3874:THR:HG23	2.57	0.40
1:A:3846:LEU:HD13	1:A:3854:PHE:CZ	2.56	0.40
2:H:12:ASP:OD1	2:H:68:SER:OG	2.39	0.40
1:B:70:GLU:OE2	1:B:122:ARG:HD3	2.21	0.40
1:B:891:GLU:HB3	1:B:978:PRO:HB3	2.03	0.40
1:B:977:LYS:HA	1:B:978:PRO:HD3	1.89	0.40
1:B:2760:TYR:O	1:B:2763:LEU:HB2	2.21	0.40
1:B:4891:CYS:HB3	1:B:4913:HIS:CE1	2.56	0.40
1:C:1425:THR:HG22	1:C:1563:VAL:HG13	2.03	0.40
1:C:1948:MET:O	1:C:1951:LEU:HD22	2.21	0.40
1:C:2788:ARG:NH2	1:C:2908:LYS:HG2	2.37	0.40
1:C:3038:GLN:NE2	1:C:3107:SER:HB2	2.36	0.40
1:C:3231:MET:HE2	1:C:3234:VAL:HG23	2.03	0.40
1:C:3642:GLU:OE1	1:C:3730:ARG:NH1	2.51	0.40
1:C:4517:LEU:HD21	1:C:4736:ASN:HB3	2.03	0.40
1:C:4584:PHE:O	1:C:4588:ILE:HG13	2.21	0.40
1:D:419:ILE:HG21	1:D:492:GLU:HG3	2.04	0.40
1:D:888:ASN:C	1:D:888:ASN:HD22	2.26	0.40
1:D:1121:GLY:O	1:D:1133:ARG:HD3	2.22	0.40
1:D:1708:ASP:HA	1:D:1712:SER:HB3	2.03	0.40
1:D:3227:ARG:NH1	1:D:3228:TYR:HB3	2.36	0.40
1:D:4795:LYS:HA	1:D:4795:LYS:HD2	1.94	0.40
1:A:1788:LYS:O	1:A:1792:ILE:HG13	2.22	0.40
1:A:3067:ASP:O	1:A:3071:THR:HG23	2.22	0.40
1:A:3213:LYS:HA	1:A:3216:GLU:CD	2.47	0.40
1:A:3651:PRO:HB2	1:A:3652:PRO:HD3	2.04	0.40
1:A:3686:PHE:HA	1:A:3689:MET:HE2	2.04	0.40
1:A:4517:LEU:HD21	1:A:4736:ASN:HB3	2.03	0.40
1:A:4665:ARG:HH12	1:A:4669:LEU:HD22	1.87	0.40
1:A:4867:ILE:HG12	1:B:4864:GLY:HA2	2.04	0.40
1:A:4891:CYS:HB3	1:A:4913:HIS:CE1	2.56	0.40
2:E:23:CYS:SG	2:E:51:ILE:HD11	2.62	0.40
1:B:375:GLN:HG3	1:B:377:VAL:HG13	2.03	0.40
1:B:670:TYR:O	1:B:673:TRP:NE1	2.54	0.40
1:B:1697:LEU:HD23	1:B:1697:LEU:HA	1.95	0.40
1:B:2208:ARG:NH2	1:B:2212:LYS:HZ1	2.20	0.40
1:B:2877:LEU:HB3	1:B:2882:LYS:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2998:ASN:C	1:B:2998:ASN:HD22	2.29	0.40
1:B:3227:ARG:NH1	1:B:3228:TYR:HB3	2.36	0.40
1:B:3840:PHE:CE1	1:B:3874:THR:HG23	2.57	0.40
1:B:3926:GLY:O	1:B:3927:PRO:C	2.63	0.40
1:B:4306:PHE:HA	1:B:4309:ILE:HG12	2.03	0.40
1:B:4602:ARG:NH1	1:B:4631:ASP:OD1	2.52	0.40
1:C:1427:TYR:HB2	1:C:1563:VAL:HG11	2.02	0.40
1:C:1705:LEU:HD12	1:C:1705:LEU:HA	1.90	0.40
1:C:2988:ARG:N	1:C:2989:PRO:HD3	2.37	0.40
1:C:4781:TYR:HD1	1:C:4846:PHE:CE1	2.40	0.40
1:C:4859:LEU:O	1:C:4863:GLN:HG2	2.22	0.40
1:D:670:TYR:O	1:D:673:TRP:NE1	2.54	0.40
1:D:1788:LYS:O	1:D:1792:ILE:HG13	2.22	0.40
1:D:1892:GLY:H	1:D:1895:GLN:NE2	2.19	0.40
1:D:2998:ASN:HD22	1:D:2998:ASN:C	2.29	0.40
1:D:3662:ASP:OD1	1:D:3665:HIS:HB2	2.21	0.40
1:D:3817:LEU:HB2	1:D:3819:MET:HE1	2.03	0.40
1:D:4602:ARG:NH1	1:D:4631:ASP:OD1	2.52	0.40
1:D:4781:TYR:HD1	1:D:4846:PHE:CE1	2.40	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	4092/4967 (82%)	3982 (97%)	108 (3%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4087 (97%)	108 (3%)	3 (0%)	48	68
1	C	2662/4967 (54%)	2597 (98%)	62 (2%)	3 (0%)	48	68
1	D	4198/4967 (84%)	4087 (97%)	108 (3%)	3 (0%)	48	68
2	E	105/108 (97%)	104 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
2	G	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
2	H	105/108 (97%)	104 (99%)	1 (1%)	0	100	100
All	All	15570/20300 (77%)	15169 (97%)	390 (2%)	11 (0%)	49	68

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4641	PRO
1	B	3927	PRO
1	B	4641	PRO
1	C	3927	PRO
1	C	4641	PRO
1	D	3927	PRO
1	D	4641	PRO
1	A	3292	GLU
1	B	3292	GLU
1	C	3292	GLU
1	D	3292	GLU

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	3708/4358 (85%)	3707 (100%)	1 (0%)	100	100
1	B	3708/4358 (85%)	3707 (100%)	1 (0%)	100	100
1	C	3708/4358 (85%)	3707 (100%)	1 (0%)	100	100
1	D	1044/4358 (24%)	1044 (100%)	0	100	100
2	E	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	G	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	12520/17788 (70%)	12517 (100%)	3 (0%)	100 100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3719	MET
1	B	3719	MET
1	C	3719	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	A	544	ASN
1	A	587	ASN
1	A	621	HIS
1	A	651	HIS
1	A	658	ASN
1	A	731	HIS
1	A	932	ASN
1	A	1267	HIS
1	A	1575	HIS
1	A	1684	GLN
1	A	1905	GLN
1	A	1917	GLN
1	A	1940	GLN
1	A	1974	ASN
1	A	2059	GLN
1	A	2089	HIS
1	A	2125	GLN
1	A	2250	ASN
1	A	2704	GLN
1	A	2722	ASN
1	A	2867	ASN
1	A	3034	HIS
1	A	3038	GLN
1	A	3079	GLN
1	A	3287	ASN
1	A	3308	ASN
1	A	3775	GLN
1	A	3850	HIS

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Mol	Chain	Res	Type
1	A	3869	ASN
1	A	3901	GLN
1	A	3955	GLN
1	A	3975	GLN
1	A	3998	GLN
1	A	4055	HIS
1	A	4159	GLN
1	A	4178	ASN
1	A	4579	HIS
1	A	4762	HIS
1	A	4766	GLN
1	A	4787	ASN
1	A	4879	GLN
1	A	4903	HIS
2	E	26	HIS
2	F	26	HIS
2	G	26	HIS
2	H	26	HIS
1	B	420	GLN
1	B	544	ASN
1	B	621	HIS
1	B	651	HIS
1	B	658	ASN
1	B	731	HIS
1	B	771	ASN
1	B	1126	GLN
1	B	1267	HIS
1	B	1551	ASN
1	B	1575	HIS
1	B	1684	GLN
1	B	1844	GLN
1	B	1905	GLN
1	B	1917	GLN
1	B	1940	GLN
1	B	1974	ASN
1	B	2059	GLN
1	B	2125	GLN
1	B	2224	ASN
1	B	2250	ASN
1	B	2704	GLN
1	B	2867	ASN
1	B	2890	GLN

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Mol	Chain	Res	Type
1	B	3034	HIS
1	B	3038	GLN
1	B	3287	ASN
1	B	3308	ASN
1	B	3775	GLN
1	B	3850	HIS
1	B	3869	ASN
1	B	3901	GLN
1	B	3925	GLN
1	B	3933	GLN
1	B	3955	GLN
1	B	3975	GLN
1	B	3998	GLN
1	B	4055	HIS
1	B	4159	GLN
1	B	4489	GLN
1	B	4762	HIS
1	B	4766	GLN
1	B	4794	ASN
1	B	4879	GLN
1	B	4903	HIS
1	C	420	GLN
1	C	544	ASN
1	C	587	ASN
1	C	621	HIS
1	C	651	HIS
1	C	658	ASN
1	C	731	HIS
1	C	836	HIS
1	C	932	ASN
1	C	1267	HIS
1	C	1575	HIS
1	C	1626	GLN
1	C	1684	GLN
1	C	1844	GLN
1	C	1905	GLN
1	C	1917	GLN
1	C	1940	GLN
1	C	1974	ASN
1	C	2059	GLN
1	C	2125	GLN
1	C	2224	ASN

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Mol	Chain	Res	Type
1	C	2250	ASN
1	C	2704	GLN
1	C	2722	ASN
1	C	2867	ASN
1	C	3034	HIS
1	C	3038	GLN
1	C	3287	ASN
1	C	3308	ASN
1	C	3775	GLN
1	C	3850	HIS
1	C	3869	ASN
1	C	3901	GLN
1	C	3925	GLN
1	C	3933	GLN
1	C	3955	GLN
1	C	3975	GLN
1	C	3998	GLN
1	C	4055	HIS
1	C	4159	GLN
1	C	4489	GLN
1	C	4762	HIS
1	C	4766	GLN
1	C	4879	GLN
1	C	4903	HIS
1	D	420	GLN
1	D	544	ASN
1	D	587	ASN
1	D	621	HIS
1	D	651	HIS
1	D	658	ASN
1	D	731	HIS
1	D	836	HIS
1	D	932	ASN
1	D	1126	GLN
1	D	4879	GLN
1	D	4903	HIS

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	D	5002	-	32,33,33	0.27	0	48,52,52	0.30	0
4	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	C	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	B	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	D	5003	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	A	5002	-	32,33,33	0.27	0	48,52,52	0.30	0
4	ATP	A	5003	-	32,33,33	0.25	0	48,52,52	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	D	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	C	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	7/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5003	-	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	5002	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	B	5003	ATP	C5'-O5'-PA-O1A
4	B	5003	ATP	C5'-O5'-PA-O2A
4	B	5003	ATP	C5'-O5'-PA-O3A
4	C	5003	ATP	C5'-O5'-PA-O1A
4	C	5003	ATP	C5'-O5'-PA-O2A
4	C	5003	ATP	C5'-O5'-PA-O3A
4	D	5003	ATP	C5'-O5'-PA-O1A
4	D	5003	ATP	C5'-O5'-PA-O2A
4	D	5003	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	O4'-C4'-C5'-O5'
4	B	5003	ATP	O4'-C4'-C5'-O5'
4	C	5003	ATP	O4'-C4'-C5'-O5'
4	D	5003	ATP	O4'-C4'-C5'-O5'
4	A	5003	ATP	C3'-C4'-C5'-O5'
4	B	5003	ATP	C3'-C4'-C5'-O5'
4	C	5003	ATP	C3'-C4'-C5'-O5'
4	D	5003	ATP	C3'-C4'-C5'-O5'
4	A	5002	ATP	PG-O3B-PB-O3A
4	B	5002	ATP	PG-O3B-PB-O3A
4	C	5002	ATP	PG-O3B-PB-O3A
4	D	5002	ATP	PG-O3B-PB-O3A
4	A	5003	ATP	PA-O3A-PB-O2B
4	B	5003	ATP	PA-O3A-PB-O2B
4	C	5003	ATP	PA-O3A-PB-O2B
4	D	5003	ATP	PA-O3A-PB-O2B
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	C5'-O5'-PA-O3A

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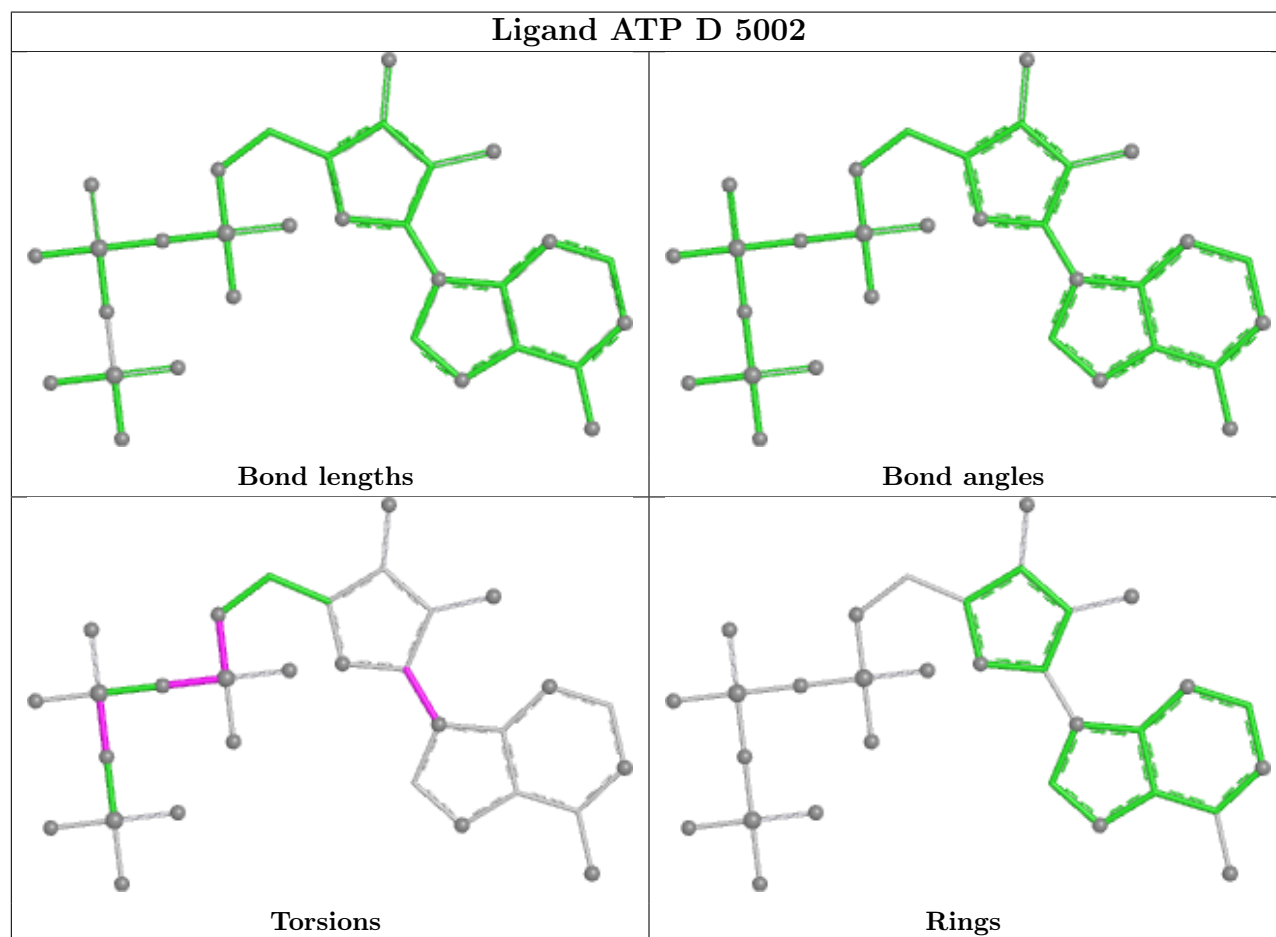
Mol	Chain	Res	Type	Atoms
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O2A
4	B	5002	ATP	C5'-O5'-PA-O3A
4	C	5002	ATP	C5'-O5'-PA-O1A
4	C	5002	ATP	C5'-O5'-PA-O2A
4	C	5002	ATP	C5'-O5'-PA-O3A
4	D	5002	ATP	C5'-O5'-PA-O1A
4	D	5002	ATP	C5'-O5'-PA-O2A
4	D	5002	ATP	C5'-O5'-PA-O3A
4	A	5002	ATP	O4'-C1'-N9-C8
4	B	5002	ATP	O4'-C1'-N9-C8
4	C	5002	ATP	O4'-C1'-N9-C8
4	D	5002	ATP	O4'-C1'-N9-C8
4	A	5002	ATP	O4'-C1'-N9-C4
4	B	5002	ATP	O4'-C1'-N9-C4
4	C	5002	ATP	O4'-C1'-N9-C4
4	D	5002	ATP	O4'-C1'-N9-C4
4	A	5003	ATP	PA-O3A-PB-O1B
4	B	5003	ATP	PA-O3A-PB-O1B
4	C	5003	ATP	PA-O3A-PB-O1B
4	D	5003	ATP	PA-O3A-PB-O1B
4	A	5002	ATP	PG-O3B-PB-O1B
4	A	5002	ATP	PG-O3B-PB-O2B
4	A	5002	ATP	PB-O3A-PA-O2A
4	B	5002	ATP	PG-O3B-PB-O1B
4	B	5002	ATP	PG-O3B-PB-O2B
4	B	5002	ATP	PB-O3A-PA-O2A
4	C	5002	ATP	PG-O3B-PB-O1B
4	C	5002	ATP	PG-O3B-PB-O2B
4	C	5002	ATP	PB-O3A-PA-O2A
4	D	5002	ATP	PG-O3B-PB-O1B
4	D	5002	ATP	PG-O3B-PB-O2B
4	D	5002	ATP	PB-O3A-PA-O2A

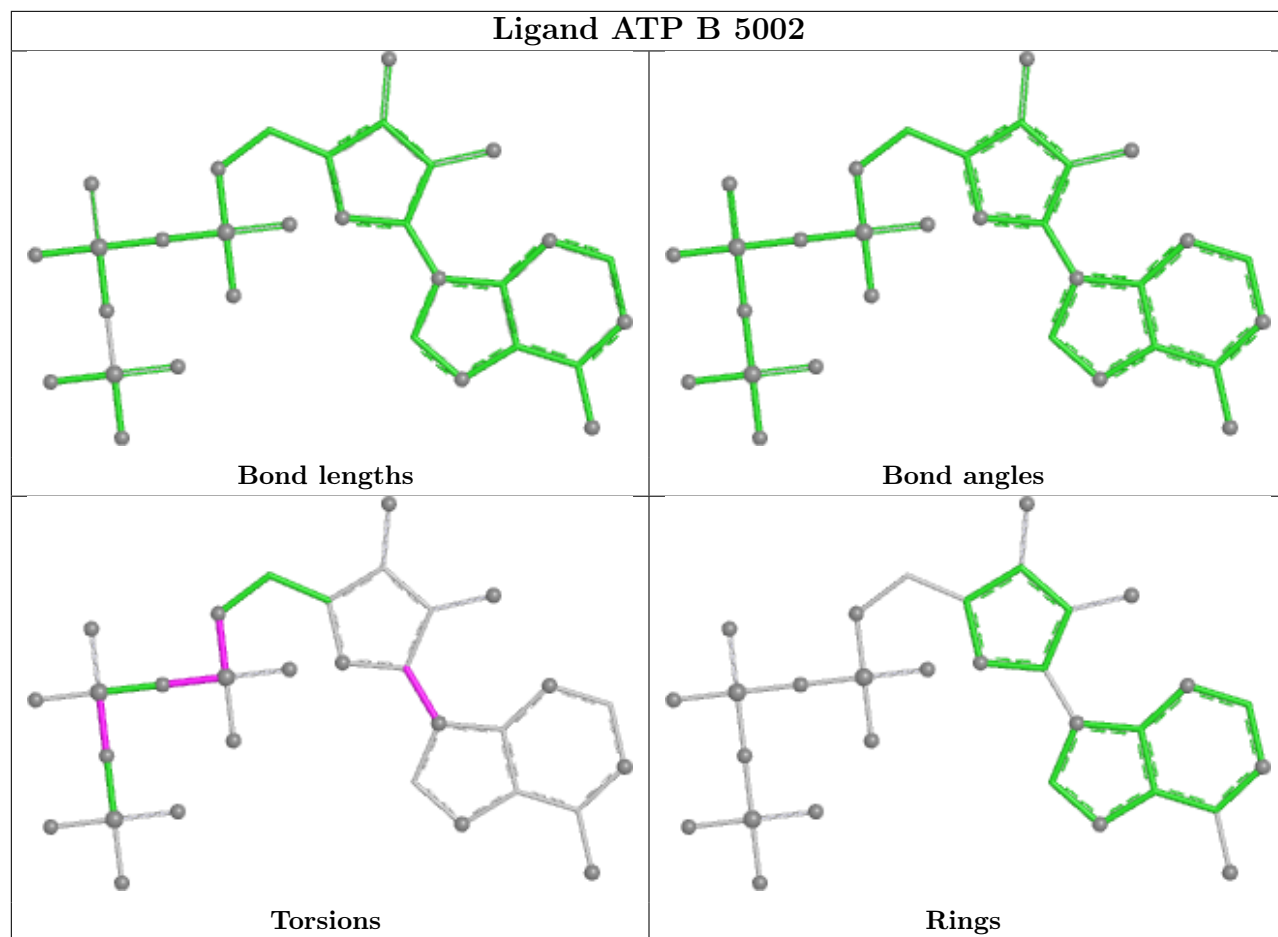
There are no ring outliers.

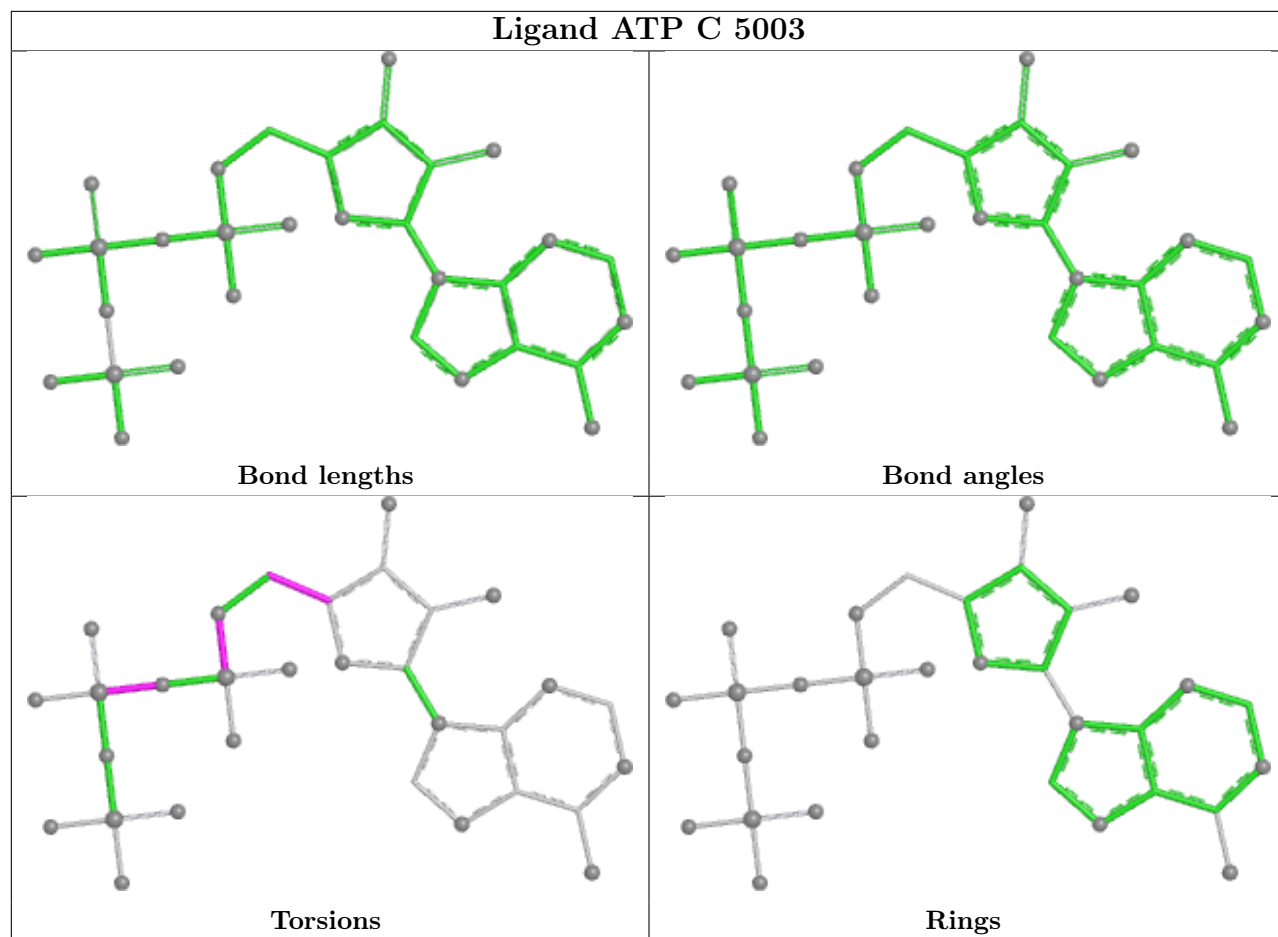
4 monomers are involved in 4 short contacts:

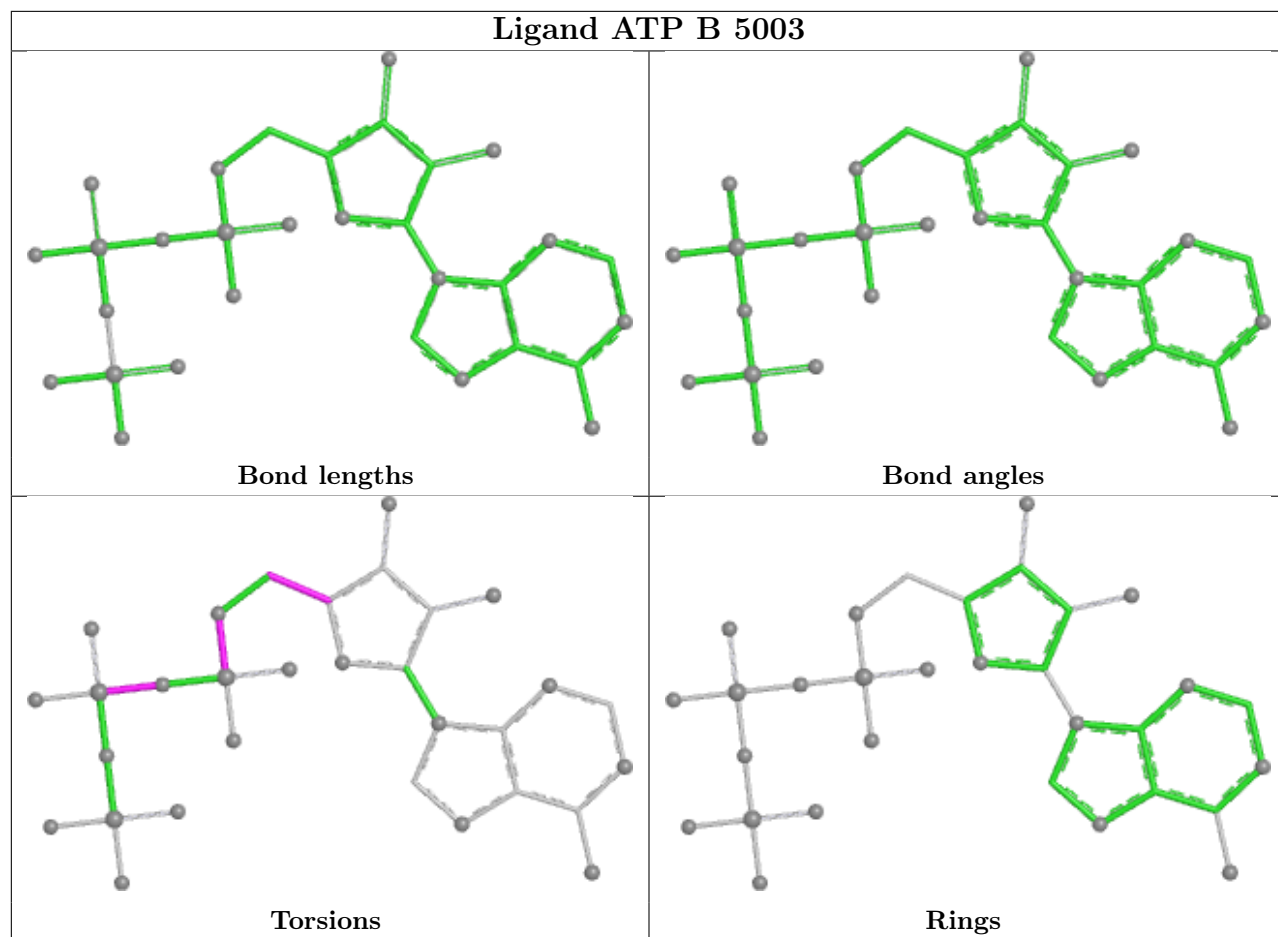
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5003	ATP	1	0
4	B	5003	ATP	1	0
4	D	5003	ATP	1	0
4	A	5003	ATP	1	0

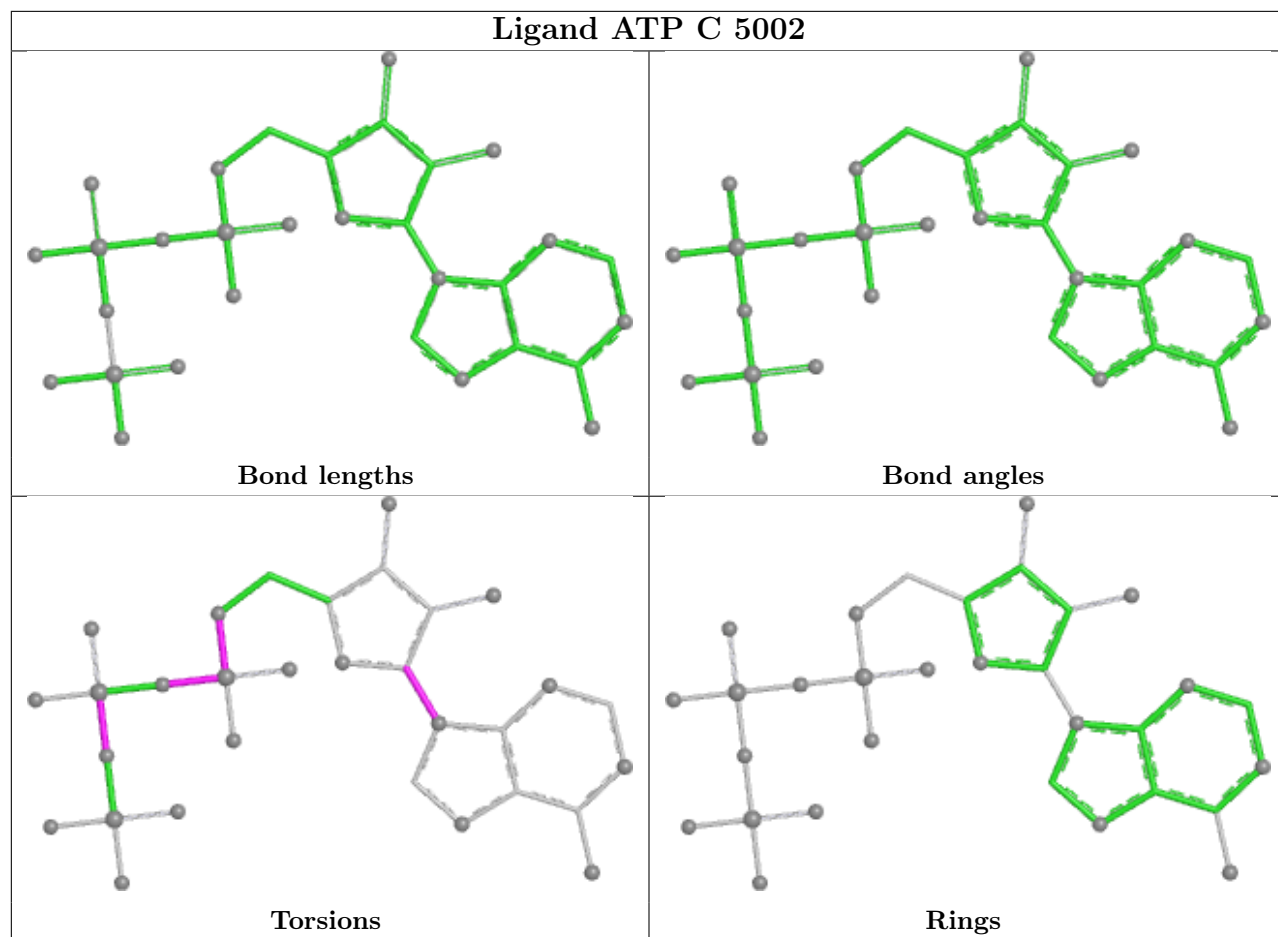
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

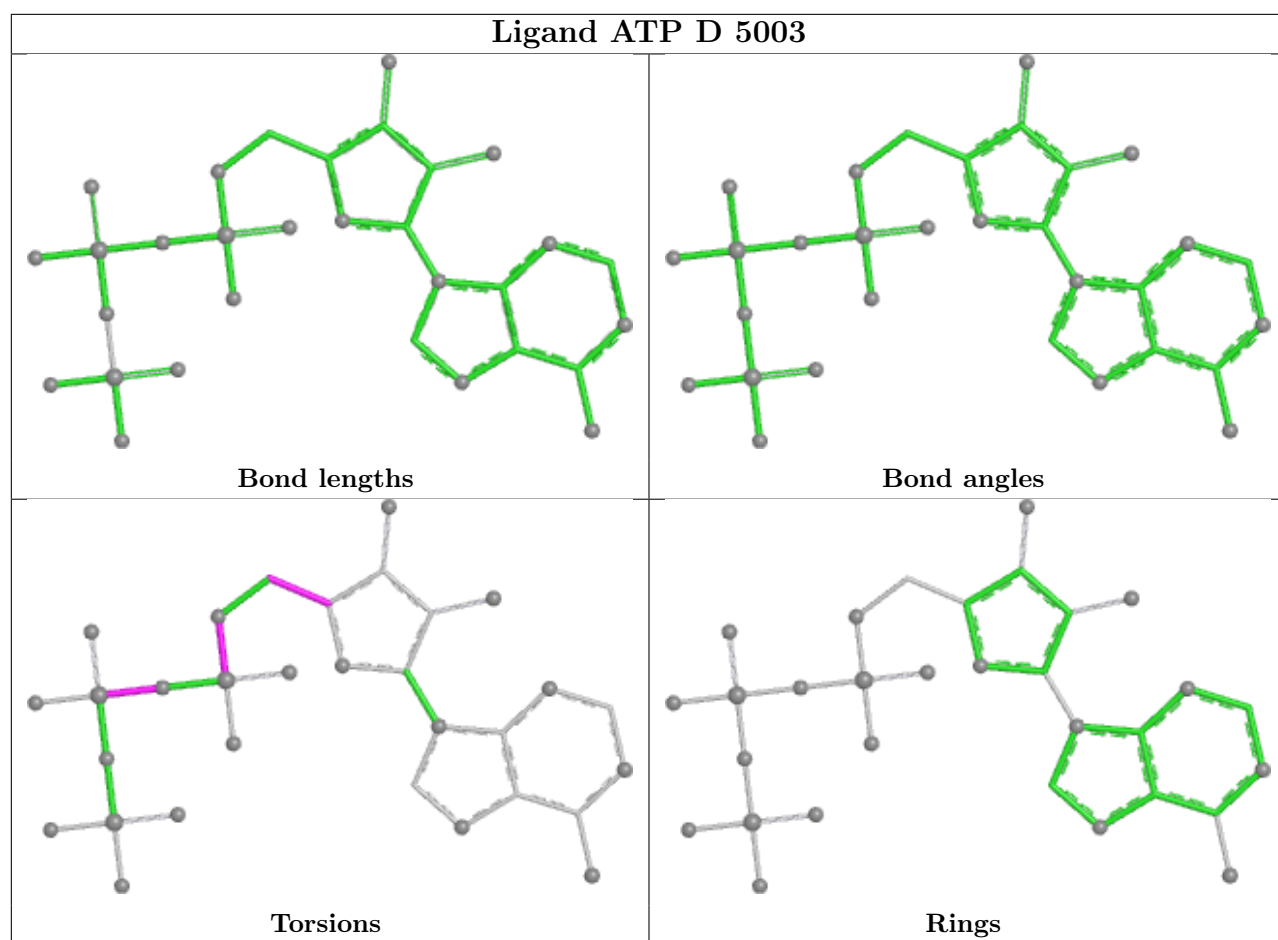


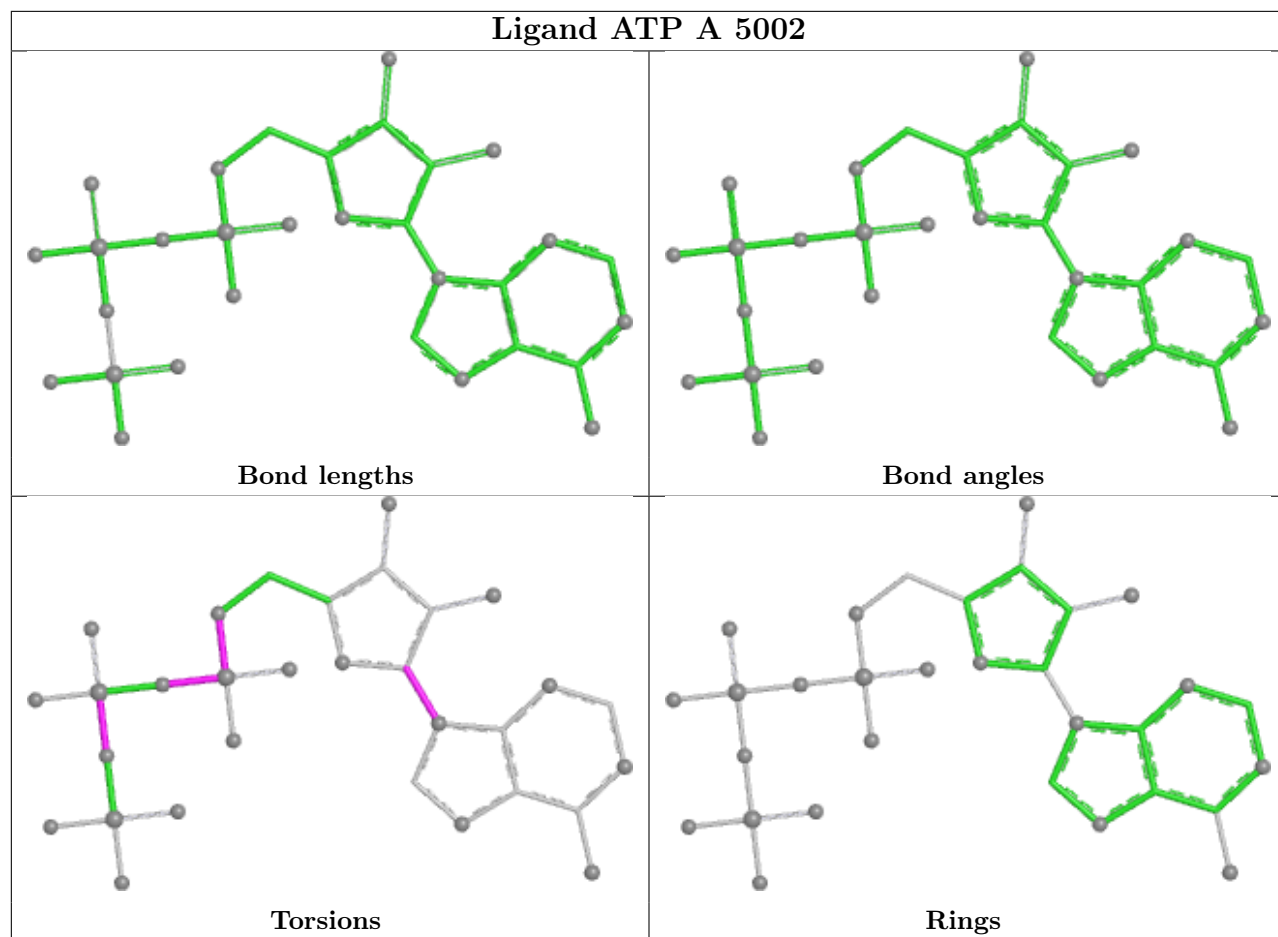


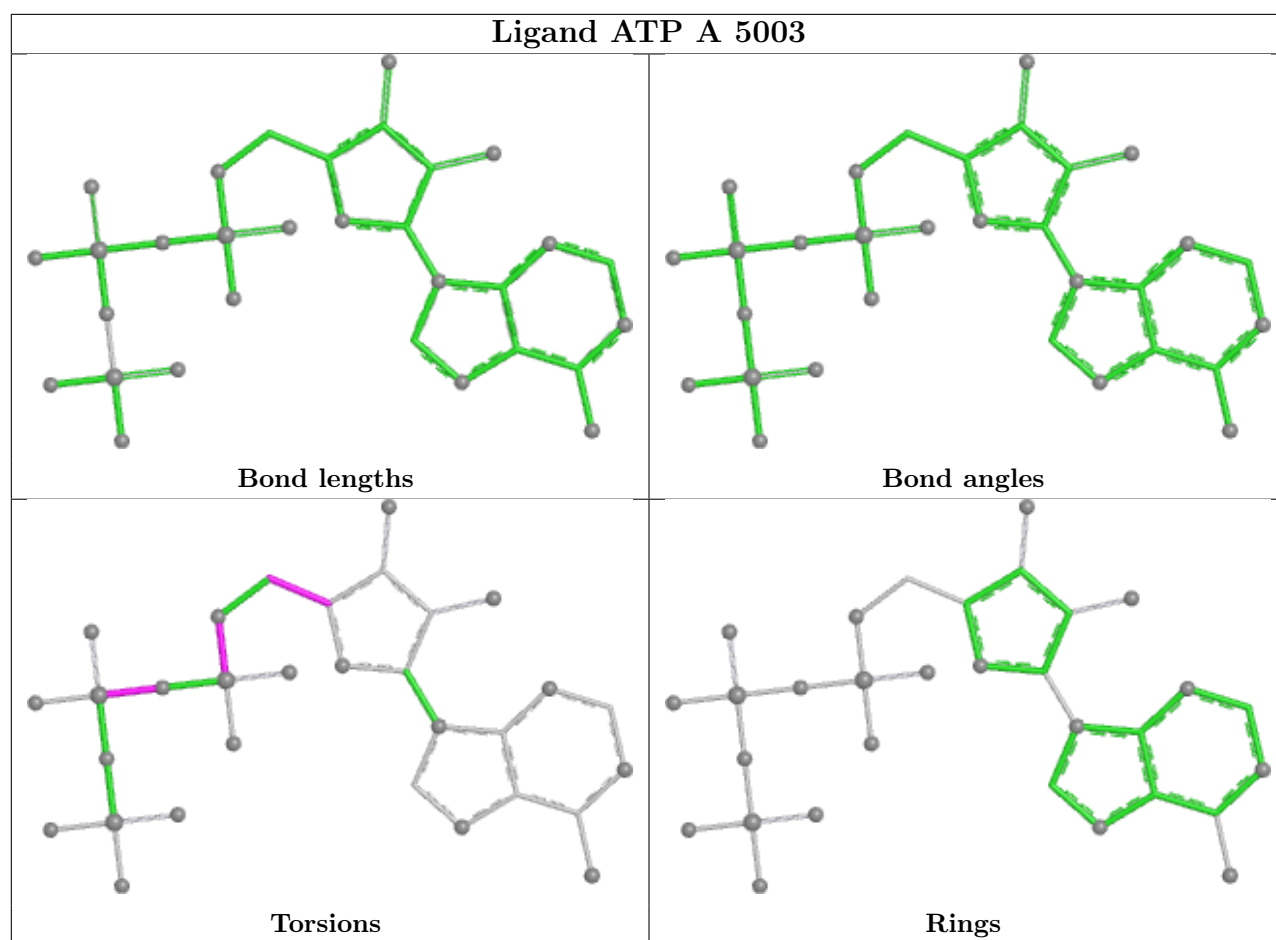












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42759. These allow visual inspection of the internal detail of the map and identification of artifacts.

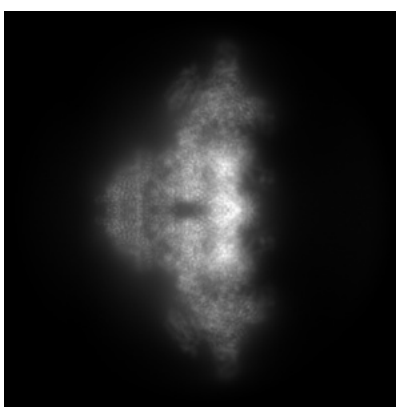
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

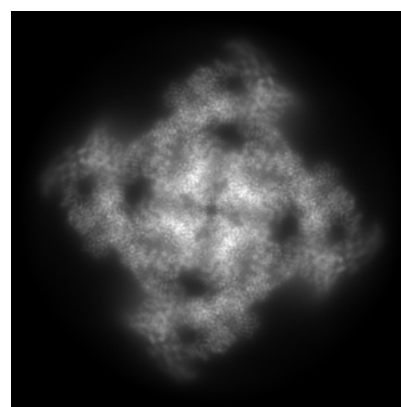
6.1.1 Primary map



X



Y



Z

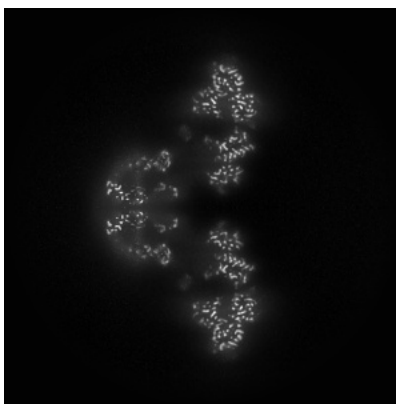
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

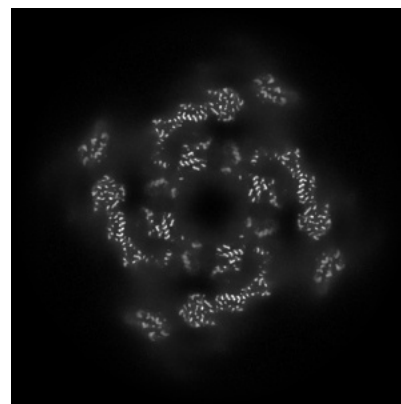
6.2.1 Primary map



X Index: 256



Y Index: 256

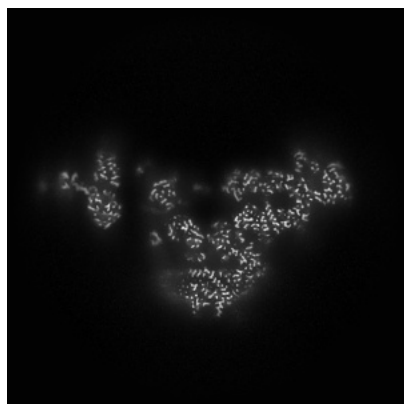


Z Index: 256

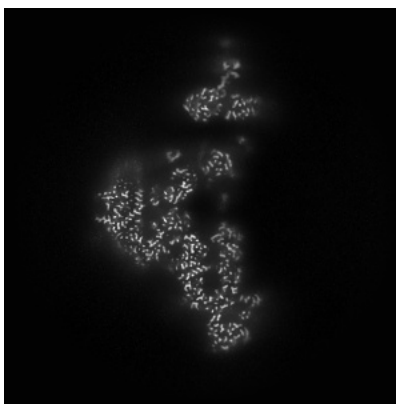
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

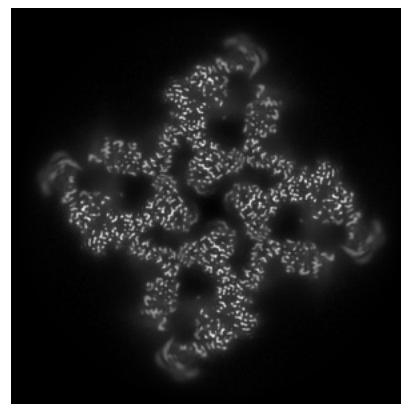
6.3.1 Primary map



X Index: 238



Y Index: 238

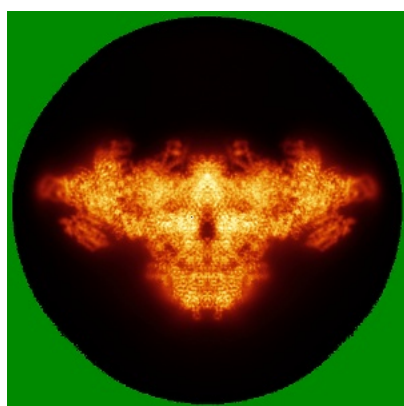


Z Index: 282

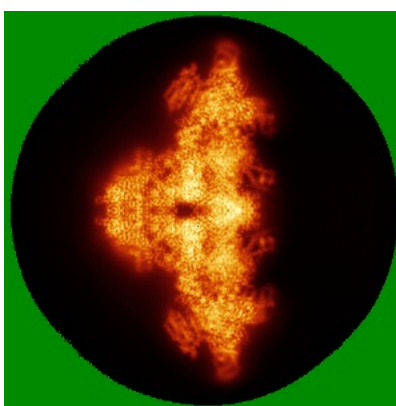
The images above show the largest variance slices of the map in three orthogonal directions.

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

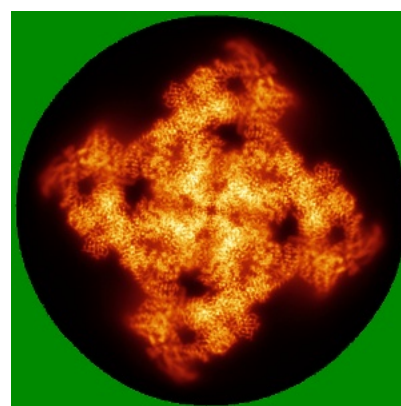
6.4.1 Primary map



X



Y

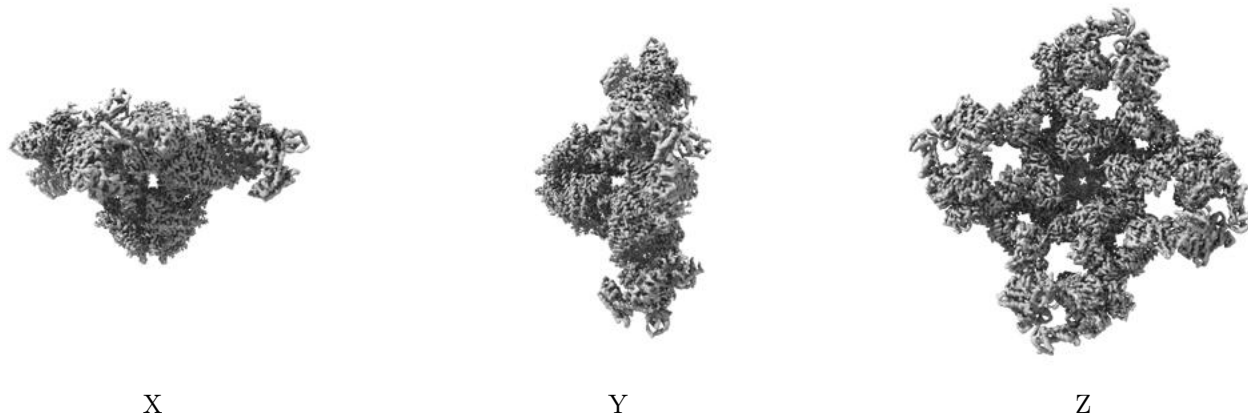


Z

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 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

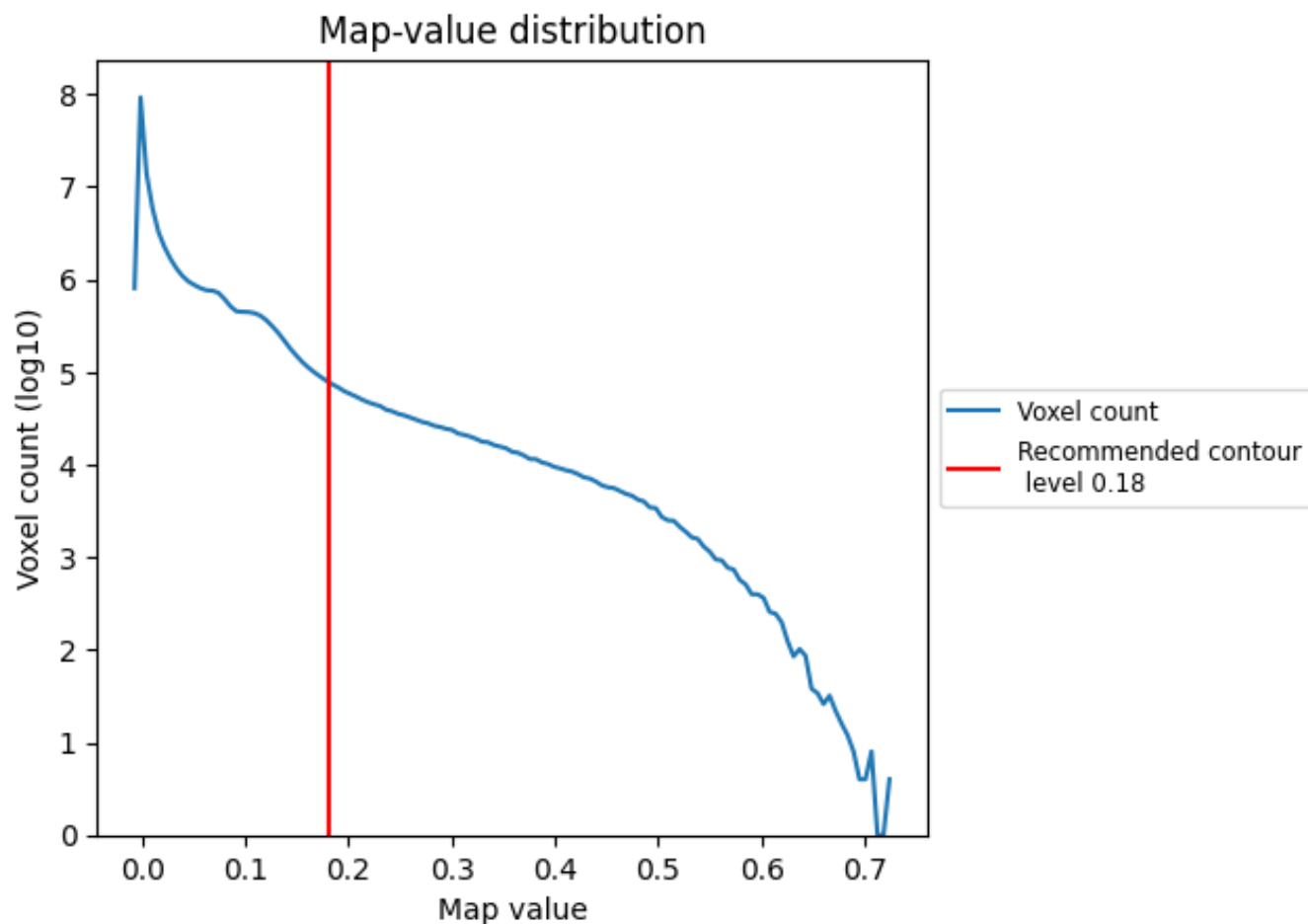
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

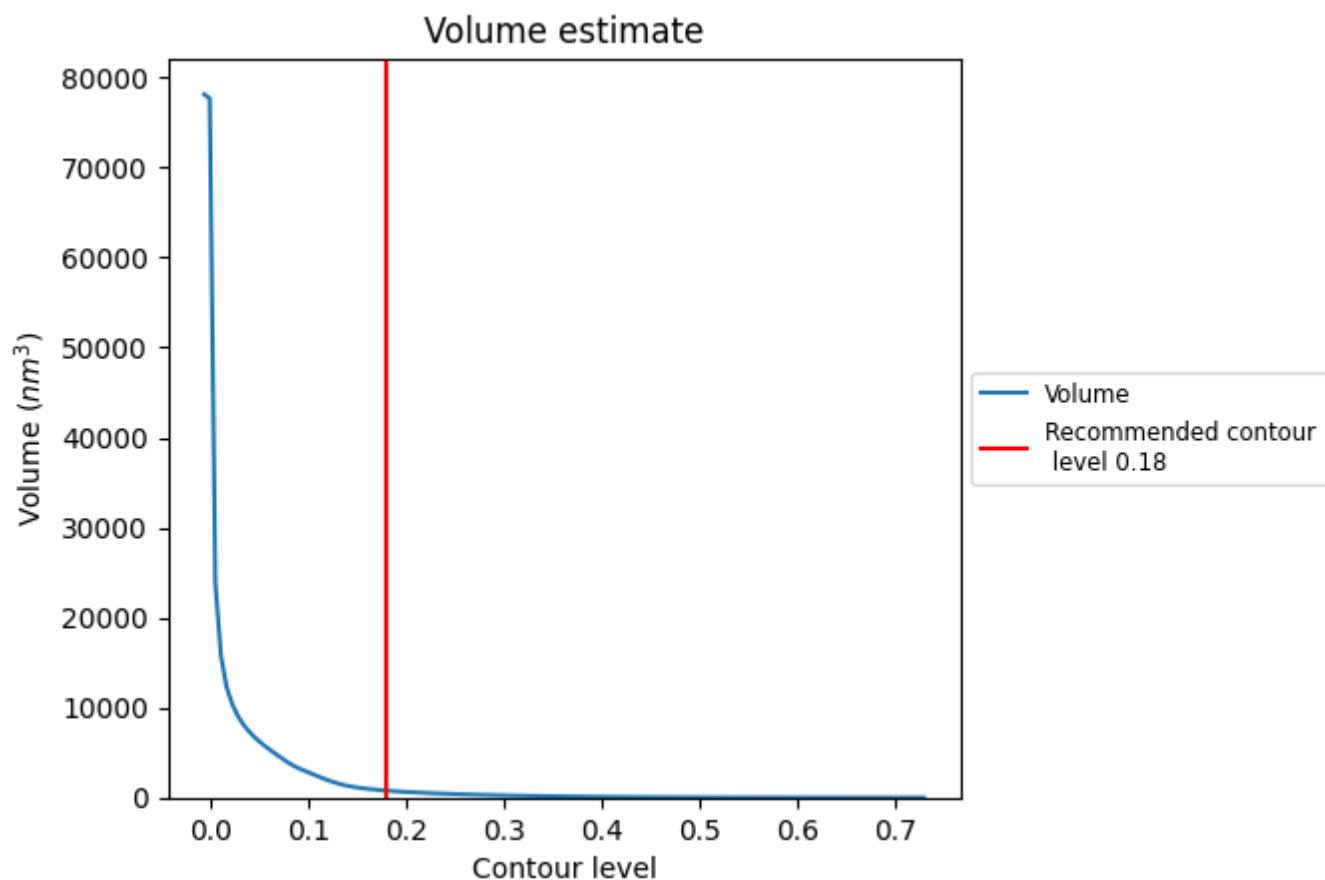
This section contains the results of statistical analysis of the map.

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.

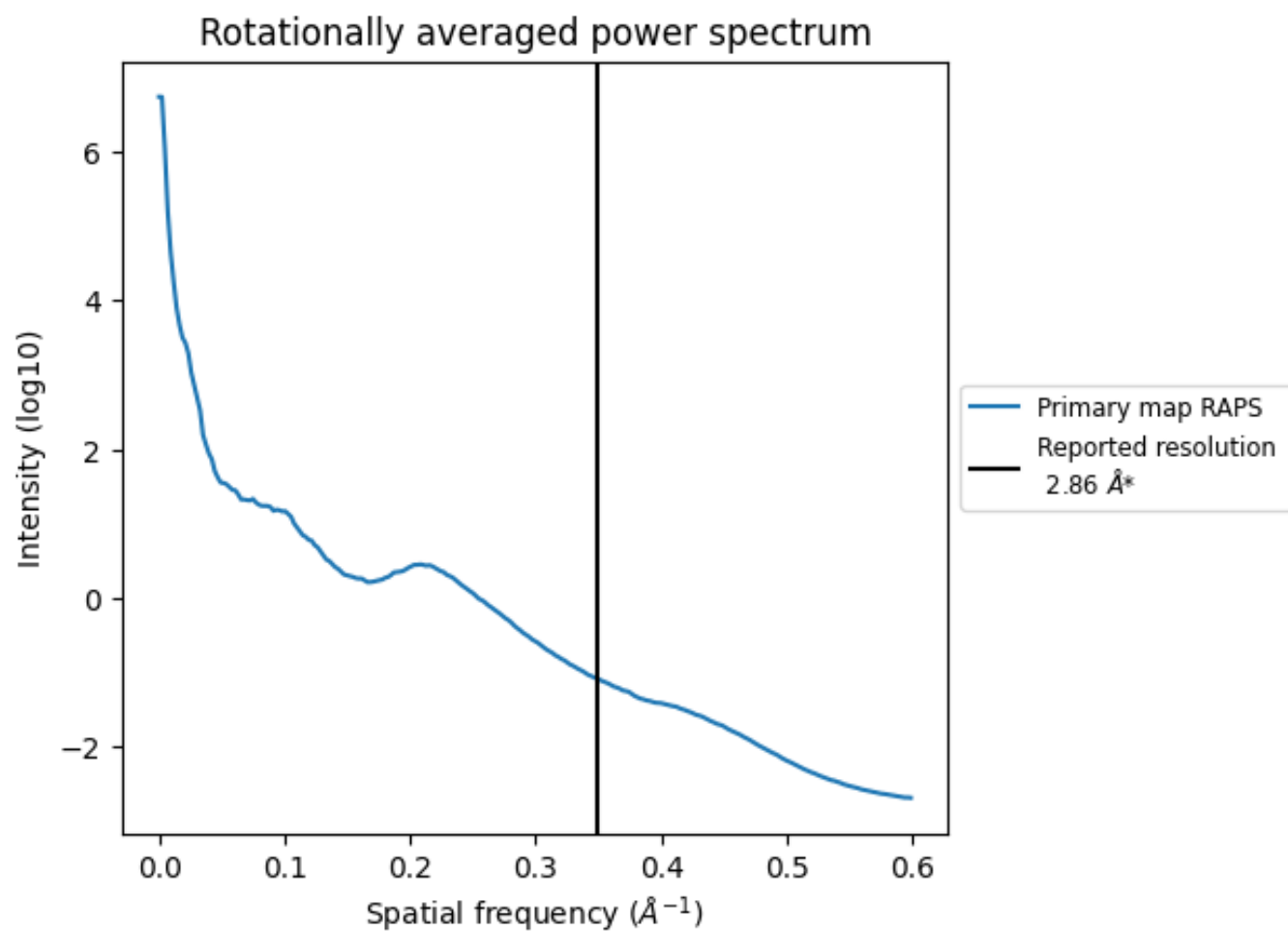
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 763 nm³; this corresponds to an approximate mass of 689 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 0.350 Å⁻¹

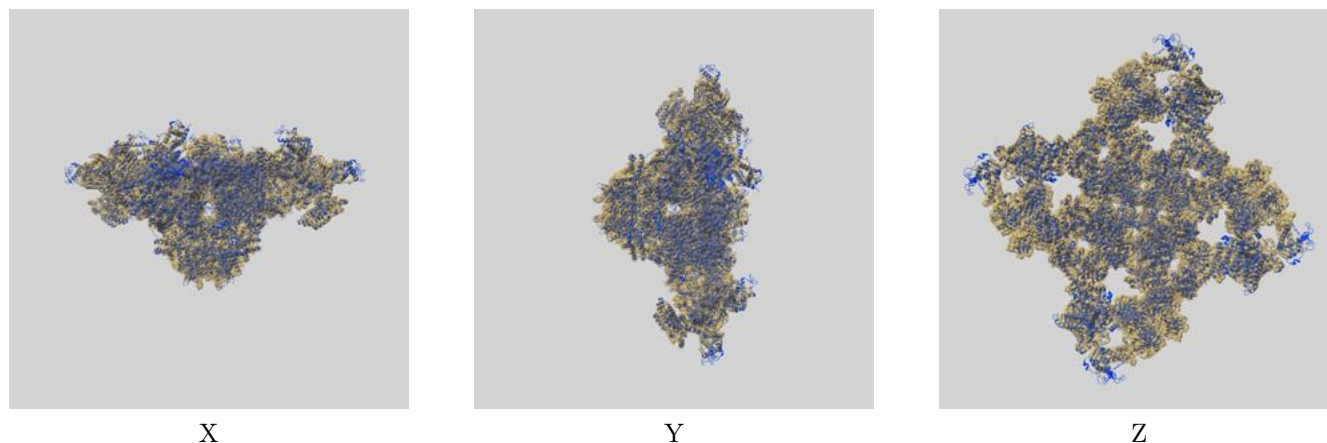
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

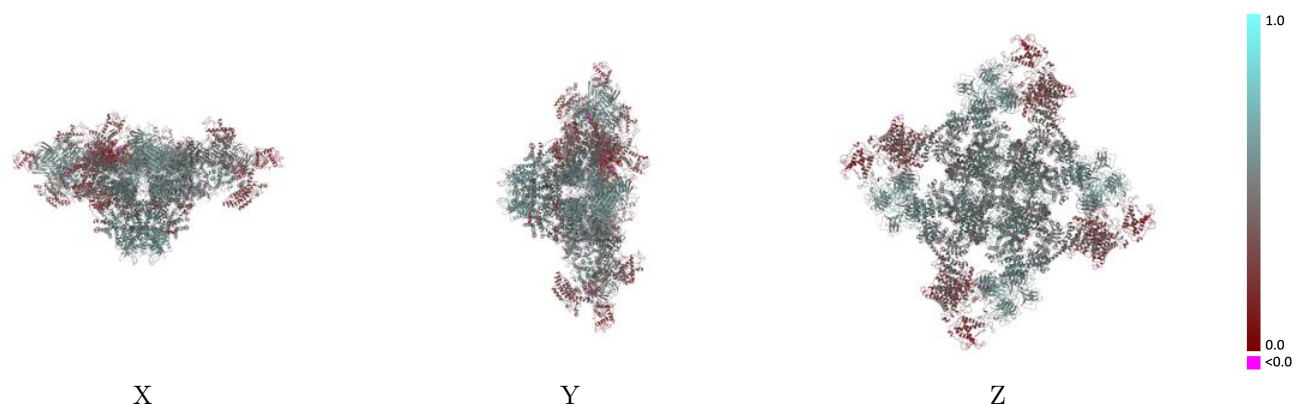
This section contains information regarding the fit between EMDB map EMD-42759 and PDB model 8UXC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



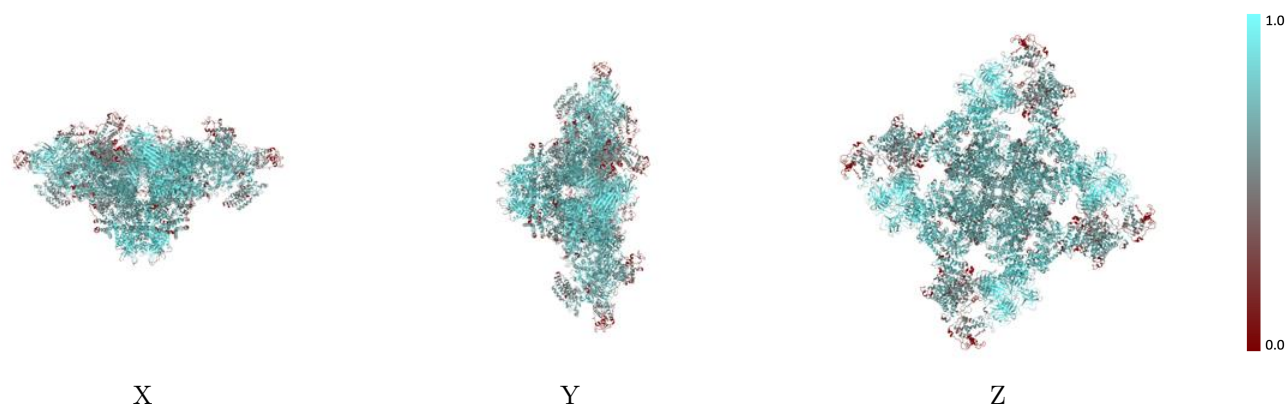
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



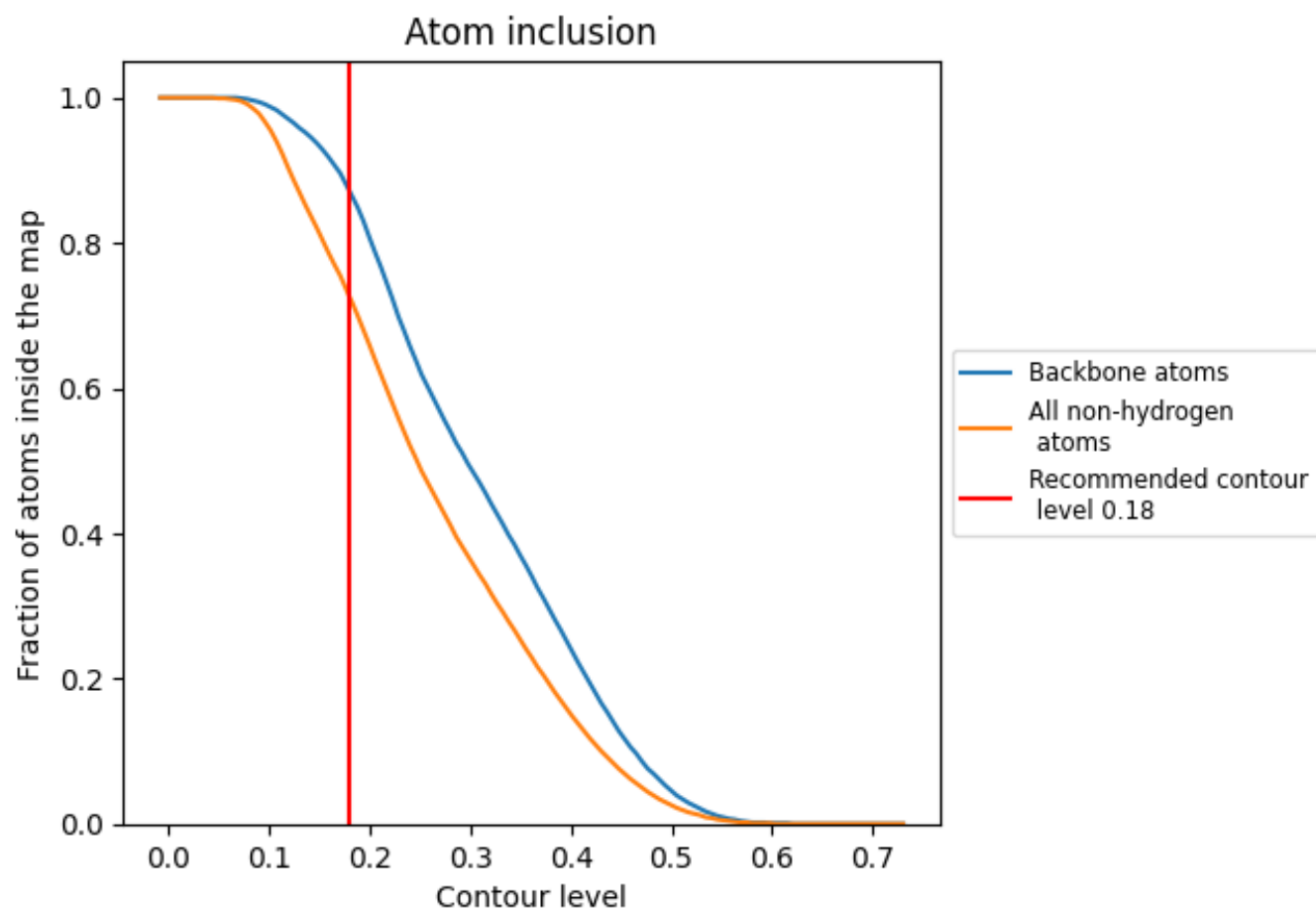
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 73% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.4660
A	0.7240	0.4640
B	0.7240	0.4640
C	0.7240	0.4640
D	0.7240	0.4640
E	0.8490	0.5520
F	0.8440	0.5520
G	0.8500	0.5520
H	0.8500	0.5510

1.0

0.0

<0.0