



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2017 – 09:01 PM EST

PDB ID : 4AKI  
Title : Dynein Motor Domain - LuAc derivative  
Authors : Schmidt, H.; Gleave, E.S.; Carter, A.P.  
Deposited on : 2012-02-22  
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

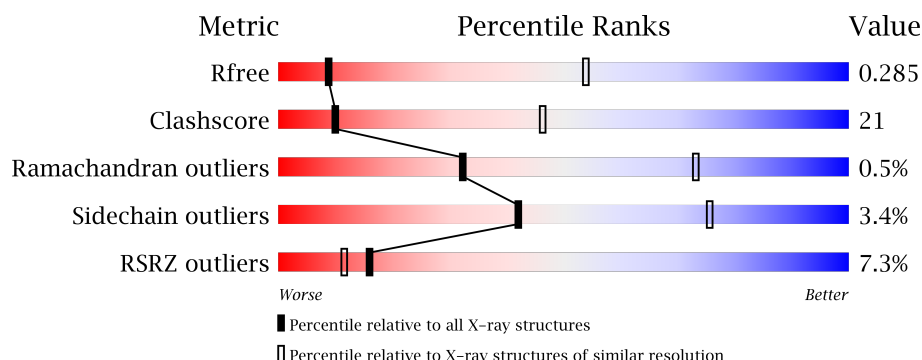
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2695	
1	B	2695	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	5094	-	-	X	-
3	SO4	A	5095	-	-	X	X
3	SO4	A	5096	-	-	X	-
3	SO4	B	5095	-	-	X	-
4	MG	A	5097	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 41590 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

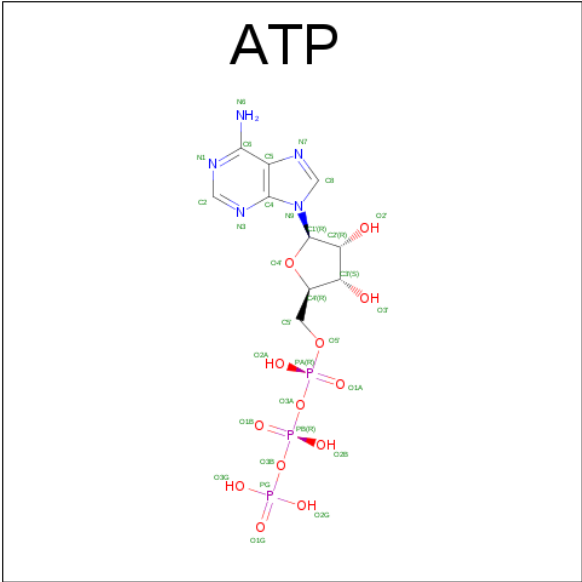
- Molecule 1 is a protein called GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			
1	B	2650	Total	C	N	O	S	0	0	0
			20748	13268	3472	3915	93			

There are 8 discrepancies between the modelled and reference sequences:

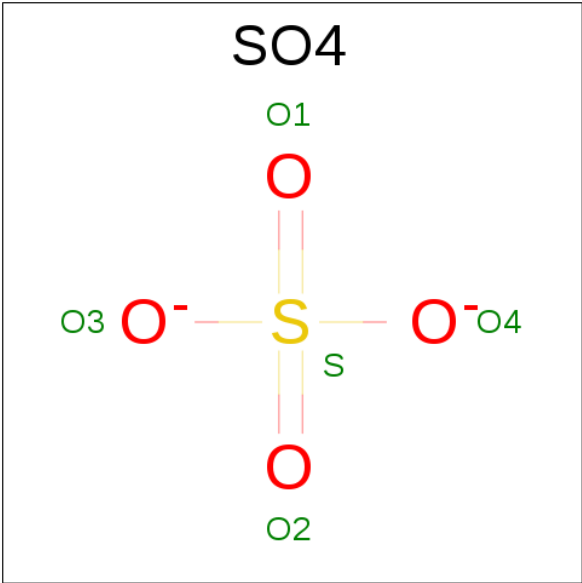
Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	-	LINKER	UNP P36022
A	219	ASP	-	LINKER	UNP P36022
A	1630	ILE	LEU	CONFLICT	UNP P36022
A	3782	ASP	GLU	CONFLICT	UNP P36022
B	218	SER	-	LINKER	UNP P36022
B	219	ASP	-	LINKER	UNP P36022
B	1630	ILE	LEU	CONFLICT	UNP P36022
B	3782	ASP	GLU	CONFLICT	UNP P36022

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

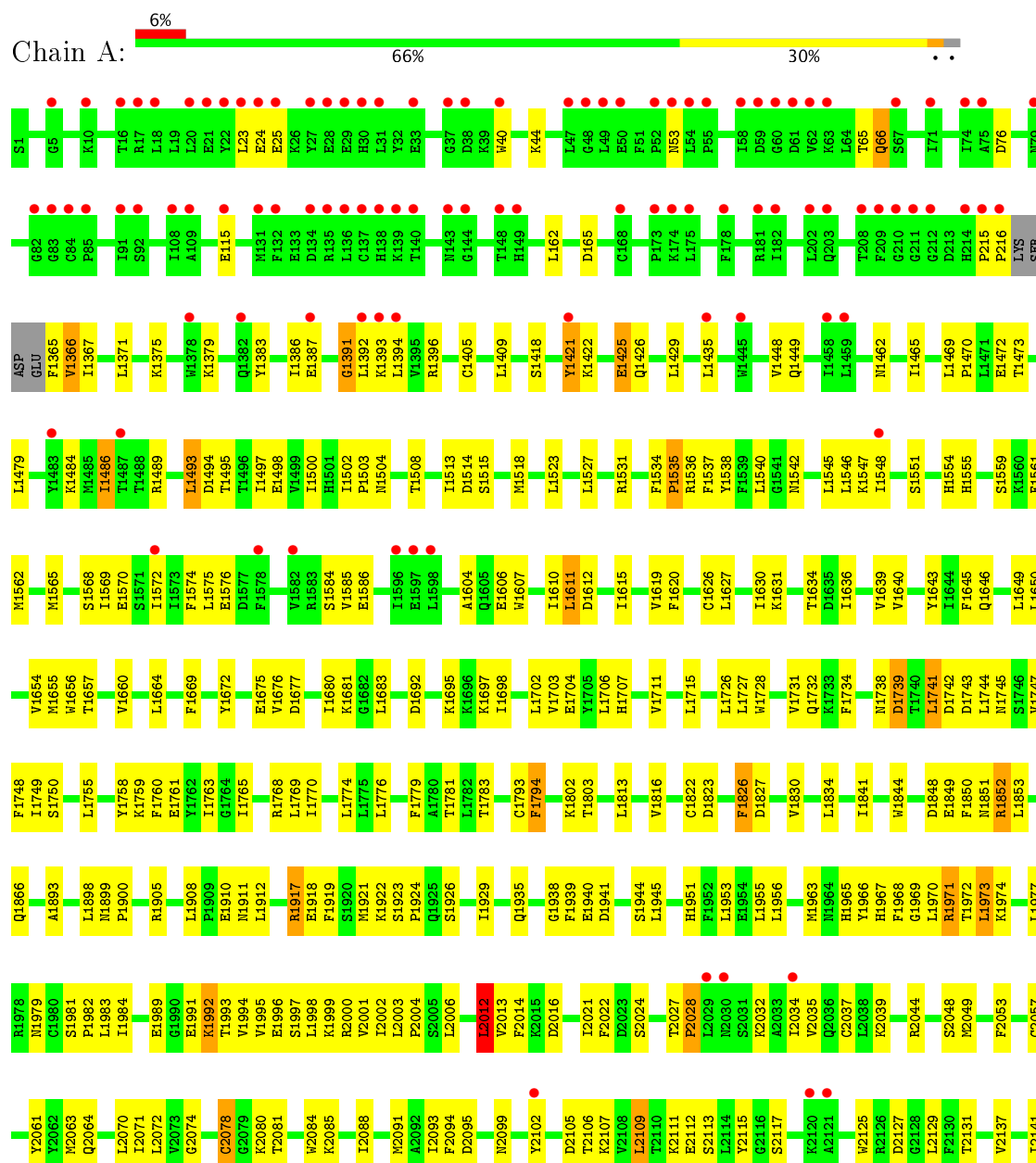
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

### 3 Residue-property plots

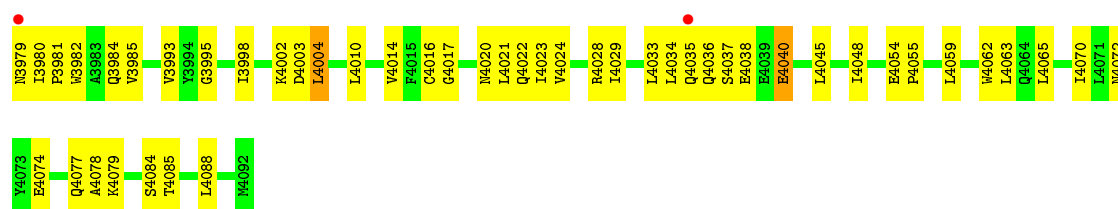
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC

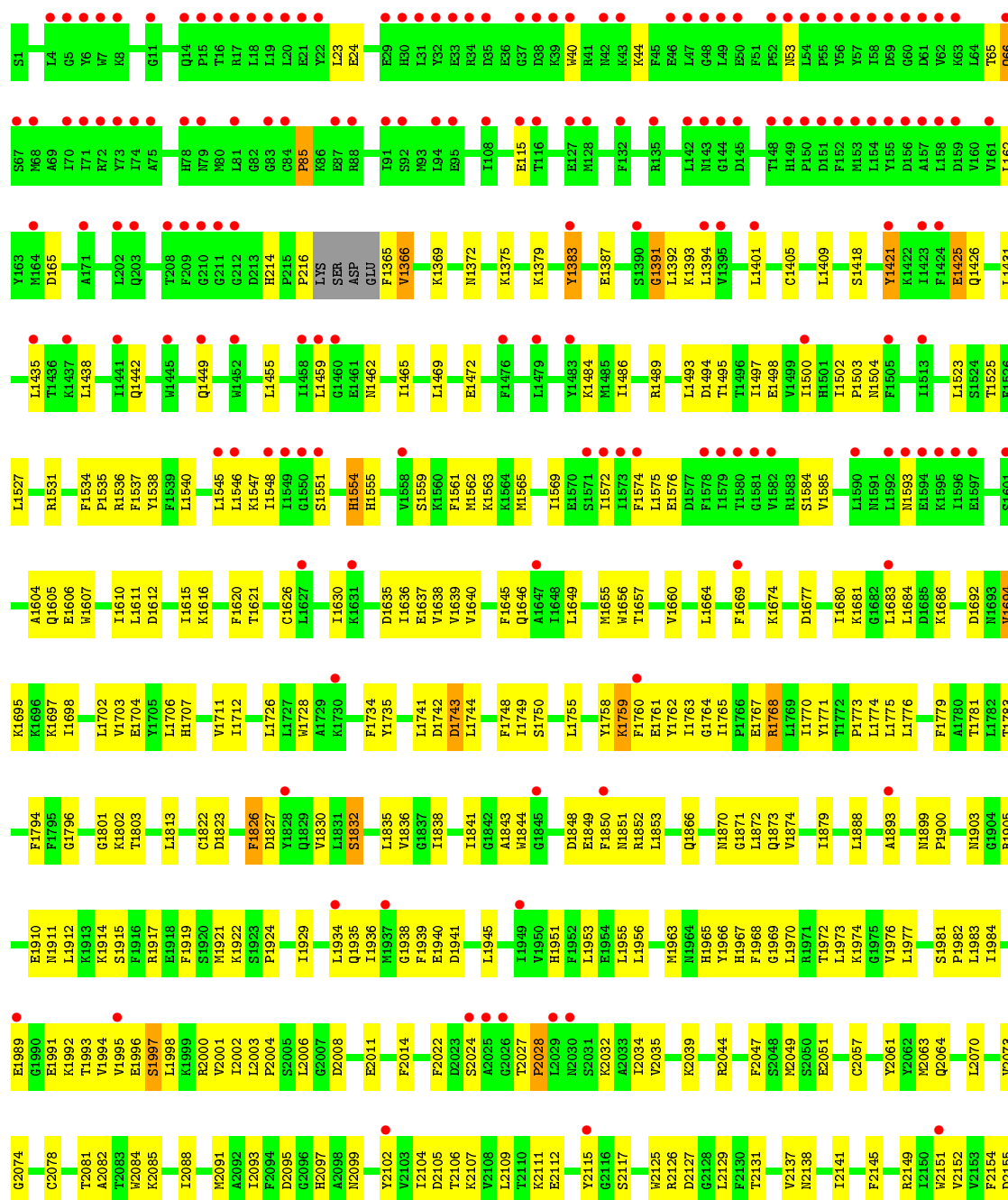


G3877	G3884	G3885	G3886	G3887	G3888	G3889	G3890	G3894	G3895	E3898	D3899	T3906	V3911	G3912	F3915	F3916	T3917	G3919	V3923	G3924	S3925	G3926	V3934	F3935	T3939	T3943	L3944	V3945	V3946	P3947	H3948	F3949	S3951	Y3955	D3960	F3963	A3964	Y3967	N3978																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
F3786	F3787	R3792	K3799	L3803	S3807	L3808	G3809	G3810	L3811	L3816	G3817	S3818	L3819	N3820	L3822	N3823	V3824	A3825	S3832	G3833	G3836	G3837	N3838	L3839	Q3845	N3846	S3847	L3848	S3849	N3850	V3851	L3853	V3854	L3855	H3858	V3859	T3862	A3865	E3869	K3870	F3871	K3872	N3873	N3874	N3875																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
L3583	N3584	L3587	N3588	N3589	L3590	K3591	L3592	E3593	A3594	N3595	L3601	F3607	D3612	N3613	L3614	V3615	Y3618	G3622	S3632	L3628	M3631	F3641	S3645	L3646	V3656	F3657	L3658	L3659	L3660	L3661	L3662	L3663	L3664	L3665	L3666	L3667	L3668	L3669	L3670	L3671	L3672	L3673	L3674	L3675	L3676	L3677	L3678	L3679	L3680	L3681	L3682	L3683	L3684	L3685	L3686	L3687																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
V3488	I3505	F3508	L3509	R3510	S3511	R3512	V3513	F3518	V3519	N3520	N3521	I3525	F3530	D3531	L3534	E3537	N3538	M3541	Q3542	R3543	K3544	D3547	L3548	L3549	K3550	Y3555	R3556	N3561	L3562	E3563	K3564	R3565	L3567	E3568	E3569	L3570	N3571	N3572	S3573	M3577	E3579	N3580	L3581	L3582																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L3353	G3354	K3355	V3358	K3359	F3360	D3361	R3365	D3368	T3372	L3373	S3400	F3406	L3407	D3409	H3413	K3414	T3415	T3416	V3417	I3418	L3419	R3439	L3440	F3446	Q3453	D3459	P3460	E3463	L3464	L3465	L3466	S3467	F3470	A3473	G3474	N3475	R3476	E3481	G3482	D3483																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
K3024	L3025	V3028	L3029	V3030	A3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053	L3054	L3055	L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L3085	L3086	L3087	L3088	L3089	L3090	L3091	L3092	L3093	L3094	L3095	L3096	L3097	L3098	L3099	L3100	L3101	L3102	L3103	L3104	L3105	L3106	L3107	L3108	L3109	L3110	L3111	L3112	L3113	L3114	L3115	L3116	L3117	L3118	L3119	L3120	L3121	L3122	L3123	L3124	L3125	L3126	L3127	L3128	L3129	L3130	L3131	L3132	L3133	L3134	L3135	L3136	L3137	L3138	L3139	L3140	L3141	L3142	L3143	L3144	L3145	L3146	L3147	L3148	L3149	L3150	L3151	L3152	L3153	L3154	L3155	L3156	L3157	L3158	L3159	L3160	L3161	L3162	L3163	L3164	L3165	L3166	L3167	L3168	L3169	L3170	L3171	L3172	L3173	L3174	L3175	L3176	L3177	L3178	L3179	L3180	L3181	L3182	L3183	L3184	L3185	L3186	L3187	L3188	L3189	L3190	L3191	L3192	L3193	L3194	L3195	L3196	L3197	L3198	L3199	L3200	L3201	L3202	L3203	L3204	L3205	L3206	L3207	L3208	L3209	L3210	L3211	L3212	L3213	L3214	L3215	L3216	L3217	L3218	L3219	L3220	L3221	L3222	L3223	L3224	L3225	L3226	L3227	L3228	L3229	L3230	L3231	L3232	L3233	L3234	L3235	L3236	L3237	L3238	L3239	L3240	L3241	L3242	L3243	L3244	L3245	L3246	L3247	L3248	L3249	L3250	L3251	L3252	L3253	L3254	L3255	L3256	L3257	L3258	L3259	L3260	L3261	L3262	L3263	L3264	L3265	L3266	L3267	L3268	L3269	L3270	L3271	L3272	L3273	L3274	L3275	L3276	L3277	L3278	L3279	L3280	L3281	L3282	L3283	L3284	L3285	L3286	L3287	L3288	L3289	L3290	L3291	L3292	L3293	L3294	L3295	L3296	L3297	L3298	L3299	L3300	L3301	L3302	L3303	L3304	L3305	L3306	L3307	L3308	L3309	L3310	L3311	L3312	L3313	L3314	L3315	L3316	L3317	L3318	L3319	L3320	L3321	L3322	L3323	L3324	L3325	L3326	L3327	L3328	L3329	L3330	L3331	L3332	L3333	L3334	L3335	L3336	L3337	L3338	L3339	L3340	L3341	L3342	L3343	L3344	L3345	L3346	L3347	L3348	L3349	L3350	L3351	L3352	L3353	L3354	L3355	L3356	L3357	L3358	L3359	L3360	L3361	L3362	L3363	L3364	L3365	L3366	L3367	L3368	L3369	L3370	L3371	L3372	L3373	L3374	L3375	L3376	L3377	L3378	L3379	L3380	L3381	L3382	L3383	L3384	L3385	L3386	L3387	L3388	L3389	L3390	L3391	L3392	L3393	L3394	L3395	L3396	L3397	L3398	L3399	L3400	L3401	L3402	L3403	L3404	L3405	L3406	L3407	L3408	L3409	L3410	L3411	L3412	L3413	L3414	L3415	L3416	L3417	L3418	L3419	L3420	L3421	L3422	L3423	L3424	L3425	L3426	L3427	L3428	L3429	L3430	L3431	L3432	L3433	L3434	L3435	L3436	L3437	L3438	L3439	L3440	L3441	L3442	L3443	L3444	L3445	L3446	L3447	L3448	L3449	L3450	L3451	L3452	L3453	L3454	L3455	L3456	L3457	L3458	L3459	L3460	L3461	L3462	L3463	L3464	L3465	L3466	L3467	L3468	L3469	L3470	L3471	L3472	L3473	L3474	L3475	L3476	L3477	L3478	L3479	L3480	L3481	L3482	L3483	L3484	L3485	L3486	L3487	L3488	L3489	L3490	L3491	L3492	L3493	L3494	L3495	L3496	L3497	L3498	L3499	L3500	L3501	L3502	L3503	L3504	L3505	L3506	L3507	L3508	L3509	L3510	L3511	L3512	L3513	L3514	L3515	L3516	L3517	L3518	L3519	L3520	L3521	L3522	L3523	L3524	L3525	L3526	L3527	L3528	L3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540	L3541	L3542	L3543	L3544	L3545	L3546	L3547	L3548	L3549	L3550	L3551	L3552	L3553	L3554	L3555	L3556	L3557	L3558	L3559	L3560	L3561	L3562	L3563	L3564	L3565	L3566	L3567	L3568	L3569	L3570	L3571	L3572	L3573	L3574	L3575	L3576	L3577	L3578	L3579	L3580	L3581	L3582	L3583	L3584	L3585	L3586	L3587	L3588	L3589	L3590	L3591	L3592	L3593	L3594	L3595	L3596	L3597	L3598	L3599	L3600	L3601	L3602	L3603	L3604	L3605	L3606	L3607	L3608	L3609	L3610	L3611	L3612	L3613	L3614	L3615	L3616	L3617	L3618	L3619	L3620	L3621	L3622	L3623	L3624	L3625	L3626	L3627	L3628	L3629	L3630	L3631	L3632	L3633	L3634	L3635	L3636	L3637	L3638	L3639	L3640	L3641	L3642	L3643	L3644	L3645	L3646	L3647	L3648	L3649	L3650	L3651	L3652	L3653	L3654	L3655	L3656	L3657	L3658	L3659	L3660	L3661	L3662	L3663	L3664	L3665	L3666	L3667	L3668	L3669	L3670	L3671	L3672	L3673	L3674	L3675	L3676	L3677	L3678	L3679	L3680	L3681	L3682	L3683	L3684	L3685	L3686	L3687	L3688	L3689	L3690	L3691	L3692	L3693	L3694	L3695	L3696	L3697	L3698	L3699	L3700	L3701	L3702	L3703	L3704	L3705	L3706	L3707	L3708	L3709	L3710	L3711	L3712	L3713	L3714	L3715	L3716	L3717	L3718	L3719	L3720	L3721	L3722	L3723	L3724	L3725	L3726	L3727	L3728	L3729	L3730	L3731	L3732	L3733	L3734	L3735	L3736	L3737	L3738	L3739	L3740	L3741	L3742	L3743	L3744	L3745	L3746	L3747	L3748	L3749	L3750	L3751	L3752	L3753	L3754	L3755	L3756	L3757	L3758	L3759	L3760	L3761	L3762	L3763	L3764	L3765	L3766	L3767	L3768	L3769	L3770	L3771	L3772	L3773	L3774	L3775	L3776	L3777	L3778	L3779	L3780	L3781	L3782	L3783	L3784	L3785	L3786	L3787	L3788	L3789	L3790	L3791	L3792	L3793	L3794	L3795	L3796	L3797	L3798	L3799	L3800	L3801	L3802	L3803	L3804	L3805	L3806	L3807	L3808	L3809	L3810	L3811	L3812	L3813	L3814	L3815	L3816	L3817	L3818	L3819	L3820	L3821	L3822	L3823	L3824	L3825	L3826	L3827	L3828	L3829	L3830	L3831	L3832	L3833	L3834	L3835	L3836	L3837	L3838	L3839	L3840	L3841	L3842	L3843	L3844	L3845	L3846	L3847	L3848	L3849	L3850	L3851	L3852	L3853	L3854	L3855	L3856	L3857	L3858	L3859	L3860	L3861	L3862	L3863	L3864	L3865	L3866	L3867	L3868	L3869	L3870	L3871	L3872	L3873	L3874	L3875	L3876	L3877	L3878	L3879	L3880	L3881	L3882	L3883	L3884	L3885	L3886	L3887	L3888	L3889	L3890	L3891	L3892	L3893	L3894	L3895	L3896	L3897	L3898	L3899	L3900	L3901	L3902	L3903	L3904	L3905	L3906	L3907	L3908	L3909	L3910	L3911	L3912	L3913	L3914	L3915	L3916	L3917	L3918	L3919	L3920	L3921	L3922	L3923	L3924	L3925	L3926	L3927	L3928	L3929	L3930	L3931	L3932	L3933	L3934	L3935	L3936	L3937	L3938	L3939	L3940	L3941	L3942	L3943	L3944	L3945	L3946	L3947	L3948	L3949	L3950	L3951	L3952	L3953	L3954	L3955	L3956	L3957	L3958	L3959	L3960	L3961	L3962	L3963	L3964	L3965	L3966	L3967	L3968	L3969	L3970	L3971	L3972	L3973	L3974	L3975	L3976	L3977	L3978	L3979	L3980	L3981	L3982	L3983	L3984	L3985	L3986	L3987	L3988	L3989	L3990	L3991	L3992	L3993	L3994	L3995	L3996	L3997	L3998	L3999	L4000	L4001	L4002	L4003	L4004	L4005	L4006	L4007	L4008	L4009	L4010	L4011	L4012	L4013	L4014	L4015	L4016	L4017	L4018	L4019	L4020	L4021	L4022	L4023	L4024	L4025	L4026	L4027	L4028	L4029	L4030	L4031	L4032	L4033	L4034	L4035	L4036	L4037	L4038	L4039	L4040	L4041	L4042	L4043	L4044	L4045	L4046	L4047	L4048	L4049	L4050	L4051	L4052	L4053	L4054	L4055	L4056	L4057	L4058	L4059	L4060	L4061	L4062	L4063	L4064	L4065	L4066	L4067	L4068	L4069	L4070	L4071	L4072	L4073	L4074	L4075	L4076	L4077	L4078	L4079	L4080	L4081	L4082	L4083	L4084	L4085	L4086	L4087	L4088	L4089	L4090	L4091	L4092	L4093	L4094	L4095	L4096	L4097	L4098	L4099	L4100	L4101	L4102	L4103	L4104	L4105	L4106	L4107	L4108	L4109	L4110	L4111	L4112	L4113	L4114	L4115	L4116	L4117	L4118	L4119	L4120	L4121	L4122	L4123	L4124	L4125	L4126	L4127	L4128	L4129	L4130	L4131	L4132	L4133	L4134	L4135	L4136	L4137	L4138	L4139	L4140	L4141	L4142	L4143	L4144	L4145	L4146	L4147	L4148	L4149	L4150	L4151	L4152	L4153	L4154	L4155





● Molecule 1: GLUTATHIONE S-TRANSFERASE CLASS-MU 26 KDA ISOZYME, DYNEIN HEAVY CHAIN CYTOPLASMIC



E3869	V3769	F3657	E3554	L3440	K3303	T2941	A2838	S2737	T2573	P2475	S2369	T2265	S2156
K3870	W3772	L3658	Y3555	F3446	W3306	D2942	D2839	H2741	T2574	K2476	S2369	F2266	E2161
F3871	N3773	LYS	Y3555	F3446	L3307	F2943	L2840	R2744	T2575	D2477	V2378	H2274	Y2162
K3872	L3774	ARG	K3560	V3449	N3308	ILE	P2841	R2744	T2576	D2478	V2378	L2275	V2169
F3873	V3777	GLU	K3564	F3458	T3309	VAL	D2842	D2746	T2577	E2488	S2379	L2276	L2170
F3874	V3778	THR	K3565	D3459	T3310	PRO	L2843	D2747	T2578	L2489	L2380	L2280	
W3875	A3779	ARG	L3566	D3460	K3311	GLU	F2844	K2748	T2579	L2490	E2381		
H3878	N3780	ALA	L3570	I3461	F3313	VAL	Q2845	A2748	K2580	L2491	A2382		
D3882	N3784	ARG	K3571	I3462	E3319	ASN	G2846	L2749	R2586	P2492	V2385	K2283	
V3785	V3785	T3669	K3574	S3463	L3320	GLU	Y2849	V2752	E2590	L2494	T2390	L2176	
F3786	F3786	K3670	K3574	L3465	L3320	LEU	L2852	H2755	T2609	P2495	V2391	L2178	
T3787	T3787	S3671	K3574	L3465	N3323	VAL	L2853	H2756	T2609	L2496	V2391	F2179	
L3887	D3672	D3672	L3578	A3473	K3323	PHE	L2853	H2756	T2609	Y2497	T2392	L2180	
L3888	D3672	D3672	L3578	A3473	K3323	THR	L2853	H2756	T2609	T2498	T2392	L2180	
L3889	R3792	E3673	E3579	G3474	I3329	GLU	L2856	L2757	Q2612	L2498	H2293	G2181	
Q3890	K3799	I3674	N3580	R3475	Y3330	PRO	L2856	L2759	S2613	S2499	L2394	L2294	
R3894		L3677	K3581	R3476	F3334	ILE	K2859	Q2760	R2620	V2502	T2396	L2295	
F3895	L3803	Y3683	K3582	E3480	F3334	GLN	T2860	A2761	R2627	V2503	T2397	L2298	
V3896	S3810	F3683	L3583	G3482	R3342	T2960	L2863	S2762	Y2630	L2506	L2407	K2299	
E3898		S3687	K3584	D3483	A3343	R2961	G2864	R2763	Y2630	L2506	L2407	F2302	
D3899	L3813	S3687	L3587	D3483	A3343	D2963	L2866	K2766	T2631	Q2508	S2410	L2186	
D3905	L3814	K3688	K3592	K3493	L3346	V2982	E2870	R2771	T2635	L2512	D2307	L2193	
T3906	L3816	L3690	E3593	S3502	V3347	G2983	E2870	R2771	T2635	K2513	D2197	D2197	
W3911	K3817	K3692	A3594	S3502	K3350	V2984	L2873	V2772	T2637	Q2514	L2310	R2199	
G3912	S3818	K3693	K3595	L3509	L3353	N2985	Y2874	L2779	T2638	K2517	L2312	D2200	
S3913	L3819	F3694	K3596	L3509	L3353	P2986	L2875	L2779	T2638	T2519	D2313	D2201	
Q3914	E3820	F3694	K3597	R3512	V3358	R2987	D2875	K2780	T2640	T2520	T2314	T2502	
F3915	N3821	K3698	E3598	V3513	K3359	P2988	V2878	Q2783	S2643	K2424	L2315	T2203	
F3916	N3822	N3700	E3605	F3518	K3361	L3010	K2883	P2784	W2653	T2425	L2316	T2204	
T3917	F3824	F3701	E3606	V3519	D3361	V3017	F2889	K2785	R2654	W2524	L2317	A2205	
G3918	A3825	K3702	F3607	T3520	T3372	K3017	T2890	L2786	L2655	T2525	L2318	R2209	
K3919	G3837	F3703	D3612	N3521	T3372	V3017	T2890	R2788	L2681	T2526	S2321	L2212	
V3923	W3838	V3719	K3613	T3525	L3391	L3024	L2891	F2795	L2681	T2438	L2326	C2220	
W3924	L3839	L3720	L3614	T3525	E3392	V3028	D2892	F2795	S2691	R2527	Q2332	S2221	
S3925	L3840	T3721	V3615	F3530	N3393	V3028	C2892	L2799	S2691	C2535	Q2335	S2224	
V3926	L3841	V3725	E3616	F3530	S3400	LEU	P2894	L2799	L2694	N2536	Q2335	K2225	
Y3927	Q3845	V3725	K3617	F3530	S3400	VAL	K2902	L2808	L2700	N2543	R2336	L2226	
W3934	M3846	S3729	L3633	T3533	F3406	ASN	K2902	L2808	L2700	R2549	T2339	L2229	
F3935	S3847	S3730	G3622	L3534	L3407	GLU	L2903	T2812	L2707	R2549	F2346	L2241	
L3848	L3848	D3731	K3631	E3537	L3408	LEU	L2908	T2812	W2707	R2549	F2346	L2241	
I3939	S3849	D3731	K3631	K3538	D3409	ASN	L2908	T2812	W2707	R2549	F2346	L2241	
T3943	K3850	L3736	G3636	K3541	H3413	LYS	R2911	L2816	L2712	R2552	L2455	Q2351	
V3946	K3852	T3740	F3641	Q3542	V3417	SER	W2916	M2821	F2723	L2559	N2463	E2345	
P3947	V3854	T3740	Y3642	R3544	L3429	ILE	M2917	L2822	C2724	P2562	Y2464	L2353	
L3855	L3855	L3744	S3645	K3544	L3429	SER	G2918	L2828	E2727	S2563	L2467	D2355	
H3858	H3858	R3745	I3646	D3547	F3431	LEU	D2919	E2829	E2727	K2564	T2467	L2356	
S3951	V3859	E3766	L3650	L3548	F3431	VAL	H2920	E2829	L2728	K2565	S2357	S2257	
Y3954	F3767	F3767	L3650	L3549	F3436	K3297	T2924	L2833	E2729	S2566	L2471	S2257	
Y3955	A3865	F3768	Y3656	L3551	R3439	E3301	T2924	L2833	W2731	Y2571	L2472	A2362	

WORLDWIDE  
 **PDB**  
PROTEIN DATA BANK

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.77Å 118.19Å 202.68Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	49.14 – 3.70 49.09 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.14-3.70) 99.9 (49.09-3.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 3.67Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.231 , 0.289 0.226 , 0.285	Depositor DCC
$R_{free}$ test set	4446 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	142.7	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 138.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	41590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, 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	0.58	1/21146 (0.0%)	0.80	12/28618 (0.0%)
1	B	0.47	0/21146	0.68	4/28618 (0.0%)
All	All	0.53	1/42292 (0.0%)	0.74	16/57236 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2872	GLU	CG-CD	7.57	1.63	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1741	LEU	CB-CG-CD1	8.44	125.34	111.00
1	A	1973	LEU	CB-CG-CD1	-7.38	98.45	111.00
1	A	2872	GLU	OE1-CD-OE2	-7.25	114.59	123.30
1	A	2866	LEU	CA-CB-CG	6.12	129.38	115.30
1	A	1769	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	2866	LEU	CB-CG-CD1	6.04	121.28	111.00
1	B	3650	LEU	CB-CG-CD1	-5.85	101.06	111.00
1	A	2012	LEU	CA-CB-CG	5.84	128.72	115.30
1	B	2866	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	3577	MET	CG-SD-CE	5.72	109.36	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1611	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	A	1776	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	A	1769	LEU	CB-CG-CD1	5.27	119.96	111.00
1	B	2620	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	2759	ILE	CG1-CB-CG2	-5.23	99.90	111.40
1	A	1917	ARG	NE-CZ-NH2	-5.09	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1739	ASP	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	20748	0	20207	891	0
1	B	20748	0	20206	851	0
2	A	31	0	12	4	0
2	B	31	0	12	7	0
3	A	15	0	0	9	0
3	B	15	0	0	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	41590	0	40437	1741	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 21.

All (1741) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PRO:C	1:A:3475:ASN:HB3	1.39	1.40
1:B:1620:PHE:HD1	1:B:1760:PHE:CZ	1.53	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1620:PHE:HD1	1:A:1760:PHE:CZ	1.58	1.21
1:B:3534:LEU:CD1	1:B:3618:TYR:HE2	1.53	1.21
1:B:1409:LEU:HD21	1:B:1435:LEU:HB3	1.24	1.18
1:A:3777:VAL:HG11	1:A:3895:PHE:HE1	1.06	1.18
1:A:4033:LEU:CD1	1:A:4035:GLN:HB2	1.76	1.16
1:A:3534:LEU:CD1	1:A:3618:TYR:HE2	1.59	1.15
1:B:1992:LYS:HG3	1:B:2024:SER:HB2	1.23	1.15
1:A:3525:ILE:HD11	1:A:3646:ILE:HG22	1.25	1.14
1:B:2111:LYS:HD3	1:B:2161:GLU:HG3	1.25	1.14
1:B:3525:ILE:HD11	1:B:3646:ILE:HG22	1.23	1.14
1:A:2111:LYS:HD3	1:A:2161:GLU:HG3	1.18	1.13
1:B:2473:LEU:HD23	1:B:2475:PRO:HD3	1.31	1.12
1:A:2707:VAL:HB	1:A:2712:LEU:HD11	1.19	1.11
1:B:2707:VAL:HB	1:B:2712:LEU:HD11	1.17	1.10
1:A:1992:LYS:HG3	1:A:2024:SER:HB2	1.17	1.09
1:A:3024:LEU:HD11	1:A:3303:LYS:HG3	1.31	1.09
1:A:2380:LEU:HD13	1:A:2390:ILE:HD11	1.34	1.08
1:B:3777:VAL:HG11	1:B:3895:PHE:HE1	0.97	1.08
1:A:2141:ILE:HD12	1:A:2146:LYS:HE2	1.20	1.07
1:A:3303:LYS:HA	1:A:3306:TRP:CD1	1.89	1.07
1:A:2494:LEU:HD13	1:A:2498:GLY:CA	1.85	1.07
1:B:1620:PHE:CD1	1:B:1760:PHE:CZ	2.42	1.06
1:A:2107:LYS:HE3	1:A:2495:ASP:OD2	1.51	1.06
1:B:2488:GLU:HB3	1:B:2491:LEU:HD12	1.12	1.06
1:A:1386:ILE:HG21	1:A:1396:ARG:HD2	1.32	1.06
1:B:1620:PHE:CD1	1:B:1760:PHE:HZ	1.73	1.06
1:B:3777:VAL:HG11	1:B:3895:PHE:CE1	1.90	1.06
1:A:3530:PHE:CD1	1:A:3618:TYR:HD2	1.71	1.06
1:B:1645:PHE:HB3	1:B:1765:ILE:HG22	1.37	1.06
1:A:1645:PHE:HB3	1:A:1765:ILE:CG2	1.86	1.05
1:B:2494:LEU:HD13	1:B:2498:GLY:CA	1.86	1.05
1:A:2380:LEU:HD22	1:A:2384:GLU:OE1	1.54	1.05
1:A:1645:PHE:HB3	1:A:1765:ILE:HG22	1.34	1.04
1:A:2494:LEU:CD1	1:A:2498:GLY:HA2	1.86	1.04
1:B:3534:LEU:CD1	1:B:3618:TYR:CE2	2.40	1.04
1:B:1645:PHE:HB3	1:B:1765:ILE:CG2	1.87	1.04
1:B:3534:LEU:HD12	1:B:3618:TYR:HE2	1.20	1.04
1:A:1983:LEU:HD22	1:A:1997:SER:OG	1.58	1.04
1:A:216:PRO:C	1:A:3475:ASN:CB	2.24	1.03
1:B:2473:LEU:CD2	1:B:2475:PRO:HD3	1.87	1.03
1:A:1992:LYS:CG	1:A:2024:SER:HB2	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2988:SER:HB3	1:A:2989:PRO:HD2	1.04	1.03
1:A:2488:GLU:HB3	1:A:2491:LEU:HD12	1.36	1.03
1:B:3303:LYS:HA	1:B:3306:TRP:CD1	1.93	1.03
1:B:1992:LYS:CG	1:B:2024:SER:HB2	1.89	1.03
1:B:2494:LEU:CD1	1:B:2498:GLY:HA2	1.89	1.02
1:A:1823:ASP:HB2	1:A:1852:ARG:O	1.56	1.02
1:A:2920:TRP:HB2	1:A:2989:PRO:HG3	1.06	1.02
1:B:1983:LEU:HD12	1:B:1997:SER:OG	1.59	1.02
1:B:3024:LEU:HD11	1:B:3303:LYS:HG3	1.39	1.01
1:A:2707:VAL:CB	1:A:2712:LEU:HD11	1.89	1.01
1:B:3530:PHE:CD1	1:B:3618:TYR:HD2	1.77	1.01
1:B:2707:VAL:CB	1:B:2712:LEU:HD11	1.88	1.01
1:A:2386:MET:HB2	1:A:2627:ARG:HD3	1.42	1.01
1:B:2107:LYS:HE3	1:B:2495:ASP:OD2	1.60	1.00
1:B:2488:GLU:CB	1:B:2491:LEU:HD12	1.91	1.00
1:A:1535:PRO:HB2	1:A:1841:ILE:HG13	1.44	1.00
1:A:2448:ASP:HB2	1:A:2829:GLU:OE2	1.59	1.00
1:A:3303:LYS:O	1:A:3306:TRP:HD1	1.43	1.00
1:B:1823:ASP:HB2	1:B:1852:ARG:O	1.61	1.00
1:A:2988:SER:HB3	1:A:2989:PRO:CD	1.90	1.00
1:A:3777:VAL:HG11	1:A:3895:PHE:CE1	1.97	0.99
1:A:1620:PHE:CD1	1:A:1760:PHE:CZ	2.50	0.99
1:B:3534:LEU:HD12	1:B:3618:TYR:CE2	1.97	0.99
1:B:2488:GLU:HB3	1:B:2491:LEU:CD1	1.92	0.99
1:A:3777:VAL:CG1	1:A:3895:PHE:HE1	1.74	0.99
1:B:2787:HIS:HA	1:B:3460:PRO:HD2	1.42	0.99
1:A:3534:LEU:CD1	1:A:3618:TYR:CE2	2.45	0.99
1:B:2064:GLN:HE22	1:B:2091:MET:CE	1.76	0.98
1:A:2380:LEU:CD1	1:A:2390:ILE:HD11	1.93	0.98
1:A:1409:LEU:HD21	1:A:1435:LEU:HB3	1.44	0.98
1:B:2745:ILE:HG23	1:B:2756:MET:HE2	1.43	0.97
1:B:2988:SER:HB3	1:B:2989:PRO:HD2	1.45	0.97
1:A:1970:LEU:HD13	1:A:1974:LYS:HE3	1.46	0.96
1:A:2064:GLN:OE1	1:A:2091:MET:HE1	1.64	0.96
1:A:3406:PHE:HB2	1:A:3513:VAL:CG1	1.94	0.96
1:A:2476:LYS:H	1:A:2476:LYS:CD	1.74	0.96
1:B:1822:CYS:HB2	1:B:1853:LEU:HD21	1.43	0.96
1:A:1822:CYS:HB2	1:A:1853:LEU:HD21	1.43	0.96
1:A:3024:LEU:CD1	1:A:3303:LYS:HG3	1.96	0.96
1:A:3534:LEU:HD12	1:A:3618:TYR:HE2	1.24	0.96
1:B:1744:LEU:HA	1:B:1760:PHE:CE2	1.99	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2112:GLU:HB3	1:B:2117:SER:HB2	1.48	0.95
1:A:1386:ILE:HG21	1:A:1396:ARG:CD	1.95	0.95
1:B:1992:LYS:HE2	1:B:2024:SER:O	1.64	0.95
1:B:1956:LEU:HB3	1:B:1968:PHE:HE2	1.31	0.95
1:A:2988:SER:CB	1:A:2989:PRO:HD2	1.97	0.95
1:A:4033:LEU:HD11	1:A:4035:GLN:HB2	1.47	0.95
1:B:1939:PHE:CD2	1:B:1940:GLU:O	2.19	0.95
1:A:3534:LEU:HD12	1:A:3618:TYR:CE2	2.01	0.95
1:B:3777:VAL:CG1	1:B:3895:PHE:HE1	1.78	0.95
1:A:1620:PHE:HD1	1:A:1760:PHE:HZ	1.07	0.94
1:A:2386:MET:CB	1:A:2627:ARG:HD3	1.95	0.94
1:B:1630:ILE:HG22	1:B:1655:MET:SD	2.06	0.94
1:A:2476:LYS:H	1:A:2476:LYS:HD3	1.26	0.94
1:A:2745:ILE:HG23	1:A:2756:MET:HE1	1.47	0.94
1:A:1645:PHE:CB	1:A:1765:ILE:HG22	1.96	0.94
1:A:1409:LEU:HD21	1:A:1435:LEU:CB	1.98	0.94
1:B:1645:PHE:CB	1:B:1765:ILE:HG22	1.97	0.94
1:B:1535:PRO:HB2	1:B:1841:ILE:HG13	1.50	0.94
1:B:2473:LEU:HD11	1:B:2527:GLU:CG	1.96	0.94
1:A:3460:PRO:O	1:A:3463:SER:HB2	1.67	0.93
1:B:1866:GLN:OE1	1:B:1911:ASN:HB2	1.68	0.93
1:B:2472:THR:CG2	1:B:2524:VAL:HG22	1.99	0.93
1:B:1774:LEU:HD21	1:B:1922:LYS:O	1.68	0.93
1:B:2494:LEU:HD13	1:B:2498:GLY:HA2	0.95	0.93
1:A:1802:LYS:HG2	1:A:1921:MET:HG3	1.47	0.93
1:A:3530:PHE:CD1	1:A:3618:TYR:CD2	2.56	0.93
1:A:2137:VAL:O	1:A:2141:ILE:HG23	1.69	0.93
1:A:3509:LEU:CD1	1:A:3513:VAL:HG21	1.98	0.93
1:B:2081:THR:HB	2:B:5093:ATP:PA	2.09	0.92
1:A:4065:LEU:HD11	1:A:4070:ILE:HD11	1.48	0.92
1:A:2111:LYS:HD3	1:A:2161:GLU:CG	2.00	0.92
1:A:2400:HIS:CD2	1:A:2559:LEU:HD13	2.06	0.91
1:B:1983:LEU:HD21	1:B:2000:ARG:NE	1.84	0.91
1:B:2787:HIS:HA	1:B:3460:PRO:CD	2.00	0.91
1:A:1992:LYS:HE2	1:A:2024:SER:O	1.71	0.91
1:B:3534:LEU:HD13	1:B:3618:TYR:HE2	1.35	0.91
1:B:2332:GLY:HA2	1:B:2335:GLN:HB2	1.50	0.91
1:B:2064:GLN:NE2	1:B:2091:MET:CE	2.33	0.91
1:A:2787:HIS:HA	1:A:3460:PRO:HD2	1.49	0.90
1:B:3534:LEU:HD11	1:B:3614:LEU:HD23	1.50	0.90
1:A:3737:THR:HB	1:A:3740:THR:OG1	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2400:HIS:NE2	1:A:2559:LEU:HD13	1.86	0.90
1:B:3737:THR:HB	1:B:3740:THR:OG1	1.69	0.90
1:B:1535:PRO:C	1:B:1841:ILE:HD11	1.90	0.90
1:A:2563:SER:HB3	1:A:2566:SER:H	1.35	0.90
1:A:2494:LEU:HD13	1:A:2498:GLY:HA2	0.94	0.90
1:B:2473:LEU:HD23	1:B:2475:PRO:CD	2.02	0.90
1:B:1726:LEU:CD1	1:B:3984:GLN:HB3	2.02	0.89
1:B:2473:LEU:HD11	1:B:2527:GLU:HG2	1.52	0.89
1:B:1802:LYS:HG2	1:B:1921:MET:HG3	1.54	0.89
1:A:1939:PHE:CD2	1:A:1940:GLU:O	2.26	0.89
1:B:2755:HIS:HB2	1:B:2911:ARG:O	1.72	0.89
1:A:4033:LEU:HD13	1:A:4035:GLN:HB2	1.54	0.88
1:A:1535:PRO:C	1:A:1841:ILE:HD11	1.92	0.88
1:A:1823:ASP:CB	1:A:1852:ARG:O	2.20	0.88
1:A:3946:VAL:HG12	1:A:3950:PHE:O	1.72	0.88
1:B:1604:ALA:HA	1:B:1607:TRP:CD1	2.09	0.88
1:A:1562:MET:HB3	1:A:1569:ILE:HD11	1.55	0.88
1:A:2787:HIS:HA	1:A:3460:PRO:CG	2.02	0.88
1:A:2920:TRP:HB2	1:A:2989:PRO:CG	1.99	0.87
1:A:2787:HIS:HA	1:A:3460:PRO:CD	2.03	0.87
1:A:2446:SER:H	1:A:2449:THR:CG2	1.86	0.87
1:A:3534:LEU:HD13	1:A:3618:TYR:HE2	1.38	0.87
1:B:1940:GLU:HB2	1:B:1989:GLU:O	1.73	0.87
1:A:1649:LEU:HD11	1:A:1704:GLU:HG3	1.56	0.87
1:A:1866:GLN:OE1	1:A:1911:ASN:HB2	1.74	0.87
1:A:2064:GLN:NE2	1:A:2091:MET:SD	2.47	0.87
1:A:2920:TRP:CB	1:A:2989:PRO:HG3	2.01	0.87
1:B:2476:LYS:CD	1:B:2476:LYS:H	1.87	0.87
1:B:2627:ARG:NH1	1:B:2631:THR:CG2	2.38	0.87
1:B:1956:LEU:HB3	1:B:1968:PHE:CE2	2.09	0.86
1:A:1924:PRO:HB2	1:A:1929:ILE:HD11	1.55	0.86
1:B:2988:SER:HB3	1:B:2989:PRO:CD	2.04	0.86
1:A:2787:HIS:HA	1:A:3460:PRO:HG2	1.56	0.86
1:B:1392:LEU:HD13	1:B:1393:LYS:N	1.90	0.86
1:B:2473:LEU:HD21	1:B:2527:GLU:HB2	1.55	0.86
1:B:2274:HIS:HE1	1:B:2326:LEU:O	1.59	0.86
1:A:2766:LYS:HE2	1:A:2890:THR:HB	1.58	0.86
1:A:1726:LEU:HD12	1:A:3984:GLN:HB3	1.55	0.85
1:B:2787:HIS:HA	1:B:3460:PRO:CG	2.06	0.85
1:B:3530:PHE:CD1	1:B:3618:TYR:CD2	2.64	0.85
1:B:3645:SER:HB3	1:B:3890:GLN:HE21	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1387:GLU:HB3	1:A:1393:LYS:HG2	1.58	0.85
1:A:1392:LEU:HD13	1:A:1393:LYS:N	1.91	0.85
1:A:2141:ILE:CD1	1:A:2146:LYS:HE2	2.06	0.85
1:B:3946:VAL:HG12	1:B:3950:PHE:O	1.76	0.85
1:A:3656:VAL:HG13	1:A:3677:LEU:HB3	1.59	0.85
1:B:2627:ARG:NH1	1:B:2630:TYR:CD2	2.45	0.85
1:A:3024:LEU:HD11	1:A:3303:LYS:CG	2.07	0.85
1:B:2131:THR:HG22	1:B:2176:LEU:HD21	1.57	0.85
1:A:1940:GLU:HB2	1:A:1989:GLU:O	1.77	0.84
1:A:2131:THR:HG22	1:A:2176:LEU:HD21	1.59	0.84
1:A:3303:LYS:O	1:A:3306:TRP:CD1	2.28	0.84
1:A:2446:SER:H	1:A:2449:THR:HG23	1.39	0.84
1:B:3406:PHE:HB2	1:B:3513:VAL:CG1	2.06	0.84
1:B:2563:SER:HB3	1:B:2566:SER:H	1.41	0.84
1:A:2112:GLU:HB3	1:A:2117:SER:HB2	1.57	0.84
1:B:1365:PHE:O	1:B:1366:VAL:HG22	1.78	0.84
1:A:2336:ARG:HD3	1:A:2355:ASP:OD2	1.77	0.84
1:B:2627:ARG:HH11	1:B:2630:TYR:HD2	1.25	0.84
1:B:2446:SER:H	1:B:2449:THR:HG23	1.43	0.83
1:B:1823:ASP:CB	1:B:1852:ARG:O	2.25	0.83
1:B:2745:ILE:HG23	1:B:2756:MET:CE	2.08	0.83
1:A:2274:HIS:HE1	1:A:2326:LEU:O	1.61	0.83
1:A:2488:GLU:CB	1:A:2491:LEU:HD12	2.09	0.83
1:B:2111:LYS:HD3	1:B:2161:GLU:CG	2.07	0.83
1:A:2106:THR:OG1	1:A:2154:PHE:HB3	1.78	0.83
1:A:1649:LEU:CD1	1:A:1704:GLU:HG3	2.07	0.83
1:B:2787:HIS:HA	1:B:3460:PRO:HG2	1.61	0.83
1:B:3024:LEU:CD1	1:B:3303:LYS:HG3	2.09	0.83
1:A:2755:HIS:HB2	1:A:2911:ARG:O	1.79	0.82
1:B:1574:PHE:HB3	1:B:1576:GLU:H	1.43	0.82
1:B:3998:ILE:HG21	1:B:4004:LEU:HG	1.59	0.82
1:A:2111:LYS:NZ	1:A:2161:GLU:HG2	1.94	0.82
1:B:1425:GLU:OE1	1:B:1426:GLN:HA	1.79	0.82
1:B:3919:LYS:HZ3	1:B:4038:GLU:CD	1.83	0.82
1:A:2488:GLU:HB3	1:A:2491:LEU:CD1	2.08	0.82
1:B:2081:THR:HB	2:B:5093:ATP:O2A	1.78	0.82
1:B:3509:LEU:CD1	1:B:3513:VAL:HG21	2.10	0.82
1:A:1425:GLU:OE1	1:A:1426:GLN:HA	1.78	0.82
1:B:2627:ARG:NH1	1:B:2631:THR:HG23	1.94	0.82
1:A:1604:ALA:HA	1:A:1607:TRP:NE1	1.95	0.81
1:A:3645:SER:HB3	1:A:3890:GLN:HE21	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PRO:O	1:A:216:PRO:CB	2.28	0.81
1:A:2476:LYS:HZ1	1:A:2528:ARG:HD2	1.43	0.81
1:B:3566:LEU:HA	1:B:3583:LEU:HD21	1.61	0.81
1:A:2362:ALA:HB3	1:A:2365:LYS:O	1.81	0.81
1:B:2106:THR:OG1	1:B:2154:PHE:HB3	1.80	0.81
1:A:1849:GLU:HG2	1:A:1899:ASN:ND2	1.95	0.81
1:A:2064:GLN:OE1	1:A:2091:MET:CE	2.29	0.81
1:A:3923:VAL:HG23	1:A:4038:GLU:HA	1.62	0.81
1:A:1630:ILE:HG22	1:A:1655:MET:SD	2.21	0.81
1:B:2627:ARG:NH1	1:B:2630:TYR:CE2	2.48	0.81
1:A:1493:LEU:HD23	1:A:1498:GLU:HB3	1.63	0.81
1:B:3566:LEU:HA	1:B:3583:LEU:CD2	2.10	0.81
1:B:3792:ARG:HB2	1:B:3955:TYR:CD1	2.15	0.81
1:B:2111:LYS:NZ	1:B:2161:GLU:HG2	1.96	0.81
1:B:1604:ALA:HA	1:B:1607:TRP:NE1	1.95	0.80
1:B:2446:SER:H	1:B:2449:THR:CG2	1.93	0.80
1:B:1939:PHE:HD2	1:B:1940:GLU:O	1.62	0.80
1:B:3998:ILE:CG2	1:B:4004:LEU:HG	2.12	0.80
1:B:2707:VAL:CG1	1:B:2712:LEU:CD1	2.59	0.80
1:A:3303:LYS:HA	1:A:3306:TRP:NE1	1.95	0.79
1:B:2473:LEU:CD2	1:B:2475:PRO:CD	2.57	0.79
1:A:3303:LYS:C	1:A:3306:TRP:HD1	1.84	0.79
1:B:2112:GLU:HB3	1:B:2117:SER:CB	2.12	0.79
1:A:1421:TYR:O	1:A:1425:GLU:CB	2.30	0.79
1:A:2476:LYS:NZ	1:A:2528:ARG:HD2	1.97	0.79
1:A:3303:LYS:CA	1:A:3306:TRP:CD1	2.65	0.79
1:A:2181:GLY:O	1:A:2182:GLU:HG3	1.83	0.79
1:A:2332:GLY:HA2	1:A:2335:GLN:HB2	1.62	0.79
1:A:1394:LEU:HD22	1:A:1449:GLN:HE22	1.48	0.79
1:B:1744:LEU:HA	1:B:1760:PHE:CD2	2.18	0.79
1:A:2707:VAL:CG1	1:A:2712:LEU:CD1	2.61	0.78
1:A:3530:PHE:HD1	1:A:3618:TYR:HD2	1.31	0.78
1:A:3799:LYS:O	1:A:3803:LEU:HG	1.82	0.78
1:A:1956:LEU:HB3	1:A:1968:PHE:CE2	2.18	0.78
1:B:1562:MET:HB3	1:B:1569:ILE:HD11	1.64	0.78
1:B:2707:VAL:HB	1:B:2712:LEU:CD1	2.08	0.78
1:B:1924:PRO:HB2	1:B:1929:ILE:HD11	1.64	0.78
1:B:1996:GLU:O	1:B:2000:ARG:HG3	1.81	0.78
1:B:2380:LEU:HD12	1:B:2577:ALA:HB1	1.65	0.78
1:B:3303:LYS:O	1:B:3306:TRP:HD1	1.66	0.78
1:B:1409:LEU:CD2	1:B:1435:LEU:HB3	2.09	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:LEU:HD12	1:A:1971:ARG:N	1.98	0.78
1:B:2137:VAL:O	1:B:2141:ILE:HG23	1.84	0.78
1:B:2493:LYS:HG3	1:B:2494:LEU:H	1.48	0.78
1:A:1386:ILE:CG2	1:A:1396:ARG:CD	2.62	0.78
1:A:1620:PHE:CD1	1:A:1760:PHE:HZ	1.96	0.78
1:B:3923:VAL:HG23	1:B:4038:GLU:HA	1.66	0.78
1:A:1604:ALA:HA	1:A:1607:TRP:CD1	2.18	0.77
1:B:2472:THR:HG21	1:B:2524:VAL:HG22	1.65	0.77
1:A:1421:TYR:O	1:A:1425:GLU:HB2	1.84	0.77
1:B:1953:LEU:CD1	1:B:1973:LEU:HB3	2.14	0.77
1:B:3473:ALA:HB3	1:B:3476:ARG:O	1.85	0.77
1:A:3509:LEU:HD12	1:A:3513:VAL:CG2	2.13	0.77
1:B:1387:GLU:HB3	1:B:1393:LYS:HG2	1.66	0.77
1:A:2476:LYS:HG2	1:A:2478:ASP:O	1.85	0.77
1:B:1405:CYS:O	1:B:1409:LEU:HG	1.85	0.77
1:A:2064:GLN:OE1	1:A:2151:TRP:HH2	1.67	0.76
1:B:1421:TYR:O	1:B:1425:GLU:CB	2.32	0.76
1:B:1849:GLU:HG2	1:B:1899:ASN:ND2	2.00	0.76
1:B:2293:HIS:CE1	1:B:2409:ASN:HB3	2.20	0.76
1:B:1409:LEU:HD21	1:B:1435:LEU:CB	2.11	0.76
1:B:1421:TYR:O	1:B:1425:GLU:HB2	1.85	0.76
1:B:1645:PHE:CB	1:B:1765:ILE:CG2	2.61	0.76
1:B:2473:LEU:HD23	1:B:2474:LEU:N	2.01	0.76
1:B:2476:LYS:HG2	1:B:2478:ASP:O	1.86	0.76
1:B:2476:LYS:NZ	1:B:2528:ARG:HD2	2.00	0.76
1:B:3871:PHE:CZ	1:B:3873:MET:HB2	2.21	0.76
1:A:3460:PRO:O	1:A:3463:SER:CB	2.32	0.76
1:B:2572:GLU:CD	1:B:2590:GLU:HG3	2.05	0.76
1:B:2787:HIS:CA	1:B:3460:PRO:HD2	2.15	0.76
1:B:2920:TRP:HB2	1:B:2989:PRO:HG3	1.67	0.76
1:A:2411:LYS:HG2	1:A:2530:HIS:HE1	1.51	0.76
1:A:1540:LEU:CD1	1:A:1548:ILE:CD1	2.64	0.75
1:A:2563:SER:HB2	1:A:2566:SER:OG	1.86	0.75
1:A:3946:VAL:CG1	1:A:3950:PHE:O	2.34	0.75
1:A:3939:ILE:HG13	1:A:4010:LEU:CD2	2.16	0.75
1:B:1366:VAL:HG13	1:B:1369:LYS:HE3	1.68	0.75
1:B:2003:LEU:HA	1:B:2006:LEU:HD12	1.69	0.75
1:B:2064:GLN:HE22	1:B:2091:MET:HE3	1.49	0.75
1:B:3534:LEU:HD13	1:B:3618:TYR:CE2	2.15	0.75
1:A:1939:PHE:HD2	1:A:1940:GLU:O	1.67	0.75
1:B:1489:ARG:HH12	1:B:1503:PRO:HG2	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2064:GLN:NE2	1:B:2091:MET:HE3	2.00	0.75
1:A:3816:LEU:HD23	1:A:3847:SER:OG	1.86	0.75
1:A:4033:LEU:CD1	1:A:4035:GLN:CB	2.60	0.75
1:B:1967:HIS:C	1:B:1968:PHE:HD1	1.90	0.75
1:B:3774:ILE:O	1:B:3778:VAL:HG23	1.86	0.75
1:A:2707:VAL:HB	1:A:2712:LEU:CD1	2.09	0.75
1:A:3777:VAL:CG1	1:A:3895:PHE:CE1	2.63	0.75
1:B:1983:LEU:HD11	1:B:2000:ARG:HD2	1.66	0.75
1:B:2707:VAL:CG1	1:B:2712:LEU:HD11	2.16	0.75
1:A:2032:LYS:O	1:A:2035:VAL:HG12	1.85	0.75
1:B:3525:ILE:CD1	1:B:3646:ILE:HG22	2.11	0.75
1:B:1392:LEU:HD13	1:B:1392:LEU:C	2.06	0.75
1:A:2107:LYS:HE2	1:A:2499:SER:HB3	1.67	0.74
1:A:3406:PHE:HB2	1:A:3513:VAL:HG11	1.68	0.74
1:B:2380:LEU:HD11	1:B:2577:ALA:CB	2.17	0.74
1:B:3799:LYS:O	1:B:3803:LEU:HG	1.87	0.74
1:A:1940:GLU:HG3	1:A:1941:ASP:H	1.52	0.74
1:B:2032:LYS:O	1:B:2035:VAL:HG12	1.85	0.74
1:B:3303:LYS:CA	1:B:3306:TRP:CD1	2.70	0.74
1:A:1983:LEU:HD21	1:A:2000:ARG:HD2	1.69	0.74
1:A:3406:PHE:HB2	1:A:3513:VAL:HG12	1.69	0.74
1:A:3525:ILE:CD1	1:A:3646:ILE:HG22	2.13	0.74
1:B:2476:LYS:HD2	1:B:2476:LYS:H	1.51	0.74
1:B:3645:SER:HB3	1:B:3890:GLN:NE2	2.00	0.74
1:A:3534:LEU:HD11	1:A:3614:LEU:HD23	1.67	0.74
1:A:1744:LEU:HA	1:A:1760:PHE:CE2	2.23	0.74
1:A:1392:LEU:HD13	1:A:1392:LEU:C	2.07	0.74
1:A:3871:PHE:CZ	1:A:3873:MET:HB2	2.22	0.74
1:B:2175:ILE:HG12	1:B:2183:ARG:HB3	1.70	0.74
1:B:2380:LEU:CD1	1:B:2577:ALA:CB	2.65	0.74
1:B:2512:LYS:HB3	1:B:2523:TRP:HH2	1.52	0.74
1:A:1956:LEU:HB3	1:A:1968:PHE:HE2	1.53	0.74
1:B:2512:LYS:O	1:B:2513:GLN:HB2	1.88	0.74
1:A:1569:ILE:HA	1:A:1584:SER:HA	1.70	0.73
1:A:2745:ILE:HG23	1:A:2756:MET:CE	2.17	0.73
1:B:1726:LEU:HD12	1:B:3984:GLN:HB3	1.66	0.73
1:B:3946:VAL:CG1	1:B:3950:PHE:O	2.36	0.73
1:B:3303:LYS:C	1:B:3306:TRP:HD1	1.91	0.73
1:A:3566:LEU:HA	1:A:3583:LEU:CD2	2.18	0.73
1:A:2112:GLU:HB3	1:A:2117:SER:CB	2.19	0.73
1:A:2707:VAL:CG1	1:A:2712:LEU:HD11	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2785:LYS:HD3	1:B:3482:GLY:O	1.89	0.73
1:B:3618:TYR:CD1	1:B:3618:TYR:N	2.54	0.73
1:A:1802:LYS:NZ	3:A:5096:SO4:S	2.61	0.73
1:A:3303:LYS:CA	1:A:3306:TRP:HD1	2.02	0.73
1:B:2203:THR:HG22	1:B:2205:ALA:H	1.54	0.73
1:A:1405:CYS:O	1:A:1409:LEU:HG	1.88	0.73
1:A:2176:LEU:O	1:A:2183:ARG:HA	1.88	0.73
1:B:2380:LEU:CD1	1:B:2577:ALA:HB1	2.18	0.73
1:B:3792:ARG:HB2	1:B:3955:TYR:CE1	2.23	0.73
1:B:1630:ILE:CG2	1:B:1655:MET:SD	2.76	0.72
1:B:1569:ILE:HA	1:B:1584:SER:HA	1.70	0.72
1:A:2201:HIS:CE1	1:A:2497:TYR:HA	2.24	0.72
1:B:3656:VAL:HG13	1:B:3677:LEU:HB3	1.70	0.72
1:B:3690:LEU:HD23	1:B:3694:PHE:HB3	1.70	0.72
1:A:1822:CYS:SG	1:A:1850:PHE:HA	2.29	0.72
1:B:1849:GLU:HG2	1:B:1899:ASN:HD22	1.54	0.72
1:B:2176:LEU:O	1:B:2183:ARG:HA	1.89	0.72
1:B:2627:ARG:NH1	1:B:2631:THR:HG22	2.04	0.72
1:B:3024:LEU:HD11	1:B:3303:LYS:CG	2.18	0.72
1:A:1849:GLU:HG2	1:A:1899:ASN:HD22	1.53	0.72
1:B:1706:LEU:HD22	1:B:1935:GLN:HG2	1.70	0.72
1:B:1726:LEU:HD13	1:B:3984:GLN:HB3	1.69	0.72
1:A:3509:LEU:CD1	1:A:3513:VAL:CG2	2.68	0.71
1:B:2476:LYS:HZ1	1:B:2528:ARG:HD2	1.54	0.71
1:A:1645:PHE:CB	1:A:1765:ILE:CG2	2.61	0.71
1:B:1620:PHE:HA	1:B:1760:PHE:HE1	1.55	0.71
1:B:216:PRO:CB	1:B:1365:PHE:HD2	2.03	0.71
1:B:2563:SER:HB2	1:B:2566:SER:OG	1.91	0.71
1:B:3737:THR:OG1	1:B:3740:THR:HB	1.90	0.71
1:A:3530:PHE:HD1	1:A:3618:TYR:CD2	2.04	0.71
1:B:3330:TYR:OH	1:B:3346:LEU:HD22	1.89	0.71
1:B:1983:LEU:HD21	1:B:2000:ARG:CZ	2.19	0.71
1:B:1983:LEU:HB3	1:B:1993:THR:HG23	1.72	0.71
1:B:2448:ASP:HB2	1:B:2829:GLU:OE1	1.91	0.71
1:B:2107:LYS:HE2	1:B:2499:SER:HB3	1.72	0.71
1:B:3631:MET:CE	1:B:3698:MET:HG3	2.21	0.71
1:B:3566:LEU:O	1:B:3570:LEU:HG	1.91	0.71
1:A:1540:LEU:HD11	1:A:1548:ILE:HD11	1.73	0.71
1:A:2960:THR:HB	1:A:2963:ASP:HB2	1.73	0.70
1:A:3774:ILE:O	1:A:3778:VAL:HG23	1.91	0.70
1:A:3792:ARG:HB2	1:A:3955:TYR:CD1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1698:ILE:O	1:B:1702:LEU:HG	1.91	0.70
1:B:1970:LEU:HD13	1:B:1974:LYS:HE2	1.72	0.70
1:A:2003:LEU:HA	1:A:2006:LEU:HD12	1.74	0.70
1:A:3871:PHE:HZ	1:A:3873:MET:HB2	1.56	0.70
1:B:2514:GLY:O	1:B:2523:TRP:CH2	2.44	0.70
1:A:1774:LEU:HD21	1:A:1922:LYS:O	1.91	0.70
1:B:1535:PRO:HB2	1:B:1841:ILE:CG1	2.19	0.70
1:B:3303:LYS:O	1:B:3306:TRP:CD1	2.44	0.70
1:B:3406:PHE:HB2	1:B:3513:VAL:HG11	1.73	0.70
1:A:1493:LEU:HD23	1:A:1498:GLU:CB	2.22	0.70
1:A:3618:TYR:CD1	1:A:3618:TYR:N	2.54	0.70
1:B:2410:SER:C	1:B:2411:LYS:HG3	2.12	0.70
1:B:2745:ILE:HG12	1:B:2756:MET:HE1	1.73	0.70
1:A:1495:THR:HG22	1:A:1497:ILE:HG22	1.73	0.70
1:A:2294:LEU:HB3	1:A:2317:LEU:HD22	1.74	0.70
1:A:3305:ARG:O	1:A:3307:LEU:N	2.24	0.70
1:B:1611:LEU:O	1:B:1615:ILE:HG23	1.91	0.70
1:B:1536:ARG:N	1:B:1841:ILE:HD11	2.07	0.70
1:A:1612:ASP:HA	1:A:1615:ILE:CD1	2.21	0.69
1:A:2203:THR:HG22	1:A:2205:ALA:H	1.56	0.69
1:A:3330:TYR:OH	1:A:3346:LEU:HD22	1.92	0.69
1:A:3645:SER:HB3	1:A:3890:GLN:NE2	2.06	0.69
1:B:1612:ASP:HA	1:B:1615:ILE:CD1	2.22	0.69
1:B:1495:THR:HG22	1:B:1497:ILE:HG22	1.73	0.69
1:B:1649:LEU:HD11	1:B:1704:GLU:HG3	1.73	0.69
1:A:3785:TYR:HE2	1:A:3859:VAL:HG22	1.57	0.69
1:B:3919:LYS:NZ	1:B:4038:GLU:CD	2.46	0.69
1:B:3871:PHE:HZ	1:B:3873:MET:HB2	1.57	0.69
1:A:3979:ASN:O	1:A:3981:PRO:HD2	1.92	0.69
1:B:1540:LEU:CD1	1:B:1548:ILE:CD1	2.71	0.69
1:A:1646:GLN:NE2	1:A:1758:TYR:OH	2.26	0.69
1:A:1970:LEU:HD13	1:A:1974:LYS:CE	2.20	0.69
1:A:2175:ILE:HG12	1:A:2183:ARG:HB3	1.74	0.69
1:A:2285:GLU:HB2	1:A:2412:ARG:NH2	2.08	0.69
1:A:2107:LYS:CE	1:A:2495:ASP:OD2	2.37	0.69
1:B:1822:CYS:SG	1:B:1849:GLU:O	2.51	0.69
1:B:1365:PHE:O	1:B:1366:VAL:CG2	2.41	0.69
1:B:2081:THR:HB	2:B:5093:ATP:O1A	1.92	0.69
1:A:2514:GLY:O	1:A:2523:TRP:CH2	2.45	0.69
1:A:2125:TRP:CZ2	1:A:2178:LEU:HD13	2.28	0.68
1:A:3534:LEU:HD13	1:A:3618:TYR:CE2	2.19	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3850:TRP:NE1	1:A:3854:TYR:HB3	2.08	0.68
1:B:1649:LEU:CD1	1:B:1704:GLU:HG3	2.23	0.68
1:B:1983:LEU:CD1	1:B:1997:SER:OG	2.39	0.68
1:B:3566:LEU:HD13	1:B:3570:LEU:CD1	2.23	0.68
1:B:3777:VAL:CG1	1:B:3895:PHE:CE1	2.65	0.68
1:B:2081:THR:CB	2:B:5093:ATP:O2A	2.41	0.68
1:A:1995:VAL:HG21	1:A:2024:SER:HB3	1.74	0.68
1:A:2419:PRO:O	1:A:2424:LYS:HE3	1.93	0.68
1:A:1967:HIS:C	1:A:1968:PHE:HD1	1.97	0.68
1:B:3303:LYS:CA	1:B:3306:TRP:HD1	2.04	0.68
1:B:3851:VAL:HG13	1:B:3855:LEU:HD23	1.76	0.68
1:A:1802:LYS:NZ	3:A:5096:SO4:O2	2.26	0.68
1:A:1983:LEU:HB3	1:A:1993:THR:HG23	1.75	0.68
1:A:3837:GLY:O	1:A:3871:PHE:HD1	1.77	0.68
1:A:4033:LEU:HD13	1:A:4035:GLN:CB	2.21	0.68
1:B:3592:LYS:O	1:B:3596:ASN:HB2	1.94	0.68
1:A:1698:ILE:O	1:A:1702:LEU:HG	1.94	0.68
1:A:3848:LEU:HD21	1:A:3852:LYS:HE3	1.75	0.68
1:B:1620:PHE:HB2	1:B:1760:PHE:CE1	2.29	0.68
1:B:3886:ALA:N	1:B:3887:PRO:HD2	2.09	0.68
1:A:2787:HIS:CA	1:A:3460:PRO:HD2	2.20	0.68
1:B:1425:GLU:OE1	1:B:1426:GLN:CA	2.42	0.68
1:B:1620:PHE:HD1	1:B:1760:PHE:HZ	0.81	0.68
1:B:2224:SER:O	2:B:5093:ATP:H2	1.76	0.68
1:A:2293:HIS:NE2	1:A:2409:ASN:HB3	2.09	0.67
1:A:3566:LEU:HA	1:A:3583:LEU:HD21	1.76	0.67
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.76	0.67
1:A:1462:ASN:HB2	1:A:1465:ILE:HG22	1.75	0.67
1:A:1744:LEU:HA	1:A:1760:PHE:CD2	2.29	0.67
1:B:1540:LEU:CD1	1:B:1548:ILE:HD11	2.25	0.67
1:A:2293:HIS:CE1	1:A:2409:ASN:HB3	2.29	0.67
1:B:2766:LYS:HE2	1:B:2890:THR:HB	1.75	0.67
1:A:1822:CYS:SG	1:A:1849:GLU:O	2.53	0.67
1:A:2080:LYS:HG2	1:A:2215:PHE:CE1	2.30	0.67
1:B:3458:PHE:CE1	1:B:3459:ASP:O	2.47	0.67
1:B:3530:PHE:HD1	1:B:3618:TYR:HD2	1.42	0.67
1:A:1630:ILE:HA	1:A:1634:THR:HG22	1.75	0.67
1:A:2305:LEU:HD11	1:A:2368:PHE:CG	2.29	0.67
1:B:1527:LEU:HD23	1:B:1545:LEU:HD22	1.75	0.67
1:B:3816:LEU:HD23	1:B:3847:SER:OG	1.94	0.67
1:A:2493:LYS:HG3	1:A:2494:LEU:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2252:LEU:HD21	1:A:2310:LEU:HD23	1.76	0.67
1:A:216:PRO:O	1:A:3475:ASN:HB3	1.95	0.67
1:A:1489:ARG:HH12	1:A:1503:PRO:HG2	1.59	0.67
1:A:2386:MET:HB3	1:A:2627:ARG:HD3	1.75	0.67
1:B:2394:THR:H	1:B:2397:THR:HB	1.58	0.67
1:B:1527:LEU:CD2	1:B:1545:LEU:HD22	2.24	0.67
1:B:3303:LYS:HA	1:B:3306:TRP:NE1	2.10	0.67
1:B:3837:GLY:O	1:B:3871:PHE:HD1	1.77	0.67
1:A:3525:ILE:HD11	1:A:3646:ILE:CG2	2.16	0.67
1:B:1531:ARG:HG2	1:B:1537:PHE:HB3	1.76	0.67
1:B:3566:LEU:CD1	1:B:3570:LEU:HD11	2.24	0.67
1:B:2941:THR:HG22	1:B:2942:ASP:H	1.60	0.66
1:A:1536:ARG:N	1:A:1841:ILE:HD11	2.09	0.66
1:A:1540:LEU:CD1	1:A:1548:ILE:HD11	2.25	0.66
1:B:1425:GLU:OE1	1:B:1426:GLN:N	2.28	0.66
1:A:3979:ASN:C	1:A:3981:PRO:HD2	2.16	0.66
1:A:1703:VAL:HG13	1:A:1770:ILE:HD13	1.78	0.66
1:B:2181:GLY:O	1:B:2182:GLU:HG3	1.96	0.66
1:B:1645:PHE:CG	1:B:1765:ILE:HG22	2.31	0.66
1:B:2779:LEU:HD23	1:B:2812:ARG:O	1.96	0.66
1:B:3819:ILE:O	1:B:3823:ASN:HB2	1.94	0.66
1:B:3850:TRP:NE1	1:B:3854:TYR:HB3	2.10	0.66
1:A:3998:ILE:HG21	1:A:4004:LEU:HG	1.77	0.66
1:A:1425:GLU:OE1	1:A:1426:GLN:CA	2.43	0.66
1:A:1493:LEU:CD2	1:A:1498:GLU:HB3	2.25	0.66
1:A:1612:ASP:HA	1:A:1615:ILE:HD11	1.78	0.66
1:B:1620:PHE:HA	1:B:1760:PHE:CE1	2.31	0.66
1:A:2631:THR:O	1:A:2635:THR:HG22	1.96	0.66
1:A:1626:CYS:SG	1:A:1639:VAL:HG11	2.35	0.65
1:A:2382:ALA:O	1:A:2385:VAL:HG12	1.96	0.65
1:B:216:PRO:CB	1:B:1365:PHE:CD2	2.79	0.65
1:B:3935:PHE:HB2	1:B:4014:VAL:HG11	1.77	0.65
1:B:2707:VAL:CG1	1:B:2712:LEU:HD12	2.27	0.65
1:A:1527:LEU:CD2	1:A:1545:LEU:HD22	2.26	0.65
1:A:2514:GLY:HA3	1:A:2523:TRP:CZ2	2.32	0.65
1:A:3998:ILE:CG2	1:A:4004:LEU:HG	2.27	0.65
1:A:2220:CYS:SG	1:A:2224:SER:HB2	2.36	0.65
1:A:3566:LEU:O	1:A:3570:LEU:HG	1.97	0.65
1:B:3406:PHE:HB2	1:B:3513:VAL:HG12	1.76	0.65
1:B:3979:ASN:O	1:B:3981:PRO:HD2	1.97	0.65
1:A:2290:LEU:HD13	1:A:2407:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2728:LEU:HD12	1:A:2771:ARG:CZ	2.27	0.65
1:B:3839:ILE:HG23	1:B:3873:MET:HG3	1.78	0.65
1:A:3459:ASP:OD2	1:A:3461:ILE:HG12	1.97	0.65
1:B:2336:ARG:HD3	1:B:2355:ASP:OD2	1.97	0.65
1:B:2489:ILE:HG22	1:B:2535:CYS:HB3	1.78	0.65
1:A:1645:PHE:CG	1:A:1765:ILE:HG22	2.32	0.65
1:A:2512:LYS:O	1:A:2513:GLN:HB2	1.97	0.65
1:A:3566:LEU:HD13	1:A:3570:LEU:CD1	2.27	0.65
1:A:2448:ASP:HB2	1:A:2829:GLU:CD	2.17	0.65
1:A:3010:LEU:HD21	1:A:3317:SER:HB3	1.79	0.65
1:A:1706:LEU:CD2	1:A:1935:GLN:HG2	2.27	0.64
1:A:2842:ASP:O	1:A:2845:GLN:HG2	1.97	0.64
1:A:3473:ALA:HB3	1:A:3476:ARG:O	1.96	0.64
1:B:2707:VAL:CB	1:B:2712:LEU:CD1	2.72	0.64
1:A:3509:LEU:HD11	1:A:3513:VAL:HG21	1.76	0.64
1:A:3819:ILE:O	1:A:3823:ASN:HB2	1.96	0.64
1:B:2112:GLU:CB	1:B:2117:SER:HB2	2.25	0.64
1:B:2920:TRP:HB2	1:B:2989:PRO:CG	2.26	0.64
1:A:2707:VAL:CG1	1:A:2712:LEU:HD12	2.26	0.64
1:B:1534:PHE:CE2	1:B:1536:ARG:HB2	2.33	0.64
1:B:3509:LEU:HD12	1:B:3513:VAL:CG2	2.28	0.64
1:A:2779:LEU:HD23	1:A:2812:ARG:O	1.97	0.64
1:A:2315:THR:HG21	1:A:2350:SER:HB3	1.80	0.64
1:B:2536:ASN:HB2	1:B:2543:ARG:HE	1.63	0.64
1:B:3530:PHE:CE1	1:B:3618:TYR:CD2	2.85	0.64
1:A:2095:ASP:CG	1:A:2149:ARG:NH2	2.50	0.64
1:A:2222:ILE:HG23	1:A:2284:LEU:HD11	1.80	0.64
1:A:3566:LEU:CD1	1:A:3570:LEU:HD11	2.26	0.64
1:A:2495:ASP:O	1:A:2498:GLY:N	2.30	0.64
1:A:3618:TYR:HD1	1:A:3618:TYR:N	1.94	0.64
1:B:2252:LEU:HD21	1:B:2310:LEU:HD23	1.79	0.64
1:A:2141:ILE:HD12	1:A:2146:LYS:CE	2.12	0.64
1:A:3785:TYR:CE2	1:A:3859:VAL:HG22	2.33	0.64
1:B:1748:PHE:CD2	1:B:1755:LEU:HD22	2.32	0.64
1:A:2111:LYS:HZ3	1:A:2161:GLU:HG2	1.60	0.63
1:A:2285:GLU:HB2	1:A:2412:ARG:HH22	1.62	0.63
1:A:3792:ARG:HB2	1:A:3955:TYR:CE1	2.33	0.63
1:B:2111:LYS:CD	1:B:2161:GLU:HG3	2.17	0.63
1:A:1953:LEU:CD1	1:A:1973:LEU:HB3	2.27	0.63
1:A:3641:PHE:HA	1:A:3889:LEU:HD21	1.81	0.63
1:B:1706:LEU:HD11	1:B:1936:ILE:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1738:ASN:O	1:A:1739:ASP:OD1	2.16	0.63
1:A:1992:LYS:HG3	1:A:2024:SER:CB	2.11	0.63
1:A:1995:VAL:HG22	1:A:2022:PHE:CE2	2.33	0.63
1:A:3737:THR:OG1	1:A:3740:THR:HB	1.98	0.63
1:A:2632:ALA:HB3	1:A:2647:LEU:HD21	1.80	0.63
1:B:2846:GLY:O	1:B:2849:TYR:HB3	1.98	0.63
1:B:3530:PHE:HD1	1:B:3618:TYR:CD2	2.17	0.63
1:A:1562:MET:CB	1:A:1569:ILE:HD11	2.29	0.63
1:A:2536:ASN:HB2	1:A:2543:ARG:HE	1.64	0.63
1:A:3409:ASP:HB3	1:A:3518:PHE:HB2	1.81	0.63
1:B:3618:TYR:HD1	1:B:3618:TYR:N	1.94	0.63
1:A:1991:GLU:O	1:A:1995:VAL:HG23	1.99	0.62
1:A:2151:TRP:HE3	1:A:2193:LEU:HD11	1.64	0.62
1:A:3700:MET:HB3	1:A:4085:THR:HG21	1.81	0.62
1:A:1938:GLY:O	1:A:1989:GLU:HB3	1.98	0.62
1:A:1421:TYR:O	1:A:1425:GLU:N	2.33	0.62
1:B:2276:LEU:HD21	1:B:2415:ILE:HG21	1.81	0.62
1:B:3566:LEU:HD13	1:B:3570:LEU:HD11	1.80	0.62
1:B:3912:GLY:O	1:B:3915:PHE:CZ	2.53	0.62
1:A:1827:ASP:HB3	1:A:1830:VAL:HG12	1.81	0.62
1:A:1826:PHE:HE1	1:A:1853:LEU:HD22	1.62	0.62
1:B:2034:ILE:HD12	1:B:2061:TYR:CZ	2.34	0.62
1:B:3951:SER:HB2	1:B:4002:LYS:HD2	1.82	0.62
1:A:1535:PRO:HB2	1:A:1841:ILE:CG1	2.25	0.62
1:A:1826:PHE:CE1	1:A:1853:LEU:HD22	2.35	0.62
1:B:1984:ILE:HG21	1:B:1989:GLU:HG3	1.80	0.62
1:A:3912:GLY:O	1:A:3915:PHE:CE2	2.53	0.62
1:B:1706:LEU:HD22	1:B:1935:GLN:CG	2.29	0.62
1:A:2394:THR:H	1:A:2397:THR:HB	1.64	0.62
1:A:3303:LYS:HD2	1:A:3306:TRP:CD1	2.33	0.62
1:A:3307:LEU:HA	1:A:3310:THR:HB	1.81	0.62
1:B:2420:PRO:HD3	1:B:2536:ASN:HD21	1.65	0.62
1:A:1421:TYR:CD2	1:A:1425:GLU:HB2	2.33	0.62
1:A:1748:PHE:CD2	1:A:1755:LEU:HD22	2.34	0.62
1:A:1970:LEU:CD1	1:A:1974:LYS:HE3	2.24	0.62
1:A:2386:MET:CB	1:A:2627:ARG:CD	2.77	0.62
1:B:1391:GLY:HA3	1:B:1484:LYS:NZ	2.14	0.62
1:B:3839:ILE:CG2	1:B:3873:MET:HG3	2.29	0.62
1:A:1996:GLU:O	1:A:2000:ARG:HG3	2.00	0.62
1:A:2563:SER:CB	1:A:2566:SER:OG	2.47	0.62
1:B:1938:GLY:O	1:B:1989:GLU:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2111:LYS:HZ2	1:B:2161:GLU:HG2	1.62	0.62
1:B:2472:THR:HG21	1:B:2524:VAL:CG2	2.30	0.62
1:B:2473:LEU:HD11	1:B:2527:GLU:HG3	1.81	0.62
1:B:2563:SER:CB	1:B:2566:SER:OG	2.48	0.62
1:B:3925:SER:HB2	1:B:3972:LEU:HD13	1.82	0.62
1:A:1692:ASP:O	1:A:1695:LYS:HB3	2.00	0.62
1:A:3583:LEU:O	1:A:3587:LEU:HG	2.00	0.62
1:B:1540:LEU:HD12	1:B:1548:ILE:CD1	2.29	0.62
1:B:2728:LEU:O	1:B:2728:LEU:HD12	1.99	0.61
1:B:3330:TYR:CE2	1:B:3346:LEU:HD13	2.34	0.61
1:B:3541:MET:HA	1:B:3544:LYS:HG2	1.82	0.61
1:B:3979:ASN:C	1:B:3981:PRO:HD2	2.20	0.61
1:A:1574:PHE:HB3	1:A:1576:GLU:H	1.65	0.61
1:B:2064:GLN:NE2	1:B:2091:MET:SD	2.73	0.61
1:B:1801:GLY:N	3:B:5096:SO4:O2	2.29	0.61
1:A:1531:ARG:HG2	1:A:1537:PHE:HB3	1.82	0.61
1:B:1493:LEU:HD23	1:B:1498:GLU:CB	2.29	0.61
1:B:1616:LYS:HE3	1:B:1761:GLU:HG3	1.82	0.61
1:B:1744:LEU:HD22	1:B:1760:PHE:CD2	2.36	0.61
1:B:2508:GLN:HG3	1:B:2512:LYS:HD2	1.81	0.61
1:B:3736:LEU:HD11	1:B:3745:ARG:HG3	1.82	0.61
1:A:1983:LEU:HD21	1:A:2000:ARG:CD	2.31	0.61
1:A:1967:HIS:O	1:A:1968:PHE:HD1	1.82	0.61
1:B:1365:PHE:C	1:B:1366:VAL:CG2	2.68	0.61
1:B:1744:LEU:HA	1:B:1760:PHE:HE2	1.61	0.61
1:B:1703:VAL:HG13	1:B:1770:ILE:HD13	1.83	0.61
1:B:2960:THR:HB	1:B:2963:ASP:HB2	1.82	0.61
1:B:2472:THR:CG2	1:B:2524:VAL:CG2	2.77	0.61
1:A:2339:ILE:HG23	1:A:2353:LEU:HB3	1.83	0.61
1:A:2785:LYS:HD3	1:A:3482:GLY:O	2.01	0.61
1:A:3429:LEU:HD21	1:A:3439:ARG:HB3	1.83	0.61
1:A:3541:MET:HA	1:A:3544:LYS:HG2	1.83	0.61
1:A:3530:PHE:CE1	1:A:3618:TYR:CD2	2.88	0.61
1:A:4065:LEU:HD11	1:A:4070:ILE:CD1	2.29	0.61
1:A:2421:GLY:N	3:A:5094:SO4:O1	2.31	0.61
1:B:2495:ASP:O	1:B:2498:GLY:N	2.34	0.61
1:B:2786:ILE:O	1:B:3460:PRO:HB2	1.99	0.61
1:A:1469:LEU:HD13	1:A:1523:LEU:HD21	1.83	0.61
1:A:2427:ILE:HD12	1:A:2559:LEU:CD2	2.31	0.61
1:A:3330:TYR:CE2	1:A:3346:LEU:HD13	2.36	0.61
1:B:2473:LEU:HD22	1:B:2475:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1612:ASP:HA	1:B:1615:ILE:HD11	1.83	0.61
1:B:2386:MET:HB2	1:B:2627:ARG:HD3	1.83	0.61
1:A:1540:LEU:HD12	1:A:1548:ILE:CD1	2.31	0.60
1:A:2293:HIS:CE1	1:A:2409:ASN:CB	2.84	0.60
1:B:1692:ASP:O	1:B:1695:LYS:HB3	2.01	0.60
1:B:1852:ARG:HG3	1:B:1852:ARG:O	2.01	0.60
1:B:3429:LEU:HD21	1:B:3439:ARG:HB3	1.82	0.60
1:B:3612:ASP:O	1:B:3615:VAL:HG22	2.00	0.60
1:A:1527:LEU:HD23	1:A:1545:LEU:HD22	1.83	0.60
1:A:1656:TRP:O	1:A:1660:VAL:HG12	2.01	0.60
1:B:2424:LYS:HA	1:B:2559:LEU:HD12	1.81	0.60
1:B:2445:PHE:HA	1:B:2449:THR:HG21	1.83	0.60
1:B:3700:MET:HB3	1:B:4085:THR:HG21	1.82	0.60
1:A:1462:ASN:CB	1:A:1465:ILE:HG22	2.31	0.60
1:B:1469:LEU:HD13	1:B:1523:LEU:CD2	2.31	0.60
1:B:2838:ALA:HB3	1:B:2878:VAL:HG13	1.83	0.60
1:B:3330:TYR:CE1	1:B:3334:PHE:CD2	2.89	0.60
1:B:3350:LYS:HA	1:B:3353:LEU:HD12	1.84	0.60
1:B:3911:TRP:HH2	1:B:3926:VAL:HG12	1.65	0.60
1:A:1969:GLY:O	1:A:1972:THR:HB	2.01	0.60
1:A:2380:LEU:HD11	1:A:2390:ILE:HD11	1.83	0.60
1:B:2332:GLY:HA2	1:B:2335:GLN:CB	2.27	0.60
1:B:3737:THR:HB	1:B:3740:THR:CB	2.31	0.60
1:A:1409:LEU:HD21	1:A:1435:LEU:HB2	1.79	0.60
1:A:1851:ASN:HD21	1:A:1899:ASN:HB2	1.66	0.60
1:A:2282:ASN:HB3	1:A:2552:ARG:HG3	1.81	0.60
1:A:3817:GLY:H	1:A:3821:ASN:HB2	1.66	0.60
1:B:3702:MET:HB3	1:B:3767:PHE:HZ	1.67	0.60
1:B:1620:PHE:CZ	1:B:1743:ASP:HB3	2.35	0.60
1:B:2125:TRP:CZ2	1:B:2178:LEU:HD13	2.36	0.60
1:B:2637:PRO:O	1:B:2639:GLN:NE2	2.35	0.60
1:B:3459:ASP:OD2	1:B:3461:ILE:HG12	2.01	0.60
1:A:1391:GLY:HA3	1:A:1484:LYS:NZ	2.17	0.60
1:A:1536:ARG:HD2	1:A:1565:MET:O	2.02	0.60
1:A:2081:THR:O	1:A:2085:LYS:HB2	2.02	0.60
1:A:3509:LEU:HD12	1:A:3513:VAL:HG21	1.75	0.60
1:B:1991:GLU:O	1:B:1995:VAL:HG23	2.02	0.60
1:B:3855:LEU:HD12	1:B:3859:VAL:HG23	1.83	0.60
1:B:4065:LEU:HD11	1:B:4070:ILE:HD11	1.84	0.60
1:A:3886:ALA:N	1:A:3887:PRO:HD2	2.17	0.59
1:B:3509:LEU:CD1	1:B:3513:VAL:CG2	2.79	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3948:HIS:NE2	1:A:4072:ASN:CG	2.55	0.59
1:B:3919:LYS:NZ	1:B:4038:GLU:CG	2.65	0.59
1:A:162:LEU:HA	1:A:165:ASP:O	2.02	0.59
1:A:1425:GLU:OE1	1:A:1426:GLN:N	2.36	0.59
1:A:2354:SER:OG	1:A:2357:SER:HB2	2.02	0.59
1:B:3692:LYS:HE3	1:B:3898:GLU:HB3	1.84	0.59
1:A:1534:PHE:HD2	1:A:1537:PHE:CE1	2.21	0.59
1:A:2755:HIS:NE2	1:A:2835:LEU:HG	2.17	0.59
1:A:2941:THR:HG22	1:A:2942:ASP:H	1.67	0.59
1:B:3845:GLN:OE1	1:B:3878:HIS:HB2	2.01	0.59
1:A:1421:TYR:CE2	1:A:1425:GLU:HG3	2.37	0.59
1:A:2677:VAL:HG11	1:A:2686:LEU:HD21	1.83	0.59
1:A:2728:LEU:HD12	1:A:2771:ARG:NH2	2.17	0.59
1:A:3537:GLU:OE1	1:A:3618:TYR:OH	2.21	0.59
1:A:3851:VAL:HG13	1:A:3855:LEU:HD23	1.85	0.59
1:A:3945:LEU:O	1:A:3948:HIS:O	2.21	0.59
1:B:2723:PHE:O	1:B:2727:GLU:HB2	2.02	0.59
1:B:2842:ASP:O	1:B:2845:GLN:HG2	2.02	0.59
1:A:1620:PHE:HA	1:A:1760:PHE:CE1	2.37	0.59
1:A:1900:PRO:HB3	1:A:1905:ARG:HA	1.83	0.59
1:B:1536:ARG:HD2	1:B:1565:MET:O	2.02	0.59
1:A:1394:LEU:CD2	1:A:1449:GLN:HE22	2.14	0.59
1:A:1630:ILE:CG2	1:A:1655:MET:SD	2.89	0.59
1:A:2784:PRO:HG2	1:A:2817:ILE:HD13	1.84	0.59
1:A:2787:HIS:CA	1:A:3460:PRO:HG2	2.32	0.59
1:A:2034:ILE:HD12	1:A:2061:TYR:CZ	2.38	0.59
1:A:2489:ILE:HG22	1:A:2535:CYS:HB3	1.84	0.59
1:A:3810:SER:O	1:A:3838:TRP:HB2	2.03	0.59
1:B:1911:ASN:OD1	1:B:1912:LEU:N	2.36	0.59
1:A:1536:ARG:HD3	1:A:1841:ILE:HD13	1.85	0.59
1:B:1998:LEU:HD11	1:B:2022:PHE:HZ	1.67	0.59
1:B:2290:LEU:HD23	1:B:2321:SER:HA	1.83	0.59
1:B:2707:VAL:HG12	1:B:2712:LEU:CD1	2.33	0.59
1:A:2549:ARG:HE	2:A:5093:ATP:PG	2.25	0.58
1:A:3737:THR:HB	1:A:3740:THR:CB	2.33	0.58
1:A:4033:LEU:HD12	1:A:4035:GLN:N	2.18	0.58
1:B:1910:GLU:HB2	1:B:3846:MET:CB	2.33	0.58
1:B:2293:HIS:CE1	1:B:2409:ASN:CB	2.86	0.58
1:B:2780:LYS:HD3	1:B:2813:THR:HG22	1.85	0.58
1:B:2761:ALA:O	1:B:2892:CYS:HB3	2.02	0.58
1:A:2332:GLY:HA2	1:A:2335:GLN:CB	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1900:PRO:HB3	1:B:1905:ARG:HA	1.85	0.58
1:B:3566:LEU:CA	1:B:3583:LEU:HD21	2.30	0.58
1:B:3583:LEU:O	1:B:3587:LEU:HG	2.04	0.58
1:B:3618:TYR:O	1:B:3622:GLY:N	2.33	0.58
1:B:3919:LYS:HZ3	1:B:4038:GLU:CG	2.16	0.58
1:A:1984:ILE:HG21	1:A:1989:GLU:HG3	1.84	0.58
1:A:2640:THR:HG23	1:A:2643:SER:H	1.67	0.58
1:B:3978:ASN:O	1:B:3981:PRO:CD	2.51	0.58
1:A:2446:SER:H	1:A:2449:THR:HG21	1.67	0.58
1:A:2745:ILE:HG12	1:A:2756:MET:HE3	1.85	0.58
1:B:1744:LEU:HD22	1:B:1760:PHE:CG	2.39	0.58
1:B:3525:ILE:HD11	1:B:3646:ILE:CG2	2.16	0.58
1:A:2155:ASP:OD1	1:A:2549:ARG:NH2	2.35	0.58
1:A:3592:LYS:O	1:A:3596:ASN:HB2	2.03	0.58
1:B:1394:LEU:HD22	1:B:1449:GLN:NE2	2.18	0.58
1:B:1849:GLU:OE2	1:B:1899:ASN:ND2	2.36	0.58
1:B:3330:TYR:CD1	1:B:3334:PHE:CD2	2.92	0.58
1:B:3631:MET:HE1	1:B:3698:MET:HG3	1.84	0.58
1:B:1620:PHE:CA	1:B:1760:PHE:CE1	2.86	0.58
1:B:3537:GLU:OE1	1:B:3618:TYR:OH	2.20	0.58
1:A:1779:PHE:O	1:A:1783:THR:HG22	2.03	0.58
1:B:2472:THR:CB	1:B:2524:VAL:HG22	2.34	0.58
1:B:3912:GLY:O	1:B:3915:PHE:CE2	2.57	0.58
1:B:4084:SER:O	1:B:4088:LEU:HG	2.03	0.58
1:B:1967:HIS:O	1:B:1968:PHE:HD1	1.86	0.58
1:B:162:LEU:HA	1:B:165:ASP:O	2.04	0.58
1:B:3330:TYR:OH	1:B:3346:LEU:HD13	2.04	0.58
1:B:3440:LEU:CD2	1:B:3462:ILE:HD12	2.33	0.58
1:B:3612:ASP:O	1:B:3615:VAL:CG2	2.52	0.58
1:B:3683:TYR:O	1:B:3687:SER:HB2	2.04	0.58
1:B:1726:LEU:CD1	1:B:3984:GLN:CB	2.79	0.58
1:A:1704:GLU:OE2	1:A:1768:ARG:NH1	2.37	0.57
1:A:2846:GLY:O	1:A:2849:TYR:HB3	2.04	0.57
1:B:1750:SER:HB2	1:B:1755:LEU:CD2	2.34	0.57
1:B:2127:ASP:O	1:B:2131:THR:OG1	2.22	0.57
1:B:2627:ARG:NH1	1:B:2630:TYR:HE2	1.98	0.57
1:A:1781:THR:HG21	1:A:1919:PHE:CD1	2.39	0.57
1:A:2201:HIS:NE2	1:A:2497:TYR:O	2.37	0.57
1:A:3839:ILE:HG23	1:A:3873:MET:HG3	1.86	0.57
1:A:3912:GLY:O	1:A:3915:PHE:CZ	2.57	0.57
1:B:1826:PHE:CE1	1:B:1853:LEU:HD22	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1981:SER:HB3	1:B:1982:PRO:HD3	1.87	0.57
1:B:2111:LYS:HZ3	1:B:2161:GLU:HG2	1.68	0.57
1:B:2891:ILE:HD11	1:B:2903:ILE:HD11	1.84	0.57
1:A:2257:PHE:HD1	1:A:2262:LEU:HD11	1.69	0.57
1:A:2437:LEU:H	1:A:2437:LEU:HD12	1.69	0.57
1:A:2808:LEU:HD21	1:A:2856:LEU:HD12	1.86	0.57
1:A:3303:LYS:C	1:A:3306:TRP:CD1	2.74	0.57
1:B:1940:GLU:HG3	1:B:1941:ASP:H	1.69	0.57
1:B:2131:THR:HG22	1:B:2176:LEU:CD2	2.30	0.57
1:B:2627:ARG:HH11	1:B:2631:THR:HG23	1.64	0.57
1:A:1493:LEU:O	1:A:1494:ASP:HB2	2.04	0.57
1:A:2137:VAL:O	1:A:2141:ILE:CG2	2.50	0.57
1:A:2476:LYS:CD	1:A:2476:LYS:N	2.52	0.57
1:A:3519:VAL:HG13	1:A:3521:ASN:ND2	2.19	0.57
1:A:3555:TYR:HE1	1:A:3593:GLU:HG2	1.68	0.57
1:B:1683:LEU:HB3	1:B:1702:LEU:HD21	1.85	0.57
1:B:2302:PHE:HA	1:B:2310:LEU:HD11	1.85	0.57
1:A:1394:LEU:HD22	1:A:1449:GLN:NE2	2.19	0.57
1:A:2111:LYS:CD	1:A:2161:GLU:HG3	2.13	0.57
1:A:1965:HIS:HD2	1:A:2212:LEU:CD2	2.18	0.57
1:B:1849:GLU:CG	1:B:1899:ASN:HD22	2.18	0.57
1:A:1559:SER:HB3	1:A:1572:ILE:HG22	1.86	0.57
1:A:2380:LEU:HD13	1:A:2390:ILE:CD1	2.23	0.57
1:A:2563:SER:CB	1:A:2566:SER:H	2.15	0.57
1:A:3303:LYS:HA	1:A:3306:TRP:HE1	1.67	0.57
1:A:3618:TYR:O	1:A:3622:GLY:N	2.34	0.57
1:A:4024:VAL:HG11	1:A:4062:TRP:CD2	2.38	0.57
1:B:1620:PHE:CB	1:B:1760:PHE:CE1	2.88	0.57
1:B:3995:GLY:HA2	1:B:3998:ILE:HD13	1.86	0.57
1:A:2419:PRO:O	1:A:2424:LYS:CE	2.52	0.57
1:A:4021:LEU:HD23	1:A:4023:ILE:HG13	1.85	0.57
1:A:2048:SER:H	2:A:5093:ATP:HN62	1.52	0.57
1:B:2382:ALA:O	1:B:2385:VAL:HG12	2.04	0.57
1:B:2472:THR:HG22	1:B:2524:VAL:HG13	1.86	0.57
1:B:2473:LEU:HG	1:B:2525:THR:O	2.05	0.57
1:B:3784:ASN:ND2	1:B:3865:ALA:O	2.37	0.57
1:B:3785:TYR:HE2	1:B:3859:VAL:HG22	1.69	0.57
1:A:1469:LEU:HB3	1:A:1472:GLU:HB2	1.87	0.57
1:A:1706:LEU:HD21	1:A:1935:GLN:HG2	1.86	0.57
1:A:1940:GLU:HG3	1:A:1941:ASP:N	2.18	0.57
1:A:2071:ILE:HB	1:A:2212:LEU:HD12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3538:ASN:HB3	1:A:3541:MET:HG2	1.87	0.57
1:A:3566:LEU:HD13	1:A:3570:LEU:HD11	1.86	0.57
1:B:2293:HIS:NE2	1:B:2409:ASN:HB3	2.19	0.57
1:A:1911:ASN:OD1	1:A:1912:LEU:N	2.38	0.56
1:A:2127:ASP:O	1:A:2131:THR:OG1	2.23	0.56
1:A:4017:GLY:HA3	1:A:4021:LEU:HD12	1.87	0.56
1:B:2106:THR:HG1	1:B:2154:PHE:HB3	1.68	0.56
1:A:2241:LEU:HD13	1:A:2299:ARG:HH11	1.68	0.56
1:A:3833:LYS:HZ3	1:A:3862:THR:HG21	1.70	0.56
1:A:3939:ILE:HG13	1:A:4010:LEU:HD22	1.86	0.56
1:B:2063:MET:HB3	1:B:2070:LEU:HD11	1.86	0.56
1:B:2755:HIS:NE2	1:B:2835:LEU:HG	2.20	0.56
1:B:3409:ASP:HB3	1:B:3518:PHE:HB2	1.87	0.56
1:A:1620:PHE:CZ	1:A:1743:ASP:HB3	2.40	0.56
1:A:1995:VAL:HG22	1:A:2022:PHE:CD2	2.40	0.56
1:A:3631:MET:CE	1:A:3698:MET:HG3	2.36	0.56
1:B:1531:ARG:HG2	1:B:1537:PHE:CB	2.36	0.56
1:A:2938:MET:SD	1:A:3321:ILE:HG21	2.45	0.56
1:A:4022:GLN:HG2	1:A:4022:GLN:O	2.05	0.56
1:A:1939:PHE:O	1:A:1940:GLU:HB3	2.05	0.56
1:B:1748:PHE:HD2	1:B:1755:LEU:HD22	1.69	0.56
1:B:2512:LYS:O	1:B:2513:GLN:CB	2.52	0.56
1:A:1726:LEU:CD1	1:A:3984:GLN:HB3	2.30	0.56
1:B:1462:ASN:HB2	1:B:1465:ILE:HG22	1.88	0.56
1:B:1493:LEU:HD23	1:B:1498:GLU:HB3	1.86	0.56
1:B:3017:VAL:HG21	1:B:3313:PHE:CE2	2.41	0.56
1:A:2627:ARG:NH1	1:A:2630:TYR:CE2	2.74	0.56
1:B:1493:LEU:O	1:B:1494:ASP:HB2	2.06	0.56
1:B:2380:LEU:HD12	1:B:2577:ALA:CB	2.31	0.56
1:A:3509:LEU:HD12	1:A:3513:VAL:HG23	1.88	0.56
1:B:1392:LEU:HD13	1:B:1393:LYS:C	2.26	0.56
1:B:1995:VAL:HG22	1:B:2022:PHE:CE2	2.41	0.56
1:A:1619:VAL:HG12	1:A:1760:PHE:HD1	1.70	0.56
1:A:2305:LEU:HD11	1:A:2368:PHE:CD1	2.41	0.56
1:A:2868:ASP:HB2	1:A:2872:GLU:OE1	2.06	0.56
1:B:3785:TYR:CE2	1:B:3859:VAL:HG22	2.41	0.56
1:B:1998:LEU:CD1	1:B:2022:PHE:HZ	2.18	0.56
1:A:1497:ILE:O	1:A:1500:ILE:HG12	2.05	0.55
1:A:2514:GLY:C	1:A:2523:TRP:CH2	2.80	0.55
1:B:3919:LYS:NZ	1:B:4038:GLU:HG3	2.21	0.55
1:B:2489:ILE:HD11	1:B:2506:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3737:THR:CB	1:B:3740:THR:HB	2.37	0.55
1:A:1983:LEU:HB3	1:A:1993:THR:CG2	2.36	0.55
1:A:2111:LYS:HZ2	1:A:2161:GLU:HG2	1.67	0.55
1:A:2220:CYS:SG	1:A:2224:SER:CB	2.94	0.55
1:B:1646:GLN:NE2	1:B:1758:TYR:OH	2.40	0.55
1:B:3911:TRP:HH2	1:B:3926:VAL:CG1	2.19	0.55
1:A:2386:MET:HB3	1:A:2627:ARG:CD	2.36	0.55
1:A:3683:TYR:O	1:A:3687:SER:HB2	2.07	0.55
1:A:2002:ILE:HB	1:A:2014:PHE:CE2	2.42	0.55
1:B:2336:ARG:HA	1:B:2339:ILE:HD12	1.88	0.55
1:B:2362:ALA:HB3	1:B:2365:LYS:O	2.07	0.55
1:B:3645:SER:CB	1:B:3890:GLN:NE2	2.69	0.55
1:A:1425:GLU:OE1	1:A:1429:LEU:HD12	2.06	0.55
1:A:1527:LEU:HD21	1:A:1546:LEU:CD2	2.36	0.55
1:A:4037:SER:HB3	1:A:4040:GLU:HB3	1.87	0.55
1:B:1563:LYS:HE2	1:B:1585:VAL:HG12	1.87	0.55
1:B:2109:LEU:CD1	1:B:2129:LEU:HD23	2.36	0.55
1:B:2155:ASP:OD1	1:B:2549:ARG:NH2	2.40	0.55
1:B:3845:GLN:NE2	1:B:3882:ASP:O	2.39	0.55
1:B:3787:THR:HG22	1:B:3875:MET:HB2	1.88	0.55
1:A:1365:PHE:C	1:A:1366:VAL:HG23	2.27	0.55
1:A:2410:SER:O	1:A:2411:LYS:HB2	2.06	0.55
1:A:2763:ARG:N	3:A:5095:SO4:O1	2.38	0.55
1:A:2151:TRP:CE3	1:A:2193:LEU:HD11	2.41	0.55
1:A:2788:ARG:HG3	1:A:3459:ASP:HA	1.89	0.55
1:B:115:GLU:CB	1:B:1372:ASN:OD1	2.55	0.55
1:A:1531:ARG:HD3	1:A:1537:PHE:O	2.07	0.55
1:A:1535:PRO:O	1:A:1841:ILE:CD1	2.55	0.55
1:A:1502:ILE:HG23	1:A:1503:PRO:HD2	1.89	0.55
1:A:2064:GLN:CD	1:A:2091:MET:CE	2.75	0.55
1:A:3440:LEU:HD23	1:A:3462:ILE:HD12	1.88	0.55
1:A:4023:ILE:HD12	1:A:4029:ILE:HD11	1.87	0.55
1:A:2078:CYS:N	2:A:5093:ATP:O2B	2.31	0.55
1:B:1421:TYR:O	1:B:1425:GLU:N	2.40	0.55
1:B:2447:LYS:HE3	1:B:2493:LYS:HD3	1.89	0.55
1:B:4024:VAL:HG11	1:B:4062:TRP:CD2	2.42	0.55
1:A:1627:LEU:HD11	1:A:1631:LYS:HE3	1.89	0.54
1:A:2786:ILE:O	1:A:3460:PRO:HB2	2.07	0.54
1:A:2002:ILE:HG22	1:A:2006:LEU:HD11	1.88	0.54
1:A:2131:THR:HG22	1:A:2176:LEU:CD2	2.34	0.54
1:A:2336:ARG:CD	1:A:2355:ASP:OD2	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2400:HIS:NE2	1:A:2559:LEU:CD1	2.67	0.54
1:B:2476:LYS:N	1:B:2476:LYS:CD	2.63	0.54
1:A:1823:ASP:HB2	1:A:1853:LEU:HD23	1.88	0.54
1:A:1940:GLU:CB	1:A:1989:GLU:O	2.51	0.54
1:A:2707:VAL:HG12	1:A:2712:LEU:CD1	2.37	0.54
1:B:1911:ASN:OD1	1:B:1912:LEU:HG	2.08	0.54
1:B:1956:LEU:CB	1:B:1968:PHE:CE2	2.88	0.54
1:B:3737:THR:CB	1:B:3740:THR:CB	2.85	0.54
1:B:3946:VAL:HA	1:B:3947:PRO:C	2.27	0.54
1:A:1604:ALA:HA	1:A:1607:TRP:HE1	1.72	0.54
1:A:1535:PRO:O	1:A:1841:ILE:HD11	2.08	0.54
1:A:2112:GLU:CB	1:A:2117:SER:HB2	2.35	0.54
1:A:2201:HIS:CE1	1:A:2497:TYR:CA	2.91	0.54
1:A:3566:LEU:CA	1:A:3583:LEU:HD21	2.37	0.54
1:B:1462:ASN:CB	1:B:1465:ILE:HG22	2.37	0.54
1:B:3924:TRP:O	1:B:3927:TYR:HB3	2.08	0.54
1:A:1392:LEU:HD13	1:A:1393:LYS:C	2.27	0.54
1:A:2063:MET:HB3	1:A:2070:LEU:HD11	1.90	0.54
1:B:1421:TYR:CD2	1:B:1425:GLU:HB2	2.42	0.54
1:B:1394:LEU:CD2	1:B:1449:GLN:HE22	2.20	0.54
1:A:1852:ARG:HG3	1:A:1852:ARG:O	2.06	0.54
1:B:1983:LEU:HD21	1:B:2000:ARG:HE	1.66	0.54
1:B:2761:ALA:O	1:B:2892:CYS:CB	2.55	0.54
1:B:2936:ILE:HG22	1:B:2962:ARG:HD3	1.89	0.54
1:B:3737:THR:OG1	1:B:3740:THR:CB	2.55	0.54
1:A:2115:TYR:OH	1:A:2162:TYR:O	2.23	0.54
1:A:2181:GLY:C	1:A:2182:GLU:HG3	2.27	0.54
1:A:2786:ILE:HG12	1:A:2821:ASN:HA	1.90	0.54
1:A:3877:CYS:SG	1:A:3884:LEU:CD2	2.96	0.54
1:B:3645:SER:CB	1:B:3890:GLN:HE21	2.18	0.54
1:A:1386:ILE:CG2	1:A:1396:ARG:HD3	2.37	0.54
1:A:3645:SER:CB	1:A:3890:GLN:HE21	2.19	0.54
1:B:2274:HIS:CE1	1:B:2326:LEU:O	2.50	0.54
1:B:2960:THR:HG22	1:B:2961:ILE:N	2.23	0.54
1:B:3330:TYR:CE1	1:B:3334:PHE:CE2	2.96	0.54
1:A:2448:ASP:CB	1:A:2829:GLU:OE2	2.47	0.54
1:B:1527:LEU:HD21	1:B:1546:LEU:HD21	1.88	0.54
1:B:2151:TRP:HE3	1:B:2193:LEU:HD11	1.73	0.54
1:B:2728:LEU:HG	1:B:2771:ARG:HH22	1.72	0.54
1:B:3323:ASN:HD21	1:B:3361:ASP:H	1.56	0.54
1:B:3656:VAL:CG1	1:B:3677:LEU:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3810:SER:O	1:B:3838:TRP:HB2	2.07	0.54
1:A:1645:PHE:CZ	1:A:1649:LEU:HD22	2.43	0.53
1:A:2064:GLN:OE1	1:A:2151:TRP:CH2	2.55	0.53
1:A:2707:VAL:HG12	1:A:2712:LEU:HD12	1.89	0.53
1:A:4059:LEU:HA	1:A:4063:LEU:HD13	1.89	0.53
1:B:1823:ASP:HB2	1:B:1853:LEU:HD23	1.90	0.53
1:B:2220:CYS:SG	1:B:2224:SER:CB	2.96	0.53
1:A:3307:LEU:O	1:A:3311:LYS:N	2.27	0.53
1:A:3440:LEU:CD2	1:A:3462:ILE:HD12	2.38	0.53
1:B:1759:LYS:HE3	1:B:1761:GLU:OE2	2.08	0.53
1:B:2074:GLY:O	1:B:2197:ASP:HA	2.09	0.53
1:B:2835:LEU:HD23	1:B:2911:ARG:HB2	1.91	0.53
1:B:3854:TYR:O	1:B:3858:HIS:HB2	2.08	0.53
1:A:2106:THR:HG1	1:A:2154:PHE:HB3	1.72	0.53
1:A:3703:PHE:CE1	1:A:3766:GLU:HG2	2.43	0.53
1:B:1953:LEU:HD11	1:B:1973:LEU:HB3	1.91	0.53
1:B:3509:LEU:HD11	1:B:3513:VAL:HG21	1.90	0.53
1:A:2141:ILE:HG22	1:A:2145:PHE:HB2	1.90	0.53
1:A:2305:LEU:CD1	1:A:2368:PHE:CD1	2.91	0.53
1:B:2741:HIS:HA	1:B:2744:ARG:HD2	1.89	0.53
1:B:1744:LEU:CD2	1:B:1760:PHE:CD2	2.92	0.53
1:A:3612:ASP:O	1:A:3615:VAL:HG22	2.08	0.53
1:B:2002:ILE:HB	1:B:2014:PHE:CE2	2.43	0.53
1:B:2181:GLY:O	1:B:2182:GLU:CG	2.57	0.53
1:B:3767:PHE:HB3	1:B:3769:VAL:HG23	1.90	0.53
1:A:1534:PHE:CE2	1:A:1536:ARG:HB2	2.43	0.53
1:A:2336:ARG:HG2	1:A:2355:ASP:OD1	2.08	0.53
1:A:2419:PRO:O	1:A:2424:LYS:NZ	2.42	0.53
1:A:3017:VAL:HG21	1:A:3313:PHE:CE2	2.44	0.53
1:B:2201:HIS:CE1	1:B:2497:TYR:HA	2.44	0.53
1:A:1409:LEU:CD2	1:A:1435:LEU:HB2	2.39	0.53
1:A:1970:LEU:C	1:A:1970:LEU:HD12	2.28	0.53
1:A:3817:GLY:H	1:A:3821:ASN:CB	2.21	0.53
1:B:1914:LYS:HD3	1:B:3959:CYS:SG	2.48	0.53
1:B:3330:TYR:CZ	1:B:3346:LEU:HD13	2.44	0.53
1:A:2488:GLU:CD	1:A:2491:LEU:HD11	2.29	0.53
1:A:2177:THR:HG22	1:A:2183:ARG:HG2	1.91	0.53
1:A:2795:PHE:CE2	1:A:2799:LEU:HD11	2.44	0.53
1:A:2048:SER:H	2:A:5093:ATP:N6	2.06	0.53
1:A:1979:ASN:O	1:A:1983:LEU:HD13	2.09	0.52
1:A:2339:ILE:HG12	1:A:2353:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2450:THR:H	1:A:2453:HIS:CE1	2.27	0.52
1:A:2788:ARG:HB2	1:A:3459:ASP:HB3	1.90	0.52
1:B:1995:VAL:HG22	1:B:2022:PHE:CD2	2.44	0.52
1:B:3308:ASN:O	1:B:3312:GLN:HB2	2.09	0.52
1:B:2201:HIS:NE2	1:B:2497:TYR:O	2.42	0.52
1:B:2476:LYS:H	1:B:2476:LYS:HD3	1.72	0.52
1:B:3772:TRP:HZ3	1:B:3780:ASN:HD22	1.56	0.52
1:A:1822:CYS:SG	1:A:1849:GLU:C	2.88	0.52
1:A:2787:HIS:HB3	1:A:3461:ILE:HG23	1.91	0.52
1:A:1981:SER:HB3	1:A:1982:PRO:HD3	1.91	0.52
1:A:2173:ASN:HB3	1:A:2175:ILE:HG22	1.90	0.52
1:A:2230:LEU:HD23	1:A:2288:VAL:HG13	1.90	0.52
1:A:2290:LEU:HD23	1:A:2321:SER:HA	1.92	0.52
1:A:3692:LYS:HE3	1:A:3898:GLU:HB3	1.91	0.52
1:A:3877:CYS:SG	1:A:3884:LEU:HD22	2.50	0.52
1:A:4021:LEU:HD23	1:A:4023:ILE:CG1	2.39	0.52
1:B:1822:CYS:HB2	1:B:1853:LEU:CD2	2.29	0.52
1:B:1939:PHE:HD1	1:B:1939:PHE:H	1.56	0.52
1:B:2493:LYS:HG3	1:B:2494:LEU:N	2.19	0.52
1:B:2860:THR:HG22	1:B:2865:LEU:O	2.09	0.52
1:A:1486:ILE:HG12	1:A:1508:THR:HG21	1.91	0.52
1:A:2285:GLU:CB	1:A:2412:ARG:NH2	2.73	0.52
1:B:2173:ASN:HB3	1:B:2175:ILE:HG22	1.91	0.52
1:B:2571:TYR:HA	1:B:2574:TYR:HB2	1.91	0.52
1:B:3461:ILE:C	1:B:3463:SER:H	2.12	0.52
1:B:3519:VAL:HG13	1:B:3521:ASN:ND2	2.24	0.52
1:A:2095:ASP:CG	1:A:2149:ARG:HH22	2.11	0.52
1:A:2462:THR:HG22	1:A:2476:LYS:HA	1.90	0.52
1:A:1926:SER:HA	1:A:1929:ILE:HD13	1.92	0.52
1:A:2012:LEU:HD13	1:A:2016:ASP:OD2	2.10	0.52
1:A:3547:ASP:HA	1:A:3550:LYS:HB3	1.90	0.52
1:A:3911:TRP:HH2	1:A:3926:VAL:CG1	2.23	0.52
1:A:3951:SER:HB2	1:A:4002:LYS:HD2	1.91	0.52
1:A:4034:LEU:O	1:A:4034:LEU:HD23	2.10	0.52
1:B:1365:PHE:C	1:B:1366:VAL:HG23	2.30	0.52
1:B:1392:LEU:C	1:B:1392:LEU:CD1	2.77	0.52
1:B:2109:LEU:HD13	1:B:2129:LEU:HD23	1.92	0.52
1:B:2220:CYS:SG	1:B:2224:SER:HB2	2.50	0.52
1:B:3641:PHE:HA	1:B:3889:LEU:HD21	1.91	0.52
1:A:1536:ARG:HB3	1:A:1565:MET:HB2	1.90	0.52
1:A:1620:PHE:HA	1:A:1760:PHE:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2833:THR:HG21	1:A:2841:PRO:HD2	1.91	0.52
1:A:3656:VAL:CG1	1:A:3677:LEU:HB3	2.36	0.52
1:A:3995:GLY:HA2	1:A:3998:ILE:HD13	1.91	0.52
1:B:1394:LEU:HD22	1:B:1449:GLN:HE22	1.74	0.52
1:A:2494:LEU:O	1:A:2494:LEU:HD12	2.10	0.52
1:A:3854:TYR:O	1:A:3858:HIS:HB2	2.10	0.52
1:B:1604:ALA:HA	1:B:1607:TRP:HE1	1.72	0.52
1:B:2631:THR:O	1:B:2635:THR:HG22	2.10	0.52
1:A:1650:LEU:HD11	1:A:1747:VAL:HG11	1.92	0.52
1:A:2578:ILE:HG21	1:A:2630:TYR:HB2	1.91	0.52
1:B:1681:LYS:HE2	1:B:1939:PHE:CZ	2.44	0.52
1:B:2064:GLN:NE2	1:B:2091:MET:HE1	2.24	0.52
1:B:3460:PRO:O	1:B:3463:SER:CB	2.58	0.52
1:B:2620:ARG:NH2	3:B:5095:SO4:O3	2.43	0.52
1:A:1514:ASP:O	1:A:1518:MET:HG3	2.10	0.51
1:A:1677:ASP:HA	1:A:1680:ILE:HD12	1.93	0.51
1:A:1707:HIS:O	1:A:1711:VAL:HG23	2.10	0.51
1:A:1963:MET:HB3	1:A:1966:TYR:CD2	2.45	0.51
1:A:2645:ILE:CD1	1:A:2686:LEU:HG	2.40	0.51
1:B:1983:LEU:HD11	1:B:2000:ARG:CD	2.39	0.51
1:B:2786:ILE:HG12	1:B:2821:ASN:HA	1.92	0.51
1:A:1645:PHE:HZ	1:A:1768:ARG:HD2	1.75	0.51
1:B:1781:THR:HG21	1:B:1919:PHE:CE1	2.45	0.51
1:B:3978:ASN:O	1:B:3981:PRO:HD3	2.10	0.51
1:B:1469:LEU:HB3	1:B:1472:GLU:HB2	1.91	0.51
1:B:1707:HIS:O	1:B:1711:VAL:HG23	2.10	0.51
1:B:1940:GLU:CB	1:B:1989:GLU:O	2.51	0.51
1:A:2780:LYS:HD3	1:A:2813:THR:HG22	1.93	0.51
1:A:3737:THR:CB	1:A:3740:THR:CB	2.89	0.51
1:A:3737:THR:OG1	1:A:3740:THR:CB	2.59	0.51
1:B:1493:LEU:CD2	1:B:1498:GLU:HB3	2.41	0.51
1:B:2061:TYR:O	1:B:2064:GLN:HG2	2.10	0.51
1:B:2312:ASP:HB3	1:B:2351:GLN:HG3	1.91	0.51
1:B:2266:PHE:HD1	1:B:2326:LEU:HD21	1.76	0.51
1:A:1939:PHE:HD1	1:A:1939:PHE:H	1.57	0.51
1:A:2302:PHE:HA	1:A:2310:LEU:HD11	1.92	0.51
1:A:65:THR:O	1:A:66:GLN:CB	2.59	0.51
1:B:2795:PHE:CE2	1:B:2799:LEU:HD11	2.46	0.51
1:A:1749:ILE:HD13	1:A:1813:LEU:HD22	1.92	0.51
1:A:3645:SER:CB	1:A:3890:GLN:NE2	2.74	0.51
1:A:3839:ILE:CG2	1:A:3873:MET:HG3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3787:THR:HG22	1:A:3875:MET:HB2	1.93	0.51
1:A:3934:TRP:CB	1:A:4023:ILE:HD13	2.41	0.51
1:A:3946:VAL:HB	1:A:3947:PRO:HA	1.91	0.51
1:B:2034:ILE:CD1	1:B:2061:TYR:CE2	2.94	0.51
1:B:2787:HIS:CA	1:B:3460:PRO:HG2	2.37	0.51
1:A:1917:ARG:HD2	1:A:3963:PHE:CE2	2.46	0.51
1:A:2427:ILE:HD12	1:A:2559:LEU:HD22	1.92	0.51
1:B:1606:GLU:O	1:B:1610:ILE:HG12	2.11	0.51
1:B:3509:LEU:O	1:B:3513:VAL:HG23	2.11	0.51
1:A:4065:LEU:O	1:A:4065:LEU:HD12	2.10	0.51
1:B:2464:TYR:HE1	1:B:2524:VAL:HG11	1.75	0.51
1:B:2708:ASN:O	1:B:2712:LEU:HD13	2.10	0.51
1:B:4022:GLN:HG2	1:B:4022:GLN:O	2.11	0.51
1:A:2084:TRP:HE3	1:A:2088:ILE:HD12	1.76	0.51
1:A:2637:PRO:O	1:A:2639:GLN:NE2	2.44	0.51
1:B:2448:ASP:HB2	1:B:2829:GLU:CD	2.31	0.51
1:B:4024:VAL:HG23	1:B:4027:VAL:H	1.75	0.51
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.91	0.51
1:A:1803:THR:HG21	1:A:1848:ASP:OD1	2.10	0.51
1:A:2102:TYR:HB2	1:A:2152:VAL:HG22	1.93	0.51
1:B:2494:LEU:HD12	1:B:2494:LEU:O	2.11	0.51
1:B:2107:LYS:CE	1:B:2499:SER:HB3	2.40	0.51
1:B:2512:LYS:HB3	1:B:2523:TRP:CH2	2.40	0.51
1:A:1706:LEU:HD22	1:A:1935:GLN:HG2	1.93	0.50
1:A:3566:LEU:HD11	1:A:3570:LEU:HD11	1.92	0.50
1:B:1635:ASP:HB2	1:B:1638:VAL:HG23	1.93	0.50
1:A:1606:GLU:O	1:A:1610:ILE:HG12	2.11	0.50
1:A:3845:GLN:OE1	1:A:3878:HIS:HB2	2.11	0.50
1:B:2640:THR:HG23	1:B:2643:SER:H	1.76	0.50
1:B:3307:LEU:HA	1:B:3310:THR:HB	1.92	0.50
1:A:2422:SER:H	1:A:2424:LYS:HZ1	1.59	0.50
1:B:1612:ASP:HA	1:B:1615:ILE:HG12	1.94	0.50
1:B:1803:THR:HG21	1:B:1848:ASP:OD1	2.11	0.50
1:B:2201:HIS:CE1	1:B:2497:TYR:HB3	2.47	0.50
1:B:3547:ASP:HA	1:B:3550:LYS:HB3	1.92	0.50
1:A:3725:VAL:HG22	1:A:3731:ASP:HA	1.93	0.50
1:B:1502:ILE:HG23	1:B:1503:PRO:HD2	1.93	0.50
1:B:1575:LEU:O	1:B:1576:GLU:HB3	2.11	0.50
1:B:2627:ARG:HH12	1:B:2631:THR:HG22	1.73	0.50
1:A:2034:ILE:CD1	1:A:2061:TYR:CZ	2.95	0.50
1:A:2982:VAL:HG12	1:A:2983:GLY:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1822:CYS:SG	1:B:1849:GLU:C	2.90	0.50
1:B:2034:ILE:HD12	1:B:2061:TYR:CE2	2.46	0.50
1:B:2488:GLU:CD	1:B:2491:LEU:HD11	2.32	0.50
1:B:2784:PRO:HG2	1:B:2817:ILE:HD13	1.93	0.50
1:B:2785:LYS:HE2	1:B:3480:GLU:OE1	2.11	0.50
1:A:3911:TRP:HH2	1:A:3926:VAL:HG12	1.77	0.50
1:B:1826:PHE:HE1	1:B:1853:LEU:HD22	1.76	0.50
1:B:2336:ARG:CD	1:B:2355:ASP:OD2	2.59	0.50
1:B:2354:SER:H	1:B:2357:SER:HB2	1.76	0.50
1:B:2749:LEU:HD12	1:B:2773:VAL:HG12	1.94	0.50
1:B:3671:VAL:O	1:B:3674:ILE:HG22	2.11	0.50
1:A:1531:ARG:CD	1:A:1538:TYR:HA	2.42	0.50
1:A:1849:GLU:CG	1:A:1899:ASN:ND2	2.70	0.50
1:A:2034:ILE:CD1	1:A:2061:TYR:CE2	2.95	0.50
1:A:2111:LYS:CD	1:A:2161:GLU:CG	2.84	0.50
1:A:2645:ILE:HD11	1:A:2686:LEU:HG	1.94	0.50
1:B:2707:VAL:HG12	1:B:2712:LEU:HD12	1.91	0.50
1:B:2788:ARG:HG3	1:B:3459:ASP:HA	1.93	0.50
1:A:2476:LYS:N	1:A:2476:LYS:HD3	2.09	0.50
1:A:3323:ASN:HD21	1:A:3361:ASP:H	1.58	0.50
1:B:3440:LEU:HD23	1:B:3462:ILE:HD12	1.93	0.50
1:A:1535:PRO:C	1:A:1841:ILE:CD1	2.75	0.50
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.93	0.50
1:A:2762:SER:O	1:A:2763:ARG:HB2	2.12	0.50
1:B:2262:LEU:HA	1:B:2265:ILE:HD12	1.94	0.50
1:B:2290:LEU:HD13	1:B:2407:LEU:HD23	1.93	0.50
1:A:3692:LYS:HE3	1:A:3898:GLU:O	2.12	0.49
1:B:1387:GLU:HA	1:B:1393:LYS:HA	1.94	0.49
1:B:4020:ASN:HB3	1:B:4028:ARG:HH11	1.77	0.49
1:A:1983:LEU:HD21	1:A:2000:ARG:NE	2.27	0.49
1:A:2002:ILE:HB	1:A:2014:PHE:HE2	1.78	0.49
1:A:2385:VAL:HG23	1:A:2574:TYR:HD1	1.77	0.49
1:A:2654:ARG:HH22	1:A:2691:SER:HB2	1.77	0.49
1:A:1392:LEU:CD1	1:A:1392:LEU:C	2.78	0.49
1:A:3979:ASN:C	1:A:3981:PRO:CD	2.80	0.49
1:B:3566:LEU:HD13	1:B:3570:LEU:HD12	1.94	0.49
1:A:1657:THR:HG21	1:A:1734:PHE:O	2.12	0.49
1:A:2295:ILE:HG12	1:A:2314:ILE:HD12	1.93	0.49
1:A:3353:LEU:HD23	1:A:3358:VAL:HG11	1.95	0.49
1:B:1995:VAL:HG21	1:B:2024:SER:HB3	1.93	0.49
1:A:1849:GLU:CG	1:A:1899:ASN:HD22	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2064:GLN:NE2	1:A:2091:MET:CE	2.76	0.49
1:A:2960:THR:HG22	1:A:2961:ILE:N	2.27	0.49
1:A:3350:LYS:HA	1:A:3353:LEU:HD12	1.94	0.49
1:A:3566:LEU:HD13	1:A:3570:LEU:HD12	1.95	0.49
1:A:4033:LEU:HD12	1:A:4036:GLN:H	1.78	0.49
1:B:1645:PHE:CD2	1:B:1765:ILE:HG22	2.47	0.49
1:B:2105:ASP:OD2	1:B:2508:GLN:HB2	2.12	0.49
1:B:3319:GLU:HA	1:B:3359:LYS:O	2.13	0.49
1:A:1421:TYR:CZ	1:A:1425:GLU:HG3	2.46	0.49
1:A:1531:ARG:HG2	1:A:1537:PHE:CB	2.42	0.49
1:A:1540:LEU:HD11	1:A:1561:PHE:HB3	1.95	0.49
1:A:3848:LEU:HD12	1:A:3884:LEU:HD12	1.93	0.49
1:B:2170:LEU:HB3	1:B:2209:ARG:HD3	1.95	0.49
1:B:2552:ARG:NH2	2:B:5093:ATP:O2G	2.45	0.49
1:A:1626:CYS:SG	1:A:1639:VAL:CG1	3.01	0.49
1:A:1748:PHE:CE2	1:A:1755:LEU:HD22	2.47	0.49
1:A:2514:GLY:CA	1:A:2523:TRP:CZ2	2.96	0.49
1:A:3855:LEU:HD12	1:A:3859:VAL:HG23	1.93	0.49
1:B:2517:LYS:NZ	1:B:2520:GLU:OE1	2.45	0.49
1:A:1448:VAL:HG22	1:A:1513:ILE:HB	1.94	0.49
1:A:2074:GLY:O	1:A:2197:ASP:HA	2.13	0.49
1:A:2364:ASP:O	1:A:2365:LYS:HG2	2.13	0.49
1:B:1838:ILE:HG13	1:B:1843:ALA:HB3	1.95	0.49
1:B:1844:TRP:CD1	1:B:1893:ALA:HB3	2.48	0.49
1:B:3459:ASP:OD2	1:B:3461:ILE:CG1	2.60	0.49
1:A:3481:ILE:O	1:A:3483:ASP:N	2.36	0.49
1:A:3737:THR:HB	1:A:3740:THR:HG1	1.77	0.49
1:B:2095:ASP:CG	1:B:2149:ARG:NH2	2.66	0.49
1:B:2472:THR:HB	1:B:2524:VAL:HG22	1.94	0.49
1:B:2385:VAL:O	1:B:2574:TYR:HE1	1.96	0.49
1:B:3817:GLY:H	1:B:3821:ASN:HB2	1.78	0.49
1:A:1626:CYS:HB2	1:A:1643:TYR:CD2	2.48	0.49
1:A:3889:LEU:HG	1:A:3894:ARG:HD3	1.95	0.49
1:A:3946:VAL:HA	1:A:3947:PRO:C	2.33	0.49
1:B:1657:THR:HG21	1:B:1734:PHE:O	2.13	0.49
1:B:3555:TYR:HE1	1:B:3593:GLU:HG2	1.77	0.49
1:A:2828:LEU:HD13	1:A:2902:MET:SD	2.53	0.48
1:A:3671:VAL:O	1:A:3674:ILE:HG22	2.13	0.48
1:A:3978:ASN:O	1:A:3981:PRO:CD	2.60	0.48
1:B:2044:ARG:HH21	1:B:2093:ILE:HD11	1.76	0.48
1:B:2737:SER:HB2	1:B:2924:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2760:GLY:O	1:B:2761:ALA:HB3	2.13	0.48
1:B:3460:PRO:O	1:B:3463:SER:HB3	2.13	0.48
1:A:76:ASP:CB	1:B:85:PRO:CB	2.90	0.48
1:A:1469:LEU:CD1	1:A:1523:LEU:HD21	2.43	0.48
1:A:1664:LEU:HD23	1:A:1669:PHE:HZ	1.77	0.48
1:A:1645:PHE:CD2	1:A:1765:ILE:HG22	2.48	0.48
1:A:2354:SER:OG	1:A:2357:SER:CB	2.61	0.48
1:A:2839:ASP:O	1:A:2841:PRO:HD3	2.12	0.48
1:B:2446:SER:H	1:B:2449:THR:HG21	1.74	0.48
1:B:23:LEU:O	1:B:24:GLU:CB	2.62	0.48
1:B:65:THR:O	1:B:66:GLN:CB	2.60	0.48
1:A:1911:ASN:OD1	1:A:1912:LEU:HG	2.13	0.48
1:A:3737:THR:CB	1:A:3740:THR:HB	2.44	0.48
1:A:2425:THR:HG23	3:A:5094:SO4:O2	2.14	0.48
1:B:2109:LEU:HD11	1:B:2129:LEU:CD2	2.44	0.48
1:B:2177:THR:HG22	1:B:2183:ARG:HG2	1.94	0.48
1:B:2654:ARG:HH22	1:B:2691:SER:HB2	1.79	0.48
1:B:2894:PRO:HG3	1:B:2916:TRP:CH2	2.49	0.48
1:B:3810:SER:HB3	1:B:3837:GLY:HA2	1.96	0.48
1:B:3946:VAL:HB	1:B:3947:PRO:HA	1.95	0.48
1:A:1683:LEU:HB3	1:A:1702:LEU:HD21	1.96	0.48
1:A:1794:PHE:HD1	1:A:1802:LYS:HB3	1.79	0.48
1:A:3721:THR:O	1:A:3725:VAL:HG23	2.14	0.48
1:B:2008:ASP:HA	1:B:2011:GLU:HB2	1.96	0.48
1:B:1531:ARG:HD3	1:B:1537:PHE:O	2.13	0.48
1:B:1559:SER:HB3	1:B:1572:ILE:HG22	1.96	0.48
1:A:2109:LEU:HD13	1:A:2129:LEU:HD23	1.94	0.48
1:A:2763:ARG:HA	3:A:5095:SO4:O1	2.14	0.48
1:A:3024:LEU:HD13	1:A:3303:LYS:HG3	1.92	0.48
1:A:3690:LEU:HD23	1:A:3694:PHE:HB3	1.96	0.48
1:B:2464:TYR:CE1	1:B:2524:VAL:HG11	2.48	0.48
1:B:2563:SER:CB	1:B:2566:SER:H	2.20	0.48
1:B:2655:ILE:HD11	1:B:2747:ARG:HH22	1.78	0.48
1:B:3612:ASP:C	1:B:3615:VAL:HG22	2.34	0.48
1:B:3934:TRP:CB	1:B:4023:ILE:HD13	2.43	0.48
1:B:3979:ASN:C	1:B:3981:PRO:CD	2.81	0.48
1:A:1826:PHE:CE1	1:A:1853:LEU:CD2	2.96	0.48
1:A:2169:VAL:HG13	1:A:2186:ILE:HG12	1.94	0.48
1:A:1967:HIS:NE2	1:A:2204:PRO:HB3	2.28	0.48
1:A:3541:MET:HB2	1:A:3607:PHE:HE1	1.78	0.48
1:B:2380:LEU:HD12	1:B:2380:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4059:LEU:HA	1:B:4063:LEU:HD13	1.95	0.48
1:A:1421:TYR:CE2	1:A:1425:GLU:CG	2.96	0.48
1:A:2084:TRP:CZ3	1:A:2085:LYS:HG3	2.49	0.48
1:A:4065:LEU:HD12	1:A:4065:LEU:C	2.33	0.48
1:B:2027:THR:HA	1:B:2028:PRO:HD3	1.49	0.48
1:B:3592:LYS:O	1:B:3596:ASN:N	2.46	0.48
1:B:3818:SER:O	1:B:3820:GLU:N	2.46	0.48
1:A:1540:LEU:CD1	1:A:1548:ILE:HD12	2.41	0.48
1:A:2860:THR:HG22	1:A:2865:LEU:O	2.13	0.48
1:B:1637:GLU:HG2	1:B:1686:LYS:HG3	1.96	0.48
1:B:1706:LEU:CD1	1:B:1936:ILE:HG12	2.43	0.48
1:B:3461:ILE:C	1:B:3463:SER:N	2.66	0.48
1:B:3566:LEU:HD11	1:B:3570:LEU:HD11	1.94	0.48
1:A:2741:HIS:O	1:A:2745:ILE:HG13	2.15	0.47
1:A:3373:LEU:O	1:A:3373:LEU:HD23	2.13	0.47
1:B:1540:LEU:HD11	1:B:1561:PHE:HB3	1.95	0.47
1:B:2316:LEU:HD13	1:B:2351:GLN:HB3	1.95	0.47
1:B:2514:GLY:HA3	1:B:2523:TRP:CZ2	2.49	0.47
1:A:1683:LEU:HD22	1:A:1698:ILE:HG23	1.96	0.47
1:A:2027:THR:HA	1:A:2028:PRO:HD3	1.48	0.47
1:A:3459:ASP:OD2	1:A:3461:ILE:CG1	2.61	0.47
1:A:3703:PHE:HE1	1:A:3766:GLU:HG2	1.79	0.47
1:B:1534:PHE:HD2	1:B:1537:PHE:CE1	2.33	0.47
1:B:1781:THR:HG21	1:B:1919:PHE:CD1	2.49	0.47
1:B:1849:GLU:CG	1:B:1899:ASN:ND2	2.74	0.47
1:B:1969:GLY:O	1:B:1972:THR:HB	2.14	0.47
1:B:2220:CYS:SG	1:B:2221:SER:N	2.88	0.47
1:B:2280:THR:HA	1:B:2283:LYS:HD2	1.95	0.47
1:A:1554:HIS:O	1:A:1555:HIS:HB2	2.15	0.47
1:A:1849:GLU:OE2	1:A:1899:ASN:ND2	2.47	0.47
1:B:1939:PHE:O	1:B:1940:GLU:HB3	2.14	0.47
1:B:1646:GLN:OE1	1:B:1763:ILE:HG12	2.14	0.47
1:B:1645:PHE:HB2	1:B:1697:LYS:HG3	1.97	0.47
1:B:2473:LEU:HD23	1:B:2475:PRO:N	2.29	0.47
1:B:2724:CYS:SG	1:B:2729:GLU:OE2	2.72	0.47
1:B:4021:LEU:HD23	1:B:4023:ILE:CG1	2.45	0.47
1:A:1542:ASN:O	1:A:1546:LEU:HG	2.14	0.47
1:A:1731:VAL:HG12	1:A:1732:GLN:N	2.28	0.47
1:B:1620:PHE:HB2	1:B:1760:PHE:CZ	2.49	0.47
1:B:2828:LEU:HD13	1:B:2902:MET:SD	2.54	0.47
1:B:2761:ALA:O	1:B:2892:CYS:SG	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TRP:O	1:B:44:LYS:N	2.47	0.47
1:A:4084:SER:O	1:A:4088:LEU:HG	2.14	0.47
1:B:1726:LEU:HD13	1:B:3984:GLN:CB	2.44	0.47
1:B:1934:LEU:HD22	1:B:1945:LEU:HD12	1.97	0.47
1:B:2380:LEU:C	1:B:2380:LEU:HD12	2.35	0.47
1:B:3010:LEU:HD22	1:B:3320:LEU:HD12	1.96	0.47
1:A:1636:ILE:O	1:A:1640:VAL:HG23	2.15	0.47
1:A:2424:LYS:H	1:A:2424:LYS:HG3	1.52	0.47
1:B:2064:GLN:OE1	1:B:2151:TRP:HH2	1.98	0.47
1:B:2452:GLU:HA	1:B:2455:LEU:HD12	1.97	0.47
1:A:1386:ILE:HD12	1:A:1396:ARG:HH11	1.80	0.47
1:A:1681:LYS:HE2	1:A:1939:PHE:CE1	2.50	0.47
1:A:2517:LYS:NZ	1:A:2520:GLU:OE1	2.48	0.47
1:A:1375:LYS:O	1:A:1379:LYS:HG2	2.15	0.47
1:A:3877:CYS:SG	1:A:3884:LEU:HD21	2.55	0.47
1:B:1392:LEU:HD13	1:B:1393:LYS:CA	2.45	0.47
1:B:3818:SER:O	1:B:3821:ASN:N	2.43	0.47
1:B:4021:LEU:HD23	1:B:4023:ILE:HG12	1.96	0.47
1:A:2580:LYS:HG2	1:A:2586:ARG:HH22	1.79	0.46
1:A:3934:TRP:HB3	1:A:4023:ILE:HD13	1.97	0.46
1:B:2494:LEU:HB2	1:B:2499:SER:N	2.30	0.46
1:B:3306:TRP:HH2	1:B:3594:ALA:HB1	1.80	0.46
1:B:3509:LEU:CG	1:B:3513:VAL:HG21	2.45	0.46
1:A:2358:THR:HG22	1:A:2359:ILE:N	2.29	0.46
1:A:2105:ASP:OD2	1:A:2508:GLN:HB2	2.15	0.46
1:A:3967:TYR:HE2	1:A:3985:VAL:HA	1.80	0.46
1:B:1459:LEU:HD23	1:B:1465:ILE:HG13	1.96	0.46
1:B:1917:ARG:HD2	1:B:3963:PHE:CE2	2.50	0.46
1:B:1973:LEU:O	1:B:1977:LEU:HG	2.15	0.46
1:B:2467:THR:O	1:B:2471:LEU:N	2.48	0.46
1:A:1422:LYS:O	1:A:1425:GLU:HB3	2.15	0.46
1:A:2878:VAL:HA	1:A:2881:ILE:HD12	1.97	0.46
1:A:3995:GLY:HA2	1:A:3998:ILE:CD1	2.46	0.46
1:A:2763:ARG:CA	3:A:5095:SO4:O1	2.64	0.46
1:B:1425:GLU:OE1	1:B:1425:GLU:C	2.53	0.46
1:B:1929:ILE:HD12	1:B:1929:ILE:H	1.81	0.46
1:B:2252:LEU:HD22	1:B:2314:ILE:HG13	1.97	0.46
1:B:3566:LEU:HA	1:B:3583:LEU:HD23	1.95	0.46
1:A:2571:TYR:HA	1:A:2574:TYR:HB2	1.97	0.46
1:A:3592:LYS:O	1:A:3596:ASN:N	2.48	0.46
1:B:2849:TYR:O	1:B:2853:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:LEU:CD2	1:A:1435:LEU:CB	2.82	0.46
1:A:2445:PHE:HA	1:A:2449:THR:HG21	1.96	0.46
1:A:2476:LYS:HZ2	1:A:2528:ARG:HB2	1.80	0.46
1:A:3415:ILE:HD13	1:A:3453:GLN:HG3	1.97	0.46
1:B:1694:VAL:HG23	1:B:1697:LYS:HE2	1.97	0.46
1:B:2201:HIS:CE1	1:B:2497:TYR:CA	2.98	0.46
1:B:2580:LYS:HG2	1:B:2586:ARG:HH22	1.79	0.46
1:A:2112:GLU:HB3	1:A:2117:SER:OG	2.16	0.46
1:A:2125:TRP:CZ2	1:A:2178:LEU:CD1	2.97	0.46
1:A:3509:LEU:CG	1:A:3513:VAL:HG21	2.45	0.46
1:A:3924:TRP:O	1:A:3927:TYR:HB3	2.15	0.46
1:B:1611:LEU:O	1:B:1615:ILE:HG12	2.15	0.46
1:B:1984:ILE:CG2	1:B:1989:GLU:HG3	2.44	0.46
1:B:3509:LEU:HG	1:B:3513:VAL:HG21	1.96	0.46
1:A:1425:GLU:OE1	1:A:1425:GLU:C	2.54	0.46
1:A:1995:VAL:HG22	1:A:2022:PHE:HE2	1.80	0.46
1:A:2654:ARG:NH1	1:A:2658:ASP:OD1	2.49	0.46
1:A:2835:LEU:HD23	1:A:2911:ARG:HB2	1.97	0.46
1:A:1418:SER:HB2	1:A:3446:PHE:HB3	1.96	0.46
1:A:40:TRP:O	1:A:44:LYS:N	2.49	0.46
1:B:1734:PHE:CD2	1:B:1749:ILE:HG12	2.50	0.46
1:B:1827:ASP:HB3	1:B:1830:VAL:HG12	1.97	0.46
1:B:2503:VAL:HA	1:B:2506:LEU:HD12	1.97	0.46
1:B:2988:SER:CB	1:B:2989:PRO:CD	2.85	0.46
1:B:3541:MET:HB2	1:B:3607:PHE:HE1	1.81	0.46
1:A:2318:ILE:O	1:A:2322:LEU:HB2	2.16	0.46
1:B:1421:TYR:CE2	1:B:1425:GLU:HG3	2.50	0.46
1:B:1547:LYS:O	1:B:1551:SER:HB3	2.16	0.46
1:B:2099:ASN:HA	1:B:2149:ARG:O	2.16	0.46
1:A:1527:LEU:HD21	1:A:1546:LEU:HD23	1.97	0.46
1:A:2627:ARG:NH1	1:A:2630:TYR:CD2	2.84	0.46
1:A:3612:ASP:O	1:A:3615:VAL:CG2	2.63	0.46
1:A:1748:PHE:HD2	1:A:1755:LEU:HD22	1.77	0.46
1:A:3508:PHE:O	1:A:3512:ARG:HG2	2.16	0.46
1:B:1612:ASP:HA	1:B:1615:ILE:CG1	2.46	0.46
1:B:3813:ILE:HG22	1:B:3840:LEU:HD23	1.98	0.46
1:A:1392:LEU:HD23	1:A:1484:LYS:HA	1.97	0.45
1:A:1462:ASN:HB2	1:A:1465:ILE:CG2	2.44	0.45
1:A:1660:VAL:HG13	1:A:1728:TRP:CH2	2.51	0.45
1:A:1586:GLU:HG3	1:A:1765:ILE:H	1.81	0.45
1:A:1945:LEU:HD13	1:A:1994:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2204:PRO:HA	1:A:2207:ILE:HD12	1.97	0.45
1:A:3807:SER:O	1:A:3808:LYS:HB2	2.16	0.45
1:B:1535:PRO:C	1:B:1841:ILE:CD1	2.75	0.45
1:B:2785:LYS:NZ	1:B:3480:GLU:CD	2.69	0.45
1:A:2199:LEU:O	1:A:2201:HIS:N	2.49	0.45
1:B:1992:LYS:HG2	1:B:2024:SER:HB2	1.88	0.45
1:B:1965:HIS:HD2	1:B:2212:LEU:HD21	1.81	0.45
1:B:2425:THR:HG23	3:B:5095:SO4:O2	2.17	0.45
1:A:1534:PHE:CD2	1:A:1537:PHE:CE1	3.02	0.45
1:A:1844:TRP:CD1	1:A:1893:ALA:HB3	2.50	0.45
1:A:1951:HIS:O	1:A:1955:LEU:HB2	2.17	0.45
1:A:2286:THR:HA	1:A:2412:ARG:NE	2.31	0.45
1:B:1535:PRO:O	1:B:1841:ILE:HD11	2.14	0.45
1:B:1968:PHE:CD1	1:B:1968:PHE:N	2.84	0.45
1:A:2458:LEU:HG	1:A:2484:LEU:HD21	1.99	0.45
1:A:3330:TYR:CE1	1:A:3334:PHE:CD2	3.05	0.45
1:B:2354:SER:OG	1:B:2357:SER:HB2	2.16	0.45
1:A:1387:GLU:HA	1:A:1393:LYS:HA	1.98	0.45
1:A:1391:GLY:HA3	1:A:1484:LYS:HZ1	1.82	0.45
1:B:1540:LEU:HD11	1:B:1548:ILE:HD11	1.99	0.45
1:B:3462:ILE:O	1:B:3465:LEU:HB3	2.17	0.45
1:A:2783:GLN:HG2	1:A:2816:ILE:HB	1.99	0.45
1:A:2766:LYS:CE	1:A:2890:THR:HB	2.39	0.45
1:B:2472:THR:HG22	1:B:2524:VAL:CG1	2.47	0.45
1:B:3343:ALA:O	1:B:3347:VAL:HG23	2.17	0.45
1:A:1822:CYS:HB2	1:A:1853:LEU:CD2	2.31	0.45
1:A:1910:GLU:HB2	1:A:3846:MET:HA	1.98	0.45
1:A:3308:ASN:O	1:A:3312:GLN:HB2	2.16	0.45
1:A:3470:PHE:CE1	1:A:3488:VAL:HG21	2.52	0.45
1:B:1535:PRO:O	1:B:1841:ILE:CD1	2.65	0.45
1:B:1684:LEU:HD21	1:B:1936:ILE:O	2.16	0.45
1:B:1750:SER:CB	1:B:1755:LEU:HD23	2.46	0.45
1:B:1826:PHE:O	1:B:1826:PHE:CG	2.70	0.45
1:B:1822:CYS:SG	1:B:1850:PHE:HA	2.56	0.45
1:B:1910:GLU:HB2	1:B:3846:MET:HB3	1.98	0.45
1:B:1968:PHE:N	1:B:1968:PHE:HD1	2.15	0.45
1:B:3584:MET:HA	1:B:3587:LEU:HD12	1.98	0.45
1:A:1759:LYS:HE3	1:A:1761:GLU:OE2	2.17	0.45
1:A:2280:THR:HA	1:A:2283:LYS:HD2	1.99	0.45
1:A:2358:THR:CG2	1:A:2359:ILE:N	2.80	0.45
1:A:2446:SER:N	1:A:2449:THR:HG23	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2494:LEU:HB2	1:A:2499:SER:N	2.32	0.45
1:A:3462:ILE:O	1:A:3465:LEU:N	2.45	0.45
1:A:3832:SER:O	1:A:3836:GLY:N	2.45	0.45
1:B:1677:ASP:HA	1:B:1680:ILE:HD12	1.99	0.45
1:A:2984:VAL:C	1:A:2986:PRO:HD3	2.37	0.45
1:A:3010:LEU:HD22	1:A:3320:LEU:HD12	1.99	0.45
1:A:3461:ILE:C	1:A:3463:SER:N	2.70	0.45
1:B:1656:TRP:HE1	1:B:1712:ILE:HD11	1.81	0.45
1:B:2354:SER:OG	1:B:2357:SER:CB	2.65	0.45
1:B:2552:ARG:HG2	1:B:2552:ARG:HH11	1.81	0.45
1:A:1527:LEU:HD21	1:A:1546:LEU:HD21	1.98	0.45
1:A:1793:CYS:SG	1:A:1918:GLU:HG2	2.57	0.45
1:A:2386:MET:HB3	1:A:2627:ARG:NE	2.32	0.45
1:A:2707:VAL:HG11	1:A:2712:LEU:CD1	2.45	0.45
1:B:2039:LYS:HG2	1:B:2049:MET:HG3	1.98	0.45
1:B:2081:THR:O	1:B:2085:LYS:HB2	2.17	0.45
1:B:3342:ARG:NH2	1:B:3393:ASN:OD1	2.47	0.45
1:A:1392:LEU:HD13	1:A:1393:LYS:CA	2.46	0.44
1:A:2099:ASN:HA	1:A:2149:ARG:O	2.17	0.44
1:A:2155:ASP:OD1	1:A:2195:GLU:HG3	2.17	0.44
1:A:3330:TYR:CD1	1:A:3334:PHE:CD2	3.05	0.44
1:B:1849:GLU:CD	1:B:1899:ASN:HD22	2.21	0.44
1:B:1826:PHE:CE1	1:B:1853:LEU:CD2	3.00	0.44
1:B:2492:PRO:HB2	1:B:2502:VAL:HG11	1.99	0.44
1:B:2707:VAL:HG11	1:B:2712:LEU:HD12	1.98	0.44
1:B:3481:ILE:O	1:B:3483:ASP:N	2.47	0.44
1:B:3725:VAL:HG22	1:B:3731:ASP:HA	1.97	0.44
1:B:4020:ASN:ND2	1:B:4028:ARG:HD3	2.32	0.44
1:A:1968:PHE:N	1:A:1968:PHE:CD1	2.84	0.44
1:B:1536:ARG:HD3	1:B:1536:ARG:HA	1.72	0.44
1:B:1562:MET:CB	1:B:1569:ILE:HD11	2.40	0.44
1:B:1681:LYS:HE2	1:B:1939:PHE:HZ	1.83	0.44
1:B:3449:VAL:HG13	1:B:3493:LYS:HB2	1.99	0.44
1:B:3462:ILE:O	1:B:3465:LEU:N	2.48	0.44
1:A:23:LEU:O	1:A:25:GLU:N	2.50	0.44
1:B:1626:CYS:SG	1:B:1639:VAL:HG11	2.57	0.44
1:B:1796:GLY:O	1:B:1900:PRO:HD3	2.17	0.44
1:B:2473:LEU:CD2	1:B:2474:LEU:N	2.76	0.44
1:A:2021:ILE:HG22	1:A:2022:PHE:HD1	1.82	0.44
1:A:2646:ARG:NH1	1:A:2687:GLY:H	2.14	0.44
1:A:2749:LEU:HD12	1:A:2773:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3579:GLU:O	1:A:3582:GLU:N	2.43	0.44
1:B:1612:ASP:CA	1:B:1615:ILE:HG12	2.48	0.44
1:B:1832:SER:O	1:B:1836:VAL:HG23	2.18	0.44
1:B:2960:THR:CG2	1:B:2961:ILE:N	2.80	0.44
1:B:3869:GLU:O	1:B:3870:LYS:C	2.56	0.44
1:A:1547:LYS:O	1:A:1551:SER:HB3	2.18	0.44
1:A:2861:ARG:HD2	1:A:2866:LEU:HD13	2.00	0.44
1:A:3407:LEU:HD23	1:A:3518:PHE:CE2	2.53	0.44
1:B:1469:LEU:HD13	1:B:1523:LEU:HD21	1.97	0.44
1:B:2002:ILE:HG22	1:B:2006:LEU:HD11	2.00	0.44
1:B:2084:TRP:HE3	1:B:2088:ILE:HD12	1.82	0.44
1:B:2437:LEU:H	1:B:2437:LEU:HD12	1.82	0.44
1:B:2728:LEU:C	1:B:2728:LEU:HD12	2.38	0.44
1:A:1559:SER:CB	1:A:1572:ILE:HG22	2.47	0.44
1:A:1826:PHE:O	1:A:1826:PHE:CG	2.70	0.44
1:B:1593:ASN:HD21	1:B:1621:THR:CB	2.30	0.44
1:B:2112:GLU:HB3	1:B:2117:SER:OG	2.18	0.44
1:B:3964:ALA:HB2	1:B:3993:VAL:HG11	2.00	0.44
1:B:4060:SER:HB3	1:B:4070:ILE:HG13	1.98	0.44
1:A:1421:TYR:O	1:A:1425:GLU:CA	2.65	0.44
1:A:1611:LEU:O	1:A:1615:ILE:HG23	2.18	0.44
1:A:3760:LEU:HD21	1:A:4078:ALA:HA	1.99	0.44
1:A:3767:PHE:HB3	1:A:3769:VAL:HG23	2.00	0.44
1:A:4034:LEU:C	1:A:4034:LEU:HD23	2.38	0.44
1:B:1664:LEU:HD23	1:B:1669:PHE:HZ	1.82	0.44
1:B:1748:PHE:CE2	1:B:1755:LEU:HD22	2.52	0.44
1:B:1870:ASN:O	1:B:1874:VAL:HG23	2.17	0.44
1:A:1646:GLN:OE1	1:A:1763:ILE:HG12	2.18	0.44
1:A:1803:THR:HG21	1:A:1848:ASP:CG	2.37	0.44
1:A:2037:CYS:SG	1:A:2094:PHE:HB2	2.57	0.44
1:A:2354:SER:H	1:A:2357:SER:HB2	1.83	0.44
1:A:2707:VAL:HG11	1:A:2712:LEU:HD12	2.00	0.44
1:A:3566:LEU:HD23	1:A:3587:LEU:HD11	1.99	0.44
1:A:3631:MET:HE1	1:A:3698:MET:HG3	2.00	0.44
1:A:3821:ASN:O	1:A:3825:ALA:HB2	2.17	0.44
1:B:1967:HIS:C	1:B:1968:PHE:CD1	2.82	0.44
1:B:2034:ILE:CD1	1:B:2061:TYR:CZ	3.00	0.44
1:B:2241:LEU:HD13	1:B:2299:ARG:HH11	1.82	0.44
1:B:2758:LEU:HD13	1:B:2766:LYS:HB2	1.99	0.44
1:B:2783:GLN:HG2	1:B:2816:ILE:HB	1.99	0.44
1:B:2755:HIS:CB	1:B:2911:ARG:O	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2788:ARG:HB2	1:B:3459:ASP:HB3	2.00	0.44
1:B:3671:VAL:HA	1:B:3674:ILE:HG22	1.99	0.44
1:A:1660:VAL:CG1	1:A:1728:TRP:CH2	3.01	0.44
1:A:1681:LYS:HE2	1:A:1939:PHE:CZ	2.53	0.44
1:A:2141:ILE:CD1	1:A:2146:LYS:CE	2.86	0.44
1:A:3702:MET:HB3	1:A:3767:PHE:HZ	1.83	0.44
1:B:1375:LYS:HE3	1:B:1431:LEU:HD13	1.99	0.44
1:B:2339:ILE:HG23	1:B:2353:LEU:HB3	2.00	0.44
1:B:2410:SER:O	1:B:2411:LYS:HG3	2.17	0.44
1:B:3458:PHE:HE1	1:B:3462:ILE:HB	1.82	0.44
1:B:3786:PHE:CD1	1:B:3895:PHE:HE2	2.36	0.44
1:A:1531:ARG:HD3	1:A:1538:TYR:HA	2.00	0.43
1:A:1926:SER:HA	1:A:1929:ILE:CD1	2.48	0.43
1:A:2266:PHE:HD1	1:A:2326:LEU:HD21	1.83	0.43
1:A:2375:ILE:HG22	1:A:2376:PRO:O	2.18	0.43
1:A:2512:LYS:O	1:A:2513:GLN:CB	2.66	0.43
1:A:3319:GLU:HA	1:A:3359:LYS:O	2.17	0.43
1:B:1531:ARG:HD2	1:B:1538:TYR:HA	2.00	0.43
1:B:1645:PHE:CZ	1:B:1649:LEU:HD22	2.52	0.43
1:B:3897:TYR:CZ	1:B:3899:ASP:HB3	2.53	0.43
1:A:2262:LEU:HA	1:A:2265:ILE:HD12	1.98	0.43
1:A:2404:PHE:CZ	1:A:2428:MET:HG2	2.53	0.43
1:A:2417:CYS:O	1:A:2558:TYR:HA	2.17	0.43
1:B:1418:SER:HB2	1:B:3446:PHE:HB3	1.99	0.43
1:B:1992:LYS:CG	1:B:2024:SER:CB	2.79	0.43
1:B:2476:LYS:HZ2	1:B:2528:ARG:HD2	1.77	0.43
1:A:1973:LEU:O	1:A:1977:LEU:HG	2.18	0.43
1:A:2197:ASP:HB3	1:A:2549:ARG:HD2	1.99	0.43
1:A:3964:ALA:HB2	1:A:3993:VAL:HG11	1.99	0.43
1:A:4033:LEU:HD13	1:A:4035:GLN:CG	2.49	0.43
1:B:1976:VAL:HG11	1:B:1998:LEU:HD23	2.00	0.43
1:B:2410:SER:O	1:B:2411:LYS:CB	2.66	0.43
1:B:2563:SER:C	1:B:2565:LYS:H	2.21	0.43
1:B:3839:ILE:HG22	1:B:3871:PHE:HE1	1.83	0.43
1:A:1531:ARG:HD2	1:A:1538:TYR:HA	2.01	0.43
1:A:1611:LEU:O	1:A:1615:ILE:HG12	2.19	0.43
1:A:2061:TYR:O	1:A:2064:GLN:HG2	2.17	0.43
1:A:2578:ILE:CG2	1:A:2630:TYR:HB2	2.48	0.43
1:A:3628:ILE:HG13	1:A:3705:LEU:HD23	2.00	0.43
1:A:3785:TYR:N	1:A:3785:TYR:CD1	2.87	0.43
1:B:1749:ILE:HD13	1:B:1813:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1835:LEU:O	1:B:1838:ILE:HG22	2.18	0.43
1:B:2984:VAL:C	1:B:2986:PRO:HD3	2.38	0.43
1:B:3544:LYS:O	1:B:3548:LEU:HB2	2.18	0.43
1:A:1540:LEU:HD12	1:A:1548:ILE:HD12	2.00	0.43
1:B:1750:SER:HB2	1:B:1755:LEU:HD23	2.01	0.43
1:B:2833:THR:CG2	1:B:2841:PRO:HD2	2.48	0.43
1:B:3939:ILE:HG12	1:B:4010:LEU:CD2	2.49	0.43
1:A:2982:VAL:CG1	1:A:2983:GLY:N	2.82	0.43
1:B:2419:PRO:O	1:B:2424:LYS:NZ	2.51	0.43
1:B:2201:HIS:CE1	1:B:2497:TYR:O	2.72	0.43
1:A:2109:LEU:CD1	1:A:2129:LEU:HD23	2.49	0.43
1:A:2274:HIS:CE1	1:A:2326:LEU:O	2.54	0.43
1:A:3338:ASN:H	1:A:3341:GLU:HB2	1.82	0.43
1:A:4033:LEU:C	1:A:4033:LEU:HD12	2.39	0.43
1:B:1383:TYR:CZ	1:B:1401:LEU:HD13	2.54	0.43
1:B:1803:THR:HG21	1:B:1848:ASP:CG	2.39	0.43
1:B:2151:TRP:CE3	1:B:2193:LEU:HD11	2.54	0.43
1:B:2653:TRP:HB3	1:B:2654:ARG:NH1	2.34	0.43
1:A:1367:ILE:HG22	1:A:1371:LEU:HD12	2.00	0.43
1:A:1650:LEU:O	1:A:1654:VAL:HG23	2.19	0.43
1:A:2178:LEU:HB3	1:A:2179:PRO:HD2	2.01	0.43
1:A:2447:LYS:HE3	1:A:2493:LYS:HD3	2.00	0.43
1:A:2503:VAL:HA	1:A:2506:LEU:HD12	2.01	0.43
1:A:2575:TYR:HD1	1:A:2578:ILE:HD11	1.83	0.43
1:A:3810:SER:HB3	1:A:3837:GLY:HA2	2.01	0.43
1:B:1391:GLY:HA3	1:B:1484:LYS:HZ1	1.81	0.43
1:B:2226:ILE:HG12	1:B:2284:LEU:HD22	2.01	0.43
1:B:2760:GLY:HA2	1:B:2917:MET:HB2	2.00	0.43
1:B:2853:LEU:HD21	1:B:2870:GLU:HG3	2.00	0.43
1:A:2072:LEU:HD11	1:A:2193:LEU:HD23	2.01	0.43
1:A:2760:GLY:O	1:A:2761:ALA:HB3	2.18	0.43
1:A:3696:MET:SD	1:A:3760:LEU:HD23	2.59	0.43
1:A:3869:GLU:O	1:A:3870:LYS:C	2.56	0.43
1:B:2081:THR:OG1	2:B:5093:ATP:O1B	2.37	0.43
1:B:2380:LEU:CD1	1:B:2577:ALA:HB2	2.46	0.43
1:B:3636:GLY:CA	1:B:3642:TYR:O	2.67	0.43
1:A:1741:LEU:O	1:A:1742:ASP:HB2	2.19	0.43
1:A:1830:VAL:O	1:A:1834:LEU:HG	2.19	0.43
1:A:2829:GLU:HA	1:A:2832:ASN:HD22	1.84	0.43
1:B:1636:ILE:O	1:B:1640:VAL:HG23	2.19	0.43
1:B:1704:GLU:OE2	1:B:1768:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1735:TYR:HB2	1:B:1748:PHE:CZ	2.53	0.43
1:B:2001:VAL:O	1:B:2004:PRO:HD2	2.19	0.43
1:B:2463:ASN:O	1:B:2475:PRO:HD2	2.19	0.43
1:B:2707:VAL:HG11	1:B:2712:LEU:CD1	2.45	0.43
1:B:2936:ILE:CG2	1:B:2962:ARG:HD3	2.48	0.43
1:B:3721:THR:O	1:B:3725:VAL:HG23	2.19	0.43
1:B:3886:ALA:N	1:B:3887:PRO:CD	2.80	0.43
1:B:4022:GLN:O	1:B:4023:ILE:C	2.57	0.43
1:A:1392:LEU:N	1:A:1484:LYS:HE2	2.34	0.42
1:A:2411:LYS:HG2	1:A:2530:HIS:CE1	2.41	0.42
1:A:2492:PRO:CB	1:A:2502:VAL:HG11	2.49	0.42
1:A:2385:VAL:HG23	1:A:2574:TYR:CD1	2.53	0.42
1:B:3889:LEU:HG	1:B:3894:ARG:HD3	2.01	0.42
1:A:1715:LEU:HG	1:A:1727:LEU:HD22	2.02	0.42
1:A:4033:LEU:CD1	1:A:4035:GLN:N	2.82	0.42
1:B:1554:HIS:O	1:B:1555:HIS:HB2	2.18	0.42
1:B:1762:TYR:CZ	1:B:1764:GLY:HA2	2.54	0.42
1:B:2410:SER:O	1:B:2411:LYS:CG	2.67	0.42
1:B:3719:VAL:HB	1:B:3744:LEU:HD11	2.01	0.42
1:A:1672:TYR:O	1:A:1676:VAL:HG23	2.19	0.42
1:A:1781:THR:HG21	1:A:1919:PHE:CE1	2.55	0.42
1:A:1953:LEU:HD11	1:A:1973:LEU:HB3	1.98	0.42
1:A:1991:GLU:O	1:A:1994:VAL:HB	2.19	0.42
1:A:1998:LEU:CD1	1:A:2022:PHE:HZ	2.32	0.42
1:A:2760:GLY:HA3	1:A:2766:LYS:HD3	2.01	0.42
1:A:3785:TYR:CE2	1:A:3859:VAL:HG13	2.54	0.42
1:A:4033:LEU:HD12	1:A:4035:GLN:H	1.84	0.42
1:A:4045:LEU:O	1:A:4048:ILE:HG22	2.19	0.42
1:B:1941:ASP:O	1:B:1945:LEU:HG	2.18	0.42
1:B:1970:LEU:CD1	1:B:1974:LYS:HE2	2.45	0.42
1:B:3566:LEU:CD2	1:B:3587:LEU:HD11	2.49	0.42
1:B:3815:PRO:O	1:B:3821:ASN:HB3	2.19	0.42
1:A:2707:VAL:CB	1:A:2712:LEU:CD1	2.72	0.42
1:A:3735:LYS:H	1:A:3735:LYS:HG2	1.69	0.42
1:B:1983:LEU:HB3	1:B:1993:THR:CG2	2.47	0.42
1:B:2104:ILE:O	1:B:2154:PHE:HA	2.19	0.42
1:A:1939:PHE:N	1:A:1939:PHE:CD1	2.87	0.42
1:A:2225:LYS:HD2	1:A:2281:PHE:CZ	2.55	0.42
1:A:2738:MET:HG2	1:A:2769:LEU:HD21	2.00	0.42
1:A:1575:LEU:O	1:A:1576:GLU:HB3	2.20	0.42
1:A:2306:ASP:HB2	1:A:2309:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2640:THR:O	1:A:2643:SER:HB3	2.20	0.42
1:A:3365:ARG:HD2	1:A:3368:ASP:OD2	2.19	0.42
1:A:3461:ILE:C	1:A:3463:SER:H	2.22	0.42
1:B:2106:THR:H	1:B:2156:SER:HB2	1.84	0.42
1:B:2073:VAL:HG21	1:B:2199:LEU:HD11	2.01	0.42
1:B:3413:HIS:O	1:B:3417:VAL:HG23	2.20	0.42
1:B:3407:LEU:HD23	1:B:3518:PHE:CE2	2.55	0.42
1:B:3701:THR:OG1	1:B:4085:THR:HG22	2.19	0.42
1:A:1620:PHE:CA	1:A:1760:PHE:CE1	3.01	0.42
1:A:1965:HIS:HD2	1:A:2212:LEU:HD23	1.85	0.42
1:A:2423:GLY:CA	3:A:5094:SO4:O3	2.68	0.42
1:A:2860:THR:HG21	1:A:2867:LEU:HD12	2.02	0.42
1:B:1645:PHE:HZ	1:B:1768:ARG:HD2	1.84	0.42
1:B:1741:LEU:O	1:B:1742:ASP:HB2	2.19	0.42
1:B:1851:ASN:HD21	1:B:1899:ASN:HB2	1.84	0.42
1:B:2141:ILE:HG22	1:B:2145:PHE:HB2	2.02	0.42
1:B:2115:TYR:OH	1:B:2162:TYR:O	2.27	0.42
1:B:2354:SER:OG	1:B:2357:SER:CA	2.68	0.42
1:B:2745:ILE:HG12	1:B:2756:MET:CE	2.45	0.42
1:B:2941:THR:HG22	1:B:2942:ASP:N	2.30	0.42
1:A:1822:CYS:SG	1:A:1850:PHE:CA	3.04	0.42
1:A:2493:LYS:HG3	1:A:2494:LEU:N	2.33	0.42
1:A:3414:MET:O	1:A:3418:ILE:HG12	2.19	0.42
1:A:4074:GLU:HA	1:A:4077:GLN:HE21	1.84	0.42
1:B:2095:ASP:HB3	1:B:2097:HIS:ND1	2.35	0.42
1:B:2730:VAL:HA	1:B:2731:PRO:HD3	1.81	0.42
1:A:1365:PHE:O	1:A:1366:VAL:CB	2.68	0.42
1:A:1540:LEU:HD23	1:A:1540:LEU:HA	1.65	0.42
1:A:1568:SER:HB2	1:A:1816:VAL:HG21	2.01	0.42
1:A:2095:ASP:OD1	1:A:2149:ARG:NH2	2.53	0.42
1:A:2178:LEU:HB2	1:A:2182:GLU:H	1.83	0.42
1:A:2563:SER:C	1:A:2565:LYS:H	2.23	0.42
1:A:2609:THR:HA	1:A:2612:GLN:O	2.20	0.42
1:A:2708:ASN:O	1:A:2712:LEU:HD13	2.20	0.42
1:A:3784:ASN:ND2	1:A:3865:ALA:O	2.52	0.42
1:B:1409:LEU:CD2	1:B:1435:LEU:CB	2.83	0.42
1:B:1612:ASP:C	1:B:1615:ILE:HG12	2.39	0.42
1:B:1871:GLY:HA3	1:B:1879:ILE:HG21	2.02	0.42
1:B:2492:PRO:CB	1:B:2502:VAL:HG11	2.49	0.42
1:A:1727:LEU:O	1:A:1731:VAL:HG23	2.20	0.42
1:A:1967:HIS:C	1:A:1968:PHE:CD1	2.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2229:LEU:HD11	1:A:2285:GLU:HG3	2.02	0.42
1:A:2510:MET:O	1:A:2513:GLN:NE2	2.53	0.42
1:A:2755:HIS:HB3	1:A:2912:CYS:SG	2.60	0.42
1:A:3590:LEU:HD12	1:A:3593:GLU:HB2	2.02	0.42
1:A:3728:GLU:CG	1:A:4079:LYS:HE2	2.49	0.42
1:A:3978:ASN:O	1:A:3981:PRO:HD3	2.20	0.42
1:B:1951:HIS:O	1:B:1955:LEU:HB2	2.20	0.42
1:B:2169:VAL:HG13	1:B:2186:ILE:HG12	2.02	0.42
1:B:3817:GLY:H	1:B:3821:ASN:CB	2.33	0.42
1:A:3505:ILE:O	1:A:3510:ARG:NH1	2.53	0.41
1:B:1375:LYS:O	1:B:1379:LYS:HG2	2.20	0.41
1:B:1392:LEU:HD23	1:B:1484:LYS:HA	2.02	0.41
1:B:1998:LEU:CD1	1:B:2022:PHE:CZ	3.02	0.41
1:B:2578:ILE:CG2	1:B:2630:TYR:HB2	2.50	0.41
1:B:2908:LEU:O	1:B:2912:CYS:HB2	2.20	0.41
1:A:2034:ILE:HD12	1:A:2061:TYR:CE2	2.55	0.41
1:A:2141:ILE:CG2	1:A:2145:PHE:HB2	2.49	0.41
1:A:2786:ILE:HD12	1:A:3460:PRO:CG	2.49	0.41
1:B:1497:ILE:O	1:B:1500:ILE:HG12	2.19	0.41
1:B:1531:ARG:CD	1:B:1538:TYR:HA	2.50	0.41
1:B:2700:LEU:HD13	1:B:2707:VAL:HG11	2.01	0.41
1:B:3017:VAL:HG21	1:B:3313:PHE:HE2	1.83	0.41
1:A:2001:VAL:O	1:A:2004:PRO:HD2	2.20	0.41
1:A:2044:ARG:HH21	1:A:2093:ILE:HD11	1.85	0.41
1:A:2758:LEU:HD22	1:A:2917:MET:SD	2.60	0.41
1:B:1540:LEU:HA	1:B:1540:LEU:HD23	1.74	0.41
1:B:3551:LEU:HA	1:B:3554:GLU:HB3	2.01	0.41
1:A:23:LEU:O	1:A:24:GLU:C	2.58	0.41
1:A:3544:LYS:HE3	1:A:3607:PHE:CD1	2.55	0.41
1:A:2424:LYS:NZ	3:A:5094:SO4:O1	2.54	0.41
1:B:1392:LEU:N	1:B:1484:LYS:HE2	2.34	0.41
1:B:1873:GLN:HE22	1:B:1915:SER:HA	1.84	0.41
1:B:2047:PHE:CE2	1:B:2082:ALA:HB1	2.55	0.41
1:B:2138:ASN:ND2	1:B:2185:PRO:O	2.53	0.41
1:B:2763:ARG:HD3	1:B:3512:ARG:NH1	2.35	0.41
1:A:1536:ARG:HA	1:A:1536:ARG:HD3	1.79	0.41
1:A:2012:LEU:HD12	1:A:2013:VAL:N	2.35	0.41
1:A:2786:ILE:HD12	1:A:3460:PRO:HG2	2.02	0.41
1:A:3413:HIS:O	1:A:3417:VAL:HG23	2.21	0.41
1:A:3544:LYS:O	1:A:3548:LEU:HB2	2.19	0.41
1:B:115:GLU:CB	1:B:1372:ASN:CG	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2609:THR:HA	1:B:2612:GLN:O	2.20	0.41
1:B:3570:LEU:HD23	1:B:3580:ASN:CG	2.40	0.41
1:A:2039:LYS:HG2	1:A:2049:MET:HG3	2.03	0.41
1:A:2109:LEU:HB3	1:A:2113:SER:HB2	2.03	0.41
1:A:2141:ILE:HG22	1:A:2145:PHE:CB	2.51	0.41
1:A:2489:ILE:HD11	1:A:2506:LEU:HD13	2.02	0.41
1:B:2102:TYR:HB2	1:B:2152:VAL:HG22	2.02	0.41
1:B:2276:LEU:CD2	1:B:2415:ILE:HG21	2.47	0.41
1:B:2508:GLN:O	1:B:2512:LYS:HB2	2.20	0.41
1:B:2517:LYS:HD2	1:B:2520:GLU:OE1	2.20	0.41
1:B:2839:ASP:O	1:B:2841:PRO:HD3	2.20	0.41
1:B:2852:LEU:HG	1:B:2856:LEU:HD13	2.03	0.41
1:A:1966:TYR:CZ	1:A:2006:LEU:HD23	2.55	0.41
1:A:2225:LYS:HG2	1:A:2229:LEU:HD12	2.02	0.41
1:A:2336:ARG:HG2	1:A:2355:ASP:CG	2.41	0.41
1:A:2568:SER:HA	1:A:2597:VAL:HG21	2.02	0.41
1:A:2761:ALA:O	1:A:2892:CYS:CB	2.69	0.41
1:A:3330:TYR:CZ	1:A:3346:LEU:HD13	2.55	0.41
1:A:3534:LEU:HD12	1:A:3618:TYR:CZ	2.52	0.41
1:A:3833:LYS:NZ	1:A:3862:THR:HG21	2.36	0.41
1:A:4020:ASN:ND2	1:A:4028:ARG:HD3	2.35	0.41
1:B:2044:ARG:NH2	1:B:2093:ILE:HD11	2.35	0.41
1:B:2982:VAL:HG12	1:B:2983:GLY:N	2.36	0.41
1:A:1479:LEU:HD11	1:A:1515:SER:HB3	2.03	0.41
1:A:1706:LEU:HD21	1:A:1935:GLN:CG	2.48	0.41
1:A:23:LEU:C	1:A:25:GLU:N	2.74	0.41
1:A:2276:LEU:HD21	1:A:2415:ILE:HG21	2.03	0.41
1:A:2476:LYS:H	1:A:2476:LYS:HD2	1.73	0.41
1:A:2762:SER:O	1:A:2763:ARG:CB	2.68	0.41
1:A:2891:ILE:HD11	1:A:2903:ILE:HD11	2.03	0.41
1:A:4054:GLU:HA	1:A:4055:PRO:HD3	1.98	0.41
1:B:1963:MET:HB3	1:B:1966:TYR:CD2	2.55	0.41
1:B:3919:LYS:HZ1	1:B:4038:GLU:HG3	1.83	0.41
1:A:1898:LEU:HD11	1:A:1908:LEU:CD2	2.50	0.41
1:A:1929:ILE:H	1:A:1929:ILE:HD12	1.86	0.41
1:A:3570:LEU:HD23	1:A:3580:ASN:CG	2.41	0.41
1:A:3772:TRP:HZ3	1:A:3780:ASN:HD22	1.68	0.41
1:A:4033:LEU:CD1	1:A:4035:GLN:H	2.34	0.41
1:B:1438:LEU:O	1:B:1442:GLN:HB2	2.20	0.41
1:B:1771:TYR:HA	1:B:1775:LEU:HD13	2.03	0.41
1:B:1939:PHE:CD1	1:B:1939:PHE:N	2.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3636:GLY:HA2	1:B:3642:TYR:O	2.20	0.41
1:A:1742:ASP:HB3	1:A:1745:ASN:HD22	1.85	0.41
1:A:2852:LEU:HG	1:A:2856:LEU:HD13	2.03	0.41
1:A:3737:THR:CB	1:A:3740:THR:OG1	2.56	0.41
1:B:1531:ARG:HD2	1:B:1538:TYR:CD1	2.55	0.41
1:B:2229:LEU:HD11	1:B:2285:GLU:HG3	2.02	0.41
1:B:2752:VAL:O	1:B:2883:LYS:HA	2.21	0.41
1:B:3839:ILE:HG22	1:B:3871:PHE:CE1	2.56	0.41
1:B:3848:LEU:HD21	1:B:3852:LYS:HE3	2.02	0.41
1:B:4033:LEU:HD23	1:B:4033:LEU:HA	1.80	0.41
1:B:4065:LEU:HD12	1:B:4065:LEU:O	2.21	0.41
1:A:2088:ILE:HG12	1:A:2151:TRP:CZ2	2.55	0.41
1:A:3464:ARG:O	1:A:3467:SER:O	2.38	0.41
1:B:1674:LYS:HA	1:B:1677:ASP:HB3	2.03	0.41
1:B:1779:PHE:O	1:B:1783:THR:HG22	2.21	0.41
1:B:1872:LEU:HG	1:B:1888:LEU:HD21	2.04	0.41
1:B:2494:LEU:HD12	1:B:2494:LEU:C	2.41	0.41
1:B:2552:ARG:HG2	1:B:2552:ARG:NH1	2.36	0.41
1:B:3688:THR:HG21	1:B:3777:VAL:CG2	2.50	0.41
1:A:1992:LYS:CG	1:A:2024:SER:CB	2.78	0.40
1:A:2488:GLU:HB3	1:A:2491:LEU:CG	2.51	0.40
1:B:1383:TYR:CE2	1:B:1401:LEU:HD13	2.57	0.40
1:B:1493:LEU:HD23	1:B:1498:GLU:HB2	2.00	0.40
1:B:1534:PHE:CZ	1:B:1536:ARG:HB2	2.57	0.40
1:B:1773:PRO:HA	1:B:1776:LEU:HD12	2.03	0.40
1:B:2111:LYS:CD	1:B:2161:GLU:CG	2.87	0.40
1:B:3353:LEU:HD23	1:B:3358:VAL:HG11	2.02	0.40
1:B:3431:PHE:CZ	1:B:3458:PHE:HD1	2.40	0.40
1:B:3785:TYR:CD1	1:B:3785:TYR:N	2.89	0.40
1:B:3978:ASN:O	1:B:3981:PRO:HD2	2.21	0.40
1:B:1469:LEU:HD13	1:B:1523:LEU:HD23	2.02	0.40
1:B:1527:LEU:HD23	1:B:1545:LEU:CD2	2.50	0.40
1:B:2109:LEU:HD11	1:B:2129:LEU:HD23	2.03	0.40
1:B:2514:GLY:CA	1:B:2523:TRP:CZ2	3.05	0.40
1:A:2819:GLU:HB3	1:A:2891:ILE:HG22	2.03	0.40
1:A:3846:MET:HG3	1:A:3847:SER:N	2.35	0.40
1:A:3951:SER:HB3	1:A:4003:ASP:OD2	2.22	0.40
1:B:1660:VAL:HG13	1:B:1728:TRP:CH2	2.57	0.40
1:B:2032:LYS:HA	1:B:2032:LYS:HD3	1.89	0.40
1:B:3703:PHE:CE1	1:B:3766:GLU:HG2	2.56	0.40
1:B:3821:ASN:O	1:B:3825:ALA:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4081:VAL:O	1:B:4085:THR:HG23	2.22	0.40
1:A:1620:PHE:HB2	1:A:1760:PHE:CE1	2.57	0.40
1:A:1750:SER:HB2	1:A:1755:LEU:CD2	2.52	0.40
1:A:2661:VAL:HG12	1:A:2916:TRP:CE2	2.57	0.40
1:A:3612:ASP:C	1:A:3615:VAL:HG22	2.41	0.40
1:A:3924:TRP:CD1	1:A:3924:TRP:C	2.95	0.40
1:B:1991:GLU:O	1:B:1994:VAL:HB	2.21	0.40
1:B:2378:VAL:HG11	1:B:2392:ILE:HD12	2.02	0.40
1:B:3772:TRP:HZ3	1:B:3780:ASN:ND2	2.20	0.40
1:A:1365:PHE:O	1:A:1366:VAL:HB	2.21	0.40
1:A:1672:TYR:O	1:A:1675:GLU:HB3	2.22	0.40
1:A:2053:PHE:HB2	1:A:2219:VAL:HB	2.02	0.40
1:A:2418:GLY:O	1:A:2424:LYS:HE3	2.21	0.40
1:A:3406:PHE:CZ	1:A:3505:ILE:HG21	2.57	0.40
1:B:1612:ASP:O	1:B:1615:ILE:HG12	2.21	0.40
1:B:2107:LYS:CD	1:B:2499:SER:HB3	2.52	0.40
1:B:2336:ARG:HG2	1:B:2355:ASP:OD1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	2640/2695 (98%)	2519 (95%)	107 (4%)	14 (0%)	32	73
1	B	2640/2695 (98%)	2522 (96%)	104 (4%)	14 (0%)	32	73
All	All	5280/5390 (98%)	5041 (96%)	211 (4%)	28 (0%)	32	73

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1391	GLY

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Mol	Chain	Res	Type
1	B	214	HIS
1	B	1366	VAL
1	B	1391	GLY
1	A	1366	VAL
1	A	2990	GLY
1	A	3306	TRP
1	A	3482	GLY
1	B	3482	GLY
1	A	53	ASN
1	B	53	ASN
1	B	2562	PRO
1	B	2731	PRO
1	A	115	GLU
1	A	2519	PRO
1	B	66	GLN
1	B	2519	PRO
1	A	66	GLN
1	B	3914	GLN
1	B	3980	ILE
1	A	3980	ILE
1	B	85	PRO
1	A	2562	PRO
1	B	3819	ILE
1	A	1470	PRO
1	A	1535	PRO
1	A	2028	PRO
1	B	2028	PRO

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	2218/2453 (90%)	2140 (96%)	78 (4%)	41	75
1	B	2218/2453 (90%)	2144 (97%)	74 (3%)	43	76
All	All	4436/4906 (90%)	4284 (97%)	152 (3%)	42	75

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1383	TYR
1	A	1421	TYR
1	A	1425	GLU
1	A	1473	THR
1	A	1486	ILE
1	A	1493	LEU
1	A	1504	ASN
1	A	1794	PHE
1	A	1826	PHE
1	A	1852	ARG
1	A	1923	SER
1	A	1944	SER
1	A	1971	ARG
1	A	1992	LYS
1	A	1999	LYS
1	A	2012	LEU
1	A	2057	CYS
1	A	2078	CYS
1	A	2109	LEU
1	A	2202	THR
1	A	2218	ASP
1	A	2295	ILE
1	A	2346	PHE
1	A	2357	SER
1	A	2386	MET
1	A	2424	LYS
1	A	2428	MET
1	A	2461	HIS
1	A	2472	THR
1	A	2476	LYS
1	A	2526	ILE
1	A	2544	ILE
1	A	2563	SER
1	A	2566	SER
1	A	2611	LEU
1	A	2638	ARG
1	A	2694	LEU
1	A	2822	ILE
1	A	2833	THR
1	A	2843	LEU
1	A	2853	LEU
1	A	2856	LEU

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Mol	Chain	Res	Type
1	A	2865	LEU
1	A	2873	LEU
1	A	2875	ASP
1	A	2911	ARG
1	A	2920	TRP
1	A	3301	PHE
1	A	3329	ILE
1	A	3332	THR
1	A	3355	LYS
1	A	3372	THR
1	A	3400	SER
1	A	3418	ILE
1	A	3531	ASP
1	A	3538	ASN
1	A	3548	LEU
1	A	3565	ARG
1	A	3601	LEU
1	A	3618	TYR
1	A	3677	LEU
1	A	3717	GLU
1	A	3729	SER
1	A	3735	LYS
1	A	3737	THR
1	A	3744	LEU
1	A	3811	LEU
1	A	3871	PHE
1	A	3884	LEU
1	A	3906	THR
1	A	3917	THR
1	A	3943	THR
1	A	3950	PHE
1	A	3960	ASP
1	A	3982	TRP
1	A	4004	LEU
1	A	4016	CYS
1	A	4040	GLU
1	B	1383	TYR
1	B	1421	TYR
1	B	1425	GLU
1	B	1455	LEU
1	B	1486	ILE
1	B	1504	ASN

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Mol	Chain	Res	Type
1	B	1525	THR
1	B	1554	HIS
1	B	1605	GLN
1	B	1694	VAL
1	B	1743	ASP
1	B	1759	LYS
1	B	1767	GLU
1	B	1768	ARG
1	B	1794	PHE
1	B	1826	PHE
1	B	1832	SER
1	B	1903	ASN
1	B	1997	SER
1	B	2051	GLU
1	B	2057	CYS
1	B	2078	CYS
1	B	2126	ARG
1	B	2229	LEU
1	B	2285	GLU
1	B	2295	ILE
1	B	2307	ASP
1	B	2346	PHE
1	B	2351	GLN
1	B	2369	SER
1	B	2390	ILE
1	B	2395	ILE
1	B	2397	THR
1	B	2424	LYS
1	B	2428	MET
1	B	2476	LYS
1	B	2566	SER
1	B	2576	LYS
1	B	2613	SER
1	B	2681	LEU
1	B	2694	LEU
1	B	2822	ILE
1	B	2843	LEU
1	B	2856	LEU
1	B	2865	LEU
1	B	2866	LEU
1	B	2873	LEU
1	B	2875	ASP

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Mol	Chain	Res	Type
1	B	2920	TRP
1	B	3301	PHE
1	B	3329	ILE
1	B	3372	THR
1	B	3391	LEU
1	B	3400	SER
1	B	3502	SER
1	B	3560	LYS
1	B	3598	GLU
1	B	3605	GLU
1	B	3673	GLU
1	B	3677	LEU
1	B	3729	SER
1	B	3737	THR
1	B	3744	LEU
1	B	3871	PHE
1	B	3899	ASP
1	B	3905	ASP
1	B	3906	THR
1	B	3917	THR
1	B	3943	THR
1	B	3960	ASP
1	B	3980	ILE
1	B	3982	TRP
1	B	4016	CYS
1	B	4024	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1449	GLN
1	A	1622	GLN
1	A	1646	GLN
1	A	1736	GLN
1	A	1745	ASN
1	A	1851	ASN
1	A	1873	GLN
1	A	1899	ASN
1	A	1951	HIS
1	A	1965	HIS
1	A	1979	ASN
1	A	2068	GLN

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Mol	Chain	Res	Type
1	A	2099	ASN
1	A	2228	HIS
1	A	2274	HIS
1	A	2282	ASN
1	A	2293	HIS
1	A	2383	HIS
1	A	2409	ASN
1	A	2459	HIS
1	A	2530	HIS
1	A	2536	ASN
1	A	2634	ASN
1	A	2683	ASN
1	A	2688	ASN
1	A	3323	ASN
1	A	3338	ASN
1	A	3497	HIS
1	A	3521	ASN
1	A	3542	GLN
1	A	3588	ASN
1	A	3624	HIS
1	A	3780	ASN
1	A	3890	GLN
1	A	4020	ASN
1	A	4077	GLN
1	B	1533	GLN
1	B	1605	GLN
1	B	1622	GLN
1	B	1646	GLN
1	B	1851	ASN
1	B	1864	ASN
1	B	1873	GLN
1	B	1899	ASN
1	B	2064	GLN
1	B	2068	GLN
1	B	2099	ASN
1	B	2228	HIS
1	B	2274	HIS
1	B	2282	ASN
1	B	2293	HIS
1	B	2383	HIS
1	B	2409	ASN
1	B	2536	ASN

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Mol	Chain	Res	Type
1	B	2598	HIS
1	B	2634	ASN
1	B	2683	ASN
1	B	2753	GLN
1	B	3323	ASN
1	B	3336	HIS
1	B	3521	ASN
1	B	3542	GLN
1	B	3624	HIS
1	B	3685	GLN
1	B	3780	ASN
1	B	3890	GLN
1	B	3962	GLN
1	B	3970	ASN
1	B	4020	ASN
1	B	4077	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 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
2	ATP	A	5093	4	27,33,33	1.16	2 (7%)	25,52,52	1.98	2 (8%)
3	SO4	A	5094	-	4,4,4	0.56	0	6,6,6	0.46	0
3	SO4	A	5095	-	4,4,4	0.56	0	6,6,6	0.70	0
3	SO4	A	5096	-	4,4,4	0.36	0	6,6,6	0.31	0
2	ATP	B	5093	4	27,33,33	0.96	2 (7%)	25,52,52	1.74	3 (12%)
3	SO4	B	5094	-	4,4,4	0.47	0	6,6,6	0.46	0
3	SO4	B	5095	-	4,4,4	0.43	0	6,6,6	0.25	0
3	SO4	B	5096	-	4,4,4	0.30	0	6,6,6	0.28	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
2	ATP	A	5093	4	-	0/18/38/38	0/3/3/3
3	SO4	A	5094	-	-	0/0/0/0	0/0/0/0
3	SO4	A	5095	-	-	0/0/0/0	0/0/0/0
3	SO4	A	5096	-	-	0/0/0/0	0/0/0/0
2	ATP	B	5093	4	-	0/18/38/38	0/3/3/3
3	SO4	B	5094	-	-	0/0/0/0	0/0/0/0
3	SO4	B	5095	-	-	0/0/0/0	0/0/0/0
3	SO4	B	5096	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5093	ATP	C2'-C1'	-2.08	1.50	1.53
2	B	5093	ATP	O4'-C1'	2.07	1.44	1.41
2	A	5093	ATP	C5-C4	2.31	1.45	1.40
2	B	5093	ATP	C5-C4	2.94	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5093	ATP	N3-C2-N1	-7.59	122.25	128.86
2	B	5093	ATP	N3-C2-N1	-6.50	123.20	128.86
2	A	5093	ATP	C4-C5-N7	-2.63	106.87	109.41
2	B	5093	ATP	C4-C5-N7	-2.22	107.26	109.41
2	B	5093	ATP	C2'-C3'-C4'	2.05	106.60	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5093	ATP	4	0
3	A	5094	SO4	4	0
3	A	5095	SO4	3	0
3	A	5096	SO4	2	0
2	B	5093	ATP	7	0
3	B	5095	SO4	2	0
3	B	5096	SO4	1	0

## 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2650/2695 (98%)	0.14	160 (6%)	23 16	80, 163, 325, 500	0
1	B	2650/2695 (98%)	0.37	229 (8%)	11 9	117, 210, 355, 500	0
All	All	5300/5390 (98%)	0.25	389 (7%)	16 11	80, 189, 342, 500	0

All (389) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	THR	18.5
1	B	155	TYR	17.3
1	B	35	ASP	17.2
1	B	143	ASN	16.5
1	B	31	LEU	16.3
1	B	67	SER	16.0
1	A	210	GLY	15.8
1	B	71	ILE	15.4
1	A	211	GLY	14.9
1	B	30	HIS	12.7
1	B	151	ASP	12.2
1	B	18	LEU	11.8
1	B	59	ASP	11.5
1	B	152	PHE	11.5
1	A	84	CYS	11.0
1	B	29	GLU	10.8
1	B	17	ARG	10.2
1	A	209	PHE	10.0
1	B	19	LEU	9.6
1	A	202	LEU	9.5
1	B	73	TYR	9.2
1	A	54	LEU	8.7
1	B	1579	ILE	8.5
1	B	154	LEU	8.5

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Mol	Chain	Res	Type	RSRZ
1	B	1581	GLY	8.0
1	B	1596	ILE	7.9
1	B	1572	ILE	7.8
1	B	34	ARG	7.8
1	B	72	ARG	7.7
1	A	216	PRO	7.7
1	B	159	ASP	7.6
1	B	158	LEU	7.6
1	B	74	ILE	7.5
1	A	215	PRO	7.5
1	A	85	PRO	7.4
1	B	1580	THR	7.1
1	B	149	HIS	7.0
1	B	1549	ILE	6.8
1	B	70	ILE	6.8
1	B	58	ILE	6.6
1	B	47	LEU	6.4
1	B	94	LEU	6.3
1	B	3580	ASN	6.3
1	B	1574	PHE	6.3
1	B	1483	TYR	6.1
1	B	20	LEU	6.1
1	A	138	HIS	5.8
1	B	14	GLN	5.8
1	B	2024	SER	5.8
1	A	1597	GLU	5.7
1	A	135	ARG	5.6
1	B	56	TYR	5.6
1	B	1452	TRP	5.5
1	B	3582	GLU	5.5
1	B	1459	LEU	5.5
1	B	2025	ALA	5.4
1	B	95	GLU	5.4
1	A	3580	ASN	5.3
1	B	2298	TYR	5.3
1	A	143	ASN	5.3
1	A	58	ILE	5.3
1	B	2844	PHE	5.3
1	B	61	ASP	5.2
1	B	75	ALA	5.2
1	A	59	ASP	5.2
1	A	3537	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	5.2
1	B	5	GLY	5.1
1	B	3581	ASP	5.1
1	A	131	MET	5.1
1	B	211	GLY	5.1
1	A	212	GLY	5.1
1	A	3594	ALA	5.1
1	A	1487	THR	5.0
1	B	87	GLU	5.0
1	B	3839	ILE	5.0
1	B	1558	VAL	5.0
1	B	1597	GLU	5.0
1	A	3584	MET	4.9
1	B	1546	LEU	4.8
1	B	81	LEU	4.8
1	A	134	ASP	4.8
1	B	22	TYR	4.7
1	A	83	GLY	4.7
1	B	144	GLY	4.7
1	B	1582	VAL	4.7
1	B	1601	SER	4.6
1	B	21	GLU	4.6
1	B	2808	LEU	4.6
1	B	108	ILE	4.6
1	B	1424	PHE	4.6
1	A	3567	LEU	4.5
1	A	208	THR	4.5
1	A	3587	LEU	4.5
1	B	53	ASN	4.5
1	A	3740	THR	4.4
1	A	1483	TYR	4.3
1	A	29	GLU	4.3
1	B	60	GLY	4.3
1	B	40	TRP	4.3
1	A	132	PHE	4.3
1	A	3563	GLU	4.3
1	B	1573	ILE	4.3
1	A	16	THR	4.3
1	B	1548	ILE	4.3
1	A	47	LEU	4.2
1	B	202	LEU	4.2
1	A	74	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	210	GLY	4.1
1	B	116	THR	4.1
1	A	3025	ASN	4.1
1	A	24	GLU	4.1
1	B	1545	LEU	4.1
1	A	203	GLN	4.1
1	A	139	LYS	4.0
1	B	6	TYR	4.0
1	B	16	THR	4.0
1	A	2364	ASP	4.0
1	A	108	ILE	4.0
1	B	33	GLU	4.0
1	A	168	CYS	4.0
1	A	27	TYR	4.0
1	B	1845	GLY	3.9
1	B	54	LEU	3.9
1	A	1598	LEU	3.9
1	A	63	LYS	3.9
1	B	145	ASP	3.9
1	A	52	PRO	3.8
1	A	109	ALA	3.8
1	A	2029	LEU	3.8
1	B	3534	LEU	3.8
1	B	1395	VAL	3.8
1	A	3744	LEU	3.7
1	B	38	ASP	3.7
1	B	43	LYS	3.7
1	B	2026	GLY	3.6
1	B	2863	LEU	3.6
1	B	1594	GLU	3.6
1	B	3540	GLU	3.6
1	B	3618	TYR	3.6
1	B	84	CYS	3.6
1	B	142	LEU	3.6
1	B	42	ASN	3.6
1	B	2115	TYR	3.6
1	B	37	GLY	3.6
1	A	61	ASP	3.6
1	A	2868	ASP	3.5
1	A	67	SER	3.5
1	A	173	PRO	3.5
1	B	3571	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	3589	ASN	3.5
1	B	91	ILE	3.5
1	B	46	GLU	3.5
1	B	1550	GLY	3.5
1	A	3581	ASP	3.5
1	B	1937	MET	3.5
1	A	3741	ASN	3.4
1	A	1572	ILE	3.4
1	A	148	THR	3.4
1	B	1592	LEU	3.4
1	B	8	LYS	3.4
1	B	2179	PRO	3.4
1	B	157	ALA	3.4
1	B	1551	SER	3.4
1	A	2030	ASN	3.3
1	B	3579	GLU	3.3
1	B	55	PRO	3.3
1	A	3784	ASN	3.3
1	B	1590	LEU	3.3
1	B	83	GLY	3.3
1	A	3731	ASP	3.3
1	A	1393	LYS	3.3
1	B	2355	ASP	3.3
1	B	1401	LEU	3.3
1	B	1647	ALA	3.3
1	A	3875	MET	3.3
1	B	52	PRO	3.2
1	B	88	ARG	3.2
1	A	37	GLY	3.2
1	A	3571	ASN	3.2
1	A	140	THR	3.2
1	A	1378	TRP	3.2
1	A	3734	PRO	3.2
1	B	132	PHE	3.2
1	B	156	ASP	3.2
1	B	1683	LEU	3.2
1	B	1500	ILE	3.2
1	A	22	TYR	3.2
1	B	3436	PHE	3.2
1	A	3566	LEU	3.1
1	A	23	LEU	3.1
1	B	3583	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	212	GLY	3.1
1	B	161	VAL	3.1
1	B	50	GLU	3.1
1	A	1458	ILE	3.1
1	B	2302	PHE	3.1
1	A	82	GLY	3.1
1	B	2241	LEU	3.1
1	B	1850	PHE	3.1
1	B	3475	ASN	3.1
1	A	3919	LYS	3.0
1	B	2859	LYS	3.0
1	A	62	VAL	3.0
1	A	5	GLY	3.0
1	B	135	ARG	3.0
1	B	164	MET	3.0
1	B	209	PHE	3.0
1	B	3840	LEU	3.0
1	A	115	GLU	3.0
1	A	79	ASN	3.0
1	B	3538	ASN	3.0
1	A	17	ARG	3.0
1	B	1669	PHE	3.0
1	A	3722	MET	2.9
1	A	60	GLY	2.9
1	B	66	GLN	2.9
1	A	18	LEU	2.9
1	A	1459	LEU	2.9
1	B	92	SER	2.9
1	A	49	LEU	2.9
1	B	1476	PHE	2.9
1	B	3578	LEU	2.9
1	A	53	ASN	2.9
1	A	31	LEU	2.9
1	A	1382	GLN	2.9
1	B	3816	LEU	2.8
1	B	203	GLN	2.8
1	B	1989	GLU	2.8
1	A	25	GLU	2.8
1	B	3841	LEU	2.8
1	B	63	LYS	2.8
1	A	30	HIS	2.8
1	B	57	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	32	TYR	2.8
1	A	3865	ALA	2.8
1	B	1394	LEU	2.8
1	A	3570	LEU	2.8
1	A	3300	THR	2.7
1	B	2029	LEU	2.7
1	B	3533	THR	2.7
1	A	55	PRO	2.7
1	B	3564	LYS	2.7
1	B	11	GLY	2.7
1	B	2795	PHE	2.7
1	A	1394	LEU	2.7
1	A	3899	ASP	2.7
1	B	150	PRO	2.7
1	A	40	TRP	2.7
1	A	91	ILE	2.7
1	B	2839	ASP	2.7
1	A	1445	TRP	2.7
1	A	3739	ASP	2.7
1	A	3321	ILE	2.7
1	B	1631	LYS	2.7
1	B	2151	TRP	2.7
1	A	174	LYS	2.7
1	B	1458	ILE	2.7
1	B	3584	MET	2.7
1	B	2030	ASN	2.7
1	A	149	HIS	2.7
1	A	2034	ILE	2.6
1	A	3556	LYS	2.6
1	A	3917	THR	2.6
1	A	20	LEU	2.6
1	B	1445	TRP	2.6
1	A	2120	LYS	2.6
1	B	3954	TYR	2.6
1	B	1595	LYS	2.6
1	A	33	GLU	2.6
1	B	3873	MET	2.6
1	B	2246	LEU	2.6
1	A	3555	TYR	2.6
1	A	3297	LYS	2.6
1	A	3024	LEU	2.6
1	B	15	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2840	ILE	2.6
1	A	2942	ASP	2.6
1	A	2363	ASN	2.5
1	A	71	ILE	2.5
1	B	3617	GLU	2.5
1	B	2102	TYR	2.5
1	B	1893	ALA	2.5
1	B	2941	THR	2.5
1	A	175	LEU	2.5
1	A	3561	ASN	2.5
1	B	1505	PHE	2.5
1	B	1760	PHE	2.5
1	B	1730	LYS	2.5
1	B	1593	ASN	2.5
1	A	3016	PHE	2.5
1	B	3541	MET	2.5
1	B	1479	LEU	2.4
1	A	3572	ASN	2.4
1	B	3359	LYS	2.4
1	B	1627	LEU	2.4
1	B	68	MET	2.4
1	A	4035	GLN	2.4
1	B	115	GLU	2.4
1	B	3874	PHE	2.4
1	B	62	VAL	2.4
1	B	2295	ILE	2.4
1	A	10	LYS	2.4
1	A	178	PHE	2.4
1	A	3018	ASN	2.4
1	A	92	SER	2.4
1	B	1934	LEU	2.4
1	A	3874	PHE	2.4
1	B	127	GLU	2.3
1	A	137	CYS	2.3
1	A	1392	LEU	2.3
1	B	1383	TYR	2.3
1	A	3299	LEU	2.3
1	B	4	LEU	2.3
1	A	3979	ASN	2.3
1	A	28	GLU	2.3
1	A	136	LEU	2.3
1	B	48	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	79	ASN	2.3
1	B	3542	GLN	2.3
1	B	1949	ILE	2.3
1	A	3542	GLN	2.3
1	A	144	GLY	2.2
1	A	38	ASP	2.2
1	B	1390	SER	2.2
1	B	2817	ILE	2.2
1	B	1435	LEU	2.2
1	B	208	THR	2.2
1	A	1596	ILE	2.2
1	A	3588	ASN	2.2
1	B	2439	ASP	2.2
1	A	48	GLY	2.2
1	B	2257	PHE	2.2
1	B	2299	ARG	2.2
1	A	2179	PRO	2.2
1	B	1828	TYR	2.2
1	B	171	ALA	2.2
1	B	3565	ARG	2.2
1	A	3021	LEU	2.2
1	A	3022	GLU	2.2
1	B	3923	VAL	2.2
1	B	2245	GLU	2.2
1	A	21	GLU	2.2
1	B	1995	VAL	2.2
1	B	2856	LEU	2.2
1	A	182	ILE	2.2
1	B	39	LYS	2.2
1	B	3566	LEU	2.2
1	A	3737	THR	2.1
1	A	3569	GLU	2.1
1	A	2102	TYR	2.1
1	B	3814	ILE	2.1
1	B	78	HIS	2.1
1	A	2121	ALA	2.1
1	B	2918	GLY	2.1
1	A	3298	SER	2.1
1	B	1449	GLN	2.1
1	A	1421	TYR	2.1
1	B	1441	ILE	2.1
1	A	2362	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	75	ALA	2.1
1	A	3573	SER	2.1
1	B	2256	SER	2.1
1	B	7	TRP	2.1
1	B	2845	GLN	2.1
1	A	1387	GLU	2.1
1	B	1421	TYR	2.1
1	B	2318	ILE	2.1
1	B	1423	ILE	2.1
1	A	181	ARG	2.1
1	B	3574	GLN	2.1
1	A	50	GLU	2.1
1	B	153	MET	2.0
1	B	2843	LEU	2.0
1	B	128	MET	2.0
1	A	1548	ILE	2.0
1	B	1571	SER	2.0
1	A	3593	GLU	2.0
1	A	1582	VAL	2.0
1	B	1460	GLY	2.0
1	A	214	HIS	2.0
1	A	1578	PHE	2.0
1	A	3723	ILE	2.0
1	A	1435	LEU	2.0
1	B	1437	LYS	2.0
1	B	1578	PHE	2.0
1	B	2889	PHE	2.0
1	B	1513	ILE	2.0
1	B	3537	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	A	5097	1/1	0.99	0.40	3.20	59,59,59,59	0
3	SO4	A	5095	5/5	0.95	0.40	2.26	108,128,132,133	0
2	ATP	A	5093	31/31	0.95	0.32	1.55	72,125,180,196	0
3	SO4	B	5095	5/5	0.90	0.24	1.14	155,178,186,207	0
3	SO4	A	5094	5/5	0.95	0.29	0.93	109,114,153,161	0
2	ATP	B	5093	31/31	0.93	0.28	0.68	115,184,238,261	0
4	MG	B	5097	1/1	0.98	0.24	0.43	127,127,127,127	0
3	SO4	B	5094	5/5	0.86	0.30	0.27	151,165,190,192	0
3	SO4	A	5096	5/5	0.83	0.22	0.14	128,136,144,154	0
3	SO4	B	5096	5/5	0.96	0.14	-0.53	158,193,224,235	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.