



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:39 PM UTC

PDB ID : 8SEP / pdb_00008sep
EMDB ID : EMD-40424
Title : Cryo-EM Structure of RyR1 + ADP
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.57 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

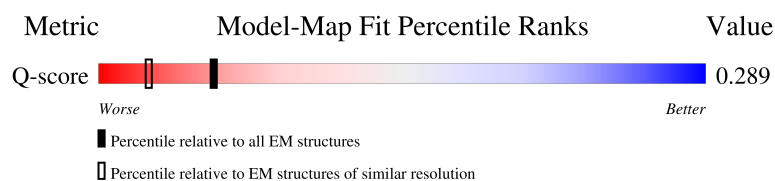
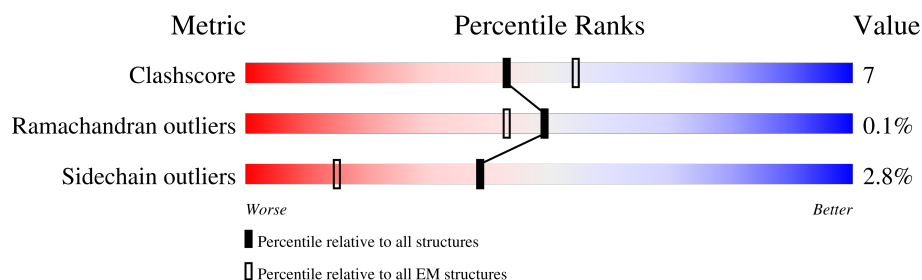
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.57 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12682 (3.07 - 4.07)

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

Mol	Chain	Length	Quality of chain
1	A	5037	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	350	 22%8%69%
2	F	350	 22%8%69%
2	G	350	 23%8%69%
2	H	350	 22%8%69%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 143100 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	B	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	C	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		
1	D	4379	Total	C	N	O	S	9	0
			34929	22223	6026	6444	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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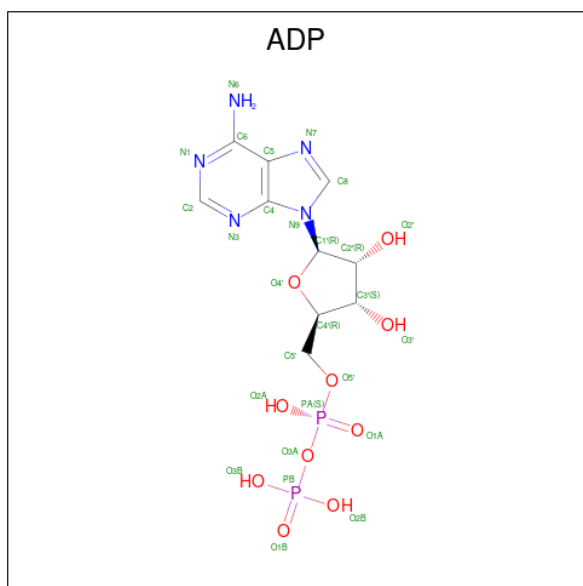
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

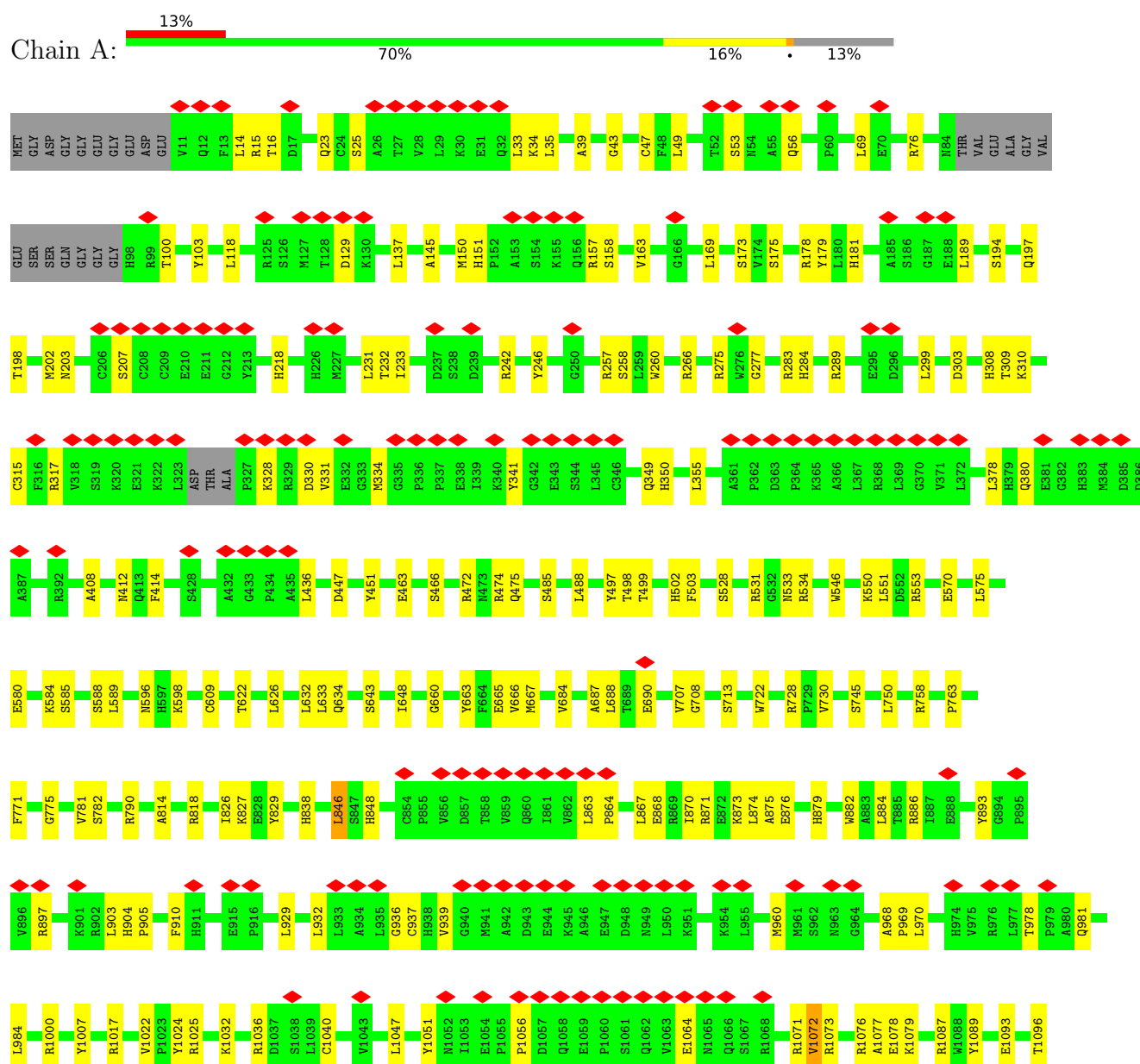


Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0

3 Residue-property plots

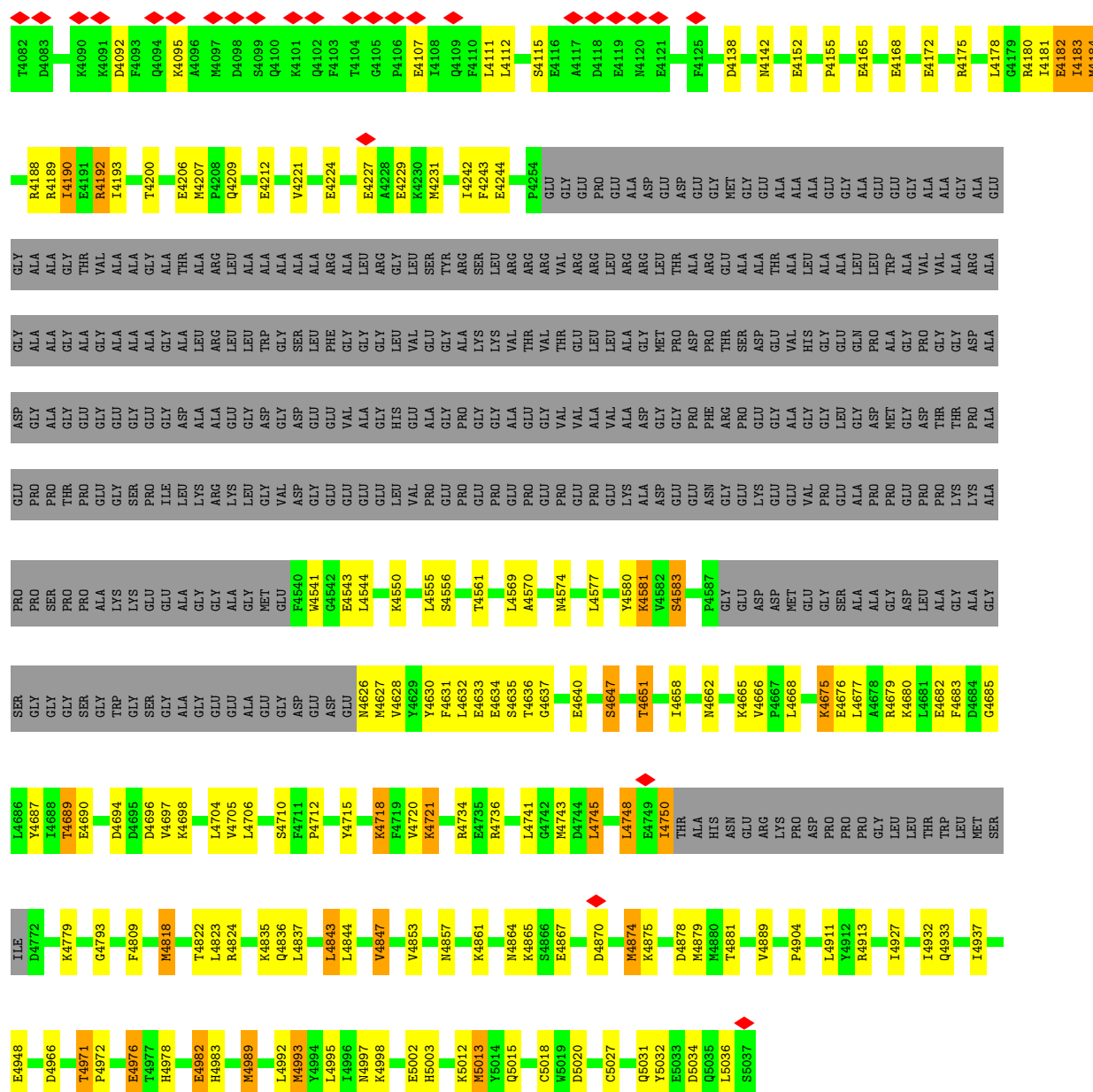
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Ryanodine receptor 1





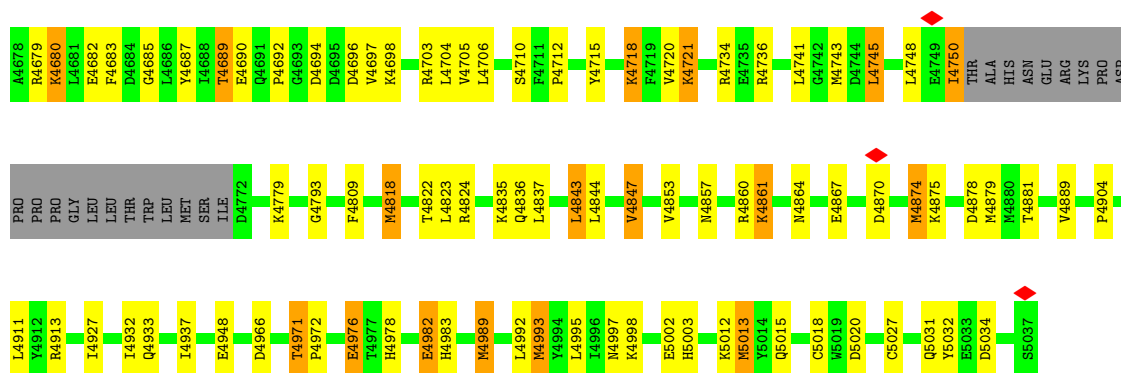
L3990	Q3766	R3637	G3561	K3477	R2448	H3146	G3028	A2936	E2876	M2816	W2755
L3891	Q3767	M3638	K3562	M3478	L3249	H3149	H3033	V2937	Q2877	L2817	W2756
F3899	R3768	L3641	V3563	A3479	M3250	H3150		T2938	L2878	A2818	K2757
L3924	H3770	M3652	E3564	LYS	S2559	Q3151	E3037	R2939	A2879	W2819	
S3929	T3772	E3655	G3565	ALA	I3270	Q3151	M3038	LEU	E2880	E2820	E2760
W3935	R3773	E3655	S3568	GLY	L3274	V3156	L3042	LYS	W2881	W2821	Y2761
W3935	M3782	A3659	Q3571	ASP	L3274	I3157		ASP	T2882	T2822	T2762
K3940	G3788	S3660	K3573	ALA	Y3280	V3161	K3045	MET	H2883	L2823	H2763
E3967	M3793	W3661	M3573	K3384	L2881	Q3162	L3046	GLY	T2884	E2824	E2764
L3980	G3801	L3662	L3579	A3386	P2882			L2946	N2885	K2825	K2765
R3984	D3676	L3663	R3582	SER	W2885	W3160	L3049	D2947	W2886	A2826	W2766
L3805	A3680	E3681	E3583	GLN	E3290	V3183	W3050	T2948	A2767	R2827	A2767
N3809	G3681	E3682	E3584	GLU	A3291	E3184	R3051	S2949	R2888	E2828	T2768
V3812	E3682	E3683	D3585	THR	P3292	K3185	R3053	E2952	K2889	G2829	D2769
L3817	Q3683	E3684	D3586	LYS	P3293	L3186	L3056	L2960	K2891	GLU	W2770
K3823	E3685	E3686	D3587	LYS	P3294	L3190	T3059	Q2961	Q2892	GLU	I2771
L3835	E3686	E3687	I3592	LYS	A3295	L3194	P3062	L2964	E2893	THR	W2773
S3840	E3688	E3689	R3595	LYS	L3296	L3197	V3065	L2965	L2894	GLU	W2774
W3841	E3690	E3691	V3596	LYS	A3298	A3204		W2966	E2895	LYS	W2775
L3842	E3692	E3693	L3606	LYS	P3297	F3205	L3068	M2967	K2896	LYS	S2776
A3846	E3694	E3695	E3607	LYS	A3300	L3206	H3069		A2897	LYS	W2777
Q3850	E3696	E3697	Q3608	LYS	P3301	E3207	L3075	S2970	G2898	ARG	Q2778
M3858	E3698	E3699	T3609	LYS	P3302	L3210	L3076	Q2971	Q2899	ILE	E2779
V3859	E3700	E3701	E3610	LYS	P3303		A3077	I2974	G2900	SER	W2780
N3860	E3702	E3703	E3611	LYS	C3304	Y3213	R3078	E2978	T2901	GLN	V2781
E3861	E3704	E3705	P3612	LYS	S3309	N3214		A2979	H2902	THR	D2782
D3862	E3706	E3707	L3613	LYS	I3322	A3215	M3081	V2980	P2903	ALA	E2783
G3863	E3708	E3709	K3614	LYS	I3323	C3216	K3082	V2981	L2904	GLN	E2784
T3864	E3710	E3711	K3615	LYS	N3324	S3217	S3083	S2982	L2905	THR	L2785
V3865	E3712	E3713	E3616	LYS	W3325	V3218	E3086	Q2984	V2906	ASP	K2786
L3866	E3714	E3715	E3617	LYS	N3326	Y3219	I3087	R2985	P2907	PIR	T2787
N3867	E3716	E3717	E3618	LYS	L3327	T3220	R3093	V2986	D2908	GLU	H2788
R3868	E3718	E3719	E3619	LYS	G3328	T3221		E2987	T2910	GLY	F2789
Q3869	E3720	E3721	E3620	LYS	I3329	K3222	M3106	K2988	L2911	Y2855	W2790
N3870	E3722	E3723	E3621	LYS	D3330	S3223	G3113	S2989	T2912	N2856	L2791
E3871	E3724	E3725	E3622	LYS	M3335	P3224	K3114	P2990	A2913	P2857	R2792
R3872	E3726	E3727	E3623	LYS	A3339	R3225	V3115	H2991	K2914	Q2858	F2793
K3873	E3728	E3729	E3624	LYS	V3340	A3228	S3116	E2992	E2915	P2860	Y2794
W3874	E3730	E3731	E3625	LYS	I3345	L3229	ALA	Q2993	K2916	D2861	T2796
M3875	E3732	E3733	E3626	LYS	I3346	L3230	ARG	F2997	A2917	L2862	F2797
E3876	E3734	E3735	E3627	LYS	R3348	G3231	THR		R2918	S2863	S2798
A3877	E3736	E3737	E3628	LYS	A3349	L3232	VAL	I3001	D2919	G2864	E2799
D3878	E3738	E3739	E3629	LYS	P3350	P3233	K3123	T3020	R2920	V2865	K2800
Q3889	E3740	E3741	E3630	LYS	L3354	E3238	L3129	P3021	E2921	L2867	D2801
			E3631	LYS	F3358	K3239	Y3131	A3022	K2922	S2868	K2802
			E3632	LYS		V3245		K3023	A2923	R2869	E2803
			E3633	LYS		L3246		V3024	Q2924	E2870	L2804
			E3634	LYS		D3247		L3025	L2926	Y2805	R2806
			E3635	LYS				G3026	L2927	Q2872	W2807
				LYS					K2928	A2873	P2808
				LYS					F2929	M2874	L2809
				LYS					L2930	E2811	K2810
				LYS					Q2931	Q2872	E2812
				LYS					M2932	L2813	L2813
				LYS					G2934	K2814	A2815



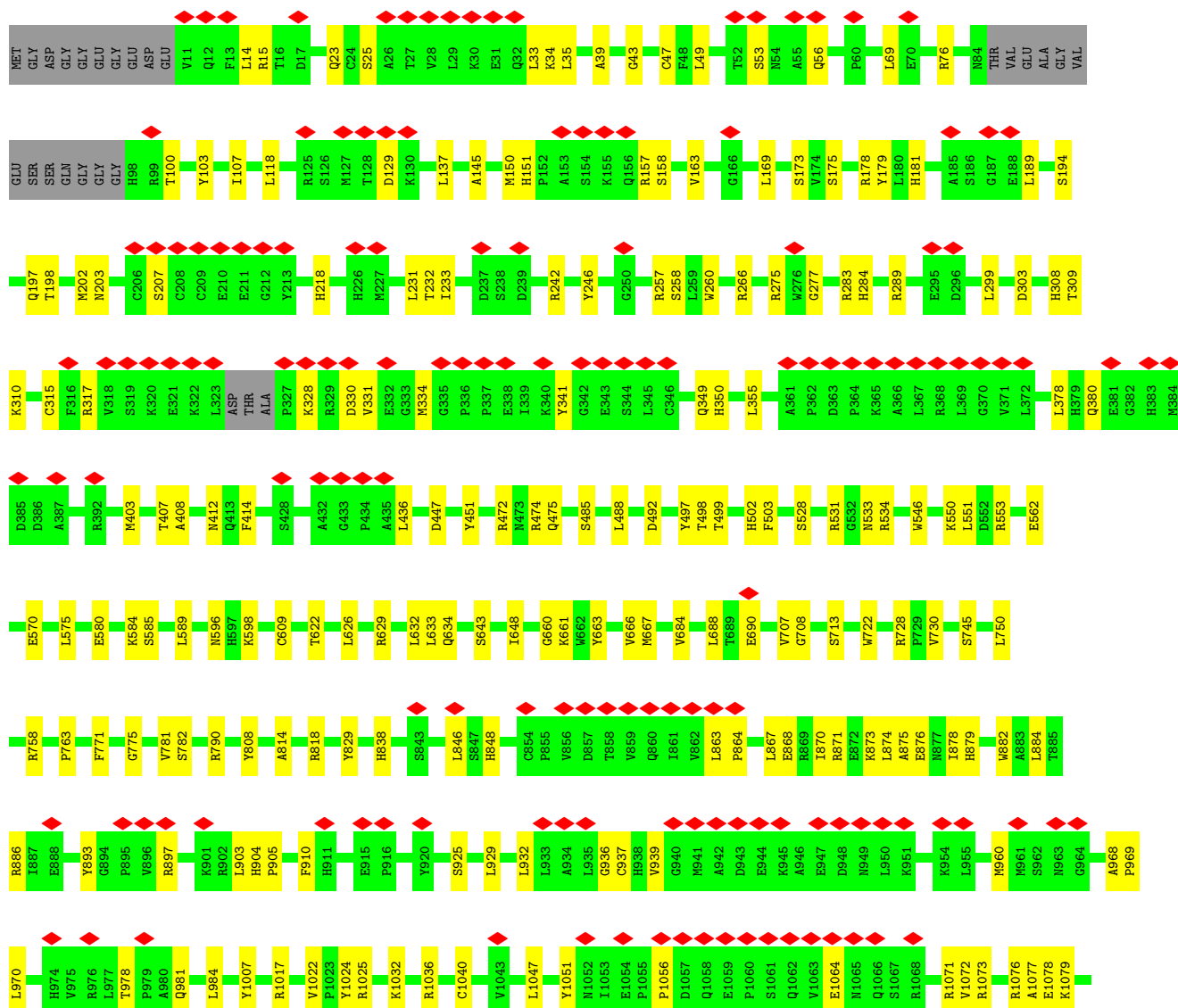








• Molecule 1: Ryanodine receptor 1



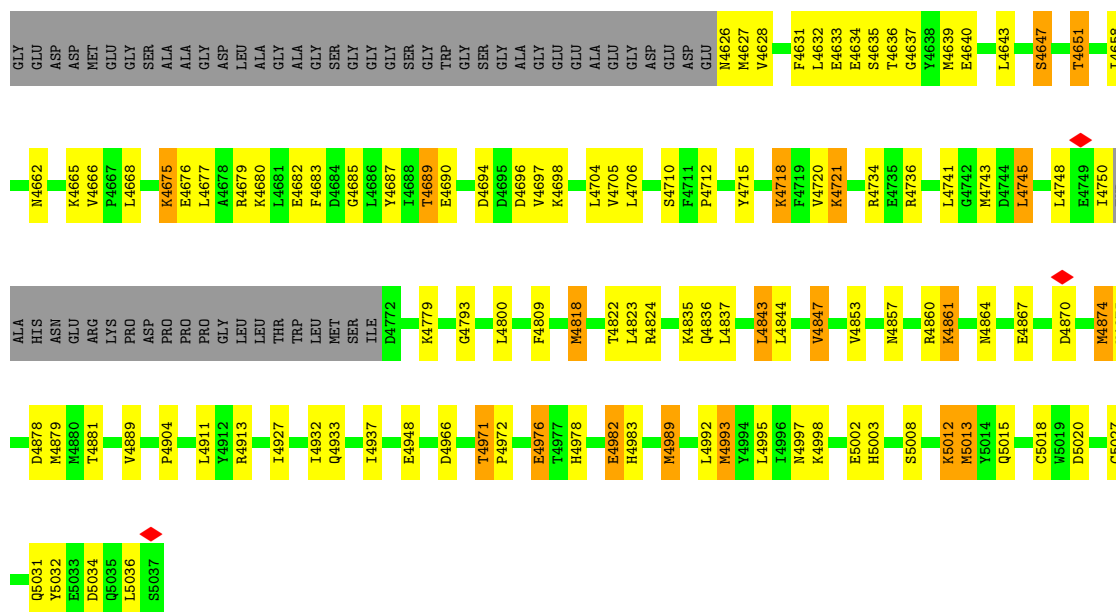


G3871	E3872	K3873	V3874	K3875	A3876	D3877	D3878	S3879	E3880	E3881	E3882	E3883	E3884	E3885	E3886	E3887	E3888	E3889	E3890	E3891	E3892	E3893	E3894	E3895	E3896	E3897	E3898	E3899	E3900	E3901	E3902	E3903	E3904	E3905	E3906	E3907	E3908	E3909	E3910	E3911	E3912	E3913	E3914	E3915	E3916	E3917	E3918	E3919	E3920										
GLU	GLU	GLU	GLU	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3757	K3760	Q3766	Q3767	Q3768	R3769	L3770	H3771	L3772	R3773	G3788	G3801	L3805	N3809	V3812	L3817	L3835	S3840	V3841	L3842	A3846	Q3850	M3858	V3859	N3860	E3861	E3862	Q3863	T3864	V3865	L3866	N3867	R3868	Q3869	N3870													
H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	H3638	L3641	M3652	E3655	A3659	A3660	V3661	L3662	L3663	D3676	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	D3696	C3703	E3736	GLU	GLY	GLU	ASN	GLY	GLU	ALA										
K3537	T3538	R3539	Y3540	A3541	L3542	K3543	E3548	V3549	R3550	E3551	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	V3563	E3564	G3565	M3573	L3579	R3582	E3583	E3584	D3585	A3586	D3587	I3589	R3595	V3596	L3603	Y3604	H3605	L3606	E3607	Q3608	T3609	E3610	H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620									
N3457	F3458	V3459	V3460	Q3461	N3462	K3463	N3464	N3465	N3466	M3467	R3468	F3469	L3470	T3471	D3472	D3473	S3474	K3475	S3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	GLY	ASP	GLN	GLU	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	Q3506	K3515	N3523	M3524	F3525	R3527	D3531	L3532	I3533	M3534					
G3328	L3329	D3330	M3335	A3339	E3340	I3345	R3348	A3349	R3350	P3351	L3354	F3358	I3362	E3377	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	R3389	R3395	R3403	D3404	L3405	L3408	Y3409	I3413	R3414	D3417	N3418	L3424	E3433	L3434	F3435	R3436	R3453	E3454																		
V3218	Y3219	T3220	K3221	K3222	K3223	P3224	R3225	A3228	I3229	L3230	G3231	L3232	P3233	E3238	M3239	V3245	L3246	D3247	R3248	L3249	M3250	S3259	I3270	L3274	Y3280	L3281	P3282	W3285	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	I3322	K3323	V3324	M3325	N3326	L3327										
R3093	M3106	V3107	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	L3129	F3130	Y3131	H3146	Q3149	H3150	Q3151	V3156	I3157	V3161	Q3162	S3171	N3180	V3183	E3184	K3185	L3186	L3190	L3194	L3197	K3204	F3205	L3206	E3207	L3210	Y3213	N3214	A3215	C3216	S3217																
E2992	Q2993	F2997	I3001	N3007	T3011	T3020	P3021	A3022	K3023	V3024	L3025	G3026	S3027	G3028	N3033	E3037	M3038	L3042	K3045	L3046	L3049	V3050	R3051	H3052	R3053	L3056	T3059	P3062	V3065	L3068	H3069	L3075	D3076	A3077	R3078	M3081	K3082	S3083	E3086	I3087																			
E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	M2933	Q2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	L2946	D2947	T2948	S2949	E2952	L2960	Q2961	Q2962	L2963	L2964	R2965	W2966	N2967	S2970	Q2971	I2974	E2978	A2979	V2980	Y2981	S2982	S2983	V2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991						
D2861	L2862	S2863	Q2864	T2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	G2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920
D2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	Y2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	
V2740	E2741	T2742	L2743	V2744	V2745	I2746	I2747	P2748	E2749	K2750	L2751	S2752	D2753	F2754	I2755	K2756	K2757	E2760	Y2761	T2762	H2763	E2764	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	E2779	N2780	W2781	D2782	E2783	L2784	L2785	K2786	T2787	H2788	P2789	K2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800			







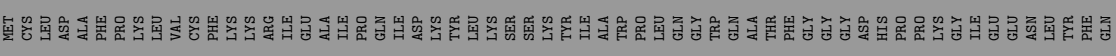
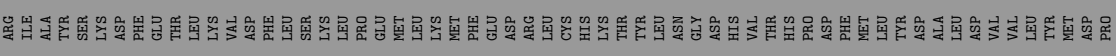
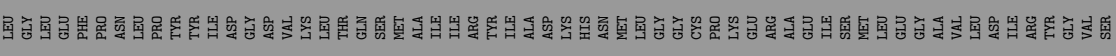
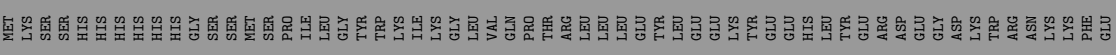


- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

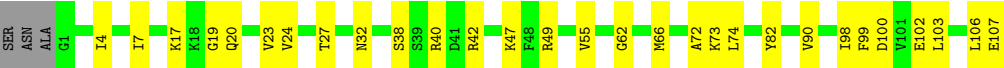
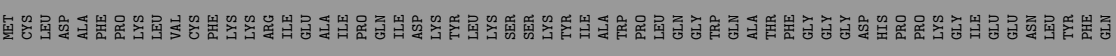
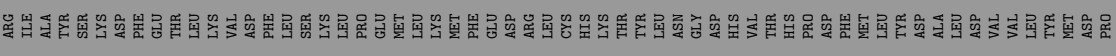
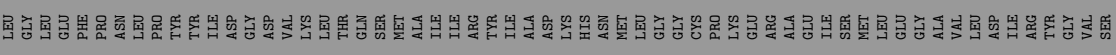
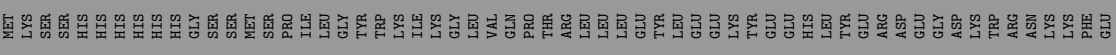
- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



● Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



● Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171805	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.602	Depositor
Minimum map value	-0.818	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.263	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.28	0/35746	0.62	7/48409 (0.0%)
1	B	0.28	0/35746	0.62	7/48409 (0.0%)
1	C	0.28	0/35746	0.62	8/48409 (0.0%)
1	D	0.28	0/35746	0.62	7/48409 (0.0%)
2	E	0.23	0/834	0.54	0/1123
2	F	0.23	0/834	0.54	0/1123
2	G	0.23	0/834	0.54	0/1123
2	H	0.23	0/834	0.54	0/1123
All	All	0.27	0/146320	0.62	29/198128 (0.0%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4581	LYS	CA-CB-CG	6.83	127.76	114.10
1	C	4581	LYS	CA-CB-CG	6.83	127.75	114.10
1	A	4581	LYS	CA-CB-CG	6.82	127.75	114.10
1	D	4581	LYS	CA-CB-CG	6.81	127.72	114.10
1	D	4184	MET	CA-C-N	-6.10	116.74	122.17
1	D	4184	MET	C-N-CA	-6.10	116.74	122.17
1	A	4184	MET	CA-C-N	-6.10	116.74	122.17
1	A	4184	MET	C-N-CA	-6.10	116.74	122.17
1	B	4184	MET	CA-C-N	-6.04	116.79	122.17
1	B	4184	MET	C-N-CA	-6.04	116.79	122.17
1	C	4184	MET	CA-C-N	-6.04	116.79	122.17
1	C	4184	MET	C-N-CA	-6.04	116.79	122.17
1	D	4581	LYS	CB-CG-CD	5.46	123.87	111.30
1	C	4581	LYS	CB-CG-CD	5.45	123.83	111.30
1	A	4581	LYS	CB-CG-CD	5.44	123.81	111.30
1	B	4581	LYS	CB-CG-CD	5.44	123.81	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1022	VAL	N-CA-C	-5.31	104.83	109.19
1	B	1022	VAL	N-CA-C	-5.26	104.88	109.19
1	C	1022	VAL	N-CA-C	-5.24	104.89	109.19
1	A	1022	VAL	N-CA-C	-5.21	104.92	109.19
1	B	905	PRO	N-CA-C	5.12	123.03	112.47
1	C	905	PRO	N-CA-C	5.12	123.03	112.47
1	D	905	PRO	N-CA-C	5.12	123.03	112.47
1	D	3622	LYS	CA-CB-CG	5.12	124.34	114.10
1	A	3622	LYS	CA-CB-CG	5.11	124.32	114.10
1	B	3622	LYS	CA-CB-CG	5.10	124.31	114.10
1	C	3622	LYS	CA-CB-CG	5.09	124.27	114.10
1	A	905	PRO	N-CA-C	5.08	122.94	112.47
1	C	4694	ASP	CB-CA-C	5.02	114.80	109.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	34929	0	34552	453	0
1	B	34929	0	34552	457	0
1	C	34929	0	34552	460	0
1	D	34929	0	34552	464	0
2	E	818	0	824	20	0
2	F	818	0	824	21	0
2	G	818	0	824	21	0
2	H	818	0	824	21	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	143100	0	141552	1879	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 7.

All (1879) 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:B:2248:ARG:HB3	1:B:2286:LEU:HD11	1.72	0.71
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.72	0.71
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.72	0.71
1:D:2248:ARG:HB3	1:D:2286:LEU:HD11	1.72	0.71
1:A:2248:ARG:HB3	1:A:2286:LEU:HD11	1.72	0.71
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.72	0.71
1:C:2248:ARG:HB3	1:C:2286:LEU:HD11	1.72	0.71
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.72	0.70
1:A:76:ARG:HG2	1:D:3935:TRP:HB3	1.72	0.70
1:B:1520:VAL:HG12	1:B:1527:MET:HG3	1.76	0.68
1:D:1520:VAL:HG12	1:D:1527:MET:HG3	1.75	0.68
1:C:1520:VAL:HG12	1:C:1527:MET:HG3	1.76	0.68
1:A:1520:VAL:HG12	1:A:1527:MET:HG3	1.76	0.67
1:C:3935:TRP:HB3	1:D:76:ARG:HG2	1.77	0.66
1:B:3935:TRP:HB3	1:C:76:ARG:HG2	1.77	0.66
1:D:3980:LEU:HD12	1:D:3985:LEU:HD22	1.77	0.66
1:A:3454:GLU:HA	1:A:3457:ASN:HB2	1.78	0.66
1:A:3935:TRP:HB3	1:B:76:ARG:HG2	1.77	0.66
1:C:3980:LEU:HD12	1:C:3985:LEU:HD22	1.77	0.66
1:B:3454:GLU:HA	1:B:3457:ASN:HB2	1.78	0.65
1:C:3454:GLU:HA	1:C:3457:ASN:HB2	1.78	0.65
1:D:3454:GLU:HA	1:D:3457:ASN:HB2	1.78	0.65
1:B:475:GLN:NE2	1:B:528:SER:O	2.30	0.65
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.78	0.65
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.78	0.65
1:A:3980:LEU:HD12	1:A:3985:LEU:HD22	1.77	0.65
1:B:3980:LEU:HD12	1:B:3985:LEU:HD22	1.77	0.65
1:A:475:GLN:NE2	1:A:528:SER:O	2.30	0.65
1:D:475:GLN:NE2	1:D:528:SER:O	2.30	0.65
1:C:475:GLN:NE2	1:C:528:SER:O	2.30	0.64
1:A:34:LYS:H	1:A:53:SER:HB3	1.63	0.64
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.78	0.64
1:C:3395:ARG:HE	1:C:3453:ARG:HH12	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3395:ARG:HE	1:B:3453:ARG:HH12	1.45	0.64
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.31	0.64
1:B:34:LYS:H	1:B:53:SER:HB3	1.63	0.64
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.78	0.64
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.31	0.64
1:C:3362:ILE:HD11	1:C:3408:LEU:HD22	1.80	0.64
1:D:3395:ARG:HE	1:D:3453:ARG:HH12	1.45	0.64
1:D:3362:ILE:HD11	1:D:3408:LEU:HD22	1.80	0.63
1:A:3362:ILE:HD11	1:A:3408:LEU:HD22	1.79	0.63
1:C:34:LYS:H	1:C:53:SER:HB3	1.63	0.63
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.31	0.63
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.72	0.63
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.80	0.63
1:B:1246:GLU:HB2	1:B:1601:MET:HE1	1.80	0.63
1:D:1064:GLU:O	1:D:1071:ARG:NH2	2.32	0.63
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.72	0.63
1:C:3753:PHE:HA	1:C:3756:LYS:HB3	1.81	0.63
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.80	0.63
1:C:4878:ASP:HB3	1:C:4881:THR:HG22	1.81	0.63
1:D:1432:THR:HA	1:D:1520:VAL:O	1.99	0.63
1:B:1432:THR:HA	1:B:1520:VAL:O	1.99	0.62
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.80	0.62
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.31	0.62
1:A:1246:GLU:HB2	1:A:1601:MET:HE1	1.80	0.62
1:B:1078:GLU:OE2	1:B:1237:TRP:NE1	2.32	0.62
1:B:3362:ILE:HD11	1:B:3408:LEU:HD22	1.80	0.62
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.80	0.62
1:C:1078:GLU:OE2	1:C:1237:TRP:NE1	2.32	0.62
1:D:1078:GLU:OE2	1:D:1237:TRP:NE1	2.32	0.62
1:D:3246:LEU:HG	1:D:3250:MET:HE1	1.81	0.62
1:B:3753:PHE:HA	1:B:3756:LYS:HB3	1.81	0.62
1:D:34:LYS:H	1:D:53:SER:HB3	1.63	0.62
1:D:1246:GLU:HB2	1:D:1601:MET:HE1	1.80	0.62
1:A:1432:THR:HA	1:A:1520:VAL:O	1.99	0.62
1:A:3395:ARG:HE	1:A:3453:ARG:HH12	1.45	0.62
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.72	0.62
1:A:3875:MET:HB3	1:A:3878:ASP:HB3	1.82	0.62
1:A:4878:ASP:HB3	1:A:4881:THR:HG22	1.81	0.62
1:B:580:GLU:HG3	1:B:584:LYS:HZ2	1.65	0.62
2:H:20:GLN:HG3	2:H:106:LEU:HD13	1.82	0.62
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:GLU:OE2	1:A:1237:TRP:NE1	2.32	0.62
1:B:3659:ALA:HA	1:B:3663:LEU:HD12	1.82	0.62
1:B:3875:MET:HB3	1:B:3878:ASP:HB3	1.82	0.62
1:D:4878:ASP:HB3	1:D:4881:THR:HG22	1.81	0.62
2:G:20:GLN:HG3	2:G:106:LEU:HD13	1.82	0.62
1:A:580:GLU:HG3	1:A:584:LYS:HZ2	1.65	0.62
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.18	0.62
1:A:3753:PHE:HA	1:A:3756:LYS:HB3	1.81	0.62
1:B:1064:GLU:O	1:B:1071:ARG:NH2	2.32	0.62
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.18	0.61
1:B:3414:ARG:O	1:B:3418:ASN:ND2	2.33	0.61
1:C:3114:LYS:HD3	1:C:3116:SER:H	1.66	0.61
1:C:3659:ALA:HA	1:C:3663:LEU:HD12	1.82	0.61
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.72	0.61
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	1.82	0.61
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.34	0.61
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.82	0.61
1:B:4878:ASP:HB3	1:B:4881:THR:HG22	1.81	0.61
1:C:1432:THR:HA	1:C:1520:VAL:O	1.99	0.61
1:C:3246:LEU:HG	1:C:3250:MET:HE1	1.81	0.61
1:A:3414:ARG:O	1:A:3418:ASN:ND2	2.33	0.61
1:B:1289:LEU:HD22	1:B:1562:ILE:HD11	1.83	0.61
1:B:3246:LEU:HG	1:B:3250:MET:HE1	1.81	0.61
1:B:3680:ALA:HB2	1:B:3696:ASP:HB3	1.83	0.61
1:B:4823:LEU:HD22	1:C:4843:LEU:HD22	1.82	0.61
1:A:3842:LEU:HB2	1:A:3929:SER:HB3	1.83	0.61
1:C:1246:GLU:HB2	1:C:1601:MET:HE1	1.80	0.61
1:C:3875:MET:HB3	1:C:3878:ASP:HB3	1.82	0.61
2:E:20:GLN:HG3	2:E:106:LEU:HD13	1.82	0.61
1:A:3114:LYS:HD3	1:A:3116:SER:H	1.66	0.61
1:A:3246:LEU:HG	1:A:3250:MET:HE1	1.81	0.61
1:C:580:GLU:HG3	1:C:584:LYS:HZ2	1.66	0.61
1:D:3680:ALA:HB2	1:D:3696:ASP:HB3	1.83	0.61
1:A:1568:LYS:HE2	1:A:1574:PRO:HD3	1.83	0.61
1:D:3875:MET:HB3	1:D:3878:ASP:HB3	1.82	0.61
2:F:20:GLN:HG3	2:F:106:LEU:HD13	1.82	0.61
1:C:4823:LEU:HD22	1:D:4843:LEU:HD22	1.82	0.61
1:D:580:GLU:HG3	1:D:584:LYS:HZ2	1.65	0.61
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.33	0.61
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	1.82	0.61
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1064:GLU:O	1:C:1071:ARG:NH2	2.32	0.60
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.18	0.60
1:C:1289:LEU:HD22	1:C:1562:ILE:HD11	1.83	0.60
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.18	0.60
1:D:3753:PHE:HA	1:D:3756:LYS:HB3	1.81	0.60
1:D:3733:CYS:O	1:D:3766:GLN:NE2	2.34	0.60
1:D:3842:LEU:HB2	1:D:3929:SER:HB3	1.83	0.60
1:D:3114:LYS:HD3	1:D:3116:SER:H	1.65	0.60
1:B:3114:LYS:HD3	1:B:3116:SER:H	1.65	0.60
1:C:3414:ARG:O	1:C:3418:ASN:ND2	2.33	0.60
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.82	0.60
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.84	0.60
1:A:3680:ALA:HB2	1:A:3696:ASP:HB3	1.83	0.60
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.83	0.60
1:D:1568:LYS:HE2	1:D:1574:PRO:HD3	1.83	0.60
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.33	0.60
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.84	0.60
1:B:3350:ARG:HE	1:B:3351:PRO:HD2	1.67	0.60
1:C:317:ARG:NH1	1:C:349:GLN:OE1	2.35	0.60
1:D:317:ARG:NH1	1:D:349:GLN:OE1	2.35	0.60
1:D:3350:ARG:HE	1:D:3351:PRO:HD2	1.67	0.60
1:A:1289:LEU:HD22	1:A:1562:ILE:HD11	1.83	0.60
1:A:3350:ARG:HE	1:A:3351:PRO:HD2	1.67	0.60
1:A:3733:CYS:O	1:A:3766:GLN:NE2	2.35	0.60
1:B:882:TRP:O	1:B:886:ARG:NH1	2.34	0.60
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.84	0.60
1:C:3842:LEU:HB2	1:C:3929:SER:HB3	1.83	0.60
1:A:1064:GLU:O	1:A:1071:ARG:NH2	2.32	0.60
1:B:3733:CYS:O	1:B:3766:GLN:NE2	2.35	0.60
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.35	0.60
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.35	0.60
1:C:882:TRP:O	1:C:886:ARG:NH1	2.34	0.60
1:D:882:TRP:O	1:D:886:ARG:NH1	2.34	0.60
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.84	0.59
1:C:3350:ARG:HE	1:C:3351:PRO:HD2	1.67	0.59
1:C:3733:CYS:O	1:C:3766:GLN:NE2	2.34	0.59
1:B:3872:GLU:HG3	1:B:3874:VAL:H	1.68	0.59
1:C:3680:ALA:HB2	1:C:3696:ASP:HB3	1.83	0.59
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.84	0.59
1:A:882:TRP:O	1:A:886:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.35	0.59
1:C:3872:GLU:HG3	1:C:3874:VAL:H	1.67	0.59
1:D:3872:GLU:HG3	1:D:3874:VAL:H	1.68	0.59
1:D:4244:GLU:HG3	1:D:4668:LEU:HD13	1.84	0.59
1:A:317:ARG:NH1	1:A:349:GLN:OE1	2.35	0.59
1:A:1545:ASN:HD21	2:E:32:ASN:HA	1.67	0.59
1:D:688:LEU:HD23	1:D:690:GLU:H	1.68	0.59
1:D:1289:LEU:HD22	1:D:1562:ILE:HD11	1.83	0.59
1:B:317:ARG:NH1	1:B:349:GLN:OE1	2.35	0.59
1:B:1175:SER:OG	1:B:1180:ARG:NH2	2.36	0.59
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.84	0.59
1:C:4244:GLU:HG3	1:C:4668:LEU:HD13	1.84	0.59
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.31	0.59
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.85	0.59
1:B:1568:LYS:HE2	1:B:1574:PRO:HD3	1.83	0.59
1:C:4039:MET:SD	1:C:4043:GLN:NE2	2.76	0.59
1:A:2974:ILE:HD13	1:A:3049:LEU:HD12	1.85	0.59
1:A:4039:MET:SD	1:A:4043:GLN:NE2	2.76	0.59
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.35	0.59
1:D:1476:MET:HB3	1:D:1485:SER:HB2	1.85	0.59
1:D:2583:LEU:HD13	1:D:2622:LEU:HB2	1.85	0.59
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.35	0.59
1:B:2974:ILE:HD13	1:B:3049:LEU:HD12	1.85	0.59
1:C:2380:ILE:HG21	1:C:2469:ILE:HG12	1.85	0.59
1:C:2974:ILE:HD13	1:C:3049:LEU:HD12	1.85	0.59
1:D:1175:SER:OG	1:D:1180:ARG:NH2	2.36	0.59
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.85	0.59
1:A:2380:ILE:HG21	1:A:2469:ILE:HG12	1.85	0.59
1:A:3872:GLU:HG3	1:A:3874:VAL:H	1.67	0.59
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.85	0.59
1:D:2380:ILE:HG21	1:D:2469:ILE:HG12	1.85	0.59
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.35	0.59
1:A:4244:GLU:HG3	1:A:4668:LEU:HD13	1.84	0.59
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.84	0.59
1:C:4904:PRO:HB3	1:C:4913:ARG:HG2	1.85	0.59
1:D:2974:ILE:HD13	1:D:3049:LEU:HD12	1.85	0.59
1:B:3842:LEU:HB2	1:B:3929:SER:HB3	1.83	0.58
1:B:4039:MET:SD	1:B:4043:GLN:NE2	2.76	0.58
1:B:4244:GLU:HG3	1:B:4668:LEU:HD13	1.84	0.58
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.84	0.58
1:B:551:LEU:HB2	1:B:589:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.85	0.58
1:B:2380:ILE:HG21	1:B:2469:ILE:HG12	1.85	0.58
1:C:1476:MET:HB3	1:C:1485:SER:HB2	1.85	0.58
1:C:1568:LYS:HE2	1:C:1574:PRO:HD3	1.83	0.58
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.35	0.58
1:A:551:LEU:HB2	1:A:589:LEU:HD21	1.85	0.58
1:A:2583:LEU:HD13	1:A:2622:LEU:HB2	1.84	0.58
1:B:688:LEU:HD23	1:B:690:GLU:H	1.68	0.58
1:A:1476:MET:HB3	1:A:1485:SER:HB2	1.85	0.58
1:D:355:LEU:HD22	1:D:380:GLN:HA	1.86	0.58
1:D:3414:ARG:O	1:D:3418:ASN:ND2	2.33	0.58
2:G:17:LYS:HG2	2:G:20:GLN:HE22	1.69	0.58
1:A:355:LEU:HD22	1:A:380:GLN:HA	1.86	0.58
1:B:1296:GLN:NE2	1:B:1545:ASN:OD1	2.37	0.58
1:D:4039:MET:SD	1:D:4043:GLN:NE2	2.76	0.58
1:A:1175:SER:OG	1:A:1180:ARG:NH2	2.36	0.58
1:A:2095:GLN:HA	1:A:2127:GLN:HE21	1.69	0.58
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.84	0.58
2:E:38:SER:O	2:E:42:ARG:NH2	2.37	0.58
2:G:38:SER:O	2:G:42:ARG:NH2	2.37	0.58
1:A:25:SER:HA	1:A:33:LEU:O	2.04	0.58
1:C:1296:GLN:NE2	1:C:1545:ASN:OD1	2.37	0.58
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.36	0.58
1:D:1296:GLN:NE2	1:D:1545:ASN:OD1	2.37	0.58
1:D:2095:GLN:HA	1:D:2127:GLN:HE21	1.69	0.58
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.36	0.58
1:D:4904:PRO:HB3	1:D:4913:ARG:HG2	1.85	0.58
2:F:17:LYS:HG2	2:F:20:GLN:HE22	1.69	0.58
1:A:688:LEU:HD23	1:A:690:GLU:H	1.68	0.58
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.86	0.58
1:B:2583:LEU:HD13	1:B:2622:LEU:HB2	1.84	0.58
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.36	0.58
1:C:355:LEU:HD22	1:C:380:GLN:HA	1.86	0.58
1:C:688:LEU:HD23	1:C:690:GLU:H	1.67	0.58
1:C:2095:GLN:HA	1:C:2127:GLN:HE21	1.69	0.58
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.85	0.58
1:B:1476:MET:HB3	1:B:1485:SER:HB2	1.85	0.58
1:B:4904:PRO:HB3	1:B:4913:ARG:HG2	1.85	0.58
1:D:25:SER:HA	1:D:33:LEU:O	2.04	0.58
1:C:2583:LEU:HD13	1:C:2622:LEU:HB2	1.84	0.58
1:D:551:LEU:HB2	1:D:589:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.69	0.57
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.85	0.57
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.84	0.57
1:A:1296:GLN:NE2	1:A:1545:ASN:OD1	2.37	0.57
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.38	0.57
1:B:1545:ASN:HD21	2:F:32:ASN:HA	1.69	0.57
1:C:25:SER:HA	1:C:33:LEU:O	2.04	0.57
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.69	0.57
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.84	0.57
1:C:551:LEU:HB2	1:C:589:LEU:HD21	1.85	0.57
1:C:1175:SER:OG	1:C:1180:ARG:NH2	2.36	0.57
1:B:1297:PHE:HD1	1:B:1522:LEU:HA	1.70	0.57
1:B:2095:GLN:HA	1:B:2127:GLN:HE21	1.69	0.57
1:C:1545:ASN:HD21	2:G:32:ASN:HA	1.69	0.57
1:D:23:GLN:OE1	1:D:203:ASN:ND2	2.38	0.57
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.69	0.57
1:D:1545:ASN:HD21	2:H:32:ASN:HA	1.69	0.57
2:H:17:LYS:HG2	2:H:20:GLN:HE22	1.69	0.57
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.69	0.57
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.85	0.57
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.70	0.57
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.37	0.57
1:B:355:LEU:HD22	1:B:380:GLN:HA	1.86	0.57
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.86	0.57
1:C:1252:HIS:O	1:C:1275:ARG:NH1	2.38	0.57
2:F:38:SER:O	2:F:42:ARG:NH2	2.37	0.57
1:A:4904:PRO:HB3	1:A:4913:ARG:HG2	1.85	0.57
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.63	0.57
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.63	0.57
2:H:38:SER:O	2:H:42:ARG:NH2	2.37	0.57
1:A:498:THR:HA	1:A:553:ARG:HH12	1.70	0.57
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.85	0.57
1:D:1252:HIS:O	1:D:1275:ARG:NH1	2.38	0.57
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.70	0.57
1:B:25:SER:HA	1:B:33:LEU:O	2.04	0.57
1:B:1252:HIS:O	1:B:1275:ARG:NH1	2.38	0.57
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.86	0.57
1:A:1255:TYR:O	1:A:1275:ARG:NH1	2.38	0.56
1:A:1259:ARG:NH2	1:A:1595:LEU:O	2.39	0.56
1:C:1297:PHE:HD1	1:C:1522:LEU:HA	1.70	0.56
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.38	0.56
2:E:17:LYS:HG2	2:E:20:GLN:HE22	1.69	0.56
1:A:23:GLN:OE1	1:A:203:ASN:ND2	2.38	0.56
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.38	0.56
1:A:3997:ALA:HB1	1:A:4057:MET:HG2	1.86	0.56
1:A:4823:LEU:HD22	1:B:4843:LEU:HD22	1.86	0.56
1:B:498:THR:HA	1:B:553:ARG:HH12	1.70	0.56
1:B:1255:TYR:O	1:B:1275:ARG:NH1	2.38	0.56
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.37	0.56
1:C:23:GLN:OE1	1:C:203:ASN:ND2	2.38	0.56
1:C:181:HIS:HD1	1:C:198:THR:HG1	1.51	0.56
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.31	0.56
1:C:3997:ALA:HB1	1:C:4057:MET:HG2	1.86	0.56
1:A:2871:LEU:HG	1:A:2927:LEU:HD11	1.88	0.56
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.70	0.56
1:B:3997:ALA:HB1	1:B:4057:MET:HG2	1.86	0.56
1:C:299:LEU:HD22	1:C:378:LEU:HB2	1.88	0.56
1:C:1259:ARG:NH2	1:C:1595:LEU:O	2.39	0.56
1:C:1277:TRP:HD1	1:C:1559:GLN:HG3	1.71	0.56
1:D:355:LEU:HB2	1:D:378:LEU:HG	1.88	0.56
1:D:1259:ARG:NH2	1:D:1595:LEU:O	2.39	0.56
1:D:2871:LEU:HG	1:D:2927:LEU:HD11	1.88	0.56
2:G:40:ARG:NH2	2:G:102:GLU:OE1	2.39	0.56
1:A:355:LEU:HB2	1:A:378:LEU:HG	1.88	0.56
1:A:1297:PHE:HD1	1:A:1522:LEU:HA	1.70	0.56
1:A:1423:ASP:HB3	1:A:1426:ILE:HB	1.87	0.56
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.38	0.56
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.31	0.56
1:D:299:LEU:HD22	1:D:378:LEU:HB2	1.88	0.56
1:D:1297:PHE:HD1	1:D:1522:LEU:HA	1.70	0.56
1:D:3997:ALA:HB1	1:D:4057:MET:HG2	1.86	0.56
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.88	0.56
1:C:498:THR:HA	1:C:553:ARG:HH12	1.70	0.56
1:C:1451:GLY:HA3	1:C:1494:MET:HA	1.88	0.56
1:D:1712:TYR:OH	1:D:1814:MET:SD	2.63	0.56
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.36	0.56
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.37	0.56
1:B:355:LEU:HB2	1:B:378:LEU:HG	1.88	0.56
1:B:2273:LEU:HD23	1:B:2330:ARG:HG2	1.88	0.56
1:C:2745:VAL:HG11	1:C:2818:ALA:HB2	1.88	0.56
1:D:2745:VAL:HG11	1:D:2818:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1277:TRP:HD1	1:B:1559:GLN:HG3	1.71	0.56
1:B:1423:ASP:HB3	1:B:1426:ILE:HB	1.87	0.56
1:B:1780:PRO:O	2:F:42:ARG:NH1	2.39	0.56
1:C:1255:TYR:O	1:C:1275:ARG:NH1	2.38	0.56
1:C:3850:GLN:NE2	1:C:3872:GLU:OE1	2.39	0.56
1:A:1780:PRO:O	2:E:42:ARG:NH1	2.39	0.56
1:B:3850:GLN:NE2	1:B:3872:GLU:OE1	2.39	0.56
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.38	0.56
1:D:498:THR:HA	1:D:553:ARG:HH12	1.70	0.56
1:D:1255:TYR:O	1:D:1275:ARG:NH1	2.38	0.56
1:D:1780:PRO:O	2:H:42:ARG:NH1	2.39	0.56
2:F:40:ARG:NH2	2:F:102:GLU:OE1	2.39	0.56
1:B:299:LEU:HD22	1:B:378:LEU:HB2	1.88	0.56
1:B:3752:SER:OG	1:B:3755:GLU:OE1	2.24	0.56
1:C:4172:GLU:HG3	1:C:4175:ARG:HE	1.71	0.56
1:D:1423:ASP:HB3	1:D:1426:ILE:HB	1.87	0.56
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.36	0.56
1:B:1451:GLY:HA3	1:B:1494:MET:HA	1.88	0.56
1:A:829:TYR:HB3	1:A:1073:ARG:HH11	1.72	0.55
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.40	0.55
1:B:4172:GLU:HG3	1:B:4175:ARG:HE	1.71	0.55
1:A:1712:TYR:OH	1:A:1814:MET:SD	2.63	0.55
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.37	0.55
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.71	0.55
1:C:2871:LEU:HG	1:C:2927:LEU:HD11	1.88	0.55
1:D:1277:TRP:HD1	1:D:1559:GLN:HG3	1.71	0.55
1:D:1451:GLY:HA3	1:D:1494:MET:HA	1.88	0.55
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.89	0.55
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.35	0.55
1:C:355:LEU:HB2	1:C:378:LEU:HG	1.88	0.55
1:C:1423:ASP:HB3	1:C:1426:ILE:HB	1.87	0.55
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.86	0.55
1:A:299:LEU:HD22	1:A:378:LEU:HB2	1.88	0.55
1:A:3752:SER:OG	1:A:3755:GLU:OE1	2.24	0.55
1:B:2871:LEU:HG	1:B:2927:LEU:HD11	1.88	0.55
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.38	0.55
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.88	0.55
1:C:1780:PRO:O	2:G:42:ARG:NH1	2.39	0.55
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.88	0.55
1:B:2745:VAL:HG11	1:B:2818:ALA:HB2	1.88	0.55
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2273:LEU:HD23	1:C:2330:ARG:HG2	1.88	0.55
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.88	0.55
1:D:3850:GLN:NE2	1:D:3872:GLU:OE1	2.39	0.55
1:B:1259:ARG:NH2	1:B:1595:LEU:O	2.39	0.55
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.40	0.55
1:D:2003:GLN:O	1:D:2007:ASN:ND2	2.40	0.55
2:E:40:ARG:NH2	2:E:102:GLU:OE1	2.39	0.55
2:H:40:ARG:NH2	2:H:102:GLU:OE1	2.39	0.55
1:A:2745:VAL:HG11	1:A:2818:ALA:HB2	1.88	0.55
1:A:2788:HIS:NE2	1:A:2790:MET:SD	2.80	0.55
1:A:2788:HIS:HD2	1:A:2791:LEU:HB2	1.72	0.55
1:B:632:LEU:O	1:B:634:GLN:NE2	2.40	0.55
1:B:829:TYR:HB3	1:B:1073:ARG:HH11	1.71	0.55
1:B:2371:GLU:HG2	1:C:129:ASP:HA	1.88	0.55
1:C:632:LEU:O	1:C:634:GLN:NE2	2.40	0.55
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.89	0.55
1:D:4172:GLU:HG3	1:D:4175:ARG:HE	1.71	0.55
1:D:4864:ASN:ND2	1:D:4874:MET:SD	2.80	0.55
1:A:2611:CYS:HA	1:A:2614:ILE:HG22	1.89	0.55
1:A:4843:LEU:HD22	1:D:4823:LEU:HD22	1.89	0.55
1:C:2371:GLU:HG2	1:D:129:ASP:HA	1.88	0.55
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.70	0.55
1:A:49:LEU:HD12	1:A:189:LEU:HB3	1.89	0.55
1:A:4172:GLU:HG3	1:A:4175:ARG:HE	1.71	0.55
1:C:2788:HIS:NE2	1:C:2790:MET:SD	2.80	0.55
1:C:4864:ASN:ND2	1:C:4874:MET:SD	2.80	0.55
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.40	0.55
1:D:1561:VAL:HG12	1:D:1562:ILE:HG23	1.89	0.55
1:A:3850:GLN:NE2	1:A:3872:GLU:OE1	2.39	0.54
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.89	0.54
1:B:3846:ALA:HB1	1:B:3873:LYS:HG3	1.90	0.54
1:D:3752:SER:OG	1:D:3755:GLU:OE1	2.24	0.54
1:A:1152:MET:HB2	1:A:1161:ILE:HB	1.89	0.54
1:A:1277:TRP:HD1	1:A:1559:GLN:HG3	1.71	0.54
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.36	0.54
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.89	0.54
1:D:49:LEU:HD12	1:D:189:LEU:HB3	1.89	0.54
2:E:73:LYS:HE2	2:E:98:ILE:HG23	1.90	0.54
1:A:1451:GLY:HA3	1:A:1494:MET:HA	1.88	0.54
1:C:1152:MET:HB2	1:C:1161:ILE:HB	1.89	0.54
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2273:LEU:HD23	1:D:2330:ARG:HG2	1.88	0.54
1:D:3846:ALA:HB1	1:D:3873:LYS:HG3	1.90	0.54
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.40	0.54
1:A:2003:GLN:O	1:A:2007:ASN:ND2	2.39	0.54
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.40	0.54
1:C:2003:GLN:O	1:C:2007:ASN:ND2	2.40	0.54
1:B:2788:HIS:NE2	1:B:2790:MET:SD	2.80	0.54
1:C:1561:VAL:HG12	1:C:1562:ILE:HG23	1.89	0.54
1:C:2788:HIS:HD2	1:C:2791:LEU:HB2	1.72	0.54
1:B:2611:CYS:HA	1:B:2614:ILE:HG22	1.88	0.54
1:B:3696:ASP:OD1	1:B:3696:ASP:N	2.41	0.54
1:B:4864:ASN:ND2	1:B:4874:MET:SD	2.80	0.54
1:D:632:LEU:O	1:D:634:GLN:NE2	2.40	0.54
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.90	0.54
1:A:632:LEU:O	1:A:634:GLN:NE2	2.40	0.54
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.36	0.54
1:D:829:TYR:HB3	1:D:1073:ARG:HH11	1.71	0.54
1:D:1152:MET:HB2	1:D:1161:ILE:HB	1.90	0.54
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.41	0.54
1:D:2788:HIS:NE2	1:D:2790:MET:SD	2.80	0.54
1:D:3990:VAL:HG23	1:D:4051:SER:HB3	1.89	0.54
1:A:1561:VAL:HG12	1:A:1562:ILE:HG23	1.90	0.54
1:A:4864:ASN:ND2	1:A:4874:MET:SD	2.80	0.54
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.90	0.54
1:B:1612:PHE:O	1:B:1614:GLN:NE2	2.41	0.54
1:B:3990:VAL:HG23	1:B:4051:SER:HB3	1.89	0.54
1:C:3846:ALA:HB1	1:C:3873:LYS:HG3	1.90	0.54
1:D:1612:PHE:O	1:D:1614:GLN:NE2	2.41	0.54
2:H:73:LYS:HE2	2:H:98:ILE:HG23	1.90	0.54
1:A:3846:ALA:HB1	1:A:3873:LYS:HG3	1.90	0.54
1:B:2523:ASP:HB3	1:B:2578:MET:HE3	1.90	0.54
1:B:2788:HIS:HD2	1:B:2791:LEU:HB2	1.72	0.54
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.36	0.54
1:D:23:GLN:HE21	1:D:34:LYS:HB3	1.72	0.54
1:D:4689:THR:OG1	1:D:4690:GLU:N	2.41	0.54
1:A:2523:ASP:HB3	1:A:2578:MET:HE3	1.90	0.53
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.37	0.53
1:D:2788:HIS:HD2	1:D:2791:LEU:HB2	1.72	0.53
1:A:2371:GLU:HG2	1:B:129:ASP:HA	1.88	0.53
1:A:2888:ARG:HD2	1:A:2891:LYS:HE3	1.90	0.53
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.90	0.53
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.41	0.53
1:C:3990:VAL:HG23	1:C:4051:SER:HB3	1.89	0.53
2:F:73:LYS:HE2	2:F:98:ILE:HG23	1.90	0.53
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.41	0.53
1:A:3540:TYR:HE1	1:A:3549:VAL:HG21	1.74	0.53
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.90	0.53
1:B:23:GLN:HE21	1:B:34:LYS:HB3	1.72	0.53
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.90	0.53
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.89	0.53
1:A:129:ASP:HA	1:D:2371:GLU:HG2	1.91	0.53
1:A:2273:LEU:HD23	1:A:2330:ARG:HG2	1.88	0.53
1:A:4689:THR:OG1	1:A:4690:GLU:N	2.41	0.53
1:C:3414:ARG:NH1	1:C:3417:ASP:OD2	2.41	0.53
1:D:3540:TYR:HE1	1:D:3549:VAL:HG21	1.74	0.53
1:C:2611:CYS:HA	1:C:2614:ILE:HG22	1.88	0.53
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.37	0.53
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.89	0.53
1:D:2611:CYS:HA	1:D:2614:ILE:HG22	1.89	0.53
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.90	0.53
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.31	0.53
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.41	0.53
1:B:3540:TYR:HE1	1:B:3549:VAL:HG21	1.74	0.53
1:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.89	0.53
1:C:23:GLN:HE21	1:C:34:LYS:HB3	1.72	0.53
1:C:1612:PHE:O	1:C:1614:GLN:NE2	2.41	0.53
1:C:3540:TYR:HE1	1:C:3549:VAL:HG21	1.74	0.53
1:D:173:SER:HB3	1:D:178:ARG:H	1.73	0.53
1:D:2523:ASP:HB3	1:D:2578:MET:HE3	1.90	0.53
1:A:23:GLN:HE21	1:A:34:LYS:HB3	1.72	0.53
1:B:1561:VAL:HG12	1:B:1562:ILE:HG23	1.89	0.53
1:B:2888:ARG:HD2	1:B:2891:LYS:HE3	1.90	0.53
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.91	0.53
1:C:173:SER:HB3	1:C:178:ARG:H	1.73	0.53
1:C:2888:ARG:HD2	1:C:2891:LYS:HE3	1.90	0.53
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.89	0.53
1:B:2867:LEU:HD21	1:B:2871:LEU:HD23	1.91	0.53
2:G:73:LYS:HE2	2:G:98:ILE:HG23	1.90	0.53
1:A:1612:PHE:O	1:A:1614:GLN:NE2	2.41	0.53
1:A:3990:VAL:HG23	1:A:4051:SER:HB3	1.89	0.53
1:B:49:LEU:HD12	1:B:189:LEU:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3940:LYS:O	1:B:4002:LYS:NZ	2.42	0.53
1:C:266:ARG:NH2	1:C:331:VAL:O	2.40	0.53
1:D:181:HIS:HD1	1:D:198:THR:HG1	1.54	0.53
1:D:2872:GLN:NE2	1:D:2924:GLN:OE1	2.42	0.53
1:A:1153:ILE:HG13	1:A:1160:ILE:HG12	1.91	0.53
1:B:173:SER:HB3	1:B:178:ARG:H	1.73	0.53
1:C:49:LEU:HD12	1:C:189:LEU:HB3	1.89	0.53
1:C:2867:LEU:HD21	1:C:2871:LEU:HD23	1.91	0.53
1:C:3940:LYS:O	1:C:4002:LYS:NZ	2.42	0.53
1:A:708:GLY:HA3	1:A:722:TRP:HB3	1.90	0.52
1:C:2971:GLN:NE2	1:C:3045:LYS:O	2.43	0.52
1:D:3414:ARG:NH1	1:D:3417:ASP:OD2	2.41	0.52
1:A:2872:GLN:NE2	1:A:2924:GLN:OE1	2.42	0.52
1:A:3414:ARG:NH1	1:A:3417:ASP:OD2	2.41	0.52
1:C:1153:ILE:HG13	1:C:1160:ILE:HG12	1.91	0.52
1:A:2971:GLN:NE2	1:A:3045:LYS:O	2.43	0.52
1:C:708:GLY:HA3	1:C:722:TRP:HB3	1.90	0.52
1:C:3078:ARG:NH2	1:C:3151:GLN:O	2.40	0.52
1:A:173:SER:HB3	1:A:178:ARG:H	1.73	0.52
1:A:3940:LYS:O	1:A:4002:LYS:NZ	2.42	0.52
1:B:4818:MET:N	1:B:4818:MET:SD	2.83	0.52
1:C:2523:ASP:HB3	1:C:2578:MET:HE3	1.90	0.52
1:C:2974:ILE:HD12	1:C:3053:ARG:HH12	1.75	0.52
1:C:4818:MET:SD	1:C:4818:MET:N	2.83	0.52
1:D:3065:VAL:O	1:D:3069:HIS:ND1	2.43	0.52
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.91	0.52
2:G:7:ILE:HD11	2:G:73:LYS:HB2	1.92	0.52
1:A:2653:LYS:HB3	1:A:2657:LEU:HG	1.92	0.52
1:B:2971:GLN:NE2	1:B:3045:LYS:O	2.43	0.52
1:B:3078:ARG:NH2	1:B:3151:GLN:O	2.41	0.52
1:C:3219:TYR:OH	1:C:3239:MET:SD	2.60	0.52
1:D:451:TYR:O	1:D:474:ARG:NH1	2.43	0.52
1:D:1112:ASP:HB3	1:D:1603:VAL:HB	1.92	0.52
2:H:7:ILE:HD11	2:H:73:LYS:HB2	1.92	0.52
1:A:3924:LEU:HD21	1:A:3984:ARG:HH21	1.75	0.52
1:C:2538:THR:HG23	1:C:2540:THR:H	1.75	0.52
1:C:2626:LEU:HD22	1:C:2640:PRO:HB3	1.92	0.52
1:C:2872:GLN:NE2	1:C:2924:GLN:OE1	2.42	0.52
1:C:3065:VAL:O	1:C:3069:HIS:ND1	2.43	0.52
1:D:708:GLY:HA3	1:D:722:TRP:HB3	1.90	0.52
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1652:GLU:OE2	1:A:1656:ARG:NH1	2.43	0.52
1:B:2653:LYS:HB3	1:B:2657:LEU:HG	1.92	0.52
1:C:575:LEU:HD22	1:C:609:CYS:HB3	1.92	0.52
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.40	0.52
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.90	0.52
1:B:3065:VAL:O	1:B:3069:HIS:ND1	2.43	0.52
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	1.92	0.52
1:C:451:TYR:O	1:C:474:ARG:NH1	2.43	0.52
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.91	0.52
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	1.92	0.52
1:D:2653:LYS:HB3	1:D:2657:LEU:HG	1.92	0.52
1:D:2971:GLN:NE2	1:D:3045:LYS:O	2.42	0.52
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.92	0.52
1:A:4818:MET:N	1:A:4818:MET:SD	2.83	0.52
1:B:666:VAL:HG21	1:B:684:VAL:HG11	1.92	0.52
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.92	0.52
1:C:2653:LYS:HB3	1:C:2657:LEU:HG	1.92	0.52
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.37	0.52
1:D:3924:LEU:HD21	1:D:3984:ARG:HH21	1.75	0.52
1:D:3940:LYS:O	1:D:4002:LYS:NZ	2.42	0.52
1:A:3065:VAL:O	1:A:3069:HIS:ND1	2.43	0.52
1:A:3106:MET:HE1	1:A:3129:LEU:HA	1.92	0.52
1:B:451:TYR:O	1:B:474:ARG:NH1	2.43	0.52
1:B:708:GLY:HA3	1:B:722:TRP:HB3	1.90	0.52
1:B:1153:ILE:HG13	1:B:1160:ILE:HG12	1.91	0.52
1:B:3414:ARG:NH1	1:B:3417:ASP:OD2	2.41	0.52
1:B:4689:THR:OG1	1:B:4690:GLU:N	2.41	0.52
1:D:2595:LEU:O	1:D:2600:ARG:NH2	2.43	0.52
1:D:2888:ARG:HD2	1:D:2891:LYS:HE3	1.90	0.52
1:B:3757:GLU:OE2	1:B:4718:LYS:NZ	2.44	0.51
1:C:4689:THR:OG1	1:C:4690:GLU:N	2.41	0.51
1:D:1652:GLU:OE2	1:D:1656:ARG:NH1	2.43	0.51
1:D:2538:THR:HG23	1:D:2540:THR:H	1.75	0.51
1:D:2867:LEU:HD21	1:D:2871:LEU:HD23	1.91	0.51
1:D:3106:MET:HE1	1:D:3129:LEU:HA	1.92	0.51
1:A:56:GLN:O	1:A:309:THR:OG1	2.28	0.51
1:A:643:SER:HA	1:A:781:VAL:O	2.11	0.51
1:A:1112:ASP:HB3	1:A:1603:VAL:HB	1.92	0.51
1:B:56:GLN:O	1:B:309:THR:OG1	2.28	0.51
1:B:218:HIS:HD1	1:B:341:TYR:HH	1.58	0.51
1:B:2538:THR:HG23	1:B:2540:THR:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2626:LEU:HD22	1:B:2640:PRO:HB3	1.92	0.51
1:B:2974:ILE:HD12	1:B:3053:ARG:HH12	1.75	0.51
1:C:1652:GLU:OE2	1:C:1656:ARG:NH1	2.43	0.51
1:C:2595:LEU:O	1:C:2600:ARG:NH2	2.43	0.51
1:D:666:VAL:HG21	1:D:684:VAL:HG11	1.92	0.51
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.92	0.51
1:D:2974:ILE:HD12	1:D:3053:ARG:HH12	1.75	0.51
1:A:666:VAL:HG21	1:A:684:VAL:HG11	1.92	0.51
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.91	0.51
1:A:3757:GLU:OE2	1:A:4718:LYS:NZ	2.44	0.51
1:B:3924:LEU:HD21	1:B:3984:ARG:HH21	1.75	0.51
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.92	0.51
1:C:1112:ASP:HB3	1:C:1603:VAL:HB	1.92	0.51
1:D:643:SER:HA	1:D:781:VAL:O	2.11	0.51
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.43	0.51
1:D:1153:ILE:HG13	1:D:1160:ILE:HG12	1.91	0.51
1:D:2299:VAL:HG11	1:D:2356:LEU:HB3	1.93	0.51
1:D:4818:MET:N	1:D:4818:MET:SD	2.83	0.51
2:F:7:ILE:HD11	2:F:73:LYS:HB2	1.92	0.51
1:A:451:TYR:O	1:A:474:ARG:NH1	2.43	0.51
1:A:2967:MET:HE3	1:A:3042:LEU:HD11	1.93	0.51
1:B:534:ARG:HD2	1:B:570:GLU:HG2	1.93	0.51
1:B:2872:GLN:NE2	1:B:2924:GLN:OE1	2.42	0.51
1:C:666:VAL:HG21	1:C:684:VAL:HG11	1.92	0.51
1:D:2591:ARG:HH12	1:D:2634:ASN:HD21	1.58	0.51
1:A:2595:LEU:O	1:A:2600:ARG:NH2	2.43	0.51
1:A:2867:LEU:HD21	1:A:2871:LEU:HD23	1.91	0.51
1:B:575:LEU:HD22	1:B:609:CYS:HB3	1.92	0.51
1:C:3106:MET:HE1	1:C:3129:LEU:HA	1.92	0.51
1:C:3157:ILE:HA	1:C:3161:VAL:HB	1.93	0.51
1:A:231:LEU:HA	1:A:246:TYR:O	2.11	0.51
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.43	0.51
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	1.92	0.51
1:B:3106:MET:HE1	1:B:3129:LEU:HA	1.92	0.51
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.92	0.51
1:C:1658:ASP:N	1:C:1658:ASP:OD1	2.44	0.51
1:C:2299:VAL:HG11	1:C:2356:LEU:HB3	1.93	0.51
1:D:2626:LEU:HD22	1:D:2640:PRO:HB3	1.92	0.51
1:D:3757:GLU:OE2	1:D:4718:LYS:NZ	2.44	0.51
1:A:534:ARG:HD2	1:A:570:GLU:HG2	1.93	0.51
1:B:231:LEU:HA	1:B:246:TYR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1112:ASP:HB3	1:B:1603:VAL:HB	1.92	0.51
1:B:1524:THR:O	1:B:1541:GLN:NE2	2.38	0.51
1:C:3270:ILE:HA	1:C:3274:LEU:HD12	1.93	0.51
2:E:7:ILE:HD11	2:E:73:LYS:HB2	1.92	0.51
1:A:575:LEU:HD22	1:A:609:CYS:HB3	1.92	0.51
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.92	0.51
1:B:643:SER:HA	1:B:781:VAL:O	2.11	0.51
1:B:1652:GLU:OE2	1:B:1656:ARG:NH1	2.43	0.51
1:B:2299:VAL:HG11	1:B:2356:LEU:HB3	1.93	0.51
1:B:2948:THR:OG1	1:B:2952:GLU:OE2	2.25	0.51
1:B:2967:MET:HE3	1:B:3042:LEU:HD11	1.93	0.51
1:B:3270:ILE:HA	1:B:3274:LEU:HD12	1.93	0.51
1:B:4634:GLU:OE1	1:B:4637:GLY:N	2.42	0.51
1:C:485:SER:HA	1:C:488:LEU:HD12	1.93	0.51
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.93	0.51
1:D:275:ARG:NH2	1:D:328:LYS:O	2.44	0.51
1:D:2967:MET:HE3	1:D:3042:LEU:HD11	1.93	0.51
1:A:4112:LEU:O	1:A:4115:SER:OG	2.29	0.51
1:C:1784:ALA:HA	2:G:55:VAL:HA	1.93	0.51
1:D:534:ARG:HD2	1:D:570:GLU:HG2	1.93	0.51
1:A:2974:ILE:HD12	1:A:3053:ARG:HH12	1.75	0.51
1:C:643:SER:HA	1:C:781:VAL:O	2.11	0.51
1:C:2967:MET:HE3	1:C:3042:LEU:HD11	1.93	0.51
1:C:3324:VAL:HA	1:C:3327:LEU:HB2	1.93	0.51
1:D:3270:ILE:HA	1:D:3274:LEU:HD12	1.93	0.51
1:D:3324:VAL:HA	1:D:3327:LEU:HB2	1.93	0.51
1:B:3157:ILE:HA	1:B:3161:VAL:HB	1.93	0.50
1:B:5013:MET:HE1	1:B:5020:ASP:HB2	1.93	0.50
1:C:231:LEU:HA	1:C:246:TYR:O	2.11	0.50
1:C:5013:MET:HE1	1:C:5020:ASP:HB2	1.93	0.50
1:D:4112:LEU:O	1:D:4115:SER:OG	2.29	0.50
1:A:485:SER:HA	1:A:488:LEU:HD12	1.93	0.50
1:A:3270:ILE:HA	1:A:3274:LEU:HD12	1.93	0.50
1:B:2591:ARG:HH12	1:B:2634:ASN:HD21	1.58	0.50
1:B:3463:GLU:HA	1:B:3502:ARG:HH22	1.76	0.50
1:C:2339:VAL:HG12	1:C:2349:ASN:HB3	1.93	0.50
1:C:3757:GLU:OE2	1:C:4718:LYS:NZ	2.44	0.50
1:C:4165:GLU:HA	1:C:4168:GLU:HG2	1.93	0.50
1:D:3157:ILE:HA	1:D:3161:VAL:HB	1.93	0.50
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	1.93	0.50
1:A:2538:THR:HG23	1:A:2540:THR:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2591:ARG:HH12	1:A:2634:ASN:HD21	1.58	0.50
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.92	0.50
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.92	0.50
1:B:1270:LEU:HB2	1:B:1564:PHE:HB2	1.94	0.50
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.43	0.50
1:D:1658:ASP:OD1	1:D:1658:ASP:N	2.44	0.50
1:B:4165:GLU:HA	1:B:4168:GLU:HG2	1.93	0.50
1:C:534:ARG:HD2	1:C:570:GLU:HG2	1.93	0.50
1:C:758:ARG:HG2	1:C:763:PRO:HA	1.94	0.50
1:C:3634:ALA:O	1:C:3638:MET:HB2	2.11	0.50
1:D:231:LEU:HA	1:D:246:TYR:O	2.11	0.50
1:D:575:LEU:HD22	1:D:609:CYS:HB3	1.92	0.50
1:D:3634:ALA:O	1:D:3638:MET:HB2	2.11	0.50
1:A:3607:GLU:HA	1:A:3610:GLU:HG2	1.93	0.50
1:A:4165:GLU:HA	1:A:4168:GLU:HG2	1.93	0.50
1:A:5013:MET:HE1	1:A:5020:ASP:HB2	1.93	0.50
1:B:2595:LEU:O	1:B:2600:ARG:NH2	2.43	0.50
1:C:275:ARG:NH2	1:C:328:LYS:O	2.44	0.50
1:D:207:SER:H	1:D:334:MET:HE2	1.77	0.50
1:D:758:ARG:HG2	1:D:763:PRO:HA	1.94	0.50
1:B:485:SER:HA	1:B:488:LEU:HD12	1.93	0.50
1:B:3607:GLU:HA	1:B:3610:GLU:HG2	1.93	0.50
1:C:207:SER:H	1:C:334:MET:HE2	1.77	0.50
1:D:218:HIS:ND1	1:D:341:TYR:OH	2.44	0.50
1:D:485:SER:HA	1:D:488:LEU:HD12	1.93	0.50
1:D:3607:GLU:HA	1:D:3610:GLU:HG2	1.93	0.50
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	1.92	0.50
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.93	0.50
1:D:5013:MET:HE1	1:D:5020:ASP:HB2	1.93	0.50
1:A:758:ARG:HG2	1:A:763:PRO:HA	1.94	0.50
1:A:2716:ASP:OD1	1:A:2716:ASP:N	2.45	0.50
1:A:3157:ILE:HA	1:A:3161:VAL:HB	1.93	0.50
1:A:3634:ALA:O	1:A:3638:MET:HB2	2.11	0.50
1:B:758:ARG:HG2	1:B:763:PRO:HA	1.94	0.50
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.43	0.50
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.44	0.50
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.93	0.50
1:A:275:ARG:NH2	1:A:328:LYS:O	2.44	0.50
1:B:181:HIS:HD1	1:B:198:THR:HG1	1.54	0.50
1:B:2534:ALA:HB2	1:B:2589:LEU:HG	1.94	0.50
1:B:1784:ALA:HA	2:F:55:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2339:VAL:HG12	1:B:2349:ASN:HB3	1.93	0.50
1:B:3634:ALA:O	1:B:3638:MET:HB2	2.11	0.50
1:C:1270:LEU:HB2	1:C:1564:PHE:HB2	1.94	0.50
1:C:2591:ARG:HH12	1:C:2634:ASN:HD21	1.58	0.50
1:C:3924:LEU:HD21	1:C:3984:ARG:HH21	1.75	0.50
1:D:4165:GLU:HA	1:D:4168:GLU:HG2	1.93	0.50
1:B:275:ARG:NH2	1:B:328:LYS:O	2.44	0.49
1:C:3752:SER:OG	1:C:3755:GLU:OE1	2.24	0.49
1:C:4634:GLU:OE1	1:C:4637:GLY:N	2.42	0.49
1:D:3459:VAL:HG13	1:D:3464:ILE:HB	1.94	0.49
1:D:3463:GLU:HA	1:D:3502:ARG:HH22	1.76	0.49
1:C:2144:ILE:HG12	1:C:2152:THR:HG21	1.94	0.49
1:C:3459:VAL:HG13	1:C:3464:ILE:HB	1.94	0.49
1:D:2128:TYR:OH	1:D:3676:ASP:OD2	2.30	0.49
1:A:546:TRP:CE2	1:A:550:LYS:HE2	2.48	0.49
1:A:1808:ARG:NH1	1:A:1853:ILE:O	2.45	0.49
1:B:4112:LEU:O	1:B:4115:SER:OG	2.29	0.49
1:C:2534:ALA:HB2	1:C:2589:LEU:HG	1.94	0.49
1:C:3463:GLU:HA	1:C:3502:ARG:HH22	1.76	0.49
1:C:3607:GLU:HA	1:C:3610:GLU:HG2	1.93	0.49
1:D:1270:LEU:HB2	1:D:1564:PHE:HB2	1.94	0.49
1:D:1784:ALA:HA	2:H:55:VAL:HA	1.93	0.49
1:D:3078:ARG:NH2	1:D:3151:GLN:O	2.40	0.49
1:A:218:HIS:ND1	1:A:341:TYR:OH	2.44	0.49
1:A:2339:VAL:HG12	1:A:2349:ASN:HB3	1.93	0.49
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.94	0.49
1:A:3463:GLU:HA	1:A:3502:ARG:HH22	1.76	0.49
1:D:266:ARG:NH2	1:D:331:VAL:O	2.40	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.94	0.49
1:A:1658:ASP:OD1	1:A:1658:ASP:N	2.44	0.49
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.93	0.49
1:B:546:TRP:CE2	1:B:550:LYS:HE2	2.48	0.49
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.94	0.49
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.95	0.49
1:B:1864:LYS:NZ	1:B:1873:GLU:OE1	2.37	0.49
1:C:2531:ARG:HG2	1:C:2585:THR:HG21	1.94	0.49
1:C:4112:LEU:O	1:C:4115:SER:OG	2.29	0.49
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.95	0.49
1:D:2144:ILE:HG12	1:D:2152:THR:HG21	1.94	0.49
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.95	0.49
1:A:1270:LEU:HB2	1:A:1564:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2519:LEU:HD13	1:A:2522:LEU:HD12	1.95	0.49
1:A:3324:VAL:HA	1:A:3327:LEU:HB2	1.93	0.49
1:B:2519:LEU:HD13	1:B:2522:LEU:HD12	1.95	0.49
1:B:3324:VAL:HA	1:B:3327:LEU:HB2	1.93	0.49
1:D:2531:ARG:HG2	1:D:2585:THR:HG21	1.95	0.49
1:A:2534:ALA:HB2	1:A:2589:LEU:HG	1.94	0.49
1:B:207:SER:H	1:B:334:MET:HE2	1.77	0.49
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.94	0.49
1:C:475:GLN:OE1	1:C:533:ASN:ND2	2.41	0.49
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.94	0.49
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.48	0.49
1:A:3405:LEU:O	1:A:3409:TYR:HB2	2.13	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.94	0.49
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.95	0.49
1:C:3696:ASP:OD1	1:C:3696:ASP:N	2.41	0.49
1:D:43:GLY:N	1:D:447:ASP:OD2	2.46	0.49
1:D:875:ALA:O	1:D:879:HIS:ND1	2.46	0.49
1:A:414:PHE:HE1	1:A:436:LEU:HD13	1.77	0.49
1:A:1524:THR:O	1:A:1541:GLN:NE2	2.38	0.49
1:B:2144:ILE:HG12	1:B:2152:THR:HG21	1.94	0.49
1:B:3405:LEU:O	1:B:3409:TYR:HB2	2.13	0.49
1:B:3459:VAL:HG13	1:B:3464:ILE:HB	1.94	0.49
1:C:4190:ILE:H	1:C:5031:GLN:HE22	1.61	0.49
1:C:4818:MET:O	1:C:4824:ARG:NH1	2.46	0.49
1:D:3219:TYR:OH	1:D:3239:MET:SD	2.60	0.49
1:D:3537:LYS:HG3	1:D:3604:TYR:HB2	1.95	0.49
1:D:4190:ILE:H	1:D:5031:GLN:HE22	1.61	0.49
1:A:2144:ILE:HG12	1:A:2152:THR:HG21	1.94	0.48
1:A:4818:MET:O	1:A:4824:ARG:NH1	2.46	0.48
1:B:414:PHE:HE1	1:B:436:LEU:HD13	1.77	0.48
1:B:667:MET:HB3	1:B:790:ARG:HB2	1.95	0.48
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.48	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.46	0.48
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.48	0.48
1:D:660:GLY:HA2	1:D:750:LEU:HB2	1.95	0.48
1:D:2339:VAL:HG12	1:D:2349:ASN:HB3	1.93	0.48
1:D:4818:MET:O	1:D:4824:ARG:NH1	2.46	0.48
1:A:43:GLY:N	1:A:447:ASP:OD2	2.46	0.48
1:A:181:HIS:HD1	1:A:198:THR:HG1	1.54	0.48
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.95	0.48
1:A:3078:ARG:NH2	1:A:3151:GLN:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:THR:HG22	1:B:258:SER:HB3	1.94	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.46	0.48
1:C:408:ALA:O	1:C:412:ASN:HB2	2.14	0.48
1:D:232:THR:HG22	1:D:258:SER:HB3	1.94	0.48
1:D:546:TRP:CE2	1:D:550:LYS:HE2	2.48	0.48
1:A:207:SER:H	1:A:334:MET:HE2	1.77	0.48
1:A:266:ARG:NH2	1:A:331:VAL:O	2.40	0.48
1:B:1089:TYR:HA	1:B:1151:CYS:O	2.14	0.48
1:B:3537:LYS:HG3	1:B:3604:TYR:HB2	1.95	0.48
1:C:667:MET:HB3	1:C:790:ARG:HB2	1.95	0.48
1:D:2534:ALA:HB2	1:D:2589:LEU:HG	1.94	0.48
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.94	0.48
1:A:1089:TYR:HA	1:A:1151:CYS:O	2.14	0.48
1:A:2013:LYS:NZ	1:A:3661:TRP:O	2.39	0.48
1:A:2531:ARG:HG2	1:A:2585:THR:HG21	1.95	0.48
1:A:3459:VAL:HG13	1:A:3464:ILE:HB	1.94	0.48
1:B:1189:LEU:HD12	1:B:1190:PRO:HD2	1.96	0.48
1:D:1089:TYR:HA	1:D:1151:CYS:O	2.14	0.48
1:D:1189:LEU:HD12	1:D:1190:PRO:HD2	1.96	0.48
1:A:232:THR:HG22	1:A:258:SER:HB3	1.94	0.48
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.93	0.48
1:C:232:THR:HG22	1:C:258:SER:HB3	1.94	0.48
1:C:4152:GLU:OE1	1:C:4192:ARG:NH1	2.47	0.48
1:D:408:ALA:O	1:D:412:ASN:HB2	2.14	0.48
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.48	0.48
1:A:4190:ILE:H	1:A:5031:GLN:HE22	1.61	0.48
1:C:56:GLN:O	1:C:309:THR:OG1	2.28	0.48
1:C:546:TRP:CE2	1:C:550:LYS:HE2	2.48	0.48
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.40	0.48
1:C:3405:LEU:O	1:C:3409:TYR:HB2	2.13	0.48
1:D:3329:ILE:O	1:D:3403:ARG:NH2	2.42	0.48
1:D:5013:MET:HE2	1:D:5018:CYS:HB3	1.95	0.48
1:A:660:GLY:HA2	1:A:750:LEU:HB2	1.95	0.48
1:A:667:MET:HB3	1:A:790:ARG:HB2	1.95	0.48
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.95	0.48
1:B:3817:LEU:HD13	1:B:3899:PHE:HD1	1.79	0.48
1:B:4152:GLU:OE1	1:B:4192:ARG:NH1	2.47	0.48
1:B:4190:ILE:H	1:B:5031:GLN:HE22	1.61	0.48
1:D:56:GLN:O	1:D:309:THR:OG1	2.28	0.48
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.95	0.48
1:D:3405:LEU:O	1:D:3409:TYR:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:LEU:HD12	1:A:1190:PRO:HD2	1.96	0.48
1:A:4152:GLU:OE1	1:A:4192:ARG:NH1	2.47	0.48
1:C:2519:LEU:HD13	1:C:2522:LEU:HD12	1.95	0.48
1:A:875:ALA:O	1:A:879:HIS:ND1	2.46	0.48
1:A:2856:ASN:ND2	1:A:2858:GLN:OE1	2.43	0.48
1:B:179:TYR:HD2	1:B:197:GLN:HA	1.79	0.48
1:B:660:GLY:HA2	1:B:750:LEU:HB2	1.95	0.48
1:B:5013:MET:HE2	1:B:5018:CYS:HB3	1.95	0.48
1:C:43:GLY:N	1:C:447:ASP:OD2	2.46	0.48
1:C:660:GLY:HA2	1:C:750:LEU:HB2	1.95	0.48
1:C:1189:LEU:HD12	1:C:1190:PRO:HD2	1.96	0.48
1:D:414:PHE:HE1	1:D:436:LEU:HD13	1.77	0.48
1:A:15:ARG:HE	1:A:100:THR:HG22	1.79	0.48
1:A:818:ARG:NH2	1:A:1025:ARG:O	2.47	0.48
1:A:2615:ARG:HD3	1:A:2618:MET:HE1	1.96	0.48
1:A:2869:ARG:NH2	1:A:2870[B]:GLU:OE2	2.47	0.48
1:C:414:PHE:HE1	1:C:436:LEU:HD13	1.77	0.48
1:C:2638:LYS:NZ	1:C:2694:GLU:OE2	2.47	0.48
1:C:2869:ARG:NH2	1:C:2870[B]:GLU:OE2	2.47	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.94	0.48
1:D:2869:ARG:NH2	1:D:2870[B]:GLU:OE2	2.47	0.48
1:D:3788:GLY:HA2	1:D:3835:LEU:HD12	1.96	0.48
1:A:3523:ASN:OD1	1:A:3582:ARG:NH2	2.46	0.47
1:A:3537:LYS:HG3	1:A:3604:TYR:HB2	1.95	0.47
1:A:3817:LEU:HD13	1:A:3899:PHE:HD1	1.79	0.47
1:B:15:ARG:HE	1:B:100:THR:HG22	1.79	0.47
1:B:2531:ARG:HG2	1:B:2585:THR:HG21	1.94	0.47
1:B:2869:ARG:NH2	1:B:2870[B]:GLU:OE2	2.47	0.47
1:C:3788:GLY:HA2	1:C:3835:LEU:HD12	1.96	0.47
1:D:1808:ARG:NH1	1:D:1853:ILE:O	2.45	0.47
1:B:218:HIS:ND1	1:B:341:TYR:OH	2.44	0.47
1:C:1116:GLY:O	1:C:1134:LEU:N	2.47	0.47
1:C:2615:ARG:HD3	1:C:2618:MET:HE1	1.96	0.47
1:D:1116:GLY:O	1:D:1134:LEU:N	2.47	0.47
1:D:2519:LEU:HD13	1:D:2522:LEU:HD12	1.95	0.47
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.79	0.47
1:B:1116:GLY:O	1:B:1134:LEU:N	2.47	0.47
1:B:4818:MET:O	1:B:4824:ARG:NH1	2.46	0.47
1:C:179:TYR:HD2	1:C:197:GLN:HA	1.79	0.47
1:C:1154:ASP:OD1	1:C:1156:THR:OG1	2.28	0.47
1:C:2856:ASN:ND2	1:C:2858:GLN:OE1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3817:LEU:HD13	1:D:3899:PHE:HD1	1.79	0.47
1:A:299:LEU:HD13	1:A:378:LEU:HD22	1.96	0.47
1:B:408:ALA:O	1:B:412:ASN:HB2	2.14	0.47
1:B:2615:ARG:HD3	1:B:2618:MET:HE1	1.96	0.47
1:C:3046:LEU:HB3	1:C:3068:LEU:HD21	1.96	0.47
1:C:3537:LYS:HG3	1:C:3604:TYR:HB2	1.95	0.47
1:C:4583:SER:HB2	1:C:4631:PHE:HE1	1.79	0.47
2:E:27:THR:HB	2:E:100:ASP:HB3	1.97	0.47
1:A:3548:GLU:HA	1:A:3551:GLU:HG3	1.96	0.47
1:A:3801:GLY:O	1:A:3805:LEU:HB2	2.14	0.47
1:B:3046:LEU:HB3	1:B:3068:LEU:HD21	1.97	0.47
1:B:3329:ILE:O	1:B:3403:ARG:NH2	2.42	0.47
1:B:3788:GLY:HA2	1:B:3835:LEU:HD12	1.96	0.47
1:C:1089:TYR:HA	1:C:1151:CYS:O	2.14	0.47
1:C:3801:GLY:O	1:C:3805:LEU:HB2	2.14	0.47
1:C:5013:MET:HE2	1:C:5018:CYS:HB3	1.95	0.47
1:D:179:TYR:HD2	1:D:197:GLN:HA	1.79	0.47
1:D:667:MET:HB3	1:D:790:ARG:HB2	1.95	0.47
1:D:818:ARG:NH2	1:D:1025:ARG:O	2.47	0.47
1:D:3204:ALA:HB1	1:D:3207:GLU:HB2	1.97	0.47
1:D:4190:ILE:N	1:D:5031:GLN:HE22	2.12	0.47
1:A:408:ALA:O	1:A:412:ASN:HB2	2.14	0.47
1:A:730:VAL:HG12	1:A:1476:MET:HE2	1.96	0.47
1:A:1116:GLY:O	1:A:1134:LEU:N	2.47	0.47
1:A:3788:GLY:HA2	1:A:3835:LEU:HD12	1.96	0.47
1:A:4190:ILE:N	1:A:5031:GLN:HE22	2.12	0.47
1:A:4583:SER:HB2	1:A:4631:PHE:HE1	1.79	0.47
1:A:4634:GLU:OE1	1:A:4637:GLY:N	2.42	0.47
1:B:551:LEU:HD21	1:B:585:SER:HB3	1.97	0.47
1:B:730:VAL:HG12	1:B:1476:MET:HE2	1.97	0.47
1:C:15:ARG:HE	1:C:100:THR:HG22	1.79	0.47
1:C:818:ARG:NH2	1:C:1025:ARG:O	2.47	0.47
1:C:3809:ASN:HB3	1:C:3812:VAL:HB	1.96	0.47
1:C:3817:LEU:HD13	1:C:3899:PHE:HD1	1.79	0.47
1:C:4182:GLU:HG3	1:C:4192:ARG:HG3	1.97	0.47
1:D:15:ARG:HE	1:D:100:THR:HG22	1.79	0.47
1:D:551:LEU:HD21	1:D:585:SER:HB3	1.97	0.47
1:A:2507:ASP:HB3	1:A:2561:LEU:HD13	1.97	0.47
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.97	0.47
1:A:3527:PRO:HD2	1:A:3573:MET:HE1	1.96	0.47
1:A:4182:GLU:HG3	1:A:4192:ARG:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:HD13	1:B:378:LEU:HD22	1.96	0.47
1:B:622:THR:HA	1:B:626:LEU:HD23	1.96	0.47
1:B:818:ARG:NH2	1:B:1025:ARG:O	2.47	0.47
1:B:1076:ARG:NH1	1:B:1077:ALA:O	2.48	0.47
1:B:2740:VAL:HG21	1:B:2819:TRP:HE1	1.80	0.47
1:B:2863:SER:HB2	1:B:2924:GLN:HB3	1.96	0.47
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	1.97	0.47
1:B:4679:ARG:O	1:B:4683:PHE:HB2	2.15	0.47
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.95	0.47
1:C:2948:THR:OG1	1:C:2952:GLU:OE2	2.25	0.47
1:C:3527:PRO:HD2	1:C:3573:MET:HE1	1.96	0.47
1:C:4190:ILE:N	1:C:5031:GLN:HE22	2.12	0.47
1:C:4679:ARG:O	1:C:4683:PHE:HB2	2.15	0.47
1:D:2615:ARG:HD3	1:D:2618:MET:HE1	1.96	0.47
1:D:2716:ASP:OD1	1:D:2716:ASP:N	2.45	0.47
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.79	0.47
1:D:3527:PRO:HD2	1:D:3573:MET:HE1	1.96	0.47
1:D:3548:GLU:HA	1:D:3551:GLU:HG3	1.97	0.47
1:D:4182:GLU:HG3	1:D:4192:ARG:HG3	1.97	0.47
2:H:27:THR:HB	2:H:100:ASP:HB3	1.97	0.47
1:A:551:LEU:HD21	1:A:585:SER:HB3	1.97	0.47
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.27	0.47
1:A:1864:LYS:NZ	1:A:1873:GLU:OE1	2.37	0.47
1:A:3046:LEU:HB3	1:A:3068:LEU:HD21	1.97	0.47
1:A:4853:VAL:O	1:A:4857:ASN:ND2	2.48	0.47
1:B:1927:LEU:HD13	1:B:2101:MET:HG3	1.97	0.47
1:B:2507:ASP:HB3	1:B:2561:LEU:HD13	1.97	0.47
1:B:3548:GLU:HA	1:B:3551:GLU:HG3	1.97	0.47
1:B:4011:GLU:O	1:B:4014:LYS:N	2.48	0.47
1:A:475:GLN:OE1	1:A:533:ASN:ND2	2.41	0.47
1:A:3219:TYR:OH	1:A:3239:MET:SD	2.60	0.47
1:A:4011:GLU:O	1:A:4014:LYS:N	2.48	0.47
1:B:3801:GLY:O	1:B:3805:LEU:HB2	2.15	0.47
1:B:4626:ASN:OD1	1:B:4626:ASN:N	2.48	0.47
1:C:1927:LEU:HD13	1:C:2101:MET:HG3	1.97	0.47
1:C:2128:TYR:OH	1:C:3676:ASP:OD2	2.30	0.47
1:C:2585:THR:HG22	1:C:2588:ARG:HH12	1.80	0.47
1:C:4680:LYS:HE3	1:C:4680:LYS:HB3	1.66	0.47
1:D:179:TYR:N	1:D:194:SER:O	2.48	0.47
1:D:3801:GLY:O	1:D:3805:LEU:HB2	2.14	0.47
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2740:VAL:HG21	1:A:2819:TRP:HE1	1.80	0.47
1:A:5013:MET:HE2	1:A:5018:CYS:HB3	1.95	0.47
1:B:1154:ASP:OD1	1:B:1156:THR:OG1	2.28	0.47
1:C:179:TYR:N	1:C:194:SER:O	2.48	0.47
1:C:2507:ASP:HB3	1:C:2561:LEU:HD13	1.97	0.47
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	1.97	0.47
1:D:3046:LEU:HB3	1:D:3068:LEU:HD21	1.97	0.47
1:D:3603:LEU:HA	1:D:3606:LEU:HD12	1.97	0.47
1:A:3206:LEU:HB2	1:A:3280:TYR:CZ	2.50	0.46
1:B:103:TYR:HE2	1:B:157:ARG:HG2	1.81	0.46
1:B:475:GLN:OE1	1:B:533:ASN:ND2	2.41	0.46
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.27	0.46
1:B:1769:THR:N	1:B:1956:GLU:OE2	2.48	0.46
1:B:2585:THR:HG22	1:B:2588:ARG:HH12	1.80	0.46
1:B:4190:ILE:N	1:B:5031:GLN:HE22	2.12	0.46
1:B:4583:SER:HB2	1:B:4631:PHE:HE1	1.80	0.46
1:C:299:LEU:HD13	1:C:378:LEU:HD22	1.96	0.46
1:A:2573:GLU:OE2	1:A:2615:ARG:NE	2.49	0.46
1:B:2716:ASP:OD1	1:B:2716:ASP:N	2.45	0.46
1:D:1154:ASP:OD1	1:D:1156:THR:OG1	2.28	0.46
1:D:1769:THR:N	1:D:1956:GLU:OE2	2.48	0.46
1:D:2573:GLU:OE2	1:D:2615:ARG:NE	2.49	0.46
1:D:2863:SER:HB2	1:D:2924:GLN:HB3	1.96	0.46
1:D:4011:GLU:O	1:D:4014:LYS:N	2.48	0.46
1:D:4976:GLU:H	1:D:4976:GLU:HG2	1.50	0.46
1:A:2863:SER:HB2	1:A:2924:GLN:HB3	1.96	0.46
1:A:3204:ALA:HB1	1:A:3207:GLU:HB2	1.96	0.46
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.97	0.46
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.15	0.46
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	1.97	0.46
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.15	0.46
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	1.97	0.46
1:C:2522:LEU:HD23	1:C:2526:PHE:HD2	1.80	0.46
1:C:4878:ASP:OD1	1:C:4879:MET:N	2.49	0.46
1:D:4878:ASP:OD1	1:D:4879:MET:N	2.49	0.46
1:A:179:TYR:HD2	1:A:197:GLN:HA	1.79	0.46
1:A:179:TYR:N	1:A:194:SER:O	2.48	0.46
1:A:350:HIS:HB2	1:A:378:LEU:HD21	1.98	0.46
1:A:1111:PRO:HB2	1:A:1603:VAL:HG12	1.98	0.46
1:A:1769:THR:N	1:A:1956:GLU:OE2	2.49	0.46
1:A:3592:ILE:HA	1:A:3595:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2522:LEU:HD23	1:B:2526:PHE:HD2	1.80	0.46
1:B:3051:ARG:HA	1:B:3131:TYR:CZ	2.50	0.46
1:B:3523:ASN:OD1	1:B:3582:ARG:NH2	2.46	0.46
1:C:622:THR:HA	1:C:626:LEU:HD23	1.96	0.46
1:C:1769:THR:N	1:C:1956:GLU:OE2	2.48	0.46
1:D:299:LEU:HD13	1:D:378:LEU:HD22	1.96	0.46
1:D:2522:LEU:HD23	1:D:2526:PHE:HD2	1.80	0.46
2:F:27:THR:HB	2:F:100:ASP:HB3	1.97	0.46
2:H:4:ILE:HD12	2:H:66:MET:HE2	1.97	0.46
1:A:3282:PRO:HA	1:A:3285:TRP:HB2	1.98	0.46
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.79	0.46
1:B:3527:PRO:HD2	1:B:3573:MET:HE1	1.96	0.46
1:B:4182:GLU:HG3	1:B:4192:ARG:HG3	1.97	0.46
1:C:103:TYR:HE2	1:C:157:ARG:HG2	1.81	0.46
1:D:350:HIS:HB2	1:D:378:LEU:HD21	1.98	0.46
1:D:622:THR:HA	1:D:626:LEU:HD23	1.96	0.46
1:D:730:VAL:HG12	1:D:1476:MET:HE2	1.97	0.46
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.97	0.46
1:D:1927:LEU:HD13	1:D:2101:MET:HG3	1.97	0.46
1:D:2507:ASP:HB3	1:D:2561:LEU:HD13	1.97	0.46
1:D:3206:LEU:HB2	1:D:3280:TYR:CZ	2.50	0.46
1:A:2128:TYR:OH	1:A:3676:ASP:OD2	2.30	0.46
1:A:2288:LEU:HD13	1:A:2346:VAL:HG21	1.98	0.46
1:A:2522:LEU:HD23	1:A:2526:PHE:HD2	1.80	0.46
1:A:3051:ARG:HA	1:A:3131:TYR:CZ	2.50	0.46
1:A:3603:LEU:HA	1:A:3606:LEU:HD12	1.97	0.46
1:A:4878:ASP:OD1	1:A:4879:MET:N	2.49	0.46
1:B:350:HIS:HB2	1:B:378:LEU:HD21	1.98	0.46
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.45	0.46
1:B:2013:LYS:NZ	1:B:3661:TRP:O	2.39	0.46
1:B:3282:PRO:HA	1:B:3285:TRP:HB2	1.98	0.46
1:B:3809:ASN:HB3	1:B:3812:VAL:HB	1.96	0.46
1:B:4878:ASP:OD1	1:B:4879:MET:N	2.49	0.46
1:C:1116:GLY:H	1:C:1121:ALA:HB3	1.81	0.46
1:C:3282:PRO:HA	1:C:3285:TRP:HB2	1.98	0.46
1:C:3523:ASN:OD1	1:C:3582:ARG:NH2	2.46	0.46
1:D:1111:PRO:HB2	1:D:1603:VAL:HG12	1.98	0.46
1:D:3282:PRO:HA	1:D:3285:TRP:HB2	1.98	0.46
1:D:3592:ILE:HA	1:D:3595:ARG:HG2	1.97	0.46
1:D:4583:SER:HB2	1:D:4631:PHE:HE1	1.79	0.46
1:D:4679:ARG:O	1:D:4683:PHE:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:THR:HA	1:A:626:LEU:HD23	1.96	0.46
1:B:179:TYR:N	1:B:194:SER:O	2.48	0.46
1:B:266:ARG:NH2	1:B:331:VAL:O	2.40	0.46
1:B:3206:LEU:HB2	1:B:3280:TYR:CZ	2.50	0.46
1:C:551:LEU:HD21	1:C:585:SER:HB3	1.97	0.46
1:C:1291:LEU:HB3	1:C:1595:LEU:HD11	1.98	0.46
1:C:2740:VAL:HG21	1:C:2819:TRP:HE1	1.80	0.46
1:C:2863:SER:HB2	1:C:2924:GLN:HB3	1.96	0.46
1:C:3051:ARG:HA	1:C:3131:TYR:CZ	2.50	0.46
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	1.97	0.46
1:C:3204:ALA:HB1	1:C:3207:GLU:HB2	1.96	0.46
1:C:3548:GLU:HA	1:C:3551:GLU:HG3	1.97	0.46
1:C:3592:ILE:HA	1:C:3595:ARG:HG2	1.97	0.46
1:C:4063:ASP:OD1	1:C:4064:MET:N	2.49	0.46
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.15	0.46
1:D:2948:THR:OG1	1:D:2952:GLU:OE2	2.25	0.46
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	1.97	0.46
1:D:3809:ASN:HB3	1:D:3812:VAL:HB	1.96	0.46
1:D:4152:GLU:OE1	1:D:4192:ARG:NH1	2.47	0.46
1:D:4634:GLU:OE1	1:D:4637:GLY:N	2.42	0.46
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.97	0.46
1:A:103:TYR:HE2	1:A:157:ARG:HG2	1.81	0.46
1:A:2638:LYS:NZ	1:A:2694:GLU:OE2	2.47	0.46
1:A:3809:ASN:HB3	1:A:3812:VAL:HB	1.96	0.46
1:C:218:HIS:ND1	1:C:341:TYR:OH	2.44	0.46
1:C:350:HIS:HB2	1:C:378:LEU:HD21	1.98	0.46
1:C:1111:PRO:HB2	1:C:1603:VAL:HG12	1.98	0.46
1:C:4011:GLU:O	1:C:4014:LYS:N	2.48	0.46
1:D:585:SER:O	1:D:588:SER:OG	2.28	0.46
1:D:629:ARG:NH1	2:H:90:VAL:O	2.45	0.46
1:A:2008:MET:HE1	1:A:2022:PRO:HD3	1.98	0.46
1:A:4679:ARG:O	1:A:4683:PHE:HB2	2.15	0.46
1:B:2128:TYR:OH	1:B:3676:ASP:OD2	2.30	0.46
1:B:3862:ASP:OD1	1:B:3862:ASP:N	2.49	0.46
1:C:730:VAL:HG12	1:C:1476:MET:HE2	1.97	0.46
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.79	0.46
1:C:3206:LEU:HB2	1:C:3280:TYR:CZ	2.50	0.46
1:C:3603:LEU:HA	1:C:3606:LEU:HD12	1.97	0.46
1:D:475:GLN:OE1	1:D:533:ASN:ND2	2.41	0.46
1:D:1093:GLU:HB3	1:D:1201:HIS:HB3	1.98	0.46
1:D:2585:THR:HG22	1:D:2588:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2740:VAL:HG21	1:D:2819:TRP:HE1	1.80	0.46
1:D:3610:GLU:HG3	1:D:3611:HIS:CE1	2.51	0.46
1:D:3696:ASP:OD1	1:D:3696:ASP:N	2.41	0.46
2:G:27:THR:HB	2:G:100:ASP:HB3	1.97	0.46
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.98	0.46
1:A:1927:LEU:HD13	1:A:2101:MET:HG3	1.97	0.46
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.49	0.46
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.29	0.46
1:A:4063:ASP:OD1	1:A:4064:MET:N	2.49	0.46
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.49	0.46
1:B:3610:GLU:HG3	1:B:3611:HIS:CE1	2.51	0.46
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.97	0.46
1:C:4853:VAL:O	1:C:4857:ASN:ND2	2.48	0.46
1:D:499:THR:HG23	1:D:502:HIS:H	1.81	0.46
1:D:1116:GLY:H	1:D:1121:ALA:HB3	1.81	0.46
1:D:4063:ASP:OD1	1:D:4064:MET:N	2.49	0.46
2:E:66:MET:HG2	2:E:72:ALA:HB2	1.98	0.46
2:G:66:MET:HG2	2:G:72:ALA:HB2	1.98	0.46
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.15	0.45
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.98	0.45
1:A:1784:ALA:HA	2:E:55:VAL:HA	1.98	0.45
1:B:2573:GLU:OE2	1:B:2615:ARG:NE	2.49	0.45
1:C:472:ARG:NH2	1:C:531:ARG:O	2.49	0.45
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	1.98	0.45
1:C:2573:GLU:OE2	1:C:2615:ARG:NE	2.49	0.45
1:C:3329:ILE:O	1:C:3403:ARG:NH2	2.42	0.45
1:D:3051:ARG:HA	1:D:3131:TYR:CZ	2.50	0.45
2:F:4:ILE:HD12	2:F:66:MET:HE2	1.97	0.45
2:F:66:MET:HG2	2:F:72:ALA:HB2	1.98	0.45
1:A:2928:LYS:HD3	1:A:2928:LYS:HA	1.79	0.45
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.82	0.45
1:A:4630:TYR:OH	1:B:4860:ARG:NH2	2.49	0.45
1:B:1093:GLU:HB3	1:B:1201:HIS:HB3	1.98	0.45
1:B:1116:GLY:H	1:B:1121:ALA:HB3	1.81	0.45
1:B:1291:LEU:HB3	1:B:1595:LEU:HD11	1.98	0.45
1:B:2288:LEU:HD13	1:B:2346:VAL:HG21	1.98	0.45
1:B:4983:HIS:O	3:B:5101:ADP:N6	2.50	0.45
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.98	0.45
1:C:2008:MET:HE1	1:C:2022:PRO:HD3	1.98	0.45
1:C:4983:HIS:O	3:C:5101:ADP:N6	2.50	0.45
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4626:ASN:N	1:D:4626:ASN:OD1	2.48	0.45
1:D:4853:VAL:O	1:D:4857:ASN:ND2	2.48	0.45
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.98	0.45
1:B:2522:LEU:HB3	1:B:2582:MET:HE1	1.98	0.45
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.97	0.45
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.49	0.45
1:C:2928:LYS:HD3	1:C:2928:LYS:HA	1.79	0.45
1:D:1291:LEU:HB3	1:D:1595:LEU:HD11	1.98	0.45
1:A:1990:GLU:HG2	1:A:1994:ARG:HH21	1.81	0.45
1:A:2585:THR:HG22	1:A:2588:ARG:HH12	1.80	0.45
1:A:3329:ILE:O	1:A:3403:ARG:NH2	2.42	0.45
1:B:257:ARG:O	1:B:284:HIS:NE2	2.49	0.45
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.98	0.45
1:B:585:SER:O	1:B:588:SER:OG	2.28	0.45
1:B:1990:GLU:HG2	1:B:1994:ARG:HH21	1.81	0.45
1:B:3204:ALA:HB1	1:B:3207:GLU:HB2	1.96	0.45
1:D:1079:LYS:HG2	1:D:1107:PRO:HB3	1.97	0.45
1:D:1096:THR:OG1	1:D:1198:GLN:OE1	2.34	0.45
1:D:2008:MET:HE1	1:D:2022:PRO:HD3	1.98	0.45
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.49	0.45
1:A:1079:LYS:HG2	1:A:1107:PRO:HB3	1.97	0.45
1:A:1116:GLY:H	1:A:1121:ALA:HB3	1.81	0.45
1:A:1291:LEU:HB3	1:A:1595:LEU:HD11	1.98	0.45
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.98	0.45
1:A:1753:LYS:HB3	1:A:1758:ARG:HG3	1.99	0.45
1:A:2516:ASP:OD1	1:A:2517:PHE:N	2.50	0.45
1:A:2584[B]:HIS:HE1	1:A:2625:ARG:HB2	1.82	0.45
1:A:4983:HIS:O	3:A:5101:ADP:N6	2.50	0.45
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.98	0.45
1:B:1079:LYS:HG2	1:B:1107:PRO:HB3	1.97	0.45
1:C:289:ARG:HG2	1:C:303:ASP:HA	1.98	0.45
1:C:499:THR:HG23	1:C:502:HIS:H	1.81	0.45
1:C:1577:ALA:O	1:C:1584:ARG:NE	2.46	0.45
1:C:1808:ARG:NH1	1:C:1853:ILE:O	2.45	0.45
1:C:2522:LEU:HB3	1:C:2582:MET:HE1	1.98	0.45
1:C:2584[B]:HIS:HE1	1:C:2625:ARG:HB2	1.82	0.45
1:C:3610:GLU:HG3	1:C:3611:HIS:CE1	2.51	0.45
1:D:1864:LYS:NZ	1:D:1873:GLU:OE1	2.37	0.45
1:D:4983:HIS:O	3:D:5101:ADP:N6	2.50	0.45
2:G:4:ILE:HD12	2:G:66:MET:HE2	1.97	0.45
1:B:3592:ILE:HA	1:B:3595:ARG:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.98	0.45
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.99	0.45
1:C:1753:LYS:HB3	1:C:1758:ARG:HG3	1.99	0.45
1:C:3157:ILE:HG22	1:C:3162:GLN:HG2	1.98	0.45
1:D:472:ARG:NH2	1:D:531:ARG:O	2.49	0.45
1:D:1076:ARG:NH1	1:D:1077:ALA:O	2.48	0.45
1:D:1990:GLU:HG2	1:D:1994:ARG:HH21	1.81	0.45
1:D:2584[B]:HIS:HE1	1:D:2625:ARG:HB2	1.82	0.45
1:A:1093:GLU:HB3	1:A:1201:HIS:HB3	1.98	0.45
1:A:3610:GLU:HG3	1:A:3611:HIS:CE1	2.51	0.45
1:B:289:ARG:HG2	1:B:303:ASP:HA	1.98	0.45
1:B:499:THR:HG23	1:B:502:HIS:H	1.81	0.45
1:B:3603:LEU:HA	1:B:3606:LEU:HD12	1.97	0.45
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.99	0.45
1:C:1990:GLU:HG2	1:C:1994:ARG:HH21	1.81	0.45
1:C:2288:LEU:HD13	1:C:2346:VAL:HG21	1.98	0.45
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.99	0.45
1:D:3862:ASP:OD1	1:D:3862:ASP:N	2.49	0.45
1:A:499:THR:HG23	1:A:502:HIS:H	1.81	0.45
1:A:4976:GLU:H	1:A:4976:GLU:HG2	1.49	0.45
1:B:1111:PRO:HB2	1:B:1603:VAL:HG12	1.98	0.45
1:B:1753:LYS:HB3	1:B:1758:ARG:HG3	1.99	0.45
1:C:629:ARG:NH1	2:G:90:VAL:O	2.45	0.45
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.84	0.45
1:C:1093:GLU:HB3	1:C:1201:HIS:HB3	1.98	0.45
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.99	0.45
1:A:1577:ALA:O	1:A:1584:ARG:NE	2.46	0.45
1:A:3157:ILE:HG22	1:A:3162:GLN:HG2	1.98	0.45
1:B:3782:MET:HE2	1:B:3782:MET:HB2	1.88	0.45
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.82	0.45
1:B:4063:ASP:OD1	1:B:4064:MET:N	2.49	0.45
1:B:4658:ILE:HD11	1:B:4793:GLY:HA2	1.99	0.45
1:C:4626:ASN:OD1	1:C:4626:ASN:N	2.48	0.45
1:C:4976:GLU:H	1:C:4976:GLU:HG2	1.49	0.45
1:D:2516:ASP:OD1	1:D:2517:PHE:N	2.50	0.45
1:A:1228:ILE:HG12	1:D:3571:TRP:CE2	2.52	0.45
1:A:1436:SER:HA	1:A:1517:GLY:HA2	1.99	0.45
1:A:2677:LYS:HE2	1:A:2677:LYS:HB3	1.74	0.45
1:A:4626:ASN:N	1:A:4626:ASN:OD1	2.48	0.45
1:A:4721:LYS:HD3	1:A:4741:LEU:HB3	1.99	0.45
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.99	0.45
1:B:2008:MET:HE1	1:B:2022:PRO:HD3	1.98	0.45
1:B:3157:ILE:HG22	1:B:3162:GLN:HG2	1.98	0.45
1:B:3945:GLU:HA	1:B:3948:LYS:HZ3	1.82	0.45
1:B:4188:ARG:HE	1:B:4188:ARG:HB3	1.73	0.45
1:C:3433:GLU:OE1	1:C:3436:ARG:NH1	2.49	0.45
1:C:4721:LYS:HD3	1:C:4741:LEU:HB3	1.99	0.45
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	1.98	0.45
1:D:2856:ASN:ND2	1:D:2858:GLN:OE1	2.43	0.45
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.82	0.45
1:D:4861:LYS:H	1:D:4861:LYS:HG2	1.53	0.45
1:D:4989:MET:HB3	1:D:4989:MET:HE3	1.65	0.45
2:G:62:GLY:HA3	2:G:74:LEU:HD21	1.99	0.45
1:A:1076:ARG:NH1	1:A:1077:ALA:O	2.48	0.44
1:A:2522:LEU:HB3	1:A:2582:MET:HE1	1.98	0.44
1:A:4677:LEU:HD11	1:A:4687:TYR:HE2	1.82	0.44
1:B:43:GLY:N	1:B:447:ASP:OD2	2.46	0.44
1:B:3579:LEU:HD23	1:B:3582:ARG:HG2	1.99	0.44
1:B:4721:LYS:HD3	1:B:4741:LEU:HB3	1.99	0.44
1:C:1079:LYS:HG2	1:C:1107:PRO:HB3	1.97	0.44
1:C:4243:PHE:HD2	1:C:4668:LEU:HD12	1.83	0.44
1:D:103:TYR:HE2	1:D:157:ARG:HG2	1.81	0.44
1:D:2013:LYS:NZ	1:D:3661:TRP:O	2.39	0.44
2:E:4:ILE:HD12	2:E:66:MET:HE2	1.97	0.44
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.98	0.44
1:B:472:ARG:NH2	1:B:531:ARG:O	2.50	0.44
1:B:1784:ALA:O	2:F:82:TYR:OH	2.36	0.44
1:B:2208:MET:SD	1:B:2253:HIS:ND1	2.91	0.44
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.98	0.44
1:D:289:ARG:HG2	1:D:303:ASP:HA	1.98	0.44
1:D:1436:SER:HA	1:D:1517:GLY:HA2	1.99	0.44
1:D:3523:ASN:OD1	1:D:3582:ARG:NH2	2.46	0.44
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	1.98	0.44
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.28	0.44
1:A:4107:GLU:O	1:A:4111:LEU:HG	2.18	0.44
1:B:4243:PHE:HD2	1:B:4668:LEU:HD12	1.83	0.44
1:B:4853:VAL:O	1:B:4857:ASN:ND2	2.48	0.44
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.98	0.44
1:C:2516:ASP:OD1	1:C:2517:PHE:N	2.50	0.44
1:C:3579:LEU:HD23	1:C:3582:ARG:HG2	1.99	0.44
1:C:3862:ASP:N	1:C:3862:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3157:ILE:HG22	1:D:3162:GLN:HG2	1.98	0.44
1:C:2208:MET:SD	1:C:2253:HIS:ND1	2.91	0.44
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.97	0.44
1:D:2288:LEU:HD13	1:D:2346:VAL:HG21	1.98	0.44
1:D:4721:LYS:HD3	1:D:4741:LEU:HB3	1.99	0.44
2:E:62:GLY:HA3	2:E:74:LEU:HD21	1.99	0.44
2:H:66:MET:HG2	2:H:72:ALA:HB2	1.98	0.44
1:A:289:ARG:HG2	1:A:303:ASP:HA	1.98	0.44
1:A:472:ARG:NH2	1:A:531:ARG:O	2.50	0.44
1:A:3579:LEU:HD23	1:A:3582:ARG:HG2	1.99	0.44
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	1.98	0.44
1:B:2516:ASP:OD1	1:B:2517:PHE:N	2.50	0.44
1:B:2970:SER:OG	1:B:2971:GLN:OE1	2.36	0.44
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.99	0.44
1:D:2135:LEU:HD23	1:D:2135:LEU:HA	1.86	0.44
2:H:74:LEU:HB2	2:H:99:PHE:HB2	2.00	0.44
1:A:4658:ILE:HD11	1:A:4793:GLY:HA2	1.99	0.44
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.98	0.44
1:B:3433:GLU:OE1	1:B:3436:ARG:NH1	2.49	0.44
1:B:4090:LYS:HE2	1:B:4090:LYS:HB3	1.84	0.44
1:B:4861:LYS:H	1:B:4861:LYS:HG2	1.53	0.44
1:C:2616:PRO:HA	1:C:2619:LEU:HD12	2.00	0.44
1:D:1753:LYS:HB3	1:D:1758:ARG:HG3	1.99	0.44
1:D:2616:PRO:HA	1:D:2619:LEU:HD12	2.00	0.44
1:A:2891:LYS:HA	1:A:2894:LEU:HB3	2.00	0.44
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.99	0.44
1:C:2355:ARG:HA	1:C:2358:ILE:HG22	2.00	0.44
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.98	0.44
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.99	0.44
1:A:1782:PHE:O	2:E:82:TYR:OH	2.35	0.44
1:A:4243:PHE:HD2	1:A:4668:LEU:HD12	1.83	0.44
1:B:2891:LYS:HA	1:B:2894:LEU:HB3	2.00	0.44
1:B:4680:LYS:HE3	1:B:4680:LYS:HB3	1.66	0.44
1:C:1076:ARG:NH1	1:C:1077:ALA:O	2.48	0.44
1:C:2013:LYS:NZ	1:C:3661:TRP:O	2.39	0.44
1:C:3533:ILE:HD13	1:C:3596:VAL:HG13	2.00	0.44
1:D:1577:ALA:O	1:D:1584:ARG:NE	2.46	0.44
1:D:1782:PHE:O	2:H:82:TYR:OH	2.30	0.44
1:D:4243:PHE:HD2	1:D:4668:LEU:HD12	1.83	0.44
2:E:74:LEU:HB2	2:E:99:PHE:HB2	2.00	0.44
1:A:585:SER:O	1:A:588:SER:OG	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.99	0.44
1:A:3081:MET:HE1	1:A:3093:ARG:HH21	1.83	0.44
1:A:3335:MET:SD	1:A:3403:ARG:NH1	2.91	0.44
1:A:4092:ASP:HA	1:A:4095:LYS:HG2	2.00	0.44
1:A:4647:SER:O	1:A:4651:THR:OG1	2.35	0.44
1:B:1436:SER:HA	1:B:1517:GLY:HA2	1.99	0.44
1:B:2584[B]:HIS:HE1	1:B:2625:ARG:HB2	1.82	0.44
1:C:1784:ALA:O	2:G:82:TYR:OH	2.36	0.44
1:C:4107:GLU:O	1:C:4111:LEU:HG	2.18	0.44
1:D:257:ARG:O	1:D:284:HIS:NE2	2.49	0.44
1:D:2725:LYS:HZ1	1:D:2738:ARG:HH12	1.65	0.44
1:D:3081:MET:HE1	1:D:3093:ARG:HH21	1.83	0.44
1:A:2960:LEU:HB3	1:A:3038:MET:HE2	2.00	0.43
1:A:4971:THR:HG22	1:A:4972:PRO:HD2	2.00	0.43
1:B:2377:LEU:HA	1:B:2380:ILE:HG22	2.00	0.43
1:B:3194:LEU:HA	1:B:3197:LEU:HG	2.00	0.43
1:C:2377:LEU:HA	1:C:2380:ILE:HG22	2.00	0.43
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.82	0.43
1:C:4639:MET:O	1:C:4643:LEU:N	2.47	0.43
1:C:4647:SER:O	1:C:4651:THR:OG1	2.35	0.43
1:C:4658:ILE:HD11	1:C:4793:GLY:HA2	1.99	0.43
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.27	0.43
1:D:4647:SER:O	1:D:4651:THR:OG1	2.35	0.43
2:F:62:GLY:HA3	2:F:74:LEU:HD21	1.99	0.43
1:A:2044:ILE:HD11	1:A:2131:LEU:HD23	2.00	0.43
1:A:2911:LEU:HD13	1:A:2915:GLU:HG3	2.00	0.43
1:B:3335:MET:SD	1:B:3403:ARG:NH1	2.91	0.43
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.99	0.43
1:C:1864:LYS:NZ	1:C:1873:GLU:OE1	2.37	0.43
1:C:2891:LYS:HA	1:C:2894:LEU:HB3	2.00	0.43
1:D:2911:LEU:HD13	1:D:2915:GLU:HG3	2.00	0.43
1:D:4092:ASP:HA	1:D:4095:LYS:HG2	2.00	0.43
1:D:4107:GLU:O	1:D:4111:LEU:HG	2.18	0.43
1:D:4181:ILE:HD12	1:D:4183:ILE:HG23	2.00	0.43
1:D:4677:LEU:HD11	1:D:4687:TYR:HE2	1.82	0.43
1:D:4971:THR:HG22	1:D:4972:PRO:HD2	2.00	0.43
2:F:74:LEU:HB2	2:F:99:PHE:HB2	2.00	0.43
2:G:24:VAL:HG12	2:G:103:LEU:HA	2.00	0.43
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.99	0.43
1:A:2377:LEU:HA	1:A:2380:ILE:HG22	2.00	0.43
1:A:2725:LYS:HZ1	1:A:2738:ARG:HH12	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.53	0.43
1:B:2689:LYS:O	1:B:2993:GLN:NE2	2.51	0.43
1:B:4107:GLU:O	1:B:4111:LEU:HG	2.18	0.43
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.53	0.43
1:C:1436:SER:HA	1:C:1517:GLY:HA2	1.99	0.43
1:C:4874:MET:H	1:C:4874:MET:HG2	1.61	0.43
1:D:2208:MET:SD	1:D:2253:HIS:ND1	2.91	0.43
1:D:3579:LEU:HD23	1:D:3582:ARG:HG2	1.99	0.43
1:D:3823:LYS:HA	1:D:3823:LYS:HD3	1.78	0.43
1:D:4035:VAL:HG13	1:D:5032:TYR:HE2	1.84	0.43
2:G:74:LEU:HB2	2:G:99:PHE:HB2	2.00	0.43
1:A:257:ARG:O	1:A:284:HIS:NE2	2.49	0.43
1:A:2208:MET:SD	1:A:2253:HIS:ND1	2.91	0.43
1:A:4035:VAL:HG13	1:A:5032:TYR:HE2	1.84	0.43
1:A:4750:ILE:H	1:A:4750:ILE:HG13	1.60	0.43
1:B:260:TRP:HA	1:B:283:ARG:O	2.19	0.43
1:B:1724:CYS:SG	1:B:1728:ARG:NH1	2.92	0.43
1:B:2001:PRO:HG2	1:B:3864:THR:HB	2.01	0.43
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.51	0.43
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.29	0.43
1:B:4677:LEU:HD11	1:B:4687:TYR:HE2	1.82	0.43
1:B:4976:GLU:H	1:B:4976:GLU:HG2	1.50	0.43
1:C:2689:LYS:O	1:C:2993:GLN:NE2	2.51	0.43
1:C:2928:LYS:HB3	1:C:2932:MET:HE1	2.01	0.43
1:C:3194:LEU:HA	1:C:3197:LEU:HG	2.00	0.43
1:C:4035:VAL:HG13	1:C:5032:TYR:HE2	1.84	0.43
1:D:2377:LEU:HA	1:D:2380:ILE:HG22	2.00	0.43
1:D:2638:LYS:NZ	1:D:2694:GLU:OE2	2.47	0.43
1:D:3245:VAL:HG23	1:D:3248:ARG:H	1.84	0.43
1:D:4658:ILE:HD11	1:D:4793:GLY:HA2	1.99	0.43
1:A:260:TRP:HA	1:A:283:ARG:O	2.19	0.43
1:A:1724:CYS:SG	1:A:1728:ARG:NH1	2.92	0.43
1:A:2002:PRO:HB3	1:A:3641:LEU:HD13	2.00	0.43
1:A:2377:LEU:HA	1:A:2377:LEU:HD23	1.90	0.43
1:A:2970:SER:OG	1:A:2971:GLN:OE1	2.36	0.43
1:A:3533:ILE:HD13	1:A:3596:VAL:HG13	2.00	0.43
1:B:69:LEU:HD12	1:B:69:LEU:HA	1.87	0.43
1:B:150:MET:O	1:B:151:HIS:ND1	2.52	0.43
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.84	0.43
1:B:3533:ILE:HD13	1:B:3596:VAL:HG13	2.00	0.43
1:B:4971:THR:HG22	1:B:4972:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1699:GLU:OE2	1:C:1813:ARG:NH1	2.45	0.43
1:C:1782:PHE:O	2:G:82:TYR:OH	2.30	0.43
1:C:2002:PRO:HB3	1:C:3641:LEU:HD13	2.00	0.43
1:C:2742:THR:HB	1:C:2814:LYS:HG3	2.01	0.43
1:C:2960:LEU:HB3	1:C:3038:MET:HE2	2.00	0.43
1:D:260:TRP:HA	1:D:283:ARG:O	2.19	0.43
1:D:1524:THR:O	1:D:1541:GLN:NE2	2.38	0.43
1:D:2522:LEU:HB3	1:D:2582:MET:HE1	1.98	0.43
1:D:2928:LYS:HB3	1:D:2932:MET:HE1	2.01	0.43
1:D:2960:LEU:HB3	1:D:3038:MET:HE2	2.00	0.43
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.51	0.43
1:D:3582:ARG:HD3	1:D:3582:ARG:HA	1.84	0.43
1:A:150:MET:O	1:A:151:HIS:ND1	2.52	0.43
1:A:2355:ARG:HA	1:A:2358:ILE:HG22	2.00	0.43
1:A:2742:THR:HB	1:A:2814:LYS:HG3	2.01	0.43
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.51	0.43
1:C:403:MET:O	1:C:407:THR:OG1	2.35	0.43
1:C:1724:CYS:SG	1:C:1728:ARG:NH1	2.92	0.43
1:C:2044:ILE:HD11	1:C:2131:LEU:HD23	2.00	0.43
1:C:2962:GLN:HA	1:C:2965:ARG:HG2	2.01	0.43
1:C:3081:MET:HE1	1:C:3093:ARG:HH21	1.83	0.43
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.84	0.43
1:D:1724:CYS:SG	1:D:1728:ARG:NH1	2.92	0.43
1:D:4874:MET:H	1:D:4874:MET:HG2	1.61	0.43
1:A:463:GLU:O	1:A:466:SER:OG	2.34	0.43
1:A:2689:LYS:O	1:A:2993:GLN:NE2	2.51	0.43
1:A:2755:ILE:HD12	1:A:2813:LEU:HG	2.01	0.43
1:A:2963:LEU:O	1:A:2967:MET:HB2	2.19	0.43
1:B:2355:ARG:HA	1:B:2358:ILE:HG22	2.00	0.43
1:B:2928:LYS:HB3	1:B:2932:MET:HE1	2.01	0.43
1:B:3081:MET:HE1	1:B:3093:ARG:HH21	1.83	0.43
1:C:260:TRP:HA	1:C:283:ARG:O	2.19	0.43
1:C:3245:VAL:HG23	1:C:3248:ARG:H	1.84	0.43
1:C:3335:MET:SD	1:C:3403:ARG:NH1	2.91	0.43
1:D:1110:ARG:HE	1:D:1110:ARG:HB3	1.70	0.43
1:D:2742:THR:HB	1:D:2814:LYS:HG3	2.01	0.43
1:D:2891:LYS:HA	1:D:2894:LEU:HB3	2.00	0.43
1:D:3354:LEU:HA	1:D:3358:PHE:HD2	1.84	0.43
1:D:4639:MET:O	1:D:4643:LEU:N	2.47	0.43
1:A:2616:PRO:HA	1:A:2619:LEU:HD12	2.00	0.43
1:B:2742:THR:HB	1:B:2814:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2963:LEU:O	1:B:2967:MET:HB2	2.19	0.43
1:B:3354:LEU:HA	1:B:3358:PHE:HD2	1.84	0.43
1:B:4035:VAL:HG13	1:B:5032:TYR:HE2	1.84	0.43
1:B:4639:MET:O	1:B:4643:LEU:N	2.47	0.43
1:B:4647:SER:O	1:B:4651:THR:OG1	2.35	0.43
1:C:1096:THR:OG1	1:C:1198:GLN:OE1	2.34	0.43
1:C:2001:PRO:HG2	1:C:3864:THR:HB	2.00	0.43
1:C:2476:ILE:HG23	1:C:2536:LEU:HD21	2.01	0.43
1:D:1784:ALA:O	2:H:82:TYR:OH	2.36	0.43
1:D:2755:ILE:HD12	1:D:2813:LEU:HG	2.01	0.43
1:D:4675:LYS:HG3	1:D:4715:TYR:CE1	2.54	0.43
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.53	0.43
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.52	0.43
1:A:1158:ASN:HB3	1:A:1182:ILE:H	1.84	0.43
1:A:3862:ASP:OD1	1:A:3862:ASP:N	2.49	0.43
1:A:4675:LYS:HG3	1:A:4715:TYR:CE1	2.54	0.43
1:B:118:LEU:HA	1:B:137:LEU:HD23	2.01	0.43
1:B:2616:PRO:HA	1:B:2619:LEU:HD12	2.00	0.43
1:C:531:ARG:NH1	1:C:562:GLU:OE2	2.52	0.43
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.51	0.43
1:C:4181:ILE:HD12	1:C:4183:ILE:HG23	2.00	0.43
1:D:873:LYS:HG2	1:D:970:LEU:HD13	2.01	0.43
1:D:2689:LYS:O	1:D:2993:GLN:NE2	2.51	0.43
2:F:24:VAL:HG12	2:F:103:LEU:HA	2.00	0.43
1:A:2928:LYS:HB3	1:A:2932:MET:HE1	2.01	0.43
1:A:3354:LEU:HA	1:A:3358:PHE:HD2	1.84	0.43
1:A:4181:ILE:HD12	1:A:4183:ILE:HG23	2.00	0.43
1:B:2044:ILE:HD11	1:B:2131:LEU:HD23	2.00	0.43
1:B:2476:ILE:HG23	1:B:2536:LEU:HD21	2.01	0.43
1:B:2911:LEU:HD13	1:B:2915:GLU:HG3	2.00	0.43
1:B:2962:GLN:HA	1:B:2965:ARG:HG2	2.01	0.43
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.53	0.43
1:D:1158:ASN:HB3	1:D:1182:ILE:H	1.84	0.43
1:D:3533:ILE:HD13	1:D:3596:VAL:HG13	2.00	0.43
2:E:20:GLN:HB2	2:E:107:GLU:HG2	2.01	0.43
2:H:24:VAL:HG12	2:H:103:LEU:HA	2.00	0.43
2:H:62:GLY:HA3	2:H:74:LEU:HD21	1.99	0.43
1:A:1000:ARG:HA	1:A:1000:ARG:HD3	1.86	0.42
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.84	0.42
1:B:157:ARG:HG3	1:B:158:SER:H	1.84	0.42
1:C:69:LEU:HD12	1:C:69:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:LYS:HG2	1:C:970:LEU:HD13	2.01	0.42
1:C:1842:LEU:HD23	1:C:1842:LEU:HA	1.88	0.42
1:C:2355:ARG:O	1:C:2359:ARG:HG2	2.19	0.42
1:C:2963:LEU:O	1:C:2967:MET:HB2	2.19	0.42
1:C:3756:LYS:HG3	1:C:3760:LYS:NZ	2.34	0.42
1:D:2002:PRO:HB3	1:D:3641:LEU:HD13	2.00	0.42
1:D:2608:MET:HG3	1:D:2642:LYS:HE3	2.01	0.42
1:D:2859:PRO:HA	1:D:2860:PRO:HD3	1.94	0.42
2:H:20:GLN:HB2	2:H:107:GLU:HG2	2.01	0.42
1:A:846:LEU:HD22	1:A:846:LEU:HA	1.92	0.42
1:A:2476:ILE:HG23	1:A:2536:LEU:HD21	2.01	0.42
1:A:3245:VAL:HG23	1:A:3248:ARG:H	1.84	0.42
1:B:2319:PRO:HG3	1:B:2392:ARG:HA	2.01	0.42
1:B:2355:ARG:O	1:B:2359:ARG:HG2	2.19	0.42
1:B:4092:ASP:HA	1:B:4095:LYS:HG2	2.00	0.42
1:B:4989:MET:HE3	1:B:4989:MET:HB3	1.65	0.42
1:C:150:MET:O	1:C:151:HIS:ND1	2.52	0.42
1:C:1271:ARG:HA	1:C:1563:GLN:HA	2.01	0.42
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.27	0.42
1:C:2970:SER:OG	1:C:2971:GLN:OE1	2.36	0.42
1:C:3354:LEU:HA	1:C:3358:PHE:HD2	1.84	0.42
1:C:4677:LEU:HD11	1:C:4687:TYR:HE2	1.82	0.42
1:C:4971:THR:HG22	1:C:4972:PRO:HD2	2.00	0.42
1:D:3335:MET:SD	1:D:3403:ARG:NH1	2.91	0.42
1:A:2319:PRO:HG3	1:A:2392:ARG:HA	2.01	0.42
1:A:2608:MET:HG3	1:A:2642:LYS:HE3	2.01	0.42
1:A:2909:ASP:OD1	1:A:2909:ASP:N	2.52	0.42
1:B:2002:PRO:HB3	1:B:3641:LEU:HD13	2.00	0.42
1:B:2339:VAL:HG11	1:B:2353:VAL:HG11	2.01	0.42
1:B:2677:LYS:HB3	1:B:2677:LYS:HE2	1.74	0.42
1:C:257:ARG:O	1:C:284:HIS:NE2	2.49	0.42
1:C:4675:LYS:HG3	1:C:4715:TYR:CE1	2.54	0.42
1:D:39:ALA:HB2	1:D:47:CYS:HA	2.02	0.42
1:D:1231[B]:GLN:H	1:D:1231[B]:GLN:HG3	1.44	0.42
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.54	0.42
1:D:2530:MET:HE2	1:D:2530:MET:HB2	1.87	0.42
1:A:873:LYS:HG2	1:A:970:LEU:HD13	2.01	0.42
1:A:2001:PRO:HG2	1:A:3864:THR:HB	2.01	0.42
1:A:2962:GLN:HA	1:A:2965:ARG:HG2	2.01	0.42
1:B:145:ALA:HA	1:B:175:SER:HB3	2.02	0.42
1:B:873:LYS:HG2	1:B:970:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1815:LEU:HD22	1:B:1845:VAL:HG21	2.02	0.42
1:B:3756:LYS:HG3	1:B:3760:LYS:NZ	2.35	0.42
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.54	0.42
1:C:2339:VAL:HG11	1:C:2353:VAL:HG11	2.01	0.42
1:C:2755:ILE:HD12	1:C:2813:LEU:HG	2.01	0.42
1:C:2911:LEU:HD13	1:C:2915:GLU:HG3	2.00	0.42
1:D:150:MET:O	1:D:151:HIS:ND1	2.52	0.42
1:D:2355:ARG:HA	1:D:2358:ILE:HG22	2.00	0.42
1:D:2970:SER:OG	1:D:2971:GLN:OE1	2.36	0.42
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.84	0.42
1:A:157:ARG:HG3	1:A:158:SER:H	1.84	0.42
1:A:596:ASN:HD21	1:A:598:LYS:HE2	1.85	0.42
1:A:863:LEU:HA	1:A:864:PRO:HD3	1.84	0.42
1:A:3756:LYS:HG3	1:A:3760:LYS:NZ	2.35	0.42
1:A:3782:MET:HE2	1:A:3782:MET:HB2	1.88	0.42
1:B:1158:ASN:HB3	1:B:1182:ILE:H	1.84	0.42
1:B:2755:ILE:HD12	1:B:2813:LEU:HG	2.01	0.42
1:B:2997:PHE:O	1:B:3001:ILE:HB	2.19	0.42
1:B:3245:VAL:HG23	1:B:3248:ARG:H	1.84	0.42
1:B:4685:GLY:HA3	1:B:4689:THR:HG23	2.01	0.42
1:C:1158:ASN:HB3	1:C:1182:ILE:H	1.84	0.42
1:D:771:PHE:HB3	1:D:1472:VAL:HG23	2.02	0.42
1:D:1619:ARG:NH2	1:D:1622:GLU:OE1	2.53	0.42
1:D:2963:LEU:O	1:D:2967:MET:HB2	2.19	0.42
1:D:3852:LYS:HE3	1:D:3852:LYS:HB3	1.97	0.42
1:A:1619:ARG:NH2	1:A:1622:GLU:OE1	2.53	0.42
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	2.02	0.42
1:A:1842:LEU:HD23	1:A:1842:LEU:HA	1.88	0.42
1:A:2309:SER:HB2	1:A:2314:LEU:HD11	2.02	0.42
1:A:3194:LEU:HA	1:A:3197:LEU:HG	2.00	0.42
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.34	0.42
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.54	0.42
1:B:2765:LYS:HD3	1:B:2765:LYS:HA	1.81	0.42
1:B:2960:LEU:HB3	1:B:3038:MET:HE2	2.00	0.42
1:B:3219:TYR:OH	1:B:3239:MET:SD	2.60	0.42
1:C:3007:ASN:O	1:C:3011:THR:OG1	2.27	0.42
1:C:4092:ASP:HA	1:C:4095:LYS:HG2	2.00	0.42
1:D:2001:PRO:HG2	1:D:3864:THR:HB	2.00	0.42
1:D:2453:ILE:HD13	1:D:2456:ILE:HD12	2.02	0.42
1:D:3046:LEU:O	1:D:3049:LEU:HB3	2.20	0.42
1:D:3756:LYS:HG3	1:D:3760:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:24:VAL:HG12	2:E:103:LEU:HA	2.00	0.42
1:A:2948:THR:OG1	1:A:2952:GLU:OE2	2.25	0.42
1:A:4685:GLY:HA3	1:A:4689:THR:HG23	2.01	0.42
1:B:1271:ARG:HA	1:B:1563:GLN:HA	2.01	0.42
1:B:2909:ASP:N	1:B:2909:ASP:OD1	2.52	0.42
1:B:4181:ILE:HD12	1:B:4183:ILE:HG23	2.00	0.42
1:B:4675:LYS:HG3	1:B:4715:TYR:CE1	2.54	0.42
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.47	0.42
1:C:775:GLY:H	1:C:848:HIS:CE1	2.38	0.42
1:C:1101:ARG:NH1	1:C:1115:LEU:O	2.52	0.42
1:C:1231[B]:GLN:H	1:C:1231[B]:GLN:HG3	1.44	0.42
1:C:1289:LEU:HD23	1:C:1597:VAL:HG11	2.01	0.42
1:C:2017:ASP:OD1	1:C:2017:ASP:N	2.53	0.42
1:C:3582:ARG:HD3	1:C:3582:ARG:HA	1.84	0.42
1:C:4989:MET:HE3	1:C:4989:MET:HB3	1.65	0.42
1:D:1000:ARG:HA	1:D:1000:ARG:HD3	1.85	0.42
1:D:1101:ARG:NH1	1:D:1115:LEU:O	2.52	0.42
1:D:1289:LEU:HD23	1:D:1597:VAL:HG11	2.01	0.42
1:D:2319:PRO:HG3	1:D:2392:ARG:HA	2.01	0.42
1:D:3194:LEU:HA	1:D:3197:LEU:HG	2.00	0.42
1:A:2453:ILE:HD13	1:A:2456:ILE:HD12	2.02	0.42
1:A:2997:PHE:O	1:A:3001:ILE:HB	2.19	0.42
1:B:1101:ARG:NH1	1:B:1115:LEU:O	2.52	0.42
1:B:1110:ARG:HE	1:B:1110:ARG:HB3	1.70	0.42
1:B:2309:SER:HB2	1:B:2314:LEU:HD11	2.02	0.42
1:B:2453:ILE:HD13	1:B:2456:ILE:HD12	2.02	0.42
1:B:2614:ILE:O	1:B:2650:ARG:NH2	2.43	0.42
1:C:771:PHE:HB3	1:C:1472:VAL:HG23	2.02	0.42
1:C:3046:LEU:O	1:C:3049:LEU:HB3	2.20	0.42
1:D:169:LEU:HB2	1:D:202:MET:HE1	2.01	0.42
1:D:1815:LEU:HD22	1:D:1845:VAL:HG21	2.02	0.42
1:D:2017:ASP:OD1	1:D:2017:ASP:N	2.53	0.42
1:A:145:ALA:HA	1:A:175:SER:HB3	2.02	0.42
1:A:1149:VAL:HG22	1:A:1164:LEU:HD13	2.01	0.42
1:A:1231[B]:GLN:H	1:A:1231[B]:GLN:HG3	1.44	0.42
1:A:2801:ASP:OD1	1:A:2801:ASP:N	2.53	0.42
1:B:596:ASN:HD21	1:B:598:LYS:HE2	1.85	0.42
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.93	0.42
1:B:884:LEU:HD13	1:B:968:ALA:H	1.85	0.42
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	2.02	0.42
1:B:2017:ASP:OD1	1:B:2017:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2965:ARG:HG3	1:B:2966:TRP:CD1	2.55	0.42
1:C:1815:LEU:HD22	1:C:1845:VAL:HG21	2.02	0.42
1:C:2319:PRO:HG3	1:C:2392:ARG:HA	2.01	0.42
1:C:2499:LYS:O	1:C:2503:VAL:HG23	2.20	0.42
1:C:2997:PHE:O	1:C:3001:ILE:HB	2.19	0.42
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.29	0.42
1:D:775:GLY:H	1:D:848:HIS:CE1	2.38	0.42
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	2.02	0.42
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	2.02	0.42
1:D:2245:GLN:HA	1:D:2248:ARG:HG2	2.02	0.42
1:D:2962:GLN:HA	1:D:2965:ARG:HG2	2.01	0.42
1:D:3616:LYS:HD3	1:D:3616:LYS:HA	1.91	0.42
1:A:838:HIS:CE1	1:A:1201:HIS:HB2	2.55	0.42
1:A:2965:ARG:HG3	1:A:2966:TRP:CD1	2.55	0.42
1:B:3888:LEU:HD23	1:B:3888:LEU:HA	1.88	0.42
1:B:4734:ARG:HB3	1:B:4745:LEU:HD11	2.02	0.42
1:C:1619:ARG:NH2	1:C:1622:GLU:OE1	2.53	0.42
1:D:2377:LEU:HA	1:D:2377:LEU:HD23	1.90	0.42
1:D:2677:LYS:HB3	1:D:2677:LYS:HE2	1.74	0.42
1:D:2765:LYS:HD3	1:D:2765:LYS:HA	1.81	0.42
1:D:2909:ASP:OD1	1:D:2909:ASP:N	2.52	0.42
1:D:3433:GLU:OE1	1:D:3436:ARG:NH1	2.49	0.42
1:D:3888:LEU:HD23	1:D:3888:LEU:HA	1.88	0.42
1:D:4685:GLY:HA3	1:D:4689:THR:HG23	2.01	0.42
1:A:1110:ARG:HE	1:A:1110:ARG:HB3	1.70	0.41
1:A:2355:ARG:O	1:A:2359:ARG:HG2	2.19	0.41
1:C:157:ARG:HG3	1:C:158:SER:H	1.85	0.41
1:C:2309:SER:HB2	1:C:2314:LEU:HD11	2.02	0.41
1:C:2879:ALA:HB2	1:C:2923:ALA:HB2	2.02	0.41
1:D:1152:MET:HE1	1:D:1218:GLY:HA2	2.02	0.41
1:D:2339:VAL:HG11	1:D:2353:VAL:HG11	2.01	0.41
1:D:2965:ARG:HG3	1:D:2966:TRP:CD1	2.55	0.41
1:D:3330:ASP:O	1:D:3403:ARG:NH2	2.45	0.41
1:D:4998:LYS:HD3	1:D:5003:HIS:HD2	1.85	0.41
1:A:687:ALA:HA	1:A:713:SER:HA	2.02	0.41
1:A:884:LEU:HD13	1:A:968:ALA:H	1.85	0.41
1:A:1087:ARG:NH1	1:A:1221:GLU:O	2.53	0.41
1:A:1096:THR:OG1	1:A:1198:GLN:OE1	2.34	0.41
1:A:1289:LEU:HD23	1:A:1597:VAL:HG11	2.01	0.41
1:A:3046:LEU:O	1:A:3049:LEU:HB3	2.20	0.41
1:B:169:LEU:HB2	1:B:202:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:ARG:NH1	2:F:90:VAL:O	2.45	0.41
1:B:1488:LYS:HE3	1:B:1488:LYS:HB2	1.88	0.41
1:B:2608:MET:HG3	1:B:2642:LYS:HE3	2.01	0.41
1:C:169:LEU:HB2	1:C:202:MET:HE1	2.01	0.41
1:C:2453:ILE:HD13	1:C:2456:ILE:HD12	2.02	0.41
1:C:2677:LYS:HB3	1:C:2677:LYS:HE2	1.74	0.41
1:C:2965:ARG:HG3	1:C:2966:TRP:CD1	2.55	0.41
1:D:2309:SER:HB2	1:D:2314:LEU:HD11	2.02	0.41
1:D:2476:ILE:HG23	1:D:2536:LEU:HD21	2.01	0.41
1:D:2879:ALA:HB2	1:D:2923:ALA:HB2	2.02	0.41
1:D:2997:PHE:O	1:D:3001:ILE:HB	2.19	0.41
1:D:4734:ARG:HB3	1:D:4745:LEU:HD11	2.02	0.41
1:A:497:TYR:HD2	1:A:503:PHE:HD1	1.69	0.41
1:A:1488:LYS:HE3	1:A:1488:LYS:HB2	1.88	0.41
1:A:3186:LEU:HB3	1:A:3190:LEU:HD23	2.02	0.41
1:A:4998:LYS:HD3	1:A:5003:HIS:HD2	1.85	0.41
1:B:1289:LEU:HD23	1:B:1597:VAL:HG11	2.01	0.41
1:B:3046:LEU:O	1:B:3049:LEU:HB3	2.20	0.41
1:B:4843:LEU:O	1:B:4847:VAL:HG13	2.20	0.41
1:C:497:TYR:HD2	1:C:503:PHE:HD1	1.69	0.41
1:C:838:HIS:CE1	1:C:1201:HIS:HB2	2.55	0.41
1:C:1149:VAL:HG22	1:C:1164:LEU:HD13	2.01	0.41
1:C:1152:MET:HE1	1:C:1218:GLY:HA2	2.02	0.41
1:C:2608:MET:HG3	1:C:2642:LYS:HE3	2.01	0.41
1:C:4239:GLU:OE2	1:C:5014:TYR:OH	2.33	0.41
1:C:4685:GLY:HA3	1:C:4689:THR:HG23	2.01	0.41
1:D:838:HIS:CE1	1:D:1201:HIS:HB2	2.55	0.41
1:D:2814:LYS:HA	1:D:2817:ILE:HG22	2.03	0.41
1:D:2928:LYS:HA	1:D:2928:LYS:HD3	1.79	0.41
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	2.03	0.41
1:D:4013:LEU:HD12	1:D:4013:LEU:HA	1.94	0.41
1:A:1152:MET:HE1	1:A:1218:GLY:HA2	2.03	0.41
1:A:1271:ARG:HA	1:A:1563:GLN:HA	2.01	0.41
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	2.02	0.41
1:A:3652:MET:HA	1:A:3655:GLU:HG2	2.03	0.41
1:B:497:TYR:HD2	1:B:503:PHE:HD1	1.69	0.41
1:B:1087:ARG:NH1	1:B:1221:GLU:O	2.53	0.41
1:B:1619:ARG:NH2	1:B:1622:GLU:OE1	2.53	0.41
1:B:2245:GLN:HA	1:B:2248:ARG:HG2	2.02	0.41
1:B:2499:LYS:O	1:B:2503:VAL:HG23	2.20	0.41
1:C:1238:PHE:HD1	1:C:1608:MET:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	2.02	0.41
1:C:2530:MET:HE2	1:C:2530:MET:HB2	1.87	0.41
1:C:4003:LEU:HD22	1:C:4009:GLN:HG2	2.02	0.41
1:C:4998:LYS:HD3	1:C:5003:HIS:HD2	1.85	0.41
1:D:884:LEU:HD13	1:D:968:ALA:H	1.85	0.41
1:D:1077:ALA:HB3	1:D:1189:LEU:HD11	2.02	0.41
1:A:771:PHE:HB3	1:A:1472:VAL:HG23	2.02	0.41
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.54	0.41
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.02	0.41
1:A:2499:LYS:O	1:A:2503:VAL:HG23	2.20	0.41
1:A:2654:TYR:HA	1:A:2661:TRP:H	1.86	0.41
1:A:3571:TRP:CE2	1:B:1228:ILE:HG12	2.56	0.41
1:A:3793:MET:HE2	1:A:3793:MET:HB3	1.91	0.41
1:A:4843:LEU:O	1:A:4847:VAL:HG13	2.20	0.41
1:B:39:ALA:HB2	1:B:47:CYS:HA	2.02	0.41
1:B:771:PHE:HB3	1:B:1472:VAL:HG23	2.02	0.41
1:B:775:GLY:H	1:B:848:HIS:CE1	2.38	0.41
1:B:1249:PRO:HA	1:B:1250:PRO:HD3	1.96	0.41
1:B:2023:LEU:O	1:B:2028:ARG:NE	2.54	0.41
1:B:2725:LYS:HZ1	1:B:2738:ARG:HH12	1.68	0.41
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.34	0.41
1:B:4646:LEU:HD23	1:B:4646:LEU:HA	1.87	0.41
1:C:118:LEU:HA	1:C:137:LEU:HD23	2.01	0.41
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	2.02	0.41
1:C:2725:LYS:HZ1	1:C:2738:ARG:HH12	1.69	0.41
1:D:118:LEU:HA	1:D:137:LEU:HD23	2.01	0.41
1:D:266:ARG:CZ	1:D:330:ASP:HB2	2.51	0.41
1:D:858:THR:OG1	1:D:927:GLU:OE2	2.31	0.41
1:D:1149:VAL:HG22	1:D:1164:LEU:HD13	2.01	0.41
1:D:2355:ARG:O	1:D:2359:ARG:HG2	2.19	0.41
1:D:2782:ASP:N	1:D:2782:ASP:OD1	2.53	0.41
1:A:39:ALA:HB2	1:A:47:CYS:HA	2.02	0.41
1:A:118:LEU:HA	1:A:137:LEU:HD23	2.01	0.41
1:A:169:LEU:HB2	1:A:202:MET:HE1	2.01	0.41
1:A:266:ARG:CZ	1:A:330:ASP:HB2	2.51	0.41
1:A:308:HIS:HD2	1:A:310:LYS:HB3	1.86	0.41
1:A:2245:GLN:HA	1:A:2248:ARG:HG2	2.02	0.41
1:A:2622:LEU:O	1:A:2626:LEU:HG	2.21	0.41
1:A:4054:ASN:O	1:A:4058:ILE:HG12	2.21	0.41
1:A:4989:MET:HE3	1:A:4989:MET:HB3	1.65	0.41
1:B:663:TYR:OH	1:B:665:GLU:OE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4003:LEU:HD22	1:B:4009:GLN:HG2	2.03	0.41
1:B:4630:TYR:OH	1:C:4860:ARG:NH2	2.54	0.41
1:C:1249:PRO:HA	1:C:1250:PRO:HD3	1.96	0.41
1:C:2814:LYS:HA	1:C:2817:ILE:HG22	2.03	0.41
1:C:4630:TYR:OH	1:D:4860:ARG:NH2	2.54	0.41
1:D:497:TYR:HD2	1:D:503:PHE:HD1	1.69	0.41
1:D:596:ASN:HD21	1:D:598:LYS:HE2	1.85	0.41
1:D:2499:LYS:O	1:D:2503:VAL:HG23	2.20	0.41
1:D:4800:LEU:HD23	1:D:4800:LEU:HA	1.89	0.41
2:E:37:ASP:OD1	2:E:42:ARG:NH2	2.54	0.41
1:A:663:TYR:OH	1:A:665:GLU:OE2	2.36	0.41
1:A:1072:VAL:HA	1:A:1194:LEU:O	2.21	0.41
1:A:1077:ALA:HB3	1:A:1189:LEU:HD11	2.02	0.41
1:A:1699:GLU:OE2	1:A:1813:ARG:NH1	2.45	0.41
1:A:2879:ALA:HB2	1:A:2923:ALA:HB2	2.02	0.41
1:A:3568:SER:HA	1:A:3571:TRP:HE1	1.85	0.41
1:B:838:HIS:CE1	1:B:1201:HIS:HB2	2.55	0.41
1:B:932:LEU:HD22	1:B:984:LEU:HD21	2.03	0.41
1:B:1155:LEU:HD12	1:B:1184:ILE:HD13	2.02	0.41
1:B:2782:ASP:OD1	1:B:2782:ASP:N	2.53	0.41
1:C:39:ALA:HB2	1:C:47:CYS:HA	2.02	0.41
1:C:145:ALA:HA	1:C:175:SER:HB3	2.02	0.41
1:C:308:HIS:HD2	1:C:310:LYS:HB3	1.86	0.41
1:C:893:TYR:HB3	1:C:960:MET:HE2	2.03	0.41
1:C:932:LEU:HD22	1:C:984:LEU:HD21	2.03	0.41
1:C:1573:MET:SD	1:C:1574:PRO:HD2	2.61	0.41
1:C:3652:MET:HA	1:C:3655:GLU:HG2	2.03	0.41
1:D:145:ALA:HA	1:D:175:SER:HB3	2.02	0.41
1:D:2044:ILE:HD11	1:D:2131:LEU:HD23	2.00	0.41
2:F:20:GLN:HB2	2:F:107:GLU:HG2	2.01	0.41
2:F:87:HIS:HA	2:F:88:PRO:HD3	1.96	0.41
2:G:20:GLN:HB2	2:G:107:GLU:HG2	2.01	0.41
1:A:69:LEU:HA	1:A:69:LEU:HD12	1.87	0.41
1:A:775:GLY:H	1:A:848:HIS:CE1	2.38	0.41
1:A:2584[B]:HIS:CE1	1:A:2625:ARG:HB2	2.56	0.41
1:A:2587:TYR:O	1:A:2590:SER:OG	2.29	0.41
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.51	0.41
1:B:1072:VAL:HA	1:B:1194:LEU:O	2.21	0.41
1:B:1149:VAL:HG22	1:B:1164:LEU:HD13	2.01	0.41
1:B:1152:MET:HE1	1:B:1218:GLY:HA2	2.02	0.41
1:B:1743[A]:ARG:HE	1:B:1743[A]:ARG:HB2	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3652:MET:HA	1:B:3655:GLU:HG2	2.03	0.41
1:B:4047:MET:HE3	1:B:4047:MET:HB3	1.97	0.41
1:C:663:TYR:HE1	1:C:745:SER:HB3	1.85	0.41
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.93	0.41
1:C:4734:ARG:HB3	1:C:4745:LEU:HD11	2.02	0.41
1:D:403:MET:O	1:D:407:THR:OG1	2.35	0.41
1:D:1087:ARG:NH1	1:D:1221:GLU:O	2.54	0.41
1:D:2474:LEU:HD23	1:D:2494:PHE:HD2	1.86	0.41
1:D:4090:LYS:HE2	1:D:4090:LYS:HB3	1.84	0.41
2:G:37:ASP:OD1	2:G:42:ARG:NH2	2.54	0.41
1:A:1155:LEU:HD12	1:A:1184:ILE:HD13	2.02	0.41
1:A:2814:LYS:HA	1:A:2817:ILE:HG22	2.03	0.41
1:A:3433:GLU:OE1	1:A:3436:ARG:NH1	2.49	0.41
1:A:3460:VAL:HA	1:A:3502:ARG:CZ	2.51	0.41
1:A:3823:LYS:HD3	1:A:3823:LYS:HA	1.78	0.41
1:A:4865:LYS:HD2	1:A:4865:LYS:HA	1.82	0.41
1:B:661:LYS:HB3	1:B:808:TYR:HA	2.02	0.41
1:B:687:ALA:HA	1:B:713:SER:HA	2.03	0.41
1:B:1238:PHE:HD1	1:B:1608:MET:HE2	1.86	0.41
1:B:1573:MET:SD	1:B:1574:PRO:HD2	2.61	0.41
1:B:1773:PRO:HA	1:B:1774:PRO:HD3	1.93	0.41
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.86	0.41
1:B:3186:LEU:HB3	1:B:3190:LEU:HD23	2.02	0.41
1:C:884:LEU:HD13	1:C:968:ALA:H	1.85	0.41
1:C:1087:ARG:NH1	1:C:1221:GLU:O	2.54	0.41
1:C:1524:THR:O	1:C:1541:GLN:NE2	2.38	0.41
1:C:1577:ALA:HB1	1:C:1584:ARG:HA	2.03	0.41
1:C:2023:LEU:O	1:C:2028:ARG:NE	2.54	0.41
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.86	0.41
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	2.03	0.41
1:C:3186:LEU:HB3	1:C:3190:LEU:HD23	2.02	0.41
1:D:863:LEU:HA	1:D:864:PRO:HD3	1.84	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.51	0.41
1:D:893:TYR:HB3	1:D:960:MET:HE2	2.03	0.41
1:D:932:LEU:HD22	1:D:984:LEU:HD21	2.03	0.41
1:D:1271:ARG:HA	1:D:1563:GLN:HA	2.01	0.41
1:D:1849:LEU:HA	1:D:1849:LEU:HD23	1.88	0.41
1:D:2023:LEU:O	1:D:2028:ARG:NE	2.54	0.41
1:D:2584[B]:HIS:CE1	1:D:2625:ARG:HB2	2.56	0.41
1:D:2654:TYR:HA	1:D:2661:TRP:H	1.86	0.41
1:D:3186:LEU:HB3	1:D:3190:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3420:ARG:NH1	1:D:3516:LYS:O	2.52	0.41
1:D:3460:VAL:HA	1:D:3502:ARG:CZ	2.51	0.41
1:D:3568:SER:HA	1:D:3571:TRP:HE1	1.85	0.41
1:D:3652:MET:HA	1:D:3655:GLU:HG2	2.03	0.41
1:D:4843:LEU:O	1:D:4847:VAL:HG13	2.20	0.41
1:A:2339:VAL:HG11	1:A:2353:VAL:HG11	2.01	0.41
1:A:2474:LEU:HD23	1:A:2494:PHE:HD2	1.86	0.41
1:A:4734:ARG:HB3	1:A:4745:LEU:HD11	2.02	0.41
1:B:2288:LEU:HD23	1:B:2288:LEU:HA	1.91	0.41
1:B:2879:ALA:HB2	1:B:2923:ALA:HB2	2.02	0.41
1:C:2245:GLN:HA	1:C:2248:ARG:HG2	2.02	0.41
1:C:2309:SER:OG	1:C:2321:ILE:O	2.28	0.41
1:C:4090:LYS:HE2	1:C:4090:LYS:HB3	1.83	0.41
1:D:826:ILE:HG22	1:D:827:LYS:HG2	2.03	0.41
1:D:1577:ALA:HB1	1:D:1584:ARG:HA	2.03	0.41
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.86	0.41
2:F:37:ASP:OD1	2:F:42:ARG:NH2	2.54	0.41
1:A:932:LEU:HD22	1:A:984:LEU:HD21	2.03	0.40
1:A:2023:LEU:O	1:A:2028:ARG:NE	2.54	0.40
1:A:4748:LEU:HD23	1:A:4748:LEU:HA	1.96	0.40
1:B:266:ARG:CZ	1:B:330:ASP:HB2	2.51	0.40
1:B:2584[B]:HIS:CE1	1:B:2625:ARG:HB2	2.56	0.40
1:B:2814:LYS:HA	1:B:2817:ILE:HG22	2.03	0.40
1:B:2978:GLU:HA	1:B:2981:VAL:HG12	2.03	0.40
1:B:3460:VAL:HA	1:B:3502:ARG:CZ	2.51	0.40
1:B:3568:SER:HA	1:B:3571:TRP:HE1	1.85	0.40
1:B:4054:ASN:O	1:B:4058:ILE:HG12	2.21	0.40
1:C:266:ARG:CZ	1:C:330:ASP:HB2	2.51	0.40
1:C:661:LYS:HB3	1:C:808:TYR:HA	2.02	0.40
1:C:2716:ASP:OD1	1:C:2716:ASP:N	2.45	0.40
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.53	0.40
1:C:3460:VAL:HA	1:C:3502:ARG:CZ	2.51	0.40
1:D:1155:LEU:HD12	1:D:1184:ILE:HD13	2.02	0.40
1:D:1488:LYS:HE3	1:D:1488:LYS:HB2	1.88	0.40
2:G:99:PHE:HB3	2:G:101:VAL:HG23	2.03	0.40
1:A:2978:GLU:HA	1:A:2981:VAL:HG12	2.03	0.40
1:B:663:TYR:HE1	1:B:745:SER:HB3	1.85	0.40
1:B:1231[B]:GLN:H	1:B:1231[B]:GLN:HG3	1.44	0.40
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	2.02	0.40
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.78	0.40
1:B:4692:PRO:HG3	1:B:4703:ARG:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.04	0.40
1:C:1077:ALA:HB3	1:C:1189:LEU:HD11	2.02	0.40
1:C:1431:THR:HG21	1:C:1523:ALA:HB2	2.03	0.40
1:C:2283:ASN:HD21	1:C:2286:LEU:HD13	1.86	0.40
1:C:2575:ARG:HA	1:C:2575:ARG:HD2	1.95	0.40
1:C:2978:GLU:HA	1:C:2981:VAL:HG12	2.03	0.40
1:C:3249:LEU:HD12	1:C:3249:LEU:HA	1.91	0.40
1:C:3891:LEU:HB3	1:C:3899:PHE:CE2	2.57	0.40
1:D:663:TYR:HE1	1:D:745:SER:HB3	1.85	0.40
1:D:1573:MET:SD	1:D:1574:PRO:HD2	2.61	0.40
1:D:4155:PRO:HG3	1:D:5036:LEU:HD23	2.04	0.40
2:E:19:GLY:C	2:E:49:ARG:HH12	2.30	0.40
1:A:826:ILE:HG22	1:A:827:LYS:HG2	2.03	0.40
1:A:1578:ALA:O	1:A:1584:ARG:NH2	2.53	0.40
1:A:2004:GLU:HA	1:A:2007:ASN:HD22	1.87	0.40
1:A:2336:ARG:HG2	1:A:2435:ARG:HD2	2.04	0.40
1:A:2752:ASP:HA	1:A:2755:ILE:HG12	2.03	0.40
1:A:2782:ASP:OD1	1:A:2782:ASP:N	2.53	0.40
1:A:3696:ASP:OD1	1:A:3696:ASP:N	2.41	0.40
1:A:3891:LEU:HB3	1:A:3899:PHE:CE2	2.57	0.40
1:B:1077:ALA:HB3	1:B:1189:LEU:HD11	2.02	0.40
1:B:2136:ARG:O	1:B:2140:ARG:NH2	2.55	0.40
1:B:2622:LEU:O	1:B:2626:LEU:HG	2.21	0.40
1:B:2654:TYR:HA	1:B:2661:TRP:H	1.86	0.40
1:B:3330:ASP:O	1:B:3403:ARG:NH2	2.45	0.40
1:C:107:ILE:HD13	1:C:107:ILE:HA	1.92	0.40
1:C:596:ASN:HD21	1:C:598:LYS:HE2	1.85	0.40
1:C:2280:VAL:HA	1:C:2287:ALA:HB1	2.04	0.40
1:C:2296:GLU:HA	1:C:2299:VAL:HG12	2.03	0.40
1:C:2474:LEU:HD23	1:C:2494:PHE:HD2	1.86	0.40
1:C:2909:ASP:OD1	1:C:2909:ASP:N	2.52	0.40
1:C:3995:VAL:O	1:C:3999:MET:HG2	2.22	0.40
1:C:4800:LEU:HD23	1:C:4800:LEU:HA	1.89	0.40
1:D:157:ARG:HG3	1:D:158:SER:H	1.84	0.40
1:D:463:GLU:O	1:D:466:SER:OG	2.34	0.40
1:D:687:ALA:HA	1:D:713:SER:HA	2.02	0.40
1:D:2283:ASN:HD21	1:D:2286:LEU:HD13	1.86	0.40
1:D:2752:ASP:HA	1:D:2755:ILE:HG12	2.03	0.40
1:D:2978:GLU:HA	1:D:2981:VAL:HG12	2.03	0.40
1:D:5008:SER:O	1:D:5012:LYS:HD2	2.21	0.40
1:A:16:THR:HA	1:A:69:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1699:GLU:OE2	1:B:1813:ARG:NH1	2.45	0.40
1:B:2283:ASN:HD21	1:B:2286:LEU:HD13	1.86	0.40
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.54	0.40
1:B:3995:VAL:O	1:B:3999:MET:HG2	2.22	0.40
1:B:4122:MET:HE3	1:B:4122:MET:HB3	2.00	0.40
1:B:4998:LYS:HD3	1:B:5003:HIS:HD2	1.85	0.40
1:C:1155:LEU:HD12	1:C:1184:ILE:HD13	2.02	0.40
1:C:2622:LEU:O	1:C:2626:LEU:HG	2.21	0.40
1:C:4059:LEU:HD13	1:C:4059:LEU:HA	1.96	0.40
1:C:4155:PRO:HG3	1:C:5036:LEU:HD23	2.04	0.40
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	2.03	0.40
1:D:1695:LEU:HB3	1:D:1810:LYS:NZ	2.37	0.40
1:D:2136:ARG:O	1:D:2140:ARG:NH2	2.55	0.40
1:D:4054:ASN:O	1:D:4058:ILE:HG12	2.21	0.40
2:F:99:PHE:HB3	2:F:101:VAL:HG23	2.03	0.40
1:A:893:TYR:HB3	1:A:960:MET:HE2	2.03	0.40
1:A:1573:MET:SD	1:A:1574:PRO:HD2	2.61	0.40
1:A:1969:LEU:HD21	1:A:2009:LEU:HD13	2.04	0.40
1:A:2208:MET:HE3	1:A:2208:MET:HB2	1.91	0.40
1:A:3290:GLU:OE1	1:A:3309:SER:N	2.54	0.40
1:A:3995:VAL:O	1:A:3999:MET:HG2	2.22	0.40
1:A:4155:PRO:HG3	1:A:5036:LEU:HD23	2.04	0.40
1:B:494:LEU:HD12	1:B:515:TRP:CD1	2.57	0.40
1:B:2336:ARG:HG2	1:B:2435:ARG:HD2	2.04	0.40
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.57	0.40
1:B:4750:ILE:H	1:B:4750:ILE:HG13	1.60	0.40
1:C:1100:MET:HE3	1:C:1198:GLN:HB3	2.03	0.40
1:C:2584[B]:HIS:CE1	1:C:2625:ARG:HB2	2.56	0.40
1:C:2801:ASP:OD1	1:C:2801:ASP:N	2.53	0.40
1:C:4054:ASN:O	1:C:4058:ILE:HG12	2.21	0.40
1:C:4706:LEU:H	1:C:4706:LEU:HG	1.73	0.40
1:C:5008:SER:O	1:C:5012:LYS:HD2	2.21	0.40
1:C:5012:LYS:O	1:C:5016:GLU:HG2	2.21	0.40
1:D:308:HIS:HD2	1:D:310:LYS:HB3	1.86	0.40
1:D:378:LEU:HD12	1:D:378:LEU:HA	1.94	0.40
1:D:733:PRO:HG2	1:D:762:CYS:HB3	2.04	0.40
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.04	0.40
1:D:3995:VAL:O	1:D:3999:MET:HG2	2.22	0.40
1:D:4003:LEU:HD22	1:D:4009:GLN:HG2	2.02	0.40
2:E:23:VAL:HG22	2:E:47:LYS:HG2	2.04	0.40
2:H:19:GLY:C	2:H:49:ARG:HH12	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:VAL:HG22	2:H:47:LYS:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	B	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	C	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
1	D	4356/5037 (86%)	4216 (97%)	137 (3%)	3 (0%)	48	79
2	E	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	F	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	G	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	H	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
All	All	17844/21548 (83%)	17272 (97%)	560 (3%)	12 (0%)	49	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3615	SER
1	A	4712	PRO
1	B	3615	SER
1	B	4712	PRO
1	C	3615	SER
1	C	4712	PRO
1	D	3615	SER
1	D	4712	PRO
1	A	3692	GLU

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Mol	Chain	Res	Type
1	B	3692	GLU
1	C	3692	GLU
1	D	3692	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3808/4276 (89%)	3700 (97%)	108 (3%)	38	61
1	B	3808/4276 (89%)	3700 (97%)	108 (3%)	38	61
1	C	3808/4276 (89%)	3700 (97%)	108 (3%)	38	61
1	D	3808/4276 (89%)	3700 (97%)	108 (3%)	38	61
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15584/18320 (85%)	15152 (97%)	432 (3%)	38	61

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	LEU
1	A	1072	VAL
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	3690	VAL
1	A	3692	GLU
1	A	4178	LEU
1	A	4180	ARG
1	A	4182	GLU
1	A	4183	ILE
1	A	4184	MET
1	A	4188	ARG

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Mol	Chain	Res	Type
1	A	4189	ARG
1	A	4190	ILE
1	A	4192	ARG
1	A	4193	ILE
1	A	4200	THR
1	A	4206	GLU
1	A	4207	MET
1	A	4209	GLN
1	A	4212	GLU
1	A	4221	VAL
1	A	4224	GLU
1	A	4227	GLU
1	A	4229	GLU
1	A	4231	MET
1	A	4541	TRP
1	A	4543	GLU
1	A	4544	LEU
1	A	4550	LYS
1	A	4555	LEU
1	A	4556	SER
1	A	4561	THR
1	A	4569	LEU
1	A	4577	LEU
1	A	4580	TYR
1	A	4581	LYS
1	A	4583	SER
1	A	4627	MET
1	A	4628	VAL
1	A	4632	LEU
1	A	4633	GLU
1	A	4635	SER
1	A	4636	THR
1	A	4640	GLU
1	A	4647	SER
1	A	4651	THR
1	A	4662	ASN
1	A	4665	LYS
1	A	4666	VAL
1	A	4675	LYS
1	A	4676	GLU
1	A	4680	LYS
1	A	4682	GLU

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Mol	Chain	Res	Type
1	A	4689	THR
1	A	4694	ASP
1	A	4696	ASP
1	A	4697	VAL
1	A	4698	LYS
1	A	4704	LEU
1	A	4705	VAL
1	A	4706	LEU
1	A	4710	SER
1	A	4718	LYS
1	A	4720	VAL
1	A	4721	LYS
1	A	4736	ARG
1	A	4743	MET
1	A	4745	LEU
1	A	4748	LEU
1	A	4750	ILE
1	A	4779	LYS
1	A	4809	PHE
1	A	4818	MET
1	A	4822	THR
1	A	4835	LYS
1	A	4836	GLN
1	A	4837	LEU
1	A	4843	LEU
1	A	4844	LEU
1	A	4847	VAL
1	A	4861	LYS
1	A	4867	GLU
1	A	4870	ASP
1	A	4874	MET
1	A	4875	LYS
1	A	4889	VAL
1	A	4911	LEU
1	A	4927	ILE
1	A	4932	ILE
1	A	4933	GLN
1	A	4937	ILE
1	A	4948	GLU
1	A	4966	ASP
1	A	4971	THR
1	A	4976	GLU

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Mol	Chain	Res	Type
1	A	4982	GLU
1	A	4989	MET
1	A	4992	LEU
1	A	4993	MET
1	A	4995	LEU
1	A	4997	ASN
1	A	5002	GLU
1	A	5012	LYS
1	A	5013	MET
1	A	5015	GLN
1	A	5027	CYS
1	A	5034	ASP
1	B	846	LEU
1	B	1072	VAL
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	3690	VAL
1	B	3692	GLU
1	B	4178	LEU
1	B	4180	ARG
1	B	4182	GLU
1	B	4183	ILE
1	B	4184	MET
1	B	4188	ARG
1	B	4189	ARG
1	B	4190	ILE
1	B	4192	ARG
1	B	4193	ILE
1	B	4200	THR
1	B	4206	GLU
1	B	4207	MET
1	B	4209	GLN
1	B	4212	GLU
1	B	4221	VAL
1	B	4224	GLU
1	B	4227	GLU
1	B	4229	GLU
1	B	4231	MET
1	B	4541	TRP
1	B	4543	GLU
1	B	4544	LEU
1	B	4550	LYS

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Mol	Chain	Res	Type
1	B	4555	LEU
1	B	4556	SER
1	B	4561	THR
1	B	4569	LEU
1	B	4577	LEU
1	B	4580	TYR
1	B	4581	LYS
1	B	4583	SER
1	B	4627	MET
1	B	4628	VAL
1	B	4632	LEU
1	B	4633	GLU
1	B	4635	SER
1	B	4636	THR
1	B	4640	GLU
1	B	4647	SER
1	B	4651	THR
1	B	4662	ASN
1	B	4665	LYS
1	B	4666	VAL
1	B	4675	LYS
1	B	4676	GLU
1	B	4680	LYS
1	B	4682	GLU
1	B	4689	THR
1	B	4694	ASP
1	B	4696	ASP
1	B	4697	VAL
1	B	4698	LYS
1	B	4704	LEU
1	B	4705	VAL
1	B	4706	LEU
1	B	4710	SER
1	B	4718	LYS
1	B	4720	VAL
1	B	4721	LYS
1	B	4736	ARG
1	B	4743	MET
1	B	4745	LEU
1	B	4748	LEU
1	B	4750	ILE
1	B	4779	LYS

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Mol	Chain	Res	Type
1	B	4809	PHE
1	B	4818	MET
1	B	4822	THR
1	B	4835	LYS
1	B	4836	GLN
1	B	4837	LEU
1	B	4843	LEU
1	B	4844	LEU
1	B	4847	VAL
1	B	4861	LYS
1	B	4867	GLU
1	B	4870	ASP
1	B	4874	MET
1	B	4875	LYS
1	B	4889	VAL
1	B	4911	LEU
1	B	4927	ILE
1	B	4932	ILE
1	B	4933	GLN
1	B	4937	ILE
1	B	4948	GLU
1	B	4966	ASP
1	B	4971	THR
1	B	4976	GLU
1	B	4982	GLU
1	B	4989	MET
1	B	4992	LEU
1	B	4993	MET
1	B	4995	LEU
1	B	4997	ASN
1	B	5002	GLU
1	B	5012	LYS
1	B	5013	MET
1	B	5015	GLN
1	B	5027	CYS
1	B	5034	ASP
1	C	846	LEU
1	C	1072	VAL
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	3690	VAL
1	C	3692	GLU

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Mol	Chain	Res	Type
1	C	4178	LEU
1	C	4180	ARG
1	C	4182	GLU
1	C	4183	ILE
1	C	4184	MET
1	C	4188	ARG
1	C	4189	ARG
1	C	4190	ILE
1	C	4192	ARG
1	C	4193	ILE
1	C	4200	THR
1	C	4206	GLU
1	C	4207	MET
1	C	4209	GLN
1	C	4212	GLU
1	C	4221	VAL
1	C	4224	GLU
1	C	4227	GLU
1	C	4229	GLU
1	C	4231	MET
1	C	4541	TRP
1	C	4543	GLU
1	C	4544	LEU
1	C	4550	LYS
1	C	4555	LEU
1	C	4556	SER
1	C	4561	THR
1	C	4569	LEU
1	C	4577	LEU
1	C	4580	TYR
1	C	4581	LYS
1	C	4583	SER
1	C	4627	MET
1	C	4628	VAL
1	C	4632	LEU
1	C	4633	GLU
1	C	4635	SER
1	C	4636	THR
1	C	4640	GLU
1	C	4647	SER
1	C	4651	THR
1	C	4662	ASN

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Mol	Chain	Res	Type
1	C	4665	LYS
1	C	4666	VAL
1	C	4675	LYS
1	C	4676	GLU
1	C	4680	LYS
1	C	4682	GLU
1	C	4689	THR
1	C	4694	ASP
1	C	4696	ASP
1	C	4697	VAL
1	C	4698	LYS
1	C	4704	LEU
1	C	4705	VAL
1	C	4706	LEU
1	C	4710	SER
1	C	4718	LYS
1	C	4720	VAL
1	C	4721	LYS
1	C	4736	ARG
1	C	4743	MET
1	C	4745	LEU
1	C	4748	LEU
1	C	4750	ILE
1	C	4779	LYS
1	C	4809	PHE
1	C	4818	MET
1	C	4822	THR
1	C	4835	LYS
1	C	4836	GLN
1	C	4837	LEU
1	C	4843	LEU
1	C	4844	LEU
1	C	4847	VAL
1	C	4861	LYS
1	C	4867	GLU
1	C	4870	ASP
1	C	4874	MET
1	C	4875	LYS
1	C	4889	VAL
1	C	4911	LEU
1	C	4927	ILE
1	C	4932	ILE

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Mol	Chain	Res	Type
1	C	4933	GLN
1	C	4937	ILE
1	C	4948	GLU
1	C	4966	ASP
1	C	4971	THR
1	C	4976	GLU
1	C	4982	GLU
1	C	4989	MET
1	C	4992	LEU
1	C	4993	MET
1	C	4995	LEU
1	C	4997	ASN
1	C	5002	GLU
1	C	5012	LYS
1	C	5013	MET
1	C	5015	GLN
1	C	5027	CYS
1	C	5034	ASP
1	D	846	LEU
1	D	1072	VAL
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	3690	VAL
1	D	3692	GLU
1	D	4178	LEU
1	D	4180	ARG
1	D	4182	GLU
1	D	4183	ILE
1	D	4184	MET
1	D	4188	ARG
1	D	4189	ARG
1	D	4190	ILE
1	D	4192	ARG
1	D	4193	ILE
1	D	4200	THR
1	D	4206	GLU
1	D	4207	MET
1	D	4209	GLN
1	D	4212	GLU
1	D	4221	VAL
1	D	4224	GLU
1	D	4227	GLU

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Mol	Chain	Res	Type
1	D	4229	GLU
1	D	4231	MET
1	D	4541	TRP
1	D	4543	GLU
1	D	4544	LEU
1	D	4550	LYS
1	D	4555	LEU
1	D	4556	SER
1	D	4561	THR
1	D	4569	LEU
1	D	4577	LEU
1	D	4580	TYR
1	D	4581	LYS
1	D	4583	SER
1	D	4627	MET
1	D	4628	VAL
1	D	4632	LEU
1	D	4633	GLU
1	D	4635	SER
1	D	4636	THR
1	D	4640	GLU
1	D	4647	SER
1	D	4651	THR
1	D	4662	ASN
1	D	4665	LYS
1	D	4666	VAL
1	D	4675	LYS
1	D	4676	GLU
1	D	4680	LYS
1	D	4682	GLU
1	D	4689	THR
1	D	4694	ASP
1	D	4696	ASP
1	D	4697	VAL
1	D	4698	LYS
1	D	4704	LEU
1	D	4705	VAL
1	D	4706	LEU
1	D	4710	SER
1	D	4718	LYS
1	D	4720	VAL
1	D	4721	LYS

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Mol	Chain	Res	Type
1	D	4736	ARG
1	D	4743	MET
1	D	4745	LEU
1	D	4748	LEU
1	D	4750	ILE
1	D	4779	LYS
1	D	4809	PHE
1	D	4818	MET
1	D	4822	THR
1	D	4835	LYS
1	D	4836	GLN
1	D	4837	LEU
1	D	4843	LEU
1	D	4844	LEU
1	D	4847	VAL
1	D	4861	LYS
1	D	4867	GLU
1	D	4870	ASP
1	D	4874	MET
1	D	4875	LYS
1	D	4889	VAL
1	D	4911	LEU
1	D	4927	ILE
1	D	4932	ILE
1	D	4933	GLN
1	D	4937	ILE
1	D	4948	GLU
1	D	4966	ASP
1	D	4971	THR
1	D	4976	GLU
1	D	4982	GLU
1	D	4989	MET
1	D	4992	LEU
1	D	4993	MET
1	D	4995	LEU
1	D	4997	ASN
1	D	5002	GLU
1	D	5012	LYS
1	D	5013	MET
1	D	5015	GLN
1	D	5027	CYS
1	D	5034	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	98	HIS
1	A	203	ASN
1	A	241	GLN
1	A	308	HIS
1	A	461	HIS
1	A	576	ASN
1	A	597	HIS
1	A	624	ASN
1	A	636	ASN
1	A	1058	GLN
1	A	1229	ASN
1	A	1420	ASN
1	A	1506	GLN
1	A	1541	GLN
1	A	1614	GLN
1	A	1631	GLN
1	A	1640	HIS
1	A	2127	GLN
1	A	2193	GLN
1	A	2420	HIS
1	A	2441	HIS
1	A	2515	GLN
1	A	2621	HIS
1	A	2634	ASN
1	A	2773	ASN
1	A	2872	GLN
1	A	2881	ASN
1	A	2924	GLN
1	A	3007	ASN
1	A	3030	HIS
1	A	3128	ASN
1	A	3325	ASN
1	A	3343	GLN
1	A	3419	ASN
1	A	3530	GLN
1	A	3611	HIS
1	A	3766	GLN
1	A	3895	HIS
1	A	3897	ASN
1	A	3960	GLN

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Mol	Chain	Res	Type
1	A	4005	GLN
1	A	4120	ASN
1	A	4201	ASN
1	A	4558	ASN
1	A	4626	ASN
1	A	4832	HIS
1	A	4857	ASN
1	A	4947	GLN
1	A	5003	HIS
1	A	5031	GLN
1	B	23	GLN
1	B	98	HIS
1	B	203	ASN
1	B	241	GLN
1	B	461	HIS
1	B	576	ASN
1	B	597	HIS
1	B	624	ASN
1	B	636	ASN
1	B	838	HIS
1	B	877	ASN
1	B	1058	GLN
1	B	1229	ASN
1	B	1420	ASN
1	B	1506	GLN
1	B	1541	GLN
1	B	1614	GLN
1	B	1631	GLN
1	B	1640	HIS
1	B	2127	GLN
1	B	2193	GLN
1	B	2420	HIS
1	B	2441	HIS
1	B	2515	GLN
1	B	2621	HIS
1	B	2634	ASN
1	B	2772	GLN
1	B	2773	ASN
1	B	2872	GLN
1	B	2881	ASN
1	B	2924	GLN
1	B	3030	HIS

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Mol	Chain	Res	Type
1	B	3128	ASN
1	B	3150	HIS
1	B	3325	ASN
1	B	3343	GLN
1	B	3611	HIS
1	B	3766	GLN
1	B	3895	HIS
1	B	3897	ASN
1	B	3960	GLN
1	B	4005	GLN
1	B	4120	ASN
1	B	4201	ASN
1	B	4558	ASN
1	B	4626	ASN
1	B	4832	HIS
1	B	4836	GLN
1	B	4947	GLN
1	B	5003	HIS
1	B	5031	GLN
1	C	23	GLN
1	C	98	HIS
1	C	203	ASN
1	C	241	GLN
1	C	308	HIS
1	C	461	HIS
1	C	576	ASN
1	C	624	ASN
1	C	636	ASN
1	C	838	HIS
1	C	877	ASN
1	C	1229	ASN
1	C	1420	ASN
1	C	1541	GLN
1	C	1614	GLN
1	C	1631	GLN
1	C	1640	HIS
1	C	2127	GLN
1	C	2420	HIS
1	C	2441	HIS
1	C	2515	GLN
1	C	2621	HIS
1	C	2634	ASN

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Mol	Chain	Res	Type
1	C	2772	GLN
1	C	2773	ASN
1	C	2872	GLN
1	C	2881	ASN
1	C	2924	GLN
1	C	3030	HIS
1	C	3128	ASN
1	C	3150	HIS
1	C	3325	ASN
1	C	3611	HIS
1	C	3766	GLN
1	C	3895	HIS
1	C	3897	ASN
1	C	3960	GLN
1	C	4005	GLN
1	C	4120	ASN
1	C	4201	ASN
1	C	4558	ASN
1	C	4626	ASN
1	C	4832	HIS
1	C	4836	GLN
1	C	4947	GLN
1	C	5003	HIS
1	C	5031	GLN
1	D	23	GLN
1	D	98	HIS
1	D	203	ASN
1	D	241	GLN
1	D	461	HIS
1	D	576	ASN
1	D	624	ASN
1	D	636	ASN
1	D	1058	GLN
1	D	1229	ASN
1	D	1420	ASN
1	D	1614	GLN
1	D	1631	GLN
1	D	1640	HIS
1	D	2127	GLN
1	D	2193	GLN
1	D	2420	HIS
1	D	2441	HIS

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Mol	Chain	Res	Type
1	D	2515	GLN
1	D	2621	HIS
1	D	2634	ASN
1	D	2772	GLN
1	D	2773	ASN
1	D	2872	GLN
1	D	2881	ASN
1	D	2924	GLN
1	D	3030	HIS
1	D	3128	ASN
1	D	3150	HIS
1	D	3325	ASN
1	D	3343	GLN
1	D	3419	ASN
1	D	3611	HIS
1	D	3766	GLN
1	D	3895	HIS
1	D	3897	ASN
1	D	3960	GLN
1	D	4005	GLN
1	D	4120	ASN
1	D	4201	ASN
1	D	4558	ASN
1	D	4626	ASN
1	D	4832	HIS
1	D	4836	GLN
1	D	4947	GLN
1	D	5003	HIS
1	D	5031	GLN
2	E	20	GLN
2	E	53	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	ADP	D	5101	-	28,29,29	1.39	6 (21%)	43,45,45	1.79	7 (16%)
3	ADP	C	5101	-	28,29,29	1.39	6 (21%)	43,45,45	1.79	7 (16%)
3	ADP	B	5101	-	28,29,29	1.39	6 (21%)	43,45,45	1.79	7 (16%)
3	ADP	A	5101	-	28,29,29	1.39	6 (21%)	43,45,45	1.79	7 (16%)

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
3	ADP	D	5101	-	-	4/16/32/32	0/3/3/3
3	ADP	C	5101	-	-	4/16/32/32	0/3/3/3
3	ADP	B	5101	-	-	4/16/32/32	0/3/3/3
3	ADP	A	5101	-	-	4/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5101	ADP	C5-C4	4.36	1.46	1.39
3	D	5101	ADP	C5-C4	4.36	1.46	1.39
3	A	5101	ADP	C5-C4	4.36	1.46	1.39
3	B	5101	ADP	C5-C4	4.36	1.46	1.39
3	D	5101	ADP	C5-N7	-2.49	1.34	1.39
3	B	5101	ADP	C5-N7	-2.49	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5101	ADP	C5-N7	-2.49	1.34	1.39
3	A	5101	ADP	C5-N7	-2.49	1.34	1.39
3	A	5101	ADP	C5-C6	2.42	1.47	1.41
3	B	5101	ADP	C5-C6	2.42	1.47	1.41
3	C	5101	ADP	C5-C6	2.42	1.47	1.41
3	D	5101	ADP	C5-C6	2.41	1.47	1.41
3	D	5101	ADP	C8-N7	2.22	1.35	1.31
3	A	5101	ADP	C8-N7	2.21	1.35	1.31
3	B	5101	ADP	C8-N7	2.21	1.35	1.31
3	C	5101	ADP	C8-N7	2.21	1.35	1.31
3	D	5101	ADP	PA-O3A	2.17	1.61	1.59
3	B	5101	ADP	PA-O3A	2.16	1.61	1.59
3	A	5101	ADP	PA-O3A	2.16	1.61	1.59
3	C	5101	ADP	PA-O3A	2.16	1.61	1.59
3	D	5101	ADP	C4-N9	-2.06	1.33	1.37
3	C	5101	ADP	C4-N9	-2.06	1.33	1.37
3	A	5101	ADP	C4-N9	-2.06	1.33	1.37
3	B	5101	ADP	C4-N9	-2.06	1.33	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5101	ADP	C5-C4-N3	-5.66	118.92	126.72
3	D	5101	ADP	C5-C4-N3	-5.66	118.92	126.72
3	A	5101	ADP	C5-C4-N3	-5.66	118.93	126.72
3	B	5101	ADP	C5-C4-N3	-5.66	118.93	126.72
3	C	5101	ADP	N3-C4-N9	4.67	135.11	127.17
3	A	5101	ADP	N3-C4-N9	4.67	135.11	127.17
3	D	5101	ADP	N3-C4-N9	4.67	135.11	127.17
3	B	5101	ADP	N3-C4-N9	4.67	135.10	127.17
3	C	5101	ADP	C2-N3-C4	3.66	120.77	111.83
3	A	5101	ADP	C2-N3-C4	3.66	120.76	111.83
3	D	5101	ADP	C2-N3-C4	3.66	120.76	111.83
3	B	5101	ADP	C2-N3-C4	3.66	120.76	111.83
3	C	5101	ADP	N3-C2-N1	-3.27	123.63	128.58
3	A	5101	ADP	N3-C2-N1	-3.27	123.64	128.58
3	D	5101	ADP	N3-C2-N1	-3.27	123.64	128.58
3	B	5101	ADP	N3-C2-N1	-3.26	123.64	128.58
3	D	5101	ADP	C4-C5-N7	-3.02	107.13	110.58
3	C	5101	ADP	C4-C5-N7	-3.02	107.13	110.58
3	B	5101	ADP	C4-C5-N7	-3.02	107.13	110.58
3	A	5101	ADP	C4-C5-N7	-3.02	107.13	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5101	ADP	C4-N9-C8	2.84	108.72	105.74
3	D	5101	ADP	C4-N9-C8	2.84	108.72	105.74
3	A	5101	ADP	C4-N9-C8	2.84	108.72	105.74
3	B	5101	ADP	C4-N9-C8	2.83	108.71	105.74
3	B	5101	ADP	C5-N7-C8	2.27	107.02	103.45
3	D	5101	ADP	C5-N7-C8	2.27	107.02	103.45
3	A	5101	ADP	C5-N7-C8	2.27	107.02	103.45
3	C	5101	ADP	C5-N7-C8	2.27	107.02	103.45

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5101	ADP	PB-O3A-PA-O5'
3	B	5101	ADP	PB-O3A-PA-O5'
3	C	5101	ADP	PB-O3A-PA-O5'
3	D	5101	ADP	PB-O3A-PA-O5'
3	A	5101	ADP	O4'-C4'-C5'-O5'
3	B	5101	ADP	O4'-C4'-C5'-O5'
3	C	5101	ADP	O4'-C4'-C5'-O5'
3	D	5101	ADP	O4'-C4'-C5'-O5'
3	A	5101	ADP	C3'-C4'-C5'-O5'
3	B	5101	ADP	C3'-C4'-C5'-O5'
3	C	5101	ADP	C3'-C4'-C5'-O5'
3	D	5101	ADP	C3'-C4'-C5'-O5'
3	A	5101	ADP	C4'-C5'-O5'-PA
3	B	5101	ADP	C4'-C5'-O5'-PA
3	C	5101	ADP	C4'-C5'-O5'-PA
3	D	5101	ADP	C4'-C5'-O5'-PA

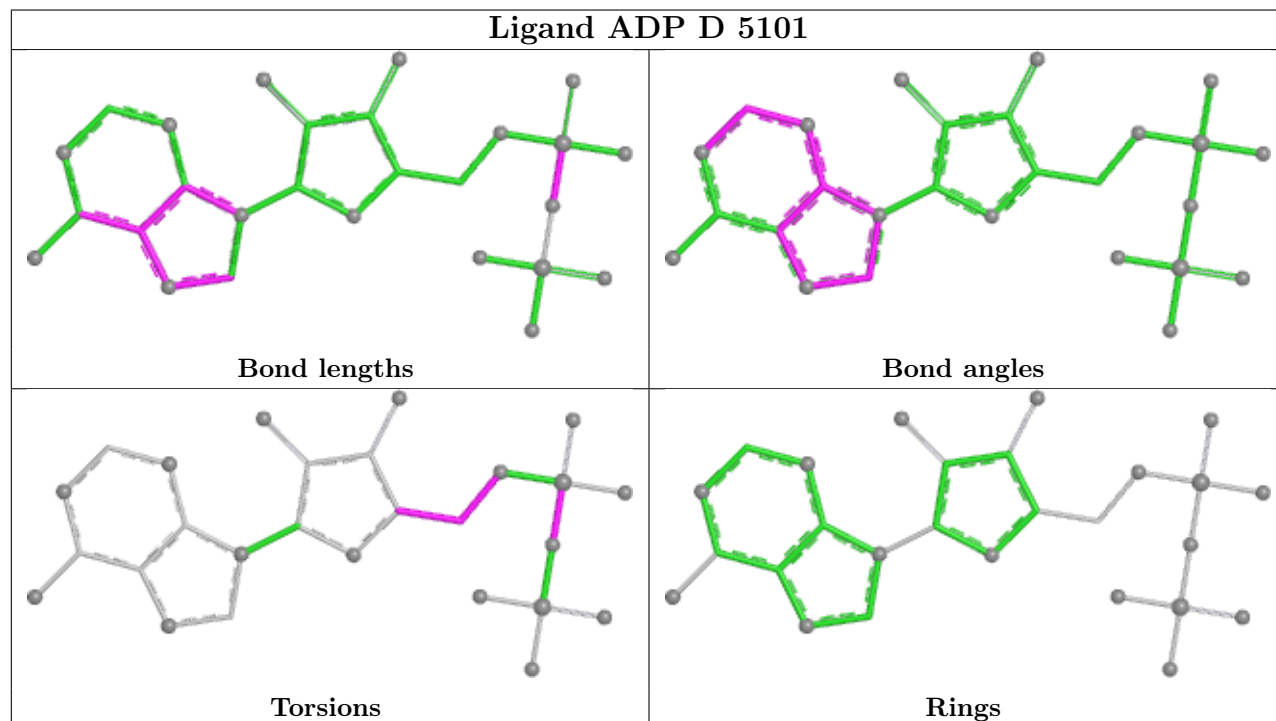
There are no ring outliers.

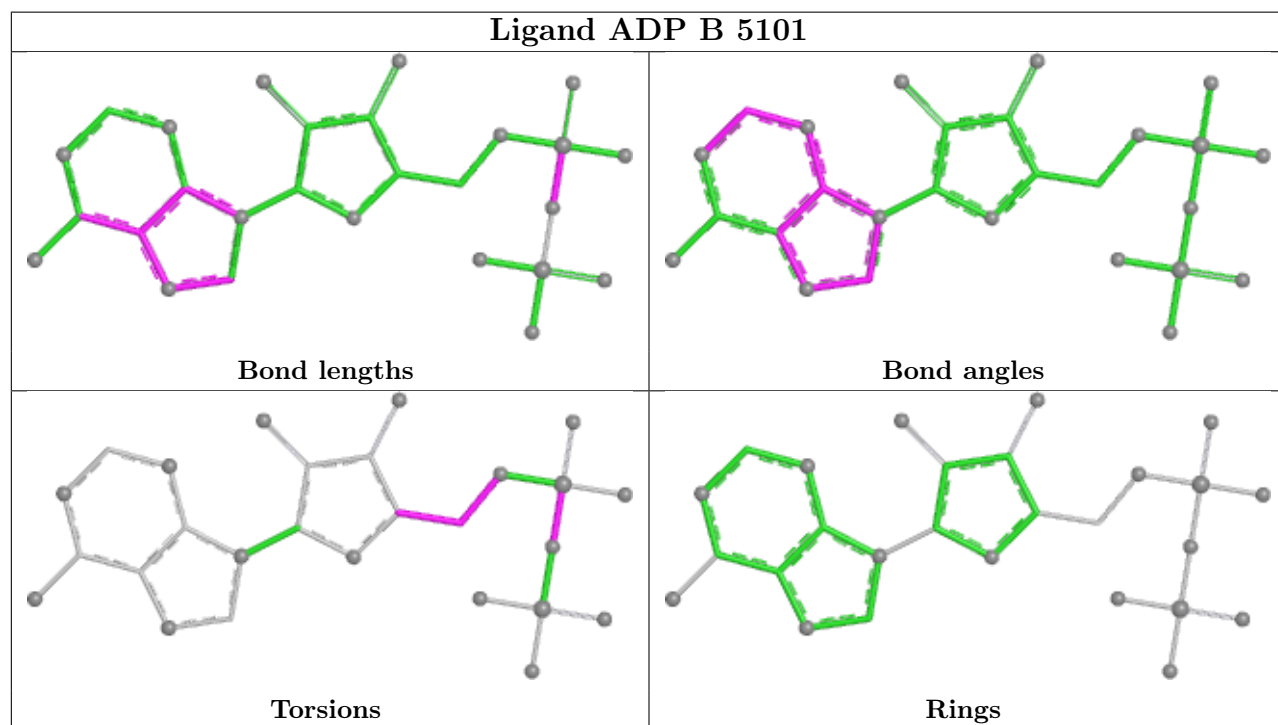
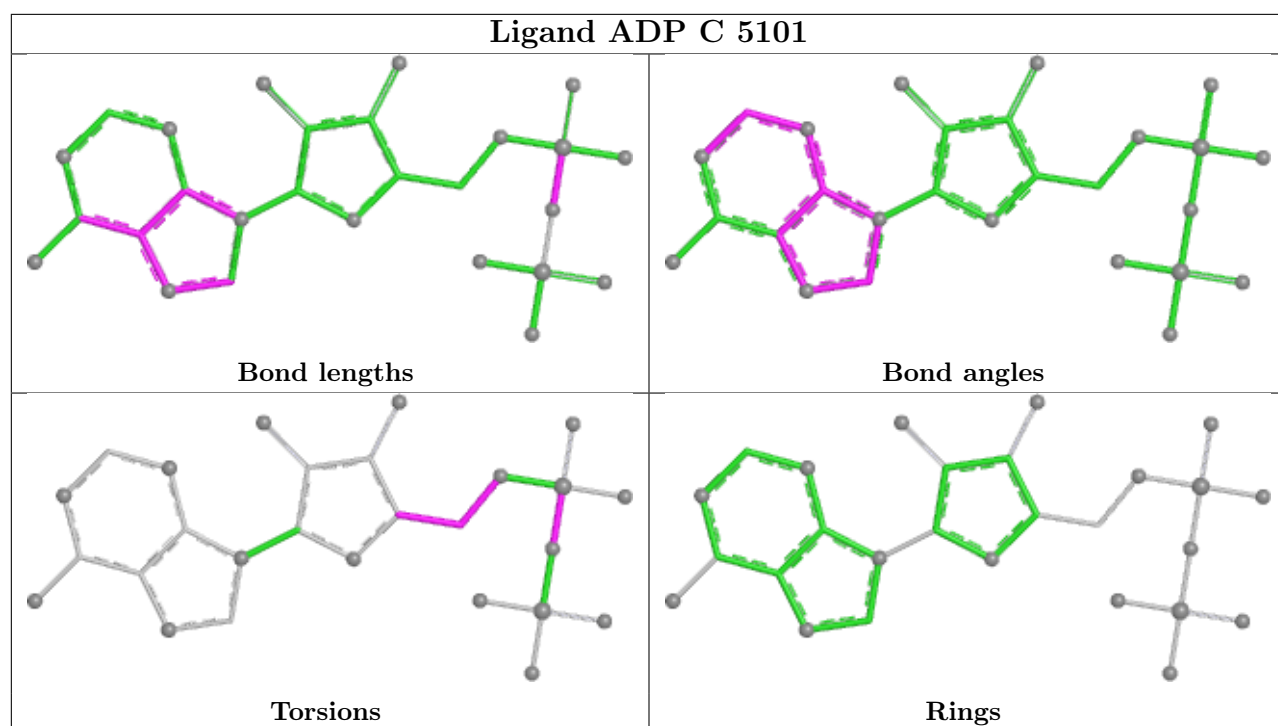
4 monomers are involved in 4 short contacts:

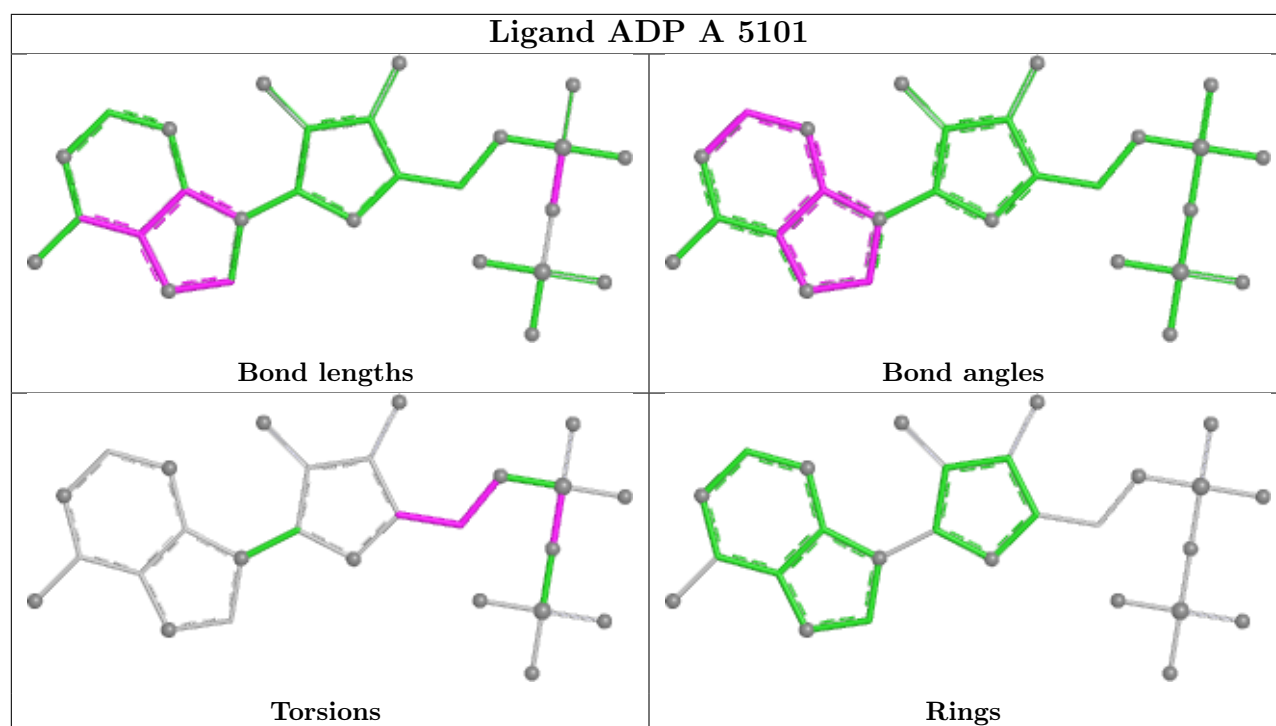
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5101	ADP	1	0
3	C	5101	ADP	1	0
3	B	5101	ADP	1	0
3	A	5101	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

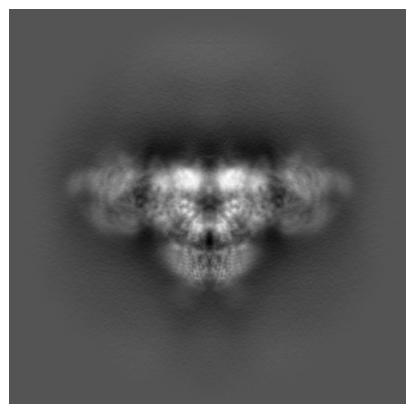
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40424. These allow visual inspection of the internal detail of the map and identification of artifacts.

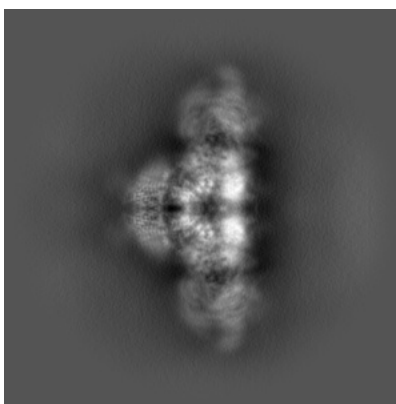
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

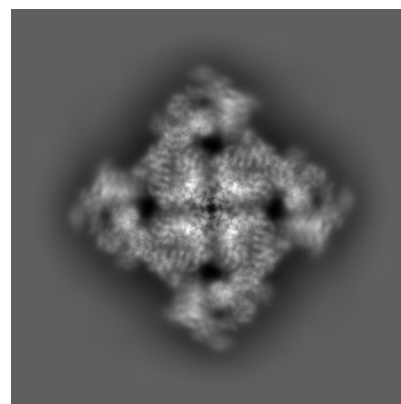
6.1.1 Primary map



X

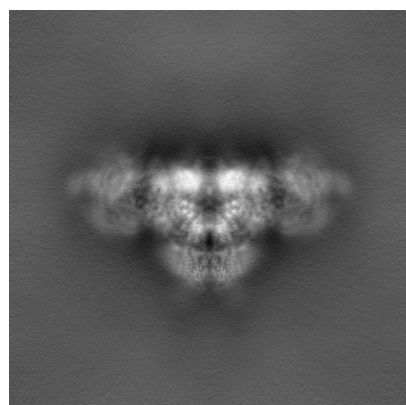


Y

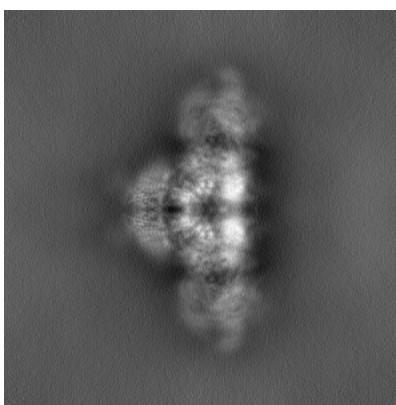


Z

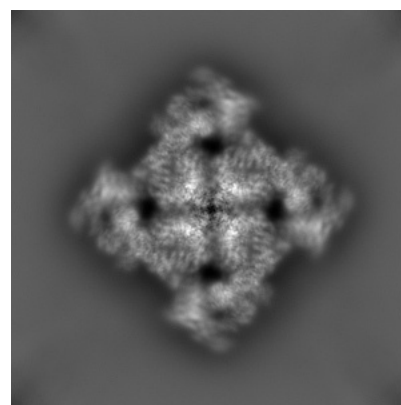
6.1.2 Raw map



X



Y

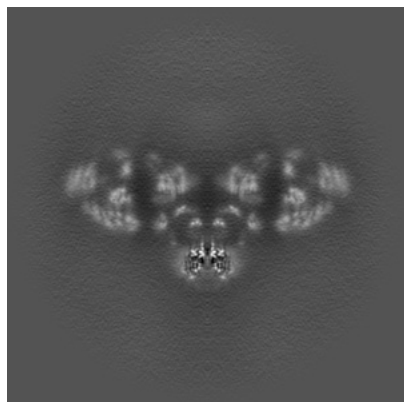


Z

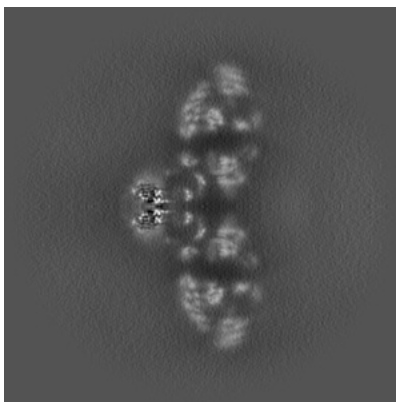
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

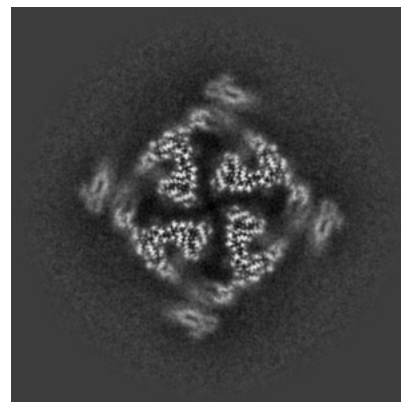
6.2.1 Primary map



X Index: 200

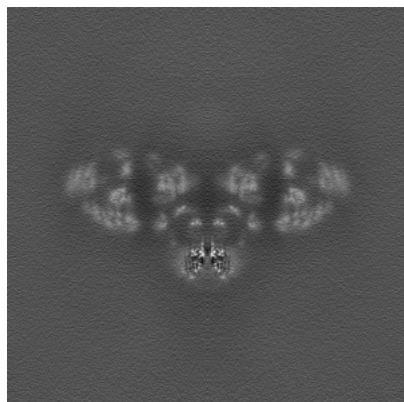


Y Index: 200

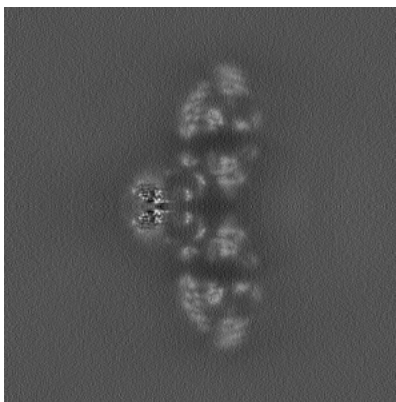


Z Index: 200

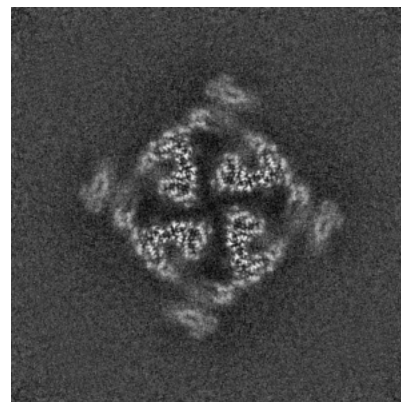
6.2.2 Raw map



X Index: 200



Y Index: 200

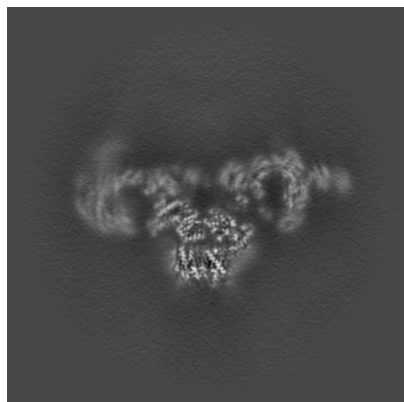


Z Index: 200

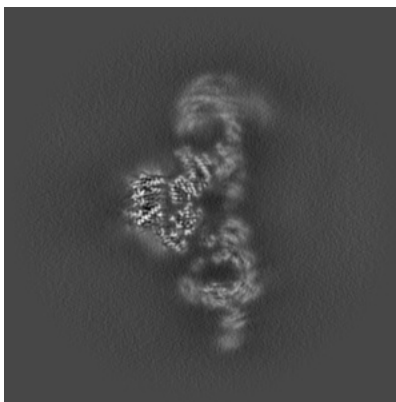
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

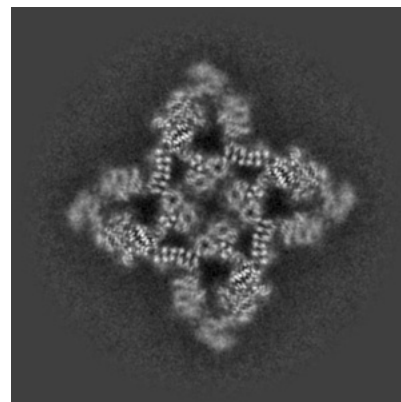
6.3.1 Primary map



X Index: 186

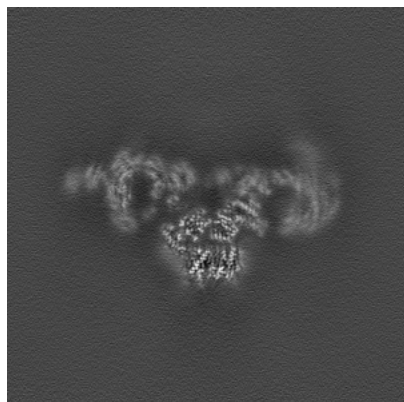


Y Index: 186

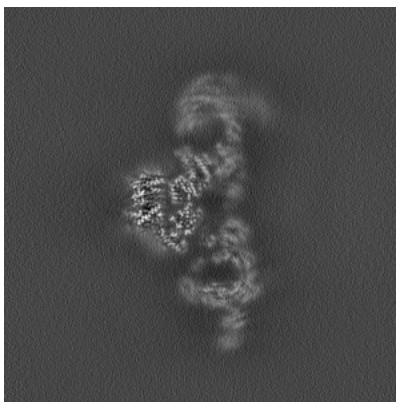


Z Index: 223

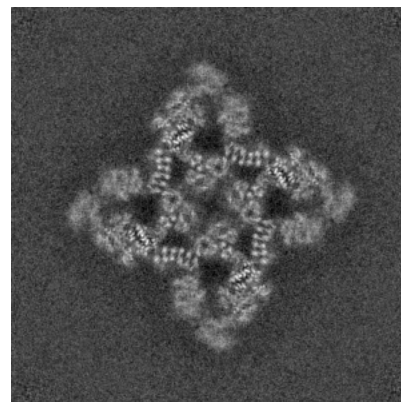
6.3.2 Raw map



X Index: 214



Y Index: 186

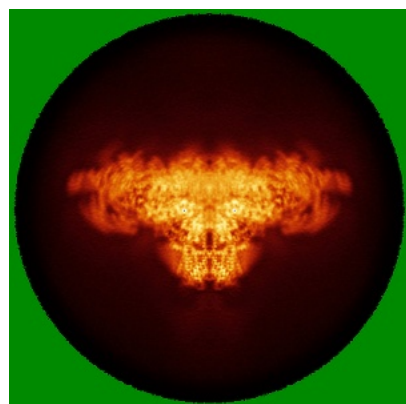


Z Index: 223

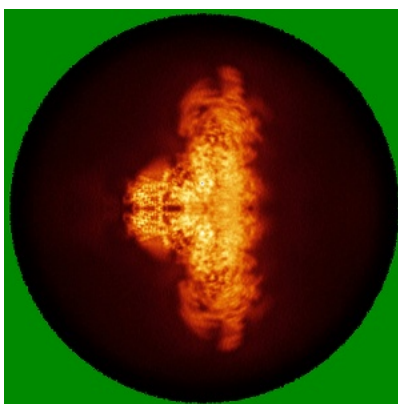
The images above show the largest variance slices of the map in three orthogonal directions.

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

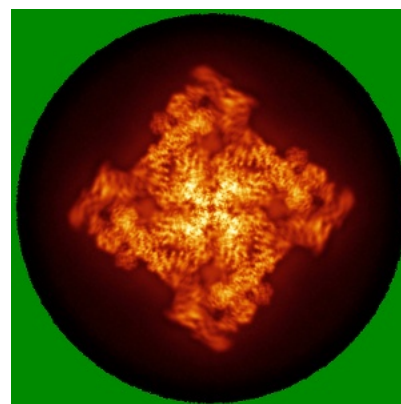
6.4.1 Primary map



X

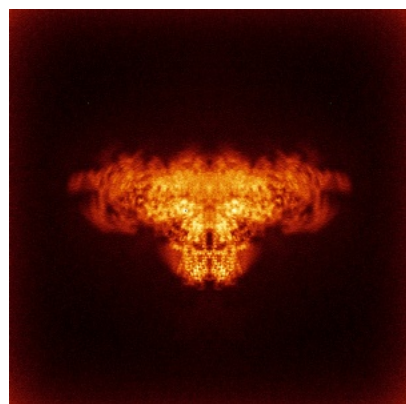


Y

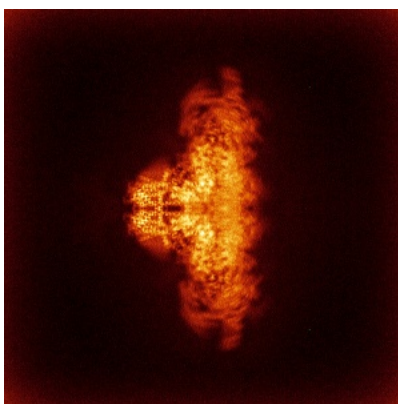


Z

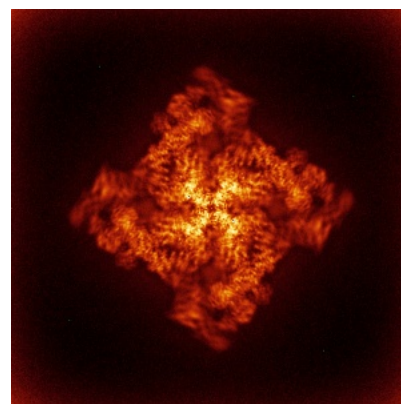
6.4.2 Raw map



X



Y

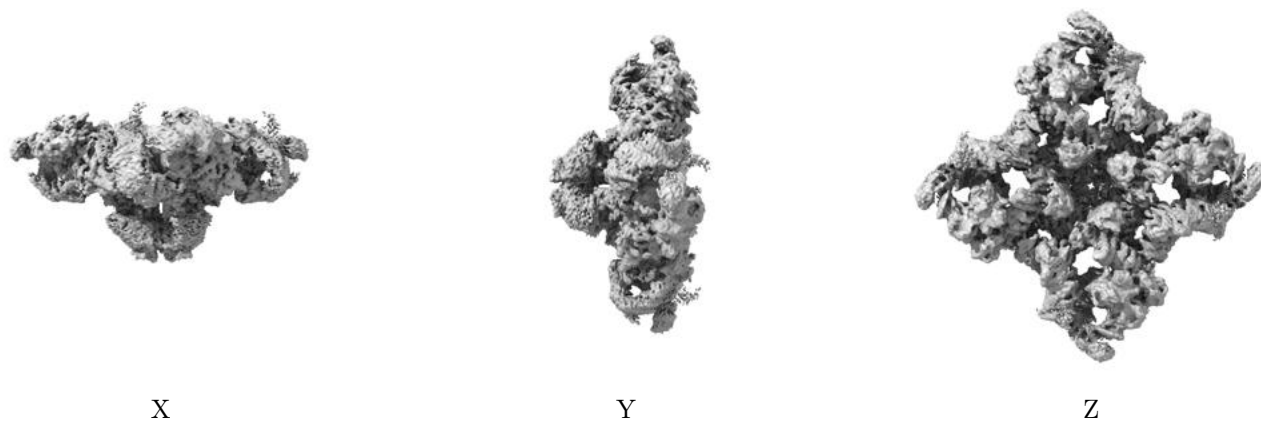


Z

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

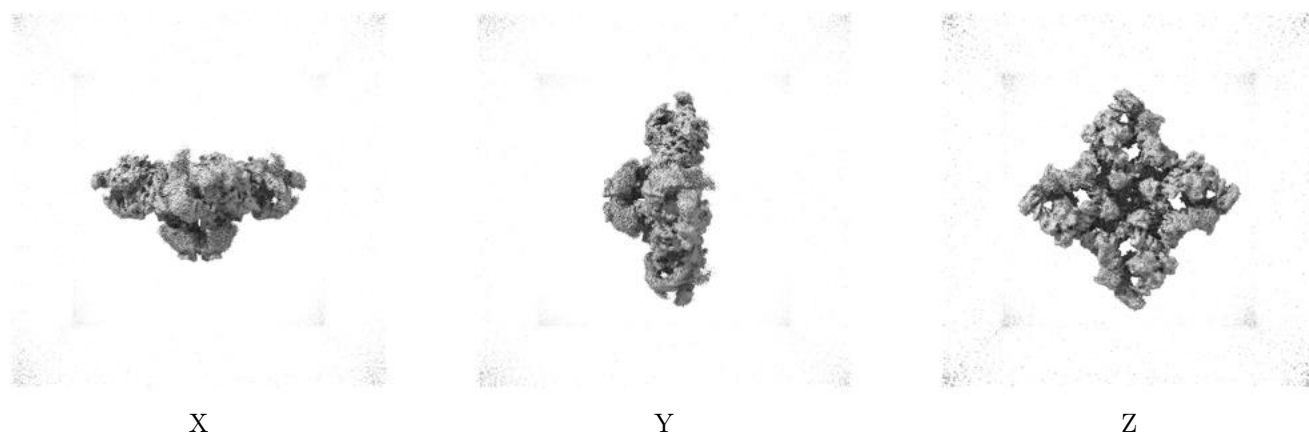
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.263. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

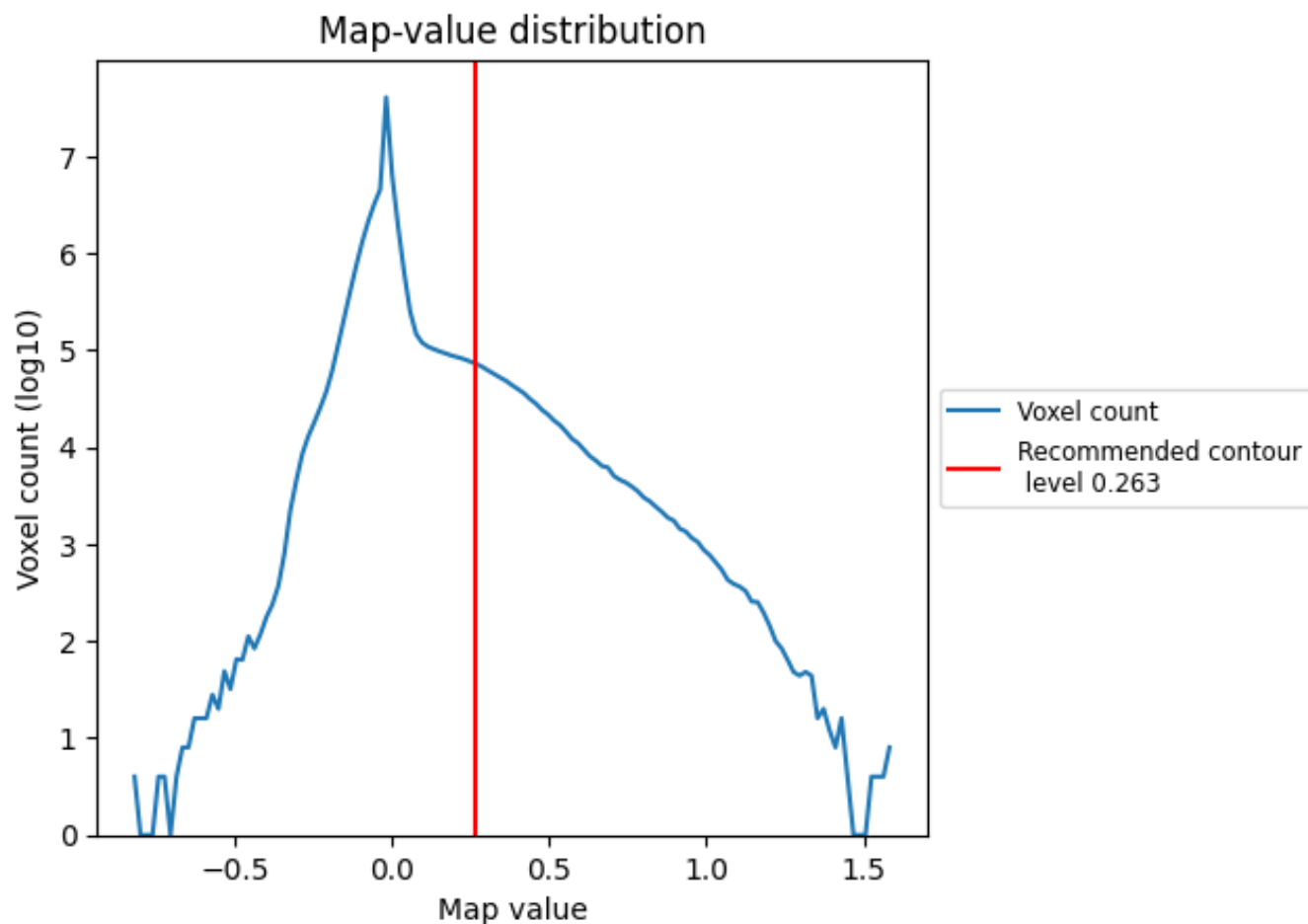
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

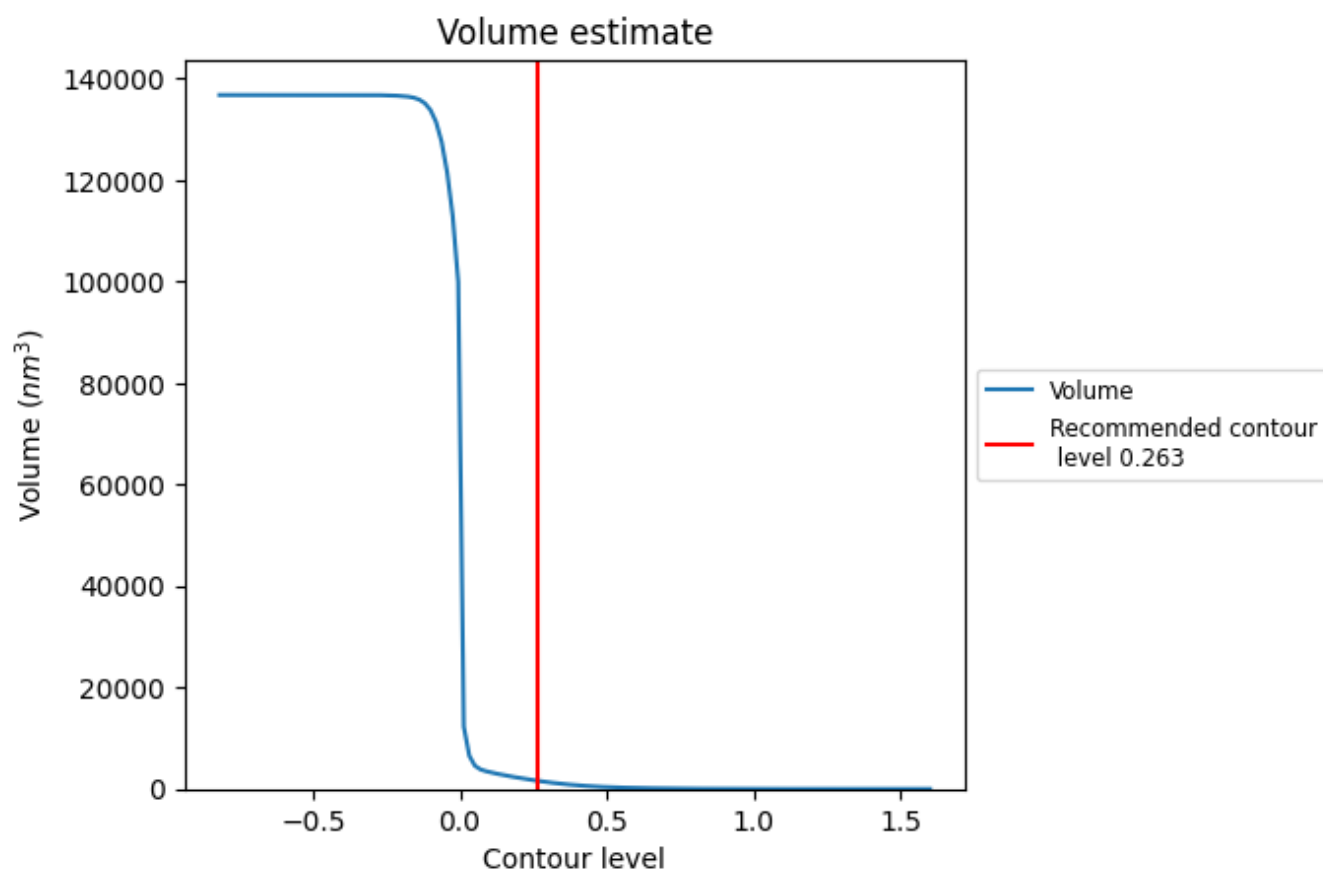
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

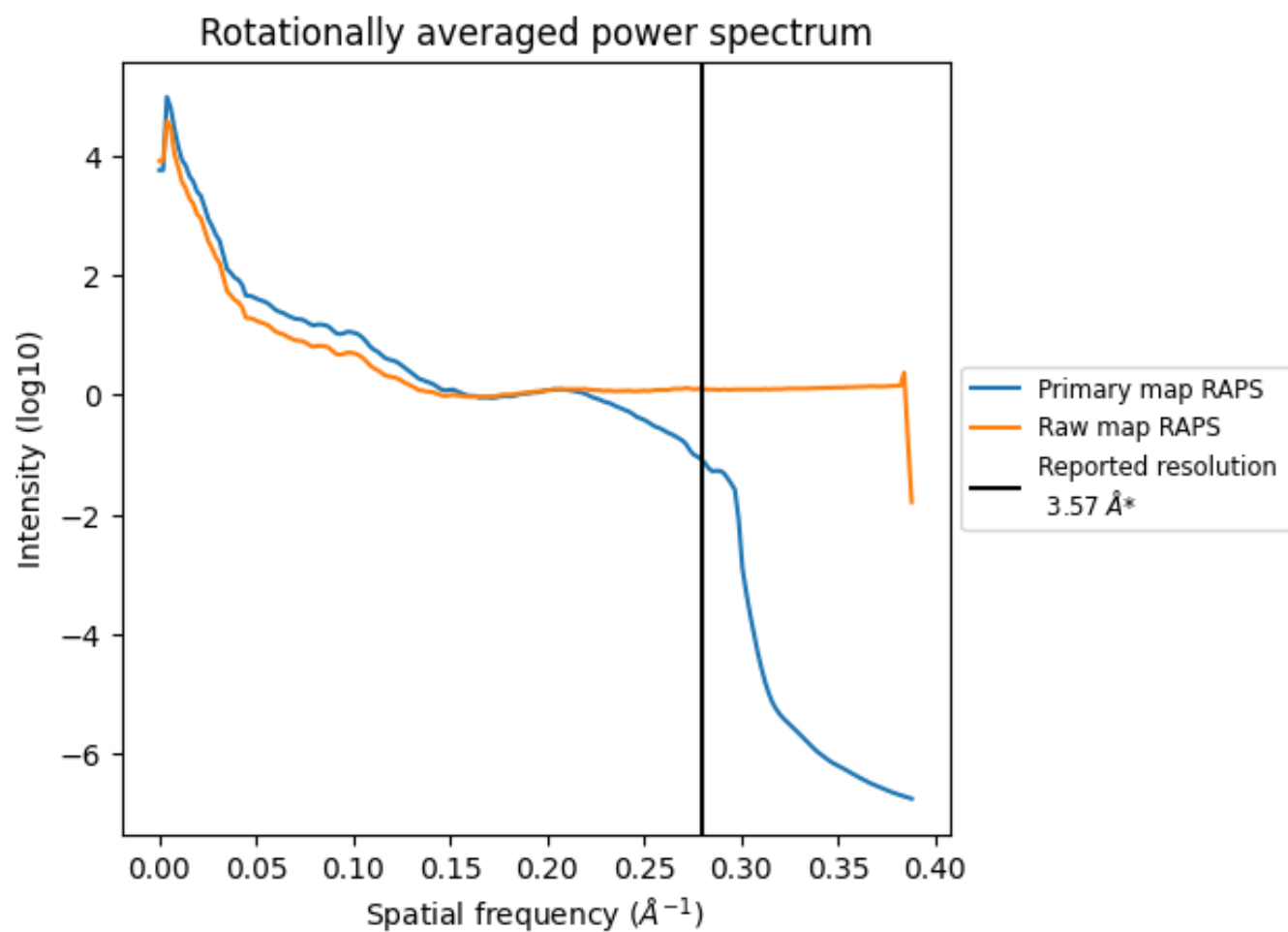
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1622 nm³; this corresponds to an approximate mass of 1465 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

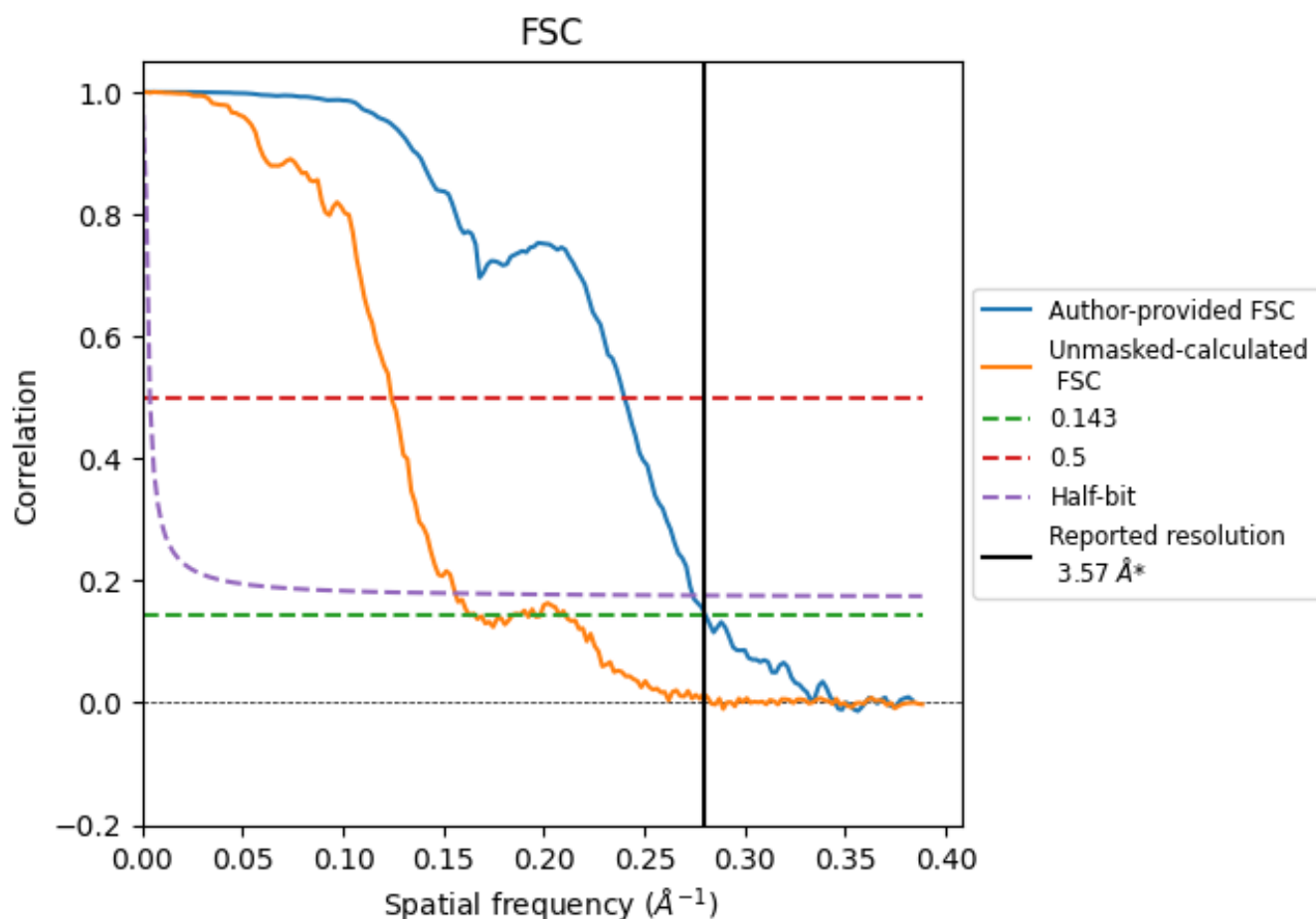


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.280 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

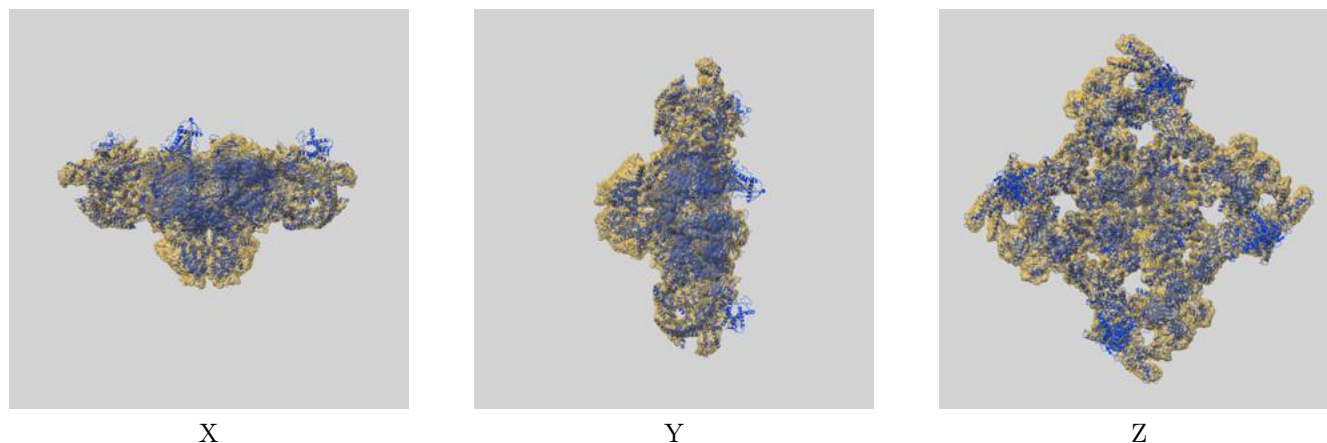
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.17	3.65
Unmasked-calculated*	6.04	8.06	6.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.04 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

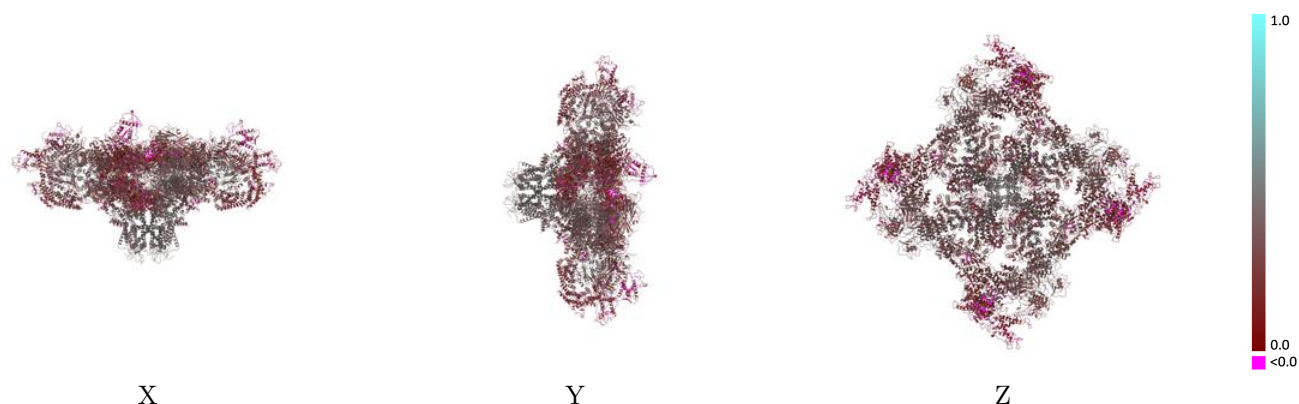
This section contains information regarding the fit between EMDB map EMD-40424 and PDB model 8SEP. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



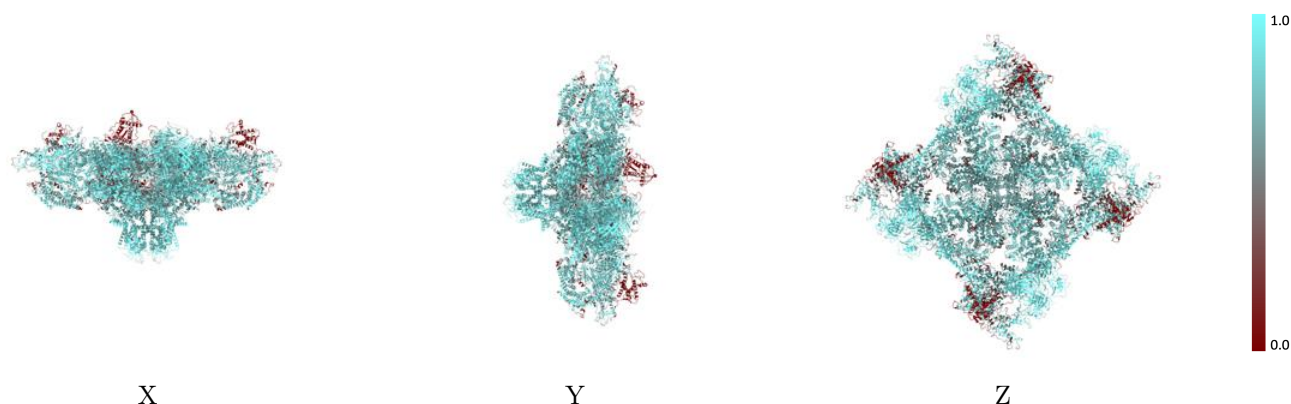
The images above show the 3D surface view of the map at the recommended contour level 0.263 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



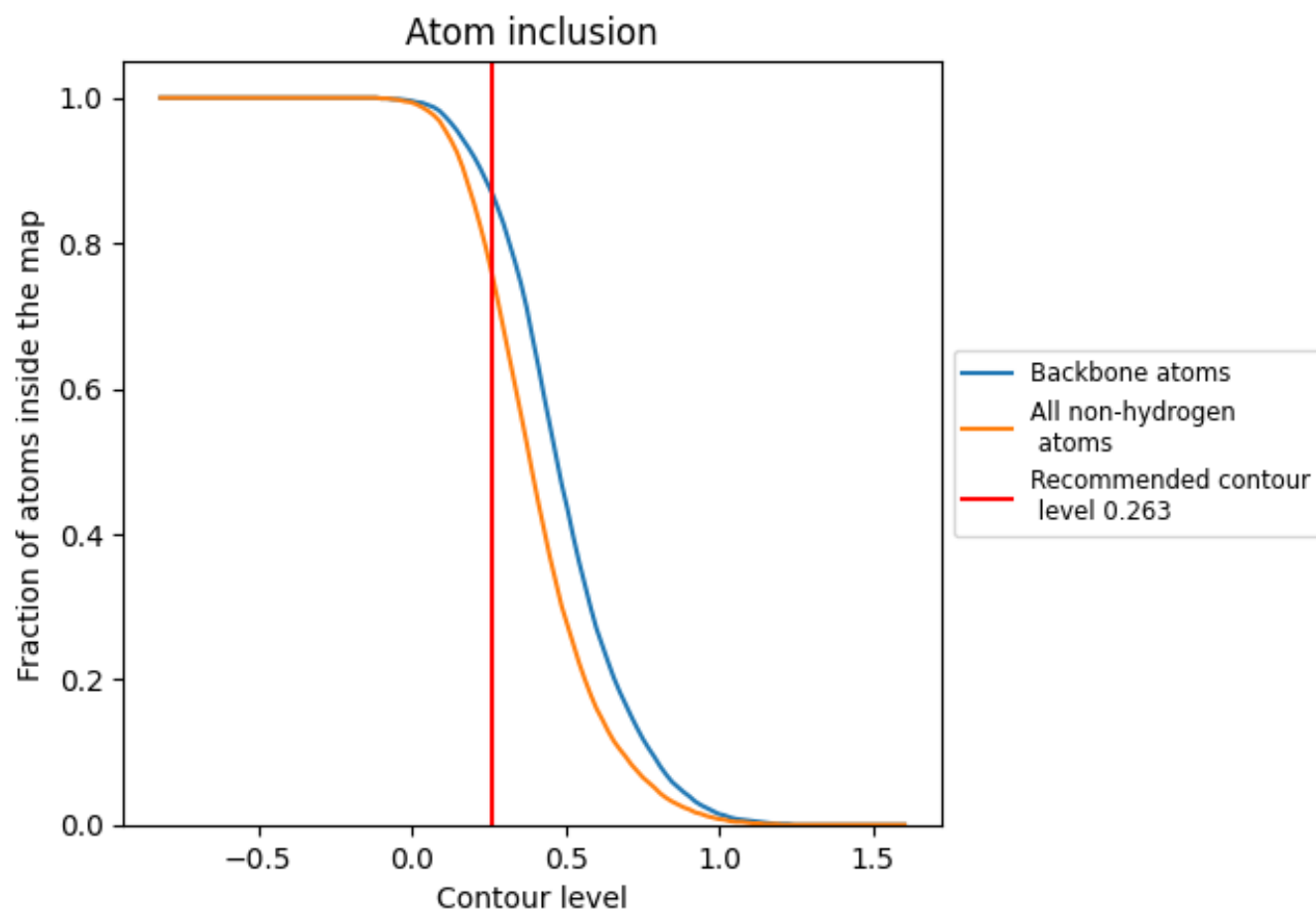
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.263).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.263) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.2890
A	0.7480	0.2870
B	0.7490	0.2880
C	0.7490	0.2880
D	0.7490	0.2880
E	0.9160	0.3620
F	0.9160	0.3620
G	0.9160	0.3620
H	0.9160	0.3620

1.0

0.0

<0.0