



## Full wwPDB EM Validation Report ⓘ

Nov 24, 2025 – 01:17 PM EST

PDB ID : 9OL6 / pdb\_00009ol6  
EMDB ID : EMD-70591  
Title : Rabbit Ryanodine Receptor 1: DMSO Control Closed Conformation  
Authors : Molinarolo, S.M.; Van Petegem, F.  
Deposited on : 2025-05-12  
Resolution : 3.11 Å(reported)  
Based on initial model : 7TZC

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

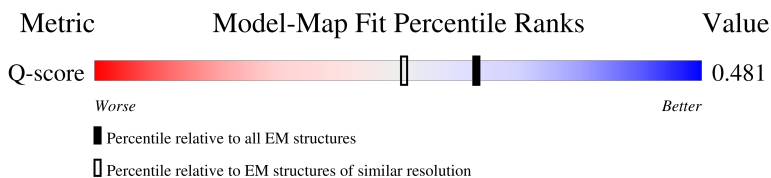
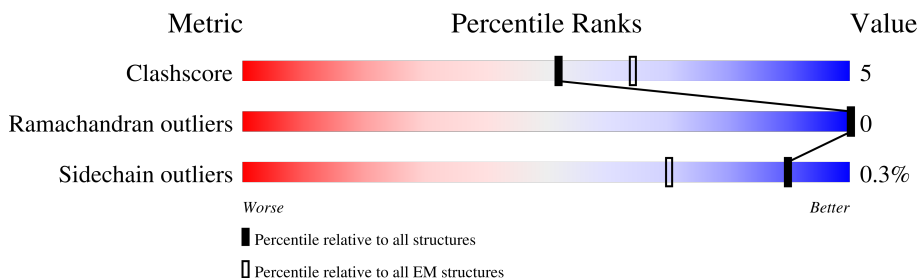
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.11 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14465 ( 2.61 - 3.61 )

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

Mol	Chain	Length	Quality of chain
1	A	5037	
1	G	5037	
1	M	5037	
1	S	5037	

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Mol	Chain	Length	Quality of chain
2	B	111	<div><div></div><div>90%</div><div>6%</div><div></div></div>
2	H	111	<div><div></div><div>90%</div><div>6%</div><div></div></div>
2	N	111	<div><div></div><div>90%</div><div>6%</div><div></div></div>
2	T	111	<div><div></div><div>90%</div><div>6%</div><div></div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 133368 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	4185	Total	C	N	O	S	0	0
			32524	20790	5626	5890	218		
1	G	4185	Total	C	N	O	S	0	0
			32524	20790	5626	5890	218		
1	M	4185	Total	C	N	O	S	0	0
			32524	20790	5626	5890	218		
1	S	4185	Total	C	N	O	S	0	0
			32524	20790	5626	5890	218		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
2	N	107	Total	C	N	O	S	0	0
			816	514	144	154	4		
2	T	107	Total	C	N	O	S	0	0
			816	514	144	154	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	SER	-	expression tag	UNP P68106
B	-2	ASN	-	expression tag	UNP P68106
B	-1	ALA	-	expression tag	UNP P68106
H	-3	SER	-	expression tag	UNP P68106
H	-2	ASN	-	expression tag	UNP P68106
H	-1	ALA	-	expression tag	UNP P68106
N	-3	SER	-	expression tag	UNP P68106
N	-2	ASN	-	expression tag	UNP P68106
N	-1	ALA	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-3	SER	-	expression tag	UNP P68106
T	-2	ASN	-	expression tag	UNP P68106
T	-1	ALA	-	expression tag	UNP P68106

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Ca 1	0
3	G	1	Total 1	Ca 1	0
3	M	1	Total 1	Ca 1	0
3	S	1	Total 1	Ca 1	0

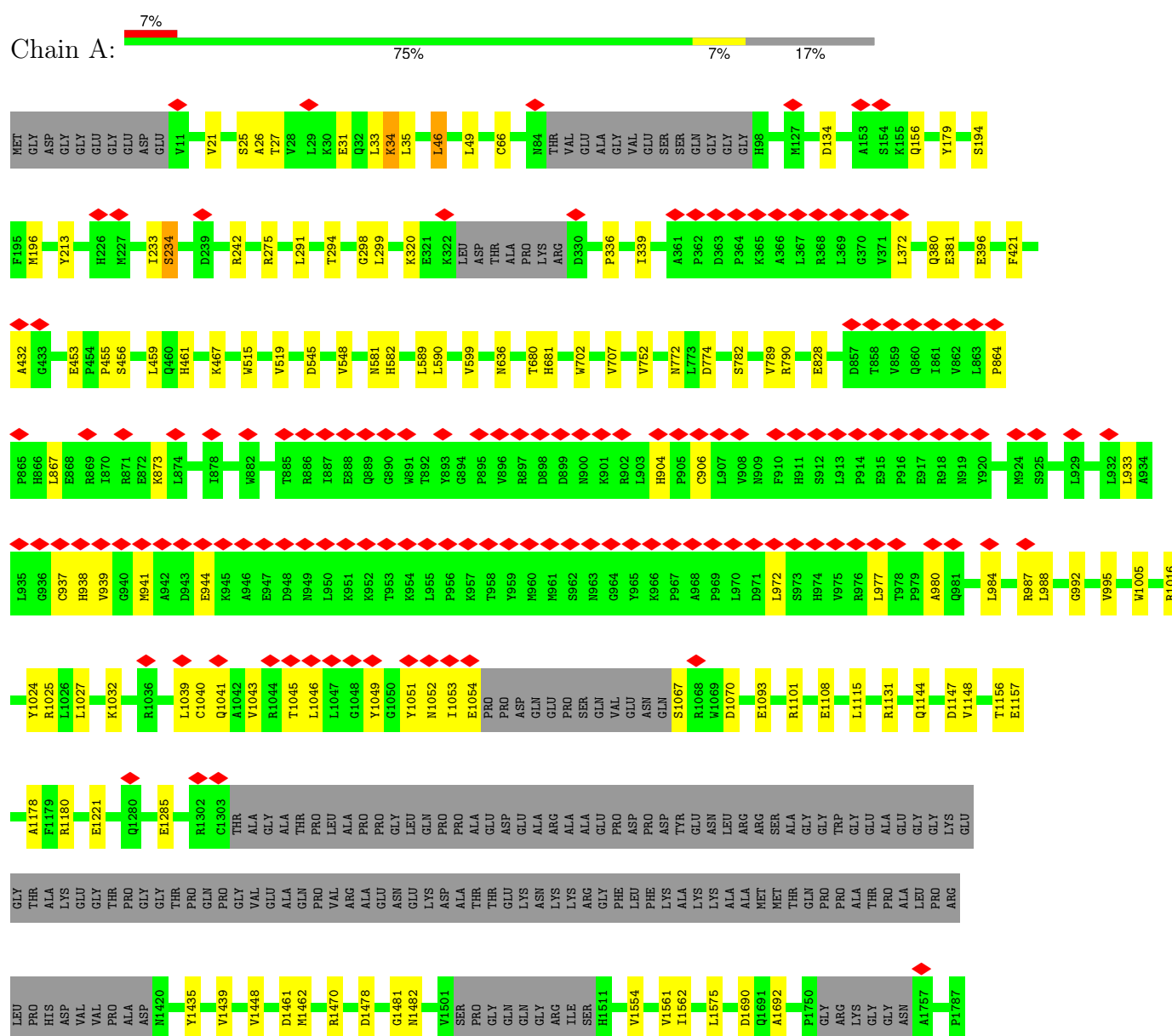
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	M	1	Total 1	Zn 1	0
4	S	1	Total 1	Zn 1	0

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

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

#### • Molecule 1: Ryanodine receptor 1





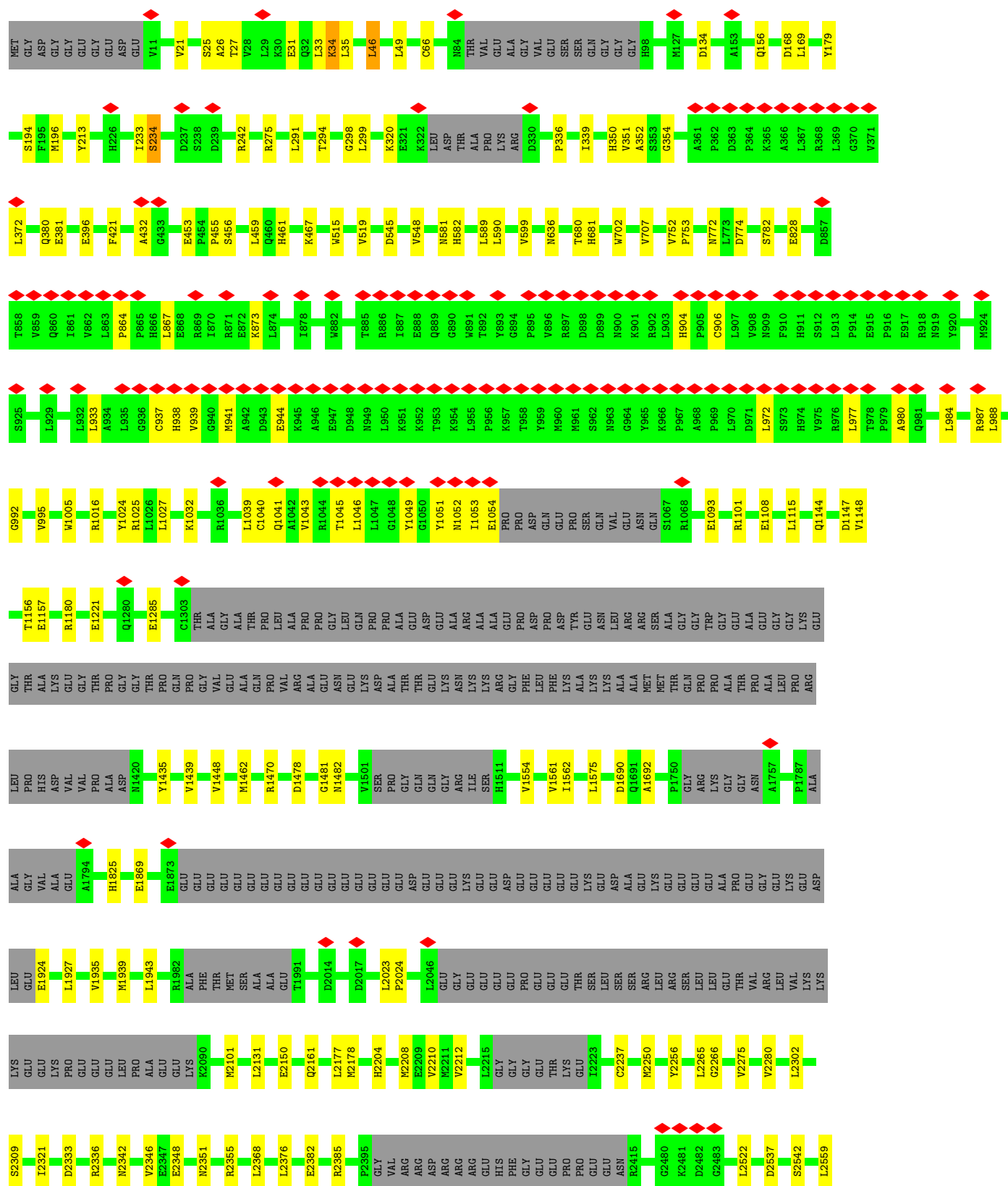
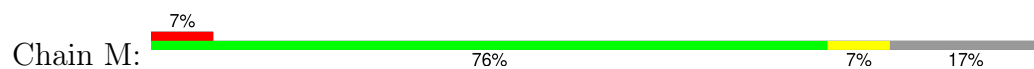




S2668	R2669	E2670	L2671	Q2672	A2673	M2674	A2675	E2676	Q2677	L2678	A2679	E2680	N2681	Y2682	H2683	T2684	N2685	W2686	G2687	A2688	K2689	K2690	K2691	Q2692	E2693	L2694	E2695	A2696	G2697	G2698	G2699	G2700	T2701	H2702	P2703	L2704	L2705	V2706	P2707	Y2708	D2709	T2710	L2711	T2712	A2713	K2714	E2715	K2716	A2717	A2718	L2719	T2720	E2721	E2722	A2723	Q2724	E2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753	L2754	L2755	L2756	L2757	L2758	L2759	L2760	L2761	L2762	L2763	L2764	L2765	L2766	L2767	L2768	L2769	L2770	L2771	Q2772	N2773	N2774	W2775	W2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	I2804	Y2805	L2806	W2807																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	I2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	Q2829	E2830	GLU	GLU	ARG	THR	L2894	E2895	A2896	G2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	A2918	D2919	A2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
D2537	S2542	M2578	V2579	D2580	S2581	R2593	S2594	V2627	F2628	D2629	V2630	P2631	N2634	A2637	E2670	L2674	Q2693	A2717	S2718	Y2719	SER	LYS	ALA	GLU	LYS	ALA	GLU	LYS	VAL	ARG	ARG	ARG	THR	ASP	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	I2746	L2747																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
V2275	V2280	L2302	S2309	L2321	D2333	R2336	M2342	V2346	E2347	E2348	M2351	R2355	L2368	L2376	E2382	R2385	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU</



● Molecule 1: Ryanodine receptor 1



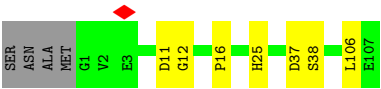
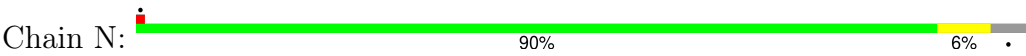
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ALA	GLY	GLY	VAL	M4097	I3917	VAL	VAL	THR	A3291	R3111	G2934	M2874	K2814	F2764	D2580
ALA	THR	VAL	GLU	E4107	D3941	GLU	GLU	ALA	PRO	LEU	Y2835	A2875	A2815	I2765	S2581
ALA	ALA	ALA	GLU	T3969	T3969	ASP	ASP	SER	PRO	GLY	Y2836	E2876	M2816	N2766	R2593
ALA	ALA	ALA	ASP	D4118	T3969	ASP	ASP	SER	PRO	VAL	Y2937	Q2877	L2817	K2767	S2594
ALA	GLY	ALA	ASP	E4119	L3980	ASP	ASP	SER	PRO	VAL	T2938	L2878	A2818	F2768	V2627
ALA	THR	ALA	ASP	E4134	L3986	ASP	ASP	ALA	GLY	THR	R2839	A2879	W2819	E2760	D2629
ALA	ALA	ALA	GLU	P4135	K3986	GLU	GLU	ALA	ALA	ALA	GLY	E2880	E2820	Y2761	V2630
ARG	ARG	ARG	GLU	E4152	M3999	GLU	GLU	LYS	P3301	THR	LYS	Y2882	W2821	T2762	P2631
LEU	LEU	LEU	GLY	Y4173	K4002	GLY	GLY	ALA	P3301	GLN	ASP	Y2882	T2822	H2763	N2634
TRP	ALA	ALA	GLU	Y4173	L4003	GLU	GLU	ASP	T3305	VAL	GLY	H2883	L2823	E2764	N2634
SER	ALA	ALA	ASN	R4192	A4004	GLY	GLY	ALA	A3306	GLY	LEU	M2884	E2824	K2765	A2637
LEU	ALA	ALA	GLY	Q4005	Q4005	GLY	GLY	SER	V3307	VAL	ASP	A2886	A2826	W2766	E2670
PHE	ARG	ARG	ALA	A4203	Q4009	ALA	ALA	GLY	D3310	G3126	THR	Q2887	R2827	A2767	L2674
GLY	ALA	ALA	ALA	W4205	W4205	GLU	GLU	SER	I3319	Q3128	GLY	R2888	Q2828	F2768	
GLY	ALA	ALA	GLY	E4206	L4013	GLY	GLY	ASP	L3320	L3129	SER	K2889	Q2829	D2769	
LEU	GLY	GLY	VAL	M4207	K4021	VAL	VAL	GLN	I3323	T3132	W2866	K2890	E2830	K2770	Q2693
LEU	SER	SER	GLU	G4225	V4024	GLU	GLU	ARG	I3323	Q3151	M2967	K2891	GLU	I2771	
THR	ARG	ARG	THR	E4226	V4024	THR	THR	THR	L3338	F3152	D2968	Q2892	ARG	Q2772	A2717
ALA	ALA	ALA	ALA	E4227	M4039	GLY	GLY	LYS	R3350	G3153	I2969	N2773	THR	N2774	S2718
VAL	ARG	ARG	VAL	E4244	Q4043	LEU	LEU	ARG	L3365	D3157	SER	W2775	LYS	W2776	Y2719
THR	ARG	ARG	THR	E4253	E4056	ARG	ARG	ASP	R3366	V3156	VAL	A2896	THR	S2777	SER
THR	ARG	ARG	THR	E4253	M4057	GLN	GLN	ASP	A3383	L3158	GLY	K2897	ARG	G2778	ALA
GLY	GLY	GLY	GLY	E4253	I4058	LYS	LYS	TYR	K3384	F3159	GLY	G2898	LYS	E2779	GLY
LEU	LEU	LEU	LEU	E4253	L4059	ARG	ARG	SER	A3385	L3175	VAL	G2900	ILE	N2780	ALA
LEU	LEU	LEU	LEU	E4253	K4060	ARG	ARG	SER	E3386	V3183	GLU	H2902	GLN	V2781	ALA
ALA	ALA	ALA	ALA	E4253	F4061	VAL	VAL	VAL	E3388	E3192	SER	L2904	ALA	D2782	THR
GLY	GLY	GLY	GLY	E4253	D4062	VAL	VAL	VAL	A3387	C3193	GLY	P2903	GLN	ASP	ALA
PRO	PRO	PRO	PRO	E4253	M4064	ALA	ALA	ALA	E3389	L3194	SER	L2905	THR	E2784	GLU
ASP	ASP	ASP	ASP	E4253	L4065	CYS	CYS	PHE	E3389	A3195	GLY	V2906	ASP	L2785	GLY
THR	THR	THR	THR	E4253	K4067	GLY	GLY	GLY	L3405	R3196	PRO	P2907	ARG	K2786	ASN
SER	SER	SER	SER	E4253	L4068	MET	MET	VAL	Y3409	K3222	GLU	Y2908	GLY	T2787	PHE
ALA	ALA	ALA	ALA	E4253	L4069	VAL	VAL	VAL	P3407	R3227	L3025	D2909	GLY	H2788	ASP
GLY	GLY	GLY	GLY	E4253	D4070	ASN	ASN	ASN	N3428	G3026	S3027	Y2910	GLY	P2737	R2738
VAL	VAL	VAL	VAL	E4253	E4075	GLY	GLY	GLY	A3429	S3027	V3050	L2911	ASP	P2739	P2739
HIS	GLY	GLY	GLY	E4253	E4075	THR	THR	THR	E3433	L3229	V3062	L2912	THR	V2740	V2740
GLY	GLY	GLY	GLY	E4253	E4075	ILE	ILE	ILE	E3433	L3229	V3065	L2913	ALA	E2741	E2741
GLN	GLN	GLN	GLN	E4253	E4075	ASN	ASN	ASN	R3436	L3232	M3081	K2914	THR	T2742	T2742
ALA	ALA	ALA	ALA	E4253	E4075	ASN	ASN	ASN	I3441	L3256	K3081	K2915	P2860	L2743	L2743
PRO	PRO	PRO	PRO	E4253	E4075	GLN	GLN	GLN	V3459	M3266	L3092	K2916	D2861	K2744	W2745
GLY	GLY	GLY	GLY	E4253	E4075	ASN	ASN	ASN	E3463	R3283	K3105	A2917	L2862	T2746	T2746
ALA	ALA	ALA	ALA	E4253	E4075	GLY	GLY	GLY	I3464			R2918	S2863	I2747	I2747
ASP	ASP	ASP	ASP	E4253	E4075	GLU	GLU	GLU				D2919	G2864	P2748	P2748
				E4253	E4075	GLU	GLU	GLU				E2799	V2865	E2749	E2749
				E4253	E4075	GLU	GLU	GLU				K2800	L2866	K2750	K2750
				E4253	E4075	GLU	GLU	GLU				K2802	T2867	L2761	L2761
				E4253	E4075	GLU	GLU	GLU				K2803	L2867		
				E4253	E4075	GLU	GLU	GLU				E2804	S2868		
				E4253	E4075	GLU	GLU	GLU				E2805	R2869		
				E4253	E4075	GLU	GLU	GLU				R2806	E2870		
				E4253	E4075	GLU	GLU	GLU				L2926	L2871		
				E4253	E4075	GLU	GLU	GLU				L2927	L2871		
				E4253	E4075	GLU	GLU	GLU				K2928			
				E4253	E4075	GLU	GLU	GLU				L2930			
				E4253	E4075	GLU	GLU	GLU				Q2931			



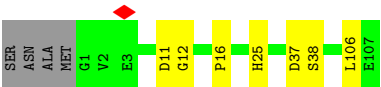
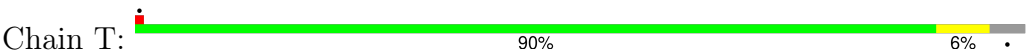




● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126217	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.269	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.047	Depositor
Map size (Å)	491.52, 491.52, 491.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	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, CA

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	0.40	0/33267	0.57	15/45152 (0.0%)
1	G	0.40	0/33267	0.57	16/45152 (0.0%)
1	M	0.40	0/33267	0.57	15/45152 (0.0%)
1	S	0.40	0/33267	0.57	16/45152 (0.0%)
2	B	0.77	0/832	0.70	0/1118
2	H	0.77	0/832	0.70	0/1118
2	N	0.78	0/832	0.70	0/1118
2	T	0.78	0/832	0.70	0/1118
All	All	0.41	0/136396	0.58	62/185080 (0.0%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4005	GLN	N-CA-C	-7.38	103.87	113.17
1	G	4005	GLN	N-CA-C	-7.37	103.88	113.17
1	S	4005	GLN	N-CA-C	-7.36	103.90	113.17
1	M	4005	GLN	N-CA-C	-7.34	103.92	113.17
1	G	3157	ILE	CA-C-O	-6.40	117.06	122.63
1	A	3157	ILE	CA-C-O	-6.39	117.07	122.63
1	S	3157	ILE	CA-C-O	-6.37	117.09	122.63
1	M	3157	ILE	CA-C-O	-6.32	117.13	122.63
1	M	3564	GLU	N-CA-C	-6.21	101.22	110.23
1	S	3564	GLU	N-CA-C	-6.20	101.24	110.23
1	G	3564	GLU	N-CA-C	-6.19	101.26	110.23
1	A	3564	GLU	N-CA-C	-6.18	101.26	110.23
1	M	3463	GLU	N-CA-C	-5.93	105.96	112.72
1	G	3463	GLU	N-CA-C	-5.89	106.01	112.72
1	S	3463	GLU	N-CA-C	-5.88	106.02	112.72
1	A	3463	GLU	N-CA-C	-5.87	106.03	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	702	TRP	CA-C-O	-5.83	114.22	120.92
1	S	702	TRP	CA-C-O	-5.82	114.23	120.92
1	G	702	TRP	CA-C-O	-5.79	114.26	120.92
1	S	4768	LEU	N-CA-C	-5.79	104.60	111.03
1	M	4768	LEU	N-CA-C	-5.78	104.61	111.03
1	M	702	TRP	CA-C-O	-5.78	114.27	120.92
1	M	4769	MET	CA-C-O	-5.78	114.39	121.67
1	S	4769	MET	CA-C-O	-5.77	114.39	121.67
1	G	4769	MET	CA-C-O	-5.76	114.41	121.67
1	A	4769	MET	CA-C-O	-5.76	114.42	121.67
1	G	4768	LEU	N-CA-C	-5.76	104.64	111.03
1	A	4768	LEU	N-CA-C	-5.74	104.66	111.03
1	A	461	HIS	CA-C-O	-5.58	114.97	120.82
1	M	461	HIS	CA-C-O	-5.55	114.99	120.82
1	S	461	HIS	CA-C-O	-5.55	114.99	120.82
1	G	461	HIS	CA-C-O	-5.55	114.99	120.82
1	A	3579	LEU	N-CA-C	-5.45	102.36	110.20
1	G	3579	LEU	N-CA-C	-5.44	102.36	110.20
1	G	589	LEU	CA-C-O	-5.42	113.97	120.10
1	M	3579	LEU	N-CA-C	-5.41	102.41	110.20
1	M	589	LEU	CA-C-O	-5.40	114.00	120.10
1	S	3579	LEU	N-CA-C	-5.40	102.42	110.20
1	S	589	LEU	CA-C-O	-5.38	114.02	120.10
1	A	589	LEU	CA-C-O	-5.38	114.02	120.10
1	M	702	TRP	N-CA-C	-5.20	101.22	109.96
1	G	702	TRP	N-CA-C	-5.19	101.24	109.96
1	A	702	TRP	N-CA-C	-5.18	101.26	109.96
1	S	702	TRP	N-CA-C	-5.17	101.27	109.96
1	A	4883	TYR	CA-C-O	-5.17	115.37	120.70
1	G	4883	TYR	CA-C-O	-5.17	115.38	120.70
1	S	3385	ALA	N-CA-C	-5.16	105.65	111.28
1	G	234	SER	CA-C-O	-5.16	116.05	121.88
1	G	3567	PRO	N-CA-C	-5.15	106.37	113.53
1	S	234	SER	CA-C-O	-5.15	116.06	121.88
1	A	3385	ALA	N-CA-C	-5.14	105.68	111.28
1	A	3567	PRO	N-CA-C	-5.14	106.39	113.53
1	M	3567	PRO	N-CA-C	-5.14	106.39	113.53
1	G	3385	ALA	N-CA-C	-5.14	105.68	111.28
1	M	3385	ALA	N-CA-C	-5.14	105.68	111.28
1	S	3567	PRO	N-CA-C	-5.13	106.41	113.53
1	A	234	SER	CA-C-O	-5.12	116.09	121.88
1	M	4883	TYR	CA-C-O	-5.11	115.44	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	4883	TYR	CA-C-O	-5.11	115.44	120.70
1	M	234	SER	CA-C-O	-5.10	116.12	121.88
1	G	768	PHE	CA-C-O	-5.04	115.30	120.54
1	S	768	PHE	CA-C-O	-5.01	115.33	120.54

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32524	0	31610	354	0
1	G	32524	0	31610	351	0
1	M	32524	0	31610	353	0
1	S	32524	0	31610	358	0
2	B	816	0	818	3	0
2	H	816	0	818	3	0
2	N	816	0	818	3	0
2	T	816	0	818	3	0
3	A	1	0	0	0	0
3	G	1	0	0	0	0
3	M	1	0	0	0	0
3	S	1	0	0	0	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
4	M	1	0	0	0	0
4	S	1	0	0	0	0
All	All	133368	0	129712	1377	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 5.

All (1377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:VAL:HA	1:A:1053:ILE:HG22	1.36	1.08
1:G:939:VAL:HA	1:G:1053:ILE:HG22	1.36	1.07
1:S:939:VAL:HA	1:S:1053:ILE:HG22	1.35	1.03
1:M:939:VAL:HA	1:M:1053:ILE:HG22	1.36	1.01
1:G:3579:LEU:HD12	1:G:3580:PRO:HD3	1.46	0.97
1:M:3579:LEU:HD12	1:M:3580:PRO:HD3	1.46	0.97
1:A:3579:LEU:HD12	1:A:3580:PRO:HD3	1.46	0.97
1:S:3579:LEU:HD12	1:S:3580:PRO:HD3	1.46	0.97
1:G:1927:LEU:HD12	1:G:2101:MET:SD	2.06	0.96
1:A:1927:LEU:HD12	1:A:2101:MET:SD	2.06	0.95
1:M:1927:LEU:HD12	1:M:2101:MET:SD	2.06	0.95
1:S:1927:LEU:HD12	1:S:2101:MET:SD	2.06	0.94
1:S:1927:LEU:CD1	1:S:2101:MET:SD	2.60	0.90
1:M:1927:LEU:CD1	1:M:2101:MET:SD	2.60	0.89
1:A:1927:LEU:CD1	1:A:2101:MET:SD	2.60	0.89
1:G:1927:LEU:CD1	1:G:2101:MET:SD	2.60	0.89
1:M:1027:LEU:HD23	1:M:1032:LYS:CG	2.03	0.89
1:A:4767:TRP:CD1	1:A:4771:ILE:HD11	2.08	0.88
1:G:1027:LEU:HD23	1:G:1032:LYS:CG	2.04	0.88
1:S:4767:TRP:CD1	1:S:4771:ILE:HD11	2.08	0.88
1:G:4767:TRP:CD1	1:G:4771:ILE:HD11	2.08	0.88
1:S:1027:LEU:HD23	1:S:1032:LYS:CG	2.04	0.88
1:M:4767:TRP:CD1	1:M:4771:ILE:HD11	2.08	0.87
1:G:3579:LEU:HG	1:G:3580:PRO:HD2	1.56	0.87
1:A:3579:LEU:HG	1:A:3580:PRO:HD2	1.55	0.86
1:A:1027:LEU:HD23	1:A:1032:LYS:CG	2.04	0.86
1:M:3579:LEU:HG	1:M:3580:PRO:HD2	1.55	0.85
1:M:275:ARG:HD3	1:M:336:PRO:HG2	1.58	0.85
1:S:275:ARG:HD3	1:S:336:PRO:HG2	1.58	0.85
1:S:3579:LEU:HG	1:S:3580:PRO:HD2	1.56	0.85
1:A:396:GLU:OE2	1:A:396:GLU:N	2.09	0.85
1:M:4767:TRP:NE1	1:M:4771:ILE:HD11	1.92	0.85
1:S:396:GLU:N	1:S:396:GLU:OE2	2.09	0.85
1:G:275:ARG:HD3	1:G:336:PRO:HG2	1.58	0.85
1:G:4767:TRP:NE1	1:G:4771:ILE:HD11	1.92	0.85
1:A:275:ARG:HD3	1:A:336:PRO:HG2	1.58	0.84
1:G:939:VAL:CA	1:G:1053:ILE:HG22	2.07	0.84
1:A:939:VAL:CA	1:A:1053:ILE:HG22	2.07	0.84
1:G:4839:MET:HG2	1:M:4823:LEU:HD22	1.60	0.84
1:A:4823:LEU:HD22	1:S:4839:MET:HG2	1.60	0.84
1:M:396:GLU:OE2	1:M:396:GLU:N	2.09	0.84
1:A:4767:TRP:NE1	1:A:4771:ILE:HD11	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4839:MET:HG3	1:S:4823:LEU:HD21	1.59	0.84
1:S:939:VAL:CA	1:S:1053:ILE:HG22	2.07	0.84
1:A:1027:LEU:HD23	1:A:1032:LYS:HG3	1.59	0.83
1:A:4839:MET:HG2	1:G:4823:LEU:HD22	1.60	0.83
1:G:1027:LEU:HD23	1:G:1032:LYS:HG3	1.59	0.83
1:A:4839:MET:HG3	1:G:4823:LEU:HD21	1.59	0.83
1:G:396:GLU:N	1:G:396:GLU:OE2	2.09	0.83
1:S:4767:TRP:NE1	1:S:4771:ILE:HD11	1.92	0.83
1:M:1027:LEU:HD23	1:M:1032:LYS:HG3	1.59	0.83
1:M:4839:MET:HG2	1:S:4823:LEU:HD22	1.60	0.83
1:A:4823:LEU:HD21	1:S:4839:MET:HG3	1.59	0.82
1:M:939:VAL:CA	1:M:1053:ILE:HG22	2.07	0.82
1:G:4839:MET:HG3	1:M:4823:LEU:HD21	1.59	0.82
1:G:1156:THR:OG1	1:G:1157:GLU:OE1	1.98	0.82
1:S:1027:LEU:HD23	1:S:1032:LYS:HG3	1.59	0.82
1:G:4917:ASP:OD2	1:M:4888:TYR:OH	1.99	0.81
1:M:2627:VAL:HG11	1:M:2910:THR:CG2	2.11	0.81
1:A:2627:VAL:HG11	1:A:2910:THR:CG2	2.11	0.81
1:S:2627:VAL:HG11	1:S:2910:THR:CG2	2.10	0.81
1:G:1561:VAL:HG12	1:G:1562:ILE:HG12	1.64	0.80
1:S:1156:THR:OG1	1:S:1157:GLU:OE1	1.98	0.80
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	1.98	0.80
1:G:2627:VAL:HG11	1:G:2910:THR:CG2	2.11	0.80
1:S:275:ARG:HH11	1:S:336:PRO:HD2	1.47	0.80
1:M:1156:THR:OG1	1:M:1157:GLU:OE1	1.98	0.80
1:A:1561:VAL:HG12	1:A:1562:ILE:HG12	1.64	0.80
1:S:1561:VAL:HG12	1:S:1562:ILE:HG12	1.64	0.80
1:M:4917:ASP:OD2	1:S:4888:TYR:OH	1.99	0.80
1:M:1561:VAL:HG12	1:M:1562:ILE:HG12	1.64	0.79
1:M:4839:MET:CG	1:S:4823:LEU:CD2	2.61	0.79
1:S:4064:MET:HE3	1:S:4107:GLU:HB3	1.65	0.79
1:G:275:ARG:HH11	1:G:336:PRO:HD2	1.47	0.79
1:A:275:ARG:HH11	1:A:336:PRO:HD2	1.47	0.79
1:G:1108:GLU:N	1:G:1108:GLU:OE1	2.16	0.79
1:M:4064:MET:HE3	1:M:4107:GLU:HB3	1.65	0.79
1:A:4839:MET:CG	1:G:4823:LEU:CD2	2.61	0.79
1:A:4823:LEU:CD2	1:S:4839:MET:CG	2.61	0.79
1:M:1108:GLU:OE1	1:M:1108:GLU:N	2.16	0.78
1:M:2627:VAL:HG11	1:M:2910:THR:HG22	1.65	0.78
1:A:4888:TYR:OH	1:S:4917:ASP:OD2	1.99	0.78
1:M:275:ARG:HH11	1:M:336:PRO:HD2	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:GLU:OE1	1:A:1108:GLU:N	2.16	0.78
1:A:2627:VAL:HG11	1:A:2910:THR:HG22	1.64	0.78
1:A:4917:ASP:OD2	1:G:4888:TYR:OH	1.99	0.78
1:G:3286:GLU:OE2	1:G:3286:GLU:N	2.17	0.78
1:G:4839:MET:CG	1:M:4823:LEU:CD2	2.61	0.78
1:S:1108:GLU:N	1:S:1108:GLU:OE1	2.16	0.78
1:G:2627:VAL:HG11	1:G:2910:THR:HG22	1.64	0.78
1:M:3286:GLU:N	1:M:3286:GLU:OE2	2.17	0.78
1:A:3286:GLU:N	1:A:3286:GLU:OE2	2.17	0.77
1:S:2627:VAL:HG11	1:S:2910:THR:HG22	1.64	0.77
1:A:4064:MET:HE3	1:A:4107:GLU:HB3	1.65	0.77
1:A:4823:LEU:HD21	1:S:4839:MET:CG	2.14	0.77
1:A:4823:LEU:CD2	1:S:4839:MET:HG2	2.15	0.77
1:A:4839:MET:CG	1:G:4823:LEU:HD21	2.14	0.77
1:G:4064:MET:HE3	1:G:4107:GLU:HB3	1.65	0.77
1:M:4839:MET:HG2	1:S:4823:LEU:CD2	2.15	0.77
1:M:4839:MET:CG	1:S:4823:LEU:HD21	2.14	0.77
1:S:3286:GLU:OE2	1:S:3286:GLU:N	2.17	0.77
1:A:1024:TYR:CE1	1:A:1032:LYS:HG2	2.20	0.76
1:S:3783:ILE:O	1:S:3786:CYS:SG	2.43	0.76
1:M:3783:ILE:O	1:M:3786:CYS:SG	2.43	0.76
1:S:1024:TYR:CE1	1:S:1032:LYS:HG2	2.20	0.76
1:A:3783:ILE:O	1:A:3786:CYS:SG	2.43	0.76
1:G:3783:ILE:O	1:G:3786:CYS:SG	2.43	0.76
1:G:4839:MET:CG	1:M:4823:LEU:HD21	2.14	0.76
1:G:1024:TYR:CE1	1:G:1032:LYS:HG2	2.20	0.76
1:A:3169:LEU:CD1	1:A:3194:LEU:HD11	2.16	0.76
1:M:3169:LEU:CD1	1:M:3194:LEU:HD11	2.16	0.76
1:A:4004:ALA:HB2	1:A:4013:LEU:HD22	1.69	0.75
1:S:3169:LEU:CD1	1:S:3194:LEU:HD11	2.16	0.75
1:M:1024:TYR:CE1	1:M:1032:LYS:HG2	2.20	0.75
1:G:3169:LEU:CD1	1:G:3194:LEU:HD11	2.16	0.75
1:G:4839:MET:HG2	1:M:4823:LEU:CD2	2.16	0.75
1:A:275:ARG:HD3	1:A:336:PRO:CG	2.17	0.75
1:G:4004:ALA:HB2	1:G:4013:LEU:HD22	1.69	0.75
1:A:4839:MET:HG2	1:G:4823:LEU:CD2	2.15	0.74
1:S:456:SER:OG	1:S:459:LEU:HG	1.88	0.74
1:G:456:SER:OG	1:G:459:LEU:HG	1.88	0.74
1:A:456:SER:OG	1:A:459:LEU:HG	1.88	0.74
1:G:275:ARG:HD3	1:G:336:PRO:CG	2.17	0.74
1:M:1435:TYR:HB3	1:M:1575:LEU:HD23	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1435:TYR:HB3	1:S:1575:LEU:HD23	1.70	0.74
1:G:3151:GLN:N	1:G:3151:GLN:OE1	2.21	0.74
1:M:456:SER:OG	1:M:459:LEU:HG	1.88	0.74
1:S:275:ARG:HD3	1:S:336:PRO:CG	2.17	0.74
1:A:3151:GLN:OE1	1:A:3151:GLN:N	2.21	0.74
1:M:275:ARG:HD3	1:M:336:PRO:CG	2.17	0.74
1:S:4004:ALA:HB2	1:S:4013:LEU:HD22	1.69	0.73
1:M:4004:ALA:HB2	1:M:4013:LEU:HD22	1.69	0.73
1:S:3151:GLN:N	1:S:3151:GLN:OE1	2.21	0.73
1:A:453:GLU:N	1:A:453:GLU:OE1	2.21	0.73
1:G:453:GLU:N	1:G:453:GLU:OE1	2.21	0.73
1:M:3151:GLN:N	1:M:3151:GLN:OE1	2.21	0.73
1:M:3753:PHE:HZ	1:M:4719:PHE:CZ	2.06	0.73
1:A:1435:TYR:HB3	1:A:1575:LEU:HD23	1.70	0.73
1:G:1943:LEU:HD11	1:G:2101:MET:HE1	1.71	0.73
1:M:1943:LEU:HD11	1:M:2101:MET:HE1	1.71	0.73
1:S:453:GLU:N	1:S:453:GLU:OE1	2.21	0.73
1:M:4207:MET:HE2	1:M:4207:MET:N	2.04	0.73
1:S:1943:LEU:HD11	1:S:2101:MET:HE1	1.71	0.73
1:M:453:GLU:N	1:M:453:GLU:OE1	2.21	0.73
1:S:3753:PHE:HZ	1:S:4719:PHE:CZ	2.07	0.73
1:G:1435:TYR:HB3	1:G:1575:LEU:HD23	1.70	0.73
1:G:4207:MET:N	1:G:4207:MET:HE2	2.04	0.73
1:G:3753:PHE:HZ	1:G:4719:PHE:CZ	2.06	0.72
1:S:3579:LEU:HD12	1:S:3580:PRO:CD	2.20	0.72
1:A:1825:HIS:CD2	1:G:3567:PRO:HG3	2.25	0.72
1:A:2670:GLU:O	1:A:2674:LEU:HD13	1.90	0.72
1:A:4207:MET:HE2	1:A:4207:MET:N	2.04	0.72
1:S:1027:LEU:HD23	1:S:1032:LYS:HG2	1.72	0.72
1:S:4207:MET:N	1:S:4207:MET:HE2	2.04	0.72
1:G:2628:PHE:CD1	1:G:2907:PRO:HG3	2.25	0.72
1:M:2628:PHE:CD1	1:M:2907:PRO:HG3	2.25	0.72
1:M:3579:LEU:HD12	1:M:3580:PRO:CD	2.20	0.72
1:G:2670:GLU:O	1:G:2674:LEU:HD13	1.90	0.72
1:M:2670:GLU:O	1:M:2674:LEU:HD13	1.90	0.72
1:A:3753:PHE:HZ	1:A:4719:PHE:CZ	2.07	0.72
1:A:1943:LEU:HD11	1:A:2101:MET:HE1	1.71	0.71
1:M:33:LEU:HD11	1:M:35:LEU:HD12	1.72	0.71
1:S:2628:PHE:CD1	1:S:2907:PRO:HG3	2.25	0.71
1:A:2628:PHE:CD1	1:A:2907:PRO:HG3	2.25	0.71
1:G:2628:PHE:HB2	1:G:2907:PRO:CD	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:LEU:HD11	1:G:35:LEU:HD12	1.72	0.71
1:A:3567:PRO:HG3	1:S:1825:HIS:CD2	2.25	0.71
1:M:2628:PHE:HB2	1:M:2907:PRO:CD	2.20	0.71
1:S:2628:PHE:HB2	1:S:2907:PRO:HD3	1.73	0.71
1:A:1027:LEU:HD23	1:A:1032:LYS:HG2	1.72	0.71
1:A:2628:PHE:HB2	1:A:2907:PRO:CD	2.20	0.71
1:G:941:MET:SD	1:G:944:GLU:HG2	2.31	0.71
1:G:1027:LEU:HD23	1:G:1032:LYS:HG2	1.72	0.71
1:A:941:MET:SD	1:A:944:GLU:HG2	2.31	0.71
1:M:1027:LEU:HD23	1:M:1032:LYS:HG2	1.72	0.71
1:S:2628:PHE:HB2	1:S:2907:PRO:CD	2.20	0.71
1:S:3427:PRO:HG2	1:S:3579:LEU:HD21	1.72	0.71
1:G:3579:LEU:HD12	1:G:3580:PRO:CD	2.20	0.71
1:M:1825:HIS:CD2	1:S:3567:PRO:HG3	2.25	0.71
1:A:3427:PRO:HG2	1:A:3579:LEU:HD21	1.72	0.70
1:G:2628:PHE:HB2	1:G:2907:PRO:HD3	1.73	0.70
1:A:980:ALA:O	1:A:984:LEU:HD13	1.92	0.70
1:S:2670:GLU:O	1:S:2674:LEU:HD13	1.90	0.70
1:S:4152:GLU:OE1	1:S:4192:ARG:NH1	2.24	0.70
1:A:33:LEU:HD11	1:A:35:LEU:HD12	1.72	0.70
1:G:1825:HIS:CD2	1:M:3567:PRO:HG3	2.25	0.70
1:G:4152:GLU:OE1	1:G:4192:ARG:NH1	2.24	0.70
1:S:980:ALA:O	1:S:984:LEU:HD13	1.92	0.70
1:M:4152:GLU:OE1	1:M:4192:ARG:NH1	2.24	0.70
1:S:941:MET:SD	1:S:944:GLU:HG2	2.31	0.70
1:A:4152:GLU:OE1	1:A:4192:ARG:NH1	2.24	0.70
1:G:980:ALA:O	1:G:984:LEU:HD13	1.92	0.70
1:M:941:MET:SD	1:M:944:GLU:HG2	2.31	0.70
1:M:3427:PRO:HG2	1:M:3579:LEU:HD21	1.72	0.70
1:A:2628:PHE:HB2	1:A:2907:PRO:HD3	1.73	0.70
1:G:3427:PRO:HG2	1:G:3579:LEU:HD21	1.72	0.70
1:S:33:LEU:HD11	1:S:35:LEU:HD12	1.72	0.70
1:M:2628:PHE:HB2	1:M:2907:PRO:HD3	1.73	0.70
1:M:3459:VAL:HG23	1:M:3464:ILE:HG23	1.73	0.70
1:G:2250:MET:HE2	1:G:2250:MET:HA	1.74	0.69
1:M:1943:LEU:CD1	1:M:2101:MET:HE1	2.22	0.69
1:S:1943:LEU:CD1	1:S:2101:MET:HE1	2.22	0.69
1:M:3579:LEU:HG	1:M:3580:PRO:CD	2.22	0.69
1:A:1943:LEU:CD1	1:A:2101:MET:HE1	2.22	0.69
1:A:3579:LEU:HD12	1:A:3580:PRO:CD	2.20	0.69
1:G:3999:MET:O	1:G:4003:LEU:HG	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:939:VAL:HA	1:S:1053:ILE:CG2	2.20	0.69
1:A:3579:LEU:HG	1:A:3580:PRO:CD	2.22	0.69
1:G:3579:LEU:HG	1:G:3580:PRO:CD	2.22	0.69
1:G:1943:LEU:CD1	1:G:2101:MET:HE1	2.22	0.69
1:M:3999:MET:O	1:M:4003:LEU:HG	1.93	0.69
1:S:3427:PRO:CG	1:S:3579:LEU:HD21	2.23	0.69
1:A:3459:VAL:HG23	1:A:3464:ILE:HG23	1.73	0.69
1:M:980:ALA:O	1:M:984:LEU:HD13	1.92	0.68
1:S:3579:LEU:HG	1:S:3580:PRO:CD	2.22	0.68
1:A:2250:MET:HE2	1:A:2250:MET:HA	1.75	0.68
1:A:3427:PRO:CG	1:A:3579:LEU:HD21	2.23	0.68
1:S:2250:MET:HE2	1:S:2250:MET:HA	1.75	0.68
1:A:4244:GLU:OE1	1:A:4668:LEU:HD13	1.93	0.68
1:G:4244:GLU:OE1	1:G:4668:LEU:HD13	1.93	0.68
1:S:4244:GLU:OE1	1:S:4668:LEU:HD13	1.93	0.68
1:G:3459:VAL:HG23	1:G:3464:ILE:HG23	1.73	0.68
1:M:2250:MET:HA	1:M:2250:MET:HE2	1.74	0.68
1:M:4767:TRP:CD2	1:M:4767:TRP:O	2.47	0.68
1:S:3459:VAL:HG23	1:S:3464:ILE:HG23	1.73	0.68
1:S:4767:TRP:O	1:S:4767:TRP:CD2	2.47	0.68
1:A:4767:TRP:CD2	1:A:4767:TRP:O	2.47	0.68
1:M:4244:GLU:OE1	1:M:4668:LEU:HD13	1.93	0.68
1:A:3999:MET:O	1:A:4003:LEU:HG	1.93	0.67
1:G:4767:TRP:O	1:G:4767:TRP:CD2	2.47	0.67
1:G:3427:PRO:CG	1:G:3579:LEU:HD21	2.23	0.67
1:M:3427:PRO:CG	1:M:3579:LEU:HD21	2.23	0.67
1:M:2333:ASP:OD1	1:M:2336:ARG:NH2	2.28	0.67
1:S:3999:MET:O	1:S:4003:LEU:HG	1.93	0.67
1:M:2537:ASP:O	1:M:2593:ARG:NH1	2.28	0.67
1:A:2537:ASP:O	1:A:2593:ARG:NH1	2.28	0.67
1:S:2333:ASP:OD1	1:S:2336:ARG:NH2	2.28	0.67
1:G:2333:ASP:OD1	1:G:2336:ARG:NH2	2.28	0.66
1:S:2537:ASP:O	1:S:2593:ARG:NH1	2.28	0.66
1:A:2333:ASP:OD1	1:A:2336:ARG:NH2	2.28	0.66
1:G:2537:ASP:O	1:G:2593:ARG:NH1	2.28	0.66
1:G:1927:LEU:HD11	1:G:2101:MET:SD	2.36	0.66
1:A:1927:LEU:HD11	1:A:2101:MET:SD	2.36	0.66
1:M:35:LEU:HD22	1:M:49:LEU:HB3	1.78	0.66
1:A:3579:LEU:CD1	1:A:3580:PRO:HD3	2.25	0.66
1:S:1927:LEU:HD11	1:S:2101:MET:SD	2.36	0.66
1:S:3283:ARG:HH22	1:S:3287:ARG:HH22	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3579:LEU:CD1	1:M:3580:PRO:CD	2.74	0.65
1:S:3579:LEU:CD1	1:S:3580:PRO:CD	2.74	0.65
1:S:275:ARG:NH1	1:S:336:PRO:HD2	2.11	0.65
1:G:35:LEU:HD22	1:G:49:LEU:HB3	1.78	0.65
1:M:3969:ILE:HD11	1:M:3980:LEU:CD1	2.27	0.65
1:A:4767:TRP:O	1:A:4767:TRP:CE3	2.50	0.65
1:G:938:HIS:O	1:G:1053:ILE:HA	1.97	0.65
1:G:3579:LEU:CG	1:G:3580:PRO:HD2	2.27	0.65
1:A:275:ARG:NH1	1:A:336:PRO:HD2	2.11	0.65
1:A:3579:LEU:CD1	1:A:3580:PRO:CD	2.74	0.65
1:G:275:ARG:NH1	1:G:336:PRO:HD2	2.11	0.65
1:G:3579:LEU:CD1	1:G:3580:PRO:CD	2.74	0.65
1:M:4767:TRP:O	1:M:4767:TRP:CE3	2.50	0.65
1:S:3579:LEU:CG	1:S:3580:PRO:HD2	2.27	0.65
1:S:4767:TRP:O	1:S:4767:TRP:CE3	2.50	0.65
1:G:939:VAL:HA	1:G:1053:ILE:CG2	2.20	0.65
1:M:937:CYS:SG	1:M:984:LEU:HG	2.37	0.65
1:A:938:HIS:O	1:A:1053:ILE:HA	1.97	0.64
1:M:938:HIS:O	1:M:1053:ILE:HA	1.97	0.64
1:G:3579:LEU:CD1	1:G:3580:PRO:HD3	2.25	0.64
1:S:984:LEU:HD12	1:S:987:ARG:HH11	1.62	0.64
1:A:3283:ARG:HH22	1:A:3287:ARG:HH22	1.44	0.64
1:M:3579:LEU:CG	1:M:3580:PRO:HD2	2.27	0.64
1:A:35:LEU:HD22	1:A:49:LEU:HB3	1.78	0.64
1:A:3579:LEU:CG	1:A:3580:PRO:HD2	2.27	0.64
1:A:3969:ILE:HD11	1:A:3980:LEU:CD1	2.27	0.64
1:M:3283:ARG:HH22	1:M:3287:ARG:HH22	1.44	0.64
1:S:3969:ILE:HD11	1:S:3980:LEU:CD1	2.27	0.64
1:G:3969:ILE:HD11	1:G:3980:LEU:CD1	2.27	0.64
1:A:984:LEU:HD12	1:A:987:ARG:HH11	1.62	0.64
1:M:1927:LEU:HD11	1:M:2101:MET:SD	2.36	0.64
1:M:275:ARG:NH1	1:M:336:PRO:HD2	2.11	0.64
1:M:3106:MET:HE3	1:M:3132:THR:HB	1.80	0.64
1:S:938:HIS:O	1:S:1053:ILE:HA	1.97	0.64
1:A:937:CYS:SG	1:A:984:LEU:HG	2.37	0.64
1:G:937:CYS:SG	1:G:984:LEU:HG	2.37	0.64
1:S:2627:VAL:CG1	1:S:2910:THR:CG2	2.76	0.64
1:S:4064:MET:CE	1:S:4107:GLU:HB3	2.28	0.64
1:G:3283:ARG:HH22	1:G:3287:ARG:HH22	1.44	0.63
1:G:3310:ASP:OD1	1:G:3350:ARG:NH2	2.32	0.63
1:S:35:LEU:HD22	1:S:49:LEU:HB3	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:937:CYS:SG	1:S:984:LEU:HG	2.37	0.63
1:G:3106:MET:HE3	1:G:3132:THR:HB	1.80	0.63
1:G:2627:VAL:CG1	1:G:2910:THR:CG2	2.76	0.63
1:G:4064:MET:HA	1:G:4067:LYS:HD3	1.81	0.63
1:M:581:ASN:OD1	1:M:582:HIS:CD2	2.52	0.63
1:M:4064:MET:HA	1:M:4067:LYS:HD3	1.81	0.63
1:A:2627:VAL:CG1	1:A:2910:THR:CG2	2.76	0.63
1:S:3310:ASP:OD1	1:S:3350:ARG:NH2	2.32	0.63
1:A:581:ASN:OD1	1:A:582:HIS:CD2	2.52	0.63
1:M:984:LEU:HD12	1:M:987:ARG:HH11	1.62	0.63
1:M:2627:VAL:CG1	1:M:2910:THR:CG2	2.76	0.63
1:M:4064:MET:CE	1:M:4107:GLU:HB3	2.28	0.63
1:S:581:ASN:OD1	1:S:582:HIS:CD2	2.52	0.63
1:A:3310:ASP:OD1	1:A:3350:ARG:NH2	2.31	0.63
1:S:3106:MET:HE3	1:S:3132:THR:HB	1.80	0.63
1:G:213:TYR:CD1	1:G:339:ILE:O	2.52	0.62
1:A:3106:MET:HE3	1:A:3132:THR:HB	1.80	0.62
1:G:984:LEU:HD12	1:G:987:ARG:HH11	1.63	0.62
1:G:4767:TRP:O	1:G:4767:TRP:CE3	2.50	0.62
1:S:213:TYR:CD1	1:S:339:ILE:O	2.52	0.62
1:A:2693:GLN:OE1	1:A:2693:GLN:N	2.32	0.62
1:G:581:ASN:OD1	1:G:582:HIS:CD2	2.52	0.62
1:M:3310:ASP:OD1	1:M:3350:ARG:NH2	2.32	0.62
1:A:1825:HIS:CD2	1:G:3567:PRO:HB3	2.35	0.62
1:M:1825:HIS:CD2	1:S:3567:PRO:HB3	2.35	0.62
1:M:2693:GLN:OE1	1:M:2693:GLN:N	2.32	0.62
1:A:4064:MET:CE	1:A:4107:GLU:HB3	2.28	0.62
1:G:1825:HIS:NE2	1:M:3567:PRO:HB3	2.15	0.62
1:M:213:TYR:CD1	1:M:339:ILE:O	2.52	0.62
1:A:3169:LEU:CD1	1:A:3194:LEU:CD1	2.78	0.62
1:G:2693:GLN:N	1:G:2693:GLN:OE1	2.32	0.62
1:A:1825:HIS:CD2	1:G:3567:PRO:CG	2.83	0.62
1:G:3592:ILE:O	1:G:3596:VAL:HG23	2.00	0.62
1:M:1825:HIS:CD2	1:S:3567:PRO:CG	2.83	0.62
1:A:1005:TRP:CE3	1:A:1016:ARG:C	2.78	0.62
1:G:1005:TRP:CE3	1:G:1016:ARG:C	2.78	0.62
1:S:1005:TRP:CE3	1:S:1016:ARG:C	2.78	0.62
1:A:3567:PRO:HB3	1:S:1825:HIS:CD2	2.35	0.61
1:M:1825:HIS:NE2	1:S:3567:PRO:HB3	2.14	0.61
1:A:3567:PRO:CG	1:S:1825:HIS:CD2	2.83	0.61
1:M:3169:LEU:CD1	1:M:3194:LEU:CD1	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1825:HIS:CD2	1:M:3567:PRO:CG	2.83	0.61
1:G:4064:MET:CE	1:G:4107:GLU:HB3	2.28	0.61
1:M:1005:TRP:CE3	1:M:1016:ARG:C	2.78	0.61
1:M:2862:LEU:CD1	1:M:2932:MET:HE1	2.30	0.61
1:S:4064:MET:HA	1:S:4067:LYS:HD3	1.80	0.61
1:A:1825:HIS:NE2	1:G:3567:PRO:HB3	2.14	0.61
1:A:2862:LEU:CD1	1:A:2932:MET:HE1	2.30	0.61
1:A:3567:PRO:HB3	1:S:1825:HIS:NE2	2.15	0.61
1:G:4767:TRP:CE2	1:G:4771:ILE:HD11	2.36	0.61
1:S:2693:GLN:N	1:S:2693:GLN:OE1	2.32	0.61
1:A:3433:GLU:OE1	1:A:3436:ARG:NH1	2.34	0.61
1:A:4064:MET:HA	1:A:4067:LYS:HD3	1.81	0.61
1:G:1157:GLU:OE1	1:G:1157:GLU:N	2.34	0.61
1:G:1825:HIS:CD2	1:M:3567:PRO:HB3	2.35	0.61
1:M:2580:ASP:OD1	1:M:2581:SER:N	2.33	0.61
1:S:3169:LEU:CD1	1:S:3194:LEU:CD1	2.78	0.61
1:A:213:TYR:CD1	1:A:339:ILE:O	2.52	0.61
1:A:3592:ILE:O	1:A:3596:VAL:HG23	2.00	0.61
1:M:939:VAL:HA	1:M:1053:ILE:CG2	2.20	0.61
1:M:1157:GLU:OE1	1:M:1157:GLU:N	2.34	0.61
1:S:1157:GLU:OE1	1:S:1157:GLU:N	2.34	0.61
1:S:2862:LEU:CD1	1:S:2932:MET:HE1	2.30	0.61
1:S:2580:ASP:OD1	1:S:2581:SER:N	2.33	0.61
1:G:2580:ASP:OD1	1:G:2581:SER:N	2.33	0.61
1:G:2862:LEU:CD1	1:G:2932:MET:HE1	2.30	0.61
1:A:4767:TRP:CE2	1:A:4771:ILE:HD11	2.36	0.61
1:G:3169:LEU:CD1	1:G:3194:LEU:CD1	2.78	0.61
1:S:3433:GLU:OE1	1:S:3436:ARG:NH1	2.34	0.61
1:A:581:ASN:OD1	1:A:582:HIS:N	2.34	0.60
1:A:2580:ASP:OD1	1:A:2581:SER:N	2.33	0.60
1:G:4954:MET:HA	1:G:4954:MET:HE2	1.83	0.60
1:M:581:ASN:OD1	1:M:582:HIS:N	2.34	0.60
1:M:4954:MET:HE2	1:M:4954:MET:HA	1.83	0.60
1:A:3283:ARG:HH22	1:A:3287:ARG:NH2	1.99	0.60
1:A:3573:MET:O	1:A:3574:ALA:C	2.44	0.60
1:S:3283:ARG:HH22	1:S:3287:ARG:NH2	1.99	0.60
1:S:2342:ASN:ND2	1:S:2342:ASN:O	2.35	0.60
1:A:4954:MET:HE2	1:A:4954:MET:HA	1.83	0.60
1:G:3433:GLU:OE1	1:G:3436:ARG:NH1	2.34	0.60
1:M:3433:GLU:OE1	1:M:3436:ARG:NH1	2.34	0.60
1:M:3592:ILE:O	1:M:3596:VAL:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4767:TRP:CE2	1:M:4771:ILE:HD11	2.36	0.60
1:S:4954:MET:HA	1:S:4954:MET:HE2	1.83	0.60
1:A:1157:GLU:OE1	1:A:1157:GLU:N	2.34	0.60
1:M:2342:ASN:O	1:M:2342:ASN:ND2	2.35	0.60
1:S:2280:VAL:HG22	1:S:2280:VAL:O	2.02	0.60
1:S:3592:ILE:O	1:S:3596:VAL:HG23	2.00	0.60
1:M:2628:PHE:HD1	1:M:2907:PRO:HG3	1.67	0.60
1:M:3283:ARG:HH22	1:M:3287:ARG:NH2	1.99	0.60
1:A:939:VAL:HA	1:A:1053:ILE:CG2	2.20	0.60
1:G:581:ASN:OD1	1:G:582:HIS:N	2.34	0.60
1:G:873:LYS:HB3	1:G:1049:TYR:CZ	2.37	0.60
1:G:3573:MET:O	1:G:3574:ALA:C	2.44	0.60
1:M:972:LEU:HD11	1:M:1045:THR:OG1	2.02	0.60
1:S:581:ASN:OD1	1:S:582:HIS:N	2.34	0.60
1:G:320:LYS:NZ	1:G:381:GLU:O	2.35	0.60
1:A:873:LYS:HB3	1:A:1049:TYR:CZ	2.37	0.59
1:S:972:LEU:HD11	1:S:1045:THR:OG1	2.02	0.59
1:S:3573:MET:O	1:S:3574:ALA:C	2.44	0.59
1:S:4767:TRP:CE2	1:S:4771:ILE:HD11	2.36	0.59
1:G:545:ASP:HA	1:G:548:VAL:HG22	1.85	0.59
1:G:3283:ARG:HH22	1:G:3287:ARG:NH2	1.99	0.59
1:G:972:LEU:HD11	1:G:1045:THR:OG1	2.02	0.59
1:A:2280:VAL:O	1:A:2280:VAL:HG22	2.02	0.59
1:G:2280:VAL:HG22	1:G:2280:VAL:O	2.02	0.59
1:A:545:ASP:HA	1:A:548:VAL:HG22	1.85	0.59
1:S:3671:ASP:OD2	1:S:3671:ASP:N	2.35	0.59
1:A:320:LYS:NZ	1:A:381:GLU:O	2.35	0.59
1:A:1027:LEU:CD2	1:A:1032:LYS:HG3	2.33	0.59
1:M:545:ASP:HA	1:M:548:VAL:HG22	1.84	0.59
1:M:3671:ASP:OD2	1:M:3671:ASP:N	2.35	0.59
1:S:873:LYS:HB3	1:S:1049:TYR:CZ	2.37	0.59
1:A:972:LEU:HD11	1:A:1045:THR:OG1	2.02	0.59
1:M:320:LYS:NZ	1:M:381:GLU:O	2.35	0.59
1:M:873:LYS:HB3	1:M:1049:TYR:CZ	2.37	0.59
1:M:3573:MET:O	1:M:3574:ALA:C	2.44	0.59
1:S:2628:PHE:HD1	1:S:2907:PRO:HG3	1.67	0.59
1:G:3192:GLU:OE2	1:G:3196:ARG:NE	2.36	0.59
1:M:2280:VAL:O	1:M:2280:VAL:HG22	2.02	0.59
1:A:2342:ASN:O	1:A:2342:ASN:ND2	2.35	0.58
1:G:2342:ASN:ND2	1:G:2342:ASN:O	2.35	0.58
1:G:3671:ASP:N	1:G:3671:ASP:OD2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:933:LEU:HD21	1:M:939:VAL:HG12	1.85	0.58
1:S:933:LEU:HD21	1:S:939:VAL:HG12	1.85	0.58
1:S:1052:ASN:ND2	1:S:1054:GLU:OE2	2.36	0.58
1:M:2542:SER:HG	1:M:2594:SER:HG	1.48	0.58
1:G:3154:ASP:O	1:G:3158:LEU:HD21	2.03	0.58
1:S:3154:ASP:O	1:S:3158:LEU:HD21	2.03	0.58
1:S:3192:GLU:OE2	1:S:3196:ARG:NE	2.36	0.58
1:A:1052:ASN:ND2	1:A:1054:GLU:OE2	2.36	0.58
1:S:320:LYS:NZ	1:S:381:GLU:O	2.35	0.58
1:A:3154:ASP:O	1:A:3158:LEU:HD21	2.03	0.58
1:S:2628:PHE:HB2	1:S:2907:PRO:CG	2.34	0.58
1:A:33:LEU:HD12	1:A:33:LEU:C	2.29	0.58
1:A:3579:LEU:CG	1:A:3580:PRO:CD	2.82	0.58
1:A:3986:TRP:CE3	1:A:3986:TRP:HA	2.39	0.58
1:M:3154:ASP:O	1:M:3158:LEU:HD21	2.03	0.58
1:S:27:THR:HA	1:S:31:GLU:O	2.04	0.58
1:S:33:LEU:C	1:S:33:LEU:HD12	2.29	0.58
1:S:213:TYR:HD1	1:S:339:ILE:O	1.87	0.58
1:S:545:ASP:HA	1:S:548:VAL:HG22	1.84	0.58
1:S:3579:LEU:CD1	1:S:3580:PRO:HD3	2.25	0.57
1:S:3579:LEU:CG	1:S:3580:PRO:CD	2.82	0.57
1:G:213:TYR:HD1	1:G:339:ILE:O	1.87	0.57
1:M:33:LEU:HD12	1:M:33:LEU:C	2.29	0.57
1:M:939:VAL:HG23	1:M:1053:ILE:CG2	2.34	0.57
1:M:27:THR:HA	1:M:31:GLU:O	2.04	0.57
1:M:2628:PHE:HB2	1:M:2907:PRO:CG	2.34	0.57
1:G:939:VAL:HG23	1:G:1053:ILE:CG2	2.34	0.57
1:S:864:PRO:HG2	1:S:867:LEU:HB2	1.86	0.57
1:A:2628:PHE:HD1	1:A:2907:PRO:HG3	1.67	0.57
1:G:933:LEU:HD21	1:G:939:VAL:HG12	1.85	0.57
1:G:4878:ASP:OD1	1:G:4879:MET:N	2.37	0.57
1:A:4682:GLU:OE2	1:A:4723:LYS:HE2	2.05	0.57
1:G:3579:LEU:CG	1:G:3580:PRO:CD	2.82	0.57
1:M:213:TYR:HD1	1:M:339:ILE:O	1.87	0.57
1:M:3579:LEU:CG	1:M:3580:PRO:CD	2.82	0.57
1:A:828:GLU:OE1	1:A:828:GLU:N	2.36	0.57
1:G:33:LEU:C	1:G:33:LEU:HD12	2.29	0.57
1:M:1052:ASN:ND2	1:M:1054:GLU:OE2	2.36	0.57
1:A:864:PRO:HG2	1:A:867:LEU:HB2	1.87	0.57
1:A:933:LEU:HD21	1:A:939:VAL:HG12	1.85	0.57
1:M:33:LEU:CD1	1:M:35:LEU:HD12	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:828:GLU:OE1	1:M:828:GLU:N	2.36	0.57
1:M:3986:TRP:HA	1:M:3986:TRP:CE3	2.39	0.57
1:M:4878:ASP:OD1	1:M:4879:MET:N	2.37	0.57
1:S:3986:TRP:HA	1:S:3986:TRP:CE3	2.39	0.57
1:G:864:PRO:HG2	1:G:867:LEU:HB2	1.87	0.56
1:G:2628:PHE:HD1	1:G:2907:PRO:HG3	1.67	0.56
1:A:27:THR:HA	1:A:31:GLU:O	2.04	0.56
1:A:213:TYR:HD1	1:A:339:ILE:O	1.87	0.56
1:A:939:VAL:HG23	1:A:1053:ILE:CG2	2.34	0.56
1:A:4658:ILE:HD11	1:A:4796:MET:HB2	1.88	0.56
1:A:4878:ASP:OD1	1:A:4879:MET:N	2.37	0.56
1:A:4949:GLN:C	1:A:4949:GLN:OE1	2.49	0.56
1:G:707:VAL:HG23	1:G:782:SER:HB3	1.87	0.56
1:S:939:VAL:HG23	1:S:1053:ILE:CG2	2.34	0.56
1:S:3753:PHE:CZ	1:S:4719:PHE:CZ	2.92	0.56
1:A:2628:PHE:HB2	1:A:2907:PRO:CG	2.34	0.56
1:A:3671:ASP:OD2	1:A:3671:ASP:N	2.35	0.56
1:G:27:THR:HA	1:G:31:GLU:O	2.04	0.56
1:G:33:LEU:CD1	1:G:35:LEU:HD12	2.35	0.56
1:G:2628:PHE:HB2	1:G:2907:PRO:CG	2.34	0.56
1:M:1027:LEU:CD2	1:M:1032:LYS:HG3	2.33	0.56
1:M:3753:PHE:CZ	1:M:4719:PHE:CZ	2.91	0.56
1:M:4682:GLU:OE2	1:M:4723:LYS:HE2	2.05	0.56
1:M:4949:GLN:C	1:M:4949:GLN:OE1	2.48	0.56
1:S:2807:TRP:HB3	1:S:2808:PRO:HD3	1.88	0.56
1:A:3753:PHE:CZ	1:A:4719:PHE:CZ	2.92	0.56
1:G:1052:ASN:ND2	1:G:1054:GLU:OE2	2.36	0.56
1:G:3128:ASN:OD1	1:G:3129:LEU:N	2.39	0.56
1:G:3986:TRP:HA	1:G:3986:TRP:CE3	2.39	0.56
1:S:3157:ILE:O	1:S:3158:LEU:HD13	2.06	0.56
1:S:4878:ASP:OD1	1:S:4879:MET:N	2.37	0.56
1:A:33:LEU:CD1	1:A:35:LEU:HD12	2.35	0.56
1:S:4949:GLN:C	1:S:4949:GLN:OE1	2.49	0.56
1:A:1093:GLU:HB2	1:A:1148:VAL:HG22	1.88	0.56
1:M:3192:GLU:OE2	1:M:3196:ARG:NE	2.36	0.56
1:A:3128:ASN:OD1	1:A:3129:LEU:N	2.39	0.56
1:S:33:LEU:CD1	1:S:35:LEU:HD12	2.35	0.56
1:S:4682:GLU:OE2	1:S:4723:LYS:HE2	2.05	0.56
1:G:3157:ILE:O	1:G:3158:LEU:HD13	2.06	0.56
1:G:4949:GLN:C	1:G:4949:GLN:OE1	2.49	0.56
1:M:707:VAL:HG23	1:M:782:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3128:ASN:OD1	1:S:3129:LEU:N	2.39	0.56
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.87	0.56
1:M:3157:ILE:O	1:M:3158:LEU:HD13	2.06	0.56
1:A:2212:VAL:HG11	1:A:2256:TYR:OH	2.06	0.55
1:G:3283:ARG:HH12	1:G:3287:ARG:CZ	2.19	0.55
1:M:2212:VAL:HG11	1:M:2256:TYR:OH	2.06	0.55
1:M:3128:ASN:OD1	1:M:3129:LEU:N	2.39	0.55
1:S:1093:GLU:HB2	1:S:1148:VAL:HG22	1.88	0.55
1:A:3283:ARG:HH12	1:A:3287:ARG:CZ	2.19	0.55
1:M:864:PRO:HG2	1:M:867:LEU:HB2	1.86	0.55
1:A:2807:TRP:HB3	1:A:2808:PRO:HD3	1.88	0.55
1:G:864:PRO:HG3	1:G:867:LEU:HD12	1.89	0.55
1:S:707:VAL:HG23	1:S:782:SER:HB3	1.87	0.55
1:S:2212:VAL:HG11	1:S:2256:TYR:OH	2.06	0.55
1:S:2542:SER:OG	1:S:2594:SER:OG	2.25	0.55
1:G:2212:VAL:HG11	1:G:2256:TYR:OH	2.06	0.55
1:G:2348:GLU:OE1	1:G:2348:GLU:N	2.38	0.55
1:G:2807:TRP:HB3	1:G:2808:PRO:HD3	1.88	0.55
1:S:2778:GLY:HA3	1:S:2787:THR:HB	1.89	0.55
1:S:3777:GLU:OE1	1:S:3777:GLU:N	2.39	0.55
1:A:3157:ILE:O	1:A:3158:LEU:HD13	2.06	0.55
1:G:1027:LEU:CD2	1:G:1032:LYS:HG3	2.33	0.55
1:G:3753:PHE:CZ	1:G:4719:PHE:CZ	2.91	0.55
1:M:977:LEU:HD11	1:M:1040:CYS:SG	2.47	0.55
1:M:1093:GLU:HB2	1:M:1148:VAL:HG22	1.88	0.55
1:M:4658:ILE:HD11	1:M:4796:MET:HB2	1.87	0.55
1:G:4658:ILE:HD11	1:G:4796:MET:HB2	1.87	0.55
1:G:4682:GLU:OE2	1:G:4723:LYS:HE2	2.05	0.55
1:S:828:GLU:OE1	1:S:828:GLU:N	2.36	0.55
1:S:4658:ILE:HD11	1:S:4796:MET:HB2	1.87	0.55
1:A:977:LEU:HD11	1:A:1040:CYS:SG	2.47	0.55
1:A:2627:VAL:CG1	1:A:2910:THR:HG21	2.37	0.55
1:G:977:LEU:HD11	1:G:1040:CYS:SG	2.47	0.55
1:G:1093:GLU:HB2	1:G:1148:VAL:HG22	1.88	0.55
1:M:2807:TRP:HB3	1:M:2808:PRO:HD3	1.88	0.55
1:M:3579:LEU:CD1	1:M:3580:PRO:HD3	2.25	0.54
1:A:3192:GLU:OE2	1:A:3196:ARG:NE	2.36	0.54
1:G:828:GLU:OE1	1:G:828:GLU:N	2.36	0.54
1:M:2627:VAL:CG1	1:M:2910:THR:HG21	2.37	0.54
1:M:3283:ARG:HH12	1:M:3287:ARG:CZ	2.19	0.54
1:S:864:PRO:HG3	1:S:867:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3283:ARG:HH12	1:S:3287:ARG:CZ	2.19	0.54
1:A:864:PRO:HG3	1:A:867:LEU:HD12	1.89	0.54
1:G:988:LEU:HB3	1:G:1039:LEU:HD13	1.90	0.54
1:M:26:ALA:O	1:M:33:LEU:HG	2.08	0.54
1:M:988:LEU:HB3	1:M:1039:LEU:HD13	1.90	0.54
1:M:4729:GLY:O	1:M:4733:GLY:N	2.41	0.54
1:S:977:LEU:HD11	1:S:1040:CYS:SG	2.47	0.54
1:G:2309:SER:HB3	1:G:2321:ILE:O	2.08	0.54
1:S:2627:VAL:CG1	1:S:2910:THR:HG21	2.37	0.54
1:A:4729:GLY:O	1:A:4733:GLY:N	2.41	0.54
1:G:2627:VAL:CG1	1:G:2910:THR:HG21	2.37	0.54
1:M:34:LYS:HA	1:M:34:LYS:HE2	1.90	0.54
1:M:2778:GLY:HA3	1:M:2787:THR:HB	1.89	0.54
1:S:4729:GLY:O	1:S:4733:GLY:N	2.41	0.54
1:A:2778:GLY:HA3	1:A:2787:THR:HB	1.89	0.54
1:A:3777:GLU:N	1:A:3777:GLU:OE1	2.39	0.54
1:G:4729:GLY:O	1:G:4733:GLY:N	2.41	0.54
1:M:2309:SER:HB3	1:M:2321:ILE:O	2.08	0.54
1:S:26:ALA:O	1:S:33:LEU:HG	2.08	0.54
1:S:3527:PRO:HD2	1:S:3573:MET:HE1	1.90	0.54
1:A:275:ARG:CD	1:A:336:PRO:HG2	2.36	0.53
1:A:3527:PRO:HD2	1:A:3573:MET:HE1	1.90	0.53
1:M:2348:GLU:OE1	1:M:2348:GLU:N	2.38	0.53
1:S:988:LEU:HB3	1:S:1039:LEU:HD13	1.90	0.53
1:G:3777:GLU:OE1	1:G:3777:GLU:N	2.39	0.53
1:G:4952:GLU:C	1:G:4952:GLU:OE1	2.52	0.53
1:M:4952:GLU:OE1	1:M:4952:GLU:C	2.52	0.53
1:S:196:MET:HE3	1:S:196:MET:HA	1.91	0.53
1:A:2309:SER:HB3	1:A:2321:ILE:O	2.08	0.53
1:A:4952:GLU:OE1	1:A:4952:GLU:C	2.52	0.53
1:G:2778:GLY:HA3	1:G:2787:THR:HB	1.89	0.53
1:G:3169:LEU:HD13	1:G:3194:LEU:CD1	2.38	0.53
1:M:864:PRO:HG3	1:M:867:LEU:HD12	1.88	0.53
1:M:3527:PRO:HD2	1:M:3573:MET:HE1	1.90	0.53
1:A:3169:LEU:HD13	1:A:3194:LEU:CD1	2.38	0.53
1:M:196:MET:HE3	1:M:196:MET:HA	1.91	0.53
1:S:3169:LEU:HD13	1:S:3194:LEU:CD1	2.38	0.53
1:S:4244:GLU:OE2	1:S:4244:GLU:HA	2.09	0.53
1:A:26:ALA:O	1:A:33:LEU:HG	2.08	0.53
1:G:3579:LEU:CD1	1:G:3580:PRO:HD2	2.38	0.53
1:M:3169:LEU:HD13	1:M:3194:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1027:LEU:CD2	1:S:1032:LYS:HG3	2.33	0.53
1:S:2309:SER:HB3	1:S:2321:ILE:O	2.08	0.53
1:S:4952:GLU:C	1:S:4952:GLU:OE1	2.52	0.53
2:B:16:PRO:HA	2:B:106:LEU:HD21	1.91	0.53
1:M:3579:LEU:CD1	1:M:3580:PRO:HD2	2.38	0.53
1:S:3579:LEU:CD1	1:S:3580:PRO:HD2	2.38	0.53
1:A:3579:LEU:CD1	1:A:3580:PRO:HD2	2.38	0.53
1:G:196:MET:HE3	1:G:196:MET:HA	1.91	0.53
1:G:3527:PRO:HD2	1:G:3573:MET:HE1	1.90	0.53
1:S:372:LEU:C	1:S:372:LEU:HD13	2.34	0.53
1:A:34:LYS:HA	1:A:34:LYS:HE2	1.90	0.52
1:A:988:LEU:HB3	1:A:1039:LEU:HD13	1.90	0.52
1:M:2542:SER:OG	1:M:2594:SER:OG	2.25	0.52
1:A:372:LEU:C	1:A:372:LEU:HD13	2.34	0.52
1:G:1041:GLN:HA	1:G:1041:GLN:OE1	2.10	0.52
1:M:4244:GLU:OE2	1:M:4244:GLU:HA	2.09	0.52
1:S:34:LYS:HE2	1:S:34:LYS:HA	1.90	0.52
1:A:988:LEU:HD23	1:A:1039:LEU:HD22	1.92	0.52
1:A:2542:SER:HG	1:A:2594:SER:HG	1.57	0.52
1:G:26:ALA:O	1:G:33:LEU:HG	2.08	0.52
1:A:977:LEU:HD21	1:A:1043:VAL:HG12	1.92	0.52
1:A:1041:GLN:OE1	1:A:1041:GLN:HA	2.10	0.52
1:A:4244:GLU:OE2	1:A:4244:GLU:HA	2.09	0.52
1:S:3753:PHE:HZ	1:S:4719:PHE:CE2	2.28	0.52
1:A:2542:SER:OG	1:A:2594:SER:OG	2.25	0.52
1:A:4689:THR:HG22	1:A:4732:PHE:CZ	2.45	0.52
1:M:3777:GLU:N	1:M:3777:GLU:OE1	2.39	0.52
2:T:16:PRO:HA	2:T:106:LEU:HD21	1.91	0.52
1:G:977:LEU:HD21	1:G:1043:VAL:HG12	1.92	0.52
1:M:772:ASN:ND2	1:M:1470:ARG:HA	2.25	0.52
1:M:3753:PHE:HZ	1:M:4719:PHE:CE2	2.28	0.52
1:S:988:LEU:HD23	1:S:1039:LEU:HD22	1.92	0.52
1:A:421:PHE:HB3	1:A:432:ALA:HB3	1.92	0.52
1:M:977:LEU:HD21	1:M:1043:VAL:HG12	1.92	0.52
1:M:4205:TRP:CE3	1:M:4989:MET:HE1	2.45	0.52
1:M:4689:THR:HG22	1:M:4732:PHE:CZ	2.45	0.52
1:S:1024:TYR:HE1	1:S:1032:LYS:HG2	1.74	0.52
1:A:196:MET:HE3	1:A:196:MET:HA	1.91	0.52
1:G:34:LYS:HE2	1:G:34:LYS:HA	1.90	0.52
1:G:372:LEU:C	1:G:372:LEU:HD13	2.34	0.52
1:G:3753:PHE:HZ	1:G:4719:PHE:CE2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:772:ASN:ND2	1:S:1470:ARG:HA	2.25	0.52
1:G:275:ARG:CD	1:G:336:PRO:HG2	2.36	0.51
1:G:4205:TRP:CE3	1:G:4989:MET:HE1	2.45	0.51
1:S:2542:SER:HG	1:S:2594:SER:HG	1.57	0.51
1:M:372:LEU:HD13	1:M:372:LEU:C	2.35	0.51
2:N:16:PRO:HA	2:N:106:LEU:HD21	1.91	0.51
2:H:16:PRO:HA	2:H:106:LEU:HD21	1.91	0.51
1:M:1041:GLN:OE1	1:M:1041:GLN:HA	2.10	0.51
1:S:977:LEU:HD21	1:S:1043:VAL:HG12	1.92	0.51
2:B:11:ASP:OD2	2:B:12:GLY:N	2.44	0.51
1:G:4244:GLU:OE2	1:G:4244:GLU:HA	2.09	0.51
1:G:4689:THR:HG22	1:G:4732:PHE:CZ	2.45	0.51
1:M:1046:LEU:C	1:M:1046:LEU:HD13	2.36	0.51
1:M:2150:GLU:OE1	1:M:2150:GLU:N	2.44	0.51
1:M:3528:THR:HG23	1:M:3573:MET:HE3	1.93	0.51
1:S:1046:LEU:HD13	1:S:1046:LEU:C	2.36	0.51
1:A:772:ASN:ND2	1:A:1470:ARG:HA	2.25	0.51
1:A:4206:GLU:C	1:A:4207:MET:HE2	2.36	0.51
1:G:233:ILE:HD12	1:G:242:ARG:HB3	1.93	0.51
1:G:4063:ASP:O	1:G:4067:LYS:HG3	2.11	0.51
1:S:4205:TRP:CE3	1:S:4989:MET:HE1	2.45	0.51
1:S:4689:THR:HG22	1:S:4732:PHE:CZ	2.45	0.51
1:A:3753:PHE:HZ	1:A:4719:PHE:CE2	2.28	0.51
1:S:3528:THR:HG23	1:S:3573:MET:HE3	1.93	0.51
1:S:4004:ALA:CB	1:S:4013:LEU:HD22	2.40	0.51
1:S:4730:ASP:OD1	1:S:4731:ILE:N	2.44	0.51
1:A:3105:LYS:HD3	1:A:3105:LYS:O	2.11	0.51
1:G:988:LEU:HD23	1:G:1039:LEU:HD22	1.92	0.51
1:M:3105:LYS:HD3	1:M:3105:LYS:O	2.11	0.51
1:S:421:PHE:HB3	1:S:432:ALA:HB3	1.92	0.51
1:S:4206:GLU:C	1:S:4207:MET:HE2	2.36	0.51
2:T:11:ASP:OD2	2:T:12:GLY:N	2.44	0.51
1:A:1046:LEU:C	1:A:1046:LEU:HD13	2.36	0.51
1:M:988:LEU:HD23	1:M:1039:LEU:HD22	1.92	0.51
1:M:421:PHE:HB3	1:M:432:ALA:HB3	1.92	0.51
1:M:4063:ASP:O	1:M:4067:LYS:HG3	2.11	0.51
1:M:4836:GLN:N	1:M:4836:GLN:OE1	2.44	0.51
1:A:2634:ASN:OD1	1:A:2637:ALA:N	2.44	0.51
1:G:4836:GLN:OE1	1:G:4836:GLN:N	2.44	0.51
2:N:11:ASP:OD2	2:N:12:GLY:N	2.44	0.51
1:S:1041:GLN:HA	1:S:1041:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:ASP:OD2	2:H:12:GLY:N	2.44	0.50
1:M:3156:VAL:HG13	1:M:3157:ILE:N	2.27	0.50
1:S:3105:LYS:O	1:S:3105:LYS:HD3	2.11	0.50
1:S:4063:ASP:O	1:S:4067:LYS:HG3	2.11	0.50
1:A:4063:ASP:O	1:A:4067:LYS:HG3	2.11	0.50
1:G:421:PHE:HB3	1:G:432:ALA:HB3	1.92	0.50
1:G:2634:ASN:OD1	1:G:2637:ALA:N	2.44	0.50
1:G:4206:GLU:C	1:G:4207:MET:HE2	2.36	0.50
1:M:1869:GLU:OE1	1:M:1869:GLU:N	2.40	0.50
1:A:4205:TRP:CE3	1:A:4989:MET:HE1	2.45	0.50
1:S:2634:ASN:OD1	1:S:2637:ALA:N	2.44	0.50
1:G:772:ASN:ND2	1:G:1470:ARG:HA	2.25	0.50
1:S:233:ILE:HD12	1:S:242:ARG:HB3	1.93	0.50
1:S:2150:GLU:N	1:S:2150:GLU:OE1	2.44	0.50
1:A:4767:TRP:O	1:A:4767:TRP:CG	2.65	0.50
1:G:3528:THR:HG23	1:G:3573:MET:HE3	1.93	0.50
1:M:941:MET:HA	1:M:1051:TYR:HA	1.94	0.50
1:S:3156:VAL:HG13	1:S:3157:ILE:N	2.27	0.50
1:A:939:VAL:O	1:A:939:VAL:HG13	2.11	0.50
1:G:4730:ASP:OD1	1:G:4731:ILE:N	2.44	0.50
1:S:941:MET:HA	1:S:1051:TYR:HA	1.94	0.50
1:G:939:VAL:HG13	1:G:939:VAL:O	2.11	0.50
1:S:1869:GLU:OE1	1:S:1869:GLU:N	2.40	0.50
1:G:1046:LEU:HD13	1:G:1046:LEU:C	2.36	0.50
1:G:3283:ARG:NH1	1:G:3287:ARG:CZ	2.75	0.50
1:M:2634:ASN:OD1	1:M:2637:ALA:N	2.44	0.50
1:M:3110:LEU:C	1:M:3110:LEU:HD13	2.37	0.50
1:S:939:VAL:HG13	1:S:939:VAL:O	2.12	0.50
1:G:275:ARG:HD3	1:G:336:PRO:CD	2.42	0.50
1:S:3283:ARG:NH1	1:S:3287:ARG:CZ	2.75	0.50
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.93	0.49
1:G:4767:TRP:O	1:G:4767:TRP:CG	2.65	0.49
1:G:291:LEU:HD11	1:G:299:LEU:HD11	1.93	0.49
1:G:1024:TYR:HE1	1:G:1032:LYS:HG2	1.74	0.49
1:G:3110:LEU:HD13	1:G:3110:LEU:C	2.37	0.49
1:M:233:ILE:HD12	1:M:242:ARG:HB3	1.93	0.49
1:M:275:ARG:HD3	1:M:336:PRO:CD	2.42	0.49
1:M:4767:TRP:O	1:M:4767:TRP:CG	2.65	0.49
1:S:275:ARG:HD3	1:S:336:PRO:CD	2.42	0.49
1:A:275:ARG:HD3	1:A:336:PRO:CD	2.42	0.49
1:A:977:LEU:CD2	1:A:1043:VAL:CG1	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2542:SER:OG	1:G:2594:SER:OG	2.25	0.49
1:G:3105:LYS:O	1:G:3105:LYS:HD3	2.11	0.49
1:M:4066:LEU:HD11	1:M:4173:TYR:CD1	2.47	0.49
1:S:291:LEU:HD11	1:S:299:LEU:HD11	1.93	0.49
1:S:939:VAL:CB	1:S:1053:ILE:HG22	2.43	0.49
1:A:2150:GLU:OE1	1:A:2150:GLU:N	2.44	0.49
1:A:3283:ARG:NH1	1:A:3287:ARG:CZ	2.75	0.49
1:G:2542:SER:HG	1:G:2594:SER:HG	1.57	0.49
1:G:4066:LEU:HD11	1:G:4173:TYR:CE1	2.48	0.49
1:M:2628:PHE:C	1:M:2628:PHE:CD2	2.90	0.49
1:M:4730:ASP:OD1	1:M:4731:ILE:N	2.44	0.49
1:S:4066:LEU:HD11	1:S:4173:TYR:CE1	2.48	0.49
1:A:3110:LEU:HD11	1:A:3183:VAL:CG1	2.43	0.49
1:A:3528:THR:HG23	1:A:3573:MET:HE3	1.93	0.49
1:G:1478:ASP:OD1	1:G:1482:ASN:N	2.45	0.49
1:M:2382:GLU:OE1	1:M:2385:ARG:NH1	2.45	0.49
1:M:3283:ARG:NH1	1:M:3287:ARG:CZ	2.75	0.49
1:M:4066:LEU:HD11	1:M:4173:TYR:CE1	2.48	0.49
1:M:4206:GLU:C	1:M:4207:MET:HE2	2.36	0.49
1:G:941:MET:HA	1:G:1051:TYR:HA	1.94	0.49
1:G:2150:GLU:N	1:G:2150:GLU:OE1	2.44	0.49
1:G:4066:LEU:HD11	1:G:4173:TYR:CD1	2.47	0.49
1:M:939:VAL:HG13	1:M:939:VAL:O	2.11	0.49
1:S:4767:TRP:O	1:S:4767:TRP:CG	2.65	0.49
1:A:941:MET:HA	1:A:1051:TYR:HA	1.94	0.49
1:A:1024:TYR:HE1	1:A:1032:LYS:HG2	1.74	0.49
1:A:2348:GLU:OE1	1:A:2348:GLU:N	2.38	0.49
1:A:2966:TRP:HA	1:A:2969:ILE:HD12	1.95	0.49
1:A:4004:ALA:CB	1:A:4013:LEU:HD22	2.40	0.49
1:G:3110:LEU:HD11	1:G:3183:VAL:CG1	2.43	0.49
1:M:4003:LEU:HD23	1:M:4009:GLN:NE2	2.28	0.49
1:S:2966:TRP:HA	1:S:2969:ILE:HD12	1.95	0.49
1:G:1285:GLU:HB2	1:G:1462:MET:HE1	1.95	0.49
1:M:291:LEU:HD11	1:M:299:LEU:HD11	1.93	0.49
1:M:939:VAL:CB	1:M:1053:ILE:HG22	2.43	0.49
1:S:3110:LEU:HD13	1:S:3110:LEU:C	2.37	0.49
1:S:3110:LEU:HD11	1:S:3183:VAL:CG1	2.43	0.49
1:S:4836:GLN:N	1:S:4836:GLN:OE1	2.44	0.49
1:A:4066:LEU:HD11	1:A:4173:TYR:CD1	2.47	0.49
1:G:1435:TYR:CB	1:G:1575:LEU:HD23	2.41	0.49
1:G:4056:GLU:C	1:G:4060:LYS:HE2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:937:CYS:SG	1:M:984:LEU:CG	3.01	0.49
1:A:939:VAL:CB	1:A:1053:ILE:HG22	2.43	0.49
1:A:1435:TYR:CB	1:A:1575:LEU:HD23	2.41	0.49
1:A:3110:LEU:C	1:A:3110:LEU:HD13	2.37	0.49
1:A:4003:LEU:HD23	1:A:4009:GLN:NE2	2.28	0.49
1:A:4836:GLN:N	1:A:4836:GLN:OE1	2.44	0.49
1:M:1285:GLU:HB2	1:M:1462:MET:HE1	1.95	0.49
1:A:291:LEU:HD11	1:A:299:LEU:HD11	1.93	0.48
1:A:4730:ASP:OD1	1:A:4731:ILE:N	2.44	0.48
1:M:2967:MET:HE3	1:M:2967:MET:HA	1.95	0.48
1:S:977:LEU:CD2	1:S:1043:VAL:CG1	2.91	0.48
1:S:2522:LEU:O	1:S:2522:LEU:HD23	2.13	0.48
1:S:4056:GLU:C	1:S:4060:LYS:HE2	2.38	0.48
1:A:937:CYS:SG	1:A:984:LEU:CG	3.01	0.48
1:A:2628:PHE:C	1:A:2628:PHE:CD2	2.90	0.48
1:G:275:ARG:HD3	1:G:336:PRO:HD2	1.95	0.48
1:G:937:CYS:SG	1:G:984:LEU:CG	3.01	0.48
1:S:4066:LEU:HD11	1:S:4173:TYR:CD1	2.48	0.48
1:A:3156:VAL:HG13	1:A:3157:ILE:N	2.27	0.48
1:A:4066:LEU:HD11	1:A:4173:TYR:CE1	2.48	0.48
1:G:3156:VAL:HG13	1:G:3157:ILE:N	2.27	0.48
1:M:977:LEU:CD2	1:M:1043:VAL:CG1	2.91	0.48
1:S:2628:PHE:C	1:S:2628:PHE:CD2	2.90	0.48
1:A:275:ARG:HD3	1:A:336:PRO:HD2	1.95	0.48
1:G:977:LEU:CD2	1:G:1043:VAL:CG1	2.91	0.48
1:G:4003:LEU:HD23	1:G:4009:GLN:NE2	2.28	0.48
1:M:3428:ASN:OD1	1:M:3429:ALA:N	2.46	0.48
1:S:3514:LEU:HD13	1:S:3514:LEU:O	2.14	0.48
1:A:4911:LEU:HA	1:A:4914:VAL:HG22	1.95	0.48
1:G:939:VAL:CB	1:G:1053:ILE:HG22	2.43	0.48
1:G:2522:LEU:O	1:G:2522:LEU:HD23	2.13	0.48
1:G:3169:LEU:HD13	1:G:3194:LEU:HD11	1.95	0.48
1:M:46:LEU:HD11	1:M:134:ASP:HB3	1.96	0.48
1:A:1285:GLU:HB2	1:A:1462:MET:HE1	1.95	0.48
1:A:3428:ASN:OD1	1:A:3429:ALA:N	2.46	0.48
1:A:4056:GLU:C	1:A:4060:LYS:HE2	2.38	0.48
1:G:3514:LEU:HD13	1:G:3514:LEU:O	2.14	0.48
1:M:2966:TRP:HA	1:M:2969:ILE:HD12	1.95	0.48
1:M:3110:LEU:HD11	1:M:3183:VAL:CG1	2.42	0.48
1:A:3514:LEU:HD13	1:A:3514:LEU:O	2.14	0.48
1:G:2628:PHE:CD2	1:G:2628:PHE:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3428:ASN:OD1	1:G:3429:ALA:N	2.46	0.48
1:S:937:CYS:SG	1:S:984:LEU:CG	3.01	0.48
1:A:2967:MET:HE3	1:A:2967:MET:HA	1.95	0.48
1:M:977:LEU:HD21	1:M:1043:VAL:CG1	2.44	0.48
1:M:2522:LEU:HD23	1:M:2522:LEU:O	2.13	0.48
1:S:3428:ASN:OD1	1:S:3429:ALA:N	2.46	0.48
1:A:1478:ASP:OD1	1:A:1482:ASN:N	2.45	0.48
1:G:2966:TRP:HA	1:G:2969:ILE:HD12	1.95	0.48
1:A:2522:LEU:HD23	1:A:2522:LEU:O	2.13	0.48
1:S:1285:GLU:HB2	1:S:1462:MET:HE1	1.95	0.48
1:A:977:LEU:HD21	1:A:1043:VAL:CG1	2.44	0.47
1:A:2368:LEU:HD11	1:A:2376:LEU:HD11	1.96	0.47
1:A:3157:ILE:C	1:A:3158:LEU:HD22	2.39	0.47
1:A:3169:LEU:HD13	1:A:3194:LEU:HD11	1.95	0.47
1:A:3528:THR:HG23	1:A:3573:MET:CE	2.44	0.47
1:G:2368:LEU:HD11	1:G:2376:LEU:HD11	1.96	0.47
1:G:4901:ILE:HG22	1:G:4902:GLU:N	2.29	0.47
1:S:46:LEU:HD11	1:S:134:ASP:HB3	1.96	0.47
1:S:275:ARG:HD3	1:S:336:PRO:HD2	1.95	0.47
1:A:46:LEU:HD11	1:A:134:ASP:HB3	1.96	0.47
1:A:4901:ILE:HG22	1:A:4902:GLU:N	2.29	0.47
1:G:4911:LEU:HA	1:G:4914:VAL:HG22	1.95	0.47
1:M:4056:GLU:C	1:M:4060:LYS:HE2	2.38	0.47
1:M:4911:LEU:HA	1:M:4914:VAL:HG22	1.95	0.47
1:S:937:CYS:SG	1:S:984:LEU:CD2	3.02	0.47
1:S:2382:GLU:OE1	1:S:2385:ARG:NH1	2.45	0.47
1:S:4003:LEU:HD23	1:S:4009:GLN:NE2	2.28	0.47
1:G:977:LEU:HD21	1:G:1043:VAL:CG1	2.44	0.47
1:M:3528:THR:HG23	1:M:3573:MET:CE	2.44	0.47
1:S:1180:ARG:HB2	1:S:1180:ARG:NH1	2.29	0.47
1:S:1561:VAL:O	1:S:1562:ILE:HD13	2.14	0.47
1:A:2131:LEU:C	1:A:2131:LEU:HD12	2.40	0.47
1:A:2382:GLU:OE1	1:A:2385:ARG:NH1	2.45	0.47
1:M:275:ARG:HD3	1:M:336:PRO:HD2	1.95	0.47
1:M:2131:LEU:C	1:M:2131:LEU:HD12	2.40	0.47
1:M:4702:ASP:O	1:M:4705:VAL:HG12	2.15	0.47
1:A:3459:VAL:HG23	1:A:3464:ILE:CG2	2.44	0.47
1:G:1180:ARG:HB2	1:G:1180:ARG:NH1	2.29	0.47
1:G:3157:ILE:C	1:G:3158:LEU:HD22	2.39	0.47
1:G:3409:TYR:CE1	1:G:3513:THR:HG21	2.50	0.47
1:M:1825:HIS:CD2	1:S:3567:PRO:CB	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:977:LEU:HD21	1:S:1043:VAL:CG1	2.44	0.47
1:S:3157:ILE:C	1:S:3158:LEU:HD22	2.39	0.47
1:A:1825:HIS:CD2	1:G:3567:PRO:CB	2.98	0.47
1:M:3283:ARG:HH12	1:M:3287:ARG:NH2	2.12	0.47
1:A:941:MET:HE3	1:A:944:GLU:OE2	2.14	0.47
1:A:1180:ARG:NH1	1:A:1180:ARG:HB2	2.29	0.47
1:A:3539:ARG:NH1	1:A:3552:PHE:CE2	2.83	0.47
1:A:3567:PRO:CB	1:S:1825:HIS:CD2	2.98	0.47
1:A:4666:VAL:N	1:A:4667:PRO:HD2	2.30	0.47
1:G:46:LEU:HD11	1:G:134:ASP:HB3	1.96	0.47
1:G:380:GLN:OE1	1:G:380:GLN:N	2.47	0.47
1:G:941:MET:HE3	1:G:944:GLU:OE2	2.14	0.47
1:G:2382:GLU:OE1	1:G:2385:ARG:NH1	2.45	0.47
1:G:2967:MET:HE3	1:G:2967:MET:HA	1.95	0.47
1:G:3283:ARG:HH12	1:G:3287:ARG:NH2	2.12	0.47
1:G:3539:ARG:NH1	1:G:3552:PHE:CE2	2.83	0.47
1:G:3753:PHE:HZ	1:G:4719:PHE:HZ	1.61	0.47
1:G:4702:ASP:O	1:G:4705:VAL:HG12	2.15	0.47
1:M:941:MET:HE3	1:M:944:GLU:OE2	2.15	0.47
1:M:3157:ILE:C	1:M:3158:LEU:HD22	2.39	0.47
1:M:3409:TYR:CE1	1:M:3513:THR:HG21	2.50	0.47
1:S:941:MET:HE3	1:S:944:GLU:OE2	2.15	0.47
1:S:1478:ASP:OD1	1:S:1482:ASN:N	2.45	0.47
1:S:3283:ARG:HH12	1:S:3287:ARG:NH2	2.12	0.47
1:S:4666:VAL:N	1:S:4667:PRO:HD2	2.30	0.47
1:S:4911:LEU:HA	1:S:4914:VAL:HG22	1.95	0.47
1:G:937:CYS:SG	1:G:984:LEU:CD2	3.03	0.47
1:G:1561:VAL:O	1:G:1562:ILE:HD13	2.14	0.47
1:G:4004:ALA:CB	1:G:4013:LEU:HD22	2.40	0.47
1:G:4666:VAL:N	1:G:4667:PRO:HD2	2.30	0.47
1:M:3514:LEU:HD13	1:M:3514:LEU:O	2.14	0.47
1:S:2368:LEU:HD11	1:S:2376:LEU:HD11	1.96	0.47
1:S:2967:MET:HE3	1:S:2967:MET:HA	1.95	0.47
1:A:977:LEU:CD2	1:A:1043:VAL:HG12	2.45	0.47
1:A:2522:LEU:HD23	1:A:2522:LEU:C	2.40	0.47
1:G:3528:THR:HG23	1:G:3573:MET:CE	2.44	0.47
1:M:2368:LEU:HD11	1:M:2376:LEU:HD11	1.96	0.47
1:M:3753:PHE:HZ	1:M:4719:PHE:HZ	1.61	0.47
1:A:4058:ILE:O	1:A:4061:PHE:HB3	2.15	0.47
1:M:1561:VAL:O	1:M:1562:ILE:HD13	2.14	0.47
1:S:4901:ILE:HG22	1:S:4902:GLU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLN:OE1	1:A:380:GLN:N	2.47	0.46
1:A:1561:VAL:O	1:A:1562:ILE:HD13	2.14	0.46
1:A:3283:ARG:HH12	1:A:3287:ARG:NH2	2.12	0.46
1:A:3941:ASP:O	1:A:4002:LYS:NZ	2.48	0.46
1:G:2131:LEU:HD12	1:G:2131:LEU:C	2.40	0.46
1:M:275:ARG:CD	1:M:336:PRO:HG2	2.36	0.46
1:M:937:CYS:SG	1:M:984:LEU:CD2	3.03	0.46
1:M:1180:ARG:NH1	1:M:1180:ARG:HB2	2.29	0.46
1:S:275:ARG:CD	1:S:336:PRO:HG2	2.36	0.46
1:A:937:CYS:SG	1:A:984:LEU:CD2	3.03	0.46
1:A:3409:TYR:CE1	1:A:3513:THR:HG21	2.50	0.46
1:G:4658:ILE:HD12	1:G:4796:MET:HE3	1.97	0.46
1:M:977:LEU:CD2	1:M:1043:VAL:HG12	2.45	0.46
1:M:2862:LEU:HD11	1:M:2932:MET:HE1	1.97	0.46
1:M:3941:ASP:O	1:M:4002:LYS:NZ	2.48	0.46
1:A:1869:GLU:OE1	1:A:1869:GLU:N	2.40	0.46
1:A:2302:LEU:HD23	1:A:2302:LEU:O	2.16	0.46
1:G:977:LEU:CD2	1:G:1043:VAL:HG12	2.45	0.46
1:M:1435:TYR:CB	1:M:1575:LEU:HD23	2.41	0.46
1:M:3539:ARG:NH1	1:M:3552:PHE:CE2	2.83	0.46
1:S:977:LEU:CD2	1:S:1043:VAL:HG12	2.45	0.46
1:S:3528:THR:HG23	1:S:3573:MET:CE	2.44	0.46
1:S:3539:ARG:NH1	1:S:3552:PHE:CE2	2.83	0.46
1:S:4702:ASP:O	1:S:4705:VAL:HG12	2.15	0.46
1:A:3999:MET:HG3	1:A:4003:LEU:HD11	1.98	0.46
1:S:2131:LEU:HD12	1:S:2131:LEU:C	2.40	0.46
1:S:3156:VAL:HG13	1:S:3157:ILE:HG13	1.98	0.46
1:A:4658:ILE:HD12	1:A:4796:MET:HE3	1.97	0.46
1:G:2302:LEU:O	1:G:2302:LEU:HD23	2.16	0.46
1:G:4705:VAL:HG22	1:G:4705:VAL:O	2.15	0.46
1:M:1024:TYR:HE1	1:M:1032:LYS:HG2	1.74	0.46
1:M:3156:VAL:HG13	1:M:3157:ILE:HG13	1.98	0.46
1:S:2348:GLU:OE1	1:S:2348:GLU:N	2.38	0.46
1:S:2522:LEU:HD23	1:S:2522:LEU:C	2.40	0.46
1:A:992:GLY:O	1:A:995:VAL:HG12	2.16	0.46
1:A:2825:LYS:HE3	1:A:2827:ARG:O	2.16	0.46
1:A:4580:TYR:O	1:S:4878:ASP:OD1	2.34	0.46
1:A:4702:ASP:O	1:A:4705:VAL:HG12	2.15	0.46
1:G:156:GLN:OE1	1:G:156:GLN:N	2.48	0.46
1:G:992:GLY:O	1:G:995:VAL:HG12	2.16	0.46
1:G:2522:LEU:HD23	1:G:2522:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4878:ASP:OD1	1:M:4580:TYR:O	2.34	0.46
1:A:2862:LEU:HD11	1:A:2932:MET:HE1	1.97	0.46
1:G:2897:LYS:O	1:G:2897:LYS:HG2	2.16	0.46
1:G:4058:ILE:O	1:G:4061:PHE:HB3	2.15	0.46
1:M:992:GLY:O	1:M:995:VAL:HG12	2.16	0.46
1:S:2825:LYS:HE3	1:S:2827:ARG:O	2.16	0.46
1:S:4658:ILE:HD12	1:S:4796:MET:HE3	1.97	0.46
1:M:1478:ASP:OD1	1:M:1482:ASN:N	2.45	0.46
1:M:2825:LYS:HE3	1:M:2827:ARG:O	2.16	0.46
1:S:3409:TYR:CE1	1:S:3513:THR:HG21	2.50	0.46
1:S:4058:ILE:O	1:S:4061:PHE:HB3	2.15	0.46
1:G:3999:MET:HG3	1:G:4003:LEU:HD11	1.98	0.46
1:M:2522:LEU:HD23	1:M:2522:LEU:C	2.40	0.46
1:M:4705:VAL:O	1:M:4705:VAL:HG22	2.15	0.46
1:M:4785:THR:O	1:M:4785:THR:HG22	2.16	0.46
1:S:4039:MET:HE3	1:S:4043:GLN:OE1	2.15	0.46
1:S:4785:THR:HG22	1:S:4785:THR:O	2.16	0.46
1:A:1690:ASP:OD1	1:A:1692:ALA:N	2.49	0.46
1:A:4705:VAL:O	1:A:4705:VAL:HG22	2.15	0.46
1:S:992:GLY:O	1:S:995:VAL:HG12	2.16	0.46
1:S:2161:GLN:NE2	1:S:2177:LEU:HD12	2.31	0.46
1:G:1825:HIS:CD2	1:M:3567:PRO:CB	2.98	0.45
1:G:2161:GLN:NE2	1:G:2177:LEU:HD12	2.31	0.45
1:G:2825:LYS:HE3	1:G:2827:ARG:O	2.16	0.45
1:G:4039:MET:HE3	1:G:4043:GLN:OE1	2.15	0.45
1:M:2897:LYS:HG2	1:M:2897:LYS:O	2.16	0.45
1:S:1435:TYR:CB	1:S:1575:LEU:HD23	2.41	0.45
1:S:2897:LYS:O	1:S:2897:LYS:HG2	2.16	0.45
1:A:2897:LYS:O	1:A:2897:LYS:HG2	2.16	0.45
1:A:4878:ASP:OD1	1:G:4580:TYR:O	2.33	0.45
1:G:3222:LYS:O	1:G:3227:ARG:NH1	2.49	0.45
1:M:1575:LEU:HD12	1:M:1575:LEU:C	2.42	0.45
1:M:2302:LEU:HD23	1:M:2302:LEU:O	2.16	0.45
1:M:4666:VAL:N	1:M:4667:PRO:HD2	2.30	0.45
1:M:4878:ASP:OD1	1:S:4580:TYR:O	2.33	0.45
1:M:4901:ILE:HG22	1:M:4902:GLU:N	2.30	0.45
1:S:1575:LEU:C	1:S:1575:LEU:HD12	2.42	0.45
1:S:3169:LEU:HD11	1:S:3194:LEU:HD11	1.96	0.45
1:M:4039:MET:HE3	1:M:4043:GLN:OE1	2.15	0.45
1:M:4058:ILE:O	1:M:4061:PHE:HB3	2.15	0.45
1:A:1575:LEU:HD12	1:A:1575:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2822:THR:OG1	1:A:2938:THR:OG1	2.34	0.45
1:A:3222:LYS:O	1:A:3227:ARG:NH1	2.49	0.45
1:S:3222:LYS:O	1:S:3227:ARG:NH1	2.49	0.45
1:S:4705:VAL:HG22	1:S:4705:VAL:O	2.15	0.45
1:A:2237:CYS:SG	1:A:2275:VAL:HG12	2.57	0.45
1:G:2212:VAL:HG11	1:G:2256:TYR:CZ	2.52	0.45
1:G:2237:CYS:SG	1:G:2275:VAL:HG12	2.57	0.45
1:G:2862:LEU:HD11	1:G:2932:MET:HE1	1.97	0.45
1:G:3941:ASP:O	1:G:4002:LYS:NZ	2.48	0.45
1:M:156:GLN:OE1	1:M:156:GLN:N	2.48	0.45
1:M:3222:LYS:O	1:M:3227:ARG:NH1	2.49	0.45
1:M:3663:LEU:HD12	1:M:3663:LEU:C	2.42	0.45
1:M:4203:ALA:O	1:M:4207:MET:HE3	2.16	0.45
1:M:4658:ILE:HD12	1:M:4796:MET:HE3	1.97	0.45
1:S:294:THR:O	1:S:298:GLY:N	2.46	0.45
1:S:2023:LEU:HB3	1:S:2024:PRO:HD2	1.99	0.45
1:G:772:ASN:HD21	1:G:1470:ARG:HA	1.82	0.45
1:G:4203:ALA:O	1:G:4207:MET:HE3	2.16	0.45
1:M:2822:THR:OG1	1:M:2938:THR:OG1	2.35	0.45
1:M:4004:ALA:CB	1:M:4013:LEU:HD22	2.40	0.45
1:S:2862:LEU:HD11	1:S:2932:MET:HE1	1.97	0.45
1:S:3999:MET:HG3	1:S:4003:LEU:HD11	1.98	0.45
1:A:772:ASN:HD21	1:A:1470:ARG:HA	1.82	0.45
1:A:2023:LEU:HB3	1:A:2024:PRO:HD2	1.99	0.45
1:A:4203:ALA:O	1:A:4207:MET:HE3	2.16	0.45
1:A:4785:THR:O	1:A:4785:THR:HG22	2.16	0.45
1:G:3081:MET:HE1	1:G:3092:LEU:HD23	1.99	0.45
1:S:4203:ALA:O	1:S:4207:MET:HE3	2.16	0.45
1:G:1869:GLU:OE1	1:G:1869:GLU:N	2.40	0.45
1:M:3999:MET:HG3	1:M:4003:LEU:HD11	1.98	0.45
1:S:2302:LEU:O	1:S:2302:LEU:HD23	2.16	0.45
1:A:3663:LEU:C	1:A:3663:LEU:HD12	2.42	0.45
1:G:1478:ASP:OD1	1:G:1481:GLY:N	2.50	0.45
1:G:1575:LEU:C	1:G:1575:LEU:HD12	2.42	0.45
1:M:3459:VAL:HG23	1:M:3464:ILE:CG2	2.44	0.45
1:S:774:ASP:OD1	1:S:774:ASP:N	2.50	0.45
1:A:1439:VAL:HG13	1:A:1439:VAL:O	2.17	0.45
1:A:2212:VAL:HG11	1:A:2256:TYR:CZ	2.52	0.45
1:A:3105:LYS:HD3	1:A:3105:LYS:C	2.42	0.45
1:A:4773:VAL:HG22	1:A:4777:ILE:HD11	1.99	0.45
1:G:3156:VAL:HG13	1:G:3157:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3366:ARG:HA	1:G:3441:ILE:HD11	1.99	0.45
1:A:2161:GLN:NE2	1:A:2177:LEU:HD12	2.31	0.44
1:G:294:THR:O	1:G:298:GLY:N	2.46	0.44
1:G:372:LEU:HD13	1:G:372:LEU:O	2.18	0.44
1:G:2768:PHE:O	1:G:2772:GLN:HG2	2.17	0.44
1:G:4900:GLU:O	1:G:4901:ILE:HD13	2.17	0.44
1:M:2161:GLN:NE2	1:M:2177:LEU:HD12	2.31	0.44
1:M:2212:VAL:HG11	1:M:2256:TYR:CZ	2.52	0.44
1:M:3050:VAL:O	1:M:3050:VAL:HG12	2.17	0.44
1:M:3366:ARG:HA	1:M:3441:ILE:HD11	1.99	0.44
1:S:2212:VAL:HG11	1:S:2256:TYR:CZ	2.52	0.44
1:S:2237:CYS:SG	1:S:2275:VAL:HG12	2.57	0.44
1:A:1478:ASP:OD1	1:A:1481:GLY:N	2.50	0.44
1:A:3156:VAL:HG13	1:A:3157:ILE:HG13	1.98	0.44
1:A:4039:MET:HE3	1:A:4043:GLN:OE1	2.15	0.44
1:G:1690:ASP:OD1	1:G:1692:ALA:N	2.49	0.44
1:G:4773:VAL:HG22	1:G:4777:ILE:HD11	1.99	0.44
1:M:1439:VAL:O	1:M:1439:VAL:HG13	2.17	0.44
1:M:1690:ASP:OD1	1:M:1692:ALA:N	2.49	0.44
1:S:1690:ASP:OD1	1:S:1692:ALA:N	2.49	0.44
1:S:4773:VAL:HG22	1:S:4777:ILE:HD11	1.99	0.44
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.99	0.44
1:G:2822:THR:OG1	1:G:2938:THR:OG1	2.35	0.44
1:G:3158:LEU:HD22	1:G:3158:LEU:N	2.33	0.44
1:G:3319:ILE:HD11	1:G:3338:LEU:HD21	2.00	0.44
1:M:2763:HIS:HE1	1:M:2790:MET:O	2.01	0.44
1:S:179:TYR:N	1:S:194:SER:O	2.50	0.44
1:S:3663:LEU:C	1:S:3663:LEU:HD12	2.42	0.44
1:A:2351:ASN:O	1:A:2355:ARG:HG3	2.18	0.44
1:A:3081:MET:HE1	1:A:3092:LEU:HD23	1.99	0.44
1:A:3655:GLU:O	1:A:3655:GLU:OE1	2.35	0.44
1:G:179:TYR:N	1:G:194:SER:O	2.51	0.44
1:M:3655:GLU:O	1:M:3655:GLU:OE1	2.35	0.44
1:M:2237:CYS:SG	1:M:2275:VAL:HG12	2.57	0.44
1:M:3081:MET:HE1	1:M:3092:LEU:HD23	1.99	0.44
1:M:4900:GLU:O	1:M:4901:ILE:HD13	2.17	0.44
1:S:3050:VAL:O	1:S:3050:VAL:HG12	2.17	0.44
1:A:2768:PHE:O	1:A:2772:GLN:HG2	2.17	0.44
1:A:3319:ILE:HD11	1:A:3338:LEU:HD21	2.00	0.44
1:A:4900:GLU:O	1:A:4901:ILE:HD13	2.17	0.44
1:G:3062:PRO:HA	1:G:3065:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3655:GLU:OE1	1:G:3655:GLU:O	2.35	0.44
1:G:4785:THR:HG22	1:G:4785:THR:O	2.16	0.44
1:M:380:GLN:OE1	1:M:380:GLN:N	2.47	0.44
1:S:156:GLN:OE1	1:S:156:GLN:N	2.48	0.44
1:S:2768:PHE:O	1:S:2772:GLN:HG2	2.17	0.44
1:S:3105:LYS:HD3	1:S:3105:LYS:C	2.42	0.44
1:S:3158:LEU:HD22	1:S:3158:LEU:N	2.33	0.44
1:S:3655:GLU:OE1	1:S:3655:GLU:O	2.35	0.44
1:A:1144:GLN:N	1:A:1147:ASP:OD2	2.47	0.44
1:A:2763:HIS:HE1	1:A:2790:MET:O	2.01	0.44
1:A:3232:LEU:HD22	1:A:3232:LEU:N	2.33	0.44
1:A:3366:ARG:HA	1:A:3441:ILE:HD11	1.99	0.44
1:G:515:TRP:O	1:G:519:VAL:HG23	2.18	0.44
1:M:372:LEU:HD13	1:M:372:LEU:O	2.18	0.44
1:M:3169:LEU:HD13	1:M:3194:LEU:HD11	1.95	0.44
1:S:3105:LYS:HE2	1:S:3105:LYS:HA	2.00	0.44
1:A:3050:VAL:HG12	1:A:3050:VAL:O	2.17	0.44
1:G:1439:VAL:HG13	1:G:1439:VAL:O	2.17	0.44
1:G:3105:LYS:HD3	1:G:3105:LYS:C	2.42	0.44
1:G:3232:LEU:N	1:G:3232:LEU:HD22	2.33	0.44
1:S:772:ASN:HD21	1:S:1470:ARG:HA	1.82	0.44
1:S:1478:ASP:OD1	1:S:1481:GLY:N	2.50	0.44
1:S:2351:ASN:O	1:S:2355:ARG:HG3	2.18	0.44
1:A:372:LEU:HD13	1:A:372:LEU:O	2.18	0.44
1:A:774:ASP:N	1:A:774:ASP:OD1	2.50	0.44
1:M:1478:ASP:OD1	1:M:1481:GLY:N	2.50	0.44
1:M:2768:PHE:O	1:M:2772:GLN:HG2	2.18	0.44
1:S:372:LEU:HD13	1:S:372:LEU:O	2.18	0.44
1:S:2874:MET:HE1	1:S:2937:VAL:HG12	2.00	0.44
1:S:3003:LEU:HB2	1:S:3004:PRO:HD3	2.00	0.44
1:S:3366:ARG:HA	1:S:3441:ILE:HD11	1.99	0.44
1:S:3539:ARG:NH1	1:S:3552:PHE:CD2	2.86	0.44
1:S:3941:ASP:O	1:S:4002:LYS:NZ	2.48	0.44
1:A:179:TYR:N	1:A:194:SER:O	2.51	0.43
1:A:3158:LEU:HD22	1:A:3158:LEU:N	2.33	0.43
1:G:590:LEU:HD13	1:G:599:VAL:HB	2.00	0.43
1:G:2023:LEU:HB3	1:G:2024:PRO:HD2	1.99	0.43
1:G:3663:LEU:C	1:G:3663:LEU:HD12	2.42	0.43
1:M:772:ASN:HD21	1:M:1470:ARG:HA	1.82	0.43
1:S:380:GLN:OE1	1:S:380:GLN:N	2.47	0.43
1:A:515:TRP:O	1:A:519:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:VAL:CB	1:A:1053:ILE:CG2	2.97	0.43
1:A:3169:LEU:HD11	1:A:3194:LEU:HD11	1.96	0.43
1:M:3169:LEU:HD11	1:M:3194:LEU:HD11	1.96	0.43
1:S:3152:PHE:O	1:S:3156:VAL:HG12	2.18	0.43
1:G:2204:HIS:O	1:G:2208:MET:HG3	2.18	0.43
1:M:939:VAL:CB	1:M:1053:ILE:CG2	2.96	0.43
1:M:2023:LEU:HB3	1:M:2024:PRO:HD2	1.99	0.43
1:M:3105:LYS:HD3	1:M:3105:LYS:C	2.42	0.43
1:M:3539:ARG:NH1	1:M:3552:PHE:CD2	2.86	0.43
1:S:3062:PRO:HA	1:S:3065:VAL:HG22	1.99	0.43
1:S:4900:GLU:O	1:S:4901:ILE:HD13	2.17	0.43
1:G:3003:LEU:HB2	1:G:3004:PRO:HD3	2.00	0.43
1:G:3050:VAL:O	1:G:3050:VAL:HG12	2.17	0.43
1:M:590:LEU:HD13	1:M:599:VAL:HB	2.00	0.43
1:M:4244:GLU:OE1	1:M:4668:LEU:HD22	2.18	0.43
1:S:234:SER:HB2	1:S:242:ARG:HG2	2.00	0.43
1:S:1448:VAL:HG22	1:S:1554:VAL:HG23	2.01	0.43
1:S:1935:VAL:O	1:S:1939:MET:HG2	2.18	0.43
1:A:2204:HIS:O	1:A:2208:MET:HG3	2.18	0.43
1:A:3105:LYS:HE2	1:A:3105:LYS:HA	2.00	0.43
1:A:3152:PHE:O	1:A:3156:VAL:HG12	2.18	0.43
1:A:4244:GLU:OE1	1:A:4668:LEU:HD22	2.18	0.43
1:G:1935:VAL:O	1:G:1939:MET:HG2	2.18	0.43
1:G:4244:GLU:OE1	1:G:4668:LEU:HD22	2.19	0.43
1:M:3003:LEU:HB2	1:M:3004:PRO:HD3	2.00	0.43
1:M:3062:PRO:HA	1:M:3065:VAL:HG22	1.99	0.43
1:M:3158:LEU:HD22	1:M:3158:LEU:N	2.33	0.43
1:M:4773:VAL:HG22	1:M:4777:ILE:HD11	1.99	0.43
1:S:1439:VAL:O	1:S:1439:VAL:HG13	2.17	0.43
1:M:515:TRP:O	1:M:519:VAL:HG23	2.18	0.43
1:M:4134:GLU:HB3	1:M:4135:PRO:HD3	2.01	0.43
1:S:1221:GLU:N	1:S:1221:GLU:OE1	2.52	0.43
1:S:2204:HIS:O	1:S:2208:MET:HG3	2.18	0.43
1:S:2763:HIS:HE1	1:S:2790:MET:O	2.01	0.43
1:S:3081:MET:HE1	1:S:3092:LEU:HD23	1.99	0.43
1:G:2351:ASN:O	1:G:2355:ARG:HG3	2.18	0.43
1:M:179:TYR:N	1:M:194:SER:O	2.51	0.43
1:M:234:SER:HB2	1:M:242:ARG:HG2	2.00	0.43
1:M:2204:HIS:O	1:M:2208:MET:HG3	2.18	0.43
1:S:4134:GLU:HB3	1:S:4135:PRO:HD3	2.01	0.43
1:A:234:SER:HB2	1:A:242:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1924:GLU:N	1:A:1924:GLU:OE1	2.52	0.43
1:A:4655:PHE:N	1:A:4796:MET:HE1	2.34	0.43
1:G:3719:ASP:OD1	1:G:3719:ASP:O	2.37	0.43
1:M:1935:VAL:O	1:M:1939:MET:HG2	2.18	0.43
1:M:3152:PHE:O	1:M:3156:VAL:HG12	2.18	0.43
1:M:4655:PHE:N	1:M:4796:MET:HE1	2.34	0.43
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	2.01	0.43
1:G:234:SER:HB2	1:G:242:ARG:HG2	2.00	0.43
1:G:2763:HIS:HE1	1:G:2790:MET:O	2.01	0.43
1:G:3539:ARG:NH1	1:G:3552:PHE:CD2	2.86	0.43
1:G:4655:PHE:N	1:G:4796:MET:HE1	2.34	0.43
1:M:1448:VAL:HG22	1:M:1554:VAL:HG23	2.01	0.43
1:M:3232:LEU:N	1:M:3232:LEU:HD22	2.33	0.43
1:S:3169:LEU:HD13	1:S:3194:LEU:HD11	1.95	0.43
1:S:3719:ASP:O	1:S:3719:ASP:OD1	2.37	0.43
1:A:707:VAL:HG23	1:A:782:SER:CB	2.48	0.43
1:A:1935:VAL:O	1:A:1939:MET:HG2	2.18	0.43
1:G:707:VAL:HG23	1:G:782:SER:CB	2.48	0.43
1:G:774:ASP:OD1	1:G:774:ASP:N	2.50	0.43
1:G:1101:ARG:NH1	1:G:1115:LEU:O	2.52	0.43
1:G:1924:GLU:N	1:G:1924:GLU:OE1	2.52	0.43
1:G:4134:GLU:HB3	1:G:4135:PRO:HD3	2.01	0.43
1:M:707:VAL:HG23	1:M:782:SER:CB	2.48	0.43
1:S:4244:GLU:OE1	1:S:4668:LEU:HD22	2.19	0.43
1:A:34:LYS:HA	1:A:34:LYS:CE	2.49	0.42
1:A:156:GLN:OE1	1:A:156:GLN:N	2.48	0.42
1:A:2346:VAL:HG13	1:A:2346:VAL:O	2.19	0.42
1:A:3539:ARG:NH1	1:A:3552:PHE:CD2	2.86	0.42
1:A:4063:ASP:OD1	1:A:4064:MET:N	2.52	0.42
1:A:4134:GLU:HB3	1:A:4135:PRO:HD3	2.01	0.42
1:G:3105:LYS:HE2	1:G:3105:LYS:HA	2.00	0.42
1:G:3152:PHE:O	1:G:3156:VAL:HG12	2.18	0.42
1:M:864:PRO:CG	1:M:867:LEU:HD12	2.49	0.42
1:M:3719:ASP:OD1	1:M:3719:ASP:O	2.37	0.42
1:S:590:LEU:HD13	1:S:599:VAL:HB	2.00	0.42
1:S:937:CYS:SG	1:S:984:LEU:HD21	2.59	0.42
1:S:939:VAL:CB	1:S:1053:ILE:CG2	2.97	0.42
1:S:3232:LEU:N	1:S:3232:LEU:HD22	2.33	0.42
1:S:3319:ILE:HD11	1:S:3338:LEU:HD21	2.00	0.42
1:S:3365:LEU:HD21	1:S:3405:LEU:HD23	2.01	0.42
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3610:GLU:OE1	1:A:3610:GLU:N	2.52	0.42
1:G:864:PRO:CG	1:G:867:LEU:HD12	2.50	0.42
1:G:939:VAL:CB	1:G:1053:ILE:CG2	2.97	0.42
1:G:1448:VAL:HG22	1:G:1554:VAL:HG23	2.01	0.42
1:G:3365:LEU:HD21	1:G:3405:LEU:HD23	2.01	0.42
1:S:33:LEU:HD11	1:S:35:LEU:CD1	2.47	0.42
1:S:515:TRP:O	1:S:519:VAL:HG23	2.18	0.42
1:G:2265:LEU:O	1:G:2266:GLY:C	2.63	0.42
1:M:21:VAL:HG12	1:M:66:CYS:HA	2.01	0.42
1:M:680:THR:HG22	1:M:681:HIS:N	2.34	0.42
1:M:774:ASP:OD1	1:M:774:ASP:N	2.50	0.42
1:S:4655:PHE:N	1:S:4796:MET:HE1	2.34	0.42
1:S:4880:MET:HE2	1:S:4880:MET:HB2	1.97	0.42
1:A:2874:MET:HE1	1:A:2937:VAL:HG12	2.00	0.42
1:A:3365:LEU:HD21	1:A:3405:LEU:HD23	2.01	0.42
1:A:3719:ASP:OD1	1:A:3719:ASP:O	2.37	0.42
1:G:2874:MET:HE1	1:G:2937:VAL:HG12	2.00	0.42
1:M:937:CYS:SG	1:M:984:LEU:HD21	2.59	0.42
1:M:1221:GLU:OE1	1:M:1221:GLU:N	2.52	0.42
1:M:4063:ASP:OD1	1:M:4064:MET:N	2.52	0.42
1:M:5000:GLU:OE1	1:M:5000:GLU:N	2.50	0.42
1:S:3917:ILE:HD13	1:S:3917:ILE:N	2.34	0.42
1:G:1221:GLU:N	1:G:1221:GLU:OE1	2.52	0.42
1:G:3110:LEU:HD12	1:G:3175:LEU:HD21	2.02	0.42
1:G:3459:VAL:HG23	1:G:3464:ILE:CG2	2.44	0.42
1:G:4063:ASP:OD1	1:G:4064:MET:N	2.52	0.42
1:M:2351:ASN:O	1:M:2355:ARG:HG3	2.18	0.42
1:S:2822:THR:OG1	1:S:2938:THR:OG1	2.35	0.42
1:A:590:LEU:HD13	1:A:599:VAL:HB	2.00	0.42
1:A:937:CYS:SG	1:A:984:LEU:HD21	2.59	0.42
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.52	0.42
1:A:2750:LYS:HG2	1:A:2750:LYS:O	2.19	0.42
1:G:3917:ILE:N	1:G:3917:ILE:HD13	2.34	0.42
1:M:1924:GLU:N	1:M:1924:GLU:OE1	2.52	0.42
1:M:2874:MET:HE1	1:M:2937:VAL:HG12	2.00	0.42
1:S:34:LYS:HA	1:S:34:LYS:CE	2.49	0.42
1:S:1101:ARG:NH1	1:S:1115:LEU:O	2.52	0.42
1:S:4063:ASP:OD1	1:S:4064:MET:N	2.52	0.42
1:A:3917:ILE:HD13	1:A:3917:ILE:N	2.34	0.42
1:G:33:LEU:HD11	1:G:35:LEU:CD1	2.47	0.42
1:G:2178:MET:SD	1:G:2210:VAL:HG11	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2967:MET:HE3	1:G:2967:MET:CA	2.49	0.42
1:M:3319:ILE:HD11	1:M:3338:LEU:HD21	2.00	0.42
1:S:4887:MET:HE3	1:S:4887:MET:HB3	1.97	0.42
1:A:1221:GLU:OE1	1:A:1221:GLU:N	2.52	0.42
1:A:2178:MET:SD	1:A:2210:VAL:HG11	2.60	0.42
1:A:2630:VAL:N	1:A:2631:PRO:HD2	2.35	0.42
1:G:21:VAL:HG12	1:G:66:CYS:HA	2.01	0.42
1:G:680:THR:HG22	1:G:681:HIS:N	2.34	0.42
1:G:2750:LYS:O	1:G:2750:LYS:HG2	2.20	0.42
1:M:2265:LEU:O	1:M:2266:GLY:C	2.62	0.42
1:M:2346:VAL:O	1:M:2346:VAL:HG13	2.19	0.42
1:A:455:PRO:HG3	1:A:467:LYS:HB3	2.02	0.42
1:A:680:THR:HG22	1:A:681:HIS:N	2.34	0.42
1:A:2967:MET:HE3	1:A:2967:MET:CA	2.49	0.42
1:A:3753:PHE:O	1:A:3757:GLU:HG2	2.20	0.42
1:G:2346:VAL:HG13	1:G:2346:VAL:O	2.19	0.42
1:G:2628:PHE:HD1	1:G:2907:PRO:CG	2.33	0.42
1:M:3110:LEU:HD12	1:M:3175:LEU:HD21	2.02	0.42
1:M:3917:ILE:HD13	1:M:3917:ILE:N	2.34	0.42
1:S:680:THR:HG22	1:S:681:HIS:N	2.34	0.42
1:S:2178:MET:SD	1:S:2210:VAL:HG11	2.60	0.42
1:S:2288:LEU:O	1:S:3849:ARG:NH1	2.51	0.42
1:S:3320:LEU:HA	1:S:3323:ILE:HG22	2.02	0.42
1:A:294:THR:O	1:A:298:GLY:N	2.46	0.42
1:G:34:LYS:HA	1:G:34:LYS:CE	2.49	0.42
1:G:2630:VAL:N	1:G:2631:PRO:HD2	2.35	0.42
1:M:1101:ARG:NH1	1:M:1115:LEU:O	2.52	0.42
1:M:2630:VAL:N	1:M:2631:PRO:HD2	2.35	0.42
1:M:2967:MET:HE3	1:M:2967:MET:CA	2.49	0.42
1:M:3105:LYS:HA	1:M:3105:LYS:HE2	2.00	0.42
1:A:977:LEU:CD2	1:A:1043:VAL:HG11	2.50	0.41
1:M:455:PRO:HG3	1:M:467:LYS:HB3	2.02	0.41
1:M:1144:GLN:N	1:M:1147:ASP:OD2	2.47	0.41
1:S:2630:VAL:N	1:S:2631:PRO:HD2	2.35	0.41
1:S:2967:MET:HE3	1:S:2967:MET:CA	2.49	0.41
1:S:3459:VAL:HG23	1:S:3464:ILE:CG2	2.44	0.41
1:A:904:HIS:HE1	1:A:906:CYS:SG	2.43	0.41
1:G:1131:ARG:NH1	1:G:1178:ALA:O	2.54	0.41
1:M:2178:MET:SD	1:M:2210:VAL:HG11	2.60	0.41
1:M:4093:PHE:O	1:M:4097:MET:HG2	2.20	0.41
1:S:3110:LEU:HD12	1:S:3175:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD11	1:A:35:LEU:CD1	2.47	0.41
1:A:1024:TYR:O	1:A:1025:ARG:C	2.63	0.41
1:A:3305:THR:HG22	1:A:3307:VAL:H	1.85	0.41
1:G:937:CYS:SG	1:G:984:LEU:HD21	2.60	0.41
1:G:977:LEU:CD2	1:G:1043:VAL:HG11	2.50	0.41
1:M:3320:LEU:HA	1:M:3323:ILE:HG22	2.02	0.41
1:M:3610:GLU:OE1	1:M:3610:GLU:N	2.52	0.41
1:S:2750:LYS:O	1:S:2750:LYS:HG2	2.19	0.41
1:S:3999:MET:HE2	1:S:3999:MET:HA	2.02	0.41
1:A:984:LEU:HD12	1:A:987:ARG:NH1	2.34	0.41
1:G:456:SER:HG	1:G:459:LEU:HG	1.79	0.41
1:G:3610:GLU:OE1	1:G:3610:GLU:N	2.52	0.41
2:H:37:ASP:OD1	2:H:38:SER:N	2.54	0.41
1:S:1039:LEU:HD23	1:S:1039:LEU:HA	1.95	0.41
1:S:2265:LEU:O	1:S:2266:GLY:C	2.62	0.41
1:S:2346:VAL:O	1:S:2346:VAL:HG13	2.19	0.41
1:A:864:PRO:CG	1:A:867:LEU:HD12	2.50	0.41
1:A:3110:LEU:HD12	1:A:3175:LEU:HD21	2.02	0.41
1:G:350:HIS:O	1:G:354:GLY:N	2.48	0.41
1:G:904:HIS:HE1	1:G:906:CYS:SG	2.43	0.41
1:G:2580:ASP:OD1	1:G:2580:ASP:C	2.64	0.41
1:G:3169:LEU:HD11	1:G:3194:LEU:HD11	1.96	0.41
1:G:3753:PHE:O	1:G:3757:GLU:HG2	2.20	0.41
1:M:1024:TYR:O	1:M:1025:ARG:C	2.63	0.41
1:M:2750:LYS:HG2	1:M:2750:LYS:O	2.19	0.41
1:M:3365:LEU:HD21	1:M:3405:LEU:HD23	2.01	0.41
1:M:3999:MET:HE2	1:M:3999:MET:HA	2.02	0.41
1:S:3610:GLU:OE1	1:S:3610:GLU:N	2.52	0.41
1:S:3753:PHE:HZ	1:S:4719:PHE:HZ	1.62	0.41
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.54	0.41
1:A:3320:LEU:HA	1:A:3323:ILE:HG22	2.02	0.41
1:G:1024:TYR:O	1:G:1025:ARG:C	2.63	0.41
1:G:2522:LEU:HD22	1:G:2578:MET:HE3	2.03	0.41
1:M:25:SER:HB3	1:M:34:LYS:HE3	2.02	0.41
1:M:3753:PHE:O	1:M:3757:GLU:HG2	2.20	0.41
1:S:21:VAL:HG12	1:S:66:CYS:HA	2.01	0.41
1:S:864:PRO:CG	1:S:867:LEU:HD12	2.50	0.41
1:S:1924:GLU:N	1:S:1924:GLU:OE1	2.52	0.41
1:A:4911:LEU:O	1:A:4914:VAL:HG22	2.21	0.41
2:B:37:ASP:OD1	2:B:38:SER:N	2.54	0.41
1:M:33:LEU:HD11	1:M:35:LEU:CD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:752:VAL:O	1:M:752:VAL:HG13	2.21	0.41
1:M:3986:TRP:HA	1:M:3986:TRP:HE3	1.86	0.41
1:S:3753:PHE:O	1:S:3757:GLU:HG2	2.20	0.41
1:S:4767:TRP:CZ2	1:S:4771:ILE:HG12	2.56	0.41
1:A:21:VAL:HG12	1:A:66:CYS:HA	2.01	0.41
1:A:25:SER:HB3	1:A:34:LYS:HE3	2.03	0.41
1:A:752:VAL:HG13	1:A:752:VAL:O	2.21	0.41
1:A:4839:MET:HG3	1:G:4823:LEU:CD2	2.32	0.41
1:A:5000:GLU:OE1	1:A:5000:GLU:N	2.49	0.41
1:G:4767:TRP:CZ2	1:G:4771:ILE:HG12	2.56	0.41
1:M:2628:PHE:HD1	1:M:2907:PRO:CG	2.33	0.41
1:M:4091:LYS:HB2	1:M:4091:LYS:HE2	1.89	0.41
1:M:4767:TRP:CE2	1:M:4771:ILE:CD1	3.04	0.41
1:S:33:LEU:CD1	1:S:35:LEU:CD1	2.99	0.41
1:A:1067:SER:OG	1:A:1070:ASP:OD2	2.34	0.41
1:A:1461:ASP:OD1	1:A:1462:MET:N	2.54	0.41
1:A:2628:PHE:HD1	1:A:2907:PRO:CG	2.32	0.41
1:A:4767:TRP:CZ2	1:A:4771:ILE:HG12	2.56	0.41
1:G:455:PRO:HG3	1:G:467:LYS:HB3	2.02	0.41
1:G:4911:LEU:O	1:G:4914:VAL:HG22	2.21	0.41
1:M:34:LYS:HA	1:M:34:LYS:CE	2.49	0.41
1:M:977:LEU:CD2	1:M:1043:VAL:HG11	2.50	0.41
1:M:2580:ASP:OD1	1:M:2580:ASP:C	2.64	0.41
1:M:2994:GLU:OE1	1:M:2994:GLU:N	2.52	0.41
1:M:3256:LEU:HD21	1:M:3266:MET:SD	2.61	0.41
1:M:3768:SER:HA	1:M:3771:HIS:CD2	2.56	0.41
1:S:168:ASP:C	1:S:169:LEU:HD12	2.46	0.41
1:S:453:GLU:OE1	1:S:453:GLU:CA	2.68	0.41
1:S:455:PRO:HG3	1:S:467:LYS:HB3	2.02	0.41
1:S:977:LEU:CD2	1:S:1043:VAL:HG11	2.50	0.41
1:S:1119:GLU:OE1	1:S:1119:GLU:N	2.48	0.41
1:S:4021:LYS:O	1:S:4024:VAL:HG12	2.21	0.41
1:A:2522:LEU:HD22	1:A:2578:MET:HE3	2.03	0.41
1:A:3256:LEU:HD21	1:A:3266:MET:SD	2.61	0.41
1:A:3999:MET:HE2	1:A:3999:MET:HA	2.02	0.41
1:A:4067:LYS:HA	1:A:4070:ASP:OD2	2.21	0.41
1:G:168:ASP:C	1:G:169:LEU:HD12	2.46	0.41
1:G:752:VAL:HG13	1:G:752:VAL:O	2.21	0.41
1:G:4093:PHE:O	1:G:4097:MET:HG2	2.20	0.41
1:G:4704:LEU:O	1:G:4704:LEU:HD23	2.21	0.41
1:M:3305:THR:HG22	1:M:3307:VAL:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:752:VAL:O	1:S:753:PRO:C	2.63	0.41
1:S:1461:ASP:OD1	1:S:1462:MET:N	2.54	0.41
1:S:2138:LEU:N	1:S:2139:PRO:CD	2.84	0.41
1:S:3362:ILE:HB	1:S:3437:MET:HE2	2.03	0.41
1:G:3362:ILE:HB	1:G:3437:MET:HE2	2.03	0.40
1:G:3768:SER:HA	1:G:3771:HIS:CD2	2.56	0.40
1:M:168:ASP:C	1:M:169:LEU:HD12	2.46	0.40
1:M:904:HIS:HE1	1:M:906:CYS:SG	2.43	0.40
1:M:3753:PHE:CE2	1:M:3757:GLU:HG3	2.56	0.40
1:S:904:HIS:HE1	1:S:906:CYS:SG	2.43	0.40
1:S:4093:PHE:O	1:S:4097:MET:HG2	2.20	0.40
1:A:33:LEU:CD1	1:A:35:LEU:CD1	2.99	0.40
1:A:2138:LEU:N	1:A:2139:PRO:CD	2.84	0.40
1:A:3324:VAL:O	1:A:3327:LEU:HD23	2.21	0.40
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.56	0.40
1:A:4090:LYS:HG2	1:A:4123:ILE:HD11	2.03	0.40
1:G:752:VAL:O	1:G:753:PRO:C	2.63	0.40
1:G:2865:VAL:HG21	1:G:2932:MET:HE2	2.04	0.40
1:M:752:VAL:O	1:M:753:PRO:C	2.63	0.40
1:S:25:SER:HB3	1:S:34:LYS:HE3	2.03	0.40
1:S:752:VAL:O	1:S:752:VAL:HG13	2.21	0.40
1:S:3156:VAL:CG1	1:S:3157:ILE:N	2.84	0.40
1:S:3256:LEU:HD21	1:S:3266:MET:SD	2.61	0.40
1:S:3305:THR:HG22	1:S:3307:VAL:H	1.85	0.40
1:S:4911:LEU:O	1:S:4914:VAL:HG22	2.21	0.40
1:A:939:VAL:HG23	1:A:1053:ILE:HG23	2.03	0.40
1:A:2265:LEU:O	1:A:2266:GLY:C	2.62	0.40
1:A:3567:PRO:CB	1:S:1825:HIS:NE2	2.83	0.40
1:G:25:SER:HB3	1:G:34:LYS:HE3	2.03	0.40
1:G:1461:ASP:OD1	1:G:1462:MET:N	2.54	0.40
1:G:4767:TRP:CE2	1:G:4771:ILE:CD1	3.04	0.40
1:M:294:THR:O	1:M:298:GLY:N	2.46	0.40
1:M:351:VAL:HG23	1:M:352:ALA:N	2.37	0.40
1:M:2522:LEU:HD22	1:M:2578:MET:HE3	2.03	0.40
1:M:3156:VAL:CG1	1:M:3157:ILE:N	2.85	0.40
1:M:4704:LEU:O	1:M:4704:LEU:HD23	2.22	0.40
1:M:4767:TRP:CZ2	1:M:4771:ILE:HG12	2.56	0.40
2:N:37:ASP:OD1	2:N:38:SER:N	2.54	0.40
1:S:2580:ASP:OD1	1:S:2580:ASP:C	2.63	0.40
1:S:3324:VAL:O	1:S:3327:LEU:HD23	2.21	0.40
1:S:3753:PHE:CE2	1:S:3757:GLU:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:4767:TRP:CE2	1:S:4771:ILE:CD1	3.04	0.40
2:T:37:ASP:OD1	2:T:38:SER:N	2.54	0.40
1:A:789:VAL:HG12	1:A:790:ARG:N	2.37	0.40
1:A:4704:LEU:HD23	1:A:4704:LEU:O	2.21	0.40
1:G:585:SER:O	1:G:588:SER:HB2	2.22	0.40
1:G:2994:GLU:OE1	1:G:2994:GLU:N	2.52	0.40
1:M:350:HIS:O	1:M:354:GLY:N	2.48	0.40
1:M:1825:HIS:NE2	1:S:3567:PRO:CB	2.83	0.40
1:M:4021:LYS:O	1:M:4024:VAL:HG12	2.21	0.40
1:S:1131:ARG:NH1	1:S:1178:ALA:O	2.54	0.40
1:S:2995:ILE:N	1:S:2995:ILE:HD12	2.37	0.40
1:S:3934:TYR:CD1	1:S:3999:MET:HE1	2.57	0.40
1:A:2995:ILE:N	1:A:2995:ILE:HD12	2.37	0.40
1:A:4021:LYS:O	1:A:4024:VAL:HG12	2.21	0.40
1:A:4044:MET:HE3	1:A:4044:MET:HB2	2.01	0.40
1:G:3087:ILE:HG23	1:G:3088:VAL:N	2.37	0.40
1:G:3156:VAL:CG1	1:G:3157:ILE:N	2.85	0.40
1:G:3305:THR:HG22	1:G:3307:VAL:H	1.85	0.40
1:G:4067:LYS:HA	1:G:4070:ASP:OD2	2.21	0.40
1:M:4911:LEU:O	1:M:4914:VAL:HG22	2.21	0.40
1:S:707:VAL:HG23	1:S:782:SER:CB	2.48	0.40
1:S:3768:SER:HA	1:S:3771:HIS:CD2	2.56	0.40
1:S:3959:LYS:HE3	1:S:4022:ASP:OD2	2.22	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	4129/5037 (82%)	4034 (98%)	95 (2%)	0	100	100
1	G	4129/5037 (82%)	4034 (98%)	95 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	4129/5037 (82%)	4034 (98%)	95 (2%)	0	100	100
1	S	4129/5037 (82%)	4035 (98%)	94 (2%)	0	100	100
2	B	105/111 (95%)	102 (97%)	3 (3%)	0	100	100
2	H	105/111 (95%)	102 (97%)	3 (3%)	0	100	100
2	N	105/111 (95%)	102 (97%)	3 (3%)	0	100	100
2	T	105/111 (95%)	102 (97%)	3 (3%)	0	100	100
All	All	16936/20592 (82%)	16545 (98%)	391 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3402/4276 (80%)	3393 (100%)	9 (0%)	91	95
1	G	3402/4276 (80%)	3394 (100%)	8 (0%)	92	96
1	M	3402/4276 (80%)	3393 (100%)	9 (0%)	91	95
1	S	3402/4276 (80%)	3394 (100%)	8 (0%)	92	96
2	B	87/91 (96%)	86 (99%)	1 (1%)	70	83
2	H	87/91 (96%)	86 (99%)	1 (1%)	70	83
2	N	87/91 (96%)	86 (99%)	1 (1%)	70	83
2	T	87/91 (96%)	86 (99%)	1 (1%)	70	83
All	All	13956/17468 (80%)	13918 (100%)	38 (0%)	90	95

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	46	LEU
1	A	636	ASN
1	A	2559	LEU

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Mol	Chain	Res	Type
1	A	3025	LEU
1	A	3569	LEU
1	A	3899	PHE
1	A	4876	CYS
1	A	4953	ASP
2	B	25	HIS
1	G	34	LYS
1	G	46	LEU
1	G	636	ASN
1	G	3025	LEU
1	G	3569	LEU
1	G	3899	PHE
1	G	4876	CYS
1	G	4953	ASP
2	H	25	HIS
1	M	34	LYS
1	M	46	LEU
1	M	636	ASN
1	M	2559	LEU
1	M	3025	LEU
1	M	3569	LEU
1	M	3899	PHE
1	M	4876	CYS
1	M	4953	ASP
2	N	25	HIS
1	S	34	LYS
1	S	46	LEU
1	S	636	ASN
1	S	3025	LEU
1	S	3569	LEU
1	S	3899	PHE
1	S	4876	CYS
1	S	4953	ASP
2	T	25	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (162) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	54	ASN
1	A	57	ASN
1	A	151	HIS

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Mol	Chain	Res	Type
1	A	460	GLN
1	A	461	HIS
1	A	582	HIS
1	A	736	HIS
1	A	772	ASN
1	A	866	HIS
1	A	909	ASN
1	A	911	HIS
1	A	1158	ASN
1	A	1281	ASN
1	A	1560	ASN
1	A	1571	ASN
1	A	1640	HIS
1	A	1775	HIS
1	A	1953	HIS
1	A	2125	HIS
1	A	2194	HIS
1	A	2441	HIS
1	A	2520	HIS
1	A	2773	ASN
1	A	2780	ASN
1	A	2877	GLN
1	A	2931	GLN
1	A	2991	HIS
1	A	3150	HIS
1	A	3326	ASN
1	A	3449	HIS
1	A	3450	ASN
1	A	3927	GLN
1	A	3994	HIS
1	A	3998	HIS
1	A	4009	GLN
1	A	4034	ASN
1	A	4109	GLN
1	A	4223	ASN
1	A	4997	ASN
2	B	94	ASN
1	G	23	GLN
1	G	54	ASN
1	G	57	ASN
1	G	151	HIS
1	G	460	GLN

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Mol	Chain	Res	Type
1	G	461	HIS
1	G	582	HIS
1	G	736	HIS
1	G	772	ASN
1	G	866	HIS
1	G	909	ASN
1	G	911	HIS
1	G	1158	ASN
1	G	1560	ASN
1	G	1571	ASN
1	G	1611	HIS
1	G	1640	HIS
1	G	1775	HIS
1	G	1953	HIS
1	G	2125	HIS
1	G	2194	HIS
1	G	2284	ASN
1	G	2520	HIS
1	G	2773	ASN
1	G	2780	ASN
1	G	2877	GLN
1	G	2931	GLN
1	G	2991	HIS
1	G	3150	HIS
1	G	3326	ASN
1	G	3450	ASN
1	G	3994	HIS
1	G	3998	HIS
1	G	4009	GLN
1	G	4034	ASN
1	G	4109	GLN
1	G	4691	GLN
1	G	4997	ASN
2	H	65	GLN
2	H	94	ASN
1	M	23	GLN
1	M	54	ASN
1	M	57	ASN
1	M	151	HIS
1	M	460	GLN
1	M	461	HIS
1	M	582	HIS

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Mol	Chain	Res	Type
1	M	736	HIS
1	M	772	ASN
1	M	866	HIS
1	M	909	ASN
1	M	911	HIS
1	M	1158	ASN
1	M	1560	ASN
1	M	1571	ASN
1	M	1611	HIS
1	M	1640	HIS
1	M	1660	GLN
1	M	1775	HIS
1	M	1953	HIS
1	M	2125	HIS
1	M	2194	HIS
1	M	2441	HIS
1	M	2520	HIS
1	M	2773	ASN
1	M	2780	ASN
1	M	2877	GLN
1	M	2931	GLN
1	M	2991	HIS
1	M	3150	HIS
1	M	3268	HIS
1	M	3326	ASN
1	M	3449	HIS
1	M	3450	ASN
1	M	3994	HIS
1	M	3998	HIS
1	M	4009	GLN
1	M	4034	ASN
1	M	4109	GLN
1	M	4223	ASN
1	M	4997	ASN
2	N	94	ASN
1	S	23	GLN
1	S	54	ASN
1	S	57	ASN
1	S	151	HIS
1	S	460	GLN
1	S	461	HIS
1	S	582	HIS

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Mol	Chain	Res	Type
1	S	736	HIS
1	S	772	ASN
1	S	866	HIS
1	S	909	ASN
1	S	911	HIS
1	S	1158	ASN
1	S	1560	ASN
1	S	1571	ASN
1	S	1611	HIS
1	S	1640	HIS
1	S	1775	HIS
1	S	1953	HIS
1	S	2125	HIS
1	S	2194	HIS
1	S	2284	ASN
1	S	2441	HIS
1	S	2520	HIS
1	S	2773	ASN
1	S	2780	ASN
1	S	2877	GLN
1	S	2931	GLN
1	S	2991	HIS
1	S	3150	HIS
1	S	3326	ASN
1	S	3449	HIS
1	S	3450	ASN
1	S	3994	HIS
1	S	3998	HIS
1	S	4034	ASN
1	S	4109	GLN
1	S	4997	ASN
2	T	94	ASN

### 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, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

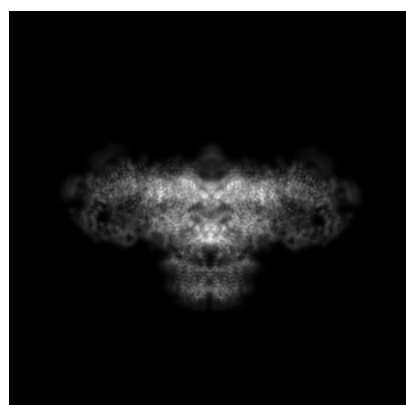
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70591. These allow visual inspection of the internal detail of the map and identification of artifacts.

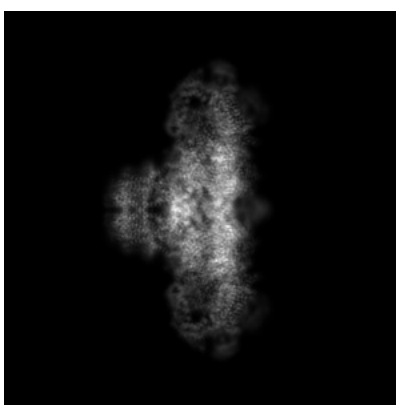
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

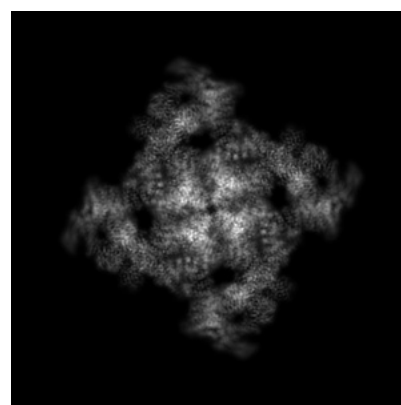
#### 6.1.1 Primary map



X



Y



Z

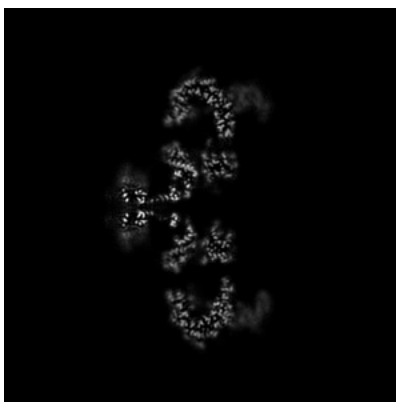
The images above show the map projected in three orthogonal directions.

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

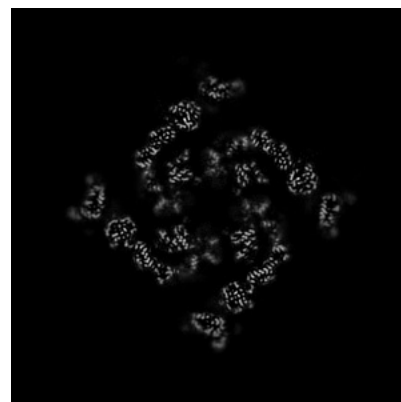
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

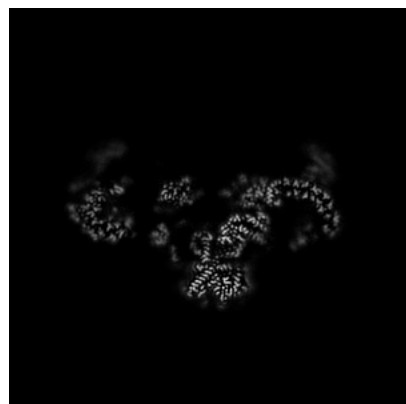


Z Index: 256

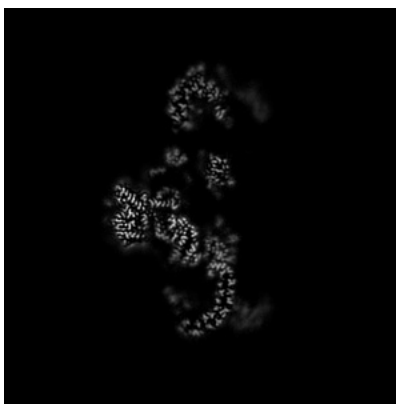
The images above show central slices of the map in three orthogonal directions.

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

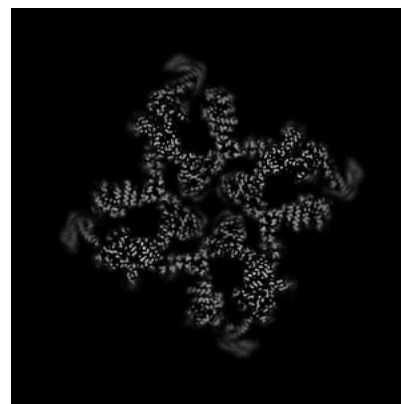
### 6.3.1 Primary map



X Index: 266



Y Index: 267

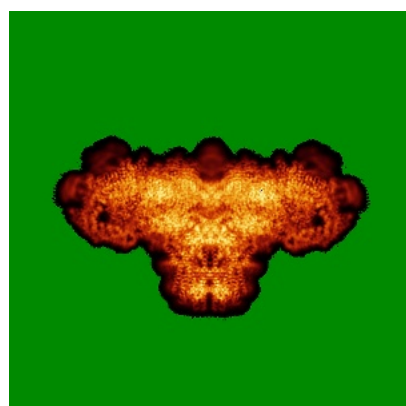


Z Index: 277

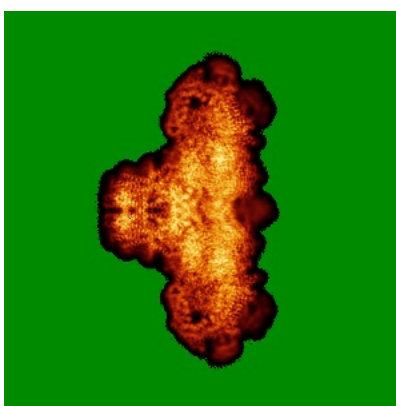
The images above show the largest variance slices of the map in three orthogonal directions.

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

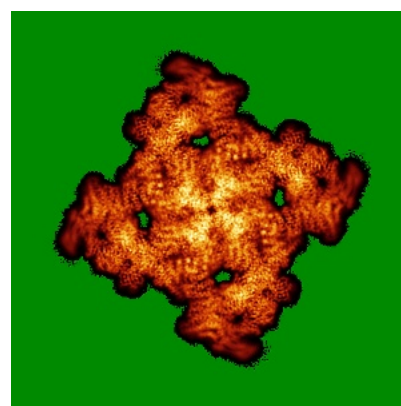
### 6.4.1 Primary map



X



Y

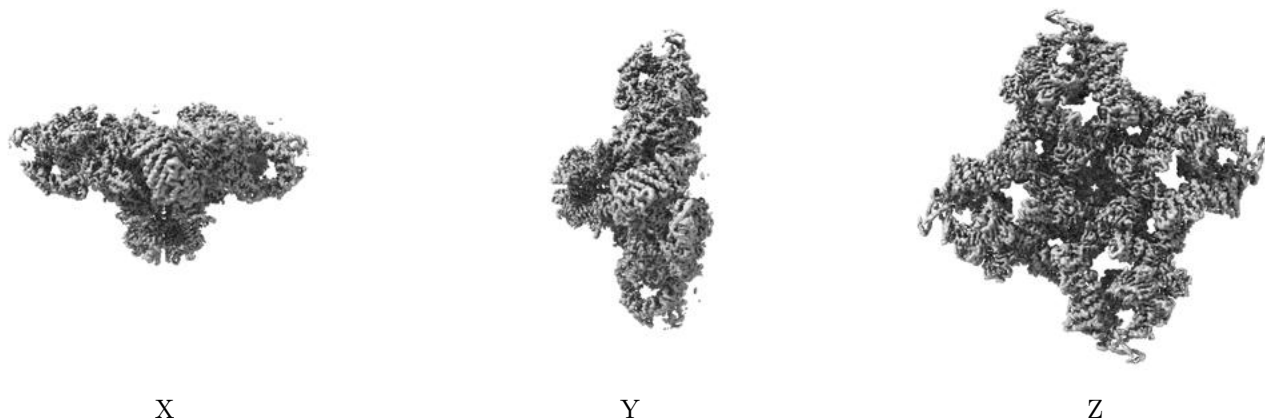


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.047. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

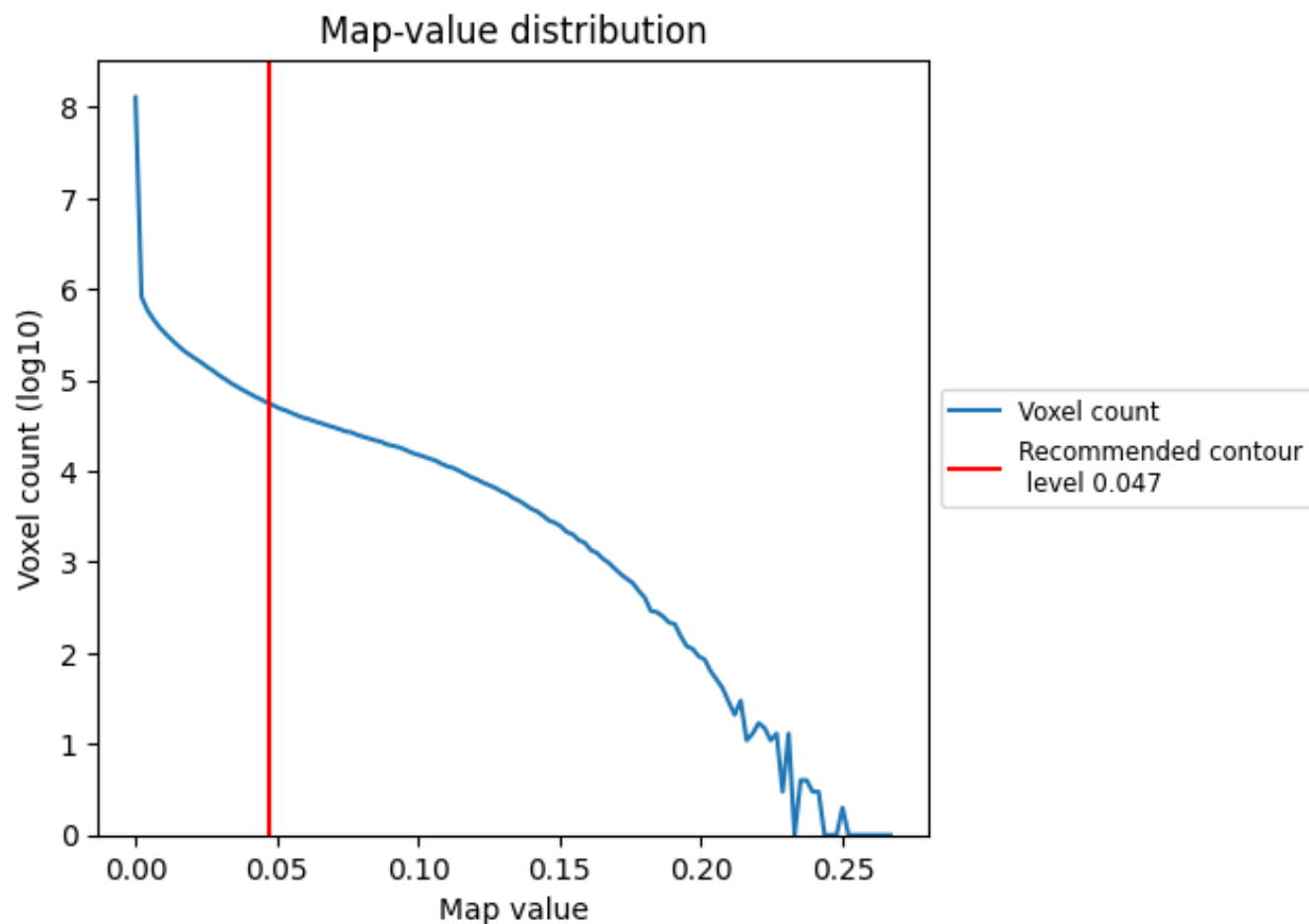
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

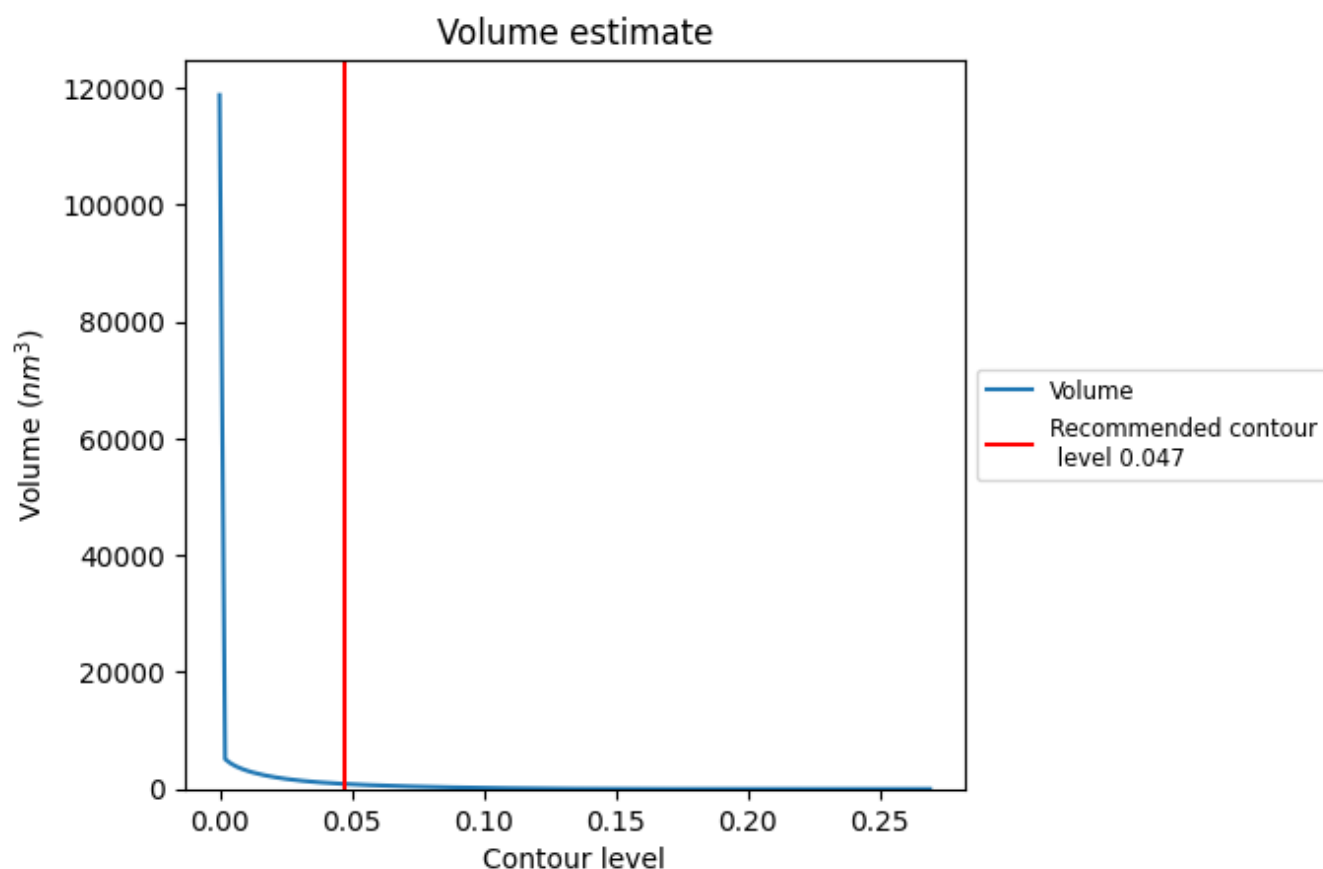
This section contains the results of statistical analysis of the map.

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



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

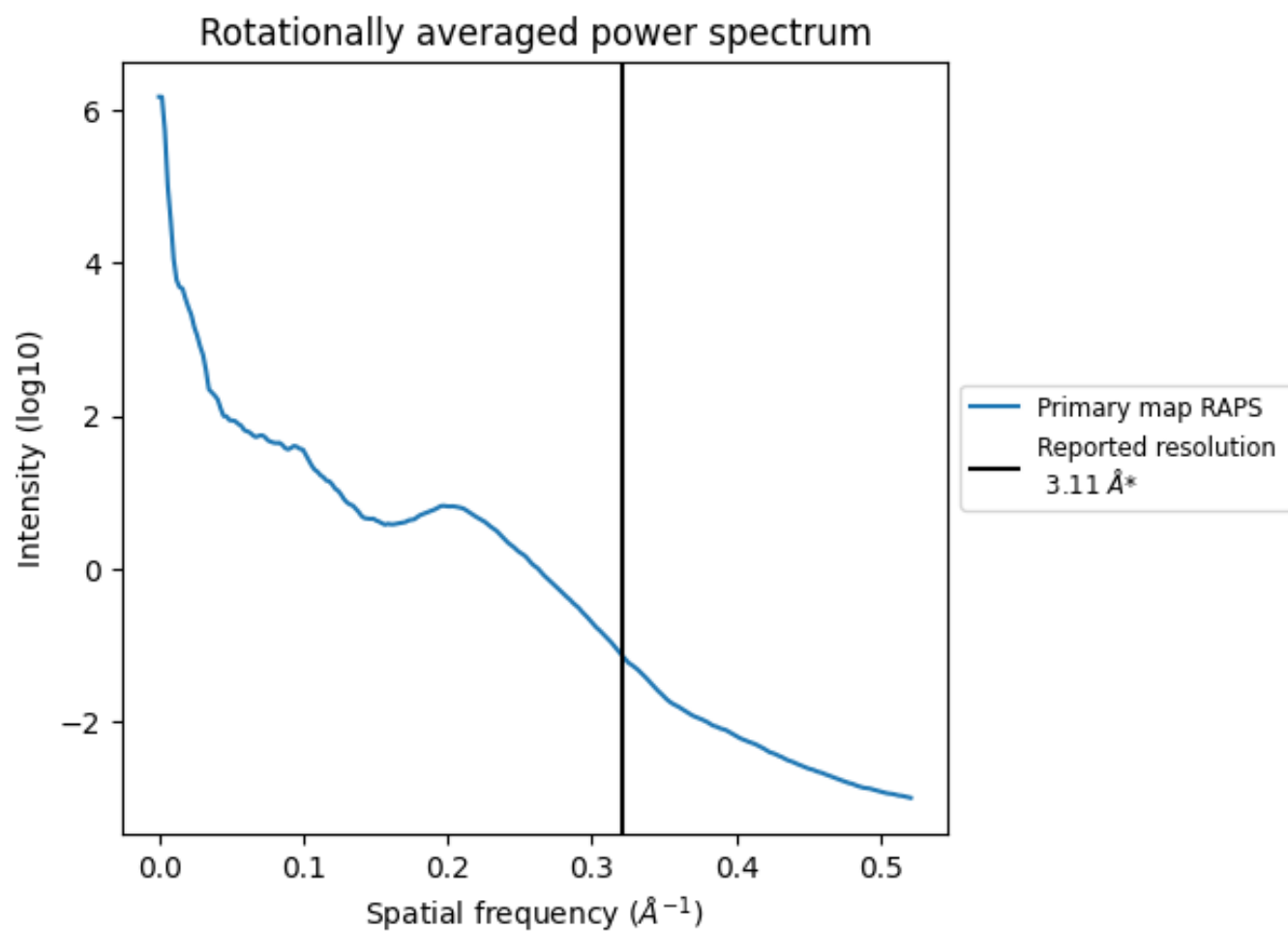
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $871 \text{ nm}^3$ ; this corresponds to an approximate mass of 787 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 0.322 Å<sup>-1</sup>

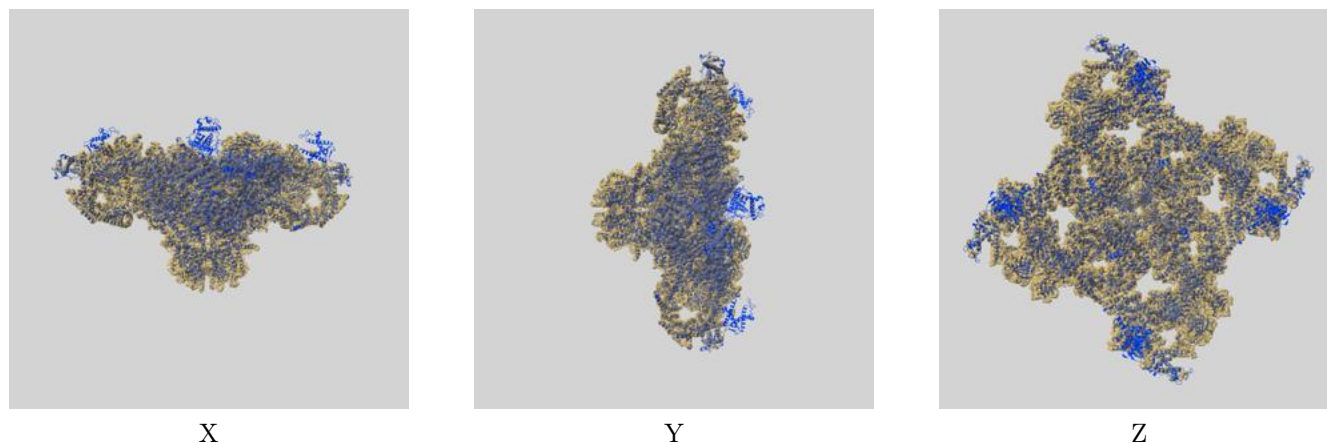
## 8 Fourier-Shell correlation

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

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

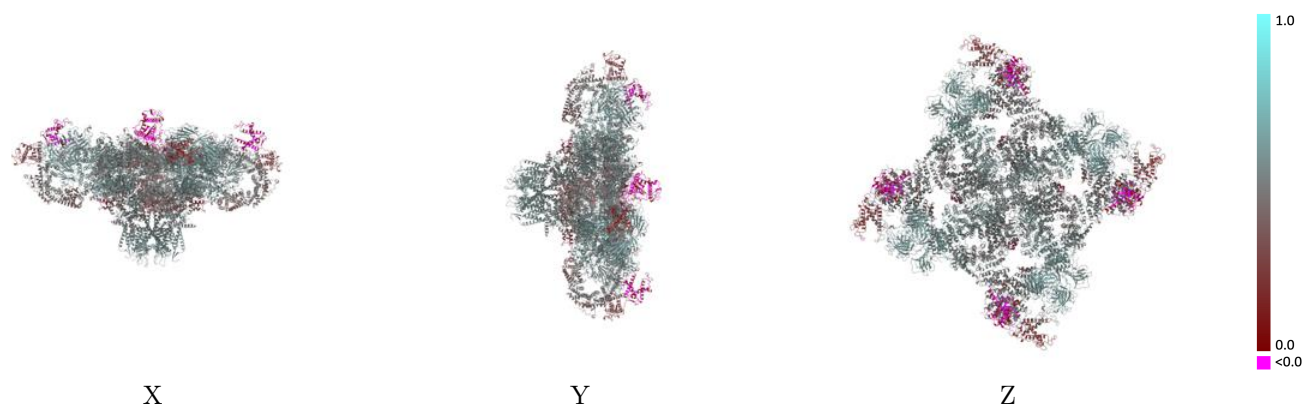
This section contains information regarding the fit between EMDB map EMD-70591 and PDB model 9OL6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

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



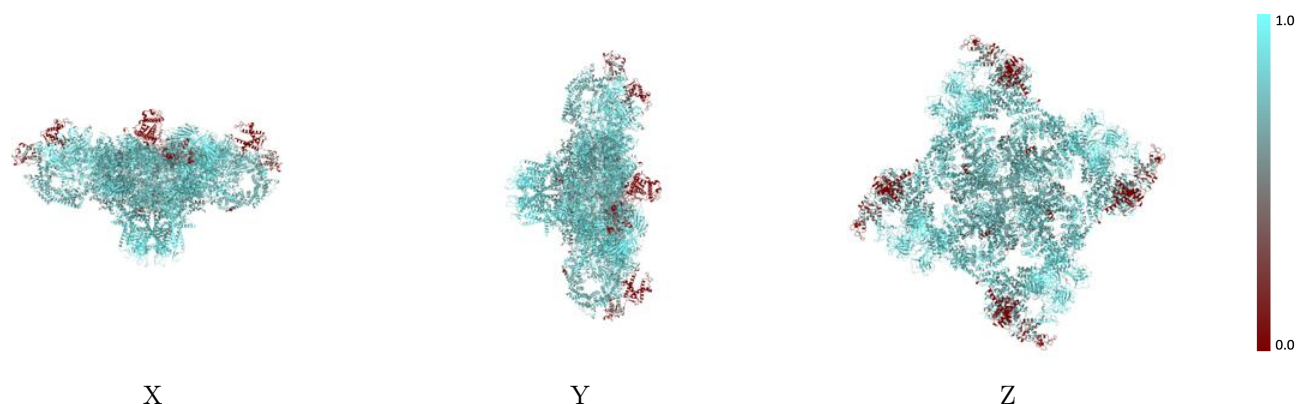
The images above show the 3D surface view of the map at the recommended contour level 0.047 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



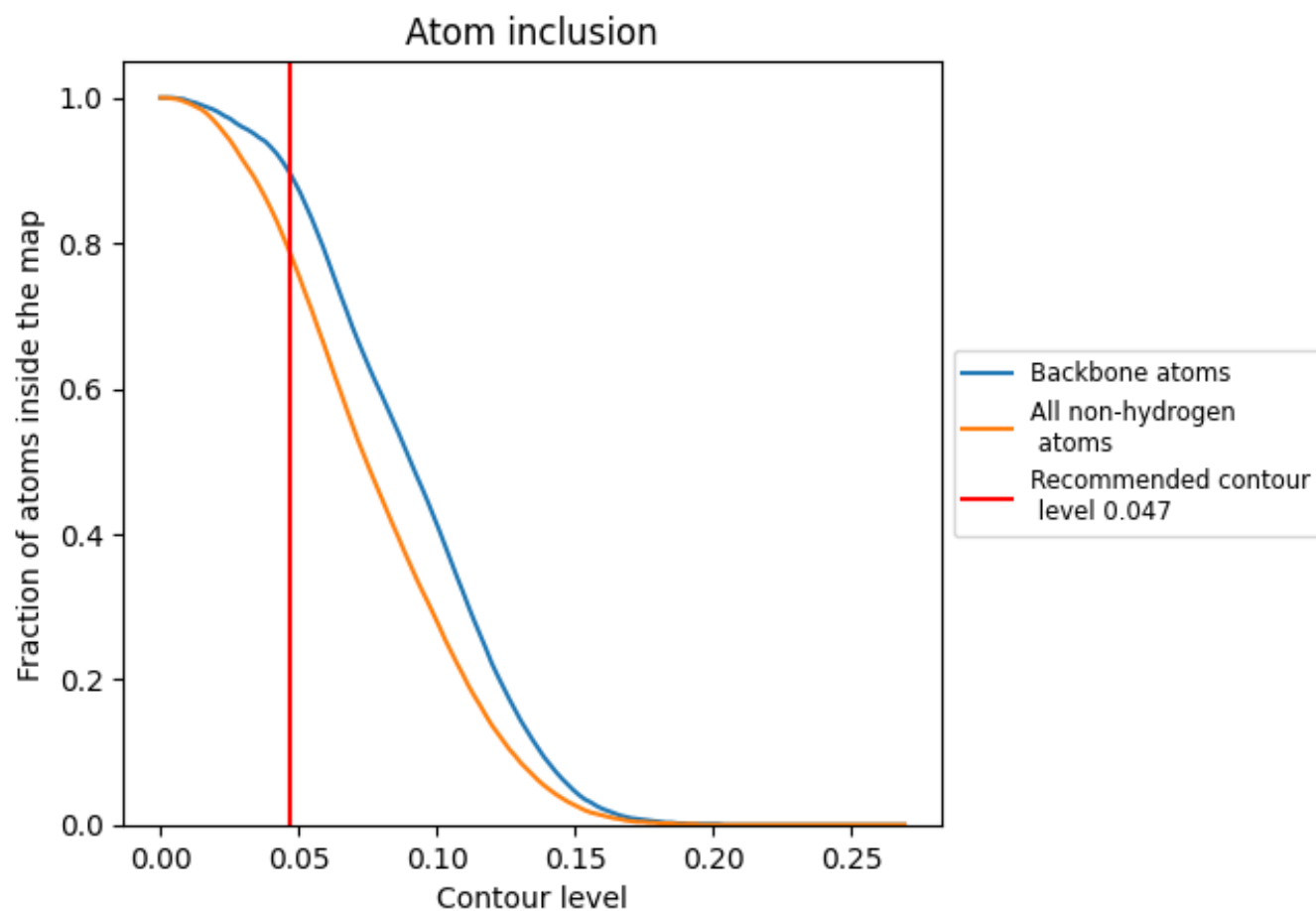
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.047).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 78% 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 (0.047) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7850	<div><div></div></div> 0.4810
A	<div><div></div></div> 0.7820	<div><div></div></div> 0.4790
B	<div><div></div></div> 0.8660	<div><div></div></div> 0.5590
G	<div><div></div></div> 0.7830	<div><div></div></div> 0.4800
H	<div><div></div></div> 0.8690	<div><div></div></div> 0.5620
M	<div><div></div></div> 0.7830	<div><div></div></div> 0.4800
N	<div><div></div></div> 0.8690	<div><div></div></div> 0.5600
S	<div><div></div></div> 0.7820	<div><div></div></div> 0.4790
T	<div><div></div></div> 0.8680	<div><div></div></div> 0.5630

1.0

0.0

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