



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:19 AM UTC

PDB ID : 6PV6 / pdb_00006pv6
EMDB ID : EMD-20486
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on : 2019-07-19
Resolution : 4.50 Å (reported)
Based on initial model : 5TB4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

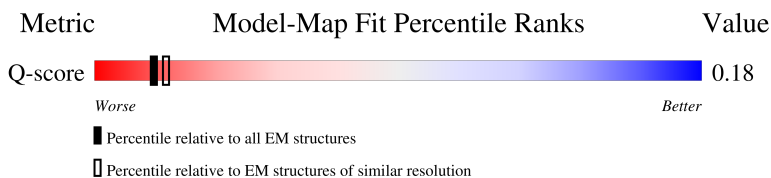
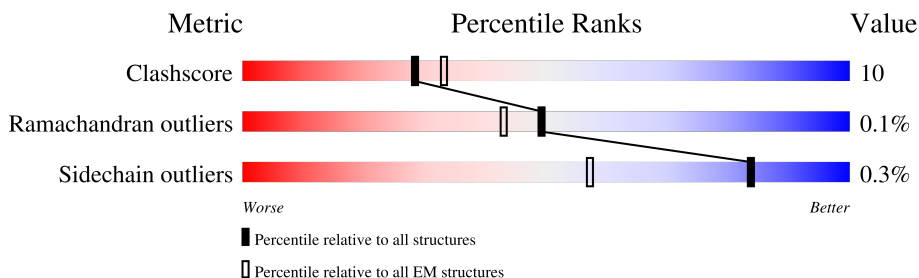
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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

Mol	Chain	Length	Quality of chain
1	B	4687	33% 70% 19% 11%
1	E	4687	37% 70% 19% 11%
1	G	4687	40% 70% 19% 11%
1	I	4687	36% 70% 19% 11%

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Mol	Chain	Length	Quality of chain
2	A	108	37%67%31%..
2	F	108	47%69%30%. .
2	H	108	54%69%30%..
2	J	108	43%69%30%..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
1	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

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

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest")

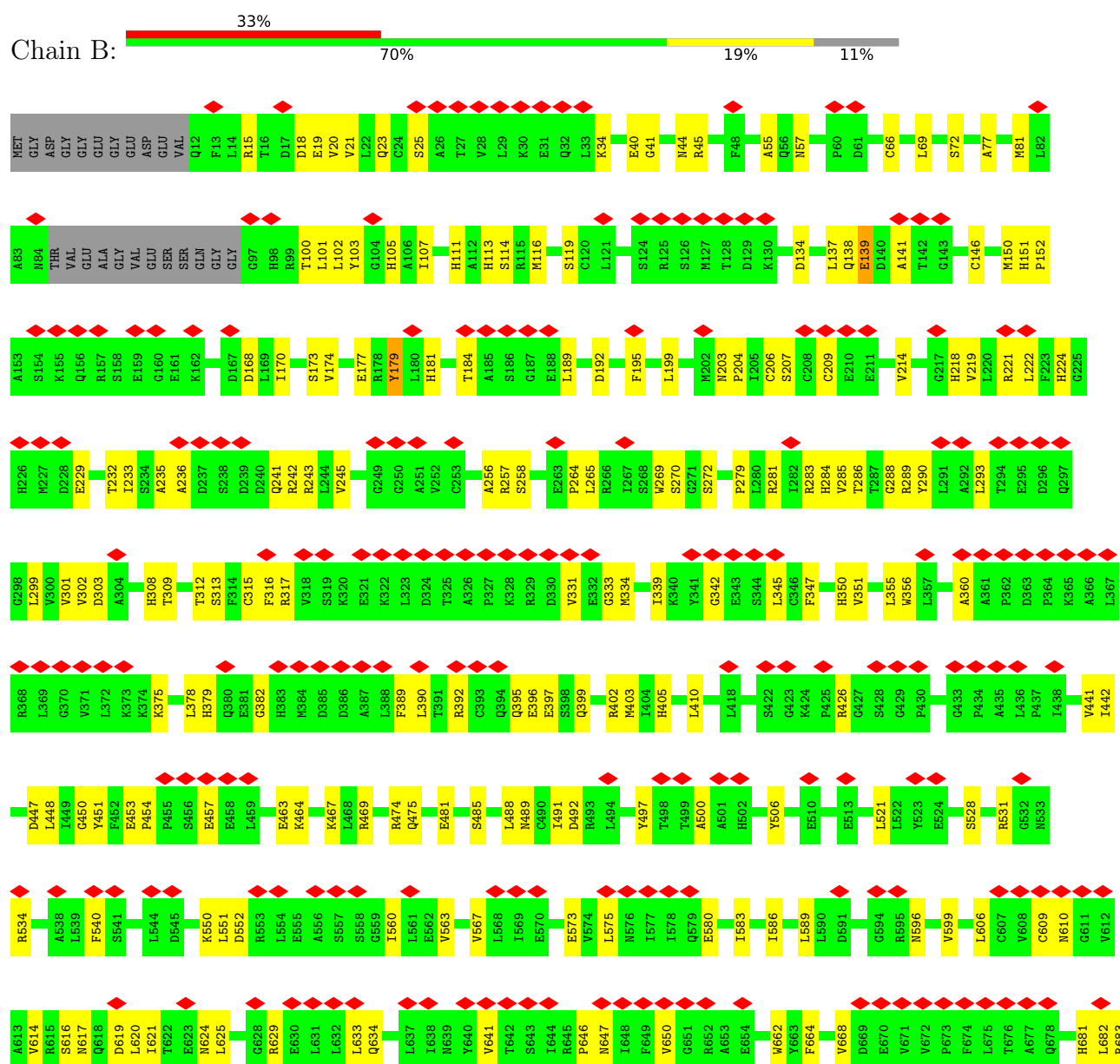
by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0

3 Residue-property plots

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

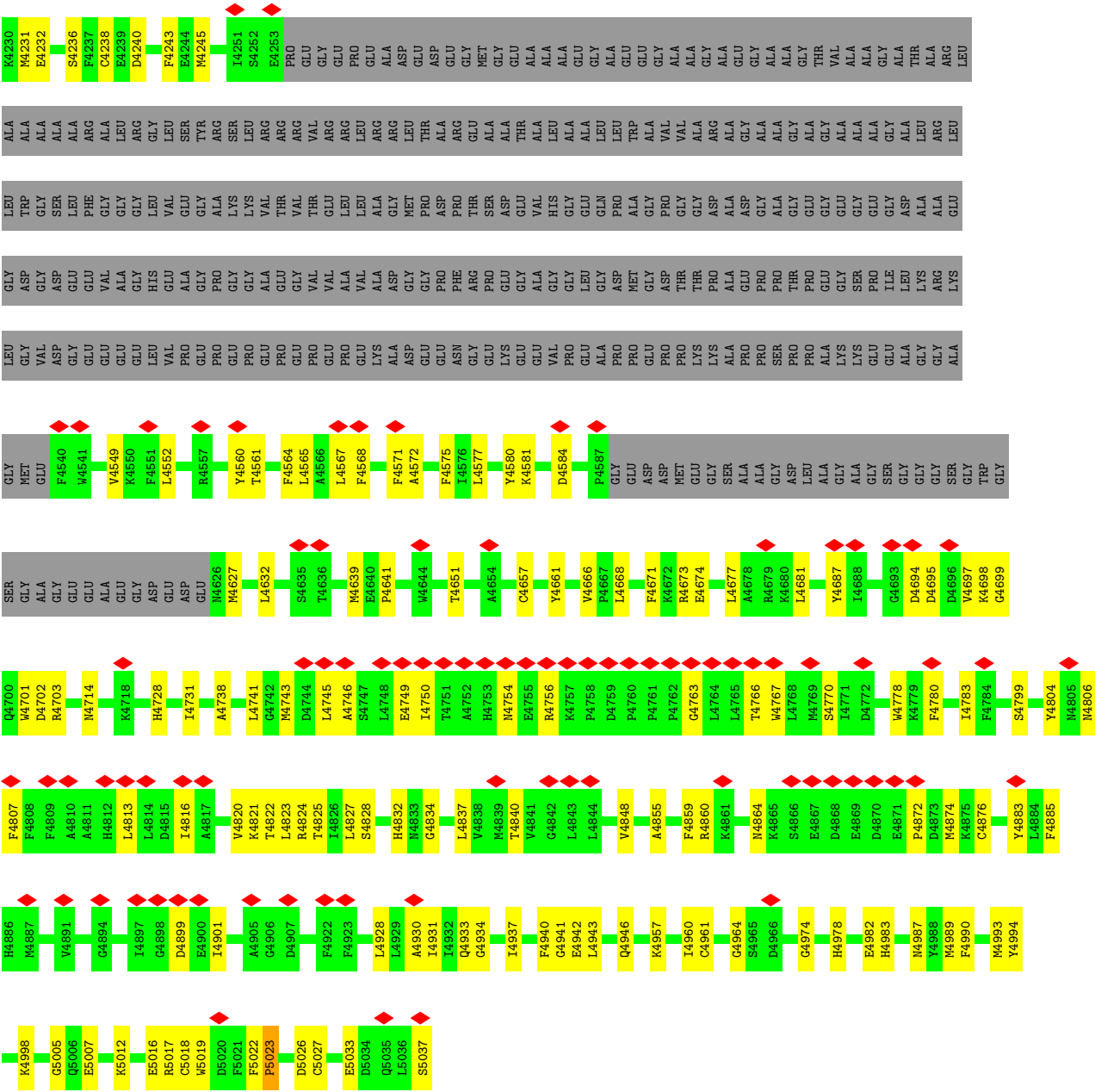
• Molecule 1: Ryanodine receptor 1



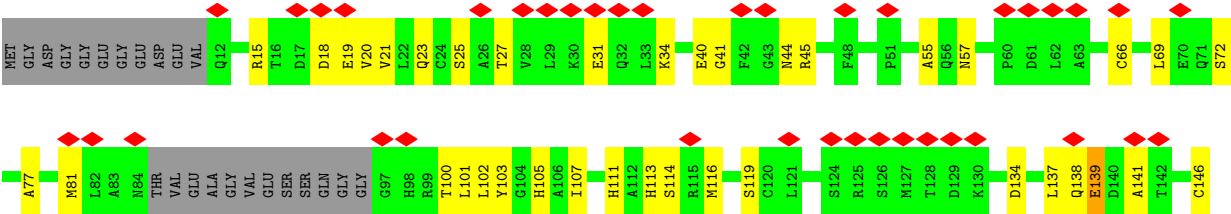


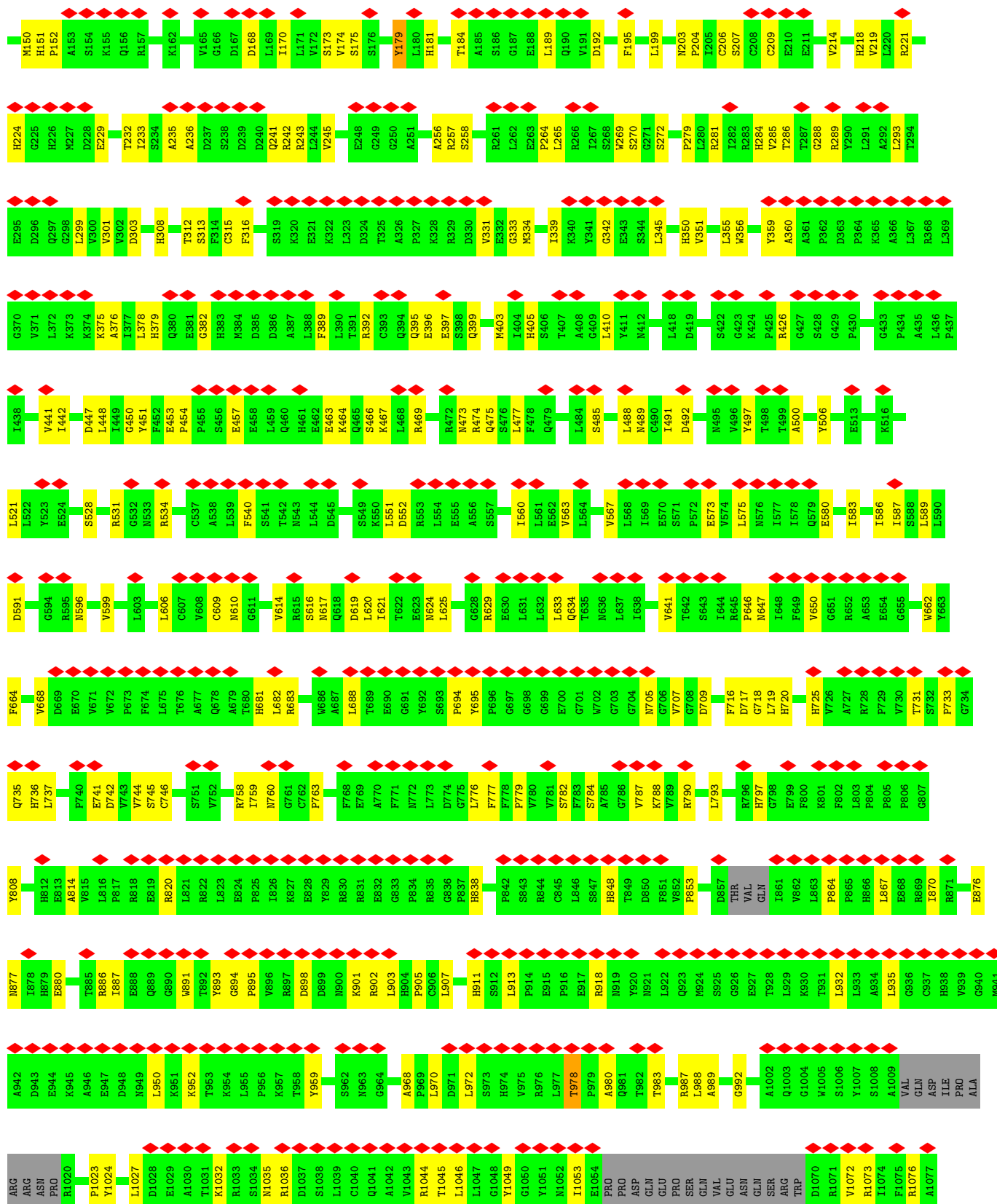
THR	L2774	N2774	X2683	X2583	L2451	A2367	L2295	N2188	GLU	H2011	LYS	D1858	F1777
GLU	W2775	W2775	X2686	X2584	R2452	L2368	E2296	F2191	LEU	F2012	GLU	V1859	S1778
LYS	S2776	S2776	X2687	X2585	A2455	R2369	K2297	Y2192	PRO	A2016	ASP	K1860	P1779
LYS	Y2777	Y2777	X2688	X2586	L2456	E2370	V2298	Y2192	ALA	D2017	L1922	I1861	P1780
THR	G2778	G2778	X2689	X2587	L2457	E2371	Y2301	Y2193	GLU	E2018	E1923	I1862	C1781
ARG	E2779	E2779	X2690	X2588	L2457	G2372	Y2302	Y2198	GLU	E2019	E1924	I1863	F1782
LYS	N2780	N2780	X2691	X2589	S2458	G2373	A2303	R2199	GLU	E2020	G1925	K1864	V1783
ILE	V2781	V2781	X2692	X2590	S2459	G2374	G2304	R2199	GLU	C2021	L1926	M1865	I1784
GLN	D2782	D2782	X2693	X2591	G2375	G2376	G2305	V2212	GLU	P2022	I1927	E1867	A1785
THR	E2783	E2783	X2694	X2592	L2376	L2377	G2306	G2216	GLU	L2023	L1931	V1870	L1786
ALA	D2784	D2784	X2695	X2593	P2462	A2378	L2307	G2217	GLU	P2024	P1932	F1871	L1787
GLN	E2785	E2785	X2696	X2594	L2463	A2379	Q2308	G2218	GLU	E2025	P1932	T1872	P1787
THR	L2786	L2786	X2697	X2595	D2464	A2380	S2309	G2219	GLU	D2026	V1935	E1873	A1788
TYR	K2787	K2787	X2698	X2596	D2465	L2380	C2310	E2219	GLU	E2027	E1946	E1874	ALA
ASP	T2788	T2788	X2699	X2597	L2466	E2381	C2311	T2220	GLU	R2028	F1946	GLY	VAL
PRO	H2788	H2788	X2699	X2598	L2469	T2384	M2312	K2221	GLU	L2039	E1950	GLU	ALA
GLU	P2789	P2789	X2699	X2599	L2470	E2388	A2315	E2222	GLU	C2042	E1951	GLU	E1793
GLY	M2790	M2790	X2700	X2600	S2471	E2389	K2316	V2111	GLU	G2043	L1952	GLU	A1794
Y2855	L2791	L2791	X2701	X2601	L2472	P2390	G2317	L2116	GLU	T2044	H1953	GLU	P1795
P2857	R2792	R2792	X2702	X2602	P2473	A2391	Y2318	M2120	GLU	Q2045	R1954	GLU	A1796
Q2858	P2793	P2793	X2703	X2603	Q2475	P2395	P2319	F2121	GLU	L2046	V1955	GLU	R1797
Y2794	N2794	N2794	X2703	X2604	Q2475	GLY	D2320	L2124	GLU	E2047	R1964	GLU	L1798
K2795	N2734	N2734	X2735	X2605	L2476	VAL	I2321	L2124	GLU	GLU	Y1965	GLU	S1799
F2735	F2735	F2735	X2736	X2606	P2477	ARG	C2326	Q2127	GLU	GLU	K1968	GLU	P1803
D2736	D2736	D2736	X2737	X2607	L2477	ARG	G2327	Y2128	GLU	GLU	L1969	GLU	L1804
Y2737	Y2737	Y2737	X2738	X2608	L2478	ARG	R2330	Q2127	GLU	GLU	Q1970	GLU	E1805
R2738	R2738	R2738	X2739	X2609	L2479	ASP	G2327	Y2128	GLU	GLU	Q1973	GLU	A1806
P2739	P2739	P2739	X2740	X2610	X2487	ARG	R2330	G2132	GLU	PRO	GLU	ASP	L1807
V2740	V2740	V2740	X2741	X2611	X2488	ARG	R2330	G2132	GLU	GLU	GLU	GLU	R1808
E2741	E2741	E2741	X2742	X2612	X2489	ARG	Y2331	R2136	GLU	GLU	Y1976	GLU	L1812
T2742	T2742	T2742	X2743	X2613	X2490	ARG	L2332	R2140	GLU	GLU	Y1977	GLU	R1813
L2743	L2743	L2743	X2744	X2614	X2503	HIS	L2335	A2141	GLU	GLU	A1978	GLU	M1814
N2744	N2744	N2744	X2745	X2615	GLY	GLY	L2335	S2147	GLU	GLU	M1981	GLU	L1815
V2745	V2745	V2745	X2746	X2616	GLU	GLU	A2338	R2147	GLU	GLU	R1982	GLU	G1822
Y2746	Y2746	Y2746	X2747	X2617	GLU	GLU	V2339	S2147	GLU	GLU	A1983	GLU	G1823
L2747	L2747	L2747	X2748	X2618	GLU	GLU	F2340	L2155	GLU	GLU	F1984	GLU	Q1824
P2748	P2748	P2748	X2749	X2619	GLU	GLU	V2341	L2155	GLU	GLU	T1985	GLU	Q1824
E2749	E2749	E2749	X2750	X2620	GLU	GLU	N2342	C2158	GLU	GLU	S1987	GLU	H1825
K2750	K2750	K2750	X2751	X2621	GLU	GLU	G2343	C2158	GLU	GLU	M1986	GLU	D1828
L2751	L2751	L2751	X2752	X2622	N2414	R2415	E2344	R2163	GLU	GLU	F1987	GLU	P1829
D2752	D2752	D2752	X2753	X2623	R2415	R2415	S2345	L2166	GLU	GLU	A1988	GLU	V1830
S2753	S2753	S2753	X2754	X2624	H2420	A2428	E2347	L2166	GLU	GLU	A1989	GLU	F1838
F2754	F2754	F2754	X2755	X2625	A2428	A2428	N2349	Q2169	GLU	GLU	E1990	GLU	V1839
L2755	L2755	L2755	X2756	X2626	L2432	L2432	A2350	M2170	GLU	GLU	T1991	GLU	P1840
N2756	N2756	N2756	X2757	X2627	L2432	L2432	N2351	M2170	GLU	GLU	F1998	GLU	V1841
K2757	K2757	K2757	X2758	X2628	C2436	C2436	R2355	Q2173	GLU	GLU	P2002	GLU	L1842
F2758	F2758	F2758	X2759	X2629	A2437	A2437	L2356	Q2173	GLU	GLU	E2003	GLU	K1843
A2759	A2759	A2759	X2760	X2630	P2438	P2438	R2359	Q2180	GLU	GLU	Q2005	GLU	L1844
E2760	E2760	E2760	X2761	X2631	H2441	H2441	K2360	N2184	GLU	GLU	Q2006	GLU	L1848
Y2761	Y2761	Y2761	X2762	X2632	H2441	H2441	L2366	Q2180	GLU	GLU	N2007	GLU	L1848
T2762	T2762	T2762	X2763	X2633	A2445	A2445	R2361	Q2180	GLU	GLU	W2008	GLU	G1852
H2763	H2763	H2763	X2764	X2634	G2446	G2446	E2362	N2187	GLU	GLU	L2009	GLU	I1853
K2764	K2764	K2764	X2765	X2635	K2447	K2447	C2363	N2187	GLU	GLU	L2010	GLU	D1856
E2765	E2765	E2765	X2766	X2636	X2564	X2564	F2364	N2187	GLU	GLU	E1857	GLU	E1857
Y2766	Y2766	Y2766	X2767	X2637	X2564	X2564			GLU	GLU		GLU	
A2767	A2767	A2767	X2768	X2638	X2564	X2564			GLU	GLU		GLU	
F2768	F2768	F2768	X2769	X2639	X2564	X2564			GLU	GLU		GLU	
K2770	K2770	K2770	X2770	X2640	X2564	X2564			GLU	GLU		GLU	
L2771	L2771	L2771	X2771	X2641	X2564	X2564			GLU	GLU		GLU	
Q2772	Q2772	Q2772	X2772	X2642	X2564	X2564			GLU	GLU		GLU	
N2773	N2773	N2773	X2773	X2643	X2564	X2564			GLU	GLU		GLU	

F4128	F4129	N4130	R4131	F4132	Q4133	R4137	D4138	N4142	V4145	L4146	L4147	L4150	S4151	H4152	H4153	V4154	H4155	H4156	R4159	L4164	S4169	E4172	Y4173	F4174	R4175	R4180	T4181	E4182	R4188	R4192	T4193	Y4194	T4200	N4201	Q4204	R4215	T4218	E4224	Q4225	Q4226	E4227	N4228	E4229	E4127																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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T3864	V3865	I3866	N3867	K3868	Q3869	N3870	G3871	E3872	K3873	V3874	M3875	D3876	D3877	E3878	F3885	R3886	F3887	L3888	Q3889	L3890	L3891	C3892	E3893	N3896	N3897	D3898	F3899	Q3900	N3901	Y3902	Q3906	T3912	Y3922	L3926	Q3927	E3928	S3929	I3930	S3931	D3932	W3935	Y3936	Y3937	S3938	G3939	K3940	D3941	E3945	Q3946																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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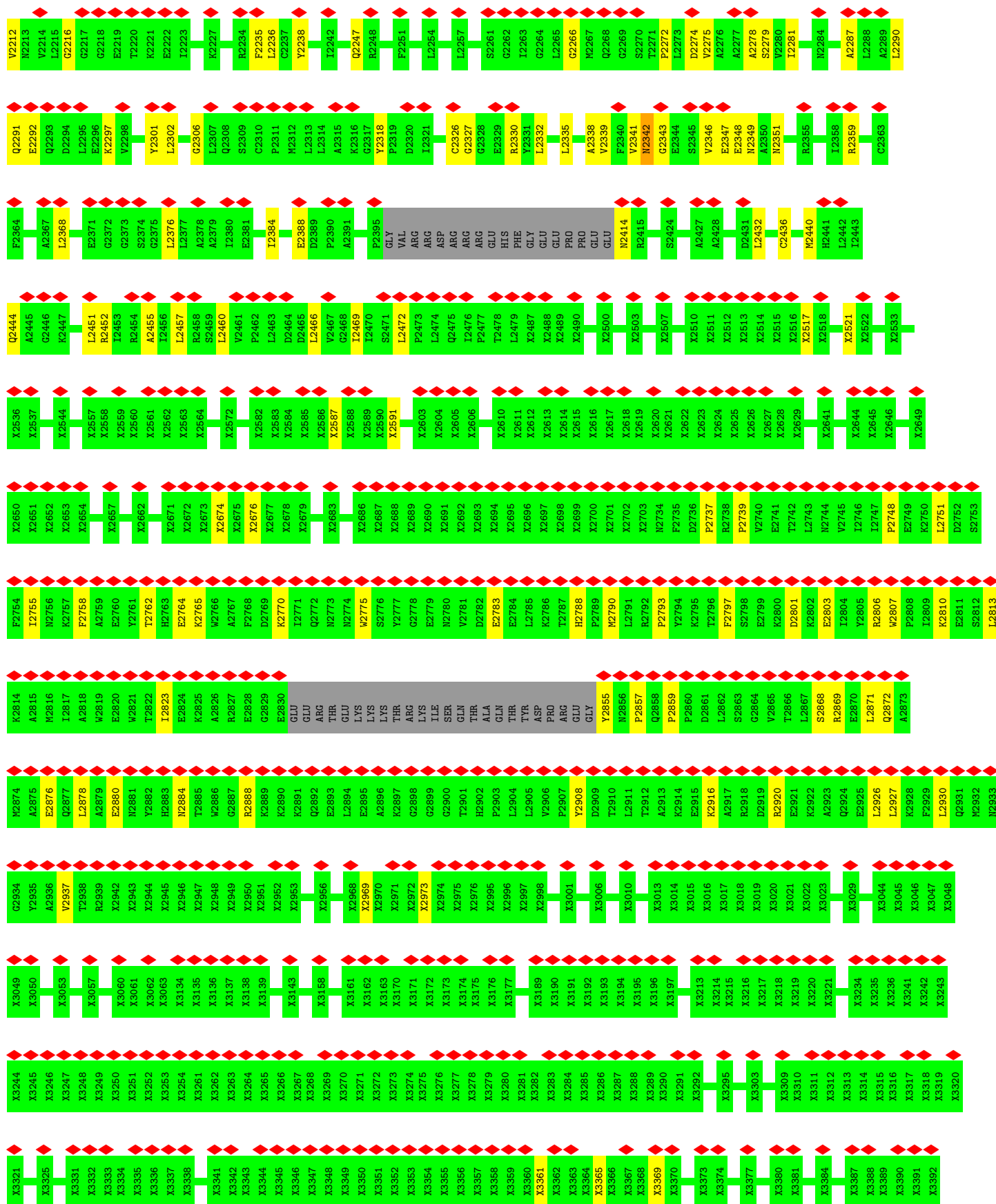


● Molecule 1: Ryanodine receptor 1

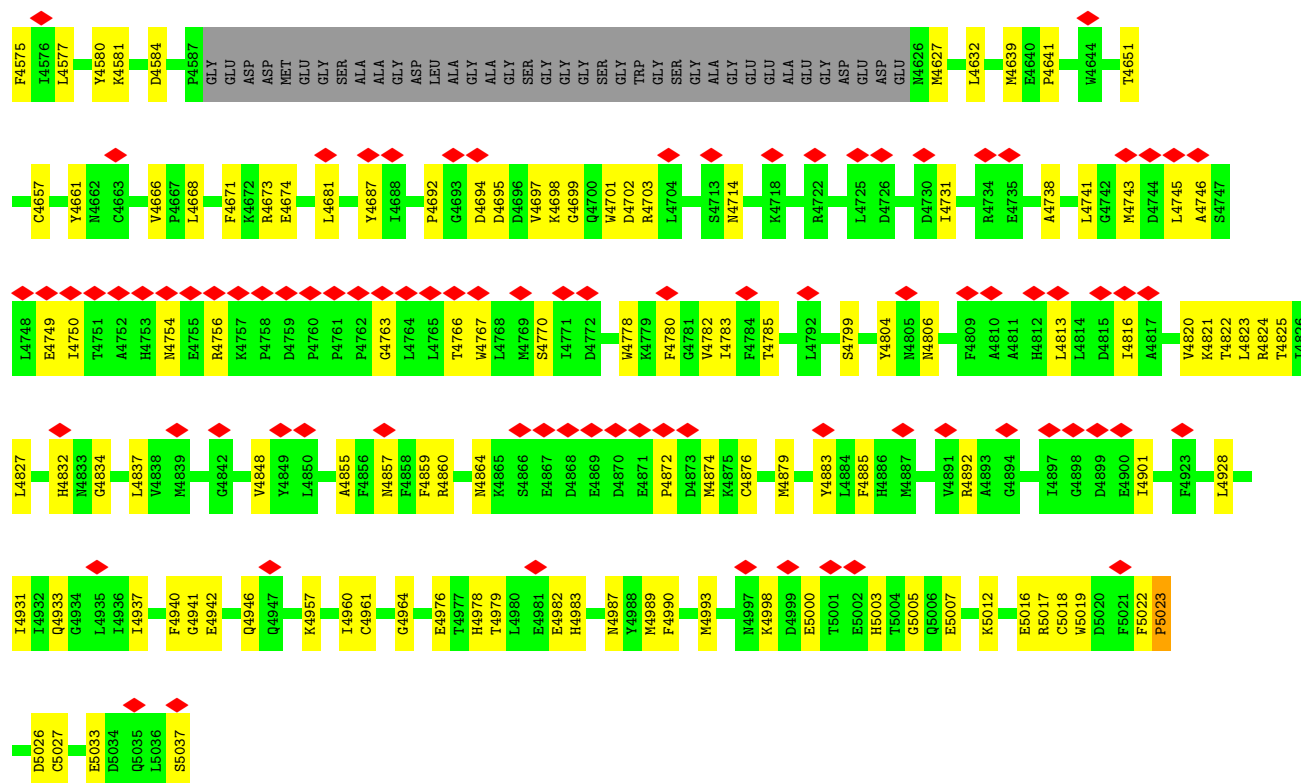




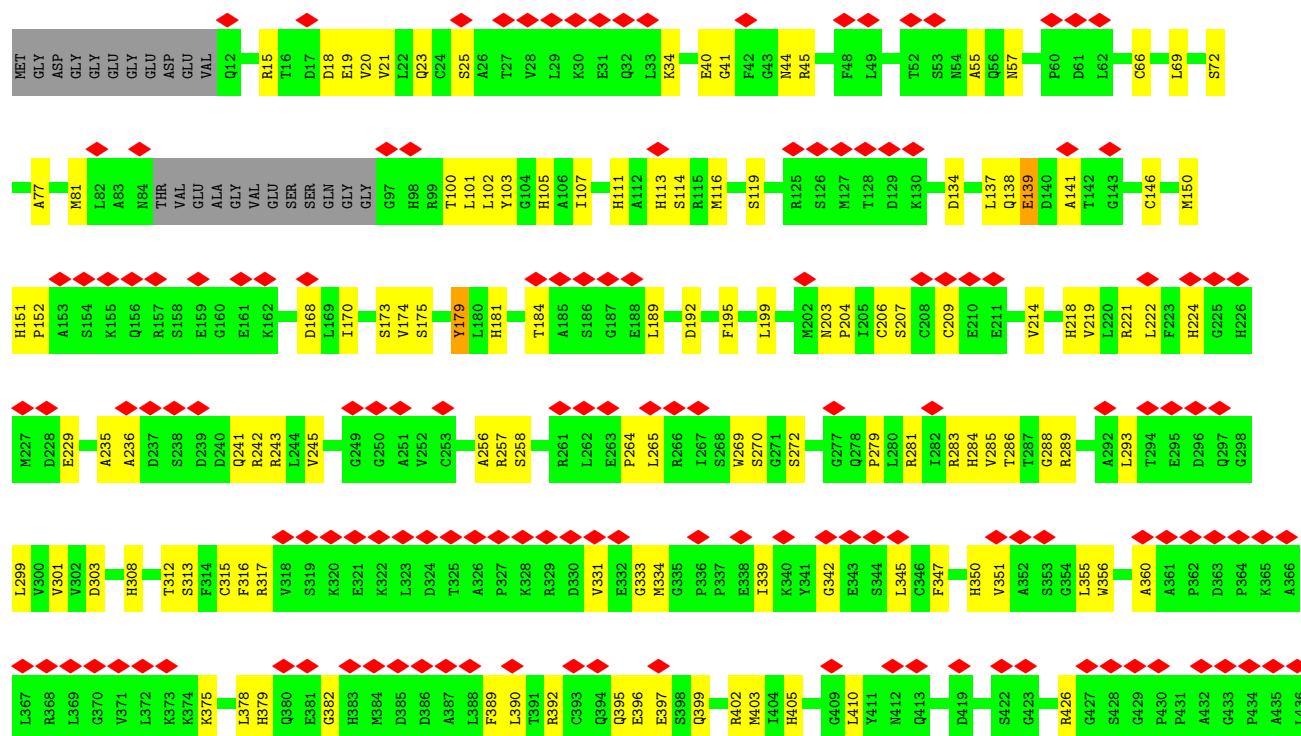


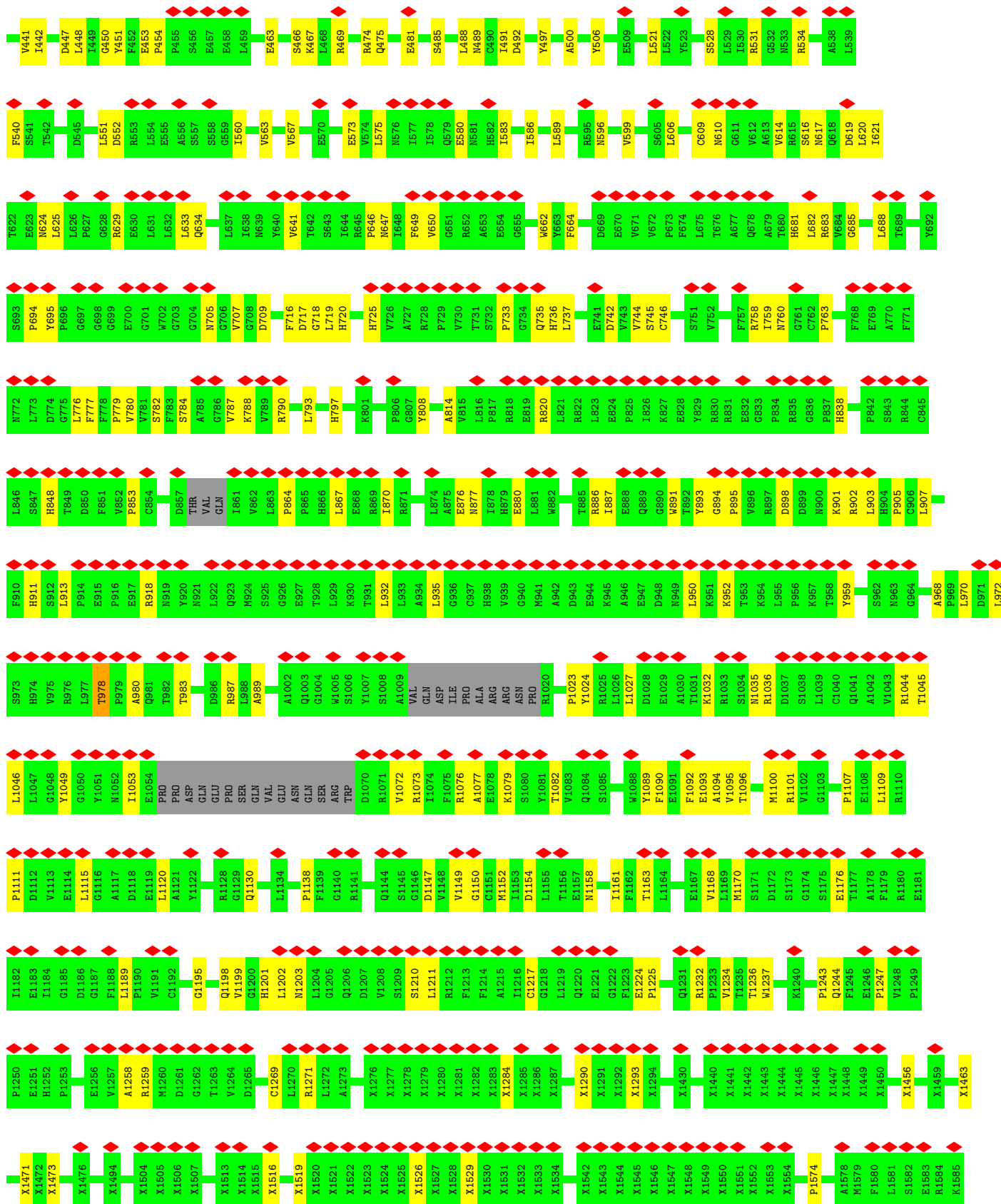






• Molecule 1: Ryanodine receptor 1

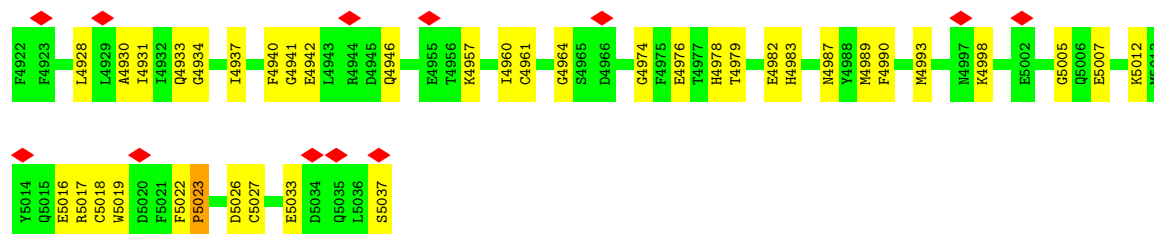




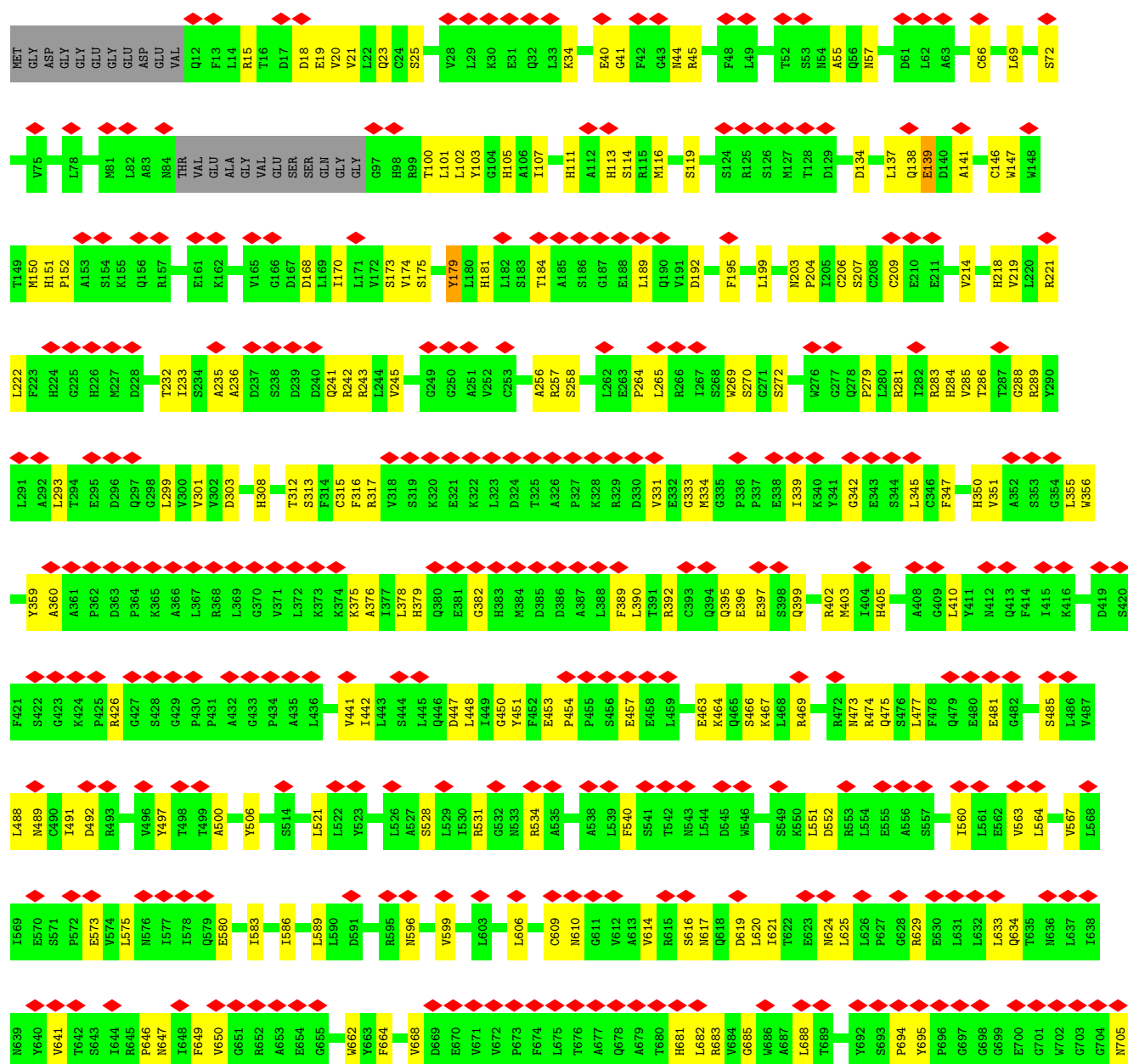
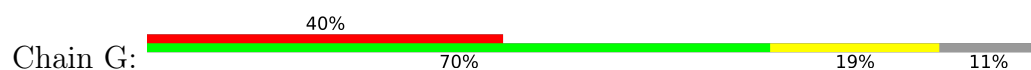








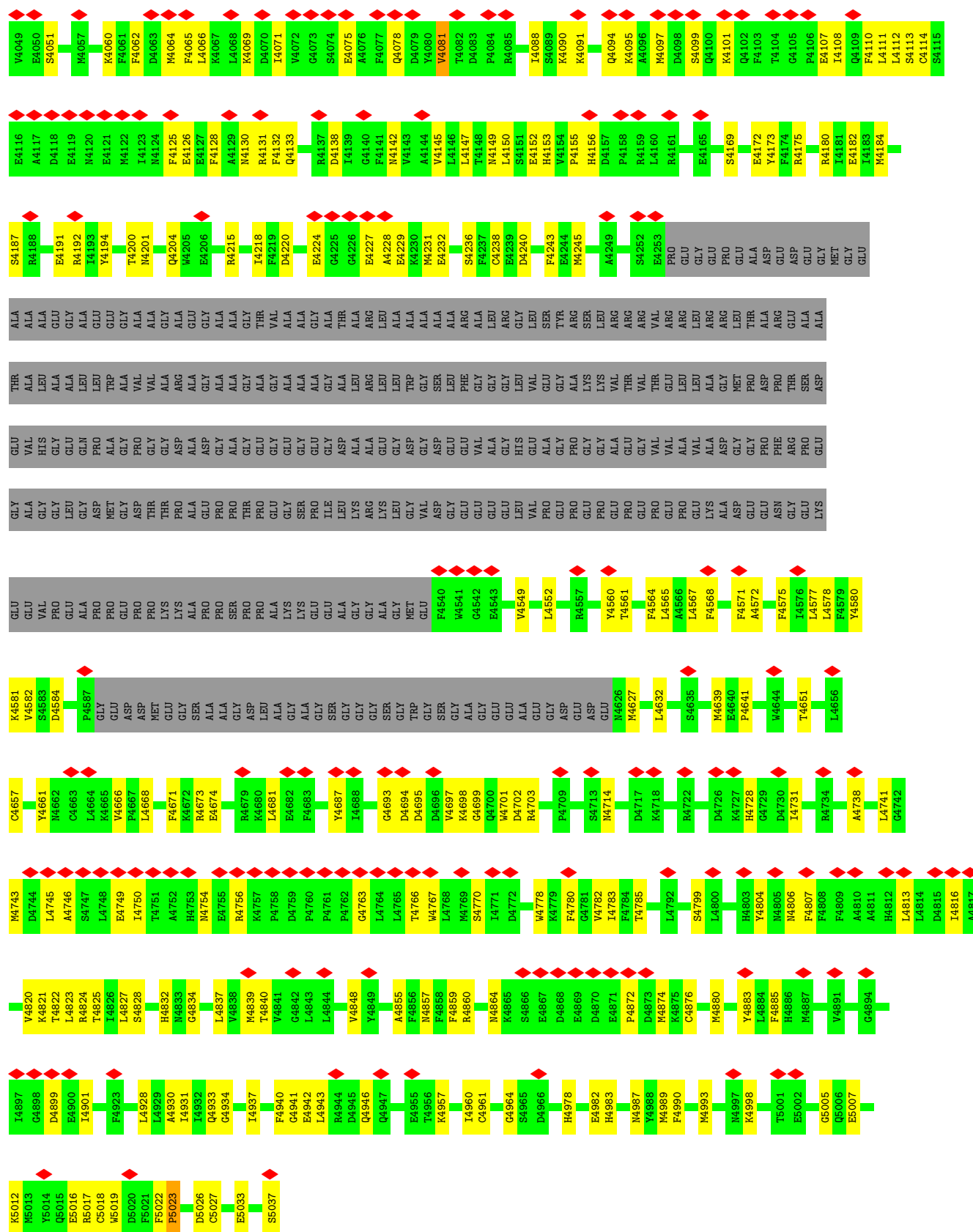
• Molecule 1: Ryanodine receptor 1

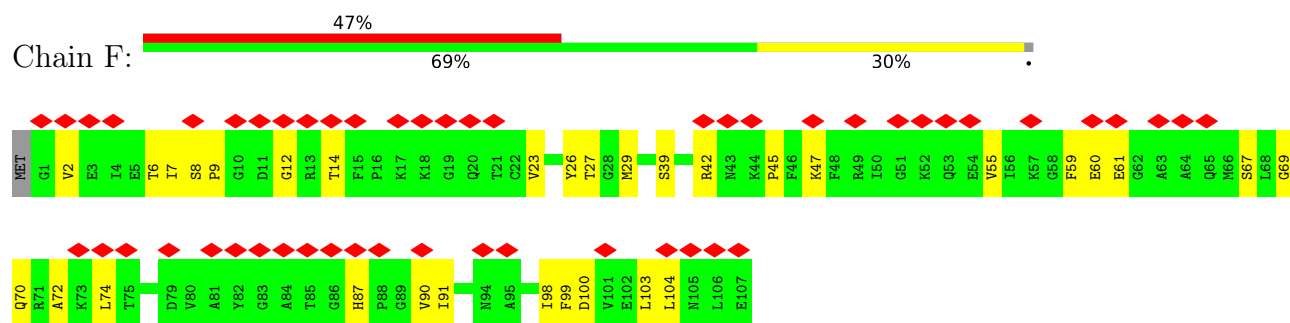




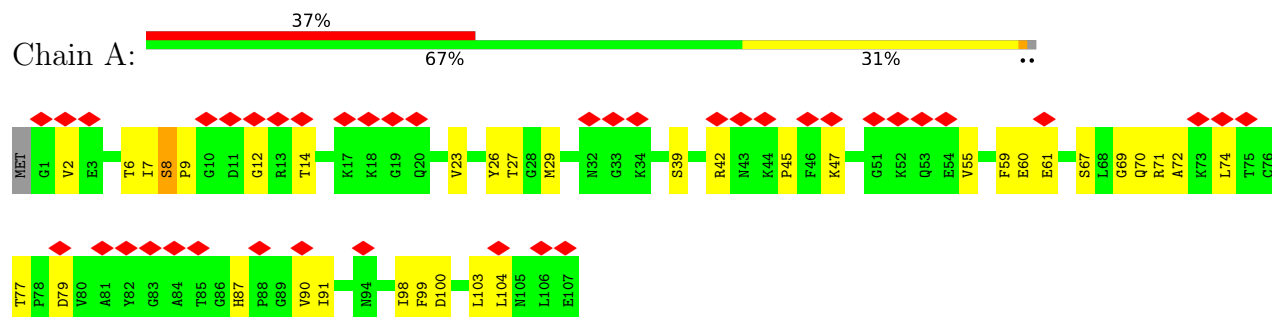


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X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3029	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142	X3143	X3158	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3186	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197										
A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	R2929	L2930	Q2931	M2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2961	X2964	X2965	X2968	X2971	X2972	X2975	X2976	X2995	V2996	X2997	X2998	X3010	X3013	X3014	X3015									
P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916		
F2797	S2798	E2799	K2800	D2801	K2802	E2803	T2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	W2816	L2817	L2818	K2819	E2820	K2821	T2822	E2823	E2824	K2825	A2826	K2827	E2828	G2829	E2830	GLU	GLU	THR	GLU	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856		

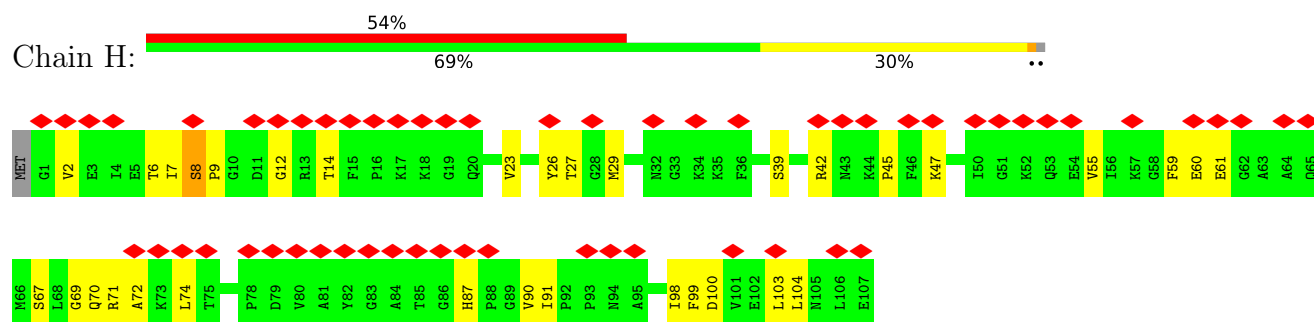




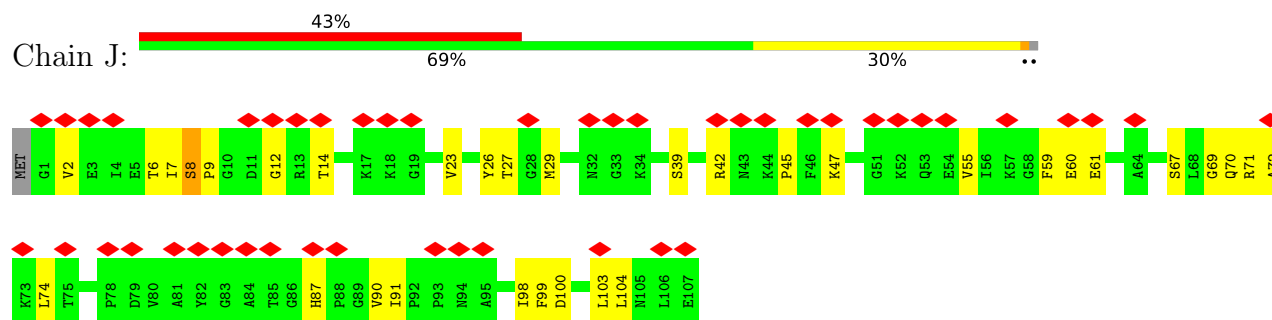
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.535	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.166	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	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	B	0.30	0/25428	0.66	13/34534 (0.0%)
1	E	0.30	0/25428	0.66	11/34534 (0.0%)
1	G	0.30	0/25428	0.66	15/34534 (0.0%)
1	I	0.30	0/25428	0.66	13/34534 (0.0%)
2	A	0.27	0/834	0.62	1/1123 (0.1%)
2	F	0.27	0/834	0.63	1/1123 (0.1%)
2	H	0.27	0/834	0.62	1/1123 (0.1%)
2	J	0.27	0/834	0.62	1/1123 (0.1%)
All	All	0.30	0/105048	0.66	56/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	22
1	E	0	22
1	G	0	22
1	I	0	22
All	All	0	88

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4153	HIS	CA-C-N	-7.64	116.68	123.33
1	B	4153	HIS	C-N-CA	-7.64	116.68	123.33
1	E	4153	HIS	CA-C-N	-7.57	116.74	123.33
1	E	4153	HIS	C-N-CA	-7.57	116.74	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4153	HIS	CA-C-N	-7.56	116.75	123.33
1	G	4153	HIS	C-N-CA	-7.56	116.75	123.33
1	I	4153	HIS	CA-C-N	-7.52	116.79	123.33
1	I	4153	HIS	C-N-CA	-7.52	116.79	123.33
1	I	4872	PRO	N-CA-C	-7.46	103.15	113.53
1	E	4872	PRO	N-CA-C	-7.44	103.19	113.53
1	G	4872	PRO	N-CA-C	-7.43	103.19	113.53
1	B	4872	PRO	N-CA-C	-7.43	103.20	113.53
2	A	8	SER	N-CA-C	5.70	121.38	113.45
2	J	8	SER	N-CA-C	5.67	121.34	113.45
2	H	8	SER	N-CA-C	5.66	121.32	113.45
2	F	8	SER	N-CA-C	5.66	121.31	113.45
1	B	4695	ASP	N-CA-C	-5.39	101.44	109.96
1	E	4695	ASP	N-CA-C	-5.37	101.47	109.96
1	G	4695	ASP	N-CA-C	-5.37	101.47	109.96
1	I	4695	ASP	N-CA-C	-5.35	101.51	109.96
1	I	1828	ASP	CA-C-N	5.31	125.30	119.89
1	I	1828	ASP	C-N-CA	5.31	125.30	119.89
1	B	1829	PRO	N-CA-C	5.30	119.54	111.11
1	G	1829	PRO	N-CA-C	5.30	119.53	111.11
1	E	1828	ASP	CA-C-N	5.27	125.27	119.89
1	E	1828	ASP	C-N-CA	5.27	125.27	119.89
1	E	1829	PRO	N-CA-C	5.25	119.46	111.11
1	I	1829	PRO	N-CA-C	5.25	119.45	111.11
1	B	1828	ASP	CA-C-N	5.22	125.22	119.89
1	B	1828	ASP	C-N-CA	5.22	125.22	119.89
1	I	2291	GLN	CA-C-N	5.22	135.41	126.32
1	I	2291	GLN	C-N-CA	5.22	135.41	126.32
1	E	2291	GLN	CA-C-N	5.22	135.40	126.32
1	E	2291	GLN	C-N-CA	5.22	135.40	126.32
1	G	1828	ASP	CA-C-N	5.22	125.21	119.89
1	G	1828	ASP	C-N-CA	5.22	125.21	119.89
1	B	2291	GLN	CA-C-N	5.20	135.37	126.32
1	B	2291	GLN	C-N-CA	5.20	135.37	126.32
1	E	4639	MET	CA-C-N	5.20	134.50	121.80
1	E	4639	MET	C-N-CA	5.20	134.50	121.80
1	G	2291	GLN	CA-C-N	5.19	135.35	126.32
1	G	2291	GLN	C-N-CA	5.19	135.35	126.32
1	G	4639	MET	CA-C-N	5.19	134.47	121.80
1	G	4639	MET	C-N-CA	5.19	134.47	121.80
1	B	4639	MET	CA-C-N	5.18	134.45	121.80
1	B	4639	MET	C-N-CA	5.18	134.45	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	4639	MET	CA-C-N	5.17	134.41	121.80
1	I	4639	MET	C-N-CA	5.17	134.41	121.80
1	G	1838	PHE	CA-C-N	5.04	131.45	122.13
1	G	1838	PHE	C-N-CA	5.04	131.45	122.13
1	B	1838	PHE	CA-C-N	5.03	131.44	122.13
1	B	1838	PHE	C-N-CA	5.03	131.44	122.13
1	I	4693	GLY	CA-C-N	5.03	131.14	121.54
1	I	4693	GLY	C-N-CA	5.03	131.14	121.54
1	G	4693	GLY	CA-C-N	5.03	131.14	121.54
1	G	4693	GLY	C-N-CA	5.03	131.14	121.54

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	GLU	Peptide
1	B	1676	LEU	Peptide
1	B	1690	ASP	Peptide
1	B	1712	TYR	Peptide
1	B	179	TYR	Peptide
1	B	1828	ASP	Peptide
1	B	1840	PRO	Peptide
1	B	2169	GLN	Peptide
1	B	2292	GLU	Peptide
1	B	2342	ASN	Peptide
1	B	2343	GLY	Peptide
1	B	2472	LEU	Peptide
1	B	2807	TRP	Peptide
1	B	3760	LYS	Peptide
1	B	3771	HIS	Peptide
1	B	3786	CYS	Peptide
1	B	3971	GLY	Peptide
1	B	4666	VAL	Peptide
1	B	4694	ASP	Peptide
1	B	552	ASP	Peptide
1	B	694	PRO	Peptide
1	B	808	TYR	Peptide
1	E	139	GLU	Peptide
1	E	1676	LEU	Peptide
1	E	1690	ASP	Peptide
1	E	1712	TYR	Peptide
1	E	179	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	E	1828	ASP	Peptide
1	E	1840	PRO	Peptide
1	E	2169	GLN	Peptide
1	E	2292	GLU	Peptide
1	E	2342	ASN	Peptide
1	E	2343	GLY	Peptide
1	E	2472	LEU	Peptide
1	E	2807	TRP	Peptide
1	E	3760	LYS	Peptide
1	E	3771	HIS	Peptide
1	E	3786	CYS	Peptide
1	E	3971	GLY	Peptide
1	E	4666	VAL	Peptide
1	E	4694	ASP	Peptide
1	E	552	ASP	Peptide
1	E	694	PRO	Peptide
1	E	808	TYR	Peptide
1	G	139	GLU	Peptide
1	G	1676	LEU	Peptide
1	G	1690	ASP	Peptide
1	G	1712	TYR	Peptide
1	G	179	TYR	Peptide
1	G	1828	ASP	Peptide
1	G	1840	PRO	Peptide
1	G	2169	GLN	Peptide
1	G	2292	GLU	Peptide
1	G	2342	ASN	Peptide
1	G	2343	GLY	Peptide
1	G	2472	LEU	Peptide
1	G	2807	TRP	Peptide
1	G	3760	LYS	Peptide
1	G	3771	HIS	Peptide
1	G	3786	CYS	Peptide
1	G	3971	GLY	Peptide
1	G	4666	VAL	Peptide
1	G	4694	ASP	Peptide
1	G	552	ASP	Peptide
1	G	694	PRO	Peptide
1	G	808	TYR	Peptide
1	I	139	GLU	Peptide
1	I	1676	LEU	Peptide
1	I	1690	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	I	1712	TYR	Peptide
1	I	179	TYR	Peptide
1	I	1828	ASP	Peptide
1	I	1840	PRO	Peptide
1	I	2169	GLN	Peptide
1	I	2292	GLU	Peptide
1	I	2342	ASN	Peptide
1	I	2343	GLY	Peptide
1	I	2472	LEU	Peptide
1	I	2807	TRP	Peptide
1	I	3760	LYS	Peptide
1	I	3771	HIS	Peptide
1	I	3786	CYS	Peptide
1	I	3971	GLY	Peptide
1	I	4666	VAL	Peptide
1	I	4694	ASP	Peptide
1	I	552	ASP	Peptide
1	I	694	PRO	Peptide
1	I	808	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	29369	0	24717	514	0
1	E	29369	0	24716	515	0
1	G	29369	0	24717	527	0
1	I	29369	0	24717	516	0
2	A	818	0	824	20	0
2	F	818	0	824	19	0
2	H	818	0	824	19	0
2	J	818	0	824	19	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102163	2122	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (2122) 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:G:2318:TYR:HH	1:G:2414:ASN:N	1.80	0.79
1:I:2318:TYR:HH	1:I:2414:ASN:N	1.80	0.79
1:E:2318:TYR:HH	1:E:2414:ASN:N	1.81	0.79
1:B:2318:TYR:HH	1:B:2414:ASN:N	1.81	0.79
1:E:179:TYR:OH	1:G:2359:ARG:NH1	2.18	0.76
1:E:4674:GLU:HG3	1:E:4714:ASN:HB3	1.73	0.71
1:E:4731:ILE:HA	1:G:4101:LYS:HG3	1.71	0.71
1:B:4674:GLU:HG3	1:B:4714:ASN:HB3	1.73	0.70
1:G:4674:GLU:HG3	1:G:4714:ASN:HB3	1.73	0.70
1:G:1671:ARG:NH2	1:G:1710:GLY:O	2.25	0.70
1:I:4674:GLU:HG3	1:I:4714:ASN:HB3	1.73	0.69
1:E:1671:ARG:NH2	1:E:1710:GLY:O	2.25	0.69
1:I:1671:ARG:NH2	1:I:1710:GLY:O	2.25	0.69
1:B:1671:ARG:NH2	1:B:1710:GLY:O	2.25	0.69
1:G:4855:ALA:HA	1:G:4859:PHE:HB2	1.75	0.69
1:I:4855:ALA:HA	1:I:4859:PHE:HB2	1.75	0.69
1:B:2266:GLY:O	1:B:2330:ARG:NH2	2.27	0.68
1:B:4855:ALA:HA	1:B:4859:PHE:HB2	1.75	0.68
1:E:4855:ALA:HA	1:E:4859:PHE:HB2	1.75	0.68
1:I:219:VAL:HG13	1:I:285:VAL:HG21	1.75	0.68
1:G:646:PRO:HD2	1:G:779:PRO:HB2	1.76	0.68
1:I:2266:GLY:O	1:I:2330:ARG:NH2	2.27	0.68
1:G:2266:GLY:O	1:G:2330:ARG:NH2	2.26	0.68
1:E:646:PRO:HD2	1:E:779:PRO:HB2	1.76	0.67
1:B:219:VAL:HG13	1:B:285:VAL:HG21	1.75	0.67
1:E:219:VAL:HG13	1:E:285:VAL:HG21	1.75	0.67
1:B:788:LYS:HG2	1:B:1630:CYS:H	1.59	0.67
1:E:2266:GLY:O	1:E:2330:ARG:NH2	2.27	0.67
1:I:646:PRO:HD2	1:I:779:PRO:HB2	1.76	0.67
1:E:788:LYS:HG2	1:E:1630:CYS:H	1.59	0.67
1:G:331:VAL:HG12	1:G:333:GLY:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:PRO:HD2	1:B:779:PRO:HB2	1.76	0.67
1:G:219:VAL:HG13	1:G:285:VAL:HG21	1.75	0.67
1:I:331:VAL:HG12	1:I:333:GLY:H	1.60	0.66
1:E:331:VAL:HG12	1:E:333:GLY:H	1.60	0.66
1:G:788:LYS:HG2	1:G:1630:CYS:H	1.59	0.66
1:B:151:HIS:HB2	1:B:170:ILE:HB	1.78	0.66
1:I:788:LYS:HG2	1:I:1630:CYS:H	1.59	0.65
1:B:103:TYR:HB3	1:B:152:PRO:HD3	1.79	0.65
1:B:2755:ILE:HD13	1:B:2810:LYS:HG2	1.77	0.65
1:G:2755:ILE:HD13	1:G:2810:LYS:HG2	1.78	0.65
1:I:1092:PHE:HB3	1:I:1149:VAL:HB	1.77	0.65
1:E:2755:ILE:HD13	1:E:2810:LYS:HG2	1.77	0.65
1:E:1777:PHE:HA	1:E:1799:SER:HB2	1.78	0.65
1:I:103:TYR:HB3	1:I:152:PRO:HD3	1.79	0.65
1:I:151:HIS:HB2	1:I:170:ILE:HB	1.78	0.65
1:I:2755:ILE:HD13	1:I:2810:LYS:HG2	1.78	0.65
1:G:103:TYR:HB3	1:G:152:PRO:HD3	1.79	0.65
1:G:742:ASP:HA	1:G:760:ASN:HD21	1.62	0.65
1:E:103:TYR:HB3	1:E:152:PRO:HD3	1.79	0.65
1:G:1092:PHE:HB3	1:G:1149:VAL:HB	1.77	0.65
1:B:331:VAL:HG12	1:B:333:GLY:H	1.60	0.65
1:B:1092:PHE:HB3	1:B:1149:VAL:HB	1.77	0.65
1:E:4961:CYS:SG	1:E:4978:HIS:NE2	2.70	0.65
1:E:2287:ALA:HA	1:E:2290:LEU:HD13	1.79	0.64
1:I:1519:UNK:HA	1:I:1526:UNK:HA	1.79	0.64
1:E:745:SER:HB2	1:E:758:ARG:HB3	1.79	0.64
1:G:4961:CYS:SG	1:G:4978:HIS:NE2	2.70	0.64
1:B:1777:PHE:HA	1:B:1799:SER:HB2	1.78	0.64
1:E:151:HIS:HB2	1:E:170:ILE:HB	1.79	0.64
1:I:742:ASP:HA	1:I:760:ASN:HD21	1.62	0.64
1:B:4813:LEU:HD12	1:B:4816:ILE:HD11	1.79	0.64
1:I:1777:PHE:HA	1:I:1799:SER:HB2	1.78	0.64
1:G:151:HIS:HB2	1:G:170:ILE:HB	1.79	0.64
1:G:4813:LEU:HD12	1:G:4816:ILE:HD11	1.79	0.64
1:B:742:ASP:HA	1:B:760:ASN:HD21	1.62	0.64
1:E:742:ASP:HA	1:E:760:ASN:HD21	1.62	0.64
1:E:1092:PHE:HB3	1:E:1149:VAL:HB	1.77	0.64
1:I:2287:ALA:HA	1:I:2290:LEU:HD13	1.79	0.64
1:G:745:SER:HB2	1:G:758:ARG:HB3	1.79	0.64
1:G:1777:PHE:HA	1:G:1799:SER:HB2	1.78	0.64
1:G:2095:GLN:O	1:G:2127:GLN:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2876:GLU:OE1	1:G:2920:ARG:NH2	2.31	0.64
1:B:745:SER:HB2	1:B:758:ARG:HB3	1.79	0.64
1:G:1519:UNK:HA	1:G:1526:UNK:HA	1.80	0.64
1:B:4961:CYS:SG	1:B:4978:HIS:NE2	2.71	0.63
1:E:1079:LYS:NZ	1:E:1107:PRO:O	2.31	0.63
1:I:745:SER:HB2	1:I:758:ARG:HB3	1.79	0.63
1:I:4961:CYS:SG	1:I:4978:HIS:NE2	2.71	0.63
1:B:1079:LYS:NZ	1:B:1107:PRO:O	2.31	0.63
1:E:4813:LEU:HD12	1:E:4816:ILE:HD11	1.79	0.63
1:I:2095:GLN:O	1:I:2127:GLN:NE2	2.31	0.63
1:I:1079:LYS:NZ	1:I:1107:PRO:O	2.31	0.63
2:F:26:TYR:OH	2:F:42:ARG:NH2	2.32	0.63
1:G:454:PRO:HG2	1:G:531:ARG:HH12	1.64	0.63
2:H:74:LEU:HB2	2:H:99:PHE:HB2	1.80	0.63
1:I:2876:GLU:OE1	1:I:2920:ARG:NH2	2.31	0.63
2:A:26:TYR:OH	2:A:42:ARG:NH2	2.32	0.63
1:B:853:PRO:HB3	1:B:1024:TYR:H	1.64	0.63
1:I:4807:PHE:HZ	1:G:4857:ASN:HB2	1.64	0.63
1:G:853:PRO:HB3	1:G:1024:TYR:H	1.64	0.63
1:B:2876:GLU:OE1	1:B:2920:ARG:NH2	2.31	0.63
1:E:454:PRO:HG2	1:E:531:ARG:HH12	1.64	0.63
1:I:454:PRO:HG2	1:I:531:ARG:HH12	1.64	0.63
1:G:2287:ALA:HA	1:G:2290:LEU:HD13	1.79	0.63
1:B:454:PRO:HG2	1:B:531:ARG:HH12	1.64	0.62
1:E:2876:GLU:OE1	1:E:2920:ARG:NH2	2.31	0.62
1:I:101:LEU:HB3	1:I:150:MET:HE1	1.81	0.62
1:G:1079:LYS:NZ	1:G:1107:PRO:O	2.31	0.62
1:B:101:LEU:HB3	1:B:150:MET:HE1	1.81	0.62
2:F:74:LEU:HB2	2:F:99:PHE:HB2	1.80	0.62
2:A:6:THR:HA	2:A:72:ALA:HA	1.82	0.62
1:B:609:CYS:SG	1:B:610:ASN:N	2.72	0.62
1:B:3993:LEU:HA	1:B:3996:PHE:HB2	1.82	0.62
1:E:2095:GLN:O	1:E:2127:GLN:NE2	2.31	0.62
1:G:101:LEU:HB3	1:G:150:MET:HE1	1.81	0.62
1:G:609:CYS:SG	1:G:610:ASN:N	2.72	0.62
2:H:26:TYR:OH	2:H:42:ARG:NH2	2.32	0.62
1:B:2287:ALA:HA	1:B:2290:LEU:HD13	1.79	0.62
1:I:609:CYS:SG	1:I:610:ASN:N	2.72	0.62
1:I:4892:ARG:NH2	1:G:4899:ASP:OD1	2.28	0.62
1:E:606:LEU:O	1:E:617:ASN:ND2	2.33	0.62
1:I:606:LEU:O	1:I:617:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:74:LEU:HB2	2:J:99:PHE:HB2	1.80	0.62
1:B:2095:GLN:O	1:B:2127:GLN:NE2	2.31	0.62
1:E:101:LEU:HB3	1:E:150:MET:HE1	1.81	0.62
1:I:4813:LEU:HD12	1:I:4816:ILE:HD11	1.79	0.62
1:E:853:PRO:HB3	1:E:1024:TYR:H	1.64	0.62
1:E:3993:LEU:HA	1:E:3996:PHE:HB2	1.82	0.62
1:G:3993:LEU:HA	1:G:3996:PHE:HB2	1.82	0.62
1:B:606:LEU:O	1:B:617:ASN:ND2	2.33	0.62
1:E:3937:TYR:O	1:E:4002:LYS:NZ	2.33	0.62
1:I:3973:CYS:SG	1:I:3976:ASN:ND2	2.73	0.62
1:G:606:LEU:O	1:G:617:ASN:ND2	2.33	0.62
1:I:853:PRO:HB3	1:I:1024:TYR:H	1.64	0.61
2:J:6:THR:HA	2:J:72:ALA:HA	1.82	0.61
2:J:26:TYR:OH	2:J:42:ARG:NH2	2.32	0.61
1:I:1244:GLN:HB3	1:I:1646:ARG:HH12	1.65	0.61
1:G:3937:TYR:O	1:G:4002:LYS:NZ	2.33	0.61
1:G:3973:CYS:SG	1:G:3976:ASN:ND2	2.73	0.61
1:B:1244:GLN:HB3	1:B:1646:ARG:HH12	1.65	0.61
1:B:3937:TYR:O	1:B:4002:LYS:NZ	2.33	0.61
2:H:6:THR:HA	2:H:72:ALA:HA	1.82	0.61
1:B:3973:CYS:SG	1:B:3976:ASN:ND2	2.73	0.61
1:E:609:CYS:SG	1:E:610:ASN:N	2.72	0.61
1:E:1247:PRO:HA	1:E:1598:GLN:HA	1.83	0.61
1:I:3937:TYR:O	1:I:4002:LYS:NZ	2.33	0.61
2:A:74:LEU:HB2	2:A:99:PHE:HB2	1.80	0.61
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.83	0.61
1:B:575:LEU:HD22	1:B:609:CYS:HB3	1.83	0.61
1:G:4673:ARG:HH22	1:G:4698:LYS:HB2	1.66	0.61
2:J:87:HIS:N	2:J:91:ILE:O	2.34	0.61
1:B:1808:ARG:NH1	1:B:1853:ILE:O	2.34	0.60
1:I:575:LEU:HD22	1:I:609:CYS:HB3	1.83	0.60
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.83	0.60
2:F:87:HIS:N	2:F:91:ILE:O	2.34	0.60
2:F:6:THR:HA	2:F:72:ALA:HA	1.82	0.60
2:A:87:HIS:N	2:A:91:ILE:O	2.34	0.60
1:B:1247:PRO:HA	1:B:1598:GLN:HA	1.83	0.60
1:E:4673:ARG:HH22	1:E:4698:LYS:HB2	1.66	0.60
1:I:1203:ASN:ND2	1:I:1210:SER:O	2.35	0.60
1:B:1203:ASN:ND2	1:B:1210:SER:O	2.34	0.60
1:E:3973:CYS:SG	1:E:3976:ASN:ND2	2.73	0.60
1:I:4673:ARG:HH22	1:I:4698:LYS:HB2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:GLY:O	1:G:45:ARG:NH1	2.35	0.60
1:G:1244:GLN:HB3	1:G:1646:ARG:HH12	1.65	0.60
1:I:1247:PRO:HA	1:I:1598:GLN:HA	1.83	0.60
1:B:1519:UNK:HA	1:B:1526:UNK:HA	1.84	0.60
1:E:1203:ASN:ND2	1:E:1210:SER:O	2.35	0.60
1:E:1244:GLN:HB3	1:E:1646:ARG:HH12	1.65	0.60
1:I:3993:LEU:HA	1:I:3996:PHE:HB2	1.82	0.60
1:G:1101:ARG:HE	1:G:1115:LEU:HB3	1.66	0.60
1:B:4741:LEU:HB2	1:B:4743:MET:HE2	1.83	0.60
1:E:575:LEU:HD22	1:E:609:CYS:HB3	1.82	0.60
1:B:4673:ARG:HH22	1:B:4698:LYS:HB2	1.66	0.60
1:E:1808:ARG:NH1	1:E:1853:ILE:O	2.34	0.60
1:I:4821:LYS:HA	1:I:4824:ARG:HE	1.67	0.60
2:A:23:VAL:HG22	2:A:47:LYS:HG2	1.83	0.60
2:H:87:HIS:N	2:H:91:ILE:O	2.34	0.60
1:B:2338:ALA:HB1	1:B:2349:ASN:HB3	1.84	0.60
1:E:4741:LEU:HB2	1:E:4743:MET:HE2	1.83	0.60
1:I:1808:ARG:NH1	1:I:1853:ILE:O	2.34	0.60
1:G:1808:ARG:NH1	1:G:1853:ILE:O	2.34	0.60
1:G:2748:PRO:HD2	1:G:2751:LEU:HD12	1.84	0.60
1:G:3762:ARG:H	1:G:4754:ASN:HA	1.67	0.60
1:G:4821:LYS:HA	1:G:4824:ARG:HE	1.67	0.60
1:B:256:ALA:HB1	1:B:286:THR:HG21	1.84	0.60
1:E:1101:ARG:HE	1:E:1115:LEU:HB3	1.66	0.60
1:I:1101:ARG:HE	1:I:1115:LEU:HB3	1.66	0.60
2:J:23:VAL:HG22	2:J:47:LYS:HG2	1.82	0.60
1:E:2338:ALA:HB1	1:E:2349:ASN:HB3	1.84	0.59
1:E:4821:LYS:HA	1:E:4824:ARG:HE	1.67	0.59
1:G:256:ALA:HB1	1:G:286:THR:HG21	1.83	0.59
1:G:1203:ASN:ND2	1:G:1210:SER:O	2.35	0.59
1:E:3762:ARG:H	1:E:4754:ASN:HA	1.67	0.59
1:I:2338:ALA:HB1	1:I:2349:ASN:HB3	1.84	0.59
1:I:4848:VAL:HG23	1:I:4883:TYR:HE1	1.66	0.59
1:G:575:LEU:HD22	1:G:609:CYS:HB3	1.83	0.59
1:B:4848:VAL:HG23	1:B:4883:TYR:HE1	1.66	0.59
1:E:1641:ILE:HG13	1:E:1643:GLU:H	1.68	0.59
1:I:41:GLY:O	1:I:45:ARG:NH1	2.35	0.59
2:F:90:VAL:HG12	2:F:91:ILE:HG12	1.84	0.59
1:E:41:GLY:O	1:E:45:ARG:NH1	2.35	0.59
1:E:175:SER:O	1:G:2452:ARG:NH1	2.32	0.59
1:E:718:GLY:HA3	1:E:737:LEU:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2359:ARG:NH1	1:G:179:TYR:OH	2.35	0.59
1:G:718:GLY:HA3	1:G:737:LEU:HA	1.84	0.59
1:G:1247:PRO:HA	1:G:1598:GLN:HA	1.83	0.59
1:G:315:CYS:SG	1:G:316:PHE:N	2.76	0.59
2:A:90:VAL:HG12	2:A:91:ILE:HG12	1.84	0.59
1:I:4238:CYS:HA	1:I:4989:MET:HE3	1.85	0.59
1:B:718:GLY:HA3	1:B:737:LEU:HA	1.84	0.59
1:E:4848:VAL:HG23	1:E:4883:TYR:HE1	1.66	0.59
1:I:19:GLU:HB2	1:I:206:CYS:HB3	1.84	0.59
1:I:315:CYS:SG	1:I:316:PHE:N	2.76	0.59
1:G:4848:VAL:HG23	1:G:4883:TYR:HE1	1.66	0.59
1:B:41:GLY:O	1:B:45:ARG:NH1	2.35	0.59
1:B:1101:ARG:HE	1:B:1115:LEU:HB3	1.66	0.59
1:B:4075:GLU:HA	1:B:4078:GLN:HB2	1.85	0.59
1:E:256:ALA:HB1	1:E:286:THR:HG21	1.83	0.59
1:I:3762:ARG:H	1:I:4754:ASN:HA	1.67	0.59
1:I:4741:LEU:HB2	1:I:4743:MET:HE2	1.83	0.59
1:G:1641:ILE:HG13	1:G:1643:GLU:H	1.68	0.59
1:B:19:GLU:HB2	1:B:206:CYS:HB3	1.84	0.59
1:E:1519:UNK:HA	1:E:1526:UNK:HA	1.84	0.59
1:E:2748:PRO:HD2	1:E:2751:LEU:HD12	1.84	0.59
1:E:4075:GLU:HA	1:E:4078:GLN:HB2	1.85	0.59
1:G:2420:HIS:ND1	1:G:2493:UNK:O	2.25	0.59
1:G:4741:LEU:HB2	1:G:4743:MET:HE2	1.83	0.59
1:I:2748:PRO:HD2	1:I:2751:LEU:HD12	1.84	0.58
1:B:4238:CYS:HA	1:B:4989:MET:HE3	1.85	0.58
1:E:315:CYS:SG	1:E:316:PHE:N	2.76	0.58
1:I:256:ALA:HB1	1:I:286:THR:HG21	1.83	0.58
1:I:716:PHE:HE2	1:I:759:ILE:HD11	1.68	0.58
1:G:19:GLU:HB2	1:G:206:CYS:HB3	1.84	0.58
1:G:716:PHE:HE2	1:G:759:ILE:HD11	1.68	0.58
1:B:315:CYS:SG	1:B:316:PHE:N	2.76	0.58
1:E:2871:LEU:HD22	1:E:2927:LEU:HD22	1.85	0.58
1:B:4821:LYS:HA	1:B:4824:ARG:HE	1.67	0.58
1:E:281:ARG:HG2	1:E:312:THR:HG21	1.85	0.58
1:I:718:GLY:HA3	1:I:737:LEU:HA	1.84	0.58
1:I:1641:ILE:HG13	1:I:1643:GLU:H	1.67	0.58
1:I:3805:LEU:HA	1:I:3809:ASN:HD22	1.68	0.58
1:G:2347:GLU:O	1:G:2351:ASN:N	2.37	0.58
1:G:2871:LEU:HD22	1:G:2927:LEU:HD22	1.85	0.58
1:E:265:LEU:HD12	1:E:279:PRO:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:LEU:O	1:E:492:ASP:N	2.36	0.58
1:G:281:ARG:HG2	1:G:312:THR:HG21	1.85	0.58
1:G:2338:ALA:HB1	1:G:2349:ASN:HB3	1.84	0.58
1:B:2347:GLU:O	1:B:2351:ASN:N	2.37	0.58
1:B:2748:PRO:HD2	1:B:2751:LEU:HD12	1.84	0.58
1:B:3762:ARG:H	1:B:4754:ASN:HA	1.67	0.58
1:I:21:VAL:HG12	1:I:66:CYS:HA	1.86	0.58
1:G:21:VAL:HG12	1:G:66:CYS:HA	1.86	0.58
1:I:683:ARG:HB2	1:I:782:SER:HB3	1.86	0.58
1:E:19:GLU:HB2	1:E:206:CYS:HB3	1.84	0.58
1:I:650:VAL:HB	1:I:777:PHE:HB2	1.85	0.58
1:B:265:LEU:HD12	1:B:279:PRO:HB2	1.85	0.58
1:B:716:PHE:HE2	1:B:759:ILE:HD11	1.68	0.58
1:B:1641:ILE:HG13	1:B:1643:GLU:H	1.68	0.58
1:E:3758:MET:HE2	1:E:3762:ARG:HB2	1.86	0.58
1:E:4238:CYS:HA	1:E:4989:MET:HE3	1.85	0.58
1:I:1109:LEU:HA	1:I:1120:LEU:HD21	1.86	0.58
1:I:4228:ALA:O	1:I:4232:GLU:N	2.37	0.58
1:I:4232:GLU:OE1	1:I:5019:TRP:NE1	2.37	0.58
1:I:4933:GLN:NE2	1:G:4933:GLN:OE1	2.36	0.58
1:G:3758:MET:HE2	1:G:3762:ARG:HB2	1.86	0.58
1:G:4065:PHE:O	1:G:4133:GLN:NE2	2.37	0.58
1:B:4228:ALA:O	1:B:4232:GLU:N	2.36	0.58
1:I:3758:MET:HE2	1:I:3762:ARG:HB2	1.86	0.58
1:I:4065:PHE:O	1:I:4133:GLN:NE2	2.37	0.58
1:G:1743:ARG:O	1:G:1964:ARG:NH2	2.37	0.58
1:B:3758:MET:HE2	1:B:3762:ARG:HB2	1.86	0.57
1:B:4065:PHE:O	1:B:4133:GLN:NE2	2.37	0.57
1:E:3932:ASP:HA	1:E:3935:TRP:HD1	1.69	0.57
1:I:4075:GLU:HA	1:I:4078:GLN:HB2	1.85	0.57
1:G:3932:ASP:HA	1:G:3935:TRP:HD1	1.69	0.57
2:H:90:VAL:HG12	2:H:91:ILE:HG12	1.84	0.57
1:B:3805:LEU:HA	1:B:3809:ASN:HD22	1.68	0.57
1:E:21:VAL:HG12	1:E:66:CYS:HA	1.86	0.57
1:I:265:LEU:HD12	1:I:279:PRO:HB2	1.85	0.57
1:I:1271:ARG:HA	1:I:1471:UNK:HA	1.86	0.57
1:I:2871:LEU:HD22	1:I:2927:LEU:HD22	1.85	0.57
1:G:1109:LEU:HA	1:G:1120:LEU:HD21	1.86	0.57
1:G:4075:GLU:HA	1:G:4078:GLN:HB2	1.85	0.57
1:B:206:CYS:SG	1:B:207:SER:N	2.78	0.57
1:B:3990:VAL:HG13	1:B:4051:SER:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:650:VAL:HB	1:E:777:PHE:HB2	1.85	0.57
1:E:3890:LEU:HA	1:E:3893:GLU:HB2	1.86	0.57
1:G:206:CYS:SG	1:G:207:SER:N	2.78	0.57
1:G:265:LEU:HD12	1:G:279:PRO:HB2	1.85	0.57
1:G:650:VAL:HB	1:G:777:PHE:HB2	1.85	0.57
1:G:683:ARG:HB2	1:G:782:SER:HB3	1.86	0.57
1:B:281:ARG:HG2	1:B:312:THR:HG21	1.85	0.57
1:B:3890:LEU:HA	1:B:3893:GLU:HB2	1.86	0.57
1:E:716:PHE:HE2	1:E:759:ILE:HD11	1.68	0.57
1:I:281:ARG:HG2	1:I:312:THR:HG21	1.85	0.57
1:I:2347:GLU:O	1:I:2351:ASN:N	2.37	0.57
1:I:3932:ASP:HA	1:I:3935:TRP:HD1	1.69	0.57
1:B:683:ARG:HB2	1:B:782:SER:HB3	1.86	0.57
1:B:4182:GLU:OE2	1:B:4983:HIS:NE2	2.38	0.57
1:E:4182:GLU:OE2	1:E:4983:HIS:NE2	2.38	0.57
1:I:206:CYS:SG	1:I:207:SER:N	2.78	0.57
1:I:4182:GLU:OE2	1:I:4983:HIS:NE2	2.38	0.57
1:G:4238:CYS:HA	1:G:4989:MET:HE3	1.85	0.57
1:B:2871:LEU:HD22	1:B:2927:LEU:HD22	1.85	0.57
1:I:235:ALA:HA	1:I:257:ARG:HD3	1.86	0.57
1:I:3990:VAL:HG13	1:I:4051:SER:HB2	1.86	0.57
1:G:3805:LEU:HA	1:G:3809:ASN:HD22	1.68	0.57
1:G:3890:LEU:HA	1:G:3893:GLU:HB2	1.86	0.57
2:J:90:VAL:HG12	2:J:91:ILE:HG12	1.84	0.57
1:B:650:VAL:HB	1:B:777:PHE:HB2	1.85	0.57
1:B:1109:LEU:HA	1:B:1120:LEU:HD21	1.86	0.57
1:B:4232:GLU:OE1	1:B:5019:TRP:NE1	2.37	0.57
1:G:4232:GLU:OE1	1:G:5019:TRP:NE1	2.37	0.57
1:E:641:VAL:HG21	1:E:705:ASN:HA	1.86	0.57
1:I:4126:GLU:O	1:I:4130:ASN:ND2	2.38	0.57
1:G:4182:GLU:OE2	1:G:4983:HIS:NE2	2.38	0.57
1:B:1973:GLN:O	1:B:1977:TYR:N	2.38	0.57
1:E:4228:ALA:O	1:E:4232:GLU:N	2.36	0.57
1:E:4232:GLU:OE1	1:E:5019:TRP:NE1	2.37	0.57
1:G:475:GLN:NE2	1:G:528:SER:O	2.38	0.57
1:B:21:VAL:HG12	1:B:66:CYS:HA	1.86	0.57
1:E:4065:PHE:O	1:E:4133:GLN:NE2	2.37	0.57
1:B:488:LEU:O	1:B:492:ASP:N	2.37	0.56
1:B:1237:TRP:HH2	1:B:1652:GLU:HA	1.70	0.56
1:B:3932:ASP:HA	1:B:3935:TRP:HD1	1.69	0.56
1:B:4933:GLN:OE1	1:E:4933:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:GLN:NE2	1:E:528:SER:O	2.38	0.56
1:I:1237:TRP:HH2	1:I:1652:GLU:HA	1.70	0.56
1:B:4152:GLU:OE1	1:B:4192:ARG:NH2	2.38	0.56
1:E:683:ARG:HB2	1:E:782:SER:HB3	1.86	0.56
1:E:3805:LEU:HA	1:E:3809:ASN:HD22	1.68	0.56
1:E:4126:GLU:O	1:E:4130:ASN:ND2	2.38	0.56
1:I:641:VAL:HG21	1:I:705:ASN:HA	1.86	0.56
1:G:4126:GLU:O	1:G:4130:ASN:ND2	2.38	0.56
1:G:4228:ALA:O	1:G:4232:GLU:N	2.36	0.56
1:B:683:ARG:NH1	1:B:707:VAL:O	2.39	0.56
1:B:1100:MET:HE2	1:B:1198:GLN:HB3	1.87	0.56
1:B:2359:ARG:NH1	1:I:179:TYR:OH	2.38	0.56
1:B:3830:GLN:HA	1:B:3833:GLN:HG2	1.88	0.56
1:B:4126:GLU:O	1:B:4130:ASN:ND2	2.38	0.56
1:E:1109:LEU:HA	1:E:1120:LEU:HD21	1.86	0.56
1:E:4152:GLU:OE1	1:E:4192:ARG:NH2	2.38	0.56
1:I:475:GLN:NE2	1:I:528:SER:O	2.38	0.56
1:I:3830:GLN:HA	1:I:3833:GLN:HG2	1.88	0.56
1:I:4152:GLU:OE1	1:I:4192:ARG:NH2	2.38	0.56
1:G:20:VAL:HG12	1:G:204:PRO:HA	1.87	0.56
1:G:235:ALA:HA	1:G:257:ARG:HD3	1.86	0.56
1:B:257:ARG:O	1:B:284:HIS:NE2	2.37	0.56
1:E:1743:ARG:O	1:E:1964:ARG:NH2	2.37	0.56
1:E:3971:GLY:H	1:E:5005:GLY:HA3	1.71	0.56
1:E:3990:VAL:HG13	1:E:4051:SER:HB2	1.87	0.56
1:G:744:VAL:HG22	1:G:759:ILE:HG12	1.88	0.56
1:G:2003:GLN:O	1:G:2007:ASN:ND2	2.38	0.56
2:A:27:THR:HB	2:A:100:ASP:HB3	1.87	0.56
1:B:972:LEU:O	1:B:1044:ARG:NH2	2.39	0.56
1:E:2003:GLN:O	1:E:2007:ASN:ND2	2.39	0.56
1:I:683:ARG:NH1	1:I:707:VAL:O	2.38	0.56
1:I:1743:ARG:O	1:I:1964:ARG:NH2	2.37	0.56
1:I:4581:LYS:HB2	1:I:4632:LEU:HB2	1.88	0.56
1:G:4152:GLU:OE1	1:G:4192:ARG:NH2	2.38	0.56
1:B:641:VAL:HG21	1:B:705:ASN:HA	1.86	0.56
1:I:2003:GLN:O	1:I:2007:ASN:ND2	2.38	0.56
1:I:2368:LEU:HB2	1:I:2376:LEU:HD23	1.87	0.56
1:G:972:LEU:O	1:G:1044:ARG:NH2	2.39	0.56
1:G:1237:TRP:HH2	1:G:1652:GLU:HA	1.70	0.56
1:G:1973:GLN:O	1:G:1977:TYR:N	2.38	0.56
1:B:744:VAL:HG22	1:B:759:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2003:GLN:O	1:B:2007:ASN:ND2	2.38	0.56
1:E:20:VAL:HG12	1:E:204:PRO:HA	1.87	0.56
1:E:683:ARG:HG2	1:E:717:ASP:HB3	1.88	0.56
1:E:1973:GLN:O	1:E:1977:TYR:N	2.38	0.56
1:G:1965:TYR:HA	1:G:1968:LYS:HE3	1.88	0.56
1:G:3830:GLN:HA	1:G:3833:GLN:HG2	1.88	0.56
2:J:27:THR:HB	2:J:100:ASP:HB3	1.87	0.56
1:B:2104:ARG:HA	1:B:2107:GLN:HB3	1.88	0.56
1:B:4581:LYS:HB2	1:B:4632:LEU:HB2	1.88	0.56
1:E:1237:TRP:HH2	1:E:1652:GLU:HA	1.70	0.56
1:E:3830:GLN:HA	1:E:3833:GLN:HG2	1.88	0.56
1:G:683:ARG:HG2	1:G:717:ASP:HB3	1.88	0.56
1:B:235:ALA:HA	1:B:257:ARG:HD3	1.86	0.56
1:B:3971:GLY:H	1:B:5005:GLY:HA3	1.71	0.56
1:I:4998:LYS:NZ	1:I:5007:GLU:OE1	2.39	0.56
1:G:2235:PHE:HA	1:G:2238:TYR:HD2	1.71	0.56
2:H:27:THR:HB	2:H:100:ASP:HB3	1.87	0.56
1:B:683:ARG:HG2	1:B:717:ASP:HB3	1.88	0.55
1:B:1965:TYR:HA	1:B:1968:LYS:HE3	1.88	0.55
1:E:2104:ARG:HA	1:E:2107:GLN:HB3	1.88	0.55
1:E:2235:PHE:HA	1:E:2238:TYR:HD2	1.71	0.55
1:I:3890:LEU:HA	1:I:3893:GLU:HB2	1.86	0.55
1:E:2368:LEU:HB2	1:E:2376:LEU:HD23	1.88	0.55
1:I:1973:GLN:O	1:I:1977:TYR:N	2.38	0.55
1:G:3990:VAL:HG13	1:G:4051:SER:HB2	1.87	0.55
1:E:4998:LYS:NZ	1:E:5007:GLU:OE1	2.39	0.55
1:I:683:ARG:HG2	1:I:717:ASP:HB3	1.88	0.55
1:G:2104:ARG:HA	1:G:2107:GLN:HB3	1.88	0.55
1:B:1271:ARG:HA	1:B:1471:UNK:HA	1.88	0.55
1:B:1743:ARG:O	1:B:1964:ARG:NH2	2.37	0.55
1:E:235:ALA:HA	1:E:257:ARG:HD3	1.86	0.55
1:I:972:LEU:O	1:I:1044:ARG:NH2	2.39	0.55
1:I:4071:ILE:HG21	1:I:4097:MET:HE1	1.89	0.55
1:G:257:ARG:O	1:G:284:HIS:NE2	2.37	0.55
1:G:695:TYR:OH	1:G:1073:ARG:NH1	2.39	0.55
1:G:1100:MET:HE2	1:G:1198:GLN:HB3	1.87	0.55
1:E:257:ARG:O	1:E:284:HIS:NE2	2.37	0.55
1:E:683:ARG:NH1	1:E:707:VAL:O	2.38	0.55
1:I:887:ILE:HG21	1:I:959:TYR:HA	1.88	0.55
1:E:709:ASP:O	1:E:725:HIS:ND1	2.40	0.55
1:E:972:LEU:O	1:E:1044:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1100:MET:HE2	1:E:1198:GLN:HB3	1.87	0.55
1:I:20:VAL:HG12	1:I:204:PRO:HA	1.87	0.55
1:I:1232:ARG:HD2	1:I:1702:HIS:HB3	1.89	0.55
1:G:641:VAL:HG21	1:G:705:ASN:HA	1.86	0.55
1:B:709:ASP:O	1:B:725:HIS:ND1	2.40	0.55
1:B:2235:PHE:HA	1:B:2238:TYR:HD2	1.71	0.55
1:B:2368:LEU:HB2	1:B:2376:LEU:HD23	1.88	0.55
1:E:744:VAL:HG22	1:E:759:ILE:HG12	1.88	0.55
1:I:709:ASP:O	1:I:725:HIS:ND1	2.40	0.55
1:G:4071:ILE:HG21	1:G:4097:MET:HE1	1.89	0.55
1:G:4581:LYS:HB2	1:G:4632:LEU:HB2	1.88	0.55
1:B:4071:ILE:HG21	1:B:4097:MET:HE1	1.89	0.55
1:E:695:TYR:OH	1:E:1073:ARG:NH1	2.39	0.55
1:E:2803:GLU:OE2	1:E:2806:ARG:NH1	2.40	0.55
1:I:695:TYR:OH	1:I:1073:ARG:NH1	2.39	0.55
1:G:3971:GLY:H	1:G:5005:GLY:HA3	1.71	0.55
1:E:580:GLU:HG3	1:E:620:LEU:HD22	1.88	0.55
1:I:1965:TYR:HA	1:I:1968:LYS:HE3	1.88	0.55
1:I:2235:PHE:HA	1:I:2238:TYR:HD2	1.71	0.55
1:G:4998:LYS:NZ	1:G:5007:GLU:OE1	2.39	0.55
2:F:27:THR:HB	2:F:100:ASP:HB3	1.87	0.55
1:B:20:VAL:HG12	1:B:204:PRO:HA	1.87	0.55
1:B:887:ILE:HG21	1:B:959:TYR:HA	1.88	0.55
1:B:1659:LEU:O	1:B:1663:HIS:N	2.37	0.55
1:B:2042:CYS:SG	1:B:2043:GLY:N	2.80	0.55
1:B:4125:PHE:HA	1:B:4128:PHE:HB3	1.89	0.55
1:E:1965:TYR:HA	1:E:1968:LYS:HE3	1.88	0.55
1:E:2347:GLU:O	1:E:2351:ASN:N	2.37	0.55
1:I:1659:LEU:O	1:I:1663:HIS:N	2.37	0.55
1:I:2104:ARG:HA	1:I:2107:GLN:HB3	1.88	0.55
1:G:4229:GLU:HA	1:G:4232:GLU:HB3	1.89	0.55
1:B:580:GLU:HG3	1:B:620:LEU:HD22	1.88	0.54
1:I:1100:MET:HE2	1:I:1198:GLN:HB3	1.87	0.54
1:G:887:ILE:HG21	1:G:959:TYR:HA	1.88	0.54
1:G:1970:GLN:NE2	1:G:3646:THR:OG1	2.40	0.54
1:G:2803:GLU:OE2	1:G:2806:ARG:NH1	2.40	0.54
1:E:887:ILE:HG21	1:E:959:TYR:HA	1.89	0.54
1:E:1232:ARG:HD2	1:E:1702:HIS:HB3	1.89	0.54
1:E:2758:PHE:O	1:E:2762:THR:N	2.39	0.54
1:E:4071:ILE:HG21	1:E:4097:MET:HE1	1.89	0.54
1:G:55:ALA:O	1:G:281:ARG:NH1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2368:LEU:HB2	1:G:2376:LEU:HD23	1.88	0.54
1:B:1232:ARG:HD2	1:B:1702:HIS:HB3	1.89	0.54
1:E:2042:CYS:SG	1:E:2043:GLY:N	2.80	0.54
1:E:4581:LYS:HB2	1:E:4632:LEU:HB2	1.88	0.54
1:I:3762:ARG:HG2	1:I:4756:ARG:HA	1.88	0.54
1:I:3971:GLY:H	1:I:5005:GLY:HA3	1.71	0.54
1:I:4125:PHE:HA	1:I:4128:PHE:HB3	1.89	0.54
1:I:4229:GLU:HA	1:I:4232:GLU:HB3	1.89	0.54
1:B:469:ARG:HH21	1:B:3712:GLU:HB3	1.72	0.54
1:E:18:ASP:H	1:E:69:LEU:HB2	1.73	0.54
1:E:1970:GLN:NE2	1:E:3646:THR:OG1	2.40	0.54
1:I:744:VAL:HG22	1:I:759:ILE:HG12	1.88	0.54
1:G:469:ARG:HH21	1:G:3712:GLU:HB3	1.72	0.54
1:G:3762:ARG:HG2	1:G:4756:ARG:HA	1.88	0.54
1:B:293:LEU:HB2	1:B:378:LEU:HD12	1.90	0.54
1:B:475:GLN:NE2	1:B:528:SER:O	2.38	0.54
1:B:2803:GLU:OE2	1:B:2806:ARG:NH1	2.40	0.54
1:B:4998:LYS:NZ	1:B:5007:GLU:OE1	2.39	0.54
1:G:683:ARG:NH1	1:G:707:VAL:O	2.38	0.54
1:G:2042:CYS:SG	1:G:2043:GLY:N	2.80	0.54
1:I:463:GLU:OE2	1:I:467:LYS:NZ	2.41	0.54
1:I:2318:TYR:OH	1:I:2414:ASN:N	2.41	0.54
1:G:463:GLU:OE2	1:G:467:LYS:NZ	2.41	0.54
1:B:695:TYR:OH	1:B:1073:ARG:NH1	2.39	0.54
1:B:1812:LEU:HD21	1:B:1861:GLN:HG2	1.90	0.54
1:E:293:LEU:HB2	1:E:378:LEU:HD12	1.90	0.54
1:E:469:ARG:HH21	1:E:3712:GLU:HB3	1.73	0.54
1:I:580:GLU:HG3	1:I:620:LEU:HD22	1.88	0.54
1:I:1970:GLN:NE2	1:I:3646:THR:OG1	2.40	0.54
1:G:2318:TYR:OH	1:G:2414:ASN:N	2.41	0.54
1:E:1812:LEU:HD21	1:E:1861:GLN:HG2	1.90	0.54
1:E:4885:PHE:HE2	1:E:4901:ILE:HD11	1.73	0.54
1:I:469:ARG:HH21	1:I:3712:GLU:HB3	1.72	0.54
1:G:1865:MET:HB3	1:G:1926:LEU:HB2	1.90	0.54
1:E:3762:ARG:HG2	1:E:4756:ARG:HA	1.88	0.54
1:I:293:LEU:HB2	1:I:378:LEU:HD12	1.90	0.54
1:G:580:GLU:HG3	1:G:620:LEU:HD22	1.88	0.54
1:E:776:LEU:HG	1:E:848:HIS:HA	1.90	0.54
1:E:4125:PHE:HA	1:E:4128:PHE:HB3	1.90	0.54
1:E:4229:GLU:HA	1:E:4232:GLU:HB3	1.89	0.54
1:I:1812:LEU:HD21	1:I:1861:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3752:SER:O	1:I:3756:LYS:N	2.38	0.54
1:G:709:ASP:O	1:G:725:HIS:ND1	2.40	0.54
1:B:776:LEU:HG	1:B:848:HIS:HA	1.90	0.53
1:B:1679:ASN:ND2	1:B:1798:LEU:O	2.41	0.53
1:B:1865:MET:HB3	1:B:1926:LEU:HB2	1.90	0.53
1:B:2770:LYS:HB3	1:B:2775:TRP:HB2	1.90	0.53
1:B:4229:GLU:HA	1:B:4232:GLU:HB3	1.89	0.53
1:I:2803:GLU:OE2	1:I:2806:ARG:NH1	2.40	0.53
1:G:293:LEU:HB2	1:G:378:LEU:HD12	1.90	0.53
1:G:4125:PHE:HA	1:G:4128:PHE:HB3	1.89	0.53
1:I:488:LEU:O	1:I:492:ASP:N	2.36	0.53
1:I:776:LEU:HG	1:I:848:HIS:HA	1.90	0.53
1:G:18:ASP:HB2	1:G:69:LEU:HD12	1.90	0.53
1:G:2770:LYS:HB3	1:G:2775:TRP:HB2	1.90	0.53
1:B:1841:VAL:HA	1:B:1844:LEU:HB3	1.91	0.53
1:B:1970:GLN:NE2	1:B:3646:THR:OG1	2.40	0.53
1:B:4885:PHE:HE2	1:B:4901:ILE:HD11	1.73	0.53
1:E:1679:ASN:ND2	1:E:1798:LEU:O	2.41	0.53
1:I:1865:MET:HB3	1:I:1926:LEU:HB2	1.90	0.53
1:I:2927:LEU:HD23	1:I:2930:LEU:HD12	1.90	0.53
1:G:18:ASP:H	1:G:69:LEU:HB2	1.73	0.53
1:B:2318:TYR:OH	1:B:2414:ASN:N	2.41	0.53
1:E:2770:LYS:HB3	1:E:2775:TRP:HB2	1.91	0.53
1:I:1841:VAL:HA	1:I:1844:LEU:HB3	1.91	0.53
1:I:2042:CYS:SG	1:I:2043:GLY:N	2.80	0.53
1:I:2770:LYS:HB3	1:I:2775:TRP:HB2	1.91	0.53
1:G:776:LEU:HG	1:G:848:HIS:HA	1.90	0.53
1:G:1679:ASN:ND2	1:G:1798:LEU:O	2.41	0.53
1:G:1778:SER:N	1:G:1799:SER:O	2.41	0.53
1:B:463:GLU:OE2	1:B:467:LYS:NZ	2.41	0.53
1:E:463:GLU:OE2	1:E:467:LYS:NZ	2.41	0.53
1:E:1841:VAL:HA	1:E:1844:LEU:HB3	1.91	0.53
1:G:1841:VAL:HA	1:G:1844:LEU:HB3	1.91	0.53
1:E:1865:MET:HB3	1:E:1926:LEU:HB2	1.90	0.53
1:I:485:SER:O	1:I:489:ASN:N	2.41	0.53
1:G:241:GLN:O	1:G:289:ARG:NH1	2.37	0.53
1:G:1812:LEU:HD21	1:G:1861:GLN:HG2	1.90	0.53
1:B:3762:ARG:HG2	1:B:4756:ARG:HA	1.88	0.53
1:B:4687:TYR:OH	1:B:4699:GLY:O	2.26	0.53
1:E:168:ASP:HB3	1:E:199:LEU:HD22	1.91	0.53
1:I:426:ARG:HB2	1:I:506:TYR:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:ASP:HB3	1:G:199:LEU:HD22	1.91	0.53
1:G:4885:PHE:HE2	1:G:4901:ILE:HD11	1.73	0.53
1:B:18:ASP:H	1:B:69:LEU:HB2	1.73	0.53
1:B:1778:SER:N	1:B:1799:SER:O	2.41	0.53
1:I:1679:ASN:ND2	1:I:1798:LEU:O	2.41	0.53
1:I:4138:ASP:O	1:I:4142:ASN:ND2	2.42	0.53
1:G:1232:ARG:HD2	1:G:1702:HIS:HB3	1.89	0.53
1:G:4138:ASP:O	1:G:4142:ASN:ND2	2.42	0.53
1:B:426:ARG:HB2	1:B:506:TYR:HA	1.91	0.53
1:E:1727:ARG:HH12	1:E:1772:ARG:HB3	1.74	0.53
1:E:2318:TYR:OH	1:E:2414:ASN:N	2.41	0.53
1:G:485:SER:O	1:G:489:ASN:N	2.41	0.53
1:G:1931:LEU:HB3	1:G:1935:VAL:HB	1.91	0.53
1:G:4746:ALA:O	1:G:4750:ILE:N	2.42	0.53
1:B:488:LEU:HA	1:B:491:ILE:HB	1.91	0.53
1:B:621:ILE:O	1:B:625:LEU:N	2.38	0.53
1:E:4138:ASP:O	1:E:4142:ASN:ND2	2.42	0.53
1:I:257:ARG:O	1:I:284:HIS:NE2	2.37	0.53
1:I:4746:ALA:O	1:I:4750:ILE:N	2.42	0.53
1:G:4687:TYR:OH	1:G:4699:GLY:O	2.26	0.53
1:B:168:ASP:HB3	1:B:199:LEU:HD22	1.91	0.52
1:E:18:ASP:HB2	1:E:69:LEU:HD12	1.90	0.52
1:E:978:THR:HB	1:E:980:ALA:H	1.74	0.52
1:I:1931:LEU:HB3	1:I:1935:VAL:HB	1.91	0.52
1:B:647:ASN:ND2	1:B:820:ARG:O	2.42	0.52
1:B:1931:LEU:HB3	1:B:1935:VAL:HB	1.91	0.52
1:B:4172:GLU:HA	1:B:4175:ARG:HE	1.74	0.52
1:I:18:ASP:H	1:I:69:LEU:HB2	1.73	0.52
1:I:360:ALA:N	1:I:375:LYS:O	2.38	0.52
1:I:1152:MET:HB2	1:I:1161:ILE:HB	1.91	0.52
1:I:4687:TYR:OH	1:I:4699:GLY:O	2.26	0.52
1:G:2927:LEU:HD23	1:G:2930:LEU:HD12	1.90	0.52
1:B:1727:ARG:HH12	1:B:1772:ARG:HB3	1.74	0.52
1:E:1931:LEU:HB3	1:E:1935:VAL:HB	1.91	0.52
1:E:4172:GLU:HA	1:E:4175:ARG:HE	1.74	0.52
1:E:4687:TYR:OH	1:E:4699:GLY:O	2.26	0.52
1:I:168:ASP:HB3	1:I:199:LEU:HD22	1.91	0.52
1:G:4928:LEU:HA	1:G:4931:ILE:HD12	1.91	0.52
1:I:3832:ILE:O	1:I:3836:MET:N	2.42	0.52
1:I:4681:LEU:HD21	1:I:4687:TYR:HD2	1.75	0.52
1:I:4928:LEU:HA	1:I:4931:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASP:HB2	1:B:69:LEU:HD12	1.90	0.52
1:B:1764:GLY:HA3	1:B:1859:VAL:HG11	1.91	0.52
1:B:4928:LEU:HA	1:B:4931:ILE:HD12	1.91	0.52
1:I:4822:THR:OG1	1:G:4839:MET:SD	2.63	0.52
1:G:1764:GLY:HA3	1:G:1859:VAL:HG11	1.91	0.52
1:G:2758:PHE:O	1:G:2762:THR:N	2.39	0.52
1:E:360:ALA:N	1:E:375:LYS:O	2.38	0.52
1:I:488:LEU:HA	1:I:491:ILE:HB	1.91	0.52
1:I:4957:LYS:HG2	1:I:4964:GLY:HA2	1.92	0.52
1:G:4172:GLU:HA	1:G:4175:ARG:HE	1.74	0.52
1:B:395:GLN:NE2	1:B:397:GLU:OE1	2.43	0.52
1:E:1764:GLY:HA3	1:E:1859:VAL:HG11	1.91	0.52
1:I:1764:GLY:HA3	1:I:1859:VAL:HG11	1.91	0.52
1:G:146:CYS:HG	1:G:147:TRP:CD1	2.28	0.52
1:G:4957:LYS:HG2	1:G:4964:GLY:HA2	1.92	0.52
1:B:45:ARG:NH2	1:B:447:ASP:OD1	2.37	0.52
1:B:2927:LEU:HD23	1:B:2930:LEU:HD12	1.90	0.52
1:B:4681:LEU:HD21	1:B:4687:TYR:HD2	1.75	0.52
1:B:4957:LYS:HG2	1:B:4964:GLY:HA2	1.92	0.52
1:E:2927:LEU:HD23	1:E:2930:LEU:HD12	1.90	0.52
1:E:4957:LYS:HG2	1:E:4964:GLY:HA2	1.92	0.52
1:I:1727:ARG:HH12	1:I:1772:ARG:HB3	1.74	0.52
1:I:4069:LYS:HB2	1:I:4133:GLN:HG3	1.92	0.52
1:G:426:ARG:HB2	1:G:506:TYR:HA	1.90	0.52
1:G:1152:MET:HB2	1:G:1161:ILE:HB	1.91	0.52
1:G:3752:SER:O	1:G:3756:LYS:N	2.38	0.52
1:G:4005:GLN:HE21	1:G:4110:PHE:HE1	1.57	0.52
1:B:40:GLU:HB3	1:B:44:ASN:HB3	1.92	0.52
1:B:877:ASN:HD22	1:B:1045:THR:HG23	1.75	0.52
1:B:978:THR:HB	1:B:980:ALA:H	1.75	0.52
1:B:1978:ALA:O	1:B:1983:ALA:N	2.40	0.52
1:B:2002:PRO:HA	1:B:2005:GLN:HB3	1.92	0.52
1:E:485:SER:O	1:E:489:ASN:N	2.41	0.52
1:I:395:GLN:NE2	1:I:397:GLU:OE1	2.43	0.52
1:G:488:LEU:HA	1:G:491:ILE:HB	1.91	0.52
1:G:1727:ARG:HH12	1:G:1772:ARG:HB3	1.74	0.52
1:G:4572:ALA:HA	1:G:4575:PHE:HB3	1.92	0.52
1:B:457:GLU:OE1	1:B:464:LYS:NZ	2.40	0.52
1:B:4763:GLY:O	1:B:4766:THR:OG1	2.24	0.52
1:E:184:THR:HA	1:E:189:LEU:HA	1.92	0.52
1:E:426:ARG:HB2	1:E:506:TYR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4681:LEU:HD21	1:E:4687:TYR:HD2	1.75	0.52
1:I:40:GLU:HB3	1:I:44:ASN:HB3	1.92	0.52
1:I:1713:ASP:O	1:I:1717:SER:N	2.39	0.52
1:G:45:ARG:NH2	1:G:447:ASP:OD1	2.37	0.52
1:B:55:ALA:O	1:B:281:ARG:NH1	2.35	0.51
1:B:4069:LYS:HB2	1:B:4133:GLN:HG3	1.92	0.51
1:E:1659:LEU:O	1:E:1663:HIS:N	2.37	0.51
1:E:4069:LYS:HB2	1:E:4133:GLN:HG3	1.92	0.51
1:I:18:ASP:HB2	1:I:69:LEU:HD12	1.90	0.51
1:I:978:THR:HB	1:I:980:ALA:H	1.75	0.51
1:I:4885:PHE:HE2	1:I:4901:ILE:HD11	1.73	0.51
1:G:719:LEU:HD22	1:G:735:GLN:HG2	1.92	0.51
1:B:629:ARG:HB3	1:B:634:GLN:HE21	1.76	0.51
1:B:1970:GLN:HA	1:B:3641:LEU:HG	1.92	0.51
1:B:3898:ASP:O	1:B:3902:TYR:N	2.43	0.51
1:B:4138:ASP:O	1:B:4142:ASN:ND2	2.42	0.51
1:B:4697:VAL:O	1:B:4701:TRP:N	2.42	0.51
1:E:488:LEU:HA	1:E:491:ILE:HB	1.91	0.51
1:E:647:ASN:ND2	1:E:820:ARG:O	2.42	0.51
1:E:877:ASN:HD22	1:E:1045:THR:HG23	1.75	0.51
1:E:1978:ALA:O	1:E:1983:ALA:N	2.40	0.51
1:E:4062:PHE:HA	1:E:4132:PHE:HZ	1.76	0.51
1:I:4572:ALA:HA	1:I:4575:PHE:HB3	1.92	0.51
1:G:978:THR:HB	1:G:980:ALA:H	1.75	0.51
1:G:4095:LYS:O	1:G:4099:SER:N	2.43	0.51
1:B:399:GLN:HG2	1:B:403:MET:HE3	1.92	0.51
1:B:2116:LEU:O	1:B:2120:MET:N	2.43	0.51
1:E:206:CYS:SG	1:E:207:SER:N	2.78	0.51
1:I:719:LEU:HD22	1:I:735:GLN:HG2	1.92	0.51
1:I:3898:ASP:O	1:I:3902:TYR:N	2.43	0.51
1:G:184:THR:HA	1:G:189:LEU:HA	1.93	0.51
1:G:221:ARG:NE	1:G:258:SER:OG	2.44	0.51
1:G:399:GLN:HG2	1:G:403:MET:HE3	1.92	0.51
1:G:1970:GLN:HA	1:G:3641:LEU:HG	1.92	0.51
1:G:3885:PHE:O	1:G:3889:GLN:N	2.41	0.51
1:B:3885:PHE:O	1:B:3889:GLN:N	2.41	0.51
1:B:4107:GLU:O	1:B:4111:LEU:N	2.40	0.51
1:E:1694:LEU:O	1:E:1712:TYR:OH	2.22	0.51
1:I:399:GLN:HG2	1:I:403:MET:HE3	1.92	0.51
1:I:4095:LYS:O	1:I:4099:SER:N	2.43	0.51
1:G:4069:LYS:HB2	1:G:4133:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:THR:HA	1:B:189:LEU:HA	1.93	0.51
1:E:3927:GLN:O	1:E:3931:SER:N	2.42	0.51
1:I:629:ARG:O	1:I:634:GLN:NE2	2.44	0.51
1:I:3840:SER:OG	1:I:3875:MET:O	2.26	0.51
1:G:1659:LEU:O	1:G:1663:HIS:N	2.37	0.51
1:G:3927:GLN:O	1:G:3931:SER:N	2.42	0.51
1:B:1152:MET:HB2	1:B:1161:ILE:HB	1.91	0.51
1:I:1089:TYR:N	1:I:1224:GLU:O	2.41	0.51
1:I:1111:PRO:HD3	1:I:1605:TRP:HE1	1.76	0.51
1:I:4172:GLU:HA	1:I:4175:ARG:HE	1.74	0.51
1:G:989:ALA:O	1:G:1035:ASN:ND2	2.44	0.51
1:B:3832:ILE:O	1:B:3836:MET:N	2.42	0.51
1:E:4857:ASN:HB2	1:G:4807:PHE:HZ	1.74	0.51
1:E:4928:LEU:HA	1:E:4931:ILE:HD12	1.91	0.51
1:I:877:ASN:HD22	1:I:1045:THR:HG23	1.75	0.51
1:I:1970:GLN:HA	1:I:3641:LEU:HG	1.92	0.51
1:G:488:LEU:O	1:G:492:ASP:N	2.36	0.51
1:G:621:ILE:O	1:G:625:LEU:N	2.38	0.51
1:G:877:ASN:HD22	1:G:1045:THR:HG23	1.75	0.51
1:G:1111:PRO:HD3	1:G:1605:TRP:HE1	1.76	0.51
1:B:2758:PHE:O	1:B:2762:THR:N	2.39	0.51
1:B:4572:ALA:HA	1:B:4575:PHE:HB3	1.91	0.51
1:E:1152:MET:HB2	1:E:1161:ILE:HB	1.91	0.51
1:E:3898:ASP:O	1:E:3902:TYR:N	2.43	0.51
1:I:1778:SER:N	1:I:1799:SER:O	2.42	0.51
1:I:2272:PRO:HA	1:I:2275:VAL:HG12	1.93	0.51
1:G:3832:ILE:O	1:G:3836:MET:N	2.42	0.51
1:I:173:SER:OG	1:I:174:VAL:N	2.44	0.51
1:I:184:THR:HA	1:I:189:LEU:HA	1.93	0.51
1:B:4095:LYS:O	1:B:4099:SER:N	2.44	0.51
1:E:719:LEU:HD22	1:E:735:GLN:HG2	1.92	0.51
1:E:793:LEU:HG	1:E:1625:GLY:HA2	1.93	0.51
1:E:1970:GLN:HA	1:E:3641:LEU:HG	1.92	0.51
1:E:2326:CYS:SG	1:E:2327:GLY:N	2.84	0.51
1:E:4572:ALA:HA	1:E:4575:PHE:HB3	1.92	0.51
1:I:629:ARG:HB3	1:I:634:GLN:HE21	1.76	0.51
1:I:2002:PRO:HA	1:I:2005:GLN:HB3	1.92	0.51
1:I:4081:VAL:HB	1:I:4088:ILE:HD12	1.92	0.51
1:G:4081:VAL:HB	1:G:4088:ILE:HD12	1.92	0.51
1:G:5012:LYS:O	1:G:5016:GLU:N	2.42	0.51
1:B:2326:CYS:SG	1:B:2327:GLY:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:GLN:NE2	1:E:397:GLU:OE1	2.43	0.50
1:E:1032:LYS:O	1:E:1036:ARG:N	2.39	0.50
1:I:1152:MET:HE1	1:I:1217:CYS:HB3	1.93	0.50
1:I:4005:GLN:HE21	1:I:4110:PHE:HE1	1.57	0.50
1:G:629:ARG:O	1:G:634:GLN:NE2	2.44	0.50
1:G:2272:PRO:HA	1:G:2275:VAL:HG12	1.93	0.50
1:B:629:ARG:O	1:B:634:GLN:NE2	2.44	0.50
1:B:864:PRO:HD2	1:B:867:LEU:HD12	1.93	0.50
1:E:173:SER:OG	1:E:174:VAL:N	2.44	0.50
1:E:629:ARG:HB3	1:E:634:GLN:HE21	1.75	0.50
1:I:45:ARG:NH2	1:I:447:ASP:OD1	2.37	0.50
1:G:2002:PRO:HA	1:G:2005:GLN:HB3	1.92	0.50
1:G:4062:PHE:HA	1:G:4132:PHE:HZ	1.76	0.50
1:B:2272:PRO:HA	1:B:2275:VAL:HG12	1.93	0.50
1:E:3885:PHE:O	1:E:3889:GLN:N	2.41	0.50
1:E:4937:ILE:O	1:E:4941:GLY:N	2.41	0.50
1:I:2326:CYS:SG	1:I:2327:GLY:N	2.84	0.50
1:I:4820:VAL:HB	1:I:4823:LEU:HD23	1.94	0.50
1:G:4681:LEU:HD21	1:G:4687:TYR:HD2	1.75	0.50
1:G:4820:VAL:HB	1:G:4823:LEU:HD23	1.94	0.50
1:B:221:ARG:NE	1:B:258:SER:OG	2.44	0.50
1:B:1111:PRO:HD3	1:B:1605:TRP:HE1	1.76	0.50
1:B:4860:ARG:HG3	1:B:4876:CYS:HB3	1.94	0.50
1:E:40:GLU:HB3	1:E:44:ASN:HB3	1.92	0.50
1:E:399:GLN:HG2	1:E:403:MET:HE3	1.92	0.50
1:E:989:ALA:O	1:E:1035:ASN:ND2	2.44	0.50
1:E:2002:PRO:HA	1:E:2005:GLN:HB3	1.92	0.50
1:E:4024:VAL:HG23	1:E:4027:LEU:HD12	1.94	0.50
1:E:4820:VAL:HB	1:E:4823:LEU:HD23	1.94	0.50
1:I:221:ARG:NE	1:I:258:SER:OG	2.44	0.50
1:I:989:ALA:O	1:I:1035:ASN:ND2	2.44	0.50
1:I:4062:PHE:HA	1:I:4132:PHE:HZ	1.76	0.50
1:G:40:GLU:HB3	1:G:44:ASN:HB3	1.92	0.50
1:G:245:VAL:HG21	1:G:299:LEU:HG	1.93	0.50
1:G:629:ARG:HB3	1:G:634:GLN:HE21	1.75	0.50
1:G:685:GLY:N	1:G:780:VAL:O	2.35	0.50
1:G:793:LEU:HG	1:G:1625:GLY:HA2	1.93	0.50
1:G:864:PRO:HD2	1:G:867:LEU:HD12	1.93	0.50
1:G:3840:SER:OG	1:G:3875:MET:O	2.26	0.50
1:B:4824:ARG:HA	1:B:4827:LEU:HB2	1.94	0.50
1:E:4005:GLN:HE21	1:E:4110:PHE:HE1	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4081:VAL:HB	1:E:4088:ILE:HD12	1.92	0.50
1:E:4152:GLU:OE1	1:E:4194:TYR:OH	2.29	0.50
1:E:4860:ARG:HG3	1:E:4876:CYS:HB3	1.94	0.50
1:I:1163:THR:HA	1:I:1168:VAL:HA	1.94	0.50
1:G:647:ASN:ND2	1:G:820:ARG:O	2.42	0.50
1:G:2326:CYS:SG	1:G:2327:GLY:N	2.84	0.50
1:E:4651:THR:HA	1:E:4799:SER:HB3	1.92	0.50
1:I:4169:SER:O	1:I:4173:TYR:N	2.45	0.50
1:G:173:SER:OG	1:G:174:VAL:N	2.44	0.50
1:G:596:ASN:HB3	1:G:599:VAL:HG22	1.94	0.50
1:G:736:HIS:HB3	2:H:8:SER:H	1.77	0.50
1:G:2116:LEU:O	1:G:2120:MET:N	2.43	0.50
1:G:3898:ASP:O	1:G:3902:TYR:N	2.43	0.50
1:B:245:VAL:HG21	1:B:299:LEU:HG	1.93	0.50
1:B:596:ASN:HB3	1:B:599:VAL:HG22	1.94	0.50
1:B:1931:LEU:HD22	1:B:1935:VAL:HG11	1.94	0.50
1:B:4005:GLN:HE21	1:B:4110:PHE:HE1	1.57	0.50
1:B:4081:VAL:HB	1:B:4088:ILE:HD12	1.92	0.50
1:B:4169:SER:O	1:B:4173:TYR:N	2.45	0.50
1:B:4820:VAL:HB	1:B:4823:LEU:HD23	1.94	0.50
1:E:221:ARG:NE	1:E:258:SER:OG	2.44	0.50
1:E:621:ILE:O	1:E:625:LEU:N	2.39	0.50
1:E:2116:LEU:O	1:E:2120:MET:N	2.43	0.50
1:E:4746:ALA:O	1:E:4750:ILE:N	2.42	0.50
1:I:1965:TYR:OH	1:I:2027:ILE:O	2.27	0.50
1:G:3781:GLN:O	1:G:3785:ALA:N	2.45	0.50
1:G:4860:ARG:HG3	1:G:4876:CYS:HB3	1.94	0.50
1:B:932:LEU:HD23	1:B:935:LEU:HD12	1.94	0.50
1:B:2823:ILE:HG12	1:B:2937:VAL:HG22	1.94	0.50
1:B:3927:GLN:O	1:B:3931:SER:N	2.42	0.50
1:E:269:TRP:HB3	1:E:272:SER:HB3	1.94	0.50
1:E:629:ARG:O	1:E:634:GLN:NE2	2.44	0.50
1:E:2457:LEU:HD23	1:E:2460:LEU:HD12	1.94	0.50
1:E:4697:VAL:O	1:E:4701:TRP:N	2.42	0.50
1:I:551:LEU:HD21	1:I:589:LEU:HB2	1.94	0.50
1:I:596:ASN:HB3	1:I:599:VAL:HG22	1.94	0.50
1:G:4824:ARG:HA	1:G:4827:LEU:HB2	1.94	0.50
1:B:4822:THR:O	1:B:4825:THR:OG1	2.29	0.50
1:E:1778:SER:N	1:E:1799:SER:O	2.41	0.50
1:E:2272:PRO:HA	1:E:2275:VAL:HG12	1.93	0.50
1:I:793:LEU:HG	1:I:1625:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1721:GLU:OE2	1:I:1725:ARG:NH2	2.39	0.50
1:G:1978:ALA:O	1:G:1983:ALA:N	2.40	0.50
1:B:173:SER:OG	1:B:174:VAL:N	2.44	0.49
1:B:1032:LYS:O	1:B:1036:ARG:N	2.39	0.49
1:B:1152:MET:HE1	1:B:1217:CYS:HB3	1.93	0.49
1:B:3676:ASP:OD1	1:B:3676:ASP:N	2.45	0.49
1:B:4024:VAL:HG23	1:B:4027:LEU:HD12	1.94	0.49
1:E:448:LEU:HA	1:E:451:TYR:HB3	1.94	0.49
1:E:864:PRO:HD2	1:E:867:LEU:HD12	1.93	0.49
1:I:1931:LEU:HD22	1:I:1935:VAL:HG11	1.94	0.49
1:I:2342:ASN:OD1	1:I:2342:ASN:N	2.45	0.49
1:I:4651:THR:HA	1:I:4799:SER:HB3	1.93	0.49
1:G:1032:LYS:O	1:G:1036:ARG:N	2.39	0.49
1:G:2868:SER:O	1:G:2872:GLN:N	2.45	0.49
1:G:4169:SER:O	1:G:4173:TYR:N	2.45	0.49
1:B:719:LEU:HD22	1:B:735:GLN:HG2	1.92	0.49
1:B:793:LEU:HG	1:B:1625:GLY:HA2	1.93	0.49
1:B:989:ALA:O	1:B:1035:ASN:ND2	2.44	0.49
1:B:4062:PHE:HA	1:B:4132:PHE:HZ	1.76	0.49
1:E:1950:GLU:O	1:E:1954:ARG:N	2.45	0.49
1:E:4095:LYS:O	1:E:4099:SER:N	2.44	0.49
1:E:4822:THR:O	1:E:4825:THR:OG1	2.28	0.49
1:E:5012:LYS:O	1:E:5016:GLU:N	2.42	0.49
1:I:245:VAL:HG21	1:I:299:LEU:HG	1.93	0.49
1:B:1163:THR:HA	1:B:1168:VAL:HA	1.94	0.49
1:E:2823:ILE:HG12	1:E:2937:VAL:HG22	1.94	0.49
1:I:4152:GLU:OE1	1:I:4194:TYR:OH	2.29	0.49
1:G:269:TRP:HB3	1:G:272:SER:HB3	1.94	0.49
1:G:1163:THR:HA	1:G:1168:VAL:HA	1.94	0.49
1:G:4152:GLU:OE1	1:G:4194:TYR:OH	2.29	0.49
1:B:1679:ASN:HA	1:B:1682:ALA:HB3	1.94	0.49
1:B:2737:PRO:O	1:B:2888:ARG:NH2	2.46	0.49
1:E:596:ASN:HB3	1:E:599:VAL:HG22	1.94	0.49
1:I:911:HIS:O	1:I:918:ARG:NH2	2.45	0.49
1:I:2457:LEU:HD23	1:I:2460:LEU:HD12	1.94	0.49
1:I:3842:LEU:O	1:I:3929:SER:OG	2.31	0.49
1:I:4976:GLU:O	1:I:4979:THR:OG1	2.29	0.49
1:G:72:SER:HB2	1:G:107:ILE:HG13	1.95	0.49
1:G:551:LEU:HD21	1:G:589:LEU:HB2	1.94	0.49
1:B:911:HIS:O	1:B:918:ARG:NH2	2.45	0.49
1:B:1698:LEU:N	1:B:1712:TYR:OH	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1111:PRO:HD3	1:E:1605:TRP:HE1	1.76	0.49
1:E:2006:ILE:O	1:E:2010:LEU:N	2.43	0.49
1:E:2868:SER:O	1:E:2872:GLN:N	2.45	0.49
1:E:3781:GLN:O	1:E:3785:ALA:N	2.45	0.49
1:I:864:PRO:HD2	1:I:867:LEU:HD12	1.93	0.49
1:I:932:LEU:HD23	1:I:935:LEU:HD12	1.94	0.49
1:I:2823:ILE:HG12	1:I:2937:VAL:HG22	1.94	0.49
1:I:2880:GLU:O	1:I:2884:ASN:N	2.42	0.49
1:I:3885:PHE:O	1:I:3889:GLN:N	2.41	0.49
1:I:4822:THR:O	1:I:4825:THR:OG1	2.29	0.49
1:G:3676:ASP:OD1	1:G:3676:ASP:N	2.45	0.49
1:G:4024:VAL:HG23	1:G:4027:LEU:HD12	1.94	0.49
1:B:4152:GLU:OE1	1:B:4194:TYR:OH	2.29	0.49
1:B:4651:THR:HA	1:B:4799:SER:HB3	1.93	0.49
1:E:245:VAL:HG21	1:E:299:LEU:HG	1.93	0.49
1:E:395:GLN:HG3	1:E:397:GLU:H	1.78	0.49
1:E:551:LEU:HD21	1:E:589:LEU:HB2	1.94	0.49
1:E:4702:ASP:OD1	1:E:4778:TRP:NE1	2.44	0.49
1:I:1679:ASN:HA	1:I:1682:ALA:HB3	1.94	0.49
1:I:2176:ASN:O	1:I:2180:GLN:N	2.42	0.49
1:I:2346:VAL:HG22	1:I:2348:GLU:H	1.78	0.49
1:I:4860:ARG:HG3	1:I:4876:CYS:HB3	1.94	0.49
1:G:395:GLN:HG3	1:G:397:GLU:H	1.78	0.49
1:G:3707:ARG:HA	1:G:3710:LEU:HD23	1.94	0.49
1:G:3842:LEU:O	1:G:3929:SER:OG	2.30	0.49
1:B:1636:MET:HE2	1:B:1638:ALA:HB2	1.95	0.49
1:B:3752:SER:O	1:B:3756:LYS:N	2.38	0.49
1:B:3780:LEU:HD11	1:B:3816:MET:HG3	1.95	0.49
1:E:838:HIS:HA	1:E:1201:HIS:HB3	1.94	0.49
1:E:1698:LEU:N	1:E:1712:TYR:OH	2.46	0.49
1:E:1713:ASP:O	1:E:1717:SER:N	2.39	0.49
1:E:4107:GLU:O	1:E:4111:LEU:N	2.40	0.49
1:I:580:GLU:OE2	1:I:624:ASN:ND2	2.46	0.49
1:I:1698:LEU:N	1:I:1712:TYR:OH	2.46	0.49
1:I:3927:GLN:O	1:I:3931:SER:N	2.42	0.49
1:I:4824:ARG:HA	1:I:4827:LEU:HB2	1.94	0.49
1:G:717:ASP:OD1	1:G:720:HIS:ND1	2.46	0.49
1:G:2346:VAL:HG22	1:G:2348:GLU:H	1.78	0.49
1:G:3897:ASN:O	1:G:3901:ASN:ND2	2.46	0.49
1:G:4201:ASN:HA	1:G:4204:GLN:HB3	1.95	0.49
1:G:4651:THR:HA	1:G:4799:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2176:ASN:O	1:B:2180:GLN:N	2.42	0.49
1:B:2880:GLU:O	1:B:2884:ASN:N	2.42	0.49
1:B:3840:SER:OG	1:B:3875:MET:O	2.26	0.49
1:E:45:ARG:NH2	1:E:447:ASP:OD1	2.37	0.49
1:E:3897:ASN:O	1:E:3901:ASN:ND2	2.46	0.49
1:I:395:GLN:HG3	1:I:397:GLU:H	1.78	0.49
1:I:838:HIS:HA	1:I:1201:HIS:HB3	1.94	0.49
1:I:3707:ARG:HA	1:I:3710:LEU:HD23	1.94	0.49
1:I:4697:VAL:O	1:I:4701:TRP:N	2.42	0.49
1:G:1516:UNK:N	1:G:1529:UNK:O	2.45	0.49
1:G:1931:LEU:HD22	1:G:1935:VAL:HG11	1.94	0.49
1:G:2737:PRO:O	1:G:2888:ARG:NH2	2.46	0.49
1:G:3946:GLN:OE1	1:G:3950:ASN:ND2	2.46	0.49
1:B:580:GLU:OE2	1:B:624:ASN:ND2	2.46	0.49
1:B:1089:TYR:N	1:B:1224:GLU:O	2.41	0.49
1:B:2346:VAL:HG22	1:B:2348:GLU:H	1.78	0.49
1:B:3842:LEU:O	1:B:3929:SER:OG	2.31	0.49
1:B:4066:LEU:HA	1:B:4133:GLN:HE22	1.78	0.49
1:E:1152:MET:HE1	1:E:1217:CYS:HB3	1.93	0.49
1:E:1931:LEU:HD22	1:E:1935:VAL:HG11	1.94	0.49
1:E:3780:LEU:HD11	1:E:3816:MET:HG3	1.95	0.49
1:I:269:TRP:HB3	1:I:272:SER:HB3	1.94	0.49
1:I:952:LYS:HB3	1:I:968:ALA:HB1	1.95	0.49
1:I:4107:GLU:O	1:I:4111:LEU:N	2.40	0.49
1:G:111:HIS:N	1:G:116:MET:O	2.46	0.49
1:G:395:GLN:NE2	1:G:397:GLU:OE1	2.43	0.49
1:G:838:HIS:HA	1:G:1201:HIS:HB3	1.94	0.49
1:B:838:HIS:HA	1:B:1201:HIS:HB3	1.94	0.49
1:B:1516:UNK:N	1:B:1529:UNK:O	2.46	0.49
1:B:2751:LEU:HD11	1:B:2823:ILE:HG21	1.95	0.49
1:E:23:GLN:OE1	1:E:203:ASN:ND2	2.46	0.49
1:E:619:ASP:OD1	1:E:1680:ARG:NH1	2.46	0.49
1:E:2737:PRO:O	1:E:2888:ARG:NH2	2.46	0.49
1:E:4832:HIS:NE2	1:E:4942:GLU:OE1	2.46	0.49
1:I:647:ASN:ND2	1:I:820:ARG:O	2.42	0.49
1:I:2009:LEU:HD23	1:I:2012:PHE:HE2	1.78	0.49
1:I:3781:GLN:O	1:I:3785:ALA:N	2.45	0.49
1:I:3897:ASN:O	1:I:3901:ASN:ND2	2.46	0.49
1:I:4024:VAL:HG23	1:I:4027:LEU:HD12	1.94	0.49
1:I:4702:ASP:OD1	1:I:4778:TRP:NE1	2.44	0.49
1:G:3780:LEU:HD11	1:G:3816:MET:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLN:HE21	1:B:34:LYS:HB3	1.78	0.48
1:B:395:GLN:HG3	1:B:397:GLU:H	1.78	0.48
1:B:551:LEU:HD21	1:B:589:LEU:HB2	1.94	0.48
1:B:583:ILE:HA	1:B:586:ILE:HD12	1.95	0.48
1:B:717:ASP:OD1	1:B:720:HIS:ND1	2.46	0.48
1:B:2868:SER:O	1:B:2872:GLN:N	2.45	0.48
1:B:3781:GLN:O	1:B:3785:ALA:N	2.45	0.48
1:E:932:LEU:HD23	1:E:935:LEU:HD12	1.94	0.48
1:I:72:SER:HB2	1:I:107:ILE:HG13	1.95	0.48
1:I:717:ASP:OD1	1:I:720:HIS:ND1	2.46	0.48
1:I:1770:SER:OG	1:I:1772:ARG:NE	2.46	0.48
1:I:1863:LEU:HB3	1:I:1870:VAL:HG11	1.95	0.48
1:I:2432:LEU:O	1:I:2436:CYS:N	2.46	0.48
1:G:23:GLN:HE21	1:G:34:LYS:HB3	1.77	0.48
1:G:1093:GLU:OE1	1:G:1201:HIS:NE2	2.46	0.48
1:G:2823:ILE:HG12	1:G:2937:VAL:HG22	1.94	0.48
1:B:269:TRP:HB3	1:B:272:SER:HB3	1.94	0.48
1:B:870:ILE:HD11	1:B:1049:TYR:CG	2.48	0.48
1:B:983:THR:O	1:B:987:ARG:N	2.45	0.48
1:B:1154:ASP:O	1:B:1158:ASN:N	2.46	0.48
1:B:1671:ARG:HE	1:B:1713:ASP:HB3	1.79	0.48
1:B:2006:ILE:O	1:B:2010:LEU:N	2.43	0.48
1:B:2009:LEU:HD23	1:B:2012:PHE:HE2	1.78	0.48
1:E:870:ILE:HD11	1:E:1049:TYR:CG	2.48	0.48
1:E:1163:THR:HA	1:E:1168:VAL:HA	1.94	0.48
1:E:3832:ILE:O	1:E:3836:MET:N	2.42	0.48
1:I:243:ARG:NH2	1:I:303:ASP:OD1	2.29	0.48
1:I:396:GLU:HG2	1:I:399:GLN:HB3	1.95	0.48
1:I:540:PHE:HD2	1:I:567:VAL:HG11	1.78	0.48
1:I:3946:GLN:OE1	1:I:3950:ASN:ND2	2.46	0.48
1:G:23:GLN:OE1	1:G:203:ASN:ND2	2.46	0.48
1:B:485:SER:O	1:B:489:ASN:N	2.41	0.48
1:E:4022:ASP:HA	1:E:4025:VAL:HG22	1.95	0.48
1:E:4201:ASN:HA	1:E:4204:GLN:HB3	1.95	0.48
1:E:4824:ARG:HA	1:E:4827:LEU:HB2	1.94	0.48
1:I:2737:PRO:O	1:I:2888:ARG:NH2	2.46	0.48
1:I:3365:UNK:O	1:I:3369:UNK:N	2.45	0.48
1:I:3676:ASP:N	1:I:3676:ASP:OD1	2.45	0.48
1:I:3780:LEU:HD11	1:I:3816:MET:HG3	1.95	0.48
1:G:15:ARG:HG2	1:G:100:THR:HA	1.96	0.48
1:G:396:GLU:HG2	1:G:399:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1271:ARG:HA	1:G:1471:UNK:HA	1.95	0.48
1:G:2302:LEU:O	1:G:2306:GLY:N	2.46	0.48
1:G:2457:LEU:HD23	1:G:2460:LEU:HD12	1.94	0.48
1:G:3365:UNK:O	1:G:3369:UNK:N	2.46	0.48
1:B:3946:GLN:OE1	1:B:3950:ASN:ND2	2.46	0.48
1:B:4180:ARG:O	1:B:4987:ASN:ND2	2.47	0.48
1:E:580:GLU:OE2	1:E:624:ASN:ND2	2.46	0.48
1:E:1154:ASP:O	1:E:1158:ASN:N	2.46	0.48
1:E:1671:ARG:HE	1:E:1713:ASP:HB3	1.78	0.48
1:E:4169:SER:O	1:E:4173:TYR:N	2.45	0.48
1:I:1636:MET:HE2	1:I:1638:ALA:HB2	1.95	0.48
1:G:1698:LEU:N	1:G:1712:TYR:OH	2.46	0.48
1:G:4822:THR:O	1:G:4825:THR:OG1	2.28	0.48
1:B:3897:ASN:O	1:B:3901:ASN:ND2	2.46	0.48
1:B:4807:PHE:HZ	1:I:4857:ASN:HB2	1.79	0.48
1:E:396:GLU:HG2	1:E:399:GLN:HB3	1.95	0.48
1:E:1679:ASN:HA	1:E:1682:ALA:HB3	1.94	0.48
1:E:3365:UNK:O	1:E:3369:UNK:N	2.46	0.48
1:E:3707:ARG:HA	1:E:3710:LEU:HD23	1.94	0.48
1:E:3946:GLN:OE1	1:E:3950:ASN:ND2	2.46	0.48
1:E:4028:LEU:HD11	1:E:4142:ASN:HB3	1.96	0.48
1:E:4702:ASP:HA	1:E:4778:TRP:HE1	1.78	0.48
1:I:57:ASN:HD22	1:I:308:HIS:HB2	1.79	0.48
1:I:442:ILE:HG23	1:I:521:LEU:HD11	1.96	0.48
1:I:2751:LEU:HD11	1:I:2823:ILE:HG21	1.95	0.48
1:I:2868:SER:O	1:I:2872:GLN:N	2.45	0.48
1:I:4832:HIS:NE2	1:I:4942:GLU:OE1	2.46	0.48
1:G:448:LEU:HA	1:G:451:TYR:HB3	1.94	0.48
1:G:580:GLU:OE2	1:G:624:ASN:ND2	2.46	0.48
1:G:619:ASP:OD1	1:G:1680:ARG:NH1	2.47	0.48
1:G:932:LEU:HD23	1:G:935:LEU:HD12	1.94	0.48
1:G:2342:ASN:N	1:G:2342:ASN:OD1	2.45	0.48
1:G:4091:LYS:HA	1:G:4094:GLN:HB3	1.96	0.48
1:G:4702:ASP:HA	1:G:4778:TRP:HE1	1.78	0.48
1:B:111:HIS:HD2	1:B:114:SER:H	1.62	0.48
1:B:2128:TYR:HB3	1:B:3669:PHE:HB3	1.95	0.48
1:B:3945:GLU:O	1:B:3949:ARG:N	2.45	0.48
1:B:4091:LYS:HA	1:B:4094:GLN:HB3	1.96	0.48
1:B:4201:ASN:HA	1:B:4204:GLN:HB3	1.95	0.48
1:E:15:ARG:HG2	1:E:100:THR:HA	1.96	0.48
1:E:72:SER:HB2	1:E:107:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4091:LYS:HA	1:E:4094:GLN:HB3	1.96	0.48
1:I:621:ILE:O	1:I:625:LEU:N	2.38	0.48
1:I:870:ILE:HD11	1:I:1049:TYR:CG	2.48	0.48
1:I:4022:ASP:HA	1:I:4025:VAL:HG22	1.95	0.48
1:G:1089:TYR:N	1:G:1224:GLU:O	2.41	0.48
1:G:1950:GLU:O	1:G:1954:ARG:N	2.45	0.48
1:B:2342:ASN:N	1:B:2342:ASN:OD1	2.45	0.48
1:B:5012:LYS:O	1:B:5016:GLU:N	2.42	0.48
1:E:540:PHE:HD2	1:E:567:VAL:HG11	1.78	0.48
1:E:717:ASP:OD1	1:E:720:HIS:ND1	2.46	0.48
1:E:2751:LEU:HD11	1:E:2823:ILE:HG21	1.95	0.48
1:I:241:GLN:O	1:I:289:ARG:NH1	2.37	0.48
1:I:2758:PHE:O	1:I:2762:THR:N	2.39	0.48
1:I:3889:GLN:OE1	1:I:3960:GLN:NE2	2.47	0.48
1:I:4091:LYS:HA	1:I:4094:GLN:HB3	1.96	0.48
1:I:4201:ASN:HA	1:I:4204:GLN:HB3	1.95	0.48
1:G:111:HIS:HD2	1:G:114:SER:H	1.62	0.48
1:G:870:ILE:HD11	1:G:1049:TYR:CG	2.48	0.48
1:G:1636:MET:HE2	1:G:1638:ALA:HB2	1.95	0.48
1:G:2009:LEU:HD23	1:G:2012:PHE:HE2	1.78	0.48
1:G:2128:TYR:HB3	1:G:3669:PHE:HB3	1.95	0.48
1:G:3945:GLU:O	1:G:3949:ARG:N	2.45	0.48
1:G:4236:SER:O	1:G:4240:ASP:N	2.43	0.48
1:G:4697:VAL:O	1:G:4701:TRP:N	2.42	0.48
1:B:236:ALA:HA	1:B:242:ARG:HD2	1.95	0.48
1:B:1863:LEU:HB3	1:B:1870:VAL:HG11	1.95	0.48
1:B:2432:LEU:O	1:B:2436:CYS:N	2.46	0.48
1:B:4832:HIS:NE2	1:B:4942:GLU:OE1	2.46	0.48
1:E:23:GLN:HE21	1:E:34:LYS:HB3	1.78	0.48
1:E:3752:SER:O	1:E:3756:LYS:N	2.38	0.48
1:E:3842:LEU:O	1:E:3929:SER:OG	2.30	0.48
1:E:4180:ARG:O	1:E:4987:ASN:ND2	2.47	0.48
1:I:111:HIS:HD2	1:I:114:SER:H	1.62	0.48
1:I:448:LEU:HA	1:I:451:TYR:HB3	1.94	0.48
1:I:2302:LEU:O	1:I:2306:GLY:N	2.46	0.48
1:I:4180:ARG:O	1:I:4987:ASN:ND2	2.47	0.48
1:G:1152:MET:HE1	1:G:1217:CYS:HB3	1.93	0.48
1:G:1863:LEU:HB3	1:G:1870:VAL:HG11	1.95	0.48
2:F:7:ILE:HG22	2:F:9:PRO:HD2	1.96	0.48
1:B:540:PHE:HD2	1:B:567:VAL:HG11	1.78	0.48
1:B:2457:LEU:HD23	1:B:2460:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:952:LYS:HB3	1:E:968:ALA:HB1	1.95	0.48
1:E:2302:LEU:O	1:E:2306:GLY:N	2.46	0.48
1:I:1671:ARG:HE	1:I:1713:ASP:HB3	1.78	0.48
1:G:209:CYS:HA	1:G:334:MET:HE2	1.96	0.48
1:G:236:ALA:HA	1:G:242:ARG:HD2	1.95	0.48
1:G:1713:ASP:O	1:G:1717:SER:N	2.39	0.48
1:G:2432:LEU:O	1:G:2436:CYS:N	2.46	0.48
2:A:7:ILE:HG22	2:A:9:PRO:HD2	1.96	0.48
1:B:15:ARG:HG2	1:B:100:THR:HA	1.96	0.48
1:B:1770:SER:OG	1:B:1772:ARG:NE	2.46	0.48
1:B:3707:ARG:HA	1:B:3710:LEU:HD23	1.94	0.48
1:B:4567:LEU:HD12	1:B:4816:ILE:HD12	1.96	0.48
1:E:2009:LEU:HD23	1:E:2012:PHE:HE2	1.78	0.48
1:I:23:GLN:HE21	1:I:34:LYS:HB3	1.78	0.48
1:I:410:LEU:HD21	1:I:441:VAL:HA	1.96	0.48
1:I:619:ASP:OD1	1:I:1680:ARG:NH1	2.47	0.48
1:I:2452:ARG:NH1	1:G:175:SER:O	2.44	0.48
1:I:4066:LEU:HA	1:I:4133:GLN:HE22	1.78	0.48
1:G:1770:SER:OG	1:G:1772:ARG:NE	2.46	0.48
1:G:2451:LEU:O	1:G:2455:ALA:N	2.42	0.48
1:G:2751:LEU:HD11	1:G:2823:ILE:HG21	1.95	0.48
1:G:4022:ASP:HA	1:G:4025:VAL:HG22	1.95	0.48
2:H:7:ILE:HG22	2:H:9:PRO:HD2	1.96	0.48
1:B:410:LEU:HD21	1:B:441:VAL:HA	1.96	0.47
1:B:682:LEU:HD13	1:B:787:VAL:HG11	1.96	0.47
1:B:913:LEU:HD13	1:B:918:ARG:HA	1.96	0.47
1:B:3365:UNK:O	1:B:3369:UNK:N	2.46	0.47
1:B:4022:ASP:HA	1:B:4025:VAL:HG22	1.95	0.47
1:E:241:GLN:O	1:E:289:ARG:NH1	2.37	0.47
1:E:2342:ASN:OD1	1:E:2342:ASN:N	2.45	0.47
1:E:4200:THR:O	1:E:4204:GLN:N	2.37	0.47
1:I:23:GLN:OE1	1:I:203:ASN:ND2	2.46	0.47
1:I:209:CYS:HA	1:I:334:MET:HE2	1.96	0.47
1:I:4567:LEU:HD12	1:I:4816:ILE:HD12	1.96	0.47
1:I:4584:ASP:HA	1:I:4627:MET:HA	1.96	0.47
1:G:1679:ASN:HA	1:G:1682:ALA:HB3	1.94	0.47
1:G:2281:ILE:HA	1:G:2341:VAL:HG11	1.96	0.47
1:G:3829:PHE:HA	1:G:3832:ILE:HD12	1.96	0.47
1:G:4028:LEU:HD11	1:G:4142:ASN:HB3	1.96	0.47
1:G:4738:ALA:HA	1:G:4743:MET:HE3	1.96	0.47
1:G:4832:HIS:NE2	1:G:4942:GLU:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:HB2	1:B:107:ILE:HG13	1.95	0.47
1:B:448:LEU:HA	1:B:451:TYR:HB3	1.94	0.47
1:B:619:ASP:OD1	1:B:1680:ARG:NH1	2.47	0.47
1:E:236:ALA:HA	1:E:242:ARG:HD2	1.95	0.47
1:E:736:HIS:HB2	2:F:7:ILE:HG23	1.95	0.47
1:E:1863:LEU:HB3	1:E:1870:VAL:HG11	1.95	0.47
1:I:3994:HIS:O	1:I:3998:HIS:ND1	2.42	0.47
1:G:57:ASN:HD22	1:G:308:HIS:HB2	1.79	0.47
1:G:451:TYR:O	1:G:474:ARG:NH1	2.44	0.47
1:G:583:ILE:HA	1:G:586:ILE:HD12	1.95	0.47
1:G:731:THR:OG1	1:G:1519:UNK:O	2.32	0.47
1:G:4180:ARG:O	1:G:4987:ASN:ND2	2.47	0.47
2:J:7:ILE:HG22	2:J:9:PRO:HD2	1.96	0.47
1:B:396:GLU:HG2	1:B:399:GLN:HB3	1.95	0.47
1:B:891:TRP:HA	1:B:902:ARG:HB3	1.96	0.47
1:B:4746:ALA:O	1:B:4750:ILE:N	2.42	0.47
1:B:4942:GLU:O	1:B:4946:GLN:N	2.47	0.47
1:E:583:ILE:HA	1:E:586:ILE:HD12	1.95	0.47
1:E:1636:MET:HE2	1:E:1638:ALA:HB2	1.95	0.47
1:E:3840:SER:OG	1:E:3875:MET:O	2.27	0.47
1:E:4738:ALA:HA	1:E:4743:MET:HE3	1.97	0.47
1:I:15:ARG:HG2	1:I:100:THR:HA	1.96	0.47
1:I:236:ALA:HA	1:I:242:ARG:HD2	1.95	0.47
1:I:583:ILE:HA	1:I:586:ILE:HD12	1.95	0.47
1:I:1516:UNK:N	1:I:1529:UNK:O	2.46	0.47
1:I:4937:ILE:O	1:I:4941:GLY:N	2.41	0.47
1:G:4937:ILE:O	1:G:4941:GLY:N	2.41	0.47
2:A:39:SER:HB2	2:A:45:PRO:HA	1.96	0.47
1:B:23:GLN:OE1	1:B:203:ASN:ND2	2.46	0.47
1:B:3994:HIS:O	1:B:3998:HIS:ND1	2.43	0.47
1:B:4560:TYR:O	1:B:4564:PHE:N	2.44	0.47
1:E:2128:TYR:HB3	1:E:3669:PHE:HB3	1.95	0.47
1:E:2346:VAL:HG22	1:E:2348:GLU:H	1.78	0.47
1:I:1848:LEU:HB3	1:I:1853:ILE:HB	1.97	0.47
1:G:442:ILE:HG23	1:G:521:LEU:HD11	1.96	0.47
1:G:540:PHE:HD2	1:G:567:VAL:HG11	1.78	0.47
1:G:1867:GLU:HA	1:G:1870:VAL:HB	1.96	0.47
1:B:111:HIS:N	1:B:116:MET:O	2.46	0.47
1:B:350:HIS:N	1:B:355:LEU:O	2.48	0.47
1:B:360:ALA:N	1:B:375:LYS:O	2.38	0.47
1:B:1950:GLU:O	1:B:1954:ARG:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:LEU:HD21	1:E:441:VAL:HA	1.96	0.47
1:I:682:LEU:HD13	1:I:787:VAL:HG11	1.96	0.47
1:G:3889:GLN:OE1	1:G:3960:GLN:NE2	2.47	0.47
1:B:3889:GLN:OE1	1:B:3960:GLN:NE2	2.47	0.47
1:B:4204:GLN:NE2	1:B:4245:MET:SD	2.70	0.47
1:B:4236:SER:O	1:B:4240:ASP:N	2.43	0.47
1:B:4702:ASP:HA	1:B:4778:TRP:HE1	1.78	0.47
1:E:57:ASN:HD22	1:E:308:HIS:HB2	1.79	0.47
1:E:891:TRP:HA	1:E:902:ARG:HB3	1.97	0.47
1:E:2281:ILE:HA	1:E:2341:VAL:HG11	1.96	0.47
1:E:3676:ASP:OD1	1:E:3676:ASP:N	2.45	0.47
1:I:1032:LYS:O	1:I:1036:ARG:N	2.39	0.47
1:I:1950:GLU:O	1:I:1954:ARG:N	2.45	0.47
1:I:4702:ASP:HA	1:I:4778:TRP:HE1	1.78	0.47
1:G:342:GLY:HA2	1:G:389:PHE:HD2	1.80	0.47
1:G:410:LEU:HD21	1:G:441:VAL:HA	1.96	0.47
1:G:1671:ARG:HE	1:G:1713:ASP:HB3	1.79	0.47
1:G:4066:LEU:HA	1:G:4133:GLN:HE22	1.78	0.47
1:B:57:ASN:HD22	1:B:308:HIS:HB2	1.79	0.47
1:B:209:CYS:HA	1:B:334:MET:HE2	1.96	0.47
1:B:442:ILE:HG23	1:B:521:LEU:HD11	1.96	0.47
1:B:886:ARG:HB2	1:B:907:LEU:HD21	1.97	0.47
1:B:952:LYS:HB3	1:B:968:ALA:HB1	1.95	0.47
1:B:1093:GLU:OE1	1:B:1201:HIS:NE2	2.46	0.47
1:B:1848:LEU:HB3	1:B:1853:ILE:HB	1.97	0.47
1:B:2302:LEU:O	1:B:2306:GLY:N	2.46	0.47
1:B:3552:UNK:O	1:B:3556:UNK:N	2.48	0.47
1:B:4028:LEU:HD11	1:B:4142:ASN:HB3	1.96	0.47
1:E:442:ILE:HG23	1:E:521:LEU:HD11	1.96	0.47
1:E:886:ARG:HB2	1:E:907:LEU:HD21	1.97	0.47
1:E:911:HIS:O	1:E:918:ARG:NH2	2.45	0.47
1:E:983:THR:O	1:E:987:ARG:N	2.45	0.47
1:E:1516:UNK:N	1:E:1529:UNK:O	2.47	0.47
1:E:4066:LEU:HA	1:E:4133:GLN:HE22	1.78	0.47
1:E:4584:ASP:HA	1:E:4627:MET:HA	1.96	0.47
1:I:2116:LEU:O	1:I:2120:MET:N	2.43	0.47
1:I:2128:TYR:HB3	1:I:3669:PHE:HB3	1.95	0.47
1:I:3552:UNK:O	1:I:3556:UNK:N	2.48	0.47
1:I:3702:VAL:O	1:I:3706:SER:N	2.43	0.47
1:I:4738:ALA:HA	1:I:4743:MET:HE3	1.97	0.47
1:G:886:ARG:HB2	1:G:907:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:911:HIS:O	1:G:918:ARG:NH2	2.45	0.47
1:G:983:THR:O	1:G:987:ARG:N	2.45	0.47
1:G:1848:LEU:HB3	1:G:1853:ILE:HB	1.97	0.47
1:G:2176:ASN:O	1:G:2180:GLN:N	2.42	0.47
1:G:4231:MET:HE1	1:G:4960:ILE:HA	1.96	0.47
1:G:4584:ASP:HA	1:G:4627:MET:HA	1.96	0.47
1:B:709:ASP:HB3	1:B:725:HIS:CE1	2.50	0.47
1:B:4584:ASP:HA	1:B:4627:MET:HA	1.96	0.47
1:B:4738:ALA:HA	1:B:4743:MET:HE3	1.96	0.47
1:E:560:ILE:HA	1:E:563:VAL:HG12	1.97	0.47
1:E:4567:LEU:HD12	1:E:4816:ILE:HD12	1.96	0.47
1:I:342:GLY:HA2	1:I:389:PHE:HD2	1.80	0.47
1:I:1093:GLU:OE1	1:I:1201:HIS:NE2	2.46	0.47
1:G:560:ILE:HA	1:G:563:VAL:HG12	1.97	0.47
1:G:1154:ASP:O	1:G:1158:ASN:N	2.46	0.47
1:G:4763:GLY:O	1:G:4766:THR:OG1	2.24	0.47
2:H:69:GLY:N	2:H:103:LEU:O	2.47	0.47
1:B:4231:MET:HE1	1:B:4960:ILE:HA	1.96	0.47
1:E:1867:GLU:HA	1:E:1870:VAL:HB	1.96	0.47
1:E:2739:PRO:HB3	1:E:2884:ASN:HB3	1.97	0.47
1:E:3829:PHE:HA	1:E:3832:ILE:HD12	1.96	0.47
1:I:3829:PHE:HA	1:I:3832:ILE:HD12	1.96	0.47
1:I:4028:LEU:HD11	1:I:4142:ASN:HB3	1.96	0.47
1:I:4231:MET:HE1	1:I:4960:ILE:HA	1.96	0.47
1:G:2739:PRO:HB3	1:G:2884:ASN:HB3	1.97	0.47
1:G:4567:LEU:HD12	1:G:4816:ILE:HD12	1.96	0.47
2:H:39:SER:HB2	2:H:45:PRO:HA	1.96	0.47
1:B:342:GLY:HA2	1:B:389:PHE:HD2	1.80	0.47
1:B:1076:ARG:NH2	1:B:1107:PRO:O	2.40	0.47
1:E:709:ASP:HB3	1:E:725:HIS:CE1	2.50	0.47
1:E:1952:GLN:HA	1:E:1955:VAL:HG12	1.97	0.47
1:I:2420:HIS:ND1	1:I:2493:UNK:O	2.30	0.47
1:I:4236:SER:O	1:I:4240:ASP:N	2.43	0.47
1:G:876:GLU:O	1:G:880:GLU:N	2.42	0.47
1:G:952:LYS:HB3	1:G:968:ALA:HB1	1.95	0.47
1:G:1952:GLN:HA	1:G:1955:VAL:HG12	1.97	0.47
1:G:3781:GLN:HA	1:G:3784:SER:HB3	1.97	0.47
2:F:39:SER:HB2	2:F:45:PRO:HA	1.96	0.47
2:J:39:SER:HB2	2:J:45:PRO:HA	1.96	0.47
1:B:614:VAL:HG22	1:B:616:SER:H	1.80	0.46
1:B:1713:ASP:O	1:B:1717:SER:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:HIS:HD2	1:E:114:SER:H	1.62	0.46
1:E:209:CYS:HA	1:E:334:MET:HE2	1.96	0.46
1:E:342:GLY:HA2	1:E:389:PHE:HD2	1.80	0.46
1:E:4090:LYS:HD3	1:E:4112:LEU:HD13	1.96	0.46
1:I:895:PRO:HA	1:I:905:PRO:HB3	1.97	0.46
1:I:2281:ILE:HA	1:I:2341:VAL:HG11	1.96	0.46
1:I:4101:LYS:HG3	1:G:4731:ILE:HA	1.96	0.46
1:G:891:TRP:HA	1:G:902:ARG:HB3	1.96	0.46
1:G:913:LEU:HD13	1:G:918:ARG:HA	1.96	0.46
1:B:731:THR:OG1	1:B:1519:UNK:O	2.33	0.46
1:B:3829:PHE:HA	1:B:3832:ILE:HD12	1.96	0.46
1:E:895:PRO:HA	1:E:905:PRO:HB3	1.97	0.46
1:E:1770:SER:OG	1:E:1772:ARG:NE	2.46	0.46
1:E:4231:MET:HE1	1:E:4960:ILE:HA	1.96	0.46
1:I:886:ARG:HB2	1:I:907:LEU:HD21	1.97	0.46
1:I:2739:PRO:HB3	1:I:2884:ASN:HB3	1.97	0.46
1:G:4942:GLU:O	1:G:4946:GLN:N	2.47	0.46
1:B:2281:ILE:HA	1:B:2341:VAL:HG11	1.96	0.46
1:E:1089:TYR:N	1:E:1224:GLU:O	2.41	0.46
1:E:3986:TRP:NE1	1:E:4043:GLN:OE1	2.48	0.46
1:E:4560:TYR:O	1:E:4564:PHE:N	2.44	0.46
1:I:709:ASP:HB3	1:I:725:HIS:CE1	2.50	0.46
1:I:3781:GLN:HA	1:I:3784:SER:HB3	1.97	0.46
1:I:3891:LEU:HB3	1:I:3899:PHE:CE2	2.51	0.46
1:G:709:ASP:HB3	1:G:725:HIS:CE1	2.50	0.46
1:G:3986:TRP:NE1	1:G:4043:GLN:OE1	2.48	0.46
1:B:1211:LEU:HD11	1:B:1225:PRO:HB3	1.97	0.46
1:B:1867:GLU:HA	1:B:1870:VAL:HB	1.96	0.46
1:E:55:ALA:O	1:E:281:ARG:NH1	2.35	0.46
1:E:1093:GLU:OE1	1:E:1201:HIS:NE2	2.46	0.46
1:E:1211:LEU:HD11	1:E:1225:PRO:HB3	1.97	0.46
1:E:2432:LEU:O	1:E:2436:CYS:N	2.46	0.46
1:I:350:HIS:N	1:I:355:LEU:O	2.48	0.46
1:I:356:TRP:O	1:I:379:HIS:N	2.43	0.46
1:I:451:TYR:O	1:I:474:ARG:NH1	2.44	0.46
1:I:891:TRP:HA	1:I:902:ARG:HB3	1.97	0.46
1:I:983:THR:O	1:I:987:ARG:N	2.45	0.46
1:I:1090:PHE:HD2	1:I:1202:LEU:HD11	1.81	0.46
1:I:3770:LEU:HD13	1:I:3770:LEU:HA	1.81	0.46
1:G:356:TRP:O	1:G:379:HIS:N	2.43	0.46
1:G:1284:UNK:HA	1:G:1463:UNK:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4204:GLN:NE2	1:G:4245:MET:SD	2.70	0.46
2:F:59:PHE:HD1	2:F:74:LEU:HD11	1.81	0.46
1:B:497:TYR:HB3	1:B:500:ALA:HB2	1.98	0.46
1:B:895:PRO:HA	1:B:905:PRO:HB3	1.98	0.46
1:B:3986:TRP:NE1	1:B:4043:GLN:OE1	2.48	0.46
1:B:4090:LYS:HD3	1:B:4112:LEU:HD13	1.96	0.46
1:E:1848:LEU:HB3	1:E:1853:ILE:HB	1.97	0.46
1:E:3645:PRO:O	1:E:3649:ALA:N	2.46	0.46
1:E:3994:HIS:O	1:E:3998:HIS:ND1	2.42	0.46
1:I:1211:LEU:HD11	1:I:1225:PRO:HB3	1.97	0.46
1:I:1867:GLU:HA	1:I:1870:VAL:HB	1.96	0.46
1:I:2440:MET:O	1:I:2444:GLN:N	2.39	0.46
1:G:682:LEU:HD13	1:G:787:VAL:HG11	1.96	0.46
1:G:1090:PHE:HD2	1:G:1202:LEU:HD11	1.81	0.46
1:G:3891:LEU:HB3	1:G:3899:PHE:CE2	2.51	0.46
1:B:25:SER:HA	1:B:34:LYS:HA	1.98	0.46
1:B:179:TYR:OH	1:E:2359:ARG:NH1	2.49	0.46
1:E:485:SER:HA	1:E:488:LEU:HB2	1.98	0.46
1:E:1271:ARG:HA	1:E:1471:UNK:HA	1.97	0.46
1:E:3945:GLU:O	1:E:3949:ARG:N	2.45	0.46
1:I:3658:LYS:HA	1:I:3661:TRP:CD2	2.51	0.46
1:I:3986:TRP:NE1	1:I:4043:GLN:OE1	2.48	0.46
1:G:113:HIS:CE1	1:G:399:GLN:HA	2.51	0.46
1:G:617:ASN:HA	1:G:620:LEU:HB2	1.98	0.46
1:G:2880:GLU:O	1:G:2884:ASN:N	2.42	0.46
1:G:4060:LYS:HE3	1:G:4064:MET:HB2	1.97	0.46
1:G:4090:LYS:HD3	1:G:4112:LEU:HD13	1.96	0.46
1:B:3702:VAL:O	1:B:3706:SER:N	2.43	0.46
1:E:614:VAL:HG22	1:E:616:SER:H	1.80	0.46
1:E:617:ASN:HA	1:E:620:LEU:HB2	1.98	0.46
1:E:4041:ALA:HA	1:E:4044:MET:HB2	1.98	0.46
1:I:497:TYR:HB3	1:I:500:ALA:HB2	1.98	0.46
1:G:1211:LEU:HD11	1:G:1225:PRO:HB3	1.97	0.46
1:G:3552:UNK:O	1:G:3556:UNK:N	2.48	0.46
2:H:59:PHE:HD1	2:H:74:LEU:HD11	1.81	0.46
1:B:224:HIS:N	1:B:229:GLU:O	2.42	0.46
1:B:3891:LEU:HB3	1:B:3899:PHE:CE2	2.51	0.46
1:E:913:LEU:HD13	1:E:918:ARG:HA	1.96	0.46
1:E:3781:GLN:HA	1:E:3784:SER:HB3	1.98	0.46
1:I:25:SER:HA	1:I:34:LYS:HA	1.98	0.46
1:I:113:HIS:CE1	1:I:399:GLN:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:485:SER:HA	1:I:488:LEU:HB2	1.98	0.46
1:I:1154:ASP:O	1:I:1158:ASN:N	2.46	0.46
1:I:1284:UNK:HA	1:I:1463:UNK:HA	1.98	0.46
1:B:485:SER:HA	1:B:488:LEU:HB2	1.98	0.46
1:B:1952:GLN:HA	1:B:1955:VAL:HG12	1.97	0.46
1:B:2297:LYS:O	1:B:2301:TYR:N	2.44	0.46
1:B:4060:LYS:HE3	1:B:4064:MET:HB2	1.97	0.46
1:E:451:TYR:O	1:E:474:ARG:NH1	2.44	0.46
1:E:633:LEU:HB3	1:E:1639:LEU:HD22	1.98	0.46
1:E:4942:GLU:O	1:E:4946:GLN:N	2.47	0.46
1:I:218:HIS:HB3	1:I:392:ARG:HD3	1.98	0.46
1:I:1952:GLN:HA	1:I:1955:VAL:HG12	1.97	0.46
1:I:4060:LYS:HE3	1:I:4064:MET:HB2	1.97	0.46
1:I:4864:ASN:H	1:I:4874:MET:HG2	1.81	0.46
1:G:1269:CYS:HA	1:G:1473:UNK:HA	1.98	0.46
1:B:560:ILE:HA	1:B:563:VAL:HG12	1.97	0.46
1:B:876:GLU:O	1:B:880:GLU:N	2.42	0.46
1:B:2739:PRO:HB3	1:B:2884:ASN:HB3	1.97	0.46
1:B:3781:GLN:HA	1:B:3784:SER:HB3	1.97	0.46
1:E:1721:GLU:OE2	1:E:1725:ARG:NH2	2.39	0.46
1:E:2297:LYS:O	1:E:2301:TYR:N	2.44	0.46
1:E:3552:UNK:O	1:E:3556:UNK:N	2.49	0.46
1:E:3889:GLN:OE1	1:E:3960:GLN:NE2	2.47	0.46
1:I:633:LEU:HB3	1:I:1639:LEU:HD22	1.98	0.46
1:I:913:LEU:HD13	1:I:918:ARG:HA	1.96	0.46
1:I:2212:VAL:O	1:I:2216:GLY:N	2.44	0.46
1:I:5012:LYS:O	1:I:5016:GLU:N	2.42	0.46
1:G:218:HIS:HB3	1:G:392:ARG:HD3	1.98	0.46
1:G:360:ALA:N	1:G:375:LYS:O	2.38	0.46
1:G:2155:LEU:HD21	1:G:2188:ASN:HD22	1.81	0.46
1:G:4041:ALA:HA	1:G:4044:MET:HB2	1.98	0.46
1:G:4864:ASN:H	1:G:4874:MET:HG2	1.81	0.46
2:A:59:PHE:HD1	2:A:74:LEU:HD11	1.81	0.46
1:B:3658:LYS:HA	1:B:3661:TRP:CD2	2.51	0.45
1:E:2176:ASN:O	1:E:2180:GLN:N	2.42	0.45
1:E:2764:GLU:HG3	1:E:2857:PRO:HB2	1.98	0.45
1:E:2878:LEU:HD13	1:E:2926:LEU:HD23	1.98	0.45
1:E:4040:ILE:HG22	1:E:4044:MET:HE3	1.98	0.45
1:I:2327:GLY:HA2	1:I:2330:ARG:HD3	1.98	0.45
1:I:2451:LEU:O	1:I:2455:ALA:N	2.42	0.45
1:G:3461:UNK:O	1:G:3465:UNK:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4937:ILE:HA	1:G:4940:PHE:HD2	1.81	0.45
2:J:59:PHE:HD1	2:J:74:LEU:HD11	1.81	0.45
1:B:134:ASP:HA	1:B:192:ASP:HA	1.98	0.45
1:B:2102:VAL:HB	1:B:2124:LEU:HD12	1.99	0.45
1:B:2420:HIS:ND1	1:B:2493:UNK:O	2.30	0.45
1:E:25:SER:HA	1:E:34:LYS:HA	1.98	0.45
1:E:111:HIS:N	1:E:116:MET:O	2.46	0.45
1:E:682:LEU:HD13	1:E:787:VAL:HG11	1.96	0.45
1:E:1243:PRO:HB2	1:E:1600:LEU:HD13	1.98	0.45
1:E:1965:TYR:HE1	1:E:2027:ILE:HB	1.82	0.45
1:E:3730:ALA:O	1:E:3734:HIS:N	2.50	0.45
1:I:55:ALA:O	1:I:281:ARG:NH1	2.35	0.45
1:I:560:ILE:HA	1:I:563:VAL:HG12	1.97	0.45
1:I:614:VAL:HG22	1:I:616:SER:H	1.80	0.45
1:I:617:ASN:HA	1:I:620:LEU:HB2	1.98	0.45
1:I:4090:LYS:HD3	1:I:4112:LEU:HD13	1.96	0.45
1:G:134:ASP:HA	1:G:192:ASP:HA	1.98	0.45
1:G:485:SER:HA	1:G:488:LEU:HB2	1.98	0.45
1:G:664:PHE:HB2	1:G:746:CYS:HB2	1.98	0.45
1:G:895:PRO:HA	1:G:905:PRO:HB3	1.97	0.45
1:G:1095:VAL:HB	1:G:1199:VAL:HG23	1.98	0.45
1:G:1456:UNK:HA	1:G:1498:UNK:HA	1.98	0.45
1:G:2121:PHE:O	1:G:3725:TYR:OH	2.33	0.45
1:G:2327:GLY:HA2	1:G:2330:ARG:HD3	1.98	0.45
1:G:4006:ASP:HB3	1:G:4009:GLN:HB2	1.98	0.45
1:G:4200:THR:O	1:G:4204:GLN:N	2.37	0.45
1:B:2384:ILE:O	1:B:2388:GLU:N	2.49	0.45
1:B:2878:LEU:HD13	1:B:2926:LEU:HD23	1.98	0.45
1:B:4040:ILE:HG22	1:B:4044:MET:HE3	1.98	0.45
1:E:463:GLU:O	1:E:466:SER:OG	2.29	0.45
1:E:1076:ARG:NH2	1:E:1107:PRO:O	2.40	0.45
1:E:3658:LYS:HA	1:E:3661:TRP:CD2	2.51	0.45
1:E:3885:PHE:HA	1:E:3888:LEU:HB2	1.98	0.45
1:E:4236:SER:O	1:E:4240:ASP:N	2.43	0.45
1:I:793:LEU:HD12	1:I:797:HIS:HB2	1.99	0.45
1:I:2878:LEU:HD13	1:I:2926:LEU:HD23	1.98	0.45
1:G:790:ARG:HG2	1:G:1627:ALA:HA	1.98	0.45
1:G:4561:THR:O	1:G:4565:LEU:N	2.50	0.45
1:B:633:LEU:HB3	1:B:1639:LEU:HD22	1.98	0.45
1:B:1716:ILE:HD11	1:B:1844:LEU:HD13	1.99	0.45
1:B:2155:LEU:HD21	1:B:2188:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4041:ALA:HA	1:B:4044:MET:HB2	1.98	0.45
1:B:4702:ASP:OD1	1:B:4778:TRP:NE1	2.44	0.45
1:B:4864:ASN:H	1:B:4874:MET:HG2	1.81	0.45
1:E:113:HIS:CE1	1:E:399:GLN:HA	2.51	0.45
1:E:790:ARG:HG2	1:E:1627:ALA:HA	1.99	0.45
1:E:4006:ASP:HB3	1:E:4009:GLN:HB2	1.98	0.45
1:E:4060:LYS:HE3	1:E:4064:MET:HB2	1.97	0.45
1:I:1076:ARG:NH2	1:I:1107:PRO:O	2.40	0.45
1:I:2102:VAL:HB	1:I:2124:LEU:HD12	1.99	0.45
1:I:4745:LEU:O	1:I:4749:GLU:N	2.50	0.45
1:I:4937:ILE:HA	1:I:4940:PHE:HD2	1.81	0.45
1:G:25:SER:HA	1:G:34:LYS:HA	1.98	0.45
1:G:633:LEU:HB3	1:G:1639:LEU:HD22	1.98	0.45
1:G:2517:UNK:O	1:G:2521:UNK:N	2.50	0.45
1:G:4107:GLU:O	1:G:4111:LEU:N	2.40	0.45
1:B:2451:LEU:O	1:B:2455:ALA:N	2.42	0.45
1:E:1284:UNK:HA	1:E:1463:UNK:HA	1.98	0.45
1:E:4215:ARG:HA	1:E:4218:ILE:HD12	1.99	0.45
1:I:3959:LYS:O	1:I:3963:ASN:N	2.48	0.45
1:B:1090:PHE:HD2	1:B:1202:LEU:HD11	1.81	0.45
1:B:1965:TYR:HE1	1:B:2027:ILE:HB	1.82	0.45
1:B:2764:GLU:HG3	1:B:2857:PRO:HB2	1.98	0.45
1:B:4200:THR:O	1:B:4204:GLN:N	2.37	0.45
1:B:4243:PHE:HE2	1:B:4668:LEU:HA	1.82	0.45
1:E:1090:PHE:HD2	1:E:1202:LEU:HD11	1.81	0.45
1:E:1095:VAL:HB	1:E:1199:VAL:HG23	1.98	0.45
1:E:2880:GLU:O	1:E:2884:ASN:N	2.42	0.45
1:E:3891:LEU:HB3	1:E:3899:PHE:HE2	1.81	0.45
1:E:4782:VAL:O	1:E:4785:THR:OG1	2.30	0.45
1:I:870:ILE:HA	1:I:870:ILE:HD12	1.79	0.45
1:I:4561:THR:O	1:I:4565:LEU:N	2.50	0.45
1:G:317:ARG:N	1:G:347:PHE:O	2.48	0.45
1:G:1721:GLU:OE2	1:G:1725:ARG:NH2	2.39	0.45
1:G:3658:LYS:HA	1:G:3661:TRP:CD2	2.51	0.45
1:G:4215:ARG:HA	1:G:4218:ILE:HD12	1.99	0.45
1:E:497:TYR:HB3	1:E:500:ALA:HB2	1.98	0.45
1:E:4232:GLU:OE2	1:E:5017:ARG:NH1	2.50	0.45
1:E:4864:ASN:H	1:E:4874:MET:HG2	1.81	0.45
1:I:3885:PHE:HA	1:I:3888:LEU:HB2	1.98	0.45
1:G:242:ARG:NH1	1:G:481:GLU:OE1	2.44	0.45
1:G:299:LEU:O	1:G:375:LYS:NZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:PHE:HB2	1:B:746:CYS:HB2	1.98	0.45
1:B:1284:UNK:HA	1:B:1463:UNK:HA	1.98	0.45
1:E:218:HIS:HB3	1:E:392:ARG:HD3	1.98	0.45
1:E:2517:UNK:O	1:E:2521:UNK:N	2.50	0.45
1:I:111:HIS:N	1:I:116:MET:O	2.46	0.45
1:I:134:ASP:HA	1:I:192:ASP:HA	1.98	0.45
1:I:1965:TYR:HE1	1:I:2027:ILE:HB	1.82	0.45
1:I:4782:VAL:O	1:I:4785:THR:OG1	2.30	0.45
1:G:2775:TRP:HZ3	1:G:2783:GLU:HA	1.82	0.45
1:G:2813:LEU:HD21	1:G:2926:LEU:HD11	1.99	0.45
2:A:69:GLY:N	2:A:103:LEU:O	2.48	0.45
1:B:113:HIS:CE1	1:B:399:GLN:HA	2.51	0.45
1:B:264:PRO:HG2	1:B:270:SER:HB2	1.99	0.45
1:B:617:ASN:HA	1:B:620:LEU:HB2	1.98	0.45
1:B:790:ARG:HG2	1:B:1627:ALA:HA	1.99	0.45
1:B:4147:LEU:HD23	1:B:4150:LEU:HD12	1.99	0.45
1:E:134:ASP:HA	1:E:192:ASP:HA	1.98	0.45
1:E:1716:ILE:HD11	1:E:1844:LEU:HD13	1.99	0.45
1:E:2775:TRP:HZ3	1:E:2783:GLU:HA	1.82	0.45
1:E:2813:LEU:HD21	1:E:2926:LEU:HD11	1.99	0.45
1:I:1290:UNK:HA	1:I:1598:GLN:HE22	1.81	0.45
1:I:2236:LEU:HD23	1:I:2275:VAL:HG21	1.98	0.45
1:I:2813:LEU:HD21	1:I:2926:LEU:HD11	1.99	0.45
1:I:3713:LYS:HG2	1:I:3715:LYS:H	1.82	0.45
1:G:1046:LEU:HD12	1:G:1053:ILE:HD11	1.99	0.45
1:G:2039:LEU:HA	1:G:2042:CYS:HB3	1.99	0.45
1:G:2212:VAL:O	1:G:2216:GLY:N	2.44	0.45
1:G:4147:LEU:HD23	1:G:4150:LEU:HD12	1.99	0.45
1:B:243:ARG:NH2	1:B:303:ASP:OD1	2.29	0.45
1:B:1243:PRO:HB2	1:B:1600:LEU:HD13	1.98	0.45
1:B:3730:ALA:O	1:B:3734:HIS:N	2.50	0.45
1:B:4215:ARG:HA	1:B:4218:ILE:HD12	1.99	0.45
1:E:1269:CYS:HA	1:E:1473:UNK:HA	1.97	0.45
1:E:3770:LEU:HD13	1:E:3770:LEU:HA	1.81	0.45
1:E:4745:LEU:O	1:E:4749:GLU:N	2.50	0.45
1:I:1978:ALA:O	1:I:1983:ALA:N	2.40	0.45
1:I:2384:ILE:O	1:I:2388:GLU:N	2.49	0.45
1:I:2517:UNK:O	1:I:2521:UNK:N	2.50	0.45
1:G:1258:ALA:HB3	1:G:1271:ARG:HB3	1.99	0.45
1:G:1653:LEU:HB3	1:G:1660:GLN:HB2	1.99	0.45
1:G:3663:LEU:H	1:G:3663:LEU:HG	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3713:LYS:HG2	1:G:3715:LYS:H	1.82	0.45
1:G:3730:ALA:O	1:G:3734:HIS:N	2.50	0.45
1:G:4040:ILE:HG22	1:G:4044:MET:HE3	1.99	0.45
1:B:2236:LEU:HD23	1:B:2275:VAL:HG21	1.99	0.44
1:B:2247:GLN:O	1:B:2279:SER:OG	2.35	0.44
1:B:3770:LEU:HD13	1:B:3770:LEU:HA	1.81	0.44
1:B:4568:PHE:HA	1:B:4571:PHE:HD2	1.83	0.44
1:E:299:LEU:O	1:E:375:LYS:NZ	2.47	0.44
1:E:2102:VAL:HB	1:E:2124:LEU:HD12	1.99	0.44
1:E:2155:LEU:HD21	1:E:2188:ASN:HD22	1.81	0.44
1:E:3891:LEU:HB3	1:E:3899:PHE:CE2	2.51	0.44
1:E:4568:PHE:HA	1:E:4571:PHE:HD2	1.83	0.44
1:E:4937:ILE:HA	1:E:4940:PHE:HD2	1.81	0.44
1:I:264:PRO:HG2	1:I:270:SER:HB2	1.99	0.44
1:I:664:PHE:HB2	1:I:746:CYS:HB2	1.98	0.44
1:I:1258:ALA:HB3	1:I:1271:ARG:HB3	1.99	0.44
1:I:2155:LEU:HD21	1:I:2188:ASN:HD22	1.81	0.44
1:I:4041:ALA:HA	1:I:4044:MET:HB2	1.98	0.44
1:I:4147:LEU:HD23	1:I:4150:LEU:HD12	1.99	0.44
1:I:4204:GLN:NE2	1:I:4245:MET:SD	2.70	0.44
1:I:4215:ARG:HA	1:I:4218:ILE:HD12	1.99	0.44
1:G:243:ARG:NH2	1:G:303:ASP:OD1	2.29	0.44
1:G:350:HIS:N	1:G:355:LEU:O	2.48	0.44
1:G:793:LEU:HD12	1:G:797:HIS:HB2	1.99	0.44
1:G:2764:GLU:HG3	1:G:2857:PRO:HB2	1.98	0.44
2:F:69:GLY:HA2	2:F:104:LEU:HD23	1.99	0.44
1:B:218:HIS:HB3	1:B:392:ARG:HD3	1.99	0.44
1:B:2039:LEU:HA	1:B:2042:CYS:HB3	1.99	0.44
1:B:2212:VAL:O	1:B:2216:GLY:N	2.44	0.44
1:B:2813:LEU:HD21	1:B:2926:LEU:HD11	1.99	0.44
1:B:4745:LEU:O	1:B:4749:GLU:N	2.50	0.44
1:E:2327:GLY:HA2	1:E:2330:ARG:HD3	1.98	0.44
1:E:2466:LEU:HA	1:E:2469:ILE:HD12	2.00	0.44
1:E:3713:LYS:HG2	1:E:3715:LYS:H	1.82	0.44
1:E:4147:LEU:HD23	1:E:4150:LEU:HD12	1.99	0.44
1:E:4243:PHE:HE2	1:E:4668:LEU:HA	1.82	0.44
1:E:4687:TYR:HE1	1:E:4703:ARG:HG2	1.82	0.44
1:I:2039:LEU:HA	1:I:2042:CYS:HB3	1.99	0.44
1:I:2121:PHE:O	1:I:3725:TYR:OH	2.33	0.44
1:I:2764:GLU:HG3	1:I:2857:PRO:HB2	1.97	0.44
1:I:4006:ASP:HB3	1:I:4009:GLN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4040:ILE:HG22	1:I:4044:MET:HE3	1.99	0.44
1:I:4243:PHE:HE2	1:I:4668:LEU:HA	1.82	0.44
1:G:497:TYR:HB3	1:G:500:ALA:HB2	1.98	0.44
1:G:614:VAL:HG22	1:G:616:SER:H	1.80	0.44
1:G:1243:PRO:HB2	1:G:1600:LEU:HD13	1.98	0.44
1:G:4243:PHE:HE2	1:G:4668:LEU:HA	1.82	0.44
1:B:241:GLN:O	1:B:289:ARG:NH1	2.37	0.44
1:B:309:THR:O	1:B:313:SER:OG	2.34	0.44
1:B:1685:LEU:HD22	1:B:1718:ILE:HD13	1.99	0.44
1:B:2327:GLY:HA2	1:B:2330:ARG:HD3	1.98	0.44
1:B:4006:ASP:HB3	1:B:4009:GLN:HB2	1.98	0.44
1:E:664:PHE:HB2	1:E:746:CYS:HB2	1.98	0.44
1:E:731:THR:OG1	1:E:1519:UNK:O	2.26	0.44
1:E:1258:ALA:HB3	1:E:1271:ARG:HB3	1.99	0.44
1:E:2236:LEU:HD23	1:E:2275:VAL:HG21	1.98	0.44
1:E:3930:ILE:HG23	1:E:3951:PHE:HE1	1.83	0.44
1:E:4763:GLY:O	1:E:4766:THR:OG1	2.25	0.44
1:E:4976:GLU:O	1:E:4979:THR:OG1	2.29	0.44
1:I:1095:VAL:HB	1:I:1199:VAL:HG23	1.98	0.44
1:I:2466:LEU:HA	1:I:2469:ILE:HD12	2.00	0.44
1:G:2878:LEU:HD13	1:G:2926:LEU:HD23	1.98	0.44
1:G:4702:ASP:OD1	1:G:4778:TRP:NE1	2.44	0.44
1:B:1258:ALA:HB3	1:B:1271:ARG:HB3	1.99	0.44
1:B:1721:GLU:OE2	1:B:1725:ARG:NH2	2.39	0.44
1:B:4687:TYR:HE1	1:B:4703:ARG:HG2	1.82	0.44
1:B:4837:LEU:O	1:B:4840:THR:OG1	2.31	0.44
1:E:356:TRP:O	1:E:379:HIS:N	2.43	0.44
1:I:317:ARG:N	1:I:347:PHE:O	2.48	0.44
1:I:3730:ALA:O	1:I:3734:HIS:N	2.50	0.44
1:I:4155:PRO:HB2	1:I:4156:HIS:CD2	2.53	0.44
1:I:4560:TYR:O	1:I:4564:PHE:N	2.44	0.44
1:B:793:LEU:HD12	1:B:797:HIS:HB2	1.99	0.44
1:B:2274:ASP:O	1:B:2278:ALA:N	2.50	0.44
1:B:4114:CYS:HB3	1:B:4131:ARG:HH22	1.82	0.44
1:B:4155:PRO:HB2	1:B:4156:HIS:CD2	2.53	0.44
1:B:4232:GLU:OE2	1:B:5017:ARG:NH1	2.50	0.44
1:B:5018:CYS:SG	1:B:5019:TRP:N	2.91	0.44
1:E:876:GLU:O	1:E:880:GLU:N	2.42	0.44
1:E:1838:PHE:HB3	1:E:1842:LEU:HD11	2.00	0.44
1:E:2451:LEU:O	1:E:2455:ALA:N	2.42	0.44
1:I:790:ARG:HG2	1:I:1627:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1269:CYS:HA	1:I:1473:UNK:HA	1.99	0.44
1:I:1970:GLN:HB2	1:I:3642:TYR:HA	2.00	0.44
1:I:5018:CYS:SG	1:I:5019:TRP:N	2.91	0.44
1:G:2102:VAL:HB	1:G:2124:LEU:HD12	1.98	0.44
1:G:2466:LEU:HA	1:G:2469:ILE:HD12	2.00	0.44
1:G:3885:PHE:HA	1:G:3888:LEU:HB2	1.98	0.44
1:G:4745:LEU:O	1:G:4749:GLU:N	2.50	0.44
1:G:5018:CYS:SG	1:G:5019:TRP:N	2.91	0.44
2:A:69:GLY:HA2	2:A:104:LEU:HD23	1.99	0.44
1:B:4987:ASN:HA	1:B:4990:PHE:HB2	2.00	0.44
1:E:1685:LEU:HD22	1:E:1718:ILE:HD13	1.99	0.44
1:E:1973:GLN:HA	1:E:1976:ARG:HB3	2.00	0.44
1:E:2039:LEU:HA	1:E:2042:CYS:HB3	1.99	0.44
1:E:5018:CYS:SG	1:E:5019:TRP:N	2.91	0.44
1:I:876:GLU:O	1:I:880:GLU:N	2.42	0.44
1:I:1046:LEU:HD12	1:I:1053:ILE:HD11	1.99	0.44
1:I:1716:ILE:HD11	1:I:1844:LEU:HD13	1.99	0.44
1:I:2274:ASP:O	1:I:2278:ALA:N	2.50	0.44
1:I:2793:PRO:HG3	1:I:2855:TYR:CZ	2.53	0.44
1:G:1838:PHE:HB3	1:G:1842:LEU:HD11	2.00	0.44
1:G:2006:ILE:O	1:G:2010:LEU:N	2.43	0.44
1:G:2236:LEU:HD23	1:G:2275:VAL:HG21	1.98	0.44
1:G:2793:PRO:HG3	1:G:2855:TYR:CZ	2.53	0.44
1:G:4568:PHE:HA	1:G:4571:PHE:HD2	1.82	0.44
1:B:1046:LEU:HD12	1:B:1053:ILE:HD11	1.99	0.44
1:B:1838:PHE:HB3	1:B:1842:LEU:HD11	2.00	0.44
1:E:793:LEU:HD12	1:E:797:HIS:HB2	1.99	0.44
1:E:2212:VAL:O	1:E:2216:GLY:N	2.44	0.44
1:E:4108:ILE:HA	1:E:4111:LEU:HD12	1.99	0.44
1:I:224:HIS:N	1:I:229:GLU:O	2.42	0.44
1:I:733:PRO:HD2	1:I:763:PRO:HD2	2.00	0.44
1:I:3930:ILE:HG23	1:I:3951:PHE:HE1	1.83	0.44
1:G:1293:UNK:N	1:G:1456:UNK:O	2.50	0.44
1:G:3960:GLN:HA	1:G:3963:ASN:HD22	1.83	0.44
2:J:29:MET:HB3	2:J:98:ILE:HB	2.00	0.44
1:B:685:GLY:N	1:B:780:VAL:O	2.35	0.44
1:B:1095:VAL:HB	1:B:1199:VAL:HG23	1.99	0.44
1:B:2517:UNK:O	1:B:2521:UNK:N	2.51	0.44
1:B:2760:GLU:O	1:B:2764:GLU:N	2.48	0.44
1:B:2788:HIS:CE1	1:B:2790:MET:HB2	2.53	0.44
1:B:3885:PHE:HA	1:B:3888:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4657:CYS:O	1:B:4661:TYR:N	2.49	0.44
1:E:2793:PRO:HG3	1:E:2855:TYR:CZ	2.53	0.44
1:E:3461:UNK:O	1:E:3465:UNK:N	2.51	0.44
1:E:4155:PRO:HB2	1:E:4156:HIS:CD2	2.53	0.44
1:I:463:GLU:O	1:I:466:SER:OG	2.29	0.44
1:I:1815:LEU:HG	1:I:1865:MET:HE2	2.00	0.44
1:I:2788:HIS:CE1	1:I:2790:MET:HB2	2.53	0.44
1:G:4108:ILE:HA	1:G:4111:LEU:HD12	1.99	0.44
1:G:4232:GLU:OE2	1:G:5017:ARG:NH1	2.50	0.44
1:G:4687:TYR:HE1	1:G:4703:ARG:HG2	1.82	0.44
1:B:733:PRO:HD2	1:B:763:PRO:HD2	2.00	0.44
1:B:1653:LEU:HB3	1:B:1660:GLN:HB2	1.99	0.44
1:B:1704:PRO:HG2	1:B:1707:LEU:HB2	2.00	0.44
1:B:1970:GLN:HB2	1:B:3642:TYR:HA	2.00	0.44
1:B:1973:GLN:HA	1:B:1976:ARG:HB3	2.00	0.44
1:B:2452:ARG:NH1	1:I:175:SER:O	2.45	0.44
1:B:2466:LEU:HA	1:B:2469:ILE:HD12	2.00	0.44
1:B:3891:LEU:HB3	1:B:3899:PHE:HE2	1.82	0.44
1:E:1735:ILE:HG23	1:E:1771:LEU:HD23	2.00	0.44
1:E:4987:ASN:HA	1:E:4990:PHE:HB2	2.00	0.44
1:I:1653:LEU:HB3	1:I:1660:GLN:HB2	1.99	0.44
1:I:1973:GLN:HA	1:I:1976:ARG:HB3	2.00	0.44
1:I:4687:TYR:HE1	1:I:4703:ARG:HG2	1.82	0.44
1:G:45:ARG:HD2	1:G:138:GLN:HB2	2.00	0.44
1:G:1023:PRO:O	1:G:1027:LEU:N	2.51	0.44
1:G:1965:TYR:HE1	1:G:2027:ILE:HB	1.82	0.44
1:G:1973:GLN:HA	1:G:1976:ARG:HB3	2.00	0.44
1:B:1234:VAL:HG12	1:B:1236:THR:H	1.83	0.43
1:E:4561:THR:O	1:E:4565:LEU:N	2.50	0.43
1:I:1234:VAL:HG12	1:I:1236:THR:H	1.83	0.43
1:I:1293:UNK:N	1:I:1456:UNK:O	2.50	0.43
1:I:3361:UNK:O	1:I:3365:UNK:N	2.51	0.43
1:I:3461:UNK:O	1:I:3465:UNK:N	2.51	0.43
1:I:3891:LEU:HB3	1:I:3899:PHE:HE2	1.81	0.43
1:I:4114:CYS:HB3	1:I:4131:ARG:HH22	1.82	0.43
1:G:264:PRO:HG2	1:G:270:SER:HB2	1.99	0.43
1:G:668:VAL:O	1:G:741:GLU:N	2.50	0.43
1:G:1716:ILE:HD11	1:G:1844:LEU:HD13	1.99	0.43
1:G:2788:HIS:CE1	1:G:2790:MET:HB2	2.53	0.43
1:G:3891:LEU:HB3	1:G:3899:PHE:HE2	1.82	0.43
1:G:3994:HIS:O	1:G:3998:HIS:ND1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4987:ASN:HA	1:G:4990:PHE:HB2	2.00	0.43
2:J:7:ILE:N	2:J:71:ARG:O	2.47	0.43
2:J:69:GLY:N	2:J:103:LEU:O	2.48	0.43
1:B:1082:THR:HG21	1:B:1107:PRO:HG3	1.99	0.43
1:B:1735:ILE:HG23	1:B:1771:LEU:HD23	2.01	0.43
1:B:2765:LYS:HA	1:B:2859:PRO:HG3	2.00	0.43
1:B:3713:LYS:HG2	1:B:3715:LYS:H	1.82	0.43
1:B:4101:LYS:HG3	1:I:4731:ILE:HA	2.00	0.43
1:E:2247:GLN:O	1:E:2279:SER:OG	2.35	0.43
1:E:4114:CYS:HB3	1:E:4131:ARG:HH22	1.82	0.43
1:E:4187:SER:OG	1:E:4191:GLU:OE2	2.36	0.43
1:I:242:ARG:NH1	1:I:481:GLU:OE1	2.44	0.43
1:I:1023:PRO:O	1:I:1027:LEU:N	2.51	0.43
1:I:1704:PRO:HG2	1:I:1707:LEU:HB2	2.00	0.43
1:I:2247:GLN:O	1:I:2279:SER:OG	2.35	0.43
1:I:2775:TRP:HZ3	1:I:2783:GLU:HA	1.82	0.43
1:I:3645:PRO:O	1:I:3649:ALA:N	2.46	0.43
1:I:3960:GLN:HA	1:I:3963:ASN:HD22	1.83	0.43
1:I:4201:ASN:ND2	1:I:4993:MET:SD	2.92	0.43
1:I:4568:PHE:HA	1:I:4571:PHE:HD2	1.83	0.43
1:G:1815:LEU:HG	1:G:1865:MET:HE2	2.00	0.43
1:G:2247:GLN:O	1:G:2279:SER:OG	2.35	0.43
1:G:3930:ILE:HG23	1:G:3951:PHE:HE1	1.83	0.43
1:G:4142:ASN:HA	1:G:4145:VAL:HG12	2.01	0.43
1:G:4187:SER:OG	1:G:4191:GLU:OE2	2.36	0.43
1:B:345:LEU:HD23	1:B:389:PHE:HB3	2.01	0.43
1:B:894:GLY:HA3	1:B:903:LEU:HD22	2.00	0.43
1:B:4108:ILE:HA	1:B:4111:LEU:HD12	1.99	0.43
1:B:4142:ASN:HA	1:B:4145:VAL:HG12	2.01	0.43
1:E:264:PRO:HG2	1:E:270:SER:HB2	1.99	0.43
1:E:2121:PHE:O	1:E:3725:TYR:OH	2.33	0.43
1:E:2440:MET:O	1:E:2444:GLN:N	2.40	0.43
1:E:2869:ARG:HA	1:E:2872:GLN:HB3	2.01	0.43
1:I:45:ARG:HD2	1:I:138:GLN:HB2	2.00	0.43
1:I:1838:PHE:HB3	1:I:1842:LEU:HD11	2.00	0.43
1:G:950:LEU:HD22	1:G:970:LEU:HB3	2.00	0.43
1:G:1970:GLN:HB2	1:G:3642:TYR:HA	2.00	0.43
1:G:2384:ILE:O	1:G:2388:GLU:N	2.49	0.43
2:F:29:MET:HB3	2:F:98:ILE:HB	2.00	0.43
1:B:356:TRP:O	1:B:379:HIS:N	2.43	0.43
1:B:1023:PRO:O	1:B:1027:LEU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2332:LEU:HA	1:B:2335:LEU:HB2	2.00	0.43
1:B:4930:ALA:O	1:B:4934:GLY:N	2.48	0.43
1:E:1970:GLN:HB2	1:E:3642:TYR:HA	2.00	0.43
1:I:4987:ASN:HA	1:I:4990:PHE:HB2	2.00	0.43
1:G:1082:THR:HG21	1:G:1107:PRO:HG3	1.99	0.43
1:G:1685:LEU:HD22	1:G:1718:ILE:HD13	1.99	0.43
1:G:4114:CYS:HB3	1:G:4131:ARG:HH22	1.83	0.43
1:G:4155:PRO:HB2	1:G:4156:HIS:CD2	2.53	0.43
2:A:29:MET:HB3	2:A:98:ILE:HB	2.00	0.43
2:J:69:GLY:HA2	2:J:104:LEU:HD23	1.99	0.43
1:B:242:ARG:NH1	1:B:481:GLU:OE1	2.44	0.43
1:B:4937:ILE:HA	1:B:4940:PHE:HD2	1.81	0.43
1:E:733:PRO:HD2	1:E:763:PRO:HD2	2.00	0.43
1:E:870:ILE:HD12	1:E:870:ILE:HA	1.80	0.43
1:E:894:GLY:HA3	1:E:903:LEU:HD22	2.00	0.43
1:E:950:LEU:HD22	1:E:970:LEU:HB3	2.00	0.43
1:E:1653:LEU:HB3	1:E:1660:GLN:HB2	1.99	0.43
1:E:1704:PRO:HG2	1:E:1707:LEU:HB2	2.00	0.43
1:E:2332:LEU:HA	1:E:2335:LEU:HB2	2.00	0.43
1:I:313:SER:HB3	1:I:351:VAL:HB	2.01	0.43
1:I:1243:PRO:HB2	1:I:1600:LEU:HD13	1.98	0.43
1:I:4142:ASN:HA	1:I:4145:VAL:HG12	2.01	0.43
1:I:4232:GLU:OE2	1:I:5017:ARG:NH1	2.50	0.43
1:G:463:GLU:O	1:G:466:SER:OG	2.29	0.43
1:G:733:PRO:HD2	1:G:763:PRO:HD2	2.00	0.43
1:B:950:LEU:HD22	1:B:970:LEU:HB3	2.00	0.43
1:B:1269:CYS:HA	1:B:1473:UNK:HA	1.99	0.43
1:B:2775:TRP:HZ3	1:B:2783:GLU:HA	1.82	0.43
1:B:2793:PRO:HG3	1:B:2855:TYR:CZ	2.53	0.43
1:E:313:SER:HB3	1:E:351:VAL:HB	2.01	0.43
1:E:345:LEU:HD23	1:E:389:PHE:HB3	2.01	0.43
1:E:2788:HIS:CE1	1:E:2790:MET:HB2	2.53	0.43
1:E:3960:GLN:HA	1:E:3963:ASN:HD22	1.83	0.43
1:I:583:ILE:HD13	1:I:621:ILE:HD13	2.01	0.43
1:I:788:LYS:HG2	1:I:1630:CYS:N	2.32	0.43
1:I:2760:GLU:O	1:I:2764:GLU:N	2.48	0.43
1:G:988:LEU:O	1:G:992:GLY:N	2.45	0.43
1:G:1747:LEU:HD13	1:G:1760:HIS:CE1	2.54	0.43
1:G:2765:LYS:HA	1:G:2859:PRO:HG3	2.00	0.43
1:G:2869:ARG:HA	1:G:2872:GLN:HB3	2.01	0.43
1:G:4048:LEU:HD23	1:G:4048:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4657:CYS:O	1:G:4661:TYR:N	2.49	0.43
1:G:4782:VAL:O	1:G:4785:THR:OG1	2.30	0.43
1:E:1046:LEU:HD12	1:E:1053:ILE:HD11	1.99	0.43
1:E:2765:LYS:HA	1:E:2859:PRO:HG3	2.00	0.43
1:E:4142:ASN:HA	1:E:4145:VAL:HG12	2.01	0.43
1:E:4201:ASN:ND2	1:E:4993:MET:SD	2.92	0.43
1:I:2765:LYS:HA	1:I:2859:PRO:HG3	2.00	0.43
1:I:3818:ASP:O	1:I:3822:ASP:N	2.52	0.43
1:G:1665:HIS:HA	1:G:1668:ARG:HG2	2.01	0.43
1:G:4560:TYR:O	1:G:4564:PHE:N	2.44	0.43
2:F:69:GLY:N	2:F:103:LEU:O	2.48	0.43
1:B:550:LYS:HD3	1:B:550:LYS:HA	1.87	0.43
1:B:668:VAL:O	1:B:741:GLU:N	2.50	0.43
1:B:3754:GLU:O	1:B:3758:MET:N	2.51	0.43
1:B:3959:LYS:O	1:B:3963:ASN:N	2.47	0.43
1:B:3960:GLN:HA	1:B:3963:ASN:HD22	1.83	0.43
1:B:4201:ASN:ND2	1:B:4993:MET:SD	2.92	0.43
1:E:457:GLU:OE1	1:E:464:LYS:NZ	2.40	0.43
1:E:988:LEU:O	1:E:992:GLY:N	2.45	0.43
1:E:3646:THR:O	1:E:3650:CYS:N	2.49	0.43
1:I:345:LEU:HD23	1:I:389:PHE:HB3	2.01	0.43
1:I:1685:LEU:HD22	1:I:1718:ILE:HD13	1.99	0.43
1:I:2006:ILE:O	1:I:2010:LEU:N	2.43	0.43
1:I:2332:LEU:HA	1:I:2335:LEU:HB2	2.00	0.43
1:G:1735:ILE:HG23	1:G:1771:LEU:HD23	2.01	0.43
1:G:2332:LEU:HA	1:G:2335:LEU:HB2	2.00	0.43
1:G:4828:SER:O	1:G:4832:HIS:N	2.51	0.43
1:B:1747:LEU:HD13	1:B:1760:HIS:CE1	2.54	0.43
1:B:1815:LEU:HG	1:B:1865:MET:HE2	2.00	0.43
1:B:2869:ARG:HA	1:B:2872:GLN:HB3	2.01	0.43
1:E:1234:VAL:HG12	1:E:1236:THR:H	1.83	0.43
1:E:3663:LEU:H	1:E:3663:LEU:HG	1.57	0.43
1:G:450:GLY:HA2	1:G:453:GLU:HB2	2.01	0.43
1:G:1094:ALA:HB3	1:G:1147:ASP:HB3	2.00	0.43
1:B:313:SER:HB3	1:B:351:VAL:HB	2.01	0.43
1:B:2969:UNK:O	1:B:2973:UNK:N	2.52	0.43
1:B:3930:ILE:HG23	1:B:3951:PHE:HE1	1.83	0.43
1:B:4019:LEU:O	1:B:4023:MET:N	2.46	0.43
1:B:4804:TYR:HB3	1:B:4806:ASN:HD22	1.84	0.43
1:E:1082:THR:HG21	1:E:1107:PRO:HG3	1.99	0.43
1:E:4780:PHE:HA	1:E:4783:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:950:LEU:HD22	1:I:970:LEU:HB3	2.00	0.43
1:I:1082:THR:HG21	1:I:1107:PRO:HG3	1.99	0.43
1:I:1150:GLY:O	1:I:1163:THR:OG1	2.34	0.43
1:I:3754:GLU:O	1:I:3758:MET:N	2.52	0.43
1:G:457:GLU:OE1	1:G:464:LYS:NZ	2.40	0.43
1:G:1130:GLN:HG2	1:G:1138:PRO:HA	2.01	0.43
1:G:2132:GLY:O	1:G:2136:ARG:N	2.52	0.43
1:G:4780:PHE:HA	1:G:4783:ILE:HD12	2.01	0.43
1:B:21:VAL:HG22	1:B:203:ASN:HB2	2.01	0.42
1:B:45:ARG:HD2	1:B:138:GLN:HB2	2.00	0.42
1:B:450:GLY:HA2	1:B:453:GLU:HB2	2.01	0.42
1:B:534:ARG:NH2	1:B:573:GLU:OE2	2.51	0.42
1:E:102:LEU:HB2	1:E:105:HIS:CE1	2.54	0.42
1:E:668:VAL:O	1:E:741:GLU:N	2.50	0.42
1:E:1094:ALA:HB3	1:E:1147:ASP:HB3	2.00	0.42
1:E:1665:HIS:HA	1:E:1668:ARG:HG2	2.01	0.42
1:E:4048:LEU:HD23	1:E:4048:LEU:HA	1.85	0.42
1:I:662:TRP:HH2	1:I:814:ALA:H	1.67	0.42
1:I:1735:ILE:HG23	1:I:1771:LEU:HD23	2.01	0.42
1:I:2297:LYS:O	1:I:2301:TYR:N	2.44	0.42
1:I:4804:TYR:HB3	1:I:4806:ASN:HD22	1.84	0.42
1:G:313:SER:HB3	1:G:351:VAL:HB	2.01	0.42
1:G:1704:PRO:HG2	1:G:1707:LEU:HB2	2.00	0.42
1:G:2297:LYS:O	1:G:2301:TYR:N	2.44	0.42
1:G:4982:GLU:OE1	1:G:4982:GLU:N	2.52	0.42
2:H:69:GLY:HA2	2:H:104:LEU:HD23	1.99	0.42
1:B:583:ILE:HD13	1:B:621:ILE:HD13	2.01	0.42
1:B:1170:MET:HE1	1:B:1176:GLU:HG3	2.02	0.42
1:B:1665:HIS:HA	1:B:1668:ARG:HG2	2.01	0.42
1:B:4780:PHE:HA	1:B:4783:ILE:HD12	2.01	0.42
1:E:1023:PRO:O	1:E:1027:LEU:N	2.51	0.42
1:E:2384:ILE:O	1:E:2388:GLU:N	2.49	0.42
1:E:4879:MET:HB3	1:G:4578:LEU:C	2.44	0.42
1:I:1130:GLN:HG2	1:I:1138:PRO:HA	2.01	0.42
1:I:1747:LEU:HD13	1:I:1760:HIS:CE1	2.54	0.42
1:I:3755:GLU:HA	1:I:3758:MET:HB3	2.02	0.42
1:I:4108:ILE:HA	1:I:4111:LEU:HD12	1.99	0.42
1:G:345:LEU:HD23	1:G:389:PHE:HB3	2.01	0.42
1:G:788:LYS:HG2	1:G:1630:CYS:N	2.32	0.42
1:G:1234:VAL:HG12	1:G:1236:THR:H	1.83	0.42
1:G:4019:LEU:O	1:G:4023:MET:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4201:ASN:ND2	1:G:4993:MET:SD	2.92	0.42
2:H:12:GLY:HA2	2:H:70:GLN:HE21	1.84	0.42
1:B:681:HIS:HB3	1:B:784:SER:HB3	2.01	0.42
1:B:3812:VAL:O	1:B:3816:MET:N	2.46	0.42
1:E:21:VAL:HG22	1:E:203:ASN:HB2	2.01	0.42
1:E:1072:VAL:HG22	1:E:1195:GLY:HA2	2.01	0.42
1:E:2274:ASP:O	1:E:2278:ALA:N	2.50	0.42
1:E:4657:CYS:O	1:E:4661:TYR:N	2.49	0.42
1:E:4982:GLU:OE1	1:E:4982:GLU:N	2.52	0.42
1:I:3906:GLN:H	1:I:3912:THR:HG23	1.85	0.42
1:G:583:ILE:HD13	1:G:621:ILE:HD13	2.01	0.42
1:G:893:TYR:HD1	1:G:907:LEU:HB2	1.84	0.42
1:G:2004:GLU:O	1:G:2008:MET:N	2.50	0.42
1:G:3818:ASP:O	1:G:3822:ASP:N	2.52	0.42
1:B:111:HIS:CD2	1:B:114:SER:H	2.38	0.42
1:B:662:TRP:HH2	1:B:814:ALA:H	1.68	0.42
1:B:1574:PRO:HB3	1:B:1589:PRO:HA	2.01	0.42
1:B:1679:ASN:O	1:B:1683:HIS:ND1	2.40	0.42
1:B:4577:LEU:HG	1:B:4580:TYR:HE2	1.85	0.42
1:E:77:ALA:O	1:E:81:MET:N	2.49	0.42
1:E:111:HIS:CD2	1:E:114:SER:H	2.38	0.42
1:E:350:HIS:N	1:E:355:LEU:O	2.48	0.42
1:E:1130:GLN:HG2	1:E:1138:PRO:HA	2.01	0.42
1:E:1574:PRO:HB3	1:E:1589:PRO:HA	2.01	0.42
1:E:1815:LEU:HG	1:E:1865:MET:HE2	2.00	0.42
1:I:102:LEU:HB2	1:I:105:HIS:CE1	2.54	0.42
1:I:894:GLY:HA3	1:I:903:LEU:HD22	2.00	0.42
1:I:4577:LEU:HG	1:I:4580:TYR:HE2	1.85	0.42
1:I:4780:PHE:HA	1:I:4783:ILE:HD12	2.01	0.42
1:I:4828:SER:O	1:I:4832:HIS:N	2.51	0.42
1:G:111:HIS:CD2	1:G:114:SER:H	2.38	0.42
1:G:1290:UNK:HA	1:G:1598:GLN:HE22	1.84	0.42
1:G:3906:GLN:H	1:G:3912:THR:HG23	1.84	0.42
1:G:4837:LEU:O	1:G:4840:THR:OG1	2.31	0.42
1:B:1130:GLN:HG2	1:B:1138:PRO:HA	2.01	0.42
1:B:3461:UNK:O	1:B:3465:UNK:N	2.52	0.42
1:B:4974:GLY:O	1:B:4978:HIS:N	2.46	0.42
1:E:224:HIS:N	1:E:229:GLU:O	2.42	0.42
1:E:379:HIS:HD2	1:E:382:GLY:H	1.68	0.42
1:E:450:GLY:HA2	1:E:453:GLU:HB2	2.01	0.42
1:E:1747:LEU:HD13	1:E:1760:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:534:ARG:NH2	1:I:573:GLU:OE2	2.51	0.42
1:I:1665:HIS:HA	1:I:1668:ARG:HG2	2.01	0.42
1:I:2132:GLY:O	1:I:2136:ARG:N	2.51	0.42
1:I:2869:ARG:HA	1:I:2872:GLN:HB3	2.01	0.42
1:I:4187:SER:OG	1:I:4191:GLU:OE2	2.36	0.42
1:I:4763:GLY:O	1:I:4766:THR:OG1	2.24	0.42
1:I:4930:ALA:O	1:I:4934:GLY:N	2.48	0.42
1:I:4982:GLU:N	1:I:4982:GLU:OE1	2.52	0.42
1:G:102:LEU:HB2	1:G:105:HIS:CE1	2.54	0.42
1:G:4184:MET:HE2	1:G:4184:MET:HB2	1.92	0.42
2:A:12:GLY:HA2	2:A:70:GLN:HE21	1.84	0.42
1:B:893:TYR:HD1	1:B:907:LEU:HB2	1.84	0.42
1:B:1094:ALA:HB3	1:B:1147:ASP:HB3	2.00	0.42
1:B:4561:THR:O	1:B:4565:LEU:N	2.50	0.42
1:I:450:GLY:HA2	1:I:453:GLU:HB2	2.01	0.42
1:I:681:HIS:HB3	1:I:784:SER:HB3	2.01	0.42
1:I:893:TYR:HD1	1:I:907:LEU:HB2	1.84	0.42
1:I:2908:TYR:CZ	1:I:2916:LYS:HG2	2.55	0.42
1:G:2760:GLU:O	1:G:2764:GLU:N	2.48	0.42
1:G:4804:TYR:HB3	1:G:4806:ASN:HD22	1.84	0.42
1:G:5022:PHE:HA	1:G:5023:PRO:HD3	1.82	0.42
2:J:2:VAL:HG21	2:J:61:GLU:HB2	2.02	0.42
2:J:12:GLY:HA2	2:J:70:GLN:HE21	1.84	0.42
1:B:102:LEU:HB2	1:B:105:HIS:CE1	2.54	0.42
1:B:1293:UNK:N	1:B:1456:UNK:O	2.52	0.42
1:B:2191:PHE:HD1	1:B:2198:MET:HG3	1.84	0.42
1:B:4937:ILE:O	1:B:4941:GLY:N	2.41	0.42
1:E:45:ARG:HD2	1:E:138:GLN:HB2	2.01	0.42
1:E:4204:GLN:NE2	1:E:4245:MET:SD	2.70	0.42
1:I:838:HIS:CE1	1:I:1201:HIS:HD2	2.38	0.42
1:I:1094:ALA:HB3	1:I:1147:ASP:HB3	2.00	0.42
1:I:2009:LEU:HA	1:I:2012:PHE:CE2	2.55	0.42
1:I:4671:PHE:HA	1:I:4674:GLU:HB2	2.02	0.42
1:I:5022:PHE:HA	1:I:5023:PRO:HD3	1.82	0.42
1:G:243:ARG:HA	1:G:301:VAL:HB	2.02	0.42
1:G:894:GLY:HA3	1:G:903:LEU:HD22	2.00	0.42
1:G:2274:ASP:O	1:G:2278:ALA:N	2.50	0.42
1:G:4549:VAL:HA	1:G:4552:LEU:HB3	2.01	0.42
1:G:4577:LEU:HG	1:G:4580:TYR:HE2	1.85	0.42
2:F:12:GLY:HA2	2:F:70:GLN:HE21	1.84	0.42
2:H:2:VAL:HG21	2:H:61:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:MET:HB3	2:H:98:ILE:HB	2.00	0.42
1:B:2009:LEU:HA	1:B:2012:PHE:CE2	2.55	0.42
1:B:4671:PHE:HA	1:B:4674:GLU:HB2	2.02	0.42
1:B:4828:SER:O	1:B:4832:HIS:N	2.51	0.42
1:B:5022:PHE:HA	1:B:5023:PRO:HD3	1.83	0.42
1:E:583:ILE:HD13	1:E:621:ILE:HD13	2.01	0.42
1:E:1679:ASN:O	1:E:1683:HIS:ND1	2.40	0.42
1:E:3959:LYS:O	1:E:3963:ASN:N	2.47	0.42
1:E:4804:TYR:HB3	1:E:4806:ASN:HD22	1.84	0.42
1:I:181:HIS:ND1	1:I:195:PHE:HB2	2.35	0.42
1:I:243:ARG:HA	1:I:301:VAL:HB	2.02	0.42
1:I:2191:PHE:HD1	1:I:2198:MET:HG3	1.84	0.42
1:G:111:HIS:HB2	1:G:137:LEU:HD11	2.02	0.42
1:G:3992:PHE:O	1:G:3996:PHE:N	2.43	0.42
2:A:2:VAL:HG21	2:A:61:GLU:HB2	2.02	0.42
1:B:1290:UNK:HA	1:B:1598:GLN:HE22	1.85	0.42
1:B:2908:TYR:CZ	1:B:2916:LYS:HG2	2.55	0.42
1:B:4899:ASP:OD1	1:E:4892:ARG:NH2	2.49	0.42
1:B:4982:GLU:OE1	1:B:4982:GLU:N	2.52	0.42
1:E:662:TRP:HH2	1:E:814:ALA:H	1.68	0.42
1:E:1170:MET:HE1	1:E:1176:GLU:HG3	2.02	0.42
1:E:3812:VAL:O	1:E:3816:MET:N	2.46	0.42
1:I:21:VAL:HG22	1:I:203:ASN:HB2	2.01	0.42
1:I:111:HIS:CD2	1:I:114:SER:H	2.38	0.42
1:I:1072:VAL:HG22	1:I:1195:GLY:HA2	2.01	0.42
1:I:4834:GLY:HA2	1:I:4837:LEU:HB2	2.02	0.42
1:G:1164:LEU:N	1:G:1167:GLU:O	2.50	0.42
1:G:4767:TRP:HE3	1:G:4770:SER:HB2	1.85	0.42
2:H:55:VAL:HG23	2:H:60:GLU:HB2	2.02	0.42
1:B:1072:VAL:HG22	1:B:1195:GLY:HA2	2.01	0.42
1:B:3755:GLU:HA	1:B:3758:MET:HB3	2.02	0.42
1:E:111:HIS:HB2	1:E:137:LEU:HD11	2.02	0.42
1:E:1164:LEU:N	1:E:1167:GLU:O	2.50	0.42
1:E:3906:GLN:H	1:E:3912:THR:HG23	1.85	0.42
1:I:1170:MET:HE1	1:I:1176:GLU:HG3	2.02	0.42
1:G:21:VAL:HG22	1:G:203:ASN:HB2	2.01	0.42
1:G:838:HIS:CE1	1:G:1201:HIS:HD2	2.38	0.42
1:B:181:HIS:ND1	1:B:195:PHE:HB2	2.35	0.41
1:B:214:VAL:HB	1:B:339:ILE:HB	2.02	0.41
1:B:3646:THR:O	1:B:3650:CYS:N	2.49	0.41
1:E:119:SER:HA	1:E:146:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2009:LEU:HA	1:E:2012:PHE:CE2	2.55	0.41
1:E:4019:LEU:O	1:E:4023:MET:N	2.45	0.41
1:E:4671:PHE:HA	1:E:4674:GLU:HB2	2.02	0.41
1:E:4767:TRP:HE3	1:E:4770:SER:HB2	1.85	0.41
1:E:4860:ARG:NH2	1:G:4582:VAL:HG21	2.34	0.41
1:I:1574:PRO:HB3	1:I:1589:PRO:HA	2.01	0.41
1:I:4220:ASP:O	1:I:4224:GLU:N	2.49	0.41
1:G:181:HIS:ND1	1:G:195:PHE:HB2	2.35	0.41
1:G:232:THR:OG1	1:G:233:ILE:N	2.53	0.41
1:G:379:HIS:HD2	1:G:382:GLY:H	1.68	0.41
1:G:534:ARG:NH2	1:G:573:GLU:OE2	2.51	0.41
1:G:662:TRP:HH2	1:G:814:ALA:H	1.68	0.41
2:J:55:VAL:HG23	2:J:60:GLU:HB2	2.02	0.41
1:B:379:HIS:HD2	1:B:382:GLY:H	1.68	0.41
1:B:3645:PRO:O	1:B:3649:ALA:N	2.46	0.41
1:E:139:GLU:O	1:E:141:ALA:N	2.53	0.41
1:E:3755:GLU:HA	1:E:3758:MET:HB3	2.02	0.41
1:I:886:ARG:HB3	1:I:891:TRP:HB2	2.02	0.41
1:I:4767:TRP:HE3	1:I:4770:SER:HB2	1.85	0.41
1:G:119:SER:HA	1:G:146:CYS:HA	2.02	0.41
1:G:1072:VAL:HG22	1:G:1195:GLY:HA2	2.01	0.41
1:G:1574:PRO:HB3	1:G:1589:PRO:HA	2.01	0.41
1:G:2908:TYR:CZ	1:G:2916:LYS:HG2	2.55	0.41
1:B:3818:ASP:O	1:B:3822:ASP:N	2.52	0.41
1:B:4677:LEU:HD13	1:B:4677:LEU:HA	1.91	0.41
1:E:232:THR:OG1	1:E:233:ILE:N	2.54	0.41
1:E:1259:ARG:NH2	1:E:1595:LEU:O	2.54	0.41
1:E:2908:TYR:CZ	1:E:2916:LYS:HG2	2.54	0.41
1:I:214:VAL:HB	1:I:339:ILE:HB	2.03	0.41
1:I:4200:THR:O	1:I:4204:GLN:N	2.37	0.41
1:B:232:THR:OG1	1:B:233:ILE:N	2.54	0.41
1:B:243:ARG:HA	1:B:301:VAL:HB	2.02	0.41
1:E:214:VAL:HB	1:E:339:ILE:HB	2.02	0.41
1:E:2191:PHE:HD1	1:E:2198:MET:HG3	1.85	0.41
1:E:3754:GLU:O	1:E:3758:MET:N	2.51	0.41
1:E:3850:GLN:HA	1:E:3853:ALA:HB3	2.03	0.41
1:E:4110:PHE:HA	1:E:4113:SER:HB3	2.03	0.41
1:I:139:GLU:O	1:I:141:ALA:N	2.54	0.41
1:I:2878:LEU:HD23	1:I:2878:LEU:HA	1.91	0.41
1:I:4710:SER:OG	1:I:4772:ASP:OD2	2.25	0.41
1:I:4942:GLU:O	1:I:4946:GLN:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:139:GLU:O	1:G:141:ALA:N	2.53	0.41
1:G:886:ARG:HB3	1:G:891:TRP:HB2	2.02	0.41
1:G:2007:ASN:OD1	1:G:3656:SER:OG	2.33	0.41
1:G:4671:PHE:HA	1:G:4674:GLU:HB2	2.02	0.41
2:J:14:THR:N	2:J:67:SER:OG	2.54	0.41
1:B:290:TYR:O	1:B:302:VAL:N	2.42	0.41
1:B:3361:UNK:O	1:B:3365:UNK:N	2.54	0.41
1:E:4577:LEU:HG	1:E:4580:TYR:HE2	1.84	0.41
1:I:685:GLY:N	1:I:780:VAL:O	2.35	0.41
1:I:1096:THR:HG23	1:I:1199:VAL:HG22	2.03	0.41
1:I:4549:VAL:HA	1:I:4552:LEU:HB3	2.01	0.41
1:I:4583:SER:O	1:I:4628:VAL:N	2.49	0.41
1:G:681:HIS:HB3	1:G:784:SER:HB3	2.01	0.41
1:G:1170:MET:HE1	1:G:1176:GLU:HG3	2.02	0.41
1:G:3361:UNK:O	1:G:3365:UNK:N	2.53	0.41
2:H:14:THR:N	2:H:67:SER:OG	2.54	0.41
1:B:139:GLU:O	1:B:141:ALA:N	2.53	0.41
1:B:838:HIS:CE1	1:B:1201:HIS:HD2	2.38	0.41
1:B:3906:GLN:H	1:B:3912:THR:HG23	1.84	0.41
1:B:4110:PHE:HA	1:B:4113:SER:HB3	2.03	0.41
1:B:4767:TRP:HE3	1:B:4770:SER:HB2	1.85	0.41
1:E:181:HIS:ND1	1:E:195:PHE:HB2	2.35	0.41
1:E:886:ARG:HB3	1:E:891:TRP:HB2	2.02	0.41
1:E:1639:LEU:N	1:E:1648:MET:O	2.54	0.41
1:E:1687:SER:OG	2:F:90:VAL:HG22	2.20	0.41
1:E:4549:VAL:HA	1:E:4552:LEU:HB3	2.01	0.41
1:G:4930:ALA:O	1:G:4934:GLY:N	2.48	0.41
1:B:77:ALA:O	1:B:81:MET:N	2.49	0.41
1:B:1774:PRO:HG2	1:B:1776:HIS:CE1	2.56	0.41
1:B:2121:PHE:O	1:B:3725:TYR:OH	2.33	0.41
1:B:3850:GLN:HA	1:B:3853:ALA:HB3	2.03	0.41
1:E:243:ARG:HA	1:E:301:VAL:HB	2.02	0.41
1:E:1286:UNK:HA	1:E:1461:UNK:HA	2.03	0.41
1:E:2132:GLY:O	1:E:2136:ARG:N	2.52	0.41
1:E:4062:PHE:O	1:E:4066:LEU:N	2.54	0.41
1:I:111:HIS:HB2	1:I:137:LEU:HD11	2.02	0.41
1:I:4242:ILE:O	1:I:4246:GLN:N	2.53	0.41
1:I:5026:ASP:OD1	1:I:5027:CYS:N	2.54	0.41
1:G:2009:LEU:HA	1:G:2012:PHE:CE2	2.55	0.41
1:B:317:ARG:N	1:B:347:PHE:O	2.48	0.41
1:B:2265:LEU:HD22	1:B:2330:ARG:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4990:PHE:O	1:B:4994:TYR:N	2.44	0.41
1:E:587:ILE:O	1:E:591:ASP:N	2.54	0.41
1:E:893:TYR:HD1	1:E:907:LEU:HB2	1.84	0.41
1:E:4834:GLY:HA2	1:E:4837:LEU:HB2	2.02	0.41
1:E:5022:PHE:HA	1:E:5023:PRO:HD3	1.82	0.41
1:I:379:HIS:HD2	1:I:382:GLY:H	1.68	0.41
1:I:649:PHE:HB3	1:I:776:LEU:HD13	2.03	0.41
1:I:1259:ARG:NH2	1:I:1595:LEU:O	2.54	0.41
1:I:3850:GLN:HA	1:I:3853:ALA:HB3	2.03	0.41
1:I:4062:PHE:O	1:I:4066:LEU:N	2.54	0.41
1:I:4657:CYS:O	1:I:4661:TYR:N	2.49	0.41
1:G:214:VAL:HB	1:G:339:ILE:HB	2.02	0.41
1:G:2199:ARG:NE	1:G:2246:ASN:OD1	2.54	0.41
1:G:3922:TYR:O	1:G:3926:LEU:N	2.47	0.41
2:A:14:THR:N	2:A:67:SER:OG	2.54	0.41
2:A:55:VAL:HG23	2:A:60:GLU:HB2	2.02	0.41
2:H:7:ILE:N	2:H:71:ARG:O	2.47	0.41
1:B:111:HIS:HB2	1:B:137:LEU:HD11	2.02	0.41
1:B:177:GLU:CD	1:E:2452:ARG:HH12	2.29	0.41
1:B:288:GLY:HA3	1:B:405:HIS:CE1	2.56	0.41
1:B:886:ARG:HB3	1:B:891:TRP:HB2	2.03	0.41
1:B:1096:THR:HG23	1:B:1199:VAL:HG22	2.02	0.41
1:B:1105:ALA:O	1:B:1189:LEU:N	2.54	0.41
1:B:1164:LEU:N	1:B:1167:GLU:O	2.50	0.41
1:B:2199:ARG:NE	1:B:2246:ASN:OD1	2.54	0.41
1:B:2674:UNK:O	1:B:2676:UNK:N	2.54	0.41
1:B:4549:VAL:HA	1:B:4552:LEU:HB3	2.01	0.41
1:B:4834:GLY:HA2	1:B:4837:LEU:HB2	2.02	0.41
1:B:5026:ASP:OD1	1:B:5027:CYS:N	2.54	0.41
1:B:5033:GLU:O	1:B:5037:SER:N	2.54	0.41
1:E:288:GLY:HA3	1:E:405:HIS:CE1	2.56	0.41
1:E:681:HIS:HB3	1:E:784:SER:HB3	2.01	0.41
1:E:3361:UNK:O	1:E:3365:UNK:N	2.54	0.41
1:E:3662:ILE:H	1:E:3662:ILE:HG13	1.79	0.41
1:E:3694:LYS:HA	1:E:3695:PRO:HD3	1.87	0.41
1:E:3818:ASP:O	1:E:3822:ASP:N	2.52	0.41
1:E:3896:ASN:ND2	1:E:3898:ASP:OD1	2.54	0.41
1:I:283:ARG:HH21	1:I:402:ARG:HH12	1.68	0.41
1:I:3945:GLU:O	1:I:3949:ARG:N	2.45	0.41
1:I:4110:PHE:HA	1:I:4113:SER:HB3	2.03	0.41
1:I:4728:HIS:HD2	1:I:4731:ILE:HD11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4987:ASN:OD1	1:I:4987:ASN:N	2.54	0.41
1:I:5033:GLU:O	1:I:5037:SER:N	2.54	0.41
1:G:222:LEU:HG	1:G:390:LEU:HD22	2.03	0.41
1:G:288:GLY:HA3	1:G:405:HIS:CE1	2.56	0.41
1:G:710:ASP:OD1	1:G:710:ASP:N	2.48	0.41
1:G:898:ASP:HB3	1:G:901:LYS:HB2	2.02	0.41
1:G:1259:ARG:NH2	1:G:1595:LEU:O	2.54	0.41
1:G:1639:LEU:N	1:G:1648:MET:O	2.54	0.41
1:G:2191:PHE:HD1	1:G:2198:MET:HG3	1.84	0.41
1:G:3542:UNK:O	1:G:3546:UNK:N	2.54	0.41
1:G:3754:GLU:O	1:G:3758:MET:N	2.51	0.41
1:G:4834:GLY:HA2	1:G:4837:LEU:HB2	2.02	0.41
2:F:2:VAL:HG21	2:F:61:GLU:HB2	2.02	0.41
2:F:14:THR:N	2:F:67:SER:OG	2.54	0.41
1:B:451:TYR:O	1:B:474:ARG:NH1	2.44	0.41
1:B:1259:ARG:NH2	1:B:1595:LEU:O	2.54	0.41
1:B:3896:ASN:ND2	1:B:3898:ASP:OD1	2.54	0.41
1:B:4062:PHE:O	1:B:4066:LEU:N	2.54	0.41
1:B:4728:HIS:HD2	1:B:4731:ILE:HD11	1.86	0.41
1:E:243:ARG:NH2	1:E:303:ASP:OD1	2.29	0.41
1:E:838:HIS:CE1	1:E:1201:HIS:HD2	2.38	0.41
1:E:898:ASP:HB3	1:E:901:LYS:HB2	2.02	0.41
1:E:1150:GLY:O	1:E:1163:THR:OG1	2.34	0.41
1:E:2004:GLU:O	1:E:2008:MET:N	2.50	0.41
1:E:2969:UNK:O	1:E:2973:UNK:N	2.54	0.41
1:E:5033:GLU:O	1:E:5037:SER:N	2.54	0.41
1:I:77:ALA:O	1:I:81:MET:N	2.49	0.41
1:I:288:GLY:HA3	1:I:405:HIS:CE1	2.56	0.41
1:I:1077:ALA:HB3	1:I:1189:LEU:HD11	2.03	0.41
1:I:1774:PRO:HG2	1:I:1776:HIS:CE1	2.56	0.41
1:I:2158:CYS:HB2	1:I:2184:ASN:HD22	1.86	0.41
1:I:3892:CYS:HB2	1:I:3900:GLN:HG2	2.03	0.41
1:I:4578:LEU:O	1:G:4880:MET:HG3	2.21	0.41
1:I:4974:GLY:O	1:I:4978:HIS:N	2.46	0.41
1:G:283:ARG:HH21	1:G:402:ARG:HH12	1.68	0.41
1:G:2158:CYS:HB2	1:G:2184:ASN:HD22	1.86	0.41
1:B:119:SER:HA	1:B:146:CYS:HA	2.02	0.40
1:B:2158:CYS:HB2	1:B:2184:ASN:HD22	1.86	0.40
1:B:4227:GLU:HG3	1:B:4228:ALA:H	1.85	0.40
1:E:359:TYR:HA	1:E:376:ALA:HA	2.03	0.40
1:E:1096:THR:HG23	1:E:1199:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2158:CYS:HB2	1:E:2184:ASN:HD22	1.86	0.40
1:I:2199:ARG:NE	1:I:2246:ASN:OD1	2.54	0.40
1:I:4227:GLU:HG3	1:I:4228:ALA:H	1.85	0.40
1:G:870:ILE:HD12	1:G:870:ILE:HA	1.79	0.40
1:G:1077:ALA:HB3	1:G:1189:LEU:HD11	2.03	0.40
1:G:1105:ALA:O	1:G:1189:LEU:N	2.54	0.40
1:G:2101:MET:HE2	1:G:2101:MET:HB3	1.98	0.40
1:G:3812:VAL:O	1:G:3816:MET:N	2.46	0.40
1:G:3850:GLN:HA	1:G:3853:ALA:HB3	2.03	0.40
1:G:4062:PHE:O	1:G:4066:LEU:N	2.54	0.40
2:A:7:ILE:N	2:A:71:ARG:O	2.47	0.40
1:B:283:ARG:HH21	1:B:402:ARG:HH12	1.68	0.40
1:B:731:THR:OG1	1:B:1520:UNK:O	2.36	0.40
1:B:988:LEU:O	1:B:992:GLY:N	2.45	0.40
1:B:2132:GLY:O	1:B:2136:ARG:N	2.52	0.40
1:E:534:ARG:NH2	1:E:573:GLU:OE2	2.51	0.40
1:E:2007:ASN:OD1	1:E:3656:SER:OG	2.33	0.40
1:E:2587:UNK:O	1:E:2591:UNK:N	2.54	0.40
1:E:4028:LEU:HD23	1:E:4146:LEU:HD13	2.04	0.40
1:E:4687:TYR:CE1	1:E:4692:PRO:HG3	2.56	0.40
1:I:736:HIS:HB3	2:J:8:SER:H	1.85	0.40
1:I:1708:ARG:HG2	1:I:1711:TYR:CE2	2.57	0.40
1:I:2265:LEU:HD22	1:I:2330:ARG:HB3	2.03	0.40
1:I:2298:VAL:HA	1:I:2301:TYR:HB2	2.04	0.40
1:I:3663:LEU:H	1:I:3663:LEU:HG	1.57	0.40
1:G:1720:LEU:HB2	1:G:1847:THR:HG23	2.03	0.40
1:G:3755:GLU:HA	1:G:3758:MET:HB3	2.02	0.40
1:G:3892:CYS:HB2	1:G:3900:GLN:HG2	2.03	0.40
1:G:3959:LYS:O	1:G:3963:ASN:N	2.47	0.40
1:G:4031:LEU:HD22	1:G:4149:ASN:ND2	2.36	0.40
2:F:55:VAL:HG23	2:F:60:GLU:HB2	2.02	0.40
1:B:736:HIS:HB3	2:A:8:SER:H	1.85	0.40
1:B:2025:GLU:HA	1:B:2028:ARG:NE	2.37	0.40
1:B:2298:VAL:HA	1:B:2301:TYR:HB2	2.04	0.40
1:B:4943:LEU:HA	1:B:4946:GLN:HB2	2.03	0.40
1:E:1774:PRO:HG2	1:E:1776:HIS:CE1	2.56	0.40
1:E:5000:GLU:HA	1:E:5003:HIS:NE2	2.37	0.40
1:E:5026:ASP:OD1	1:E:5027:CYS:N	2.54	0.40
1:I:119:SER:HA	1:I:146:CYS:HA	2.02	0.40
1:I:898:ASP:HB3	1:I:901:LYS:HB2	2.03	0.40
1:I:2674:UNK:O	1:I:2676:UNK:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3896:ASN:ND2	1:I:3898:ASP:OD1	2.54	0.40
1:I:3915:ILE:H	1:I:3915:ILE:HG13	1.67	0.40
1:I:4031:LEU:HD22	1:I:4149:ASN:ND2	2.36	0.40
1:I:4687:TYR:CE1	1:I:4692:PRO:HG3	2.56	0.40
1:G:473:ASN:O	1:G:477:LEU:N	2.53	0.40
1:G:1727:ARG:HH21	1:G:1775:HIS:CE1	2.40	0.40
1:G:1774:PRO:HG2	1:G:1776:HIS:CE1	2.56	0.40
1:G:4227:GLU:HG3	1:G:4228:ALA:H	1.85	0.40
1:G:4728:HIS:HD2	1:G:4731:ILE:HD11	1.86	0.40
1:G:4943:LEU:HA	1:G:4946:GLN:HB2	2.03	0.40
1:G:5033:GLU:O	1:G:5037:SER:N	2.54	0.40
1:B:788:LYS:HG2	1:B:1630:CYS:N	2.32	0.40
1:B:946:ALA:HA	1:B:949:ASN:HB2	2.04	0.40
1:B:2021:CYS:HA	1:B:2022:PRO:HD3	1.95	0.40
1:B:3922:TYR:O	1:B:3926:LEU:N	2.47	0.40
1:E:27:THR:OG1	1:E:31:GLU:N	2.55	0.40
1:E:1256:GLU:HG2	1:E:1273:ALA:HB3	2.04	0.40
1:E:1708:ARG:HG2	1:E:1711:TYR:CE2	2.57	0.40
1:E:1965:TYR:OH	1:E:2027:ILE:O	2.27	0.40
1:E:4031:LEU:HD22	1:E:4149:ASN:ND2	2.36	0.40
1:I:222:LEU:HG	1:I:390:LEU:HD22	2.03	0.40
1:I:4677:LEU:HD13	1:I:4677:LEU:HA	1.91	0.40
1:G:359:TYR:HA	1:G:376:ALA:HA	2.03	0.40
1:G:649:PHE:HB3	1:G:776:LEU:HD13	2.03	0.40
1:G:4110:PHE:HA	1:G:4113:SER:HB3	2.03	0.40
2:A:77:THR:OG1	2:A:79:ASP:OD1	2.34	0.40
1:B:222:LEU:HG	1:B:390:LEU:HD22	2.03	0.40
1:B:1141:ARG:H	1:B:1141:ARG:HD2	1.87	0.40
1:B:2587:UNK:O	1:B:2591:UNK:N	2.54	0.40
1:E:473:ASN:O	1:E:477:LEU:N	2.53	0.40
1:E:1105:ALA:O	1:E:1189:LEU:N	2.54	0.40
1:E:2674:UNK:O	1:E:2676:UNK:N	2.54	0.40
1:E:2797:PHE:HB3	1:E:2801:ASP:HB2	2.03	0.40
1:G:114:SER:HA	1:G:399:GLN:HE21	1.87	0.40
1:G:564:LEU:HA	1:G:567:VAL:HG22	2.03	0.40
1:G:1096:THR:HG23	1:G:1199:VAL:HG22	2.02	0.40
1:G:2025:GLU:HA	1:G:2028:ARG:NE	2.37	0.40
1:G:3462:UNK:O	1:G:3466:UNK:N	2.55	0.40
1:G:3770:LEU:HA	1:G:3770:LEU:HD13	1.80	0.40
1:G:4220:ASP:O	1:G:4224:GLU:N	2.49	0.40
1:G:5026:ASP:OD1	1:G:5027:CYS:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	B	3235/4687 (69%)	2875 (89%)	355 (11%)	5 (0%)	43	77
1	E	3235/4687 (69%)	2874 (89%)	356 (11%)	5 (0%)	43	77
1	G	3235/4687 (69%)	2876 (89%)	354 (11%)	5 (0%)	43	77
1	I	3235/4687 (69%)	2876 (89%)	354 (11%)	5 (0%)	43	77
2	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
All	All	13360/19180 (70%)	11877 (89%)	1463 (11%)	20 (0%)	49	83

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1708	ARG
1	E	1708	ARG
1	I	1708	ARG
1	G	1708	ARG
1	B	1932	PRO
1	E	1932	PRO
1	I	1932	PRO
1	G	1932	PRO
1	B	1840	PRO
1	E	1840	PRO
1	I	1840	PRO
1	G	1840	PRO
1	B	5023	PRO
1	E	5023	PRO

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Mol	Chain	Res	Type
1	I	5023	PRO
1	G	5023	PRO
1	B	4641	PRO
1	E	4641	PRO
1	I	4641	PRO
1	G	4641	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	B	2493/3209 (78%)	2485 (100%)	8 (0%)	86	84
1	E	2493/3209 (78%)	2485 (100%)	8 (0%)	86	84
1	G	2493/3209 (78%)	2485 (100%)	8 (0%)	86	84
1	I	2493/3209 (78%)	2485 (100%)	8 (0%)	86	84
2	A	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
2	J	88/89 (99%)	88 (100%)	0	100	100
All	All	10324/13192 (78%)	10292 (100%)	32 (0%)	84	84

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	688	LEU
1	B	978	THR
1	B	2010	LEU
1	B	2339	VAL
1	B	3663	LEU
1	B	3770	LEU
1	B	3805	LEU
1	B	4081	VAL
1	E	688	LEU

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Mol	Chain	Res	Type
1	E	978	THR
1	E	2010	LEU
1	E	2339	VAL
1	E	3663	LEU
1	E	3770	LEU
1	E	3805	LEU
1	E	4081	VAL
1	I	688	LEU
1	I	978	THR
1	I	2010	LEU
1	I	2339	VAL
1	I	3663	LEU
1	I	3770	LEU
1	I	3805	LEU
1	I	4081	VAL
1	G	688	LEU
1	G	978	THR
1	G	2010	LEU
1	G	2339	VAL
1	G	3663	LEU
1	G	3770	LEU
1	G	3805	LEU
1	G	4081	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (235) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	GLN
1	B	44	ASN
1	B	57	ASN
1	B	84	ASN
1	B	105	HIS
1	B	156	GLN
1	B	201	ASN
1	B	203	ASN
1	B	379	HIS
1	B	383	HIS
1	B	395	GLN
1	B	405	HIS
1	B	465	GLN
1	B	582	HIS
1	B	597	HIS

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Mol	Chain	Res	Type
1	B	838	HIS
1	B	877	ASN
1	B	1206	GLN
1	B	1220	GLN
1	B	1598	GLN
1	B	1679	ASN
1	B	1691	GLN
1	B	1693	GLN
1	B	1719	HIS
1	B	1775	HIS
1	B	1861	GLN
1	B	1941	ASN
1	B	1949	GLN
1	B	1970	GLN
1	B	2127	GLN
1	B	2194	HIS
1	B	2260	ASN
1	B	2291	GLN
1	B	2856	ASN
1	B	3766	GLN
1	B	3771	HIS
1	B	3809	ASN
1	B	3896	ASN
1	B	3946	GLN
1	B	3950	ASN
1	B	3963	ASN
1	B	3976	ASN
1	B	4005	GLN
1	B	4037	ASN
1	B	4054	ASN
1	B	4102	GLN
1	B	4120	ASN
1	B	4142	ASN
1	B	4156	HIS
1	B	4691	GLN
1	B	4728	HIS
1	B	4806	ASN
1	B	4949	GLN
1	B	5015	GLN
1	B	5031	GLN
1	E	23	GLN
1	E	44	ASN

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Mol	Chain	Res	Type
1	E	57	ASN
1	E	84	ASN
1	E	105	HIS
1	E	156	GLN
1	E	201	ASN
1	E	203	ASN
1	E	379	HIS
1	E	383	HIS
1	E	395	GLN
1	E	405	HIS
1	E	412	ASN
1	E	465	GLN
1	E	582	HIS
1	E	597	HIS
1	E	838	HIS
1	E	877	ASN
1	E	1206	GLN
1	E	1220	GLN
1	E	1598	GLN
1	E	1679	ASN
1	E	1691	GLN
1	E	1693	GLN
1	E	1719	HIS
1	E	1775	HIS
1	E	1861	GLN
1	E	1941	ASN
1	E	1970	GLN
1	E	2127	GLN
1	E	2194	HIS
1	E	2260	ASN
1	E	2291	GLN
1	E	2856	ASN
1	E	3766	GLN
1	E	3771	HIS
1	E	3809	ASN
1	E	3896	ASN
1	E	3946	GLN
1	E	3950	ASN
1	E	3963	ASN
1	E	3976	ASN
1	E	3994	HIS
1	E	4005	GLN

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Mol	Chain	Res	Type
1	E	4037	ASN
1	E	4102	GLN
1	E	4120	ASN
1	E	4142	ASN
1	E	4156	HIS
1	E	4691	GLN
1	E	4728	HIS
1	E	4806	ASN
1	E	4857	ASN
1	E	4949	GLN
1	E	5015	GLN
1	E	5031	GLN
1	I	23	GLN
1	I	44	ASN
1	I	57	ASN
1	I	84	ASN
1	I	105	HIS
1	I	156	GLN
1	I	201	ASN
1	I	203	ASN
1	I	379	HIS
1	I	383	HIS
1	I	395	GLN
1	I	405	HIS
1	I	412	ASN
1	I	465	GLN
1	I	582	HIS
1	I	597	HIS
1	I	838	HIS
1	I	877	ASN
1	I	1206	GLN
1	I	1220	GLN
1	I	1244	GLN
1	I	1598	GLN
1	I	1679	ASN
1	I	1691	GLN
1	I	1693	GLN
1	I	1719	HIS
1	I	1775	HIS
1	I	1861	GLN
1	I	1941	ASN
1	I	1949	GLN

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Mol	Chain	Res	Type
1	I	1970	GLN
1	I	2036	GLN
1	I	2127	GLN
1	I	2194	HIS
1	I	2260	ASN
1	I	2291	GLN
1	I	2856	ASN
1	I	3766	GLN
1	I	3771	HIS
1	I	3809	ASN
1	I	3896	ASN
1	I	3946	GLN
1	I	3950	ASN
1	I	3963	ASN
1	I	3976	ASN
1	I	3994	HIS
1	I	4005	GLN
1	I	4037	ASN
1	I	4102	GLN
1	I	4120	ASN
1	I	4142	ASN
1	I	4156	HIS
1	I	4691	GLN
1	I	4728	HIS
1	I	4806	ASN
1	I	4949	GLN
1	I	5015	GLN
1	I	5031	GLN
1	G	23	GLN
1	G	44	ASN
1	G	57	ASN
1	G	84	ASN
1	G	105	HIS
1	G	156	GLN
1	G	201	ASN
1	G	203	ASN
1	G	379	HIS
1	G	383	HIS
1	G	395	GLN
1	G	405	HIS
1	G	412	ASN
1	G	465	GLN

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Mol	Chain	Res	Type
1	G	582	HIS
1	G	597	HIS
1	G	838	HIS
1	G	877	ASN
1	G	1206	GLN
1	G	1220	GLN
1	G	1598	GLN
1	G	1679	ASN
1	G	1691	GLN
1	G	1693	GLN
1	G	1702	HIS
1	G	1719	HIS
1	G	1775	HIS
1	G	1861	GLN
1	G	1941	ASN
1	G	1949	GLN
1	G	1970	GLN
1	G	2005	GLN
1	G	2127	GLN
1	G	2194	HIS
1	G	2260	ASN
1	G	2291	GLN
1	G	2856	ASN
1	G	3771	HIS
1	G	3809	ASN
1	G	3896	ASN
1	G	3946	GLN
1	G	3950	ASN
1	G	3963	ASN
1	G	3976	ASN
1	G	3994	HIS
1	G	4005	GLN
1	G	4037	ASN
1	G	4102	GLN
1	G	4120	ASN
1	G	4133	GLN
1	G	4142	ASN
1	G	4156	HIS
1	G	4553	ASN
1	G	4691	GLN
1	G	4728	HIS
1	G	4806	ASN

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Mol	Chain	Res	Type
1	G	4857	ASN
1	G	4949	GLN
1	G	4973	HIS
1	G	5015	GLN
1	G	5031	GLN
2	F	65	GLN
2	A	65	GLN
2	H	32	ASN
2	H	65	GLN
2	J	65	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	12
1	B	12
1	I	12
1	G	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3613:UNK	C	3639:THR	N	45.91
1	B	3613:UNK	C	3639:THR	N	45.70
1	I	3613:UNK	C	3639:THR	N	45.65
1	G	3613:UNK	C	3639:THR	N	45.46
1	I	3163:UNK	C	3170:UNK	N	16.67
1	B	3163:UNK	C	3170:UNK	N	16.62
1	G	3163:UNK	C	3170:UNK	N	16.55
1	E	3163:UNK	C	3170:UNK	N	16.51
1	G	3063:UNK	C	3134:UNK	N	14.87
1	E	3063:UNK	C	3134:UNK	N	14.83
1	I	3063:UNK	C	3134:UNK	N	14.78
1	B	3063:UNK	C	3134:UNK	N	14.77
1	E	2703:UNK	C	2734:ASN	N	14.08
1	G	2703:UNK	C	2734:ASN	N	14.07
1	I	2703:UNK	C	2734:ASN	N	14.05
1	E	3468:UNK	C	3511:UNK	N	14.02
1	B	2703:UNK	C	2734:ASN	N	13.99
1	B	3468:UNK	C	3511:UNK	N	13.95
1	I	3468:UNK	C	3511:UNK	N	13.78
1	G	3468:UNK	C	3511:UNK	N	13.75
1	E	3236:UNK	C	3241:UNK	N	12.64
1	E	1564:UNK	C	1573:MET	N	12.60
1	G	3236:UNK	C	3241:UNK	N	12.60
1	B	3236:UNK	C	3241:UNK	N	12.55
1	B	1564:UNK	C	1573:MET	N	12.50
1	I	3236:UNK	C	3241:UNK	N	12.47
1	B	2976:UNK	C	2995:UNK	N	12.32
1	I	2976:UNK	C	2995:UNK	N	12.32
1	G	1564:UNK	C	1573:MET	N	12.32
1	I	1564:UNK	C	1573:MET	N	12.31
1	E	2976:UNK	C	2995:UNK	N	12.29
1	G	2976:UNK	C	2995:UNK	N	12.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3254:UNK	C	3261:UNK	N	8.51
1	G	3254:UNK	C	3261:UNK	N	8.49
1	B	3254:UNK	C	3261:UNK	N	8.43
1	I	3254:UNK	C	3261:UNK	N	8.39
1	I	1297:UNK	C	1430:UNK	N	5.75
1	G	1297:UNK	C	1430:UNK	N	5.72
1	B	1297:UNK	C	1430:UNK	N	5.70
1	E	1297:UNK	C	1430:UNK	N	5.49
1	I	2939:ARG	C	2942:UNK	N	4.57
1	B	2939:ARG	C	2942:UNK	N	4.45
1	G	2939:ARG	C	2942:UNK	N	4.45
1	E	2939:ARG	C	2942:UNK	N	4.41
1	I	2479:LEU	C	2487:UNK	N	4.05
1	G	2479:LEU	C	2487:UNK	N	4.02
1	B	2479:LEU	C	2487:UNK	N	4.01
1	E	2479:LEU	C	2487:UNK	N	4.00

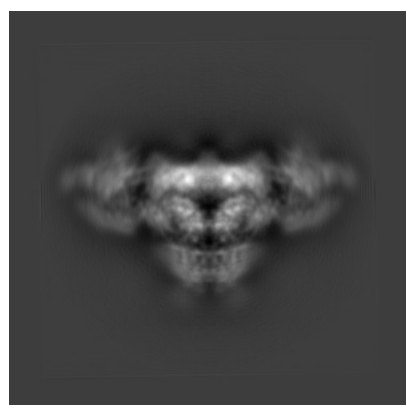
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20486. These allow visual inspection of the internal detail of the map and identification of artifacts.

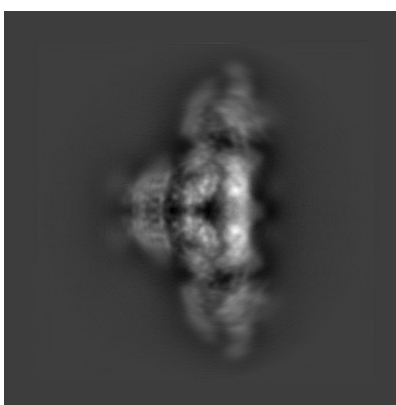
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

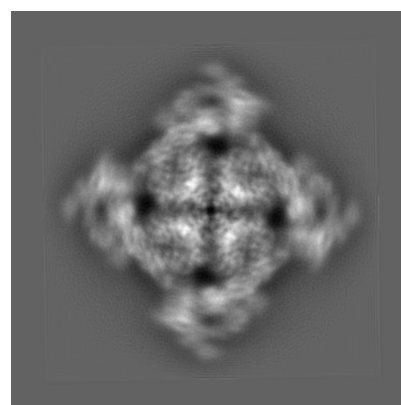
6.1.1 Primary map



X



Y

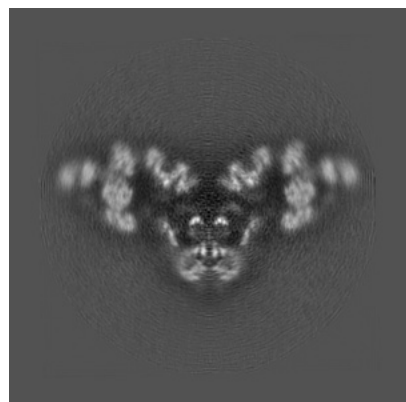


Z

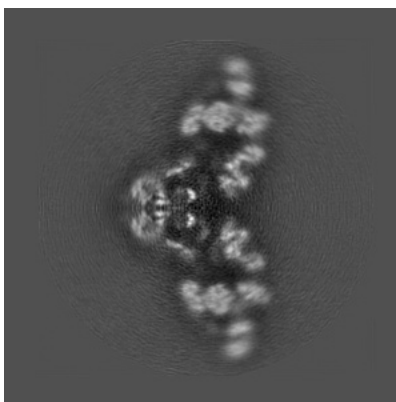
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

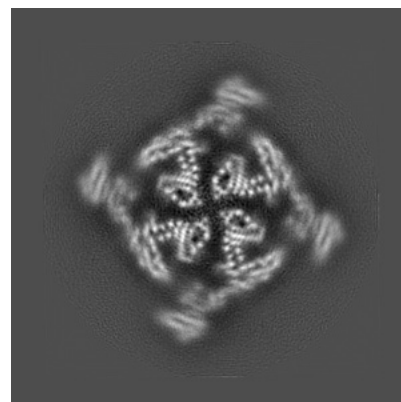
6.2.1 Primary map



X Index: 200



Y Index: 200

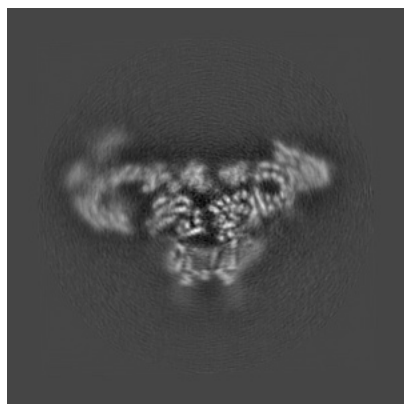


Z Index: 200

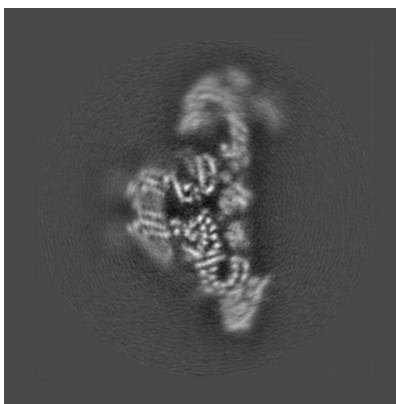
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

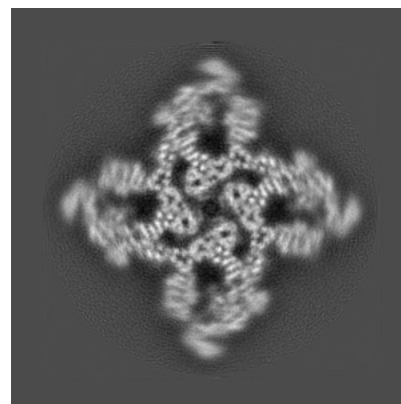
6.3.1 Primary map



X Index: 179



Y Index: 177



Z Index: 231

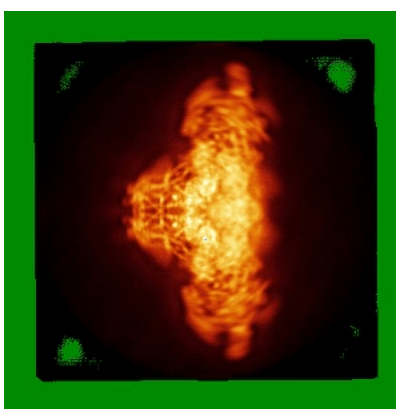
The images above show the largest variance slices of the map in three orthogonal directions.

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

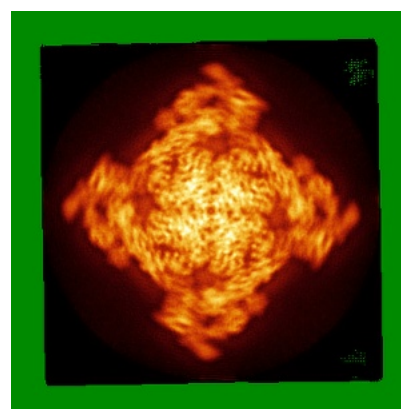
6.4.1 Primary map



X



Y

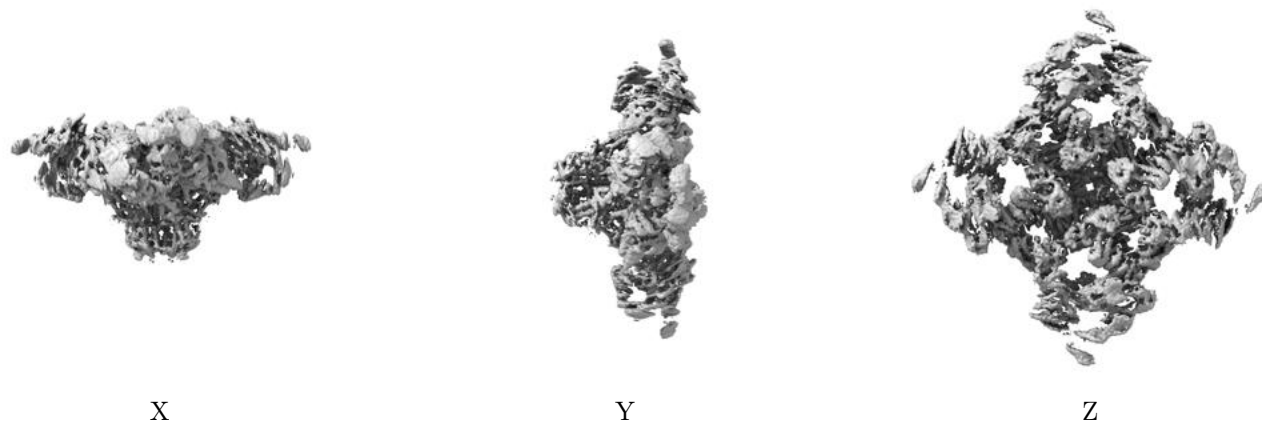


Z

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

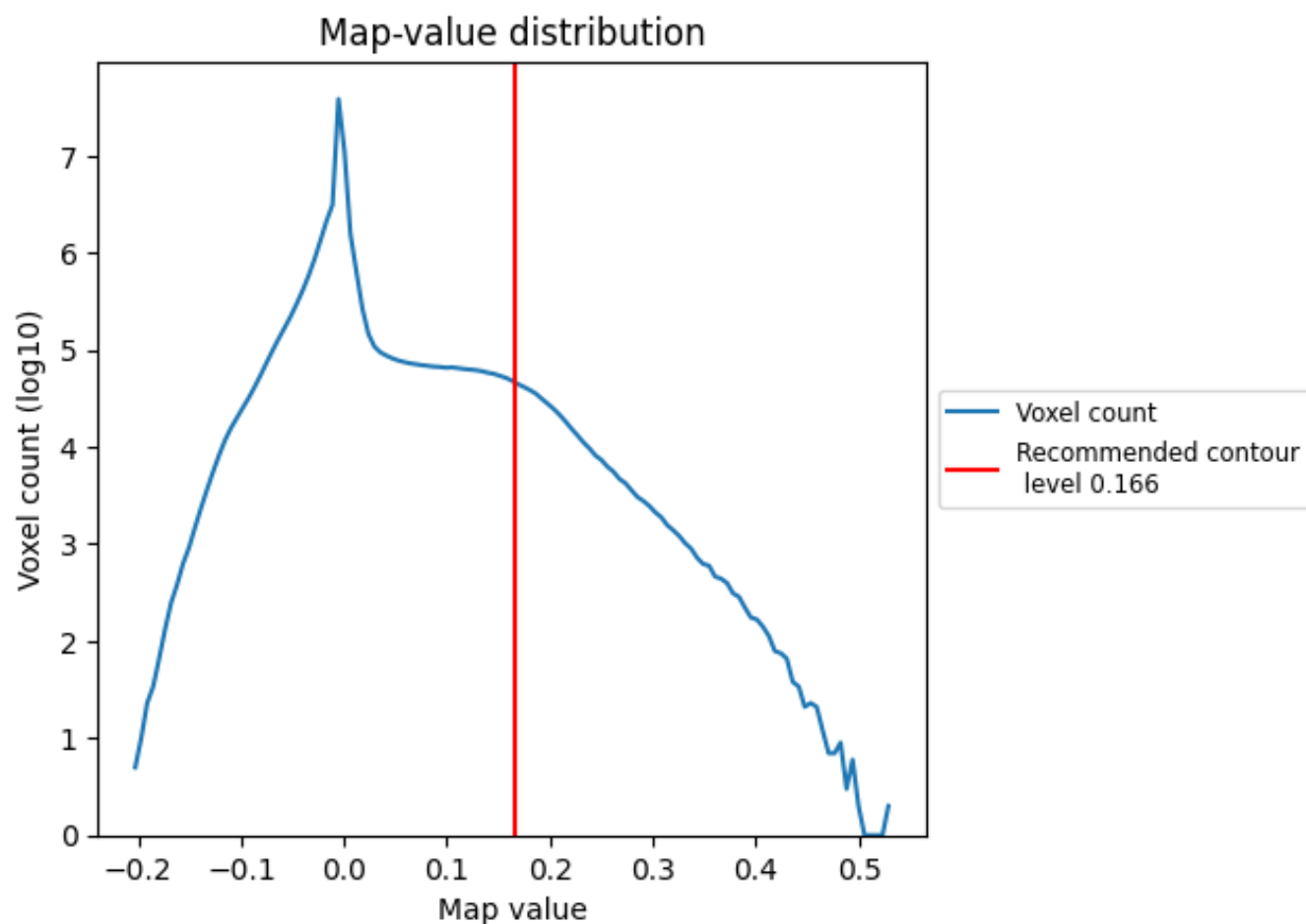
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

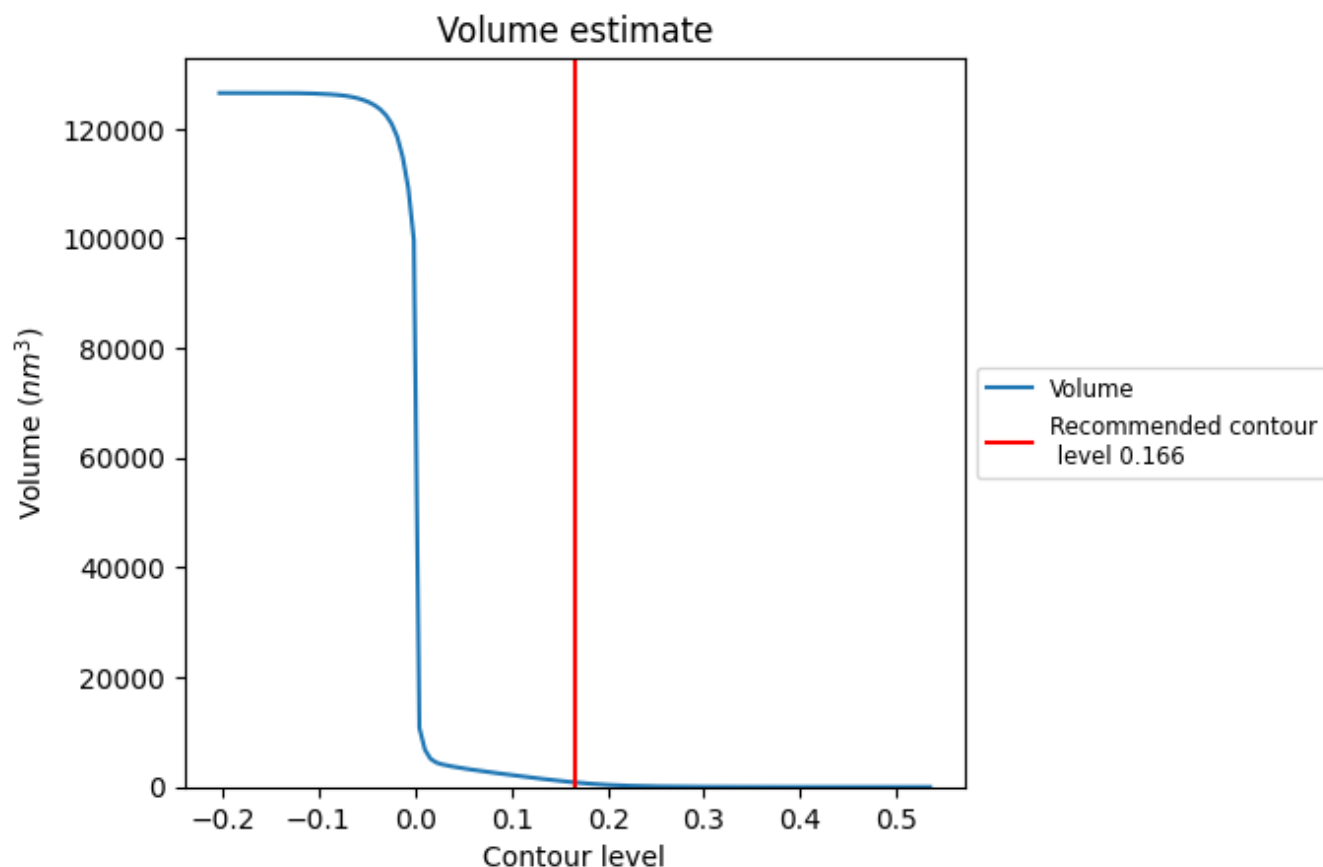
This section contains the results of statistical analysis of the map.

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.

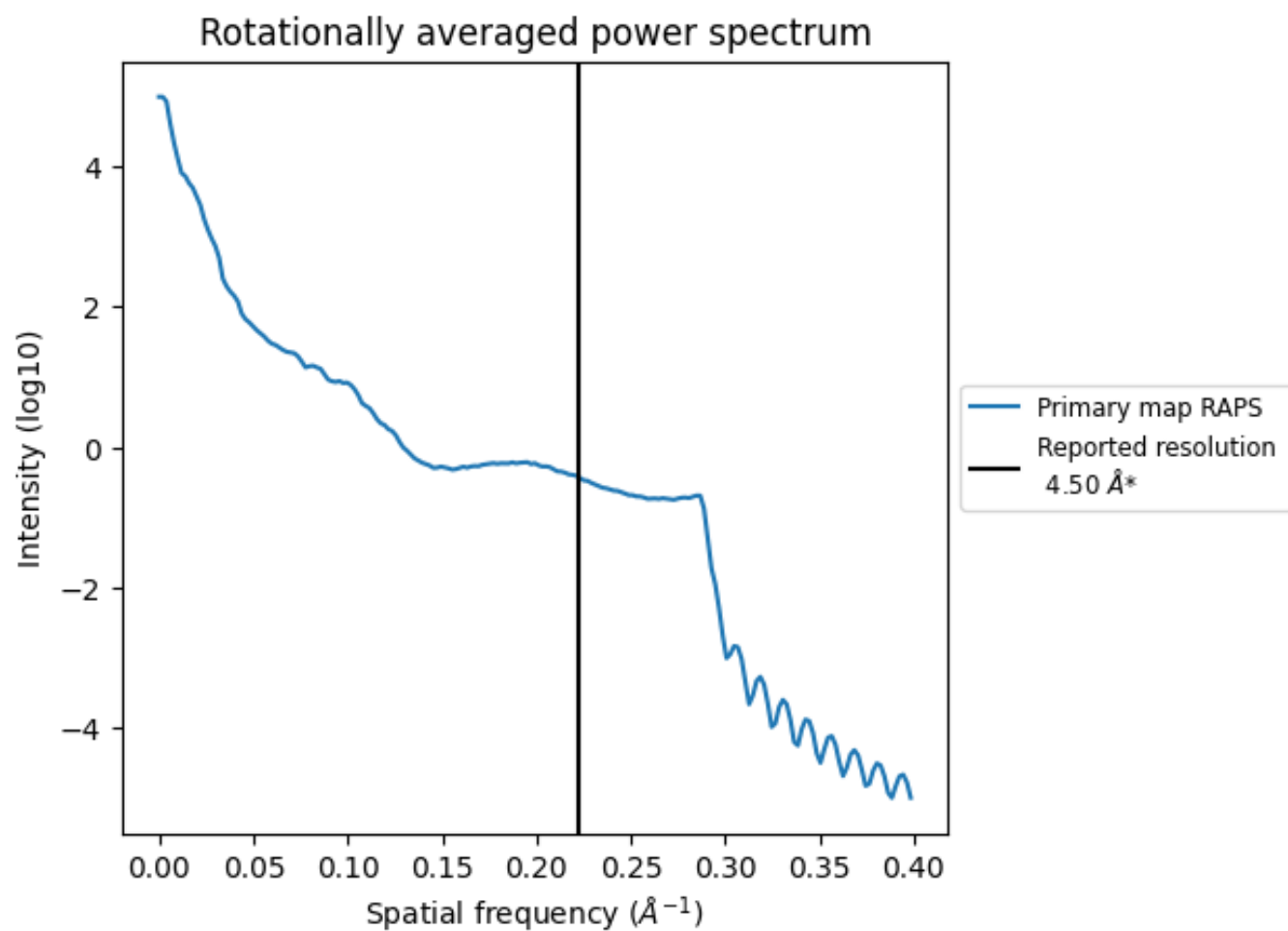
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 830 nm³; this corresponds to an approximate mass of 750 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 0.222 Å⁻¹

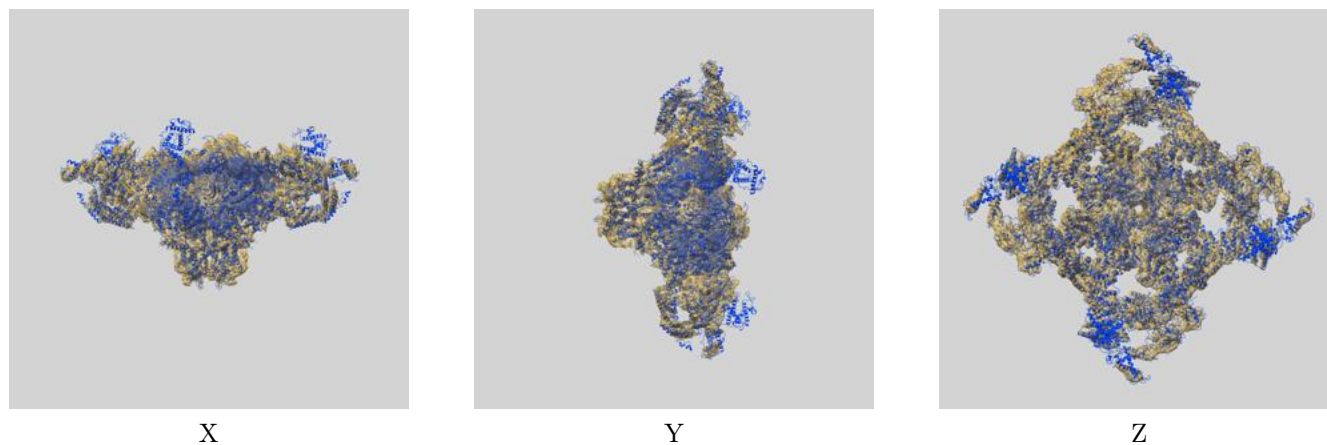
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

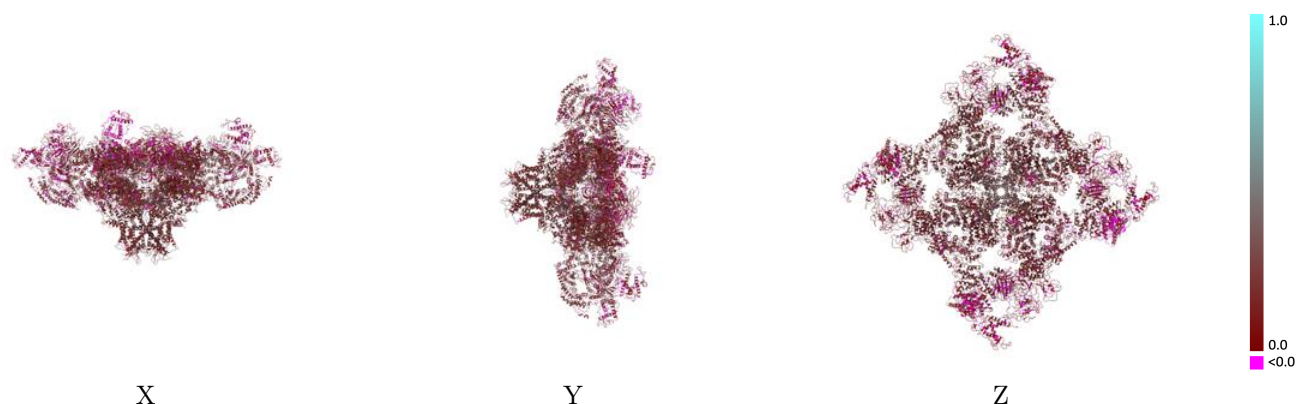
This section contains information regarding the fit between EMDB map EMD-20486 and PDB model 6PV6. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



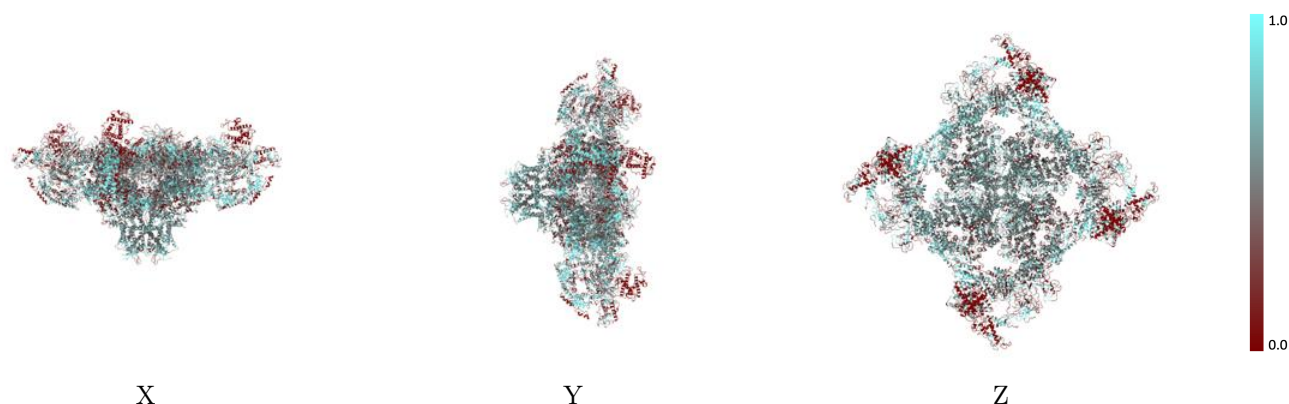
The images above show the 3D surface view of the map at the recommended contour level 0.166 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



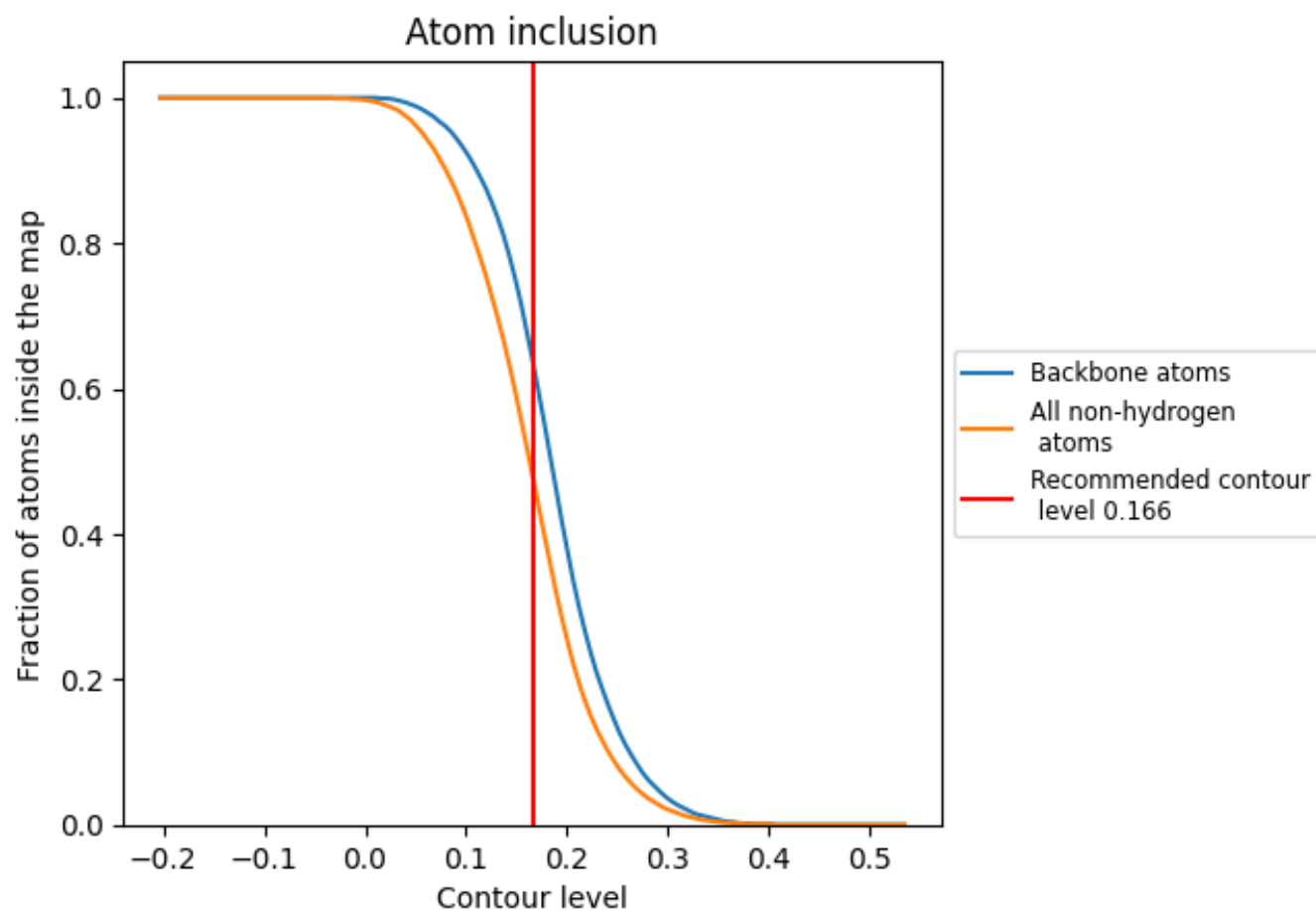
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.166).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 48% 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 (0.166) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4790	0.1800
A	0.4850	0.1850
B	0.4970	0.1950
E	0.4770	0.1780
F	0.4270	0.1320
G	0.4620	0.1660
H	0.4110	0.1400
I	0.4840	0.1860
J	0.4700	0.1810

