



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:58 PM UTC

PDB ID : 8VK3 / pdb_00008vk3
EMDB ID : EMD-43299
Title : Structure of mouse RyR1 in complex with S100A1 (EGTA-only dataset)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2024-01-08
Resolution : 3.21 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

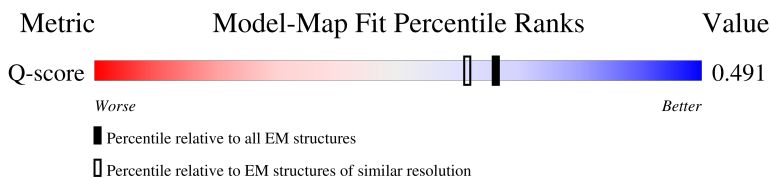
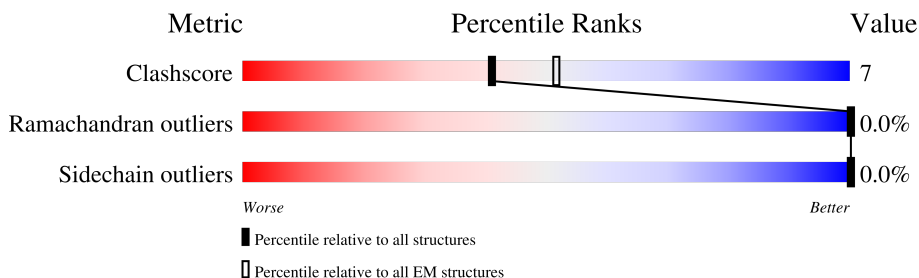
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.21 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.



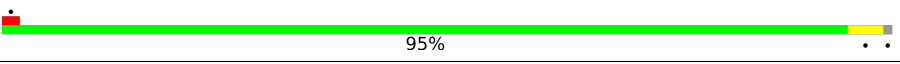
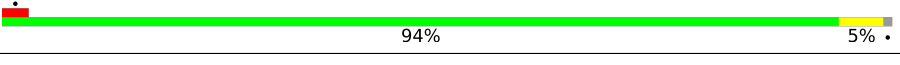
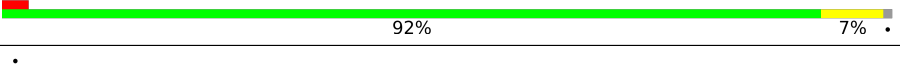
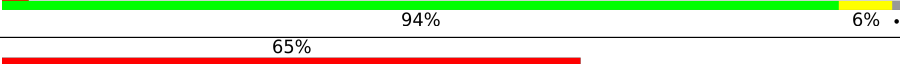
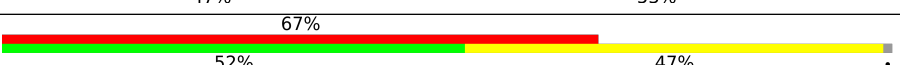
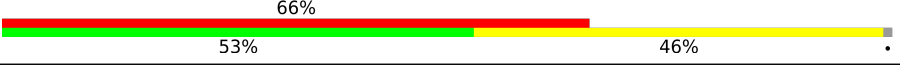
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14613 (2.71 - 3.71)

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

Mol	Chain	Length	Quality of chain
1	A	5035	15% 74% 12% 13%
1	B	5035	15% 74% 13% 13%
1	C	5035	15% 74% 13% 13%
1	D	5035	15% 74% 13% 13%

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Mol	Chain	Length	Quality of chain
2	E	108	
2	F	108	
2	G	108	
2	H	108	
3	I	94	
3	J	94	
3	K	94	
3	L	94	
3	M	94	
3	N	94	
3	O	94	
3	P	94	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 148852 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4374	Total	C	N	O	S	1	0
			34809	22140	5985	6447	237		
1	D	4374	Total	C	N	O	S	1	0
			34809	22140	5985	6447	237		
1	B	4374	Total	C	N	O	S	1	0
			34809	22140	5985	6447	237		
1	C	4374	Total	C	N	O	S	1	0
			34809	22140	5985	6447	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

- Molecule 3 is a protein called Protein S100A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
3	I	94	Total	C	N	O	S	0	0
			737	465	115	153	4		
3	K	94	Total	C	N	O	S	0	0
			737	465	115	153	4		
3	M	94	Total	C	N	O	S	0	0
			737	465	115	153	4		
3	O	94	Total	C	N	O	S	0	0
			737	465	115	153	4		

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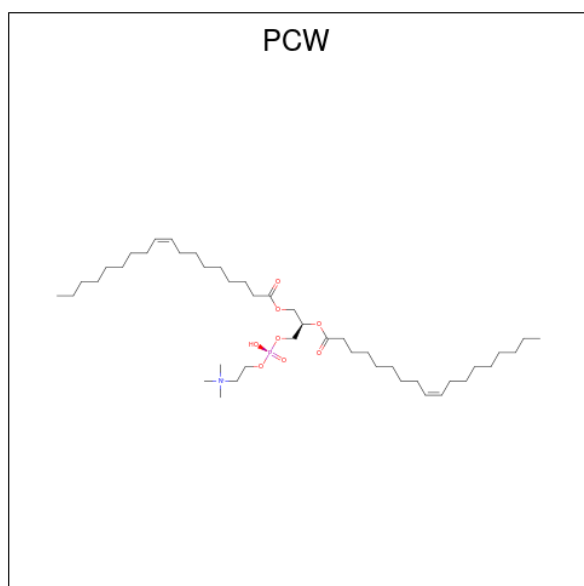
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Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
3	N	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
3	P	93	Total	C	N	O	S	0	0
			729	460	114	152	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: C₄₄H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

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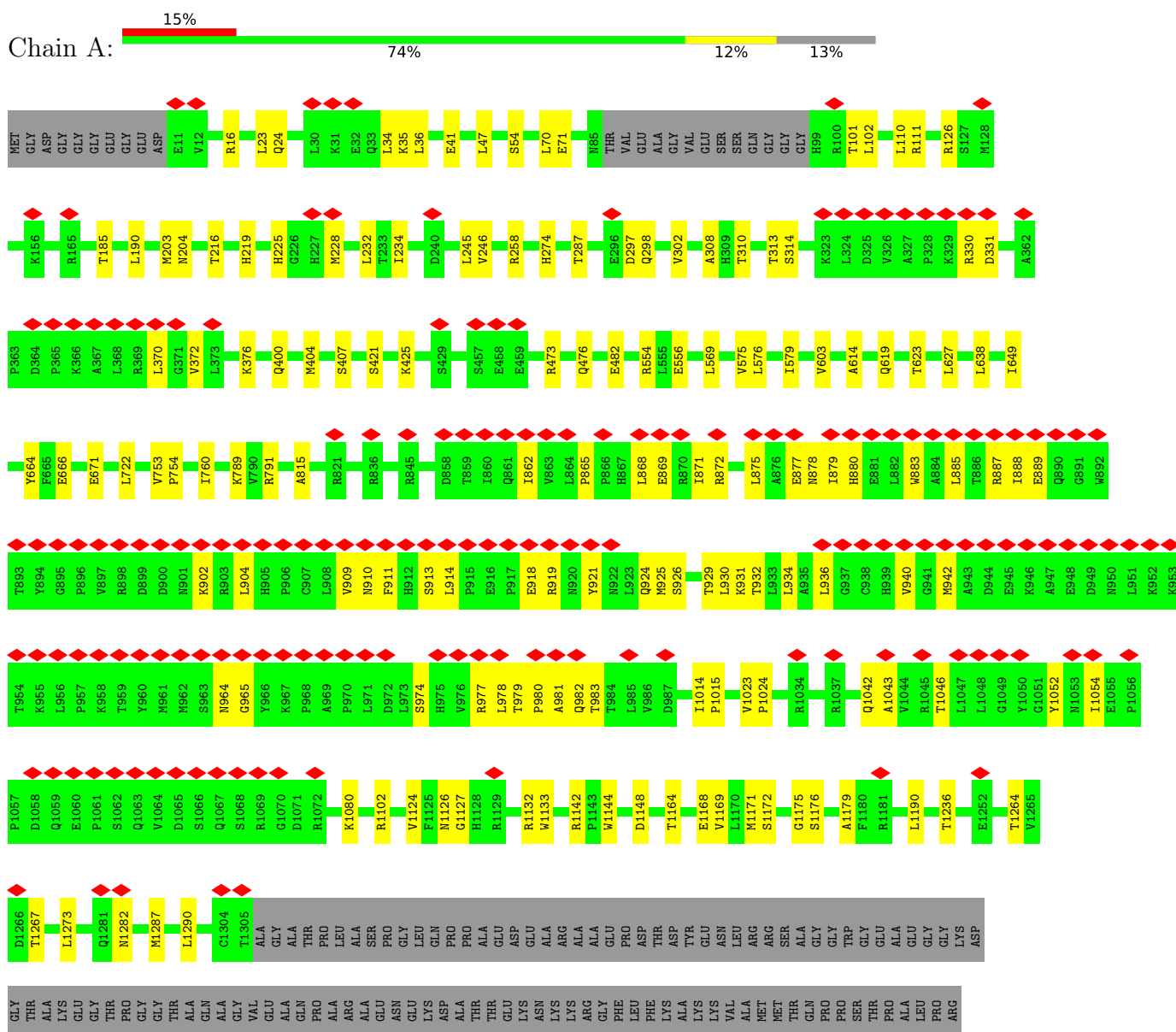
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Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

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.

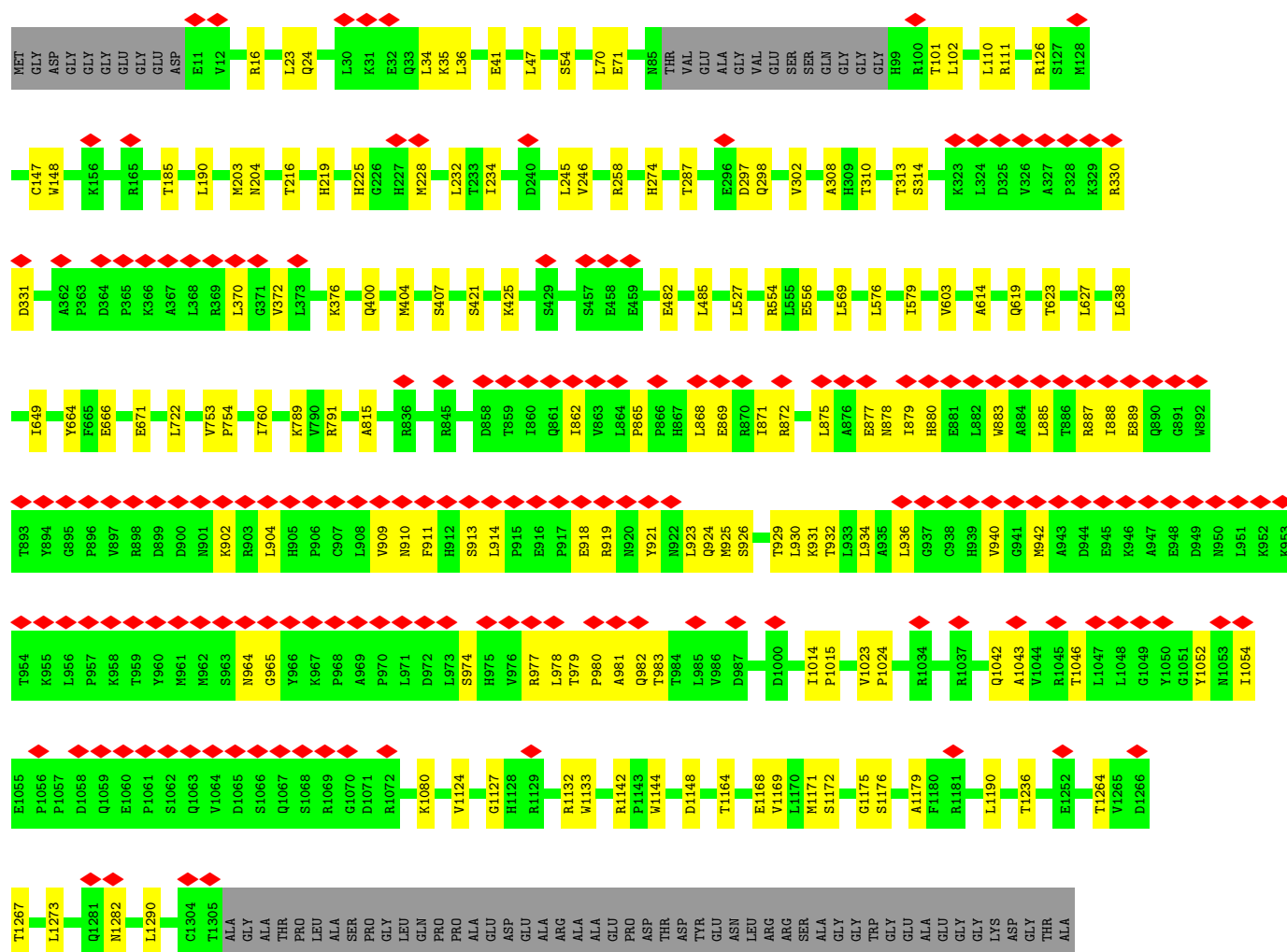
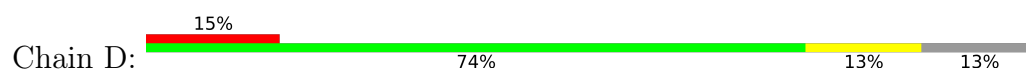
• Molecule 1: Ryanodine receptor 1





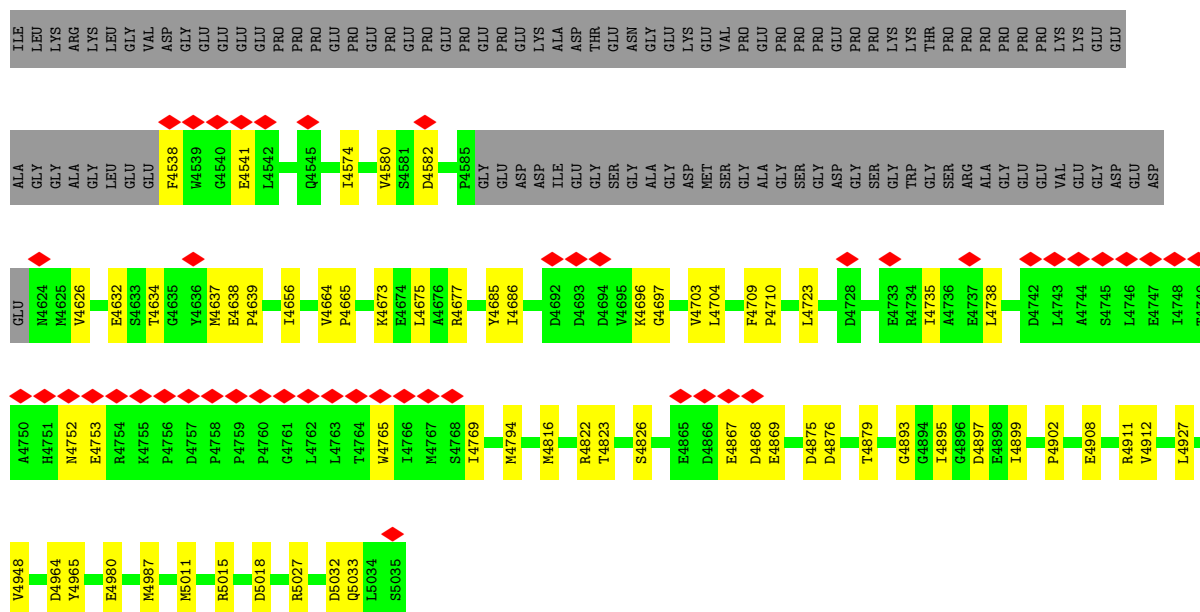


- Molecule 1: Ryanodine receptor 1

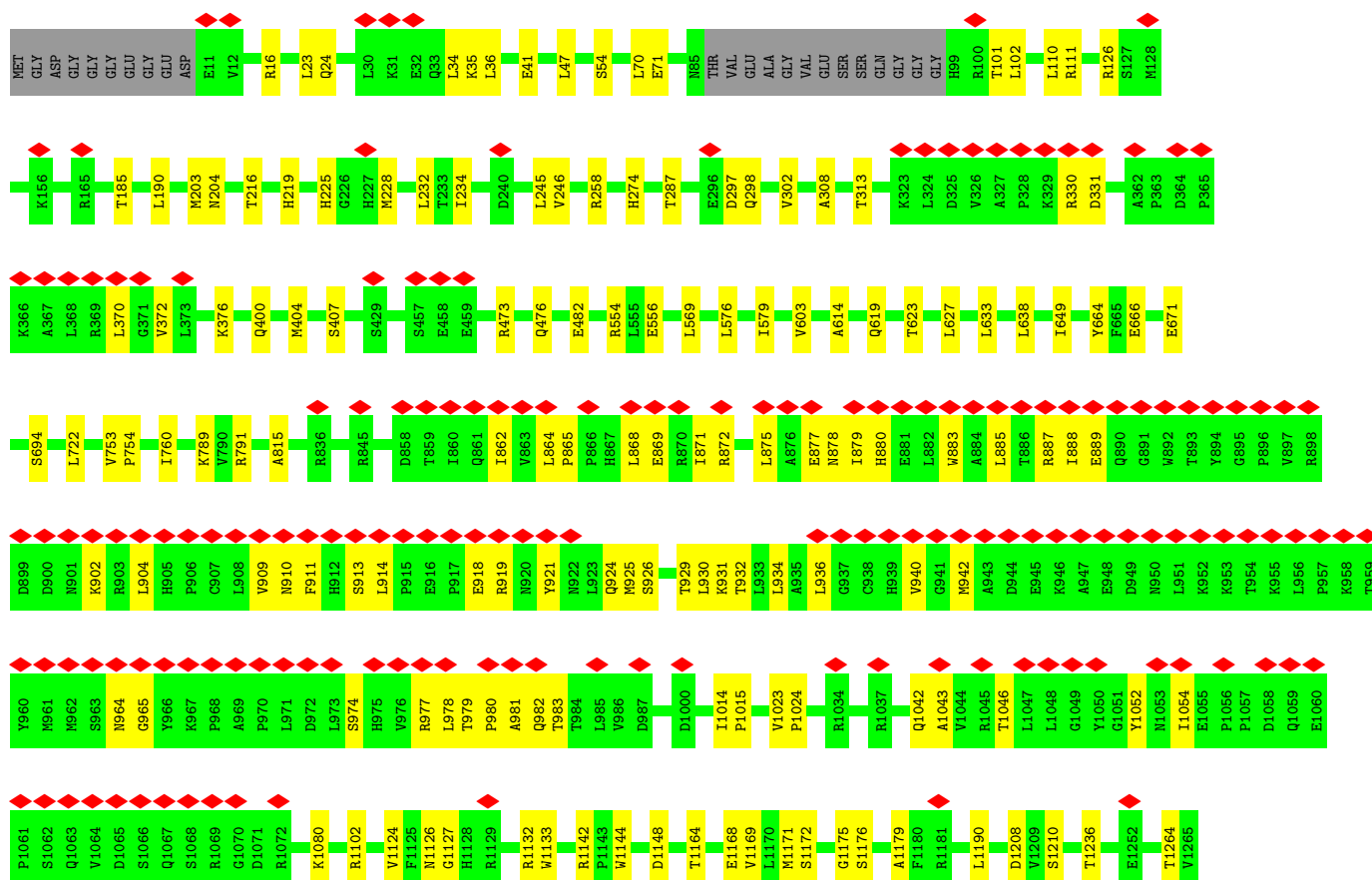
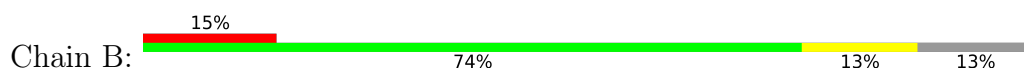


K2890	K2891	K2892	K2893	K2894	L2895	L2896	A2897	K2898	G2899	G2900	G2901	S2902	H2903	P2904	L2905	L2906	V2907	P2908	Y2909	D2910	T2911	L2912	T2913	A2914	K2915	E2916	K2917	A2918	R2919	D2920	R2921	E2922	K2923	A2924	Q2925	E2926	L2927	L2928	K2929	F2930	L2931	Q2932	Q2933	N2934	G2935	Y2936	A2937	V2938	T2939	R2940	G2941	L2942	K2943	D2944	N2945	E2946	L2947	D2948	T2949
D2770	K2771	I2772	Q2773	N2774	N2775	W2776	S2777	Y2778	G2779	E2780	N2781	L2782	D2783	E2784	E2785	L2786	K2787	T2788	H2789	P2790	M2791	L2792	R2793	P2794	Y2795	K2796	T2797	F2798	S2799	E2800	K2801	D2802	N2803	E2804	I2805	R2806	Y2807	W2808	P2809	I2810	K2811	E2812	S2813	L2814	K2815	A2816	M2817	I2818	A2819	W2820	E2821	W2822	T2823	V2824	K2825	K2826	A2827	R2828	E2829
G2830	E2831	GLU	GLU	THR	LYS	GLU	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	ASP	PRO	ARG	GLU	Y2856	N2857	P2858	Q2859	P2860	P2861	D2862	L2863	S2864	V2865	V2866	T2867	L2868	S2869	K2870	E2871	L2872	Q2873	A2874	N2875	A2876	E2877	Q2878	L2879	A2880	E2881	N2882	Y2883	H2884	N2885	T2886	G2888	R2889					
Q2694	E2695	R2698	M2701	P2702	D2717	Y2720	S2721	S2722	K2723	T2724	E2725	K2726	LYS	ALA	THR	VAL	ASP	ALA	GLU	N2735	F2736	D2737	P2738	R2739	P2740	V2741	E2742	T2743	L2744	N2745	V2746	I2747	I2748	P2749	E2750	K2751	L2752	D2753	S2754	P2755	I2756	N2757	K2758	F2759	A2760	E2761	Y2762	T2763	H2764	E2765	K2766	W2767	A2768	F2769					
H2521	V2525	D2530	A2533	L2537	D2538	T2539	E2546	F2570	T2573	E2574	H2575	R2576	A2577	I2578	M2583	T2586	L2590	A2599	V2603	L2611	L2620	L2624	R2625	R2626	L2627	V2628	N2635	E2636	F2637	P2641	E2671	L2675	S2686	K2690	K2691	Y2692	D2693	E2614	D2517	F2518																			
R2370	Q2371	E2372	E2383	I2387	D2390	Q2397	V2398	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	P2411	P2412	E2413	E2414	W2415	R2416	A2438	A2446	E2450	R2453	D2466	I2470	P2478	T2479	L2480	Q2481	D2482	Q2484	A2485	K2500	V2510	E2514	D2517	F2518																			
T2207	V2213	N2214	V2215	G2218	Q2219	E2220	S2221	K2222	E2223	L2224	R2225	M2229	F2236	Y2239	F2240	C2241	I2243	M2251	H2254	L2255	S2256	Y2257	G2263	I2264	Q2265	L2266	Q2267	M2268	Q2269	V2281	L2289	E2293	L2314	Y2319	P2320	D2321	A2351	V2355	R2356	I2359																			
LEU	MET	SER	LEU	LEU	GLY	LYS	VAL	LYS	VAL	LEU	LYS	LYS	THR	GLU	GLU	LYS	PRO	GLU	GLU	GLU	E2089	H2090	K2091	D2110	F2111	L2124	Q2128	L2132	I2145	L2156	L2167	T2183	M2187	N2188	N2189	K2190	V2191	Y2193	N2197	L2198	M2199	R2200	M2204																
N1973	Q1974	R1977	L1980	L1981	M1982	K1983	A1984	F1985	T1986	M1987	S1988	A1989	A1990	E1991	T1992	A1993	R1994	H1995	T1996	E1997	E1998	F1999	R2000	Q2006	L2010	L2011	D2018	E2019	E2020	E2021	L2024	L2032	I2045	Q2046	L2047	GLU	GLY	GLU	GLU	PRO	GLU	GLU	GLU	SER	THR	LEU	GLY	SER	ARG										
VAL	GLU	GLU	GLY	GLU	GLU	GLU	ASP	GLU	GLU	LYS	GLU	GLU	ASP	GLU	GLU	GLU	GLU	LYS	GLU	ASP	GLU	GLU	GLU	LYS	GLU	ALA	GLU	ASP	ALA	ALA	GLU	LYS	GLU	GLU	K1931	L1932	V1936	C1948	E1964	V1967	D1968	M1930																	
ASP	VAL	VAL	PRO	ALA	D1420	N1421	R1422	I1428	L1429	D1466	L1467	S1468	M1477	E1480	Q1481	G1482	H1485	S1491	N1492	G1499	V1502	S1503	P1504	G1505	Q1506	Q1507	G1508	R1509	I1510	S1511	H1512	F1540	V1562	V1563	R1619	W1627	M1636	L1677	G1678	N1679	S1688	D1691	Q1692																
L1695	L1699	L1699	R1703	Y1713	R1728	L1732	L1739	R1744	A1753	S1754	A1755	E1756	D1757	G1758	P1759	R1760	L1773	L1788	P1789	A1790	A1791	G1792	A1793	T1794	E1795	A1796	P1797	E1807	R1810	M1816	V1821	R1822	D1823	Q1826	S1857	D1860	R1874	E1875	E1876	GLU	GLU																		
LYS	GLU	THR	PRO	GLY	GLY	THR	ALA	GLN	VAL	GLU	ALA	PRO	ALA	ALA	GLU	ASN	LYS	THR	THR	GLU	LYS	ASN	LYS	ARG	GLY	PHE	LEU	PHE	LYS	ALA	LYS	VAL	ALA	MET	MET	THR	GLN	PRO	PRO	SER	THR	PRO	LEU	ARG	PRO	LEU	ARG												

GLY	ASP	GLY	VAL	R4164	S4077	L3859	E3683	R3583	ARG	G3440	R3551	S3224	I3104	S2950
ALA	ALA	ALA	TRP	N4165	F4078	G3860	Q3684	E3584	Y3504	E3441	P3225	P3225	E3105	E2953
ALA	ALA	ALA	TRP	F4166	A4079	M3861	E3685	E3585	S3505	F3442	R3226	R3226	K3106	E2953
GLY	GLY	GLY	LEU	L4167	F4080	N3862	E3686	D3586	Q3506	F3443	E3227	E3227	M3107	L2964
ALA	ALA	ALA	ALA	L4186	D4081	N3863	E3687	A3587	Q3507	Y3445	T3230	T3230	V3108	L2964
GLY	GLY	GLY	THR	L4196	D4082	N3863	E3688	D3588	T3508	Y3446	L3231	L3231	E3109	M2968
ALA	ALA	ALA	ALA	L4196	Y4083	E3864	E3689	D3589	S3509	L3510	G3232	G3232	L3111	S2971
GLY	GLY	GLY	ARG	E4202	V4084	G3865	E3690	P3590	L3510	H3450	L3233	L3233	L3112	S2971
GLY	GLY	GLY	THR	Y4225	D4085	G3866	V3691	E3591	L3515	K3453	S3236	S3236	GLY	F2974
ALA	ALA	ALA	LEU	N4226	D4086	T3867	K3592	K3592	M3525	R3454	V3237	V3237	LYS	L2978
ALA	ALA	ALA	ARG	E4227	P4087	V3868	E3692	V3593	C3526	F3455	E3238	E3238	VAL	E2979
ASP	ASP	ASP	GLY	G4228	R4088	N3870	E3693	V3594	R3595	E3456	R3367	R3367	GLN	A2980
ALA	ALA	ALA	ASP	E4229	G4089	N3871	E3694	R3595	D3530	Q3457	E3239	E3239	ALA	V2981
GLY	GLY	GLY	TYR	G4230	K4093	R3871	K3714	Q3598	Q3531	F3459	M3240	M3240	ARG	V2982
ALA	ALA	ALA	ARG	E4231	K4094	Q3872	L3717	E3599	D3532	V3460	R3249	R3249	THR	S2983
GLY	GLY	GLY	SER	E4235	D4095	G3874	D3718	V3600	L3533	V3461	L3250	L3250	GLN	S2984
ASP	ASP	ASP	ARG	E4235	P4096	E3875	L3736	V3603	V3535	Q3462	E3253	E3253	VAL	G2985
GLY	GLY	GLY	ARG	E4235	Q4097	K3876	E3737	L3604	A3537	N3463	E3259	E3259	K3124	G2985
VAL	VAL	VAL	VAL	M4248	K4098	D3901	GLY	D3608	K3538	E3464	M3267	M3267	G3125	R2986
ALA	ALA	ALA	ARG	Q4249	A4099	R3907	GLY	E3611	A3539	I3465	E3271	E3271	G3126	V2987
VAL	VAL	VAL	ARG	Q4253	M4100	T3908	GLY	H3612	R3540	N3467	I3272	I3272	V3126	E2988
ALA	ALA	ALA	ARG	E4256	D4101	T3908	GLY	P3613	R3540	M3468	E3273	E3273	G3127	K2989
GLY	GLY	GLY	THR	P4257	S4102	Q4103	ASN	TYR	L3543	F3470	T3274	T3274	Q3128	S2990
PRO	PRO	PRO	LEU	E4257	K4104	Q4103	GLY	LYS	K3544	F3471	T3275	T3275	T3133	F2999
PRO	PRO	PRO	ALA	GLY	K4105	L3927	GLY	SER	D3545	T3472	L3276	L3276	D3155	L3003
PRO	PRO	PRO	ARG	GLY	F4106	Q3930	GLY	LYS	D3547	ALA	P3276	P3276	L3004	P3005
GLY	GLY	GLY	ALA	GLY	T4107	Q3930	GLY	ALA	E3548	T3471	L3282	L3282	P3005	V3025
ASP	ASP	ASP	ALA	GLY	T4107	D3944	GLY	TRP	E3549	ALA	R3288	R3288	V3164	V3025
THR	THR	THR	THR	ASP	G4108	F3954	GLY	HIS	E3552	LYS	A3292	A3292	T3169	S3028
ALA	ALA	ALA	VAL	GLY	P4109	F3954	V3752	LEU	F3553	LYS	P3293	P3293	L3170	G3029
GLY	GLY	GLY	ALA	GLY	E4110	M3958	E3753	LEU	F3554	LYS	P3294	P3294	Y3174	K3037
ALA	ALA	ALA	ALA	GLY	I4111	M3958	E3753	SER	Q3555	LYS	P3295	P3295	L3175	I3040
LEU	LEU	LEU	LEU	ALA	L4115	T3972	F3756	LYS	N3556	LYS	P3296	P3296	G3176	I3040
LEU	LEU	LEU	TRP	GLY	E4119	Q3973	E3757	GLN	N3557	ALA	A3296	A3296	L3177	I3043
TRP	TRP	TRP	ALA	GLY	A4120	G3974	E3758	ARG	N3557	GLY	L3297	L3297	T3178	I3043
ALA	ALA	ALA	LEU	GLY	A4120	P3975	E3758	ARG	N3558	ASP	P3298	P3298	T3179	H3053
VAL	VAL	VAL	VAL	GLY	D4121	L3983	M3761	ARG	N3559	VAL	A3299	A3299	R3180	H3053
THR	THR	THR	THR	GLY	E4122	L3983	M3761	ALA	L3560	GLN	G3300	G3300	N3181	L3057
ARG	ARG	ARG	ARG	ALA	M4123	F3995	R3765	VAL	Q3561	GLY	A3301	A3301	P3182	L3057
ALA	ALA	ALA	ALA	ALA	E4124	D4009	Q3770	A3635	G3562	ASP	L3316	L3316	Y3183	D3061
GLY	GLY	GLY	GLY	GLY	M4125	D4009	S3771	C3636	K3563	SER	L3316	L3316	E3185	V3065
PRO	PRO	PRO	GLY	ASP	M4126	I4013	H3774	R3638	V3564	GLN	I3320	I3320	R3188	V3065
THR	THR	THR	GLY	GLY	I4127	I4013	N3775	R3638	E3565	ARG	L3324	L3324	L3196	L3076
ALA	ALA	ALA	ALA	GLY	C4128	L4016	N3775	M3639	G3566	THR	E3331	E3331	L3082	L3076
GLY	GLY	GLY	GLY	SER	E4129	K4017	M3785	Y3643	S3567	LYS	E3332	E3332	V3204	V3089
ALA	ALA	ALA	ALA	SER	E4130	K4017	M3785	Y3644	P3568	LYS	A3333	A3333	N3212	V3089
ALA	ALA	ALA	ALA	ALA	E4131	L4072	C3789	N3644	S3569	LYS	K3337	K3337	L3093	L3093
ALA	ALA	ALA	ALA	ALA	A4132	L4072	L3820	Y3644	R3571	ARG	E3438	E3438	L3093	L3093
ALA	ALA	ALA	ALA	ALA	A4132	L4072	L3820	Y3644	R3571	ARG	E3438	E3438	L3093	L3093
ALA	ALA	ALA	ALA	ALA	F4135	D4073	S3834	R3649	R3578	GLY	M3438	M3438	L3093	L3093
ALA	ALA	ALA	ALA	ALA	Q4136	D4073	K3855	A3650	G3579	ASP	V3439	V3439	L3093	L3093
ALA	ALA	ALA	ALA	ALA	E4137	D4073	K3855	A3650	V3580	GLY	V3439	V3439	L3093	L3093
ALA	ALA	ALA	ALA	ALA	P4138	D4073	K3855	A3650	P3581	GLY	V3439	V3439	L3093	L3093
ALA	ALA	ALA	ALA	ALA	I4142	D4073	K3855	A3650	G3582	ASP	V3439	V3439	L3093	L3093
ALA	ALA	ALA	ALA	ALA	D4160	D4073	K3855	A3650	G3582	ASP	V3439	V3439	L3093	L3093

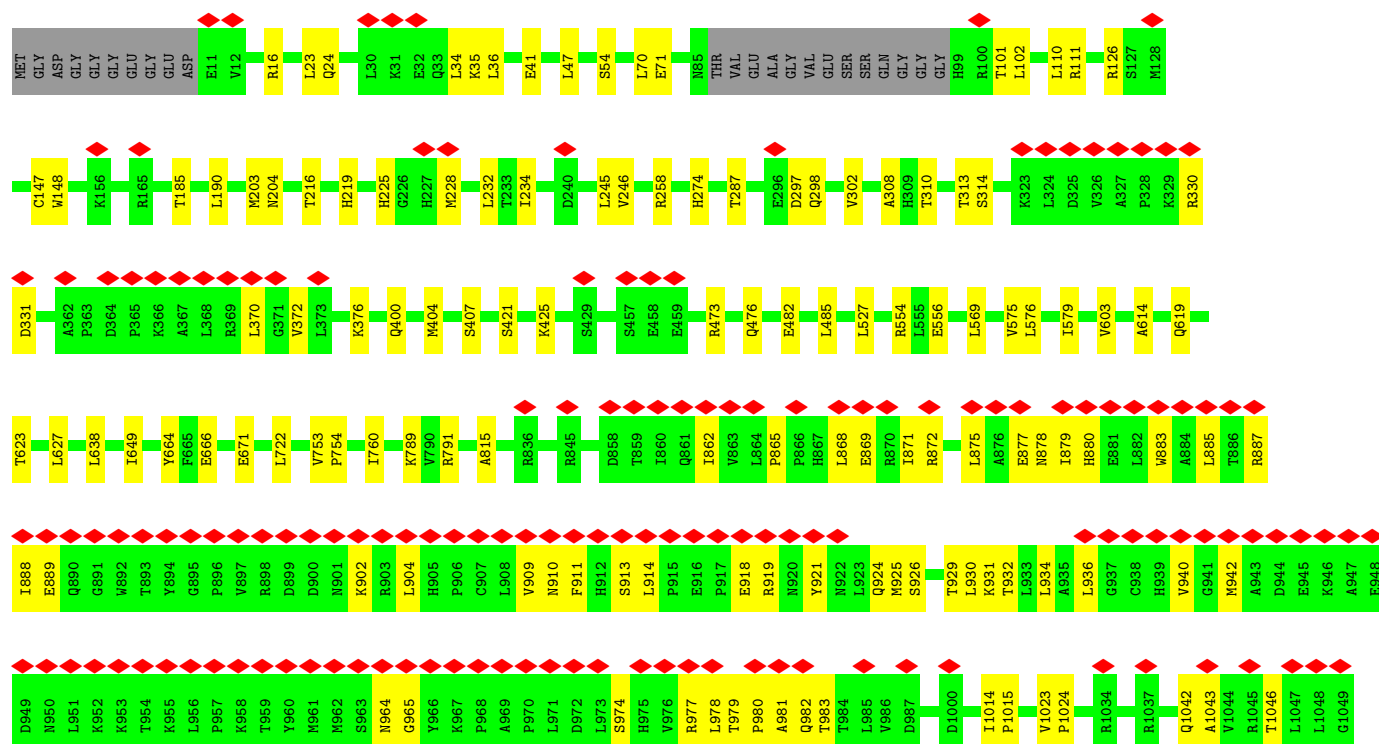


• Molecule 1: Ryanodine receptor 1



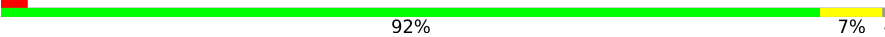


TRP	L2895	R3110	L3231	P3352	L3442	S3505	E3585	G3860	S4077	R4164
VAL	E2896	L3111	G3232	E3353	F3443	V3506	D3586	M3861	E4078	L4167
TRP	A2897	R3112	L2333	L3354	T3444	Q3507	A3587	V3862	A4079	L4167
ALA	K2898	L3113	L2336	H3358	V3446	T3508	D3588	N3863	F4080	I4186
ALA	G2900	GLY	S3237	F3359	H3450	S3509	D3589	D3865	Q4081	I4196
ALA	G2901	LYS	V3237	R3360	K3453	L3510	P3590	G3866	Y4083	E4202
GLY	S2902	VAL	E3238	P3361	R3454	L3515	F3591	T3867	A4084	V4085
TRP	H2903	SER	E3239	P3362	E3455	M3525	K3592	I3868	D4086	T4085
ALA	H2904	GLN	M3240	T3362	E3456	C3526	V3593	N3870	P4087	D4086
ALA	L2905	ARG	R3249	R3365	N3457	D3530	K3594	R3871	Q4088	P4087
TRP	L2906	THR	L3250	L3366	N3458	Q3531	R3595	N3872	G4089	G4089
ALA	V2907	GLN	E3253	R3367	F3460	D3532	E3598	N3873	K4093	K4093
ALA	G2908	VAL	E3259	R3368	V3461	L3533	E3599	N3874	D4094	D4094
ALA	S2909	THR	M3267	K3369	Q3462	V3535	V3594	E3875	D4095	D4095
ALA	V2910	ARG	Q3128	A3370	N3463	L3536	L3604	K3876	F4096	F4096
ALA	T2911	VAL	I3271	A3371	I3464	A3537	D3608	D3901	Q4097	Q4097
ALA	L2912	VAL	E3272	E3376	I3465	K3538	E3611	G3907	K4098	K4098
ALA	T2913	VAL	F3273	E3377	N3466	A3539	H3612	R3907	A4099	A4099
ALA	A2914	H3147	T3274	E3378	N3467	R3540	L3613	T3908	M4100	M4100
ALA	K2915	D3155	P3276	E3379	N3468	L3543	LYS	I3919	D4101	D4101
ALA	K2916	L3003	L3282	L3380	F3470	K3544	SER	L3927	S4102	S4102
ALA	K2917	L3004	W3286	L3381	L3471	T3545	LYS	G3927	Q4103	Q4103
ALA	A2918	V3025	E3287	L3382	L3472	T3546	LYS	G3930	K4104	K4104
ALA	R2919	S3028	R3288	L3383	ALA	D3547	ALA	D3944	Q4105	Q4105
ALA	D2920	G3029	A3292	L3384	ASP	E3548	TRP	L3944	F4106	F4106
ALA	R2921	K3037	P3293	E3387	ASN	E3549	TRP	G3954	T4107	T4107
ALA	E2922	L3040	P3294	A3388	LYS	E3552	HIS	F3954	G4108	G4108
ALA	K2923	L3043	P3295	E3389	LYS	F3553	LEU	M3958	A4109	A4109
ALA	Q2925	L3043	A3296	E3390	ALA	Q3555	LEU	I3972	E4110	E4110
ALA	E2926	H3053	L3297	G3391	LYS	N3556	SER	G3973	A4111	A4111
ALA	L2927	L3057	P3298	G3392	ALA	N3557	GLN	G3974	L4115	L4115
ALA	L2928	L3057	A3299	L3393	GLY	N3558	ARG	P3975	E4119	E4119
ALA	K2929	D3061	G3300	L3394	VAL	N3559	ARG	L3983	A4120	A4120
ALA	F2930	E3185	A3301	V3395	GLN	L3560	ALA	W3989	D4121	D4121
ALA	L2931	E3185	E3308	R3396	SER	Q3561	VAL	F3995	E4122	E4122
ALA	D2932	V3065	V3308	D3397	GLY	K3562	VAL	F3995	A4123	A4123
ALA	P2933	L3076	L3316	E3398	SER	K3563	C3636	D4009	E4124	E4124
ALA	N2934	M3082	L3320	F3399	ASP	V3564	R3637	L4013	M4125	M4125
ALA	G2935	L3088	T3324	L3406	GLN	E3565	R3638	L4016	I4126	I4126
ALA	V2936	V3089	E3331	L3409	ARG	G3566	H3639	L4017	N4127	N4127
ALA	A2937	L3093	E3332	P3411	LYS	S3567	T3640	M4050	C4128	C4128
ALA	V2938	L3104	A3333	P3428	LYS	P3568	Y3643	L4071	E4129	E4129
ALA	T2939	E3105	K3337	E3433	ARG	L3570	N3644	K4072	A4130	A4130
ALA	R2940	E3105	T3346	E3434	GLY	R3571	R3649	M4073	F4131	F4131
ALA	G2941	K3106	R3337	E3438	ASP	R3578	A3650	L4076	A4132	A4132
ALA	L2942	M3107	T3346	W3438	ARG	G3579	E3683	G4076	F4135	F4135
ALA	K2943	E3108	R3351	V3439	ARG	V3580	Q3684	Q4136	Q4136	Q4136
ALA	H2945	E3109	R3351	E3441	ARG	R3583	E3684	E4137	P4138	P4138
ALA	E2946	E3109	R3351	E3441	ARG	E3584	E3684	I4142	I4142	I4142
ALA	L2947	E3109	R3351	E3441	ARG	E3584	E3684	D4160	D4160	D4160
ALA	D2948	E3109	R3351	E3441	ARG	E3584	E3684	D4160	D4160	D4160
ALA	K2949	E3109	R3351	E3441	ARG	E3584	E3684	D4160	D4160	D4160
ALA	T2949	E3109	R3351	E3441	ARG	E3584	E3684	D4160	D4160	D4160
ALA	S2950	E3109	R3351	E3441	ARG	E3584	E3684	D4160	D4160	D4160
ALA	E2953	E3109	R3351	E3441	ARG	E3584	E3684	D4160	D4160	D4160
ALA	L2964	E3109	R3351	E3441	ARG	E3584	E3684	D4160	D4160	D4160





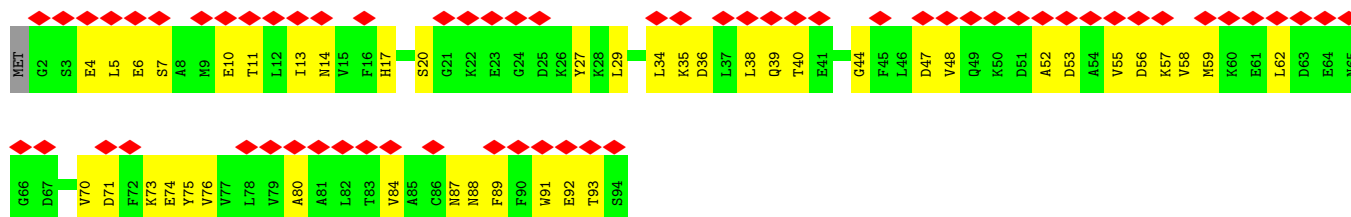


Chain G:  92% 7%



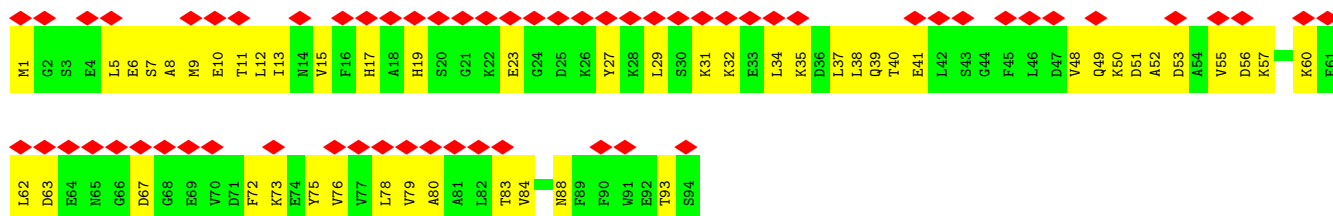
• Molecule 3: Protein S100A1

Chain J:  53% 66% 46%



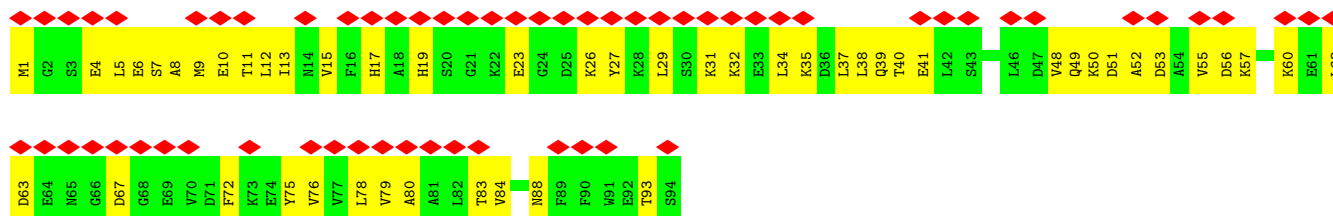
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Chain I:  48% 65% 52%



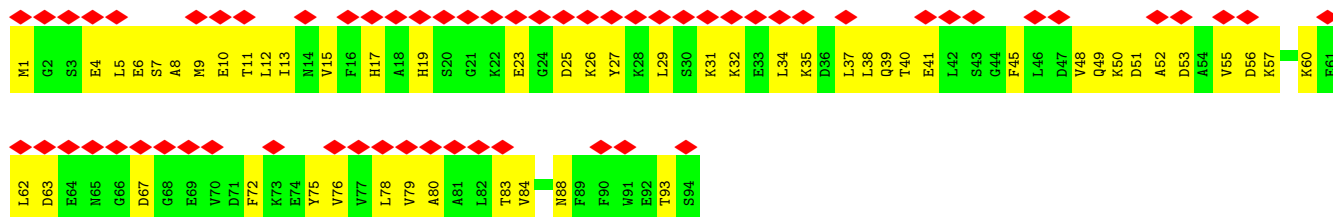
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Chain K:  47% 66% 53%

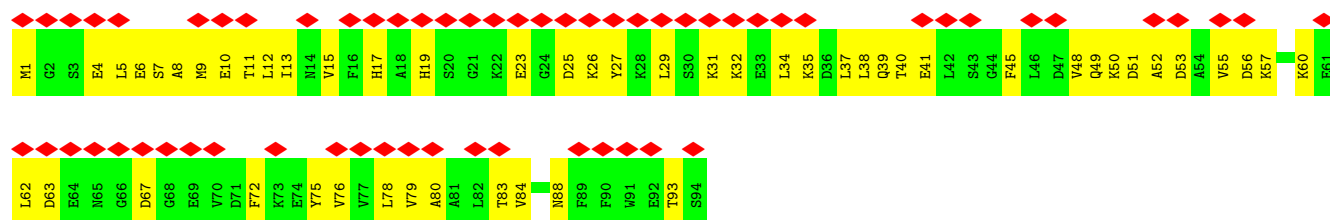


• Molecule 3: Protein S100A1

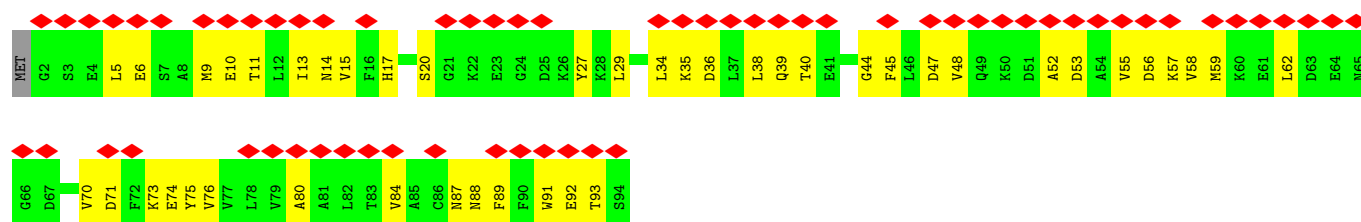
Chain M:  45% 65% 55%



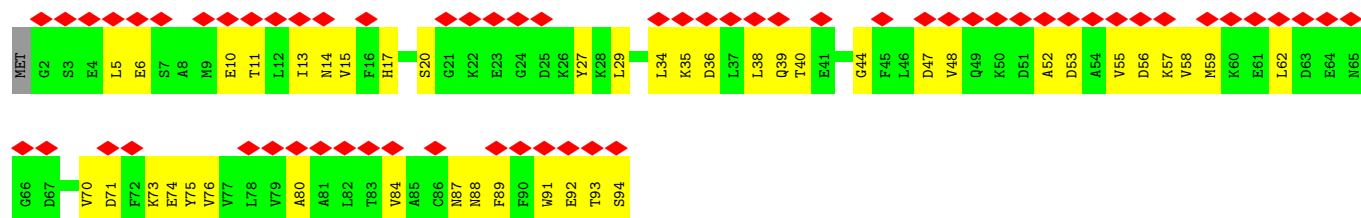
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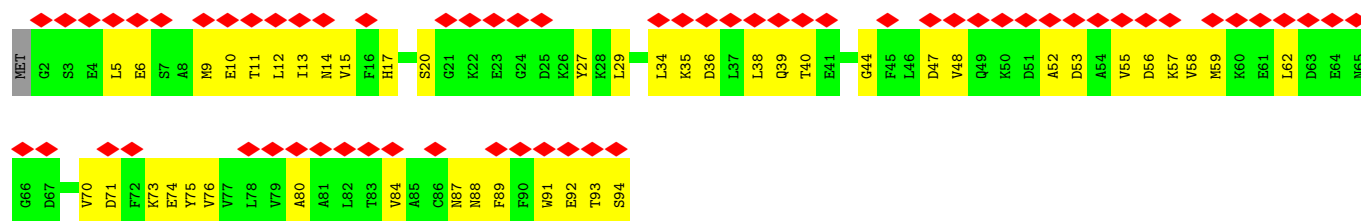
• Molecule 3: Protein S100A1



• Molecule 3: Protein S100A1



• Molecule 3: Protein S100A1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	36506	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.686	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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, PCW

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/35601	0.35	0/48224
1	B	0.14	0/35601	0.35	0/48224
1	C	0.14	0/35601	0.35	0/48224
1	D	0.14	0/35601	0.35	0/48224
2	E	0.13	0/847	0.31	0/1142
2	F	0.13	0/847	0.32	0/1142
2	G	0.13	0/847	0.31	0/1142
2	H	0.13	0/847	0.32	0/1142
3	I	0.28	0/747	0.57	0/1002
3	J	0.25	0/739	0.56	0/992
3	K	0.28	0/747	0.57	0/1002
3	L	0.25	0/739	0.56	0/992
3	M	0.28	0/747	0.57	0/1002
3	N	0.25	0/739	0.56	0/992
3	O	0.29	0/747	0.57	0/1002
3	P	0.25	0/739	0.56	0/992
All	All	0.15	0/151736	0.36	0/205440

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3240	MET	Peptide
1	B	3240	MET	Peptide
1	C	3240	MET	Peptide
1	D	3240	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34809	0	34401	425	0
1	B	34809	0	34401	432	0
1	C	34809	0	34401	431	0
1	D	34809	0	34401	433	0
2	E	829	0	826	3	0
2	F	829	0	826	3	0
2	G	829	0	826	5	0
2	H	829	0	826	4	0
3	I	737	0	717	47	0
3	J	729	0	705	41	0
3	K	737	0	717	55	0
3	L	729	0	705	48	0
3	M	737	0	717	55	0
3	N	729	0	705	47	0
3	O	737	0	717	59	0
3	P	729	0	705	52	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	108	0	167	0	0
5	B	108	0	167	0	0
5	C	108	0	167	0	0
5	D	108	0	167	0	0
All	All	148852	0	147264	2051	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2051) 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)
3:M:56:ASP:OD1	1:C:3638:ARG:NH2	1.59	1.34
1:A:3638:ARG:NH2	3:I:56:ASP:OD1	1.63	1.30
3:K:56:ASP:OD1	1:B:3638:ARG:NH2	1.63	1.30
3:O:56:ASP:OD1	1:D:3638:ARG:NH2	1.60	1.28
3:J:44:GLY:O	3:J:47:ASP:OD1	1.65	1.14
3:P:44:GLY:O	3:P:47:ASP:OD1	1.64	1.13
3:L:44:GLY:O	3:L:47:ASP:OD1	1.64	1.13
3:N:44:GLY:O	3:N:47:ASP:OD1	1.65	1.12
3:O:56:ASP:OD1	1:D:3638:ARG:CZ	2.01	1.08
3:M:5:LEU:HD23	3:M:9:MET:HE1	1.36	1.08
3:O:5:LEU:HD23	3:O:9:MET:HE1	1.36	1.06
3:K:5:LEU:HD23	3:K:9:MET:HE1	1.36	1.04
3:M:56:ASP:OD1	1:C:3638:ARG:CZ	2.05	1.03
3:K:56:ASP:OD1	1:B:3638:ARG:CZ	2.05	1.03
3:I:5:LEU:HD23	3:I:9:MET:HE1	1.36	1.01
1:D:2765:GLU:OE1	1:D:2795:TYR:OH	1.85	0.95
1:A:2765:GLU:OE1	1:A:2795:TYR:OH	1.85	0.94
1:C:2765:GLU:OE1	1:C:2795:TYR:OH	1.85	0.93
1:B:2765:GLU:OE1	1:B:2795:TYR:OH	1.85	0.93
3:J:5:LEU:HD13	3:I:15:VAL:HG11	1.52	0.92
1:C:979:THR:HG22	1:C:982:GLN:OE1	1.71	0.91
1:B:979:THR:HG22	1:B:982:GLN:OE1	1.71	0.91
1:A:3761:MET:SD	1:A:3765:ARG:NH1	2.44	0.91
1:D:979:THR:HG22	1:D:982:GLN:OE1	1.71	0.91
1:B:3761:MET:SD	1:B:3765:ARG:NH1	2.44	0.90
1:A:979:THR:HG22	1:A:982:GLN:OE1	1.71	0.90
1:C:3761:MET:SD	1:C:3765:ARG:NH1	2.44	0.90
1:D:3761:MET:SD	1:D:3765:ARG:NH1	2.44	0.89
1:C:2753:ASP:OD1	1:C:2811:LYS:NZ	2.06	0.89
3:L:47:ASP:OD2	1:B:2986:ARG:NH2	2.07	0.88
1:A:2753:ASP:OD1	1:A:2811:LYS:NZ	2.06	0.88
3:P:47:ASP:OD2	1:D:2986:ARG:NH2	2.07	0.88
1:B:2753:ASP:OD1	1:B:2811:LYS:NZ	2.06	0.87
1:D:2753:ASP:OD1	1:D:2811:LYS:NZ	2.06	0.87
1:A:3224:SER:OG	1:A:3227:GLU:OE1	1.94	0.86
1:B:3224:SER:OG	1:B:3227:GLU:OE1	1.94	0.85
1:C:3224:SER:OG	1:C:3227:GLU:OE1	1.94	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2986:ARG:NH2	3:J:47:ASP:OD2	2.08	0.85
1:D:3224:SER:OG	1:D:3227:GLU:OE1	1.94	0.85
3:K:93:THR:HG23	3:L:27:TYR:HB3	1.62	0.82
1:C:3538:LYS:NZ	1:C:3608:ASP:OD2	2.13	0.82
3:N:47:ASP:OD2	1:C:2986:ARG:NH2	2.14	0.81
1:A:1948:CYS:SG	1:A:2128:GLN:NE2	2.55	0.80
1:D:3538:LYS:NZ	1:D:3608:ASP:OD2	2.13	0.80
1:C:3761:MET:SD	1:C:3765:ARG:NH2	2.55	0.80
1:B:3761:MET:SD	1:B:3765:ARG:NH2	2.55	0.80
1:C:1948:CYS:SG	1:C:2128:GLN:NE2	2.55	0.80
3:O:26:LYS:HZ2	3:P:92:GLU:H	1.31	0.79
1:A:3714:LYS:NZ	1:A:3718:ASP:OD2	2.16	0.79
1:D:1948:CYS:SG	1:D:2128:GLN:NE2	2.55	0.79
1:D:3761:MET:SD	1:D:3765:ARG:NH2	2.55	0.79
1:C:3714:LYS:NZ	1:C:3718:ASP:OD2	2.16	0.79
1:A:3761:MET:SD	1:A:3765:ARG:NH2	2.55	0.79
1:B:1948:CYS:SG	1:B:2128:GLN:NE2	2.55	0.79
3:L:92:GLU:O	3:L:93:THR:OG1	2.01	0.79
1:A:974:SER:O	1:A:977:ARG:NH1	2.16	0.78
3:J:92:GLU:O	3:J:93:THR:OG1	2.01	0.78
1:C:974:SER:O	1:C:977:ARG:NH1	2.16	0.78
1:D:3714:LYS:NZ	1:D:3718:ASP:OD2	2.16	0.78
1:A:3538:LYS:NZ	1:A:3608:ASP:OD2	2.13	0.78
1:D:974:SER:O	1:D:977:ARG:NH1	2.16	0.78
1:B:974:SER:O	1:B:977:ARG:NH1	2.16	0.78
1:B:3714:LYS:NZ	1:B:3718:ASP:OD2	2.16	0.78
3:N:92:GLU:O	3:N:93:THR:OG1	2.01	0.78
1:A:70:LEU:HD13	1:A:102:LEU:HD11	1.65	0.77
1:A:3638:ARG:CZ	3:I:56:ASP:OD1	2.32	0.77
1:B:70:LEU:HD13	1:B:102:LEU:HD11	1.65	0.77
3:P:92:GLU:O	3:P:93:THR:OG1	2.01	0.77
1:C:1691:ASP:OD1	1:C:1692:GLN:N	2.17	0.77
1:B:1691:ASP:OD1	1:B:1692:GLN:N	2.17	0.77
1:C:70:LEU:HD13	1:C:102:LEU:HD11	1.65	0.77
1:A:3082:MET:CE	1:A:3093:LEU:HD23	2.15	0.76
1:A:2877:GLU:OE2	1:A:2921:ARG:NH1	2.18	0.76
1:D:3082:MET:CE	1:D:3093:LEU:HD23	2.15	0.76
1:D:70:LEU:HD13	1:D:102:LEU:HD11	1.65	0.76
1:A:1691:ASP:OD1	1:A:1692:GLN:N	2.17	0.76
1:D:1691:ASP:OD1	1:D:1692:GLN:N	2.17	0.76
1:B:3538:LYS:NZ	1:B:3608:ASP:OD2	2.13	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3082:MET:CE	1:C:3093:LEU:HD23	2.15	0.76
3:O:93:THR:HG23	3:P:27:TYR:HB3	1.66	0.76
1:D:2877:GLU:OE2	1:D:2921:ARG:NH1	2.18	0.76
1:B:3082:MET:CE	1:B:3093:LEU:HD23	2.15	0.76
1:B:1142:ARG:NH2	1:B:1168:GLU:OE2	2.19	0.76
1:C:2877:GLU:OE2	1:C:2921:ARG:NH1	2.18	0.76
1:C:918:GLU:OE1	1:C:918:GLU:N	2.20	0.75
1:A:1466:ASP:OD2	1:A:1468:SER:OG	2.04	0.75
1:D:877:GLU:O	1:D:880:HIS:ND1	2.20	0.75
1:C:1142:ARG:NH2	1:C:1168:GLU:OE2	2.19	0.75
1:B:877:GLU:O	1:B:880:HIS:ND1	2.20	0.75
1:B:918:GLU:OE1	1:B:918:GLU:N	2.20	0.75
1:A:1142:ARG:NH2	1:A:1168:GLU:OE2	2.19	0.75
1:C:1466:ASP:OD2	1:C:1468:SER:OG	2.04	0.75
1:A:877:GLU:O	1:A:880:HIS:ND1	2.20	0.75
1:C:877:GLU:O	1:C:880:HIS:ND1	2.20	0.75
1:B:2877:GLU:OE2	1:B:2921:ARG:NH1	2.18	0.75
3:M:15:VAL:HG11	3:N:5:LEU:HD13	1.68	0.74
1:D:1142:ARG:NH2	1:D:1168:GLU:OE2	2.19	0.74
1:A:918:GLU:N	1:A:918:GLU:OE1	2.20	0.74
3:O:15:VAL:HG11	3:P:5:LEU:HD13	1.69	0.74
1:A:2625:ARG:NH1	1:A:2907:VAL:HG21	2.03	0.74
3:O:5:LEU:HD23	3:O:9:MET:CE	2.18	0.74
1:C:2625:ARG:NH1	1:C:2907:VAL:HG21	2.03	0.74
1:B:2625:ARG:NH1	1:B:2907:VAL:HG21	2.03	0.73
1:B:2949:THR:HG22	1:B:2950:SER:H	1.53	0.73
1:D:2625:ARG:NH1	1:D:2907:VAL:HG21	2.03	0.73
1:D:918:GLU:N	1:D:918:GLU:OE1	2.20	0.73
1:A:2757:ASN:OD1	1:A:2758:LYS:N	2.22	0.73
1:B:2757:ASN:OD1	1:B:2758:LYS:N	2.22	0.73
1:D:2757:ASN:OD1	1:D:2758:LYS:N	2.22	0.73
1:C:2757:ASN:OD1	1:C:2758:LYS:N	2.22	0.72
1:B:1466:ASP:OD2	1:B:1468:SER:OG	2.04	0.72
3:M:93:THR:HG23	3:N:27:TYR:HB3	1.72	0.72
3:M:5:LEU:HD23	3:M:9:MET:CE	2.18	0.72
1:C:2949:THR:HG22	1:C:2950:SER:H	1.53	0.72
3:J:87:ASN:OD1	3:I:27:TYR:OH	2.07	0.72
3:I:5:LEU:HD23	3:I:9:MET:CE	2.18	0.72
1:D:1466:ASP:OD2	1:D:1468:SER:OG	2.04	0.72
1:A:3547:ASP:OD2	1:A:3548:GLU:N	2.23	0.72
1:D:2949:THR:HG22	1:D:2950:SER:H	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3547:ASP:OD2	1:D:3548:GLU:N	2.23	0.71
1:A:2949:THR:HG22	1:A:2950:SER:H	1.53	0.71
3:K:5:LEU:HD23	3:K:9:MET:CE	2.18	0.71
1:B:2907:VAL:HG23	1:B:2912:LEU:HD22	1.73	0.71
3:J:56:ASP:OD1	3:J:57:LYS:N	2.24	0.71
3:N:56:ASP:OD1	3:N:57:LYS:N	2.24	0.70
1:B:3547:ASP:OD2	1:B:3548:GLU:N	2.23	0.70
1:A:2907:VAL:HG23	1:A:2912:LEU:HD22	1.73	0.70
3:L:56:ASP:OD1	3:L:57:LYS:N	2.24	0.70
3:P:56:ASP:OD1	3:P:57:LYS:N	2.24	0.70
3:L:44:GLY:HA2	1:B:2986:ARG:NH2	2.06	0.70
3:K:15:VAL:HG11	3:L:5:LEU:HD13	1.73	0.70
1:C:3547:ASP:OD2	1:C:3548:GLU:N	2.23	0.69
1:C:1043:ALA:O	1:C:1046:THR:OG1	2.10	0.69
1:C:2907:VAL:HG23	1:C:2912:LEU:HD22	1.73	0.69
1:D:2907:VAL:HG23	1:D:2912:LEU:HD22	1.73	0.68
1:D:2183:ILE:HG22	1:D:2187:MET:HE2	1.75	0.68
1:A:4138:PRO:O	1:A:4142:ILE:HD12	1.94	0.68
3:K:4:GLU:OE1	3:L:11:THR:HG23	1.93	0.68
3:M:53:ASP:OD2	3:M:57:LYS:NZ	2.27	0.68
1:B:4138:PRO:O	1:B:4142:ILE:HD12	1.94	0.68
1:A:3589:ASP:OD1	1:A:3592:LYS:HB3	1.94	0.68
3:I:53:ASP:OD2	3:I:57:LYS:NZ	2.27	0.68
1:C:2183:ILE:HG22	1:C:2187:MET:HE2	1.75	0.68
1:A:2183:ILE:HG22	1:A:2187:MET:HE2	1.75	0.67
1:B:2635:ASN:OD1	1:B:2637:PHE:N	2.27	0.67
1:B:2748:ILE:HG21	1:B:2811:LYS:NZ	2.10	0.67
1:A:2635:ASN:OD1	1:A:2637:PHE:N	2.27	0.67
1:D:2635:ASN:OD1	1:D:2637:PHE:N	2.27	0.67
3:K:53:ASP:OD2	3:K:57:LYS:NZ	2.27	0.67
1:B:3869:ILE:O	1:B:3872:GLN:NE2	2.28	0.67
1:C:2635:ASN:OD1	1:C:2637:PHE:N	2.27	0.67
3:O:53:ASP:OD2	3:O:57:LYS:NZ	2.27	0.67
1:C:3869:ILE:O	1:C:3872:GLN:NE2	2.28	0.67
3:I:39:GLN:NE2	3:I:40:THR:OG1	2.28	0.67
3:M:39:GLN:NE2	3:M:40:THR:OG1	2.28	0.67
1:D:3589:ASP:OD1	1:D:3592:LYS:HB3	1.94	0.67
1:B:2183:ILE:HG22	1:B:2187:MET:HE2	1.75	0.67
1:C:3589:ASP:OD1	1:C:3592:LYS:HB3	1.94	0.67
1:B:3589:ASP:OD1	1:B:3592:LYS:HB3	1.94	0.67
1:C:4138:PRO:O	1:C:4142:ILE:HD12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3530:ASP:O	1:A:3534:ILE:HD12	1.95	0.67
3:K:39:GLN:NE2	3:K:40:THR:OG1	2.28	0.67
1:D:2748:ILE:HG21	1:D:2811:LYS:NZ	2.10	0.67
1:A:2748:ILE:HG21	1:A:2811:LYS:NZ	2.10	0.66
1:D:4138:PRO:O	1:D:4142:ILE:HD12	1.94	0.66
1:C:2748:ILE:HG21	1:C:2811:LYS:NZ	2.10	0.66
3:O:39:GLN:NE2	3:O:40:THR:OG1	2.28	0.66
1:D:3869:ILE:O	1:D:3872:GLN:NE2	2.28	0.66
1:A:3869:ILE:O	1:A:3872:GLN:NE2	2.28	0.66
1:D:3530:ASP:O	1:D:3534:ILE:HD12	1.95	0.66
1:A:1043:ALA:O	1:A:1046:THR:OG1	2.10	0.66
1:D:2197:ASN:OD1	1:D:2200:ARG:NH2	2.29	0.66
1:B:1043:ALA:O	1:B:1046:THR:OG1	2.10	0.66
1:B:3249:ARG:O	1:B:3253:GLU:OE1	2.14	0.66
3:O:56:ASP:HA	1:D:3638:ARG:HH22	1.61	0.66
1:D:3249:ARG:O	1:D:3253:GLU:OE1	2.14	0.66
1:B:3530:ASP:O	1:B:3534:ILE:HD12	1.95	0.66
1:A:3589:ASP:O	1:A:3593:ILE:HD12	1.96	0.66
1:D:3532:ASP:OD1	1:D:3533:LEU:N	2.29	0.66
3:K:1:MET:O	3:K:7:SER:OG	2.14	0.66
3:M:1:MET:O	3:M:7:SER:OG	2.14	0.66
1:A:2197:ASN:OD1	1:A:2200:ARG:NH2	2.29	0.65
3:O:1:MET:O	3:O:7:SER:OG	2.14	0.65
1:B:3532:ASP:OD1	1:B:3533:LEU:N	2.29	0.65
1:A:2814:LEU:HA	1:A:2817:MET:HE2	1.79	0.65
1:A:3249:ARG:O	1:A:3253:GLU:OE1	2.14	0.65
1:A:3457:GLN:OE1	1:A:3504:TYR:N	2.30	0.65
3:I:6:GLU:HA	3:I:9:MET:HE2	1.79	0.65
3:O:4:GLU:OE1	3:P:11:THR:HG23	1.96	0.65
1:B:2197:ASN:OD1	1:B:2200:ARG:NH2	2.29	0.65
1:C:3249:ARG:O	1:C:3253:GLU:OE1	2.14	0.65
1:C:3457:GLN:OE1	1:C:3504:TYR:N	2.30	0.65
3:I:1:MET:O	3:I:7:SER:OG	2.14	0.65
1:D:2599:ALA:O	1:D:2603:VAL:HG23	1.97	0.65
1:C:3532:ASP:OD1	1:C:3533:LEU:N	2.29	0.65
1:A:2599:ALA:O	1:A:2603:VAL:HG23	1.97	0.65
1:B:2814:LEU:HA	1:B:2817:MET:HE2	1.79	0.65
3:K:6:GLU:HA	3:K:9:MET:HE2	1.79	0.65
1:D:2814:LEU:HA	1:D:2817:MET:HE2	1.79	0.65
1:D:3589:ASP:O	1:D:3593:ILE:HD12	1.96	0.65
1:C:3589:ASP:O	1:C:3593:ILE:HD12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3457:GLN:OE1	1:D:3504:TYR:N	2.30	0.65
1:C:3082:MET:HE2	1:C:3093:LEU:HD23	1.78	0.65
1:C:3530:ASP:O	1:C:3534:ILE:HD12	1.95	0.65
1:A:2045:ILE:HG13	1:A:2132:LEU:HD23	1.79	0.65
1:D:2045:ILE:HG13	1:D:2132:LEU:HD23	1.79	0.65
1:B:3589:ASP:O	1:B:3593:ILE:HD12	1.96	0.65
3:M:6:GLU:HA	3:M:9:MET:HE2	1.79	0.65
1:D:3082:MET:HE2	1:D:3093:LEU:HD23	1.78	0.64
1:B:3457:GLN:OE1	1:B:3504:TYR:N	2.30	0.64
1:C:2814:LEU:HA	1:C:2817:MET:HE2	1.79	0.64
1:A:3532:ASP:OD1	1:A:3533:LEU:N	2.29	0.64
1:A:16:ARG:NH1	1:A:101:THR:OG1	2.31	0.64
1:B:722:LEU:HD12	1:B:1477:MET:HE1	1.80	0.64
1:A:3082:MET:HE2	1:A:3093:LEU:HD23	1.78	0.64
1:B:2599:ALA:O	1:B:2603:VAL:HG23	1.97	0.64
1:B:3082:MET:HE2	1:B:3093:LEU:HD23	1.78	0.64
1:C:3761:MET:SD	1:C:3765:ARG:CZ	2.86	0.64
1:B:1562:VAL:HG12	1:B:1563:VAL:HG13	1.80	0.64
1:C:16:ARG:NH1	1:C:101:THR:OG1	2.31	0.64
1:C:2599:ALA:O	1:C:2603:VAL:HG23	1.97	0.64
1:B:3761:MET:SD	1:B:3765:ARG:CZ	2.86	0.64
1:B:2045:ILE:HG13	1:B:2132:LEU:HD23	1.79	0.64
1:B:3170:LEU:HD12	1:B:3195:LEU:HD11	1.80	0.64
1:C:862:ILE:HG23	1:C:934:LEU:HD22	1.80	0.63
1:C:2045:ILE:HG13	1:C:2132:LEU:HD23	1.79	0.63
1:A:722:LEU:HD12	1:A:1477:MET:HE1	1.80	0.63
1:A:862:ILE:HG23	1:A:934:LEU:HD22	1.80	0.63
1:C:3564:VAL:HA	1:C:3570:LEU:HD22	1.80	0.63
1:A:1562:VAL:HG12	1:A:1563:VAL:HG13	1.80	0.63
3:O:6:GLU:HA	3:O:9:MET:HE2	1.79	0.63
1:D:1043:ALA:O	1:D:1046:THR:OG1	2.10	0.63
1:A:3170:LEU:HD12	1:A:3195:LEU:HD11	1.80	0.63
1:D:3761:MET:SD	1:D:3765:ARG:CZ	2.86	0.63
1:C:3282:LEU:HD12	1:C:3316:LEU:HD22	1.81	0.63
1:B:16:ARG:NH1	1:B:101:THR:OG1	2.31	0.63
1:B:862:ILE:HG23	1:B:934:LEU:HD22	1.80	0.63
1:B:3564:VAL:HA	1:B:3570:LEU:HD22	1.80	0.63
1:A:3282:LEU:HD12	1:A:3316:LEU:HD22	1.81	0.63
1:A:3761:MET:SD	1:A:3765:ARG:CZ	2.86	0.63
3:P:44:GLY:HA2	1:D:2986:ARG:NH2	2.14	0.63
1:B:2187:MET:O	1:B:2193:TYR:OH	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2197:ASN:OD1	1:C:2200:ARG:NH2	2.29	0.63
1:C:722:LEU:HD12	1:C:1477:MET:HE1	1.80	0.62
1:A:2828:ARG:NH2	1:A:2932:GLN:OE1	2.32	0.62
2:E:12:ASP:OD1	2:E:13:GLY:N	2.33	0.62
2:F:12:ASP:OD1	2:F:13:GLY:N	2.33	0.62
1:D:16:ARG:NH1	1:D:101:THR:OG1	2.31	0.62
1:A:3564:VAL:HA	1:A:3570:LEU:HD22	1.80	0.62
1:D:3282:LEU:HD12	1:D:3316:LEU:HD22	1.81	0.62
1:A:4100:MET:HE3	1:A:4111:ILE:HG23	1.82	0.62
2:G:12:ASP:OD1	2:G:13:GLY:N	2.33	0.62
1:B:216:THR:OG1	1:B:219:HIS:NE2	2.33	0.62
1:C:2828:ARG:NH2	1:C:2932:GLN:OE1	2.32	0.62
1:B:4100:MET:HE3	1:B:4111:ILE:HG23	1.82	0.62
3:K:56:ASP:HA	1:B:3638:ARG:HH22	1.64	0.62
1:D:1562:VAL:HG12	1:D:1563:VAL:HG13	1.80	0.62
1:C:4100:MET:HE3	1:C:4111:ILE:HG23	1.82	0.62
1:D:722:LEU:HD12	1:D:1477:MET:HE1	1.80	0.62
1:B:2828:ARG:NH2	1:B:2932:GLN:OE1	2.32	0.62
1:C:1562:VAL:HG12	1:C:1563:VAL:HG13	1.80	0.62
1:A:909:VAL:HG22	1:A:913:SER:OG	2.00	0.62
3:I:5:LEU:CD2	3:I:9:MET:HE1	2.23	0.62
2:H:12:ASP:OD1	2:H:13:GLY:N	2.33	0.62
1:D:3564:VAL:HA	1:D:3570:LEU:HD22	1.80	0.62
1:B:3282:LEU:HD12	1:B:3316:LEU:HD22	1.81	0.62
1:C:2746:VAL:HG21	1:C:2819:ALA:HB2	1.82	0.62
1:B:1857:SER:OG	1:B:1860:ASP:OD2	2.16	0.62
3:I:49:GLN:NE2	3:I:51:ASP:O	2.33	0.62
1:C:3170:LEU:HD12	1:C:3195:LEU:HD11	1.80	0.62
1:D:909:VAL:HG22	1:D:913:SER:OG	2.00	0.61
1:D:2828:ARG:NH2	1:D:2932:GLN:OE1	2.32	0.61
1:C:216:THR:OG1	1:C:219:HIS:NE2	2.33	0.61
1:C:885:LEU:O	1:C:888:ILE:HG22	2.00	0.61
1:D:3170:LEU:HD12	1:D:3195:LEU:HD11	1.80	0.61
1:D:4100:MET:HE3	1:D:4111:ILE:HG23	1.82	0.61
1:B:865:PRO:HD2	1:B:868:LEU:HD12	1.82	0.61
1:B:909:VAL:HG22	1:B:913:SER:OG	2.00	0.61
1:C:1857:SER:OG	1:C:1860:ASP:OD2	2.16	0.61
1:A:216:THR:OG1	1:A:219:HIS:NE2	2.33	0.61
3:K:5:LEU:CD2	3:K:9:MET:HE1	2.23	0.61
3:M:4:GLU:OE1	3:N:11:THR:HG23	2.00	0.61
3:M:49:GLN:NE2	3:M:51:ASP:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:862:ILE:HG23	1:D:934:LEU:HD22	1.80	0.61
1:A:2620:LEU:O	1:A:2624:LEU:HD23	2.01	0.61
3:O:49:GLN:NE2	3:O:51:ASP:O	2.33	0.61
1:A:2746:VAL:HG21	1:A:2819:ALA:HB2	1.82	0.61
1:D:216:THR:OG1	1:D:219:HIS:NE2	2.33	0.61
1:C:865:PRO:HD2	1:C:868:LEU:HD12	1.81	0.61
1:C:2620:LEU:O	1:C:2624:LEU:HD23	2.01	0.61
1:C:3771:SER:OG	1:C:3775:ASN:OD1	2.19	0.61
1:A:865:PRO:HD2	1:A:868:LEU:HD12	1.81	0.61
1:A:2624:LEU:O	1:A:2628:VAL:HG23	2.01	0.61
3:O:5:LEU:CD2	3:O:9:MET:HE1	2.23	0.61
3:P:6:GLU:O	3:P:10:GLU:OE1	2.19	0.61
1:B:1967:VAL:HG21	1:B:3650:ALA:HB1	1.83	0.61
1:B:2624:LEU:O	1:B:2628:VAL:HG23	2.01	0.61
1:C:918:GLU:HA	1:C:921:TYR:CD1	2.36	0.61
1:C:2624:LEU:O	1:C:2628:VAL:HG23	2.01	0.61
1:A:1932:LEU:HD13	1:A:1936:VAL:HG11	1.83	0.61
3:N:6:GLU:O	3:N:10:GLU:OE1	2.19	0.61
1:D:865:PRO:HD2	1:D:868:LEU:HD12	1.81	0.61
1:D:2746:VAL:HG21	1:D:2819:ALA:HB2	1.82	0.61
1:D:1967:VAL:HG21	1:D:3650:ALA:HB1	1.83	0.61
1:D:2624:LEU:O	1:D:2628:VAL:HG23	2.01	0.61
1:B:885:LEU:O	1:B:888:ILE:HG22	2.00	0.61
1:B:2907:VAL:HG23	1:B:2912:LEU:CD2	2.31	0.61
1:C:1967:VAL:HG21	1:C:3650:ALA:HB1	1.83	0.61
3:K:12:LEU:HD13	3:L:5:LEU:HD11	1.83	0.60
3:K:49:GLN:NE2	3:K:51:ASP:O	2.33	0.60
3:M:26:LYS:HZ2	3:N:92:GLU:H	1.47	0.60
3:L:35:LYS:O	3:L:39:GLN:OE1	2.20	0.60
3:L:6:GLU:O	3:L:10:GLU:OE1	2.19	0.60
1:D:918:GLU:HA	1:D:921:TYR:CD1	2.36	0.60
1:D:2204:MET:HE3	1:D:2236:PHE:HZ	1.67	0.60
1:C:909:VAL:HG22	1:C:913:SER:OG	2.00	0.60
1:A:918:GLU:HA	1:A:921:TYR:CD1	2.36	0.60
1:A:2907:VAL:HG23	1:A:2912:LEU:CD2	2.31	0.60
3:J:6:GLU:O	3:J:10:GLU:OE1	2.19	0.60
3:N:35:LYS:O	3:N:39:GLN:OE1	2.19	0.60
1:D:885:LEU:O	1:D:888:ILE:HG22	2.00	0.60
1:B:2755:PHE:CD2	1:B:2814:LEU:HD11	2.37	0.60
1:C:2907:VAL:HG23	1:C:2912:LEU:CD2	2.31	0.60
1:D:2620:LEU:O	1:D:2624:LEU:HD23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1932:LEU:HD13	1:B:1936:VAL:HG11	1.83	0.60
1:B:2620:LEU:O	1:B:2624:LEU:HD23	2.01	0.60
1:C:1932:LEU:HD13	1:C:1936:VAL:HG11	1.83	0.60
3:J:35:LYS:O	3:J:39:GLN:OE1	2.20	0.60
3:P:35:LYS:O	3:P:39:GLN:OE1	2.20	0.60
1:A:885:LEU:O	1:A:888:ILE:HG22	2.00	0.60
1:D:1932:LEU:HD13	1:D:1936:VAL:HG11	1.83	0.60
1:C:2755:PHE:CD2	1:C:2814:LEU:HD11	2.36	0.60
1:C:1264:THR:OG1	1:C:1267:THR:OG1	2.18	0.60
1:D:4823:THR:O	1:D:4826:SER:OG	2.16	0.60
1:B:918:GLU:HA	1:B:921:TYR:CD1	2.36	0.60
1:B:2438:ALA:HB2	1:B:2510:VAL:HG22	1.84	0.60
1:A:2438:ALA:HB2	1:A:2510:VAL:HG22	1.84	0.60
1:A:2755:PHE:CD2	1:A:2814:LEU:HD11	2.36	0.60
3:I:6:GLU:O	3:I:10:GLU:OE1	2.20	0.60
1:D:722:LEU:HD12	1:D:1477:MET:CE	2.32	0.60
1:D:2438:ALA:HB2	1:D:2510:VAL:HG22	1.84	0.60
1:B:2746:VAL:HG21	1:B:2819:ALA:HB2	1.82	0.59
1:C:722:LEU:HD12	1:C:1477:MET:CE	2.32	0.59
1:C:2204:MET:HE3	1:C:2236:PHE:HZ	1.67	0.59
1:A:1967:VAL:HG21	1:A:3650:ALA:HB1	1.83	0.59
1:A:2743:THR:OG1	1:A:2812:GLU:O	2.20	0.59
1:A:2204:MET:HE3	1:A:2236:PHE:HZ	1.67	0.59
3:O:6:GLU:O	3:O:10:GLU:OE1	2.20	0.59
1:B:722:LEU:HD12	1:B:1477:MET:CE	2.32	0.59
1:C:2006:GLN:NE2	1:C:3640:THR:O	2.36	0.59
1:C:2187:MET:O	1:C:2193:TYR:OH	2.14	0.59
1:C:2438:ALA:HB2	1:C:2510:VAL:HG22	1.84	0.59
1:C:5032:ASP:OD1	1:C:5033:GLN:N	2.36	0.59
3:O:72:PHE:CZ	3:O:76:VAL:HG11	2.37	0.59
1:D:2755:PHE:CD2	1:D:2814:LEU:HD11	2.36	0.59
1:C:885:LEU:O	1:C:889:GLU:OE1	2.21	0.59
1:A:1857:SER:OG	1:A:1860:ASP:OD2	2.16	0.59
3:I:72:PHE:CZ	3:I:76:VAL:HG11	2.37	0.59
3:M:56:ASP:HA	1:C:3638:ARG:HH22	1.67	0.59
3:M:72:PHE:CZ	3:M:76:VAL:HG11	2.37	0.59
1:D:3771:SER:OG	1:D:3775:ASN:OD1	2.19	0.59
1:D:5032:ASP:OD1	1:D:5033:GLN:N	2.36	0.59
1:B:2204:MET:HE3	1:B:2236:PHE:HZ	1.67	0.59
1:C:2753:ASP:HA	1:C:2756:ILE:HD12	1.85	0.59
1:A:722:LEU:HD12	1:A:1477:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:885:LEU:O	1:D:889:GLU:OE1	2.21	0.59
1:D:2907:VAL:HG23	1:D:2912:LEU:CD2	2.31	0.59
1:A:5032:ASP:OD1	1:A:5033:GLN:N	2.36	0.59
3:M:27:TYR:CD2	3:N:93:THR:HA	2.38	0.59
1:D:2753:ASP:HA	1:D:2756:ILE:HD12	1.85	0.59
1:B:885:LEU:O	1:B:889:GLU:OE1	2.21	0.58
1:C:2743:THR:OG1	1:C:2812:GLU:O	2.20	0.58
3:J:47:ASP:OD1	3:J:48:VAL:N	2.37	0.58
3:L:47:ASP:OD1	3:L:48:VAL:N	2.37	0.58
1:A:2753:ASP:HA	1:A:2756:ILE:HD12	1.85	0.58
3:K:6:GLU:O	3:K:10:GLU:OE1	2.20	0.58
3:N:34:LEU:HD11	3:N:75:TYR:CD1	2.39	0.58
1:B:71:GLU:OE2	1:B:111:ARG:NE	2.35	0.58
1:C:3865:ASP:OD1	1:C:3870:ASN:ND2	2.37	0.58
1:A:1264:THR:OG1	1:A:1267:THR:OG1	2.18	0.58
1:A:2006:GLN:NE2	1:A:3640:THR:O	2.36	0.58
1:A:3865:ASP:OD1	1:A:3870:ASN:ND2	2.37	0.58
3:P:34:LEU:HD11	3:P:75:TYR:CD1	2.39	0.58
1:B:2006:GLN:NE2	1:B:3640:THR:O	2.36	0.58
1:B:2748:ILE:HG21	1:B:2811:LYS:HZ2	1.69	0.58
1:B:2753:ASP:HA	1:B:2756:ILE:HD12	1.85	0.58
3:P:47:ASP:OD1	3:P:48:VAL:N	2.37	0.58
1:B:5032:ASP:OD1	1:B:5033:GLN:N	2.35	0.58
1:A:2156:LEU:HD13	1:A:2199:MET:HE1	1.86	0.58
1:A:3446:TRP:NE1	1:A:3456:GLU:OE2	2.37	0.58
3:J:34:LEU:HD11	3:J:75:TYR:CD1	2.39	0.58
3:K:72:PHE:CZ	3:K:76:VAL:HG11	2.37	0.58
1:D:2006:GLN:NE2	1:D:3640:THR:O	2.36	0.58
1:B:3865:ASP:OD1	1:B:3870:ASN:ND2	2.37	0.58
1:C:3366:LEU:HD23	1:C:3406:LEU:HD23	1.86	0.58
1:A:885:LEU:O	1:A:889:GLU:OE1	2.21	0.58
3:M:6:GLU:O	3:M:10:GLU:OE1	2.20	0.58
3:N:47:ASP:OD1	3:N:48:VAL:N	2.37	0.58
1:D:3865:ASP:OD1	1:D:3870:ASN:ND2	2.37	0.58
1:A:2745:ASN:OD1	1:A:2746:VAL:N	2.37	0.58
1:D:2215:VAL:HG21	1:D:2229:MET:CE	2.34	0.58
1:C:1499:GLY:O	1:C:1502:VAL:HG12	2.04	0.58
1:A:3366:LEU:HD23	1:A:3406:LEU:HD23	1.86	0.57
1:D:980:PRO:O	1:D:983:THR:OG1	2.20	0.57
1:D:3587:ALA:HA	1:D:3593:ILE:HD11	1.86	0.57
1:D:2745:ASN:OD1	1:D:2746:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3446:TRP:NE1	1:D:3456:GLU:OE2	2.37	0.57
1:B:1499:GLY:O	1:B:1502:VAL:HG12	2.04	0.57
3:L:88:ASN:OD1	3:L:89:PHE:N	2.38	0.57
3:N:88:ASN:OD1	3:N:89:PHE:N	2.37	0.57
1:C:2215:VAL:HG21	1:C:2229:MET:CE	2.34	0.57
1:C:2745:ASN:OD1	1:C:2746:VAL:N	2.37	0.57
1:A:1428:ILE:HG23	1:A:1429:LEU:HD22	1.87	0.57
1:A:2215:VAL:HG21	1:A:2229:MET:CE	2.34	0.57
3:J:88:ASN:OD1	3:J:89:PHE:N	2.38	0.57
3:O:27:TYR:CD2	3:P:93:THR:HA	2.38	0.57
1:D:2215:VAL:HG21	1:D:2229:MET:HE2	1.87	0.57
1:B:3366:LEU:HD23	1:B:3406:LEU:HD23	1.86	0.57
1:C:1428:ILE:HG23	1:C:1429:LEU:HD22	1.87	0.57
3:P:88:ASN:OD1	3:P:89:PHE:N	2.37	0.57
1:B:2745:ASN:OD1	1:B:2746:VAL:N	2.37	0.57
1:C:2156:LEU:HD13	1:C:2199:MET:HE1	1.86	0.57
3:M:48:VAL:O	3:M:50:LYS:NZ	2.38	0.57
3:N:44:GLY:HA2	1:C:2986:ARG:NH2	2.19	0.57
1:D:1499:GLY:O	1:D:1502:VAL:HG12	2.04	0.57
1:B:1428:ILE:HG23	1:B:1429:LEU:HD22	1.87	0.57
1:B:3174:TYR:O	1:B:3178:THR:HG23	2.05	0.57
1:B:3446:TRP:NE1	1:B:3456:GLU:OE2	2.37	0.57
1:C:71:GLU:OE2	1:C:111:ARG:NE	2.35	0.57
1:C:3174:TYR:O	1:C:3178:THR:HG23	2.05	0.57
3:L:34:LEU:HD11	3:L:75:TYR:CD1	2.39	0.57
1:A:2215:VAL:HG21	1:A:2229:MET:HE2	1.87	0.57
1:D:1428:ILE:HG23	1:D:1429:LEU:HD22	1.87	0.57
1:B:3587:ALA:HA	1:B:3593:ILE:HD11	1.86	0.57
1:C:3446:TRP:NE1	1:C:3456:GLU:OE2	2.37	0.57
1:D:875:LEU:O	1:D:879:ILE:HG12	2.05	0.57
1:B:1080:LYS:HA	1:B:1190:LEU:HD11	1.86	0.57
1:B:2215:VAL:HG21	1:B:2229:MET:CE	2.34	0.57
1:A:1080:LYS:HA	1:A:1190:LEU:HD11	1.86	0.57
1:A:3174:TYR:O	1:A:3178:THR:HG23	2.05	0.57
1:D:3174:TYR:O	1:D:3178:THR:HG23	2.05	0.57
1:C:875:LEU:O	1:C:879:ILE:HG12	2.05	0.57
1:C:982:GLN:HG2	1:C:1054:ILE:HD11	1.86	0.57
1:C:4902:PRO:HB3	1:C:4911:ARG:HG2	1.87	0.57
1:B:3972:ILE:HG21	1:B:3983:LEU:HD12	1.87	0.56
1:A:875:LEU:O	1:A:879:ILE:HG12	2.05	0.56
3:O:12:LEU:HD13	3:P:5:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:875:LEU:O	1:B:879:ILE:HG12	2.05	0.56
1:A:310:THR:O	1:A:314:SER:OG	2.14	0.56
1:D:1080:LYS:HA	1:D:1190:LEU:HD11	1.86	0.56
1:D:1132:ARG:NH1	1:D:1179:ALA:O	2.38	0.56
1:D:2192:PHE:HA	1:D:2199:MET:HE3	1.88	0.56
1:D:4902:PRO:HB3	1:D:4911:ARG:HG2	1.87	0.56
1:D:3366:LEU:HD23	1:D:3406:LEU:HD23	1.86	0.56
1:B:982:GLN:HG2	1:B:1054:ILE:HD11	1.86	0.56
1:C:1080:LYS:HA	1:C:1190:LEU:HD11	1.86	0.56
1:C:2215:VAL:HG21	1:C:2229:MET:HE2	1.87	0.56
1:C:3595:ARG:O	1:C:3599:GLU:OE1	2.24	0.56
1:A:3053:HIS:O	1:A:3128:GLN:NE2	2.38	0.56
1:D:2692:TYR:OH	1:D:2694:GLN:HG2	2.06	0.56
1:D:2743:THR:OG1	1:D:2812:GLU:O	2.20	0.56
1:B:1132:ARG:NH1	1:B:1179:ALA:O	2.39	0.56
3:O:25:ASP:HB3	3:P:94:SER:CB	2.36	0.56
1:D:1042:GLN:O	1:D:1046:THR:HG23	2.06	0.56
1:D:4868:ASP:OD1	1:D:4869:GLU:N	2.39	0.56
1:B:878:ASN:ND2	1:B:1046:THR:HG22	2.21	0.56
1:B:2156:LEU:HD13	1:B:2199:MET:HE1	1.86	0.56
1:A:878:ASN:ND2	1:A:1046:THR:HG22	2.21	0.56
1:A:1499:GLY:O	1:A:1502:VAL:HG12	2.04	0.56
1:A:4823:THR:O	1:A:4826:SER:OG	2.16	0.56
1:D:982:GLN:HG2	1:D:1054:ILE:HD11	1.86	0.56
1:D:2156:LEU:HD13	1:D:2199:MET:HE1	1.86	0.56
1:B:3771:SER:OG	1:B:3775:ASN:OD1	2.19	0.56
1:C:2192:PHE:HA	1:C:2199:MET:HE3	1.88	0.56
1:A:1132:ARG:NH1	1:A:1179:ALA:O	2.38	0.56
1:A:3771:SER:OG	1:A:3775:ASN:OD1	2.19	0.56
1:B:2743:THR:OG1	1:B:2812:GLU:O	2.20	0.56
1:B:4868:ASP:OD1	1:B:4869:GLU:N	2.39	0.56
1:C:3587:ALA:HA	1:C:3593:ILE:HD11	1.86	0.56
1:A:3587:ALA:HA	1:A:3593:ILE:HD11	1.86	0.56
1:B:2215:VAL:HG21	1:B:2229:MET:HE2	1.87	0.56
1:B:4235:GLU:OE2	1:B:5015:ARG:NH2	2.39	0.56
1:B:4902:PRO:HB3	1:B:4911:ARG:HG2	1.87	0.56
1:C:34:LEU:HD23	1:C:36:LEU:HD11	1.88	0.56
1:C:1132:ARG:NH1	1:C:1179:ALA:O	2.38	0.56
1:A:1042:GLN:O	1:A:1046:THR:HG23	2.06	0.56
3:I:48:VAL:O	3:I:50:LYS:NZ	2.38	0.56
1:B:1042:GLN:O	1:B:1046:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2692:TYR:OH	1:C:2694:GLN:HG2	2.06	0.56
1:A:287:THR:HG21	1:A:482:GLU:OE1	2.06	0.55
3:M:12:LEU:HD13	3:N:5:LEU:HD11	1.88	0.55
1:D:878:ASN:ND2	1:D:1046:THR:HG22	2.21	0.55
1:B:2213:VAL:HG21	1:B:2257:TYR:OH	2.06	0.55
1:C:2213:VAL:HG21	1:C:2257:TYR:OH	2.06	0.55
1:C:4235:GLU:OE2	1:C:5015:ARG:NH2	2.39	0.55
1:A:982:GLN:HG2	1:A:1054:ILE:HD11	1.86	0.55
1:A:2971:SER:HA	1:A:2974:PHE:CE1	2.41	0.55
1:A:3972:ILE:HG21	1:A:3983:LEU:HD12	1.87	0.55
1:B:3595:ARG:O	1:B:3599:GLU:OE1	2.24	0.55
1:A:4902:PRO:HB3	1:A:4911:ARG:HG2	1.87	0.55
1:D:4235:GLU:OE2	1:D:5015:ARG:NH2	2.39	0.55
1:A:3595:ARG:O	1:A:3599:GLU:OE1	2.24	0.55
1:A:4868:ASP:OD1	1:A:4869:GLU:N	2.39	0.55
3:K:84:VAL:HG23	3:L:27:TYR:CZ	2.41	0.55
1:D:287:THR:HG21	1:D:482:GLU:OE1	2.06	0.55
1:C:287:THR:HG21	1:C:482:GLU:OE1	2.06	0.55
1:D:3972:ILE:HG21	1:D:3983:LEU:HD12	1.87	0.55
1:B:287:THR:HG21	1:B:482:GLU:OE1	2.06	0.55
1:B:2971:SER:HA	1:B:2974:PHE:CE1	2.42	0.55
1:C:3972:ILE:HG21	1:C:3983:LEU:HD12	1.87	0.55
1:A:1236:THR:OG1	1:A:1703:ARG:NH1	2.40	0.55
1:D:3351:ARG:HG2	1:D:3353:GLU:OE1	2.06	0.55
1:B:34:LEU:HD23	1:B:36:LEU:HD11	1.88	0.55
1:B:3351:ARG:HG2	1:B:3353:GLU:OE1	2.06	0.55
1:A:2192:PHE:HA	1:A:2199:MET:HE3	1.87	0.55
1:B:3053:HIS:O	1:B:3128:GLN:NE2	2.38	0.55
1:C:878:ASN:ND2	1:C:1046:THR:HG22	2.21	0.55
1:C:4823:THR:O	1:C:4826:SER:OG	2.16	0.55
1:A:4235:GLU:OE2	1:A:5015:ARG:NH2	2.39	0.55
1:D:34:LEU:HD23	1:D:36:LEU:HD11	1.88	0.55
1:B:2828:ARG:NH2	1:B:2936:TYR:O	2.40	0.55
1:C:4868:ASP:OD1	1:C:4869:GLU:N	2.39	0.55
3:K:27:TYR:CD2	3:L:93:THR:HA	2.42	0.55
3:K:48:VAL:O	3:K:50:LYS:NZ	2.38	0.55
3:M:5:LEU:CD2	3:M:9:MET:HE1	2.23	0.55
1:D:2478:PRO:HD2	1:D:2537:LEU:HD21	1.89	0.55
1:D:3595:ARG:O	1:D:3599:GLU:OE1	2.24	0.55
1:B:2192:PHE:HA	1:B:2199:MET:HE3	1.88	0.55
1:C:1236:THR:OG1	1:C:1703:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3053:HIS:O	1:C:3128:GLN:NE2	2.38	0.55
1:A:71:GLU:OE2	1:A:111:ARG:NE	2.35	0.55
1:A:2045:ILE:CG1	1:A:2132:LEU:HD23	2.37	0.55
1:A:2748:ILE:HG21	1:A:2811:LYS:HZ1	1.70	0.55
1:D:3292:ALA:O	1:D:3294:PRO:HD3	2.07	0.55
1:B:1236:THR:OG1	1:B:1703:ARG:NH1	2.40	0.55
1:B:2692:TYR:OH	1:B:2694:GLN:HG2	2.06	0.55
1:C:1042:GLN:O	1:C:1046:THR:HG23	2.06	0.55
1:C:1739:LEU:HD12	1:C:1964:GLU:CD	2.32	0.55
1:C:2478:PRO:HD2	1:C:2537:LEU:HD21	1.89	0.55
1:C:3351:ARG:HG2	1:C:3353:GLU:OE1	2.06	0.55
1:B:1739:LEU:HD12	1:B:1964:GLU:CD	2.32	0.54
1:C:3460:VAL:HG23	1:C:3465:ILE:HG13	1.89	0.54
1:A:2213:VAL:HG21	1:A:2257:TYR:OH	2.06	0.54
1:A:2756:ILE:CG1	1:A:2814:LEU:HD12	2.38	0.54
1:A:2828:ARG:NH2	1:A:2936:TYR:O	2.40	0.54
1:A:3351:ARG:HG2	1:A:3353:GLU:OE1	2.06	0.54
1:D:2213:VAL:HG21	1:D:2257:TYR:OH	2.06	0.54
1:A:4964:ASP:OD1	1:A:4965:TYR:N	2.41	0.54
1:D:3053:HIS:O	1:D:3128:GLN:NE2	2.38	0.54
1:B:3460:VAL:HG23	1:B:3465:ILE:HG13	1.90	0.54
1:C:297:ASP:OD1	1:C:298:GLN:N	2.41	0.54
1:C:3292:ALA:O	1:C:3294:PRO:HD3	2.08	0.54
1:A:2692:TYR:OH	1:A:2694:GLN:HG2	2.06	0.54
1:D:1236:THR:OG1	1:D:1703:ARG:NH1	2.40	0.54
1:D:2828:ARG:NH2	1:D:2936:TYR:O	2.40	0.54
1:D:2971:SER:HA	1:D:2974:PHE:CE1	2.41	0.54
1:C:980:PRO:O	1:C:983:THR:OG1	2.20	0.54
1:C:4964:ASP:OD1	1:C:4965:TYR:N	2.41	0.54
1:A:34:LEU:HD23	1:A:36:LEU:HD11	1.88	0.54
1:A:3460:VAL:HG23	1:A:3465:ILE:HG13	1.89	0.54
1:A:3570:LEU:HD23	1:A:3570:LEU:O	2.07	0.54
3:O:27:TYR:OH	3:P:87:ASN:OD1	2.24	0.54
1:D:4964:ASP:OD1	1:D:4965:TYR:N	2.41	0.54
1:C:2045:ILE:CG1	1:C:2132:LEU:HD23	2.37	0.54
1:C:3570:LEU:O	1:C:3570:LEU:HD23	2.07	0.54
1:A:980:PRO:O	1:A:983:THR:OG1	2.20	0.54
1:D:1739:LEU:HD12	1:D:1964:GLU:CD	2.32	0.54
1:D:2045:ILE:CG1	1:D:2132:LEU:HD23	2.37	0.54
1:D:4248:MET:HE1	1:D:4987:MET:HE1	1.90	0.54
1:B:3025:VAL:HG23	1:B:3025:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3292:ALA:O	1:B:3294:PRO:HD3	2.07	0.54
1:B:3570:LEU:HD23	1:B:3570:LEU:O	2.07	0.54
1:C:2971:SER:HA	1:C:2974:PHE:CE1	2.42	0.54
1:A:2478:PRO:HD2	1:A:2537:LEU:HD21	1.89	0.54
1:A:297:ASP:OD1	1:A:298:GLN:N	2.41	0.54
3:O:5:LEU:HD12	3:P:15:VAL:HG11	1.89	0.54
1:D:71:GLU:OE2	1:D:111:ARG:NE	2.35	0.54
1:D:310:THR:O	1:D:314:SER:OG	2.14	0.54
1:D:2756:ILE:CG1	1:D:2814:LEU:HD12	2.38	0.54
1:D:3570:LEU:HD23	1:D:3570:LEU:O	2.07	0.54
1:B:980:PRO:O	1:B:983:THR:OG1	2.20	0.54
1:B:2756:ILE:CG1	1:B:2814:LEU:HD12	2.38	0.54
1:A:914:LEU:O	1:A:919:ARG:NH2	2.41	0.54
1:A:3292:ALA:O	1:A:3294:PRO:HD3	2.08	0.54
3:O:48:VAL:O	3:O:50:LYS:NZ	2.38	0.54
1:B:2045:ILE:CG1	1:B:2132:LEU:HD23	2.38	0.54
1:C:2828:ARG:NH2	1:C:2936:TYR:O	2.40	0.54
1:A:1739:LEU:HD12	1:A:1964:GLU:CD	2.32	0.54
1:A:3188:ARG:HG2	1:A:3273:ILE:HD11	1.90	0.54
1:A:4107:THR:O	1:A:4111:ILE:HD12	2.08	0.54
1:D:1857:SER:OG	1:D:1860:ASP:OD2	2.16	0.54
1:B:4107:THR:O	1:B:4111:ILE:HD12	2.08	0.54
1:B:4964:ASP:OD1	1:B:4965:TYR:N	2.41	0.54
1:C:3188:ARG:HG2	1:C:3273:ILE:HD11	1.90	0.54
1:C:914:LEU:O	1:C:919:ARG:NH2	2.41	0.53
1:A:964:ASN:OD1	1:A:965:GLY:N	2.42	0.53
1:A:4816:MET:O	1:A:4822:ARG:NH1	2.42	0.53
1:D:914:LEU:O	1:D:919:ARG:NH2	2.41	0.53
1:A:3025:VAL:HG23	1:A:3025:VAL:O	2.08	0.53
1:A:4248:MET:HE1	1:A:4987:MET:HE1	1.90	0.53
1:D:4107:THR:O	1:D:4111:ILE:HD12	2.08	0.53
1:B:2478:PRO:HD2	1:B:2537:LEU:HD21	1.89	0.53
1:B:3868:VAL:HG22	1:B:3869:ILE:H	1.74	0.53
1:B:4816:MET:O	1:B:4822:ARG:NH1	2.42	0.53
1:C:4816:MET:O	1:C:4822:ARG:NH1	2.42	0.53
1:A:2872:LEU:HB3	1:A:2928:LEU:HD21	1.91	0.53
1:A:3450:HIS:O	1:A:3454:ARG:NE	2.42	0.53
1:C:2756:ILE:CG1	1:C:2814:LEU:HD12	2.38	0.53
1:D:297:ASP:OD1	1:D:298:GLN:N	2.41	0.53
1:D:2872:LEU:HB3	1:D:2928:LEU:HD21	1.91	0.53
1:B:297:ASP:OD1	1:B:298:GLN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3188:ARG:HG2	1:B:3273:ILE:HD11	1.90	0.53
1:C:2872:LEU:HB3	1:C:2928:LEU:HD21	1.91	0.53
1:A:3868:VAL:HG22	1:A:3869:ILE:H	1.74	0.53
3:K:4:GLU:OE1	3:L:11:THR:CG2	2.56	0.53
3:O:84:VAL:HG23	3:P:27:TYR:CZ	2.43	0.53
1:D:1793:ALA:O	1:D:1794:THR:OG1	2.20	0.53
1:D:2533:ALA:O	1:D:2537:LEU:HD13	2.09	0.53
1:D:3460:VAL:HG23	1:D:3465:ILE:HG13	1.90	0.53
1:D:4083:TYR:O	1:D:4085:THR:HG23	2.09	0.53
1:B:914:LEU:O	1:B:919:ARG:NH2	2.41	0.53
1:B:2872:LEU:HB3	1:B:2928:LEU:HD21	1.91	0.53
1:B:2887:TRP:CD1	1:B:2891:LYS:HZ3	2.26	0.53
1:A:2533:ALA:O	1:A:2537:LEU:HD13	2.09	0.53
3:L:59:MET:HA	3:L:62:LEU:HD23	1.91	0.53
3:N:59:MET:HA	3:N:62:LEU:HD23	1.91	0.53
1:D:4816:MET:O	1:D:4822:ARG:NH1	2.42	0.53
1:B:2918:ALA:HA	1:B:2921:ARG:HG2	1.91	0.53
1:B:3450:HIS:O	1:B:3454:ARG:NE	2.42	0.53
1:B:4823:THR:O	1:B:4826:SER:OG	2.16	0.53
1:C:3025:VAL:HG23	1:C:3025:VAL:O	2.08	0.53
1:C:3868:VAL:HG22	1:C:3869:ILE:H	1.74	0.53
3:L:44:GLY:O	3:L:48:VAL:HG22	2.09	0.53
1:D:3188:ARG:HG2	1:D:3273:ILE:HD11	1.90	0.53
1:B:964:ASN:OD1	1:B:965:GLY:N	2.42	0.53
1:C:4083:TYR:O	1:C:4085:THR:HG23	2.09	0.53
1:C:4248:MET:HE1	1:C:4987:MET:HE1	1.90	0.53
3:J:44:GLY:O	3:J:48:VAL:HG22	2.09	0.53
1:B:2533:ALA:O	1:B:2537:LEU:HD13	2.09	0.53
1:C:2949:THR:HG22	1:C:2950:SER:N	2.23	0.53
1:D:3025:VAL:HG23	1:D:3025:VAL:O	2.08	0.53
1:D:3105:GLU:O	1:D:3109:GLU:OE1	2.27	0.53
1:D:3450:HIS:O	1:D:3454:ARG:NE	2.42	0.53
1:C:862:ILE:O	1:C:931:LYS:NZ	2.42	0.53
1:C:1793:ALA:O	1:C:1794:THR:OG1	2.20	0.53
1:C:2533:ALA:O	1:C:2537:LEU:HD13	2.08	0.53
1:C:2918:ALA:HA	1:C:2921:ARG:HG2	1.91	0.53
3:N:10:GLU:HA	3:N:13:ILE:HG22	1.91	0.52
1:D:2949:THR:HG22	1:D:2950:SER:N	2.23	0.52
1:D:3107:MET:SD	1:D:3133:THR:HG21	2.49	0.52
1:B:862:ILE:O	1:B:931:LYS:NZ	2.42	0.52
1:C:4107:THR:O	1:C:4111:ILE:HD12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3107:MET:SD	1:A:3133:THR:HG21	2.49	0.52
1:A:4083:TYR:O	1:A:4085:THR:HG23	2.09	0.52
3:J:59:MET:HA	3:J:62:LEU:HD23	1.91	0.52
3:L:47:ASP:OD1	3:L:48:VAL:HG13	2.09	0.52
3:N:44:GLY:O	3:N:48:VAL:HG22	2.09	0.52
1:D:862:ILE:O	1:D:931:LYS:NZ	2.43	0.52
1:D:964:ASN:OD1	1:D:965:GLY:N	2.42	0.52
1:C:918:GLU:HA	1:C:921:TYR:CE1	2.45	0.52
1:A:4016:LEU:HD23	1:A:4135:PHE:HE1	1.75	0.52
3:K:5:LEU:HD12	3:L:15:VAL:HG21	1.91	0.52
3:P:44:GLY:O	3:P:48:VAL:HG22	2.09	0.52
3:P:59:MET:HA	3:P:62:LEU:HD23	1.91	0.52
1:D:918:GLU:HA	1:D:921:TYR:CE1	2.45	0.52
1:D:3868:VAL:HG22	1:D:3869:ILE:H	1.74	0.52
1:D:4249:GLN:O	1:D:4253:GLN:HG3	2.10	0.52
1:C:4249:GLN:O	1:C:4253:GLN:HG3	2.10	0.52
1:A:3173:ILE:HG21	1:A:3195:LEU:HD13	1.90	0.52
3:O:5:LEU:CD1	3:P:15:VAL:HG21	2.39	0.52
1:D:147:CYS:HG	1:D:148:TRP:CD1	2.28	0.52
1:C:964:ASN:OD1	1:C:965:GLY:N	2.42	0.52
1:A:878:ASN:HD22	1:A:1046:THR:HG22	1.75	0.52
1:A:2918:ALA:HA	1:A:2921:ARG:HG2	1.91	0.52
1:A:4580:VAL:HG12	1:B:4875:ASP:O	2.10	0.52
3:P:10:GLU:HA	3:P:13:ILE:HG22	1.91	0.52
1:D:3173:ILE:HG21	1:D:3195:LEU:HD13	1.90	0.52
1:B:2167:LEU:HD11	1:B:2207:THR:HG23	1.92	0.52
1:B:4016:LEU:HD23	1:B:4135:PHE:HE1	1.75	0.52
1:A:918:GLU:HA	1:A:921:TYR:CE1	2.45	0.52
1:A:3105:GLU:O	1:A:3109:GLU:OE1	2.27	0.52
1:D:878:ASN:HD22	1:D:1046:THR:HG22	1.75	0.52
1:C:3173:ILE:HG21	1:C:3195:LEU:HD13	1.90	0.52
3:P:34:LEU:HD11	3:P:75:TYR:CE1	2.45	0.52
1:C:878:ASN:HD22	1:C:1046:THR:HG22	1.75	0.52
1:C:3547:ASP:O	1:C:3598:GLN:NE2	2.43	0.52
3:L:10:GLU:HA	3:L:13:ILE:HG22	1.91	0.52
1:D:2539:THR:HG21	1:D:2900:GLY:HA2	1.91	0.52
1:B:878:ASN:HD22	1:B:1046:THR:HG22	1.75	0.52
1:B:902:LYS:HZ2	1:B:904:LEU:HB2	1.75	0.52
1:B:3105:GLU:O	1:B:3109:GLU:OE1	2.28	0.52
1:B:3173:ILE:HG21	1:B:3195:LEU:HD13	1.91	0.52
1:B:4083:TYR:O	1:B:4085:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2625:ARG:HH11	1:C:2907:VAL:HG21	1.75	0.52
1:C:3930:GLN:HB3	1:C:3995:PHE:CE1	2.45	0.52
1:A:2887:TRP:CD1	1:A:2891:LYS:HZ3	2.27	0.52
3:I:8:ALA:O	3:I:11:THR:OG1	2.24	0.52
1:D:569:LEU:HD12	1:D:603:VAL:HG13	1.92	0.52
1:B:2539:THR:HG21	1:B:2900:GLY:HA2	1.92	0.52
1:B:3547:ASP:O	1:B:3598:GLN:NE2	2.43	0.52
1:C:2167:LEU:HD11	1:C:2207:THR:HG23	1.92	0.52
1:C:2987:VAL:O	1:C:2987:VAL:HG13	2.10	0.52
1:A:2167:LEU:HD11	1:A:2207:THR:HG23	1.92	0.52
3:O:37:LEU:O	3:O:41:GLU:OE1	2.28	0.52
1:B:4248:MET:HE1	1:B:4987:MET:HE1	1.90	0.52
1:A:2539:THR:HG21	1:A:2900:GLY:HA2	1.91	0.51
3:J:34:LEU:HD11	3:J:75:TYR:CE1	2.45	0.51
3:O:5:LEU:HD12	3:P:15:VAL:HG21	1.91	0.51
3:N:47:ASP:OD1	3:N:48:VAL:HG13	2.09	0.51
1:B:569:LEU:HD12	1:B:603:VAL:HG13	1.92	0.51
1:B:3107:MET:SD	1:B:3133:THR:HG21	2.50	0.51
1:C:554:ARG:NH2	1:C:556:GLU:OE2	2.40	0.51
1:C:3450:HIS:O	1:C:3454:ARG:NE	2.42	0.51
3:J:47:ASP:OD1	3:J:48:VAL:HG13	2.09	0.51
3:I:37:LEU:O	3:I:41:GLU:OE1	2.28	0.51
3:O:31:LYS:NZ	3:O:62:LEU:O	2.38	0.51
3:L:34:LEU:HD11	3:L:75:TYR:CE1	2.45	0.51
1:D:2918:ALA:HA	1:D:2921:ARG:HG2	1.91	0.51
1:D:3930:GLN:HB3	1:D:3995:PHE:CE1	2.45	0.51
1:B:2949:THR:HG22	1:B:2950:SER:N	2.23	0.51
1:B:4249:GLN:O	1:B:4253:GLN:HG3	2.10	0.51
1:C:147:CYS:HG	1:C:148:TRP:CD1	2.28	0.51
1:C:2517:ASP:OD2	1:C:2518:PHE:N	2.43	0.51
1:C:3107:MET:SD	1:C:3133:THR:HG21	2.50	0.51
1:A:2517:ASP:OD2	1:A:2518:PHE:N	2.43	0.51
1:A:3547:ASP:O	1:A:3598:GLN:NE2	2.43	0.51
3:K:37:LEU:O	3:K:41:GLU:OE1	2.28	0.51
3:M:37:LEU:O	3:M:41:GLU:OE1	2.28	0.51
1:D:932:THR:O	1:D:936:LEU:HD23	2.10	0.51
1:B:918:GLU:HA	1:B:921:TYR:CE1	2.45	0.51
1:B:2987:VAL:O	1:B:2987:VAL:HG13	2.10	0.51
1:C:1932:LEU:HD13	1:C:1936:VAL:CG1	2.41	0.51
1:A:2383:GLU:O	1:A:2387:ILE:HG12	2.11	0.51
1:A:4249:GLN:O	1:A:4253:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:84:VAL:HG23	3:N:27:TYR:CZ	2.45	0.51
1:D:3547:ASP:O	1:D:3598:GLN:NE2	2.43	0.51
1:B:4752:ASN:OD1	1:B:4753:GLU:N	2.42	0.51
1:C:569:LEU:HD12	1:C:603:VAL:HG13	1.92	0.51
1:C:3105:GLU:O	1:C:3109:GLU:OE1	2.27	0.51
1:A:877:GLU:O	1:A:880:HIS:CE1	2.63	0.51
1:A:2949:THR:HG22	1:A:2950:SER:N	2.23	0.51
1:A:2987:VAL:HG13	1:A:2987:VAL:O	2.10	0.51
1:D:2517:ASP:OD2	1:D:2518:PHE:N	2.43	0.51
1:B:2383:GLU:O	1:B:2387:ILE:HG12	2.11	0.51
1:C:4016:LEU:HD23	1:C:4135:PHE:HE1	1.75	0.51
1:A:569:LEU:HD12	1:A:603:VAL:HG13	1.92	0.51
1:B:877:GLU:O	1:B:880:HIS:CE1	2.63	0.51
1:B:1932:LEU:HD13	1:B:1936:VAL:CG1	2.41	0.51
1:B:2625:ARG:HH11	1:B:2907:VAL:HG21	1.75	0.51
1:B:3930:GLN:HB3	1:B:3995:PHE:CE1	2.45	0.51
3:N:34:LEU:HD11	3:N:75:TYR:CE1	2.45	0.51
3:P:47:ASP:OD1	3:P:48:VAL:HG13	2.09	0.51
1:D:877:GLU:O	1:D:880:HIS:CE1	2.63	0.51
1:A:862:ILE:O	1:A:931:LYS:NZ	2.42	0.51
3:O:38:LEU:HD12	3:O:39:GLN:N	2.26	0.51
1:D:2167:LEU:HD11	1:D:2207:THR:HG23	1.92	0.51
1:B:3250:LEU:HD23	1:B:3253:GLU:OE2	2.11	0.51
1:C:877:GLU:O	1:C:880:HIS:CE1	2.63	0.51
1:C:902:LYS:HZ2	1:C:904:LEU:HB2	1.76	0.51
1:C:932:THR:O	1:C:936:LEU:HD23	2.10	0.51
1:A:932:THR:O	1:A:936:LEU:HD23	2.10	0.51
1:A:3458:ASN:O	1:A:3459:PHE:C	2.54	0.51
3:J:10:GLU:HA	3:J:13:ILE:HG22	1.91	0.51
1:D:1932:LEU:HD13	1:D:1936:VAL:CG1	2.41	0.51
1:D:2887:TRP:CD1	1:D:2891:LYS:HZ3	2.29	0.51
1:A:3250:LEU:HD23	1:A:3253:GLU:OE2	2.11	0.51
1:A:3930:GLN:HB3	1:A:3995:PHE:CE1	2.45	0.51
3:I:31:LYS:NZ	3:I:62:LEU:O	2.38	0.51
1:D:3250:LEU:HD23	1:D:3253:GLU:OE2	2.11	0.51
1:A:2968:MET:HE1	1:A:2999:PHE:HE1	1.76	0.50
1:D:2987:VAL:HG13	1:D:2987:VAL:O	2.10	0.50
1:C:1264:THR:HG1	1:C:1267:THR:HG1	1.54	0.50
1:C:2539:THR:HG21	1:C:2900:GLY:HA2	1.91	0.50
1:A:1688:SER:OG	2:E:37:PHE:O	2.26	0.50
1:A:1932:LEU:HD13	1:A:1936:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4685:TYR:CD1	1:A:4704:LEU:HD11	2.47	0.50
3:M:31:LYS:NZ	3:M:62:LEU:O	2.38	0.50
3:M:38:LEU:HD12	3:M:39:GLN:N	2.26	0.50
1:D:2968:MET:HE1	1:D:2999:PHE:HE1	1.76	0.50
1:D:4685:TYR:CD1	1:D:4704:LEU:HD11	2.47	0.50
1:B:3433:GLU:OE1	1:B:3525:MET:CG	2.59	0.50
1:C:330:ARG:NH2	1:C:331:ASP:OD1	2.45	0.50
1:C:3467:ASN:ND2	1:C:3508:THR:O	2.44	0.50
1:A:664:TYR:OH	1:A:666:GLU:OE2	2.30	0.50
1:A:979:THR:HG22	1:A:982:GLN:CD	2.37	0.50
1:D:3169:THR:O	1:D:3173:ILE:HG12	2.11	0.50
1:C:3433:GLU:OE1	1:C:3525:MET:CG	2.59	0.50
1:A:4685:TYR:OH	1:A:4697:GLY:O	2.30	0.50
1:D:2625:ARG:HH11	1:D:2907:VAL:HG21	1.75	0.50
1:B:926:SER:O	1:B:929:THR:OG1	2.27	0.50
1:C:664:TYR:OH	1:C:666:GLU:OE2	2.30	0.50
1:C:2383:GLU:O	1:C:2387:ILE:HG12	2.11	0.50
1:A:3169:THR:O	1:A:3173:ILE:HG12	2.11	0.50
3:N:29:LEU:HD23	3:N:34:LEU:HD13	1.93	0.50
1:D:4016:LEU:HD23	1:D:4135:PHE:HE1	1.75	0.50
1:B:2517:ASP:OD2	1:B:2518:PHE:N	2.43	0.50
1:A:2755:PHE:CE2	1:A:2814:LEU:HD11	2.47	0.50
3:L:29:LEU:HD23	3:L:34:LEU:HD13	1.93	0.50
1:D:3467:ASN:ND2	1:D:3508:THR:O	2.44	0.50
1:B:3458:ASN:O	1:B:3459:PHE:C	2.54	0.50
1:C:3250:LEU:HD23	1:C:3253:GLU:OE2	2.11	0.50
1:B:664:TYR:OH	1:B:666:GLU:OE2	2.30	0.50
1:B:932:THR:O	1:B:936:LEU:HD23	2.10	0.50
1:C:3771:SER:HA	1:C:3774:HIS:CE1	2.47	0.50
1:A:2625:ARG:HH11	1:A:2907:VAL:HG21	1.75	0.50
3:J:29:LEU:HD23	3:J:34:LEU:HD13	1.93	0.50
3:I:38:LEU:HD12	3:I:39:GLN:N	2.26	0.50
1:D:4574:ILE:HG23	1:D:4637:MET:HG2	1.93	0.50
1:B:4685:TYR:CD1	1:B:4704:LEU:HD11	2.47	0.50
1:D:330:ARG:NH2	1:D:331:ASP:OD1	2.45	0.50
1:B:3467:ASN:ND2	1:B:3508:THR:O	2.44	0.50
1:C:4685:TYR:CD1	1:C:4704:LEU:HD11	2.47	0.50
3:K:5:LEU:CD1	3:L:15:VAL:HG21	2.42	0.49
3:M:8:ALA:O	3:M:11:THR:OG1	2.24	0.49
3:N:34:LEU:HD23	3:N:70:VAL:HG21	1.95	0.49
1:D:2583:MET:HE1	1:D:2611:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3433:GLU:OE1	1:D:3525:MET:CG	2.59	0.49
1:D:3554:LEU:HB2	1:D:3594:VAL:HG13	1.93	0.49
1:B:330:ARG:NH2	1:B:331:ASP:OD1	2.45	0.49
1:B:3554:LEU:HB2	1:B:3594:VAL:HG13	1.93	0.49
1:C:3316:LEU:HD23	1:C:3346:ILE:HD13	1.94	0.49
1:A:3467:ASN:ND2	1:A:3508:THR:O	2.44	0.49
3:K:26:LYS:HZ2	3:L:92:GLU:H	1.58	0.49
1:B:2583:MET:HE1	1:B:2611:LEU:HD13	1.94	0.49
1:B:2755:PHE:CE2	1:B:2814:LEU:HD11	2.47	0.49
1:B:2968:MET:HE1	1:B:2999:PHE:HE1	1.76	0.49
1:C:2755:PHE:CE2	1:C:2814:LEU:HD11	2.47	0.49
1:C:2887:TRP:CD1	1:C:2891:LYS:HZ3	2.30	0.49
1:C:2968:MET:HE1	1:C:2999:PHE:HE1	1.76	0.49
1:C:4685:TYR:OH	1:C:4697:GLY:O	2.30	0.49
1:A:2110:ASP:OD1	1:A:2111:PHE:N	2.45	0.49
1:A:3771:SER:HA	1:A:3774:HIS:CE1	2.47	0.49
3:M:5:LEU:HD12	3:N:15:VAL:HG21	1.94	0.49
3:P:29:LEU:HD23	3:P:34:LEU:HD13	1.93	0.49
1:B:2110:ASP:OD1	1:B:2111:PHE:N	2.45	0.49
1:B:2979:GLU:OE2	1:B:3057:LEU:HD22	2.13	0.49
1:C:2110:ASP:OD1	1:C:2111:PHE:N	2.45	0.49
1:A:926:SER:O	1:A:929:THR:OG1	2.27	0.49
1:A:2583:MET:HE1	1:A:2611:LEU:HD13	1.94	0.49
3:K:6:GLU:HG2	3:L:45:PHE:HE2	1.77	0.49
3:L:52:ALA:HA	3:L:55:VAL:HG12	1.95	0.49
1:D:225:HIS:O	1:D:228:MET:HE2	2.12	0.49
1:D:1264:THR:OG1	1:D:1267:THR:OG1	2.18	0.49
1:D:2383:GLU:O	1:D:2387:ILE:HG12	2.11	0.49
1:D:2755:PHE:CE2	1:D:2814:LEU:HD11	2.47	0.49
1:C:2979:GLU:OE2	1:C:3057:LEU:HD22	2.13	0.49
1:C:4574:ILE:HG23	1:C:4637:MET:HG2	1.93	0.49
1:D:2110:ASP:OD1	1:D:2111:PHE:N	2.45	0.49
1:B:234:ILE:O	1:B:258:ARG:NH1	2.46	0.49
1:B:3316:LEU:HD23	1:B:3346:ILE:HD13	1.94	0.49
1:C:2156:LEU:CD1	1:C:2199:MET:HE1	2.43	0.49
1:A:4574:ILE:HG23	1:A:4637:MET:HG2	1.93	0.49
3:K:60:LYS:O	3:K:63:ASP:OD1	2.31	0.49
1:D:4709:PHE:HB3	1:D:4710:PRO:HD3	1.94	0.49
1:B:41:GLU:OE2	1:B:407:SER:OG	2.29	0.49
1:B:3169:THR:O	1:B:3173:ILE:HG12	2.11	0.49
1:C:3927:LEU:O	1:C:3930:GLN:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:O	1:A:228:MET:HE2	2.12	0.49
1:A:234:ILE:O	1:A:258:ARG:NH1	2.46	0.49
3:K:38:LEU:HD12	3:K:39:GLN:N	2.26	0.49
1:D:41:GLU:OE2	1:D:407:SER:OG	2.29	0.49
1:D:664:TYR:OH	1:D:666:GLU:OE2	2.30	0.49
1:D:3369:ARG:O	1:D:3373:VAL:HG23	2.13	0.49
1:B:2156:LEU:CD1	1:B:2199:MET:HE1	2.43	0.49
1:B:3927:LEU:O	1:B:3930:GLN:HG3	2.13	0.49
1:B:4574:ILE:HG23	1:B:4637:MET:HG2	1.93	0.49
1:C:2748:ILE:HG21	1:C:2811:LYS:HZ2	1.78	0.49
1:C:3271:ILE:H	1:C:3271:ILE:HD12	1.78	0.49
1:A:3433:GLU:OE1	1:A:3525:MET:CG	2.59	0.49
3:J:27:TYR:HB3	3:I:93:THR:HG23	1.95	0.49
3:J:34:LEU:HD23	3:J:70:VAL:HG21	1.95	0.49
3:P:34:LEU:HD23	3:P:70:VAL:HG21	1.95	0.49
1:D:2156:LEU:CD1	1:D:2199:MET:HE1	2.43	0.49
1:B:1164:THR:HG22	1:B:1169:VAL:HA	1.94	0.49
1:B:3771:SER:HA	1:B:3774:HIS:CE1	2.47	0.49
1:C:234:ILE:O	1:C:258:ARG:NH1	2.46	0.49
3:P:53:ASP:O	3:P:57:LYS:HG2	2.13	0.49
1:D:3927:LEU:O	1:D:3930:GLN:HG3	2.13	0.49
1:B:979:THR:HG22	1:B:982:GLN:CD	2.37	0.49
1:C:41:GLU:OE2	1:C:407:SER:OG	2.29	0.49
1:C:3369:ARG:O	1:C:3373:VAL:HG23	2.13	0.49
1:A:330:ARG:NH2	1:A:331:ASP:OD1	2.45	0.49
1:A:3554:LEU:HB2	1:A:3594:VAL:HG13	1.93	0.49
3:J:53:ASP:O	3:J:57:LYS:HG2	2.13	0.49
3:M:60:LYS:O	3:M:63:ASP:OD1	2.31	0.49
1:D:2979:GLU:OE2	1:D:3057:LEU:HD22	2.13	0.49
1:B:225:HIS:O	1:B:228:MET:HE2	2.12	0.49
1:B:942:MET:HE1	1:B:1052:TYR:HE1	1.78	0.49
1:C:3169:THR:O	1:C:3173:ILE:HG12	2.11	0.49
1:C:3554:LEU:HB2	1:C:3594:VAL:HG13	1.93	0.49
1:A:3181:ASN:O	1:A:3185:GLU:OE1	2.31	0.48
1:A:3316:LEU:HD23	1:A:3346:ILE:HD13	1.94	0.48
1:A:3927:LEU:O	1:A:3930:GLN:HG3	2.13	0.48
3:I:60:LYS:O	3:I:63:ASP:OD1	2.31	0.48
3:O:60:LYS:O	3:O:63:ASP:OD1	2.31	0.48
1:D:979:THR:HG22	1:D:982:GLN:CD	2.37	0.48
1:D:1164:THR:HG22	1:D:1169:VAL:HA	1.94	0.48
1:D:3267:MET:HE3	1:D:3271:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3458:ASN:O	1:D:3459:PHE:C	2.54	0.48
1:C:225:HIS:O	1:C:228:MET:HE2	2.12	0.48
1:D:3181:ASN:O	1:D:3185:GLU:OE1	2.31	0.48
1:D:3771:SER:HA	1:D:3774:HIS:CE1	2.47	0.48
1:B:4927:LEU:O	1:B:4931:GLN:OE1	2.32	0.48
1:C:883:TRP:O	1:C:887:ARG:HD3	2.13	0.48
1:C:1164:THR:HG22	1:C:1169:VAL:HA	1.94	0.48
1:A:1164:THR:HG22	1:A:1169:VAL:HA	1.94	0.48
1:A:1973:ASN:ND2	1:A:1973:ASN:O	2.47	0.48
1:A:4875:ASP:O	1:D:4580:VAL:HG12	2.13	0.48
1:A:4927:LEU:O	1:A:4931:GLN:OE1	2.32	0.48
3:K:8:ALA:O	3:K:11:THR:OG1	2.24	0.48
3:O:19:HIS:CE1	3:O:37:LEU:HD13	2.49	0.48
1:D:883:TRP:O	1:D:887:ARG:HD3	2.13	0.48
1:B:554:ARG:NH2	1:B:556:GLU:OE2	2.40	0.48
1:B:883:TRP:O	1:B:887:ARG:HD3	2.13	0.48
1:B:3369:ARG:O	1:B:3373:VAL:HG23	2.13	0.48
1:B:4709:PHE:HB3	1:B:4710:PRO:HD3	1.94	0.48
1:C:310:THR:O	1:C:314:SER:OG	2.14	0.48
3:N:53:ASP:O	3:N:57:LYS:HG2	2.13	0.48
3:P:52:ALA:HA	3:P:55:VAL:HG12	1.94	0.48
1:D:2011:LEU:HD11	1:D:2032:LEU:HD21	1.95	0.48
1:D:3271:ILE:H	1:D:3271:ILE:HD12	1.78	0.48
1:D:3316:LEU:HD23	1:D:3346:ILE:HD13	1.94	0.48
1:C:2583:MET:HE1	1:C:2611:LEU:HD13	1.94	0.48
1:C:3458:ASN:O	1:C:3459:PHE:C	2.54	0.48
3:J:80:ALA:O	3:J:84:VAL:HG12	2.14	0.48
1:B:4580:VAL:HG12	1:C:4875:ASP:O	2.13	0.48
1:A:3369:ARG:O	1:A:3373:VAL:HG23	2.13	0.48
1:A:4908:GLU:O	1:A:4912:VAL:HG13	2.13	0.48
3:J:52:ALA:HA	3:J:55:VAL:HG12	1.95	0.48
1:D:3236:SER:OG	1:D:3238:GLU:OE1	2.32	0.48
1:D:3467:ASN:O	1:D:3471:LEU:HD13	2.14	0.48
1:B:2011:LEU:HD11	1:B:2032:LEU:HD21	1.95	0.48
1:B:3164:VAL:HG22	1:B:3233:LEU:HD21	1.96	0.48
1:C:1968:ASP:C	1:C:1968:ASP:OD2	2.57	0.48
1:A:2450:GLU:OE1	1:A:2453:ARG:NH1	2.47	0.48
1:A:2979:GLU:OE2	1:A:3057:LEU:HD22	2.13	0.48
3:I:19:HIS:CE1	3:I:37:LEU:HD13	2.49	0.48
3:N:52:ALA:HA	3:N:55:VAL:HG12	1.95	0.48
3:P:56:ASP:OD1	3:P:56:ASP:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2450:GLU:OE1	1:D:2453:ARG:NH1	2.47	0.48
1:D:4685:TYR:OH	1:D:4697:GLY:O	2.30	0.48
1:B:1973:ASN:O	1:B:1973:ASN:ND2	2.47	0.48
1:C:942:MET:HE1	1:C:1052:TYR:HE1	1.78	0.48
1:A:41:GLU:OE2	1:A:407:SER:OG	2.29	0.48
1:A:942:MET:HE1	1:A:1052:TYR:HE1	1.78	0.48
1:A:2918:ALA:O	1:A:2922:GLU:OE1	2.32	0.48
1:A:4709:PHE:HB3	1:A:4710:PRO:HD3	1.94	0.48
3:K:93:THR:HG23	3:L:27:TYR:CB	2.38	0.48
1:D:942:MET:HE1	1:D:1052:TYR:HE1	1.78	0.48
1:D:2755:PHE:HD2	1:D:2814:LEU:HD11	1.79	0.48
1:D:4908:GLU:O	1:D:4912:VAL:HG13	2.13	0.48
1:B:2686:SER:O	1:B:2690:LYS:HG2	2.14	0.48
1:B:2817:MET:SD	1:B:2879:LEU:HD12	2.54	0.48
1:A:883:TRP:O	1:A:887:ARG:HD3	2.13	0.48
1:A:2817:MET:SD	1:A:2879:LEU:HD12	2.54	0.48
1:A:3236:SER:OG	1:A:3238:GLU:OE1	2.32	0.48
3:L:56:ASP:OD1	3:L:56:ASP:C	2.57	0.48
1:B:1282:ASN:C	1:B:1282:ASN:OD1	2.57	0.48
1:B:2764:HIS:N	1:B:2806:TYR:OH	2.47	0.48
1:B:3271:ILE:H	1:B:3271:ILE:HD12	1.78	0.48
1:C:2764:HIS:N	1:C:2806:TYR:OH	2.47	0.48
1:C:3868:VAL:HG22	1:C:3869:ILE:N	2.29	0.48
3:J:56:ASP:OD1	3:J:56:ASP:C	2.57	0.48
3:L:80:ALA:O	3:L:84:VAL:HG12	2.14	0.48
1:D:2764:HIS:N	1:D:2806:TYR:OH	2.47	0.48
1:B:2450:GLU:OE1	1:B:2453:ARG:NH1	2.47	0.48
1:B:3267:MET:HE3	1:B:3271:ILE:HD11	1.95	0.48
1:B:3316:LEU:O	1:B:3320:ILE:HG12	2.14	0.48
1:B:3789:CYS:SG	1:B:3834:SER:OG	2.72	0.48
1:B:4685:TYR:OH	1:B:4697:GLY:O	2.30	0.48
1:C:2011:LEU:HD11	1:C:2032:LEU:HD21	1.96	0.48
1:C:3467:ASN:O	1:C:3471:LEU:HD13	2.14	0.48
1:C:4927:LEU:O	1:C:4931:GLN:OE1	2.32	0.48
1:A:2500:LYS:NZ	1:A:2530:ASP:OD2	2.36	0.47
3:I:7:SER:O	3:I:11:THR:HG23	2.14	0.47
3:L:34:LEU:HD23	3:L:70:VAL:HG21	1.95	0.47
1:B:3324:ILE:HG21	1:B:3409:LEU:HD21	1.96	0.47
1:B:4686:ILE:HD11	1:B:4738:LEU:HD23	1.96	0.47
1:C:2817:MET:SD	1:C:2879:LEU:HD12	2.54	0.47
1:C:3164:VAL:HG22	1:C:3233:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3181:ASN:O	1:C:3185:GLU:OE1	2.32	0.47
1:C:3236:SER:OG	1:C:3238:GLU:OE1	2.32	0.47
1:C:4709:PHE:HB3	1:C:4710:PRO:HD3	1.94	0.47
1:A:880:HIS:CE1	1:A:911:PHE:HB2	2.49	0.47
1:A:2686:SER:O	1:A:2690:LYS:HG2	2.14	0.47
1:A:3789:CYS:SG	1:A:3834:SER:OG	2.72	0.47
1:D:234:ILE:O	1:D:258:ARG:NH1	2.46	0.47
1:D:3324:ILE:HG21	1:D:3409:LEU:HD21	1.97	0.47
1:D:4875:ASP:O	1:C:4580:VAL:HG12	2.13	0.47
1:C:2671:GLU:O	1:C:2675:LEU:HD13	2.15	0.47
1:C:4752:ASN:OD1	1:C:4753:GLU:N	2.42	0.47
1:A:2011:LEU:HD11	1:A:2032:LEU:HD21	1.95	0.47
1:A:3267:MET:HE3	1:A:3271:ILE:HD11	1.95	0.47
1:A:3271:ILE:H	1:A:3271:ILE:HD12	1.78	0.47
3:K:7:SER:O	3:K:11:THR:HG23	2.14	0.47
3:O:7:SER:O	3:O:11:THR:HG23	2.14	0.47
3:L:53:ASP:O	3:L:57:LYS:HG2	2.13	0.47
3:N:56:ASP:OD1	3:N:56:ASP:C	2.57	0.47
1:D:3770:GLN:O	1:D:3774:HIS:ND1	2.47	0.47
1:D:3868:VAL:HG22	1:D:3869:ILE:N	2.29	0.47
1:D:4927:LEU:O	1:D:4931:GLN:OE1	2.32	0.47
1:B:3181:ASN:O	1:B:3185:GLU:OE1	2.31	0.47
1:B:4908:GLU:O	1:B:4912:VAL:HG13	2.13	0.47
1:C:3770:GLN:O	1:C:3774:HIS:ND1	2.47	0.47
1:C:4686:ILE:HD11	1:C:4738:LEU:HD23	1.96	0.47
1:A:3467:ASN:O	1:A:3471:LEU:HD13	2.14	0.47
1:D:980:PRO:C	1:D:983:THR:HG1	2.17	0.47
1:D:1282:ASN:C	1:D:1282:ASN:OD1	2.57	0.47
1:D:4876:ASP:OD2	1:D:4879:THR:OG1	2.28	0.47
1:B:3467:ASN:O	1:B:3471:LEU:HD13	2.14	0.47
1:C:1282:ASN:C	1:C:1282:ASN:OD1	2.57	0.47
1:C:2450:GLU:OE1	1:C:2453:ARG:NH1	2.47	0.47
1:C:3267:MET:HE3	1:C:3271:ILE:HD11	1.95	0.47
1:C:4908:GLU:O	1:C:4912:VAL:HG13	2.13	0.47
1:A:2671:GLU:O	1:A:2675:LEU:HD13	2.15	0.47
1:A:3316:LEU:O	1:A:3320:ILE:HG12	2.14	0.47
3:M:19:HIS:CE1	3:M:37:LEU:HD13	2.49	0.47
1:D:880:HIS:CE1	1:D:911:PHE:HB2	2.49	0.47
1:D:980:PRO:HA	1:D:983:THR:OG1	2.15	0.47
1:D:2686:SER:O	1:D:2690:LYS:HG2	2.14	0.47
1:D:4686:ILE:HD11	1:D:4738:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2918:ALA:O	1:B:2922:GLU:OE1	2.32	0.47
1:C:979:THR:HG22	1:C:982:GLN:CD	2.37	0.47
1:C:2747:ILE:HG22	1:C:2748:ILE:N	2.30	0.47
1:A:2755:PHE:HD2	1:A:2814:LEU:HD11	1.79	0.47
1:A:3770:GLN:O	1:A:3774:HIS:ND1	2.47	0.47
1:A:3868:VAL:HG22	1:A:3869:ILE:N	2.29	0.47
3:N:80:ALA:O	3:N:84:VAL:HG12	2.14	0.47
3:P:80:ALA:O	3:P:84:VAL:HG12	2.14	0.47
1:D:902:LYS:HZ2	1:D:904:LEU:HB2	1.79	0.47
1:D:2918:ALA:O	1:D:2922:GLU:OE1	2.32	0.47
1:D:3954:PHE:O	1:D:3958:MET:HG3	2.14	0.47
1:B:4703:VAL:HG13	1:B:4709:PHE:HE1	1.80	0.47
1:C:926:SER:O	1:C:929:THR:OG1	2.27	0.47
1:C:2930:PHE:O	1:C:2934:ASN:ND2	2.48	0.47
1:A:2156:LEU:CD1	1:A:2199:MET:HE1	2.43	0.47
1:A:2747:ILE:HG22	1:A:2748:ILE:N	2.30	0.47
1:A:2764:HIS:N	1:A:2806:TYR:OH	2.47	0.47
1:A:3164:VAL:HG22	1:A:3233:LEU:HD21	1.96	0.47
3:M:27:TYR:OH	3:N:87:ASN:OD1	2.25	0.47
3:O:8:ALA:O	3:O:11:THR:OG1	2.24	0.47
1:D:2289:LEU:HD21	1:D:3855:LYS:HD2	1.97	0.47
1:D:2671:GLU:O	1:D:2675:LEU:HD13	2.15	0.47
1:D:2747:ILE:HG22	1:D:2748:ILE:H	1.80	0.47
1:D:2747:ILE:HG22	1:D:2748:ILE:N	2.30	0.47
1:B:2930:PHE:O	1:B:2934:ASN:ND2	2.48	0.47
1:B:3868:VAL:HG22	1:B:3869:ILE:N	2.29	0.47
1:C:980:PRO:HA	1:C:983:THR:OG1	2.15	0.47
1:C:1967:VAL:CG2	1:C:3650:ALA:HB1	2.45	0.47
1:C:2918:ALA:O	1:C:2922:GLU:OE1	2.32	0.47
1:C:3316:LEU:O	1:C:3320:ILE:HG12	2.14	0.47
1:C:3324:ILE:HG21	1:C:3409:LEU:HD21	1.97	0.47
1:C:3789:CYS:SG	1:C:3834:SER:OG	2.72	0.47
1:A:2930:PHE:O	1:A:2934:ASN:ND2	2.48	0.47
1:A:3954:PHE:O	1:A:3958:MET:HG3	2.14	0.47
3:M:5:LEU:CD1	3:N:15:VAL:HG21	2.45	0.47
3:O:4:GLU:OE1	3:P:11:THR:CG2	2.63	0.47
1:D:2817:MET:SD	1:D:2879:LEU:HD12	2.54	0.47
1:D:3004:LEU:HD21	1:D:3065:VAL:HG22	1.97	0.47
1:D:3316:LEU:O	1:D:3320:ILE:HG12	2.14	0.47
1:D:3600:VAL:O	1:D:3604:LEU:HD13	2.15	0.47
1:B:1264:THR:OG1	1:B:1267:THR:OG1	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4893:GLY:N	1:C:4897:ASP:OD2	2.47	0.47
1:A:614:ALA:HB2	1:A:1677:LEU:HD12	1.97	0.47
1:A:980:PRO:HA	1:A:983:THR:OG1	2.15	0.47
1:A:3600:VAL:O	1:A:3604:LEU:HD13	2.15	0.47
1:A:4686:ILE:HD11	1:A:4738:LEU:HD23	1.96	0.47
1:A:4703:VAL:HG13	1:A:4709:PHE:HE1	1.80	0.47
2:H:37:PHE:O	1:D:1688:SER:OG	2.26	0.47
3:M:7:SER:O	3:M:11:THR:HG23	2.14	0.47
1:D:978:LEU:HD12	1:D:982:GLN:CB	2.45	0.47
1:D:2930:PHE:O	1:D:2934:ASN:ND2	2.48	0.47
1:D:3163:GLN:NE2	1:D:3204:VAL:HG11	2.30	0.47
1:B:3600:VAL:O	1:B:3604:LEU:HD13	2.15	0.47
1:C:2289:LEU:HD21	1:C:3855:LYS:HD2	1.97	0.47
1:C:3600:VAL:O	1:C:3604:LEU:HD13	2.15	0.47
1:A:1282:ASN:C	1:A:1282:ASN:OD1	2.57	0.47
1:A:1968:ASP:OD2	1:A:1968:ASP:C	2.57	0.47
1:A:3163:GLN:NE2	1:A:3204:VAL:HG11	2.30	0.47
1:A:3540:ARG:NH2	1:A:3545:ASP:OD2	2.49	0.47
3:K:19:HIS:CE1	3:K:37:LEU:HD13	2.49	0.47
3:K:31:LYS:NZ	3:K:62:LEU:O	2.38	0.47
3:K:32:LYS:HA	3:K:35:LYS:HE3	1.97	0.47
3:O:32:LYS:HA	3:O:35:LYS:HE3	1.97	0.47
3:N:13:ILE:HD11	3:N:17:HIS:HE1	1.80	0.47
1:B:880:HIS:CE1	1:B:911:PHE:HB2	2.49	0.47
1:B:978:LEU:HD12	1:B:982:GLN:CB	2.45	0.47
1:B:1968:ASP:C	1:B:1968:ASP:OD2	2.57	0.47
1:B:4100:MET:CE	1:B:4111:ILE:HG23	2.45	0.47
1:C:978:LEU:HD12	1:C:982:GLN:CB	2.45	0.47
1:A:554:ARG:NH2	1:A:556:GLU:OE2	2.40	0.46
1:A:3324:ILE:HG21	1:A:3409:LEU:HD21	1.96	0.46
3:J:93:THR:HA	3:I:27:TYR:CD2	2.50	0.46
3:L:92:GLU:C	3:L:93:THR:HG1	2.16	0.46
3:P:13:ILE:HD11	3:P:17:HIS:HE1	1.80	0.46
1:D:1713:TYR:OH	1:D:1816:MET:SD	2.73	0.46
1:D:1967:VAL:CG2	1:D:3650:ALA:HB1	2.45	0.46
1:D:1973:ASN:O	1:D:1973:ASN:ND2	2.47	0.46
1:D:2187:MET:O	1:D:2193:TYR:OH	2.14	0.46
1:B:3163:GLN:NE2	1:B:3204:VAL:HG11	2.30	0.46
1:B:3954:PHE:O	1:B:3958:MET:HG3	2.14	0.46
1:B:4107:THR:O	1:B:4110:GLU:N	2.48	0.46
1:C:2627:LEU:HD22	1:C:2641:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2747:ILE:HG22	1:C:2748:ILE:H	1.80	0.46
1:C:2748:ILE:HG21	1:C:2811:LYS:CE	2.46	0.46
1:C:3954:PHE:O	1:C:3958:MET:HG3	2.14	0.46
1:C:4107:THR:O	1:C:4110:GLU:N	2.48	0.46
3:O:93:THR:HG23	3:P:27:TYR:CB	2.41	0.46
1:D:3164:VAL:HG22	1:D:3233:LEU:HD21	1.96	0.46
1:D:3540:ARG:NH2	1:D:3545:ASP:OD2	2.49	0.46
1:D:4013:ILE:O	1:D:4017:LYS:HG2	2.16	0.46
1:B:2671:GLU:O	1:B:2675:LEU:HD13	2.15	0.46
1:B:3236:SER:OG	1:B:3238:GLU:OE1	2.32	0.46
1:C:24:GLN:OE1	1:C:204:ASN:ND2	2.49	0.46
1:C:880:HIS:CE1	1:C:911:PHE:HB2	2.49	0.46
1:C:3372:LYS:O	1:C:3376:GLU:OE1	2.33	0.46
1:A:929:THR:O	1:A:932:THR:OG1	2.28	0.46
1:A:1807:GLU:HA	1:A:1810:ARG:NH1	2.31	0.46
1:A:2747:ILE:HG22	1:A:2748:ILE:H	1.80	0.46
1:A:3559:ASN:O	1:A:3560:LEU:HB2	2.15	0.46
1:A:4107:THR:O	1:A:4110:GLU:N	2.48	0.46
1:D:3372:LYS:O	1:D:3376:GLU:OE1	2.33	0.46
1:B:2751:LYS:O	1:B:2754:SER:OG	2.31	0.46
1:B:3372:LYS:O	1:B:3376:GLU:OE1	2.33	0.46
1:C:3163:GLN:NE2	1:C:3204:VAL:HG11	2.30	0.46
1:C:4703:VAL:HG13	1:C:4709:PHE:HE1	1.80	0.46
1:A:3004:LEU:HD21	1:A:3065:VAL:HG22	1.97	0.46
3:I:32:LYS:HA	3:I:35:LYS:HE3	1.97	0.46
3:O:25:ASP:HB3	3:P:94:SER:HB3	1.96	0.46
1:D:926:SER:O	1:D:929:THR:OG1	2.27	0.46
1:D:1807:GLU:HA	1:D:1810:ARG:NH1	2.31	0.46
1:B:614:ALA:HB2	1:B:1677:LEU:HD12	1.97	0.46
1:B:2747:ILE:HG22	1:B:2748:ILE:N	2.29	0.46
1:B:2755:PHE:HD2	1:B:2814:LEU:HD11	1.79	0.46
1:B:3540:ARG:NH2	1:B:3545:ASP:OD2	2.48	0.46
1:C:1807:GLU:HA	1:C:1810:ARG:NH1	2.31	0.46
1:A:649:ILE:HG23	1:A:815:ALA:HB3	1.97	0.46
1:A:868:LEU:CD2	1:A:871:ILE:HD12	2.46	0.46
1:A:4013:ILE:O	1:A:4017:LYS:HG2	2.16	0.46
1:A:4100:MET:CE	1:A:4111:ILE:HG23	2.45	0.46
1:D:982:GLN:CG	1:D:1054:ILE:HD11	2.46	0.46
1:B:24:GLN:OE1	1:B:204:ASN:ND2	2.49	0.46
1:B:2627:LEU:HD22	1:B:2641:PRO:HB3	1.97	0.46
1:C:982:GLN:CG	1:C:1054:ILE:HD11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4013:ILE:O	1:C:4017:LYS:HG2	2.16	0.46
1:A:3372:LYS:O	1:A:3376:GLU:OE1	2.33	0.46
1:A:3567:SER:O	1:A:3571:ARG:NH1	2.49	0.46
1:D:929:THR:O	1:D:932:THR:OG1	2.29	0.46
1:D:1968:ASP:OD2	1:D:1968:ASP:C	2.57	0.46
1:B:2747:ILE:HG22	1:B:2748:ILE:H	1.80	0.46
1:B:3770:GLN:O	1:B:3774:HIS:ND1	2.47	0.46
1:C:1713:TYR:OH	1:C:1816:MET:SD	2.73	0.46
1:C:1973:ASN:O	1:C:1973:ASN:ND2	2.47	0.46
1:C:2686:SER:O	1:C:2690:LYS:HG2	2.14	0.46
1:C:3410:TYR:N	1:C:3411:PRO:HD2	2.31	0.46
1:C:3540:ARG:NH2	1:C:3545:ASP:OD2	2.49	0.46
1:A:24:GLN:OE1	1:A:204:ASN:ND2	2.49	0.46
1:A:877:GLU:HA	1:A:880:HIS:ND1	2.31	0.46
1:A:978:LEU:HD12	1:A:982:GLN:CB	2.45	0.46
3:M:32:LYS:HA	3:M:35:LYS:HE3	1.97	0.46
1:B:3373:VAL:HG12	1:B:3399:PHE:CE2	2.51	0.46
1:C:47:LEU:HD13	1:C:126:ARG:HH12	1.81	0.46
1:C:649:ILE:HG23	1:C:815:ALA:HB3	1.97	0.46
1:C:921:TYR:O	1:C:925:MET:HG2	2.16	0.46
1:A:921:TYR:O	1:A:925:MET:HG2	2.16	0.46
1:A:2627:LEU:HD22	1:A:2641:PRO:HB3	1.97	0.46
1:A:2765:GLU:OE2	1:A:2858:PRO:HA	2.16	0.46
3:J:5:LEU:HD11	3:I:12:LEU:HD13	1.98	0.46
3:J:13:ILE:HD11	3:J:17:HIS:HE1	1.80	0.46
1:D:3337:LYS:HD2	1:D:3465:ILE:CG2	2.46	0.46
1:D:4703:VAL:HG13	1:D:4709:PHE:HE1	1.80	0.46
1:B:1807:GLU:HA	1:B:1810:ARG:NH1	2.31	0.46
1:C:3559:ASN:O	1:C:3560:LEU:HB2	2.15	0.46
1:A:47:LEU:HD13	1:A:126:ARG:HH12	1.81	0.46
1:A:2757:ASN:OD1	1:A:2757:ASN:C	2.59	0.46
1:A:3820:LEU:HD21	1:A:3901:ASP:HB3	1.98	0.46
1:D:614:ALA:HB2	1:D:1677:LEU:HD12	1.97	0.46
1:D:868:LEU:CD2	1:D:871:ILE:HD12	2.46	0.46
1:D:2765:GLU:OE2	1:D:2858:PRO:HA	2.16	0.46
1:D:3789:CYS:SG	1:D:3834:SER:OG	2.72	0.46
1:D:4656:ILE:HD11	1:D:4794:MET:HB2	1.98	0.46
1:D:4765:TRP:O	1:D:4769:ILE:HG12	2.15	0.46
1:B:2204:MET:HE3	1:B:2236:PHE:CZ	2.50	0.46
1:B:2500:LYS:NZ	1:B:2530:ASP:OD2	2.36	0.46
1:C:877:GLU:HA	1:C:880:HIS:ND1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:TYR:OH	1:A:1816:MET:SD	2.73	0.46
1:A:3337:LYS:HD2	1:A:3465:ILE:CG2	2.46	0.46
1:A:3526:CYS:SG	1:A:3600:VAL:HG11	2.56	0.46
3:K:5:LEU:HD12	3:L:15:VAL:HG11	1.97	0.46
3:K:34:LEU:HD23	3:K:38:LEU:HD23	1.98	0.46
1:D:3410:TYR:N	1:D:3411:PRO:HD2	2.31	0.46
1:D:3567:SER:O	1:D:3571:ARG:NH1	2.49	0.46
1:B:980:PRO:HA	1:B:983:THR:OG1	2.15	0.46
1:B:1713:TYR:OH	1:B:1816:MET:SD	2.73	0.46
1:B:1967:VAL:CG2	1:B:3650:ALA:HB1	2.45	0.46
1:C:35:LYS:C	1:C:36:LEU:HD12	2.41	0.46
1:C:868:LEU:CD2	1:C:871:ILE:HD12	2.46	0.46
1:C:1172:SER:OG	1:C:1176:SER:N	2.47	0.46
1:C:3076:LEU:O	1:C:3147:HIS:NE2	2.48	0.46
1:A:2289:LEU:HD21	1:A:3855:LYS:HD2	1.97	0.45
1:A:4765:TRP:O	1:A:4769:ILE:HG12	2.15	0.45
2:E:7:THR:HG23	2:E:7:THR:O	2.16	0.45
1:D:47:LEU:HD13	1:D:126:ARG:HH12	1.81	0.45
1:B:47:LEU:HD13	1:B:126:ARG:HH12	1.81	0.45
1:B:2748:ILE:HG21	1:B:2811:LYS:CE	2.45	0.45
1:B:3004:LEU:HD21	1:B:3065:VAL:HG22	1.97	0.45
1:C:421:SER:O	1:C:425:LYS:NZ	2.44	0.45
1:C:2757:ASN:OD1	1:C:2757:ASN:C	2.59	0.45
1:C:3567:SER:O	1:C:3571:ARG:NH1	2.49	0.45
1:A:35:LYS:C	1:A:36:LEU:HD12	2.41	0.45
1:A:1967:VAL:CG2	1:A:3650:ALA:HB1	2.45	0.45
1:A:3756:PHE:CD1	1:A:3756:PHE:C	2.94	0.45
3:I:34:LEU:HD23	3:I:38:LEU:HD23	1.98	0.45
3:I:80:ALA:HA	3:I:83:THR:HG22	1.98	0.45
1:D:2748:ILE:HG21	1:D:2811:LYS:CE	2.45	0.45
1:D:2751:LYS:O	1:D:2754:SER:OG	2.31	0.45
1:D:2881:GLU:OE1	1:D:2909:TYR:HB3	2.17	0.45
1:D:3373:VAL:HG12	1:D:3399:PHE:CE2	2.51	0.45
1:B:35:LYS:C	1:B:36:LEU:HD12	2.41	0.45
1:B:868:LEU:CD2	1:B:871:ILE:HD12	2.46	0.45
1:B:982:GLN:CG	1:B:1054:ILE:HD11	2.46	0.45
1:B:2757:ASN:OD1	1:B:2757:ASN:C	2.59	0.45
1:B:3567:SER:O	1:B:3571:ARG:NH1	2.49	0.45
1:B:3717:LEU:HD21	1:B:3785:MET:HE1	1.98	0.45
1:A:982:GLN:CG	1:A:1054:ILE:HD11	2.46	0.45
1:D:649:ILE:HG23	1:D:815:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:921:TYR:O	1:D:925:MET:HG2	2.16	0.45
1:D:3526:CYS:SG	1:D:3600:VAL:HG11	2.56	0.45
1:D:3559:ASN:O	1:D:3560:LEU:HB2	2.15	0.45
1:D:4107:THR:O	1:D:4110:GLU:N	2.48	0.45
1:B:877:GLU:HA	1:B:880:HIS:ND1	2.31	0.45
1:B:2289:LEU:HD21	1:B:3855:LYS:HD2	1.97	0.45
1:B:3559:ASN:O	1:B:3560:LEU:HB2	2.15	0.45
1:C:3004:LEU:HD21	1:C:3065:VAL:HG22	1.97	0.45
1:C:3337:LYS:HD2	1:C:3465:ILE:CG2	2.46	0.45
1:C:3820:LEU:HD21	1:C:3901:ASP:HB3	1.98	0.45
1:C:4765:TRP:O	1:C:4769:ILE:HG12	2.15	0.45
1:A:3177:GLY:HA3	1:A:3273:ILE:HD13	1.98	0.45
3:I:67:ASP:N	3:I:67:ASP:OD1	2.49	0.45
1:D:2757:ASN:OD1	1:D:2757:ASN:C	2.59	0.45
1:D:3717:LEU:HD21	1:D:3785:MET:HE1	1.98	0.45
1:B:649:ILE:HG23	1:B:815:ALA:HB3	1.97	0.45
1:B:4013:ILE:O	1:B:4017:LYS:HG2	2.16	0.45
1:C:614:ALA:HB2	1:C:1677:LEU:HD12	1.97	0.45
1:C:3373:VAL:HG12	1:C:3399:PHE:CE2	2.51	0.45
1:C:3434:GLU:O	1:C:3438:MET:HG3	2.17	0.45
1:A:2780:GLU:OE1	1:A:2780:GLU:N	2.49	0.45
1:A:2894:GLU:OE1	1:A:2898:LYS:NZ	2.50	0.45
1:A:3717:LEU:HD21	1:A:3785:MET:HE1	1.99	0.45
3:I:12:LEU:O	3:I:15:VAL:HG12	2.17	0.45
3:M:5:LEU:HD12	3:N:15:VAL:HG11	1.98	0.45
3:O:67:ASP:OD1	3:O:67:ASP:N	2.49	0.45
3:L:13:ILE:HD11	3:L:17:HIS:HE1	1.80	0.45
1:D:24:GLN:OE1	1:D:204:ASN:ND2	2.49	0.45
1:D:1773:LEU:HD11	1:D:2145:ILE:HD11	1.99	0.45
1:D:1973:ASN:C	1:D:1973:ASN:HD22	2.24	0.45
1:D:2780:GLU:OE1	1:D:2780:GLU:N	2.49	0.45
1:B:3337:LYS:HD2	1:B:3465:ILE:CG2	2.46	0.45
1:C:3717:LEU:HD21	1:C:3785:MET:HE1	1.99	0.45
1:A:1773:LEU:HD11	1:A:2145:ILE:HD11	1.99	0.45
1:A:2881:GLU:OE1	1:A:2909:TYR:HB3	2.17	0.45
1:A:3373:VAL:HG12	1:A:3399:PHE:CE2	2.51	0.45
1:A:3410:TYR:N	1:A:3411:PRO:HD2	2.31	0.45
3:M:80:ALA:HA	3:M:83:THR:HG22	1.98	0.45
1:D:2627:LEU:HD22	1:D:2641:PRO:HB3	1.97	0.45
1:D:3434:GLU:O	1:D:3438:MET:HG3	2.17	0.45
1:D:4100:MET:CE	1:D:4111:ILE:HG23	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4893:GLY:N	1:D:4897:ASP:OD2	2.47	0.45
1:B:1773:LEU:HD11	1:B:2145:ILE:HD11	1.99	0.45
1:B:4765:TRP:O	1:B:4769:ILE:HG12	2.15	0.45
1:C:1773:LEU:HD11	1:C:2145:ILE:HD11	1.99	0.45
1:A:473:ARG:NH2	1:A:476:GLN:OE1	2.44	0.45
1:A:760:ILE:HG23	1:A:760:ILE:O	2.17	0.45
1:A:902:LYS:HZ2	1:A:904:LEU:HB2	1.81	0.45
1:A:1793:ALA:O	1:A:1794:THR:OG1	2.20	0.45
3:O:34:LEU:HD23	3:O:38:LEU:HD23	1.98	0.45
3:P:87:ASN:OD1	3:P:91:TRP:CE3	2.70	0.45
1:D:2204:MET:HE3	1:D:2236:PHE:CZ	2.50	0.45
1:B:921:TYR:O	1:B:925:MET:HG2	2.16	0.45
1:B:2193:TYR:HE1	1:B:2239:TYR:HH	1.62	0.45
1:B:3820:LEU:HD21	1:B:3901:ASP:HB3	1.98	0.45
1:C:2765:GLU:OE2	1:C:2858:PRO:HA	2.16	0.45
1:C:2964:LEU:CD2	1:C:3003:LEU:HD22	2.47	0.45
1:A:2351:ALA:O	1:A:2355:VAL:HG23	2.17	0.45
1:D:421:SER:O	1:D:425:LYS:NZ	2.44	0.45
1:D:877:GLU:HA	1:D:880:HIS:ND1	2.31	0.45
1:D:2894:GLU:OE1	1:D:2898:LYS:NZ	2.50	0.45
1:D:3282:LEU:CD1	1:D:3316:LEU:HD22	2.46	0.45
1:D:3820:LEU:HD21	1:D:3901:ASP:HB3	1.98	0.45
1:D:4225:VAL:HG11	1:D:4948:VAL:HA	1.98	0.45
1:B:3107:MET:O	1:B:3111:LEU:HD23	2.17	0.45
1:B:3526:CYS:SG	1:B:3600:VAL:HG11	2.56	0.45
1:C:3460:VAL:HG23	1:C:3465:ILE:CG1	2.47	0.45
1:C:3526:CYS:SG	1:C:3600:VAL:HG11	2.56	0.45
1:A:2204:MET:HE3	1:A:2236:PHE:CZ	2.50	0.45
3:J:20:SER:HA	3:J:29:LEU:HD13	1.99	0.45
3:J:87:ASN:OD1	3:J:91:TRP:CE3	2.70	0.45
3:M:34:LEU:HD23	3:M:38:LEU:HD23	1.98	0.45
3:L:87:ASN:OD1	3:L:91:TRP:CE3	2.70	0.45
1:D:554:ARG:NH2	1:D:556:GLU:OE2	2.40	0.45
1:D:2964:LEU:CD2	1:D:3003:LEU:HD22	2.47	0.45
1:D:3177:GLY:HA3	1:D:3273:ILE:HD13	1.98	0.45
1:B:3460:VAL:HG23	1:B:3465:ILE:CG1	2.47	0.45
1:B:3756:PHE:CD1	1:B:3756:PHE:C	2.94	0.45
1:C:2204:MET:HE3	1:C:2236:PHE:CZ	2.50	0.45
1:A:2748:ILE:HG21	1:A:2811:LYS:CE	2.46	0.45
2:H:7:THR:HG23	2:H:7:THR:O	2.17	0.45
3:K:12:LEU:O	3:K:15:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:17:HIS:CE1	3:P:87:ASN:HD21	2.35	0.45
1:D:35:LYS:C	1:D:36:LEU:HD12	2.41	0.45
1:B:2521:HIS:O	1:B:2525:VAL:HG23	2.17	0.45
1:B:3410:TYR:N	1:B:3411:PRO:HD2	2.31	0.45
1:C:929:THR:O	1:C:932:THR:OG1	2.28	0.45
1:C:2894:GLU:OE1	1:C:2898:LYS:NZ	2.50	0.45
1:C:4656:ILE:HD11	1:C:4794:MET:HB2	1.98	0.45
1:A:3107:MET:O	1:A:3111:LEU:HD23	2.17	0.44
3:K:12:LEU:HD21	3:L:9:MET:CE	2.47	0.44
3:K:34:LEU:HD21	3:K:78:LEU:HD21	2.00	0.44
1:D:3460:VAL:HG23	1:D:3465:ILE:CG1	2.47	0.44
1:D:3756:PHE:CD1	1:D:3756:PHE:C	2.94	0.44
1:B:4656:ILE:HD11	1:B:4794:MET:HB2	1.98	0.44
1:A:3434:GLU:O	1:A:3438:MET:HG3	2.17	0.44
1:A:3460:VAL:HG23	1:A:3465:ILE:CG1	2.47	0.44
1:A:3564:VAL:HG13	1:A:3565:GLU:N	2.33	0.44
1:A:4225:VAL:HG11	1:A:4948:VAL:HA	1.98	0.44
3:K:75:TYR:O	3:K:79:VAL:HG22	2.18	0.44
3:M:34:LEU:HD21	3:M:78:LEU:HD21	2.00	0.44
3:O:75:TYR:O	3:O:79:VAL:HG22	2.18	0.44
3:L:36:ASP:O	3:L:40:THR:HG23	2.17	0.44
1:D:2351:ALA:O	1:D:2355:VAL:HG23	2.17	0.44
1:B:1695:LEU:O	1:B:1699:LEU:HD13	2.17	0.44
1:B:3076:LEU:O	1:B:3147:HIS:NE2	2.48	0.44
1:B:3974:GLY:N	1:B:3975:PRO:HA	2.33	0.44
1:C:3107:MET:O	1:C:3111:LEU:HD23	2.17	0.44
1:C:4225:VAL:HG11	1:C:4948:VAL:HA	1.98	0.44
1:A:1973:ASN:C	1:A:1973:ASN:HD22	2.24	0.44
1:A:3974:GLY:N	1:A:3975:PRO:HA	2.32	0.44
3:P:36:ASP:O	3:P:40:THR:HG23	2.18	0.44
1:D:4703:VAL:HG13	1:D:4709:PHE:CE1	2.53	0.44
1:B:370:LEU:HB3	1:B:372:VAL:HG22	1.99	0.44
1:B:623:THR:HG23	1:B:627:LEU:HD12	1.99	0.44
1:B:2351:ALA:O	1:B:2355:VAL:HG23	2.17	0.44
1:B:2894:GLU:OE1	1:B:2898:LYS:NZ	2.50	0.44
1:B:3434:GLU:O	1:B:3438:MET:HG3	2.17	0.44
1:B:3564:VAL:HG13	1:B:3565:GLU:N	2.33	0.44
1:C:2351:ALA:O	1:C:2355:VAL:HG23	2.17	0.44
1:C:2881:GLU:OE1	1:C:2909:TYR:HB3	2.17	0.44
1:C:3564:VAL:HG13	1:C:3565:GLU:N	2.33	0.44
1:C:4100:MET:CE	1:C:4111:ILE:HG23	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3275:LEU:HB3	1:A:3276:PRO:HD3	2.00	0.44
1:A:4656:ILE:HD11	1:A:4794:MET:HB2	1.98	0.44
1:A:4723:LEU:HA	1:A:4735:ILE:HG21	2.00	0.44
3:K:8:ALA:O	3:K:12:LEU:HD23	2.18	0.44
3:O:34:LEU:HD21	3:O:78:LEU:HD21	1.99	0.44
3:N:87:ASN:OD1	3:N:91:TRP:CE3	2.70	0.44
1:D:3974:GLY:N	1:D:3975:PRO:HA	2.32	0.44
1:B:3282:LEU:CD1	1:B:3316:LEU:HD22	2.46	0.44
1:C:4107:THR:HG22	1:C:4109:PRO:HD2	2.00	0.44
1:A:1695:LEU:O	1:A:1699:LEU:HD13	2.18	0.44
1:A:2964:LEU:CD2	1:A:3003:LEU:HD22	2.47	0.44
3:I:8:ALA:O	3:I:12:LEU:HD23	2.18	0.44
3:M:8:ALA:O	3:M:12:LEU:HD23	2.18	0.44
3:O:12:LEU:O	3:O:15:VAL:HG12	2.17	0.44
3:N:36:ASP:O	3:N:40:THR:HG23	2.18	0.44
1:D:869:GLU:HA	1:D:872:ARG:HG2	2.00	0.44
1:D:3564:VAL:HG13	1:D:3565:GLU:N	2.33	0.44
1:B:2964:LEU:CD2	1:B:3003:LEU:HD22	2.47	0.44
1:B:3275:LEU:HB3	1:B:3276:PRO:HD3	2.00	0.44
1:B:4225:VAL:HG11	1:B:4948:VAL:HA	1.98	0.44
1:B:4893:GLY:N	1:B:4897:ASP:OD2	2.47	0.44
1:C:2755:PHE:HD2	1:C:2814:LEU:HD11	1.79	0.44
1:C:3756:PHE:C	1:C:3756:PHE:CD1	2.94	0.44
1:A:70:LEU:HD23	1:A:110:LEU:HD23	2.00	0.44
3:O:45:PHE:CE2	3:P:6:GLU:HG2	2.52	0.44
3:O:80:ALA:HA	3:O:83:THR:HG22	1.98	0.44
3:N:55:VAL:O	3:N:58:VAL:HG12	2.18	0.44
1:B:760:ILE:HG23	1:B:760:ILE:O	2.17	0.44
1:B:1172:SER:OG	1:B:1176:SER:N	2.47	0.44
1:B:3360:ILE:HB	1:B:3361:PRO:HD3	2.00	0.44
1:B:4107:THR:HG22	1:B:4109:PRO:HD2	2.00	0.44
1:B:4723:LEU:HA	1:B:4735:ILE:HG21	2.00	0.44
1:C:1695:LEU:O	1:C:1699:LEU:HD13	2.17	0.44
1:C:2521:HIS:O	1:C:2525:VAL:HG23	2.17	0.44
1:A:4703:VAL:HG13	1:A:4709:PHE:CE1	2.53	0.44
3:J:36:ASP:O	3:J:40:THR:HG23	2.17	0.44
3:M:12:LEU:O	3:M:15:VAL:HG12	2.17	0.44
1:A:623:THR:HG23	1:A:627:LEU:HD12	1.99	0.44
1:A:3282:LEU:CD1	1:A:3316:LEU:HD22	2.46	0.44
3:L:20:SER:HA	3:L:29:LEU:HD13	1.99	0.44
1:D:3107:MET:O	1:D:3111:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4107:THR:HG22	1:D:4109:PRO:HD2	2.00	0.44
1:B:473:ARG:NH2	1:B:476:GLN:OE1	2.44	0.44
1:B:869:GLU:HA	1:B:872:ARG:HG2	2.00	0.44
1:B:2765:GLU:OE2	1:B:2858:PRO:HA	2.16	0.44
1:C:3177:GLY:HA3	1:C:3273:ILE:HD13	1.98	0.44
1:C:3974:GLY:N	1:C:3975:PRO:HA	2.32	0.44
1:C:4723:LEU:HA	1:C:4735:ILE:HG21	2.00	0.44
1:A:3380:LEU:HD12	1:A:3395:VAL:HG21	2.00	0.44
3:I:75:TYR:O	3:I:79:VAL:HG22	2.18	0.44
3:K:80:ALA:HA	3:K:83:THR:HG22	1.98	0.44
3:O:8:ALA:O	3:O:12:LEU:HD23	2.18	0.44
3:P:20:SER:HA	3:P:29:LEU:HD13	1.99	0.44
1:D:70:LEU:HD23	1:D:110:LEU:HD23	2.00	0.44
1:D:1744:ARG:NE	1:D:1964:GLU:OE2	2.50	0.44
1:D:2738:PRO:O	1:D:2740:PRO:HD3	2.18	0.44
1:D:3275:LEU:HB3	1:D:3276:PRO:HD3	2.00	0.44
1:B:3443:PHE:CD2	1:B:3515:LEU:HD13	2.53	0.44
1:C:232:LEU:HD11	1:C:246:VAL:CG1	2.48	0.44
1:C:760:ILE:HG23	1:C:760:ILE:O	2.17	0.44
1:C:2749:PRO:HD2	1:C:2752:LEU:HD12	2.00	0.44
1:C:3360:ILE:HB	1:C:3361:PRO:HD3	2.00	0.44
1:C:3443:PHE:CD2	1:C:3515:LEU:HD13	2.53	0.44
1:C:4703:VAL:HG13	1:C:4709:PHE:CE1	2.53	0.44
1:A:216:THR:OG1	1:A:219:HIS:CD2	2.71	0.43
1:A:370:LEU:HB3	1:A:372:VAL:HG22	2.00	0.43
1:A:1172:SER:OG	1:A:1176:SER:N	2.47	0.43
1:A:1744:ARG:NE	1:A:1964:GLU:OE2	2.50	0.43
1:A:2738:PRO:O	1:A:2740:PRO:HD3	2.18	0.43
1:A:2749:PRO:HD2	1:A:2752:LEU:HD12	2.00	0.43
1:A:3443:PHE:CD2	1:A:3515:LEU:HD13	2.53	0.43
1:A:4096:PHE:CE1	1:A:4100:MET:HE2	2.53	0.43
3:L:88:ASN:OD1	3:L:88:ASN:C	2.61	0.43
1:D:216:THR:OG1	1:D:219:HIS:CD2	2.71	0.43
1:D:760:ILE:O	1:D:760:ILE:HG23	2.17	0.43
1:D:2749:PRO:HD2	1:D:2752:LEU:HD12	2.00	0.43
1:D:3380:LEU:HD12	1:D:3395:VAL:HG21	2.00	0.43
1:D:4723:LEU:HA	1:D:4735:ILE:HG21	2.00	0.43
1:B:2749:PRO:HD2	1:B:2752:LEU:HD12	2.00	0.43
1:C:1144:TRP:HB2	1:C:1148:ASP:HB2	2.00	0.43
1:C:3267:MET:HG3	1:C:3267:MET:O	2.18	0.43
1:C:3380:LEU:HD12	1:C:3395:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:VAL:HB	1:A:754:PRO:C	2.43	0.43
1:A:869:GLU:HA	1:A:872:ARG:HG2	2.00	0.43
1:A:2521:HIS:O	1:A:2525:VAL:HG23	2.17	0.43
3:J:84:VAL:HG11	3:I:73:LYS:HD2	2.01	0.43
3:I:34:LEU:HD21	3:I:78:LEU:HD21	1.99	0.43
3:M:48:VAL:O	3:M:48:VAL:HG12	2.18	0.43
3:O:48:VAL:O	3:O:48:VAL:HG12	2.18	0.43
3:L:55:VAL:O	3:L:58:VAL:HG12	2.18	0.43
1:D:1540:PHE:CD2	1:D:1540:PHE:C	2.97	0.43
1:D:1695:LEU:O	1:D:1699:LEU:HD13	2.18	0.43
1:B:2881:GLU:OE1	1:B:2909:TYR:HB3	2.17	0.43
1:B:3177:GLY:HA3	1:B:3273:ILE:HD13	1.98	0.43
1:B:4096:PHE:CE1	1:B:4100:MET:HE2	2.53	0.43
1:B:4664:VAL:N	1:B:4665:PRO:CD	2.81	0.43
1:C:753:VAL:HB	1:C:754:PRO:C	2.43	0.43
1:C:3275:LEU:HB3	1:C:3276:PRO:HD3	2.00	0.43
1:A:2411:PRO:N	1:A:2412:PRO:CD	2.81	0.43
1:A:2578:ILE:H	1:A:2578:ILE:HD12	1.84	0.43
1:A:3360:ILE:HB	1:A:3361:PRO:HD3	2.00	0.43
1:A:4107:THR:HG22	1:A:4109:PRO:HD2	2.00	0.43
3:N:20:SER:HA	3:N:29:LEU:HD13	1.99	0.43
1:D:2521:HIS:O	1:D:2525:VAL:HG23	2.17	0.43
1:D:3360:ILE:HB	1:D:3361:PRO:HD3	2.00	0.43
1:B:978:LEU:HD12	1:B:982:GLN:HB2	2.01	0.43
1:B:2738:PRO:O	1:B:2740:PRO:HD3	2.18	0.43
1:A:979:THR:OG1	1:A:980:PRO:HD2	2.18	0.43
1:A:3267:MET:HG3	1:A:3267:MET:O	2.19	0.43
1:A:3515:LEU:HD11	1:A:3603:VAL:HG13	2.01	0.43
3:I:48:VAL:O	3:I:48:VAL:HG12	2.18	0.43
2:F:7:THR:O	2:F:7:THR:HG23	2.18	0.43
1:D:979:THR:OG1	1:D:980:PRO:HD2	2.18	0.43
1:D:4752:ASN:OD1	1:D:4753:GLU:N	2.42	0.43
1:B:216:THR:OG1	1:B:219:HIS:CD2	2.71	0.43
1:A:2748:ILE:HG21	1:A:2811:LYS:HE3	2.01	0.43
1:A:4101:ASP:O	1:A:4104:LYS:NZ	2.45	0.43
3:J:87:ASN:HD21	3:I:17:HIS:CE1	2.36	0.43
1:D:978:LEU:HD12	1:D:982:GLN:HB2	2.01	0.43
1:D:2748:ILE:HG21	1:D:2811:LYS:HE3	2.01	0.43
1:D:3443:PHE:CD2	1:D:3515:LEU:HD13	2.53	0.43
1:B:791:ARG:HA	1:B:1627:TRP:O	2.19	0.43
1:B:979:THR:OG1	1:B:980:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2411:PRO:N	1:B:2412:PRO:CD	2.81	0.43
1:B:2792:LEU:HD12	1:B:2792:LEU:O	2.19	0.43
1:B:3380:LEU:HD12	1:B:3395:VAL:HG21	2.00	0.43
1:B:4703:VAL:HG13	1:B:4709:PHE:CE1	2.53	0.43
1:C:370:LEU:HB3	1:C:372:VAL:HG22	2.00	0.43
1:C:619:GLN:OE1	1:C:1679:ASN:ND2	2.50	0.43
1:C:868:LEU:HD21	1:C:940:VAL:HG21	2.01	0.43
1:A:978:LEU:HD12	1:A:982:GLN:HB2	2.01	0.43
1:A:3859:LEU:HB3	1:A:3871:ARG:NH2	2.34	0.43
1:D:3461:VAL:HG23	1:D:3462:GLN:OE1	2.19	0.43
1:D:3515:LEU:HD11	1:D:3603:VAL:HG13	2.01	0.43
1:B:576:LEU:HA	1:B:579:ILE:HG12	2.01	0.43
1:C:4664:VAL:N	1:C:4665:PRO:CD	2.82	0.43
1:A:1144:TRP:HB2	1:A:1148:ASP:HB2	2.00	0.43
3:P:55:VAL:O	3:P:58:VAL:HG12	2.18	0.43
1:D:2356:ARG:O	1:D:2359:ILE:HG12	2.19	0.43
1:D:4664:VAL:N	1:D:4665:PRO:CD	2.81	0.43
1:B:3267:MET:O	1:B:3267:MET:HG3	2.19	0.43
1:B:3859:LEU:HB3	1:B:3871:ARG:NH2	2.34	0.43
1:C:70:LEU:HD23	1:C:110:LEU:HD23	2.00	0.43
1:C:216:THR:OG1	1:C:219:HIS:CD2	2.71	0.43
1:C:623:THR:HG23	1:C:627:LEU:HD12	1.99	0.43
1:C:869:GLU:HA	1:C:872:ARG:HG2	2.00	0.43
1:C:1540:PHE:CD2	1:C:1540:PHE:C	2.97	0.43
1:C:1744:ARG:NE	1:C:1964:GLU:OE2	2.50	0.43
1:C:2748:ILE:HG21	1:C:2811:LYS:HE3	2.01	0.43
1:C:2769:PHE:O	1:C:2773:GLN:HG2	2.19	0.43
1:A:576:LEU:HA	1:A:579:ILE:HG12	2.01	0.43
1:A:2769:PHE:O	1:A:2773:GLN:HG2	2.19	0.43
1:A:4664:VAL:N	1:A:4665:PRO:CD	2.82	0.43
3:J:88:ASN:OD1	3:J:88:ASN:C	2.61	0.43
3:K:6:GLU:HG2	3:L:45:PHE:CE2	2.53	0.43
3:M:75:TYR:O	3:M:79:VAL:HG22	2.18	0.43
1:D:753:VAL:HB	1:D:754:PRO:C	2.43	0.43
1:D:791:ARG:HA	1:D:1627:TRP:O	2.18	0.43
1:D:1127:GLY:HA3	1:D:1144:TRP:CZ3	2.54	0.43
1:D:2411:PRO:N	1:D:2412:PRO:CD	2.81	0.43
1:D:2578:ILE:HD12	1:D:2578:ILE:H	1.84	0.43
1:D:2792:LEU:O	1:D:2792:LEU:HD12	2.19	0.43
1:D:3267:MET:HG3	1:D:3267:MET:O	2.19	0.43
1:D:4096:PHE:CE1	1:D:4100:MET:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:HD23	1:B:110:LEU:HD23	2.00	0.43
1:B:2748:ILE:HG21	1:B:2811:LYS:HE3	2.01	0.43
1:B:2780:GLU:OE1	1:B:2780:GLU:N	2.49	0.43
1:C:576:LEU:HA	1:C:579:ILE:HG12	2.01	0.43
1:C:791:ARG:HA	1:C:1627:TRP:O	2.18	0.43
1:C:868:LEU:HA	1:C:871:ILE:HD12	2.00	0.43
1:C:2356:ARG:O	1:C:2359:ILE:HG12	2.19	0.43
1:C:2411:PRO:N	1:C:2412:PRO:CD	2.81	0.43
1:C:2792:LEU:HD12	1:C:2792:LEU:O	2.19	0.43
1:A:791:ARG:HA	1:A:1627:TRP:O	2.18	0.43
1:A:5011:MET:HE1	1:A:5018:ASP:HB2	2.01	0.43
3:J:11:THR:HG21	3:I:8:ALA:HB2	2.01	0.43
3:P:88:ASN:OD1	3:P:88:ASN:C	2.61	0.43
1:D:619:GLN:OE1	1:D:1679:ASN:ND2	2.50	0.43
1:D:1491:SER:OG	1:D:1492:ASN:N	2.52	0.43
1:B:232:LEU:HD11	1:B:246:VAL:CG1	2.49	0.43
1:B:2769:PHE:O	1:B:2773:GLN:HG2	2.19	0.43
1:C:978:LEU:HD12	1:C:982:GLN:HB2	2.01	0.43
1:C:2978:LEU:HA	1:C:2981:VAL:HG22	2.01	0.43
1:C:4096:PHE:CE1	1:C:4100:MET:HE2	2.53	0.43
1:A:638:LEU:HB3	1:A:1636:MET:HE2	2.00	0.43
1:D:232:LEU:HD11	1:D:246:VAL:CG1	2.49	0.43
1:D:308:ALA:HB1	1:D:313:THR:HG21	2.01	0.43
1:B:753:VAL:HB	1:B:754:PRO:C	2.43	0.43
1:B:1540:PHE:CD2	1:B:1540:PHE:C	2.97	0.43
1:B:3461:VAL:HG23	1:B:3462:GLN:OE1	2.19	0.43
1:B:3547:ASP:OD2	1:B:3547:ASP:C	2.62	0.43
1:C:2780:GLU:OE1	1:C:2780:GLU:N	2.49	0.43
1:C:3515:LEU:C	1:C:3515:LEU:HD23	2.44	0.43
1:A:2694:GLN:NE2	3:J:4:GLU:OE2	2.52	0.42
1:A:2792:LEU:O	1:A:2792:LEU:HD12	2.19	0.42
1:A:4752:ASN:OD1	1:A:4753:GLU:N	2.42	0.42
3:J:55:VAL:O	3:J:58:VAL:HG12	2.18	0.42
2:G:7:THR:O	2:G:7:THR:HG23	2.18	0.42
3:K:67:ASP:N	3:K:67:ASP:OD1	2.49	0.42
3:M:27:TYR:HH	3:N:87:ASN:CG	2.22	0.42
1:D:623:THR:HG23	1:D:627:LEU:HD12	1.99	0.42
1:D:868:LEU:HD21	1:D:940:VAL:HG21	2.01	0.42
1:D:3765:ARG:NH2	1:D:4753:GLU:HB2	2.34	0.42
1:B:302:VAL:HG23	1:B:302:VAL:O	2.19	0.42
1:B:3515:LEU:HD23	1:B:3515:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3568:PRO:HA	1:B:3571:ARG:CZ	2.49	0.42
1:C:2738:PRO:O	1:C:2740:PRO:HD3	2.18	0.42
1:A:1540:PHE:CD2	1:A:1540:PHE:C	2.97	0.42
1:A:3547:ASP:OD2	1:A:3547:ASP:C	2.62	0.42
1:A:4893:GLY:N	1:A:4897:ASP:OD2	2.47	0.42
2:G:91:ILE:HD11	1:C:1685:ALA:HA	2.00	0.42
3:N:88:ASN:OD1	3:N:88:ASN:C	2.61	0.42
1:D:868:LEU:HA	1:D:871:ILE:HD12	2.00	0.42
1:D:4980:GLU:OE2	1:D:5027:ARG:NH2	2.53	0.42
1:D:5011:MET:HE1	1:D:5018:ASP:HB2	2.01	0.42
1:B:929:THR:O	1:B:932:THR:OG1	2.28	0.42
1:B:3515:LEU:HD11	1:B:3603:VAL:HG13	2.01	0.42
1:C:216:THR:HG22	1:C:274:HIS:HA	2.01	0.42
1:C:869:GLU:O	1:C:872:ARG:HG2	2.19	0.42
1:C:979:THR:OG1	1:C:980:PRO:HD2	2.18	0.42
1:C:2578:ILE:H	1:C:2578:ILE:HD12	1.84	0.42
1:A:619:GLN:OE1	1:A:1679:ASN:ND2	2.50	0.42
1:A:910:ASN:O	1:A:914:LEU:N	2.52	0.42
1:A:1171:MET:HE2	1:A:1175:GLY:HA2	2.02	0.42
1:A:2356:ARG:O	1:A:2359:ILE:HG12	2.19	0.42
1:A:2413:GLU:CG	1:A:2416:ARG:NH2	2.83	0.42
1:A:3104:ILE:O	1:A:3108:VAL:HG23	2.20	0.42
1:A:3570:LEU:HD23	1:A:3570:LEU:C	2.44	0.42
1:A:4895:ILE:O	1:A:4899:ILE:HG12	2.19	0.42
3:J:27:TYR:CZ	3:I:84:VAL:HG23	2.54	0.42
3:M:72:PHE:O	3:M:76:VAL:HG22	2.20	0.42
3:N:10:GLU:O	3:N:14:ASN:OD1	2.38	0.42
3:P:10:GLU:O	3:P:14:ASN:OD1	2.38	0.42
1:D:1144:TRP:HB2	1:D:1148:ASP:HB2	2.00	0.42
1:D:2635:ASN:OD1	1:D:2635:ASN:C	2.62	0.42
1:D:2953:GLU:OE1	1:D:2953:GLU:N	2.49	0.42
1:D:4895:ILE:O	1:D:4899:ILE:HG12	2.19	0.42
1:B:1144:TRP:HB2	1:B:1148:ASP:HB2	2.00	0.42
1:B:2413:GLU:CG	1:B:2416:ARG:NH2	2.83	0.42
1:B:2635:ASN:OD1	1:B:2635:ASN:C	2.62	0.42
1:B:3570:LEU:HD23	1:B:3570:LEU:C	2.44	0.42
1:B:4686:ILE:HD12	1:B:4735:ILE:CD1	2.50	0.42
1:C:1127:GLY:HA3	1:C:1144:TRP:CZ3	2.54	0.42
1:C:2635:ASN:OD1	1:C:2635:ASN:C	2.62	0.42
1:C:3461:VAL:HG23	1:C:3462:GLN:OE1	2.19	0.42
1:A:302:VAL:HG23	1:A:302:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1491:SER:OG	1:A:1492:ASN:N	2.52	0.42
1:A:3076:LEU:O	1:A:3147:HIS:NE2	2.48	0.42
3:K:48:VAL:O	3:K:48:VAL:HG12	2.18	0.42
3:K:72:PHE:O	3:K:76:VAL:HG22	2.20	0.42
3:M:67:ASP:OD1	3:M:67:ASP:N	2.49	0.42
3:O:52:ALA:HA	3:O:55:VAL:HG12	2.01	0.42
3:N:73:LYS:O	3:N:76:VAL:HG22	2.20	0.42
1:D:370:LEU:HB3	1:D:372:VAL:HG22	2.00	0.42
1:D:869:GLU:O	1:D:872:ARG:HG2	2.19	0.42
1:D:3037:LYS:O	1:D:3040:ILE:HG22	2.20	0.42
1:D:3568:PRO:HA	1:D:3571:ARG:CZ	2.49	0.42
1:B:1491:SER:OG	1:B:1492:ASN:N	2.52	0.42
1:C:638:LEU:HB3	1:C:1636:MET:HE2	2.00	0.42
1:C:910:ASN:O	1:C:914:LEU:N	2.52	0.42
1:C:2413:GLU:CG	1:C:2416:ARG:NH2	2.83	0.42
1:C:2968:MET:HG3	1:C:3043:LEU:HD12	2.02	0.42
1:C:3104:ILE:O	1:C:3108:VAL:HG23	2.20	0.42
1:C:3282:LEU:CD1	1:C:3316:LEU:HD22	2.46	0.42
1:C:3351:ARG:HG2	1:C:3352:PRO:HD2	2.02	0.42
1:C:3515:LEU:HD11	1:C:3603:VAL:HG13	2.01	0.42
1:C:3547:ASP:OD2	1:C:3547:ASP:C	2.62	0.42
1:A:3037:LYS:O	1:A:3040:ILE:HG22	2.20	0.42
3:K:23:GLU:OE2	3:K:29:LEU:HA	2.20	0.42
3:M:4:GLU:OE1	3:N:11:THR:CG2	2.65	0.42
1:D:216:THR:HG22	1:D:274:HIS:HA	2.01	0.42
1:D:1023:VAL:HG13	1:D:1024:PRO:HD2	2.02	0.42
1:D:1124:VAL:HG23	1:D:1133:TRP:HB2	2.01	0.42
1:D:2878:GLN:O	1:D:2881:GLU:HB3	2.20	0.42
1:D:3173:ILE:CG2	1:D:3195:LEU:HD13	2.50	0.42
1:D:3570:LEU:HD23	1:D:3570:LEU:C	2.44	0.42
1:B:216:THR:HG22	1:B:274:HIS:HA	2.01	0.42
1:B:619:GLN:OE1	1:B:1679:ASN:ND2	2.50	0.42
1:B:868:LEU:HA	1:B:871:ILE:HD12	2.00	0.42
1:B:1124:VAL:HG23	1:B:1133:TRP:HB2	2.01	0.42
1:B:1171:MET:HE2	1:B:1175:GLY:HA2	2.02	0.42
1:B:1793:ALA:O	1:B:1794:THR:OG1	2.20	0.42
1:B:2575:HIS:ND1	1:B:2576:ARG:HG2	2.35	0.42
1:B:2978:LEU:HA	1:B:2981:VAL:HG22	2.01	0.42
1:B:3351:ARG:HG2	1:B:3352:PRO:HD2	2.01	0.42
1:C:1973:ASN:HD22	1:C:1973:ASN:C	2.24	0.42
1:C:3037:LYS:O	1:C:3040:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3458:ASN:O	1:C:3462:GLN:OE1	2.37	0.42
1:C:3568:PRO:HA	1:C:3571:ARG:CZ	2.49	0.42
1:C:3600:VAL:HG12	1:C:3604:LEU:HD13	2.02	0.42
1:C:4980:GLU:OE2	1:C:5027:ARG:NH2	2.53	0.42
1:A:34:LEU:HD12	1:A:54:SER:HB2	2.01	0.42
1:A:232:LEU:HD11	1:A:246:VAL:CG1	2.48	0.42
1:A:2575:HIS:ND1	1:A:2576:ARG:HG2	2.35	0.42
1:A:3088:ILE:HG13	1:A:3089:VAL:N	2.35	0.42
3:M:52:ALA:HA	3:M:55:VAL:HG12	2.01	0.42
3:O:45:PHE:HE2	3:P:6:GLU:HG2	1.85	0.42
1:D:576:LEU:HA	1:D:579:ILE:HG12	2.01	0.42
1:D:1172:SER:OG	1:D:1176:SER:N	2.47	0.42
1:D:1821:VAL:HG13	1:D:1930:MET:HE1	2.02	0.42
1:D:2314:LEU:HD12	1:D:2319:TYR:CD1	2.55	0.42
1:D:2586:THR:O	1:D:2590:LEU:HD13	2.20	0.42
1:D:3104:ILE:O	1:D:3108:VAL:HG23	2.20	0.42
1:D:3458:ASN:O	1:D:3462:GLN:OE1	2.37	0.42
1:B:638:LEU:HB3	1:B:1636:MET:HE2	2.00	0.42
1:B:868:LEU:HD21	1:B:940:VAL:HG21	2.01	0.42
1:B:2578:ILE:H	1:B:2578:ILE:HD12	1.84	0.42
1:B:2878:GLN:O	1:B:2881:GLU:HB3	2.20	0.42
1:B:3104:ILE:O	1:B:3108:VAL:HG23	2.20	0.42
1:B:3181:ASN:O	1:B:3184:VAL:N	2.53	0.42
1:C:302:VAL:HG23	1:C:302:VAL:O	2.19	0.42
1:C:1124:VAL:HG23	1:C:1133:TRP:HB2	2.01	0.42
1:C:3859:LEU:HB3	1:C:3871:ARG:NH2	2.34	0.42
1:C:4074:ILE:O	1:C:4077:SER:OG	2.25	0.42
1:C:4686:ILE:HD12	1:C:4735:ILE:CD1	2.50	0.42
1:A:1124:VAL:HG23	1:A:1133:TRP:HB2	2.01	0.42
1:A:2254:HIS:O	1:A:2255:LEU:C	2.63	0.42
1:A:3181:ASN:O	1:A:3184:VAL:N	2.53	0.42
1:A:3182:PRO:HA	1:A:3185:GLU:OE1	2.20	0.42
1:A:3461:VAL:HG23	1:A:3462:GLN:OE1	2.19	0.42
1:A:4867:GLU:N	1:A:4867:GLU:OE2	2.53	0.42
1:A:4980:GLU:OE2	1:A:5027:ARG:NH2	2.53	0.42
3:J:73:LYS:O	3:J:76:VAL:HG22	2.20	0.42
3:I:52:ALA:HA	3:I:55:VAL:HG12	2.01	0.42
3:L:71:ASP:HB2	3:L:74:GLU:OE1	2.20	0.42
3:P:73:LYS:O	3:P:76:VAL:HG22	2.19	0.42
1:D:34:LEU:HD12	1:D:54:SER:HB2	2.01	0.42
1:D:2868:LEU:HD23	1:D:2873:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2978:LEU:HA	1:D:2981:VAL:HG22	2.01	0.42
1:D:3088:ILE:HG13	1:D:3089:VAL:N	2.35	0.42
1:D:3600:VAL:HG12	1:D:3604:LEU:HD13	2.02	0.42
1:D:3643:TYR:CD1	1:D:3644:ASN:OD1	2.73	0.42
1:B:869:GLU:O	1:B:872:ARG:HG2	2.19	0.42
1:B:1023:VAL:HG13	1:B:1024:PRO:HD2	2.02	0.42
1:B:1744:ARG:NE	1:B:1964:GLU:OE2	2.50	0.42
1:B:1973:ASN:C	1:B:1973:ASN:HD22	2.24	0.42
1:B:3088:ILE:HG13	1:B:3089:VAL:N	2.35	0.42
1:B:3354:LEU:HD12	1:B:3358:HIS:ND1	2.35	0.42
1:B:4895:ILE:O	1:B:4899:ILE:HG12	2.19	0.42
1:B:5011:MET:HE1	1:B:5018:ASP:HB2	2.01	0.42
1:C:2878:GLN:O	1:C:2881:GLU:HB3	2.20	0.42
1:C:3088:ILE:HG13	1:C:3089:VAL:N	2.35	0.42
1:C:4016:LEU:HD23	1:C:4135:PHE:CE1	2.54	0.42
1:A:2878:GLN:O	1:A:2881:GLU:HB3	2.20	0.42
3:M:13:ILE:O	3:M:17:HIS:ND1	2.33	0.42
1:D:1171:MET:HE2	1:D:1175:GLY:HA2	2.02	0.42
1:D:2575:HIS:ND1	1:D:2576:ARG:HG2	2.35	0.42
1:D:3076:LEU:O	1:D:3147:HIS:NE2	2.48	0.42
1:D:3547:ASP:OD2	1:D:3547:ASP:C	2.62	0.42
1:B:1821:VAL:HG13	1:B:1930:MET:HE1	2.02	0.42
1:B:2254:HIS:O	1:B:2255:LEU:C	2.63	0.42
1:A:185:THR:HG22	1:A:190:LEU:HD22	2.02	0.42
1:A:868:LEU:HA	1:A:871:ILE:HD12	2.00	0.42
1:A:1127:GLY:HA3	1:A:1144:TRP:CZ3	2.54	0.42
1:A:1273:LEU:HD22	1:A:1290:LEU:HD11	2.02	0.42
1:A:1821:VAL:HG13	1:A:1930:MET:HE1	2.02	0.42
1:A:2314:LEU:HD12	1:A:2319:TYR:CD1	2.55	0.42
1:A:3173:ILE:CG2	1:A:3195:LEU:HD13	2.50	0.42
1:A:3458:ASN:O	1:A:3462:GLN:OE1	2.37	0.42
1:A:3643:TYR:CD1	1:A:3644:ASN:OD1	2.73	0.42
1:A:3765:ARG:NH2	1:A:4753:GLU:HB2	2.34	0.42
1:A:4686:ILE:HD12	1:A:4735:ILE:CD1	2.50	0.42
3:K:52:ALA:HA	3:K:55:VAL:HG12	2.01	0.42
3:O:23:GLU:OE2	3:O:29:LEU:HA	2.20	0.42
3:L:73:LYS:O	3:L:76:VAL:HG22	2.19	0.42
3:P:38:LEU:HD12	3:P:39:GLN:N	2.35	0.42
1:D:185:THR:HG22	1:D:190:LEU:HD22	2.02	0.42
1:D:1273:LEU:HD22	1:D:1290:LEU:HD11	2.01	0.42
1:D:2769:PHE:O	1:D:2773:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3907:ARG:HG2	1:D:3908:THR:HG23	2.02	0.42
1:D:4055:SER:HG	1:D:4166:PHE:HE1	1.64	0.42
1:B:1014:ILE:HB	1:B:1015:PRO:HD3	2.02	0.42
1:B:3765:ARG:NH2	1:B:4753:GLU:HB2	2.34	0.42
1:B:4632:GLU:OE1	1:B:4634:THR:OG1	2.27	0.42
1:C:245:LEU:HD22	1:C:376:LYS:HE2	2.02	0.42
1:C:2314:LEU:HD12	1:C:2319:TYR:CD1	2.55	0.42
1:C:2586:THR:O	1:C:2590:LEU:HD13	2.19	0.42
1:C:3570:LEU:HD23	1:C:3570:LEU:C	2.44	0.42
1:C:3643:TYR:CD1	1:C:3644:ASN:OD1	2.73	0.42
1:A:868:LEU:HD21	1:A:940:VAL:HG21	2.01	0.42
1:A:942:MET:HE1	1:A:1052:TYR:CE1	2.55	0.42
3:I:23:GLU:OE2	3:I:29:LEU:HA	2.20	0.42
3:M:45:PHE:CE2	3:N:6:GLU:HG2	2.55	0.42
3:N:71:ASP:HB2	3:N:74:GLU:OE1	2.20	0.42
1:D:638:LEU:HB3	1:D:1636:MET:HE2	2.00	0.42
1:D:671:GLU:HG2	1:D:789:LYS:HB3	2.01	0.42
1:D:2413:GLU:CG	1:D:2416:ARG:NH2	2.83	0.42
1:D:3351:ARG:HG2	1:D:3352:PRO:HD2	2.01	0.42
1:D:3515:LEU:HD23	1:D:3515:LEU:C	2.44	0.42
1:D:4538:PHE:N	1:D:4541:GLU:OE1	2.53	0.42
1:B:308:ALA:HB1	1:B:313:THR:HG21	2.01	0.42
1:B:2241:CYS:SG	1:B:2251:MET:HG3	2.60	0.42
1:B:2356:ARG:O	1:B:2359:ILE:HG12	2.19	0.42
1:B:4980:GLU:OE2	1:B:5027:ARG:NH2	2.53	0.42
1:C:308:ALA:HB1	1:C:313:THR:HG21	2.01	0.42
1:C:1023:VAL:HG13	1:C:1024:PRO:HD2	2.02	0.42
1:C:2241:CYS:SG	1:C:2251:MET:HG3	2.60	0.42
1:C:3457:GLN:O	1:C:3460:VAL:HG12	2.20	0.42
1:C:4538:PHE:N	1:C:4541:GLU:OE1	2.53	0.42
1:A:3515:LEU:HD23	1:A:3515:LEU:C	2.44	0.41
1:A:3907:ARG:HG2	1:A:3908:THR:HG23	2.02	0.41
3:O:56:ASP:HA	1:D:3638:ARG:NH2	2.33	0.41
3:P:71:ASP:HB2	3:P:74:GLU:OE1	2.20	0.41
1:D:302:VAL:O	1:D:302:VAL:HG23	2.19	0.41
1:D:1793:ALA:C	1:D:1794:THR:HG23	2.45	0.41
1:D:3859:LEU:HB3	1:D:3871:ARG:NH2	2.34	0.41
1:B:3173:ILE:CG2	1:B:3195:LEU:HD13	2.50	0.41
1:C:34:LEU:HD12	1:C:54:SER:HB2	2.01	0.41
1:C:1273:LEU:HD22	1:C:1290:LEU:HD11	2.02	0.41
1:C:2575:HIS:ND1	1:C:2576:ARG:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2701:MET:HB3	1:C:2702:PRO:HD3	2.03	0.41
1:C:3765:ARG:NH2	1:C:4753:GLU:HB2	2.34	0.41
1:C:3907:ARG:HG2	1:C:3908:THR:HG23	2.02	0.41
1:C:4895:ILE:O	1:C:4899:ILE:HG12	2.20	0.41
1:C:5011:MET:HE1	1:C:5018:ASP:HB2	2.01	0.41
1:A:216:THR:HG22	1:A:274:HIS:HA	2.01	0.41
1:A:869:GLU:O	1:A:872:ARG:HG2	2.19	0.41
1:A:2413:GLU:O	1:A:2414:GLU:C	2.63	0.41
1:A:3351:ARG:HG2	1:A:3352:PRO:HD2	2.02	0.41
1:A:3855:LYS:O	1:A:3859:LEU:HD13	2.20	0.41
3:M:23:GLU:OE2	3:M:29:LEU:HA	2.20	0.41
3:N:38:LEU:HD12	3:N:39:GLN:N	2.35	0.41
1:D:3590:PRO:O	1:D:3594:VAL:HG23	2.21	0.41
1:D:3919:ILE:HG22	1:D:3983:LEU:HD21	2.02	0.41
1:D:4686:ILE:HD12	1:D:4735:ILE:CD1	2.50	0.41
1:B:910:ASN:O	1:B:914:LEU:N	2.52	0.41
1:B:1127:GLY:HA3	1:B:1144:TRP:CZ3	2.54	0.41
1:B:2755:PHE:CZ	1:B:2931:LEU:HG	2.55	0.41
1:B:4675:LEU:HD23	1:B:4709:PHE:CE1	2.55	0.41
1:C:1793:ALA:C	1:C:1794:THR:HG23	2.45	0.41
1:C:1821:VAL:HG13	1:C:1930:MET:HE1	2.02	0.41
1:C:4673:LYS:O	1:C:4677:ARG:HD3	2.20	0.41
1:A:2241:CYS:SG	1:A:2251:MET:HG3	2.60	0.41
1:A:2978:LEU:HA	1:A:2981:VAL:HG22	2.01	0.41
1:A:3108:VAL:HA	1:A:3176:LEU:HD12	2.02	0.41
3:J:10:GLU:O	3:J:14:ASN:OD1	2.38	0.41
3:I:72:PHE:O	3:I:76:VAL:HG22	2.20	0.41
2:G:24:VAL:HG22	2:G:48:LYS:HG2	2.02	0.41
1:D:245:LEU:HD22	1:D:376:LYS:HE2	2.02	0.41
1:D:910:ASN:O	1:D:914:LEU:N	2.52	0.41
1:D:3181:ASN:O	1:D:3184:VAL:N	2.53	0.41
1:D:3182:PRO:HA	1:D:3185:GLU:OE1	2.20	0.41
1:D:3354:LEU:HD12	1:D:3358:HIS:ND1	2.35	0.41
1:D:4016:LEU:HD23	1:D:4135:PHE:CE1	2.54	0.41
1:B:671:GLU:HG2	1:B:789:LYS:HB3	2.02	0.41
1:B:1974:GLN:OE1	1:B:1977:ARG:NH1	2.54	0.41
1:B:3458:ASN:O	1:B:3462:GLN:OE1	2.37	0.41
1:C:23:LEU:HD23	1:C:203:MET:HG2	2.02	0.41
1:C:1171:MET:HE2	1:C:1175:GLY:HA2	2.02	0.41
1:C:3410:TYR:HB2	1:C:3510:LEU:HD21	2.03	0.41
1:C:3919:ILE:HG22	1:C:3983:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:THR:HG23	1:A:981:ALA:HB3	2.02	0.41
1:A:2701:MET:HB3	1:A:2702:PRO:HD3	2.03	0.41
1:A:3354:LEU:HD12	1:A:3358:HIS:ND1	2.35	0.41
3:M:51:ASP:OD2	3:M:88:ASN:HB3	2.21	0.41
3:M:72:PHE:CE2	3:M:76:VAL:HG11	2.55	0.41
3:O:72:PHE:CE2	3:O:76:VAL:HG11	2.55	0.41
1:D:2968:MET:HG3	1:D:3043:LEU:HD12	2.02	0.41
1:D:3367:ARG:NH1	1:D:3441:GLU:OE2	2.53	0.41
1:B:400:GLN:O	1:B:404:MET:HG3	2.21	0.41
1:B:694:SER:O	1:B:694:SER:OG	2.31	0.41
1:B:1273:LEU:HD22	1:B:1290:LEU:HD11	2.01	0.41
1:B:2586:THR:O	1:B:2590:LEU:HD13	2.20	0.41
1:C:1974:GLN:OE1	1:C:1977:ARG:NH1	2.54	0.41
1:C:3181:ASN:O	1:C:3184:VAL:N	2.53	0.41
1:C:4675:LEU:HD23	1:C:4709:PHE:CE1	2.56	0.41
1:C:4867:GLU:N	1:C:4867:GLU:OE2	2.53	0.41
1:A:245:LEU:HD22	1:A:376:LYS:HE2	2.02	0.41
1:A:1974:GLN:OE1	1:A:1977:ARG:NH1	2.54	0.41
1:A:2635:ASN:OD1	1:A:2635:ASN:C	2.62	0.41
1:A:3568:PRO:HA	1:A:3571:ARG:CZ	2.50	0.41
1:A:4675:LEU:HD23	1:A:4709:PHE:CE1	2.55	0.41
3:J:38:LEU:HD12	3:J:39:GLN:N	2.35	0.41
3:J:71:ASP:HB2	3:J:74:GLU:OE1	2.20	0.41
1:D:3440:GLY:O	1:D:3444:ILE:HG13	2.21	0.41
1:D:4673:LYS:O	1:D:4677:ARG:HD3	2.21	0.41
1:B:1728:ARG:O	1:B:1732:LEU:HG	2.21	0.41
1:B:2570:PHE:O	1:B:2573:THR:HG23	2.21	0.41
1:B:2968:MET:HG3	1:B:3043:LEU:HD12	2.02	0.41
1:B:3182:PRO:HA	1:B:3185:GLU:OE1	2.20	0.41
1:B:3367:ARG:NH1	1:B:3441:GLU:OE2	2.53	0.41
1:B:3907:ARG:HG2	1:B:3908:THR:HG23	2.02	0.41
1:B:4538:PHE:N	1:B:4541:GLU:OE1	2.53	0.41
1:C:1014:ILE:HB	1:C:1015:PRO:HD3	2.02	0.41
1:C:3182:PRO:HA	1:C:3185:GLU:OE1	2.20	0.41
1:A:2755:PHE:CZ	1:A:2931:LEU:HG	2.55	0.41
1:A:2968:MET:HG3	1:A:3043:LEU:HD12	2.02	0.41
3:J:4:GLU:O	3:J:7:SER:OG	2.30	0.41
3:K:51:ASP:OD2	3:K:88:ASN:HB3	2.21	0.41
3:L:10:GLU:O	3:L:14:ASN:OD1	2.38	0.41
1:D:1728:ARG:O	1:D:1732:LEU:HG	2.21	0.41
1:D:1974:GLN:OE1	1:D:1977:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2254:HIS:O	1:D:2255:LEU:C	2.63	0.41
1:D:2281:VAL:O	1:D:2281:VAL:HG22	2.21	0.41
1:D:3410:TYR:HB2	1:D:3510:LEU:HD21	2.03	0.41
1:D:3457:GLN:O	1:D:3460:VAL:HG12	2.20	0.41
1:D:3855:LYS:O	1:D:3859:LEU:HD13	2.20	0.41
1:D:4675:LEU:HD23	1:D:4709:PHE:CE1	2.55	0.41
1:B:3108:VAL:HA	1:B:3176:LEU:HD12	2.02	0.41
1:C:185:THR:HG22	1:C:190:LEU:HD22	2.02	0.41
1:C:2868:LEU:HD23	1:C:2873:GLN:HG2	2.02	0.41
1:C:3590:PRO:O	1:C:3594:VAL:HG23	2.21	0.41
1:C:4703:VAL:O	1:C:4703:VAL:HG22	2.21	0.41
1:A:308:ALA:HB1	1:A:313:THR:HG21	2.01	0.41
1:A:421:SER:O	1:A:425:LYS:NZ	2.44	0.41
1:A:1014:ILE:HB	1:A:1015:PRO:HD3	2.02	0.41
1:A:1793:ALA:C	1:A:1794:THR:HG23	2.45	0.41
1:A:2189:ASN:OD1	1:A:2190:LYS:N	2.54	0.41
1:A:3590:PRO:O	1:A:3594:VAL:HG23	2.21	0.41
1:D:400:GLN:O	1:D:404:MET:HG3	2.21	0.41
1:B:34:LEU:HD12	1:B:54:SER:HB2	2.01	0.41
1:B:1287:MET:HE1	1:B:1554:PHE:HB3	2.03	0.41
1:B:2701:MET:HB3	1:B:2702:PRO:HD3	2.03	0.41
1:B:3919:ILE:HG22	1:B:3983:LEU:HD21	2.02	0.41
1:C:485:LEU:HD11	1:C:527:LEU:HD12	2.03	0.41
1:C:942:MET:HE1	1:C:1052:TYR:CE1	2.55	0.41
1:C:2413:GLU:O	1:C:2414:GLU:C	2.63	0.41
1:C:3173:ILE:CG2	1:C:3195:LEU:HD13	2.50	0.41
1:A:868:LEU:HB3	1:A:930:LEU:HD23	2.03	0.41
1:A:2239:TYR:O	1:A:2243:ILE:HG13	2.21	0.41
1:A:4186:ILE:CD1	1:A:4196:ILE:HD11	2.51	0.41
1:D:2466:ASP:O	1:D:2470:ILE:HG13	2.21	0.41
1:D:3108:VAL:HA	1:D:3176:LEU:HD12	2.02	0.41
1:B:23:LEU:HD23	1:B:203:MET:HG2	2.02	0.41
1:B:1208:ASP:OD2	1:B:1210:SER:OG	2.34	0.41
1:B:2189:ASN:OD1	1:B:2190:LYS:N	2.54	0.41
1:B:2314:LEU:HD12	1:B:2319:TYR:CD1	2.55	0.41
1:B:2625:ARG:HH12	1:B:2907:VAL:HG21	1.84	0.41
1:B:2868:LEU:HD23	1:B:2873:GLN:HG2	2.02	0.41
1:B:3600:VAL:HG12	1:B:3604:LEU:HD13	2.02	0.41
1:B:3643:TYR:CD1	1:B:3644:ASN:OD1	2.73	0.41
1:C:1491:SER:OG	1:C:1492:ASN:N	2.52	0.41
1:C:3440:GLY:O	1:C:3444:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:VAL:HG13	1:A:1024:PRO:HD2	2.02	0.41
1:A:1102:ARG:HG2	1:A:1126:ASN:HB2	2.03	0.41
1:A:1287:MET:HE1	1:A:1554:PHE:HB3	2.03	0.41
1:A:2413:GLU:HG3	1:A:2416:ARG:NH2	2.36	0.41
1:A:2466:ASP:O	1:A:2470:ILE:HG13	2.21	0.41
1:A:2570:PHE:O	1:A:2573:THR:HG23	2.21	0.41
1:A:2586:THR:O	1:A:2590:LEU:HD13	2.20	0.41
1:A:2868:LEU:HD23	1:A:2873:GLN:HG2	2.02	0.41
1:A:3457:GLN:O	1:A:3460:VAL:HG12	2.20	0.41
1:A:3758:GLU:OE1	1:A:3761:MET:CE	2.69	0.41
1:A:3919:ILE:HG22	1:A:3983:LEU:HD21	2.02	0.41
1:A:4673:LYS:O	1:A:4677:ARG:HD3	2.20	0.41
3:I:13:ILE:O	3:I:17:HIS:ND1	2.33	0.41
3:K:72:PHE:CE2	3:K:76:VAL:HG11	2.55	0.41
3:M:25:ASP:HB3	3:N:94:SER:CB	2.51	0.41
3:O:13:ILE:HG23	3:O:17:HIS:CE1	2.56	0.41
3:O:51:ASP:OD2	3:O:88:ASN:HB3	2.21	0.41
3:O:72:PHE:O	3:O:76:VAL:HG22	2.20	0.41
1:D:1795:GLU:N	1:D:1795:GLU:OE2	2.54	0.41
1:D:2701:MET:HB3	1:D:2702:PRO:HD3	2.03	0.41
1:D:3758:GLU:OE1	1:D:3761:MET:CE	2.69	0.41
1:D:4638:GLU:HB3	1:D:4639:PRO:HD3	2.03	0.41
1:D:4703:VAL:O	1:D:4703:VAL:HG22	2.21	0.41
1:D:4867:GLU:N	1:D:4867:GLU:OE2	2.53	0.41
1:B:979:THR:HG23	1:B:981:ALA:HB3	2.02	0.41
1:B:980:PRO:C	1:B:983:THR:HG1	2.21	0.41
1:B:1102:ARG:HG2	1:B:1126:ASN:HB2	2.03	0.41
1:B:1793:ALA:C	1:B:1794:THR:HG23	2.45	0.41
1:B:2754:SER:O	1:B:2757:ASN:OD1	2.39	0.41
1:B:3440:GLY:O	1:B:3444:ILE:HG13	2.21	0.41
1:B:3758:GLU:OE1	1:B:3761:MET:CE	2.69	0.41
1:B:3855:LYS:O	1:B:3859:LEU:HD13	2.20	0.41
1:B:4638:GLU:HB3	1:B:4639:PRO:HD3	2.03	0.41
1:B:4867:GLU:OE2	1:B:4867:GLU:N	2.53	0.41
1:C:400:GLN:O	1:C:404:MET:HG3	2.21	0.41
1:C:868:LEU:HB3	1:C:930:LEU:HD23	2.03	0.41
1:C:2189:ASN:OD1	1:C:2190:LYS:N	2.54	0.41
1:C:2254:HIS:O	1:C:2255:LEU:C	2.63	0.41
1:C:2754:SER:O	1:C:2757:ASN:OD1	2.39	0.41
1:C:3108:VAL:HA	1:C:3176:LEU:HD12	2.02	0.41
1:C:3354:LEU:HD12	1:C:3358:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3855:LYS:O	1:C:3859:LEU:HD13	2.20	0.41
1:C:3972:ILE:CG2	1:C:3983:LEU:HD12	2.51	0.41
1:A:671:GLU:HG2	1:A:789:LYS:HB3	2.02	0.41
1:A:868:LEU:HD22	1:A:871:ILE:HD12	2.03	0.41
1:A:4538:PHE:N	1:A:4541:GLU:OE1	2.53	0.41
1:A:4670:LYS:O	1:A:4673:LYS:HG2	2.21	0.41
3:L:38:LEU:HD12	3:L:39:GLN:N	2.35	0.41
1:D:485:LEU:HD11	1:D:527:LEU:HD12	2.03	0.41
1:D:942:MET:HE1	1:D:1052:TYR:CE1	2.55	0.41
1:D:2189:ASN:OD1	1:D:2190:LYS:N	2.54	0.41
1:D:2413:GLU:O	1:D:2414:GLU:C	2.63	0.41
1:D:2570:PHE:O	1:D:2573:THR:HG23	2.21	0.41
1:D:2695:GLU:OE1	1:D:2695:GLU:HA	2.21	0.41
1:D:4632:GLU:OE1	1:D:4634:THR:OG1	2.27	0.41
1:B:868:LEU:HD22	1:B:871:ILE:HD12	2.03	0.41
1:B:2413:GLU:O	1:B:2414:GLU:C	2.63	0.41
1:B:3457:GLN:O	1:B:3460:VAL:HG12	2.20	0.41
1:B:3590:PRO:O	1:B:3594:VAL:HG23	2.21	0.41
1:B:4186:ILE:CD1	1:B:4196:ILE:HD11	2.51	0.41
1:C:575:VAL:O	1:C:579:ILE:HG12	2.21	0.41
1:C:671:GLU:HG2	1:C:789:LYS:HB3	2.02	0.41
1:A:400:GLN:O	1:A:404:MET:HG3	2.21	0.40
1:A:575:VAL:O	1:A:579:ILE:HG12	2.21	0.40
1:A:3367:ARG:NH1	1:A:3441:GLU:OE2	2.53	0.40
1:A:3440:GLY:O	1:A:3444:ILE:HG13	2.21	0.40
1:A:4653:PHE:HB2	1:A:4794:MET:HE1	2.04	0.40
3:I:37:LEU:HD23	3:I:75:TYR:CE1	2.56	0.40
2:F:58:ARG:O	2:F:62:GLU:HG3	2.21	0.40
3:K:13:ILE:HG23	3:K:17:HIS:CE1	2.56	0.40
3:M:13:ILE:HG23	3:M:17:HIS:CE1	2.56	0.40
3:O:5:LEU:HD12	3:P:15:VAL:CB	2.52	0.40
3:O:62:LEU:HD12	3:O:63:ASP:N	2.36	0.40
1:D:2124:LEU:O	1:D:2128:GLN:HG2	2.22	0.40
1:D:2241:CYS:SG	1:D:2251:MET:HG3	2.60	0.40
1:B:245:LEU:HD22	1:B:376:LYS:HE2	2.02	0.40
1:B:1795:GLU:N	1:B:1795:GLU:OE2	2.54	0.40
1:B:3362:THR:O	1:B:3366:LEU:HD13	2.21	0.40
1:B:3593:ILE:HD12	1:B:3593:ILE:H	1.86	0.40
1:B:4703:VAL:HG22	1:B:4703:VAL:O	2.21	0.40
1:C:2695:GLU:OE1	1:C:2695:GLU:HA	2.21	0.40
1:C:3286:TRP:HA	1:C:3308:VAL:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3758:GLU:OE1	1:C:3761:MET:CE	2.69	0.40
1:C:3989:TRP:HE3	1:C:4050:MET:SD	2.44	0.40
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	2.03	0.40
1:A:3362:THR:O	1:A:3366:LEU:HD13	2.21	0.40
1:A:3593:ILE:HD12	1:A:3593:ILE:H	1.86	0.40
3:I:51:ASP:OD2	3:I:88:ASN:HB3	2.21	0.40
3:I:72:PHE:CE2	3:I:76:VAL:HG11	2.55	0.40
2:G:58:ARG:O	2:G:62:GLU:HG3	2.21	0.40
3:M:17:HIS:CE1	3:N:87:ASN:HD21	2.39	0.40
3:O:12:LEU:HD11	3:P:9:MET:CE	2.51	0.40
3:O:56:ASP:CG	1:D:3638:ARG:NH2	2.62	0.40
1:D:919:ARG:O	1:D:923:LEU:HG	2.22	0.40
1:D:3362:THR:O	1:D:3366:LEU:HD13	2.21	0.40
1:D:4186:ILE:CD1	1:D:4196:ILE:HD11	2.51	0.40
1:B:185:THR:HG22	1:B:190:LEU:HD22	2.02	0.40
1:B:942:MET:HE1	1:B:1052:TYR:CE1	2.55	0.40
1:B:3037:LYS:O	1:B:3040:ILE:HG22	2.20	0.40
1:B:3410:TYR:HB2	1:B:3510:LEU:HD21	2.03	0.40
1:B:3989:TRP:HE3	1:B:4050:MET:SD	2.44	0.40
1:B:4670:LYS:O	1:B:4673:LYS:HG2	2.21	0.40
1:B:4673:LYS:O	1:B:4677:ARG:HD3	2.20	0.40
1:A:2940:ARG:HB2	1:A:2944:ASP:CG	2.47	0.40
1:A:3406:LEU:HD22	1:A:3410:TYR:CZ	2.56	0.40
1:A:3600:VAL:HG12	1:A:3604:LEU:HD13	2.02	0.40
1:A:4876:ASP:OD2	1:A:4879:THR:OG1	2.28	0.40
3:I:31:LYS:HA	3:I:34:LEU:HB3	2.03	0.40
3:I:62:LEU:HD12	3:I:63:ASP:N	2.36	0.40
3:K:37:LEU:HD23	3:K:75:TYR:CE1	2.56	0.40
3:M:31:LYS:HA	3:M:34:LEU:HB3	2.03	0.40
1:D:23:LEU:HD23	1:D:203:MET:HG2	2.02	0.40
1:D:2500:LYS:NZ	1:D:2530:ASP:OD2	2.36	0.40
1:D:2940:ARG:HB2	1:D:2944:ASP:CG	2.47	0.40
1:D:3004:LEU:HB2	1:D:3005:PRO:HD3	2.03	0.40
1:B:4016:LEU:HD23	1:B:4135:PHE:CE1	2.54	0.40
1:C:979:THR:HG23	1:C:981:ALA:HB3	2.02	0.40
1:C:2010:LEU:O	1:C:2024:LEU:HD12	2.22	0.40
1:C:3362:THR:O	1:C:3366:LEU:HD13	2.21	0.40
1:C:4686:ILE:HG21	1:C:4726:HIS:HB3	2.03	0.40
1:A:3989:TRP:HE3	1:A:4050:MET:SD	2.44	0.40
3:K:12:LEU:HD11	3:L:9:MET:CE	2.51	0.40
3:K:31:LYS:HA	3:K:34:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:37:LEU:HD23	3:M:75:TYR:CE1	2.56	0.40
1:D:2239:TYR:O	1:D:2243:ILE:HG13	2.21	0.40
1:D:2413:GLU:HG3	1:D:2416:ARG:NH2	2.36	0.40
1:D:2755:PHE:CZ	1:D:2931:LEU:HG	2.55	0.40
1:D:3534:ILE:HD12	1:D:3534:ILE:H	1.87	0.40
1:D:4696:LYS:HA	1:D:4696:LYS:HE2	2.04	0.40
1:B:633:LEU:HD13	1:B:1667:THR:HG23	2.04	0.40
1:B:868:LEU:HB3	1:B:930:LEU:HD23	2.03	0.40
1:B:1425:PRO:O	1:B:1429:LEU:HD23	2.22	0.40
1:B:2413:GLU:HG3	1:B:2416:ARG:NH2	2.36	0.40
1:B:3286:TRP:HA	1:B:3308:VAL:HG13	2.04	0.40
1:C:473:ARG:NH2	1:C:476:GLN:OE1	2.44	0.40
1:C:1102:ARG:HG2	1:C:1126:ASN:HB2	2.03	0.40
1:C:2466:ASP:O	1:C:2470:ILE:HG13	2.21	0.40
1:C:2755:PHE:CZ	1:C:2931:LEU:HG	2.55	0.40
1:C:3367:ARG:NH1	1:C:3441:GLU:OE2	2.53	0.40
1:C:4186:ILE:CD1	1:C:4196:ILE:HD11	2.51	0.40
1:C:4638:GLU:HB3	1:C:4639:PRO:HD3	2.03	0.40
1:A:23:LEU:HD23	1:A:203:MET:HG2	2.02	0.40
1:A:902:LYS:HZ2	1:A:904:LEU:HD12	1.87	0.40
1:A:3410:TYR:HB2	1:A:3510:LEU:HD21	2.03	0.40
1:A:4638:GLU:HB3	1:A:4639:PRO:HD3	2.03	0.40
1:A:4703:VAL:HG22	1:A:4703:VAL:O	2.21	0.40
2:H:58:ARG:O	2:H:62:GLU:HG3	2.21	0.40
3:K:62:LEU:HD12	3:K:63:ASP:N	2.36	0.40
3:P:12:LEU:O	3:P:15:VAL:HG22	2.22	0.40
1:D:868:LEU:HB3	1:D:930:LEU:HD23	2.03	0.40
1:D:979:THR:HG23	1:D:981:ALA:HB3	2.02	0.40
1:D:1014:ILE:HB	1:D:1015:PRO:HD3	2.02	0.40
1:D:2010:LEU:O	1:D:2024:LEU:HD12	2.21	0.40
1:B:864:LEU:HD21	1:B:872:ARG:HD2	2.04	0.40
1:B:2210:GLU:HA	1:B:2213:VAL:HG22	2.04	0.40
1:B:2387:ILE:HD13	1:B:2393:ARG:NE	2.37	0.40
1:B:2905:LEU:HD12	1:B:2912:LEU:HD11	2.04	0.40
1:C:1728:ARG:O	1:C:1732:LEU:HG	2.21	0.40
1:C:2239:TYR:O	1:C:2243:ILE:HG13	2.21	0.40
1:C:2640:MET:HB3	1:C:2641:PRO:HD3	2.04	0.40
1:C:2905:LEU:HD12	1:C:2912:LEU:HD11	2.04	0.40
1:C:2953:GLU:OE1	1:C:2953:GLU:N	2.49	0.40
1:C:3344:GLN:HE22	1:C:3470:PHE:HD1	1.70	0.40
1:C:3446:TRP:HA	1:C:3452:PHE:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4653:PHE:HB2	1:C:4794:MET:HE1	2.04	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	A	4347/5035 (86%)	4258 (98%)	88 (2%)	1 (0%)	100	100
1	B	4347/5035 (86%)	4257 (98%)	89 (2%)	1 (0%)	100	100
1	C	4347/5035 (86%)	4257 (98%)	89 (2%)	1 (0%)	100	100
1	D	4347/5035 (86%)	4257 (98%)	89 (2%)	1 (0%)	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
3	I	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
3	J	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
3	K	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
3	L	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
3	M	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
3	N	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
3	O	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
3	P	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
All	All	18540/21324 (87%)	18125 (98%)	411 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2948	ASP
1	D	2948	ASP
1	B	2948	ASP
1	C	2948	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3808/4296 (89%)	3806 (100%)	2 (0%)	88	89
1	B	3808/4296 (89%)	3806 (100%)	2 (0%)	88	89
1	C	3808/4296 (89%)	3806 (100%)	2 (0%)	88	89
1	D	3808/4296 (89%)	3806 (100%)	2 (0%)	88	89
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
3	I	81/81 (100%)	81 (100%)	0	100	100
3	J	80/81 (99%)	80 (100%)	0	100	100
3	K	81/81 (100%)	81 (100%)	0	100	100
3	L	80/81 (99%)	80 (100%)	0	100	100
3	M	81/81 (100%)	81 (100%)	0	100	100
3	N	80/81 (99%)	80 (100%)	0	100	100
3	O	81/81 (100%)	81 (100%)	0	100	100
3	P	80/81 (99%)	80 (100%)	0	100	100
All	All	16232/18192 (89%)	16224 (100%)	8 (0%)	100	100

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4582	ASP

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Mol	Chain	Res	Type
1	A	4626	VAL
1	D	4582	ASP
1	D	4626	VAL
1	B	4582	ASP
1	B	4626	VAL
1	C	4582	ASP
1	C	4626	VAL

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

Mol	Chain	Res	Type
1	A	152	HIS
1	A	202	ASN
1	A	721	HIS
1	A	726	HIS
1	A	737	HIS
1	A	878	ASN
1	A	1059	GLN
1	A	1126	ASN
1	A	1207	GLN
1	A	1221	GLN
1	A	1483	ASN
1	A	1506	GLN
1	A	1559	HIS
1	A	1591	GLN
1	A	1950	GLN
1	A	2012	HIS
1	A	2128	GLN
1	A	2689	HIS
1	A	2694	GLN
1	A	2962	GLN
1	A	2963	GLN
1	A	3031	HIS
1	A	3429	ASN
1	A	3872	GLN
1	A	3898	HIS
1	A	3917	ASN
1	A	3973	GLN
1	A	3981	GLN
1	A	4001	HIS
1	A	4057	ASN
1	A	4207	GLN

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Mol	Chain	Res	Type
1	A	4219	GLN
3	J	14	ASN
3	J	49	GLN
3	I	19	HIS
3	I	39	GLN
3	I	65	ASN
3	I	88	ASN
2	F	95	HIS
3	K	19	HIS
3	K	39	GLN
3	K	65	ASN
3	K	88	ASN
3	M	19	HIS
3	M	39	GLN
3	M	65	ASN
3	M	88	ASN
3	O	19	HIS
3	O	39	GLN
3	O	88	ASN
3	L	49	GLN
3	N	14	ASN
3	N	49	GLN
3	P	49	GLN
1	D	152	HIS
1	D	721	HIS
1	D	726	HIS
1	D	878	ASN
1	D	1059	GLN
1	D	1126	ASN
1	D	1159	ASN
1	D	1207	GLN
1	D	1221	GLN
1	D	1483	ASN
1	D	1506	GLN
1	D	1559	HIS
1	D	1950	GLN
1	D	2012	HIS
1	D	2128	GLN
1	D	2689	HIS
1	D	2962	GLN
1	D	2963	GLN
1	D	3429	ASN

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Mol	Chain	Res	Type
1	D	3872	GLN
1	D	3898	HIS
1	D	3917	ASN
1	D	3973	GLN
1	D	4001	HIS
1	D	4057	ASN
1	D	4207	GLN
1	D	4219	GLN
1	D	5029	GLN
1	B	106	HIS
1	B	152	HIS
1	B	202	ASN
1	B	721	HIS
1	B	726	HIS
1	B	878	ASN
1	B	1059	GLN
1	B	1126	ASN
1	B	1207	GLN
1	B	1221	GLN
1	B	1483	ASN
1	B	1506	GLN
1	B	1559	HIS
1	B	1591	GLN
1	B	1950	GLN
1	B	1973	ASN
1	B	2012	HIS
1	B	2128	GLN
1	B	2622	HIS
1	B	2689	HIS
1	B	2962	GLN
1	B	2963	GLN
1	B	3009	GLN
1	B	3344	GLN
1	B	3429	ASN
1	B	3872	GLN
1	B	3898	HIS
1	B	3917	ASN
1	B	3973	GLN
1	B	4001	HIS
1	B	4057	ASN
1	B	4207	GLN
1	B	4219	GLN

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Mol	Chain	Res	Type
1	C	106	HIS
1	C	152	HIS
1	C	202	ASN
1	C	721	HIS
1	C	726	HIS
1	C	737	HIS
1	C	878	ASN
1	C	1059	GLN
1	C	1126	ASN
1	C	1207	GLN
1	C	1221	GLN
1	C	1483	ASN
1	C	1506	GLN
1	C	1559	HIS
1	C	1591	GLN
1	C	1950	GLN
1	C	1973	ASN
1	C	2012	HIS
1	C	2128	GLN
1	C	2622	HIS
1	C	2689	HIS
1	C	2962	GLN
1	C	2963	GLN
1	C	3429	ASN
1	C	3872	GLN
1	C	3898	HIS
1	C	3917	ASN
1	C	3973	GLN
1	C	3981	GLN
1	C	4001	HIS
1	C	4057	ASN
1	C	4207	GLN
1	C	4219	GLN
1	C	5029	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PCW	A	8003	-	53,53,53	1.20	6 (11%)	59,61,61	2.29	9 (15%)
5	PCW	A	8002	-	53,53,53	1.18	6 (11%)	59,61,61	2.35	9 (15%)
5	PCW	D	5101	-	53,53,53	1.20	5 (9%)	59,61,61	2.29	9 (15%)
5	PCW	C	5101	-	53,53,53	1.20	5 (9%)	59,61,61	2.29	9 (15%)
5	PCW	C	5103	-	53,53,53	1.18	6 (11%)	59,61,61	2.35	9 (15%)
5	PCW	B	8002	-	53,53,53	1.18	5 (9%)	59,61,61	2.35	9 (15%)
5	PCW	B	8003	-	53,53,53	1.20	5 (9%)	59,61,61	2.29	9 (15%)
5	PCW	D	5103	-	53,53,53	1.18	6 (11%)	59,61,61	2.35	9 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PCW	A	8003	-	-	21/57/57/57	-
5	PCW	A	8002	-	-	28/57/57/57	-
5	PCW	D	5101	-	-	21/57/57/57	-
5	PCW	C	5101	-	-	21/57/57/57	-
5	PCW	C	5103	-	-	28/57/57/57	-
5	PCW	B	8002	-	-	28/57/57/57	-
5	PCW	B	8003	-	-	21/57/57/57	-
5	PCW	D	5103	-	-	28/57/57/57	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5103	PCW	O3-C11	3.10	1.42	1.33
5	A	8002	PCW	O3-C11	3.08	1.42	1.33
5	B	8002	PCW	O3-C11	3.08	1.42	1.33
5	C	5103	PCW	O3-C11	3.08	1.42	1.33
5	D	5101	PCW	O3-C11	3.07	1.42	1.33
5	A	8003	PCW	O3-C11	3.07	1.42	1.33
5	C	5101	PCW	O3-C11	3.07	1.42	1.33
5	B	8003	PCW	O3-C11	3.07	1.42	1.33
5	D	5101	PCW	O2-C31	2.94	1.42	1.34
5	B	8003	PCW	O2-C31	2.94	1.42	1.34
5	C	5101	PCW	O2-C31	2.94	1.42	1.34
5	A	8003	PCW	O2-C31	2.92	1.42	1.34
5	A	8002	PCW	O2-C31	2.78	1.42	1.34
5	D	5103	PCW	O2-C31	2.78	1.42	1.34
5	A	8002	PCW	O2-C2	-2.78	1.40	1.46
5	D	5103	PCW	O2-C2	-2.78	1.40	1.46
5	B	8002	PCW	O2-C2	-2.78	1.40	1.46
5	C	5103	PCW	O2-C31	2.76	1.42	1.34
5	B	8002	PCW	O2-C31	2.75	1.42	1.34
5	C	5103	PCW	O2-C2	-2.75	1.40	1.46
5	A	8003	PCW	O2-C2	-2.64	1.40	1.46
5	D	5101	PCW	O2-C2	-2.64	1.40	1.46
5	B	8003	PCW	O2-C2	-2.62	1.40	1.46
5	C	5101	PCW	O2-C2	-2.62	1.40	1.46
5	C	5103	PCW	P-O4P	2.12	1.67	1.59
5	A	8002	PCW	P-O4P	2.11	1.67	1.59
5	B	8002	PCW	P-O4P	2.11	1.67	1.59
5	A	8003	PCW	P-O4P	2.09	1.67	1.59
5	D	5101	PCW	P-O4P	2.09	1.67	1.59
5	B	8003	PCW	P-O4P	2.09	1.67	1.59
5	D	5103	PCW	P-O4P	2.09	1.67	1.59
5	C	5101	PCW	P-O4P	2.07	1.67	1.59
5	A	8003	PCW	C5-C4	2.02	1.57	1.51
5	C	5103	PCW	P-O3P	2.01	1.67	1.59
5	A	8002	PCW	C5-C4	2.01	1.57	1.51
5	D	5103	PCW	C5-C4	2.01	1.57	1.51
5	C	5103	PCW	C5-C4	2.01	1.57	1.51
5	A	8002	PCW	P-O3P	2.00	1.67	1.59
5	D	5103	PCW	P-O3P	2.00	1.67	1.59
5	B	8003	PCW	P-O3P	2.00	1.67	1.59
5	C	5101	PCW	P-O3P	2.00	1.67	1.59
5	B	8002	PCW	C5-C4	2.00	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8003	PCW	P-O3P	2.00	1.67	1.59
5	D	5101	PCW	P-O3P	2.00	1.67	1.59

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5103	PCW	C8-N-C6	11.91	140.27	108.98
5	A	8002	PCW	C8-N-C6	11.89	140.21	108.98
5	B	8002	PCW	C8-N-C6	11.89	140.21	108.98
5	C	5103	PCW	C8-N-C6	11.88	140.19	108.98
5	B	8003	PCW	C8-N-C6	10.78	137.28	108.98
5	D	5101	PCW	C8-N-C6	10.77	137.28	108.98
5	C	5101	PCW	C8-N-C6	10.77	137.28	108.98
5	A	8003	PCW	C8-N-C6	10.77	137.25	108.98
5	A	8003	PCW	C7-N-C5	7.90	141.30	109.91
5	D	5101	PCW	C7-N-C5	7.89	141.29	109.91
5	C	5101	PCW	C7-N-C5	7.89	141.27	109.91
5	B	8003	PCW	C7-N-C5	7.89	141.27	109.91
5	A	8002	PCW	C7-N-C5	7.25	138.72	109.91
5	C	5103	PCW	C7-N-C5	7.25	138.72	109.91
5	B	8002	PCW	C7-N-C5	7.24	138.71	109.91
5	D	5103	PCW	C7-N-C5	7.24	138.69	109.91
5	D	5103	PCW	C8-N-C7	-5.32	95.01	108.98
5	A	8002	PCW	C8-N-C7	-5.31	95.02	108.98
5	C	5103	PCW	C8-N-C7	-5.31	95.02	108.98
5	B	8002	PCW	C8-N-C7	-5.29	95.08	108.98
5	C	5101	PCW	C8-N-C7	-4.98	95.89	108.98
5	D	5101	PCW	C8-N-C7	-4.98	95.90	108.98
5	A	8003	PCW	C8-N-C7	-4.97	95.93	108.98
5	B	8003	PCW	C8-N-C7	-4.96	95.93	108.98
5	B	8003	PCW	C7-N-C6	-4.83	96.30	108.98
5	C	5101	PCW	C7-N-C6	-4.82	96.33	108.98
5	D	5101	PCW	C7-N-C6	-4.81	96.33	108.98
5	A	8003	PCW	C7-N-C6	-4.80	96.37	108.98
5	B	8002	PCW	C7-N-C6	-4.69	96.66	108.98
5	A	8002	PCW	C7-N-C6	-4.69	96.66	108.98
5	D	5103	PCW	C7-N-C6	-4.69	96.66	108.98
5	C	5103	PCW	C7-N-C6	-4.68	96.69	108.98
5	B	8003	PCW	C21-C20-C19	4.15	155.93	124.83
5	A	8003	PCW	C21-C20-C19	4.15	155.91	124.83
5	D	5101	PCW	C21-C20-C19	4.14	155.88	124.83
5	C	5101	PCW	C21-C20-C19	4.14	155.86	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	8002	PCW	C21-C20-C19	3.98	154.65	124.83
5	D	5103	PCW	C21-C20-C19	3.98	154.65	124.83
5	B	8002	PCW	C21-C20-C19	3.98	154.65	124.83
5	C	5103	PCW	C21-C20-C19	3.97	154.59	124.83
5	B	8002	PCW	O2-C31-C32	3.72	119.54	111.48
5	C	5103	PCW	O2-C31-C32	3.72	119.53	111.48
5	A	8002	PCW	O2-C31-C32	3.72	119.52	111.48
5	D	5103	PCW	O2-C31-C32	3.70	119.48	111.48
5	A	8003	PCW	C8-N-C5	-3.56	95.75	109.91
5	D	5101	PCW	C8-N-C5	-3.55	95.81	109.91
5	C	5101	PCW	C8-N-C5	-3.54	95.82	109.91
5	B	8003	PCW	C8-N-C5	-3.54	95.83	109.91
5	B	8002	PCW	C8-N-C5	-3.36	96.57	109.91
5	D	5103	PCW	C8-N-C5	-3.35	96.59	109.91
5	A	8002	PCW	C8-N-C5	-3.35	96.61	109.91
5	C	5103	PCW	C8-N-C5	-3.35	96.61	109.91
5	A	8003	PCW	O2-C31-C32	3.31	118.64	111.48
5	D	5101	PCW	O2-C31-C32	3.30	118.62	111.48
5	B	8003	PCW	O2-C31-C32	3.29	118.59	111.48
5	C	5101	PCW	O2-C31-C32	3.29	118.59	111.48
5	C	5103	PCW	C6-N-C5	-2.70	99.18	109.91
5	B	8002	PCW	C6-N-C5	-2.70	99.19	109.91
5	A	8002	PCW	C6-N-C5	-2.70	99.19	109.91
5	D	5103	PCW	C6-N-C5	-2.69	99.20	109.91
5	C	5101	PCW	O3-C11-C12	2.59	119.73	111.83
5	B	8003	PCW	C6-N-C5	-2.59	99.63	109.91
5	A	8003	PCW	C6-N-C5	-2.58	99.64	109.91
5	D	5101	PCW	C6-N-C5	-2.58	99.64	109.91
5	A	8003	PCW	O3-C11-C12	2.58	119.71	111.83
5	C	5101	PCW	C6-N-C5	-2.58	99.65	109.91
5	D	5101	PCW	O3-C11-C12	2.57	119.66	111.83
5	B	8003	PCW	O3-C11-C12	2.55	119.62	111.83
5	B	8002	PCW	O3-C11-C12	2.37	119.06	111.83
5	C	5103	PCW	O3-C11-C12	2.37	119.06	111.83
5	A	8002	PCW	O3-C11-C12	2.36	119.03	111.83
5	D	5103	PCW	O3-C11-C12	2.35	119.00	111.83

There are no chirality outliers.

All (196) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	8002	PCW	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
5	A	8002	PCW	C1-O3P-P-O4P
5	A	8003	PCW	O4P-C4-C5-N
5	D	5101	PCW	O4P-C4-C5-N
5	D	5103	PCW	O4P-C4-C5-N
5	D	5103	PCW	C1-O3P-P-O4P
5	B	8002	PCW	O4P-C4-C5-N
5	B	8002	PCW	C1-O3P-P-O4P
5	B	8003	PCW	O4P-C4-C5-N
5	C	5101	PCW	O4P-C4-C5-N
5	C	5103	PCW	O4P-C4-C5-N
5	C	5103	PCW	C1-O3P-P-O4P
5	A	8002	PCW	C13-C14-C15-C16
5	D	5103	PCW	C13-C14-C15-C16
5	B	8002	PCW	C13-C14-C15-C16
5	C	5103	PCW	C13-C14-C15-C16
5	A	8003	PCW	C11-C12-C13-C14
5	D	5101	PCW	C11-C12-C13-C14
5	B	8003	PCW	C11-C12-C13-C14
5	C	5101	PCW	C11-C12-C13-C14
5	A	8003	PCW	C12-C13-C14-C15
5	A	8003	PCW	C44-C45-C46-C47
5	D	5101	PCW	C12-C13-C14-C15
5	D	5101	PCW	C44-C45-C46-C47
5	B	8003	PCW	C12-C13-C14-C15
5	B	8003	PCW	C44-C45-C46-C47
5	C	5101	PCW	C12-C13-C14-C15
5	C	5101	PCW	C44-C45-C46-C47
5	A	8002	PCW	C44-C45-C46-C47
5	D	5103	PCW	C44-C45-C46-C47
5	B	8002	PCW	C44-C45-C46-C47
5	C	5103	PCW	C44-C45-C46-C47
5	A	8003	PCW	C41-C42-C43-C44
5	D	5101	PCW	C41-C42-C43-C44
5	B	8003	PCW	C41-C42-C43-C44
5	C	5101	PCW	C41-C42-C43-C44
5	A	8002	PCW	C11-C12-C13-C14
5	D	5103	PCW	C11-C12-C13-C14
5	B	8002	PCW	C11-C12-C13-C14
5	C	5103	PCW	C11-C12-C13-C14
5	D	5103	PCW	C35-C36-C37-C38
5	B	8002	PCW	C35-C36-C37-C38
5	A	8002	PCW	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
5	C	5103	PCW	C35-C36-C37-C38
5	A	8002	PCW	C32-C31-O2-C2
5	D	5103	PCW	C32-C31-O2-C2
5	B	8002	PCW	C32-C31-O2-C2
5	C	5103	PCW	C32-C31-O2-C2
5	A	8003	PCW	C20-C21-C22-C23
5	D	5101	PCW	C20-C21-C22-C23
5	B	8003	PCW	C20-C21-C22-C23
5	C	5101	PCW	C20-C21-C22-C23
5	A	8003	PCW	C14-C15-C16-C17
5	D	5101	PCW	C14-C15-C16-C17
5	B	8003	PCW	C14-C15-C16-C17
5	C	5101	PCW	C14-C15-C16-C17
5	A	8003	PCW	C2-C1-O3P-P
5	D	5101	PCW	C2-C1-O3P-P
5	B	8003	PCW	C2-C1-O3P-P
5	C	5101	PCW	C2-C1-O3P-P
5	A	8003	PCW	C16-C17-C18-C19
5	D	5101	PCW	C16-C17-C18-C19
5	B	8003	PCW	C16-C17-C18-C19
5	C	5101	PCW	C16-C17-C18-C19
5	A	8003	PCW	O3P-C1-C2-C3
5	D	5101	PCW	O3P-C1-C2-C3
5	B	8003	PCW	O3P-C1-C2-C3
5	C	5101	PCW	O3P-C1-C2-C3
5	A	8002	PCW	O31-C31-O2-C2
5	D	5103	PCW	O31-C31-O2-C2
5	B	8002	PCW	O31-C31-O2-C2
5	C	5103	PCW	O31-C31-O2-C2
5	A	8002	PCW	C40-C41-C42-C43
5	D	5103	PCW	C40-C41-C42-C43
5	B	8002	PCW	C40-C41-C42-C43
5	C	5103	PCW	C40-C41-C42-C43
5	A	8002	PCW	C12-C11-O3-C3
5	D	5103	PCW	C12-C11-O3-C3
5	B	8002	PCW	C12-C11-O3-C3
5	C	5103	PCW	C12-C11-O3-C3
5	A	8002	PCW	C41-C42-C43-C44
5	D	5103	PCW	C41-C42-C43-C44
5	B	8002	PCW	C41-C42-C43-C44
5	C	5103	PCW	C41-C42-C43-C44
5	B	8002	PCW	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
5	A	8002	PCW	C21-C22-C23-C24
5	D	5103	PCW	C21-C22-C23-C24
5	C	5103	PCW	C21-C22-C23-C24
5	A	8002	PCW	C1-C2-C3-O3
5	D	5103	PCW	C1-C2-C3-O3
5	B	8002	PCW	C1-C2-C3-O3
5	C	5103	PCW	C1-C2-C3-O3
5	B	8002	PCW	C33-C34-C35-C36
5	A	8002	PCW	C33-C34-C35-C36
5	D	5103	PCW	C33-C34-C35-C36
5	C	5103	PCW	C33-C34-C35-C36
5	A	8002	PCW	C24-C25-C26-C27
5	D	5103	PCW	C24-C25-C26-C27
5	B	8002	PCW	C24-C25-C26-C27
5	C	5103	PCW	C24-C25-C26-C27
5	A	8002	PCW	O11-C11-O3-C3
5	D	5103	PCW	O11-C11-O3-C3
5	B	8002	PCW	O11-C11-O3-C3
5	C	5103	PCW	O11-C11-O3-C3
5	A	8003	PCW	O3P-C1-C2-O2
5	D	5101	PCW	O3P-C1-C2-O2
5	B	8003	PCW	O3P-C1-C2-O2
5	C	5101	PCW	O3P-C1-C2-O2
5	C	5101	PCW	C19-C20-C21-C22
5	A	8003	PCW	C19-C20-C21-C22
5	D	5101	PCW	C19-C20-C21-C22
5	B	8003	PCW	C19-C20-C21-C22
5	A	8003	PCW	C21-C22-C23-C24
5	D	5101	PCW	C21-C22-C23-C24
5	B	8003	PCW	C21-C22-C23-C24
5	C	5101	PCW	C21-C22-C23-C24
5	A	8003	PCW	C35-C36-C37-C38
5	D	5101	PCW	C35-C36-C37-C38
5	B	8003	PCW	C35-C36-C37-C38
5	C	5101	PCW	C35-C36-C37-C38
5	A	8002	PCW	O2-C2-C3-O3
5	D	5103	PCW	O2-C2-C3-O3
5	B	8002	PCW	O2-C2-C3-O3
5	C	5103	PCW	O2-C2-C3-O3
5	D	5103	PCW	C32-C33-C34-C35
5	B	8002	PCW	C32-C33-C34-C35
5	A	8002	PCW	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
5	C	5103	PCW	C32-C33-C34-C35
5	A	8003	PCW	C4-C5-N-C8
5	D	5101	PCW	C4-C5-N-C8
5	B	8003	PCW	C4-C5-N-C8
5	C	5101	PCW	C4-C5-N-C8
5	A	8002	PCW	C1-O3P-P-O1P
5	A	8002	PCW	C1-O3P-P-O2P
5	A	8002	PCW	C4-O4P-P-O2P
5	D	5103	PCW	C1-O3P-P-O1P
5	D	5103	PCW	C1-O3P-P-O2P
5	D	5103	PCW	C4-O4P-P-O2P
5	B	8002	PCW	C1-O3P-P-O1P
5	B	8002	PCW	C1-O3P-P-O2P
5	B	8002	PCW	C4-O4P-P-O2P
5	C	5103	PCW	C1-O3P-P-O1P
5	C	5103	PCW	C1-O3P-P-O2P
5	C	5103	PCW	C4-O4P-P-O2P
5	A	8003	PCW	C13-C14-C15-C16
5	D	5101	PCW	C13-C14-C15-C16
5	B	8003	PCW	C13-C14-C15-C16
5	C	5101	PCW	C13-C14-C15-C16
5	A	8003	PCW	C40-C41-C42-C43
5	D	5101	PCW	C40-C41-C42-C43
5	B	8003	PCW	C40-C41-C42-C43
5	C	5101	PCW	C40-C41-C42-C43
5	A	8002	PCW	C25-C26-C27-C28
5	D	5103	PCW	C25-C26-C27-C28
5	B	8002	PCW	C25-C26-C27-C28
5	C	5103	PCW	C25-C26-C27-C28
5	A	8002	PCW	C2-C1-O3P-P
5	D	5103	PCW	C2-C1-O3P-P
5	B	8002	PCW	C2-C1-O3P-P
5	C	5103	PCW	C2-C1-O3P-P
5	A	8003	PCW	C1-C2-O2-C31
5	D	5101	PCW	C1-C2-O2-C31
5	B	8003	PCW	C1-C2-O2-C31
5	C	5101	PCW	C1-C2-O2-C31
5	A	8002	PCW	C23-C24-C25-C26
5	D	5103	PCW	C23-C24-C25-C26
5	B	8002	PCW	C23-C24-C25-C26
5	C	5103	PCW	C23-C24-C25-C26
5	A	8002	PCW	C4-C5-N-C8

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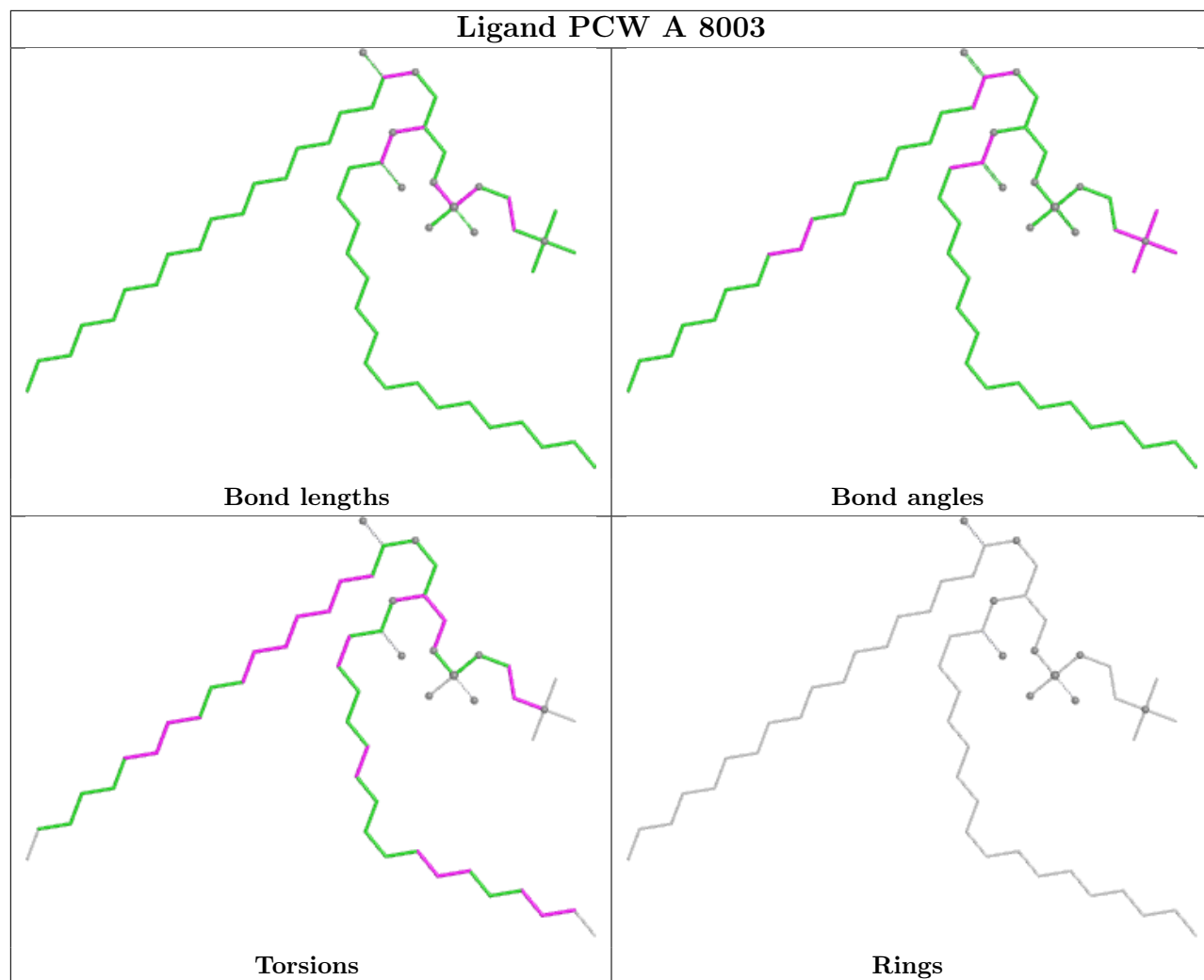
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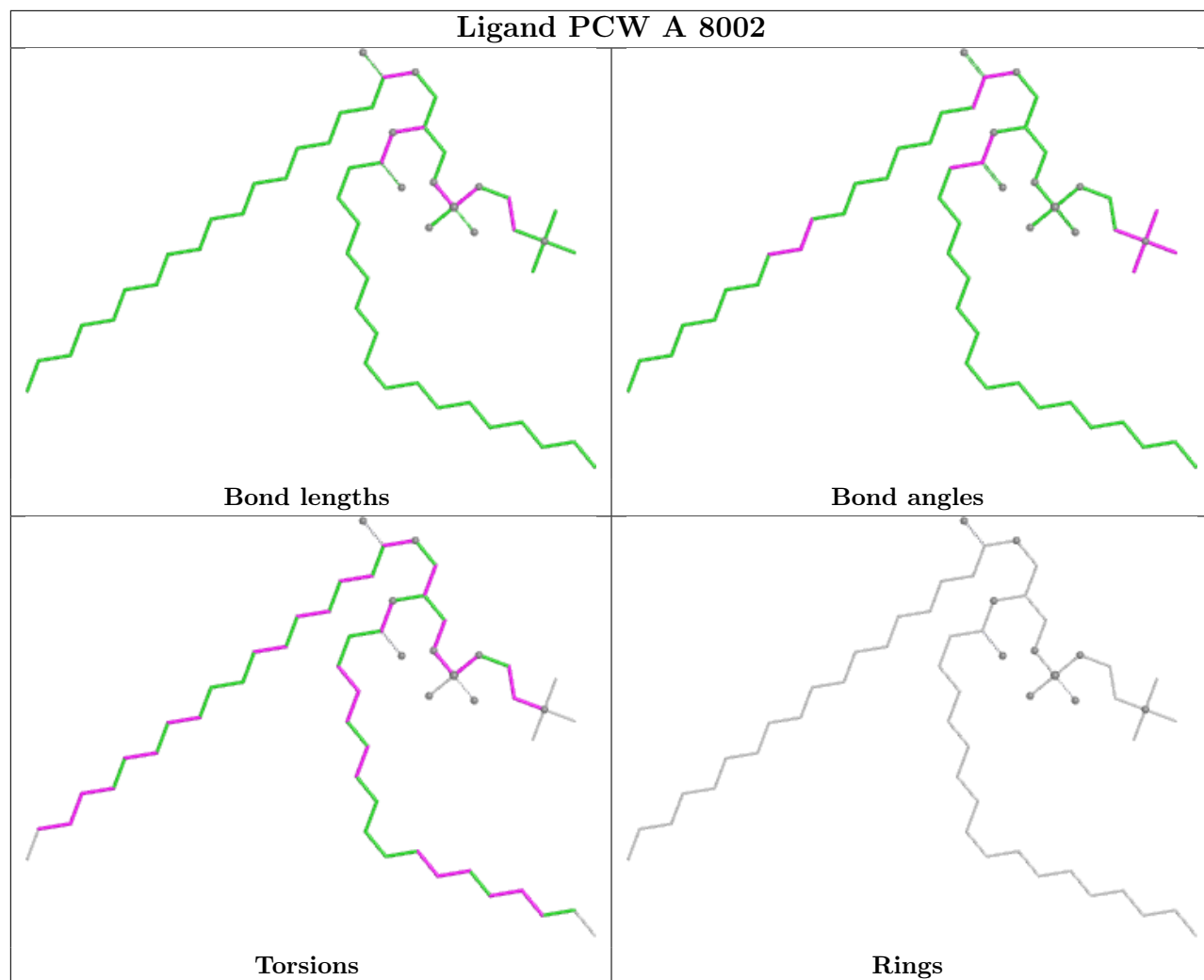
Mol	Chain	Res	Type	Atoms
5	D	5103	PCW	C4-C5-N-C8
5	B	8002	PCW	C4-C5-N-C8
5	C	5103	PCW	C4-C5-N-C8
5	C	5103	PCW	C15-C16-C17-C18
5	B	8002	PCW	C15-C16-C17-C18
5	A	8002	PCW	C15-C16-C17-C18
5	D	5103	PCW	C15-C16-C17-C18
5	C	5101	PCW	C45-C46-C47-C48
5	A	8003	PCW	C45-C46-C47-C48
5	D	5101	PCW	C45-C46-C47-C48
5	B	8003	PCW	C45-C46-C47-C48
5	A	8002	PCW	C43-C44-C45-C46
5	D	5103	PCW	C43-C44-C45-C46
5	B	8002	PCW	C43-C44-C45-C46
5	C	5103	PCW	C43-C44-C45-C46
5	A	8002	PCW	C19-C20-C21-C22
5	D	5103	PCW	C19-C20-C21-C22
5	B	8002	PCW	C19-C20-C21-C22
5	C	5103	PCW	C19-C20-C21-C22
5	D	5101	PCW	C15-C16-C17-C18
5	A	8003	PCW	C15-C16-C17-C18
5	B	8003	PCW	C15-C16-C17-C18
5	C	5101	PCW	C15-C16-C17-C18
5	A	8003	PCW	C31-C32-C33-C34
5	D	5101	PCW	C31-C32-C33-C34
5	B	8003	PCW	C31-C32-C33-C34
5	C	5101	PCW	C31-C32-C33-C34

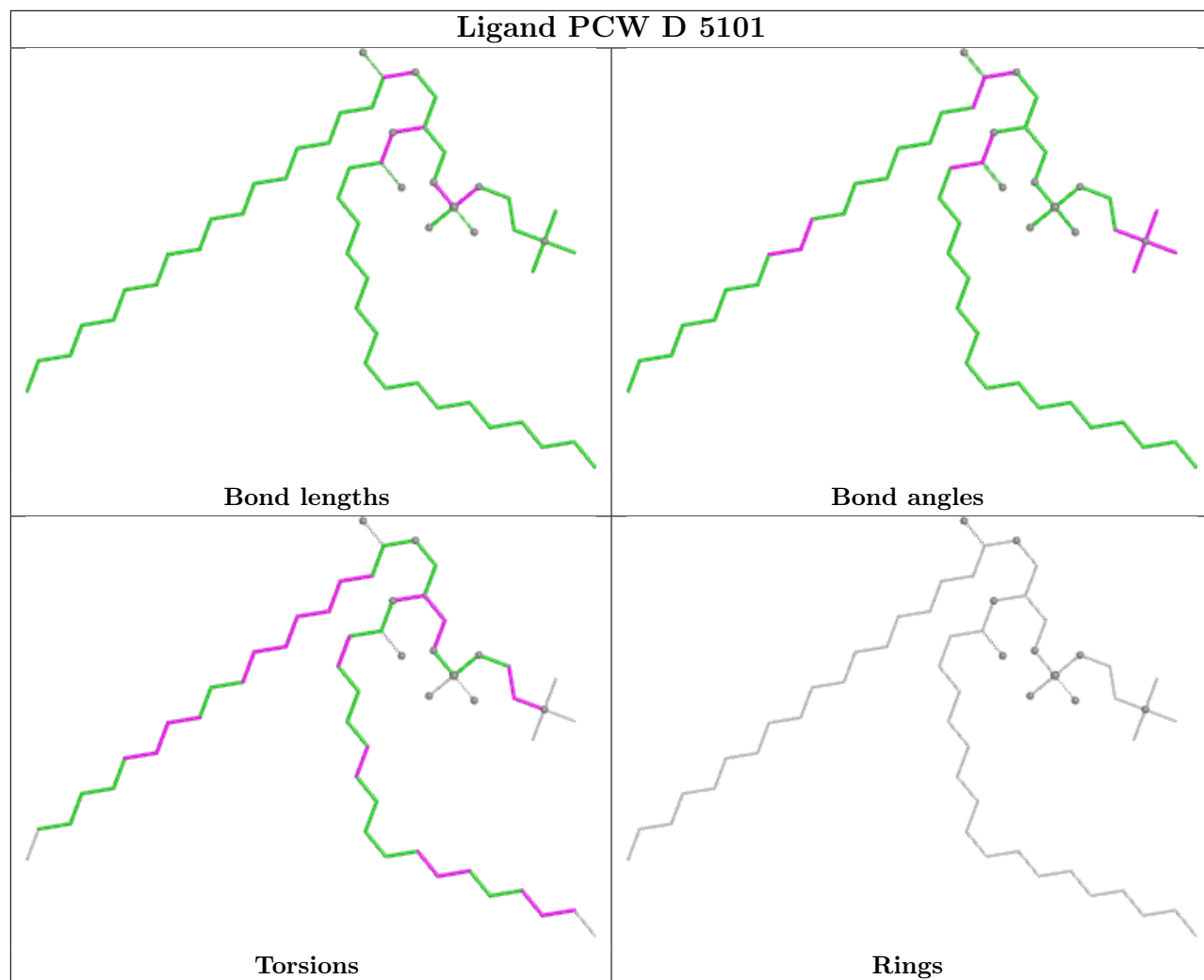
There are no ring outliers.

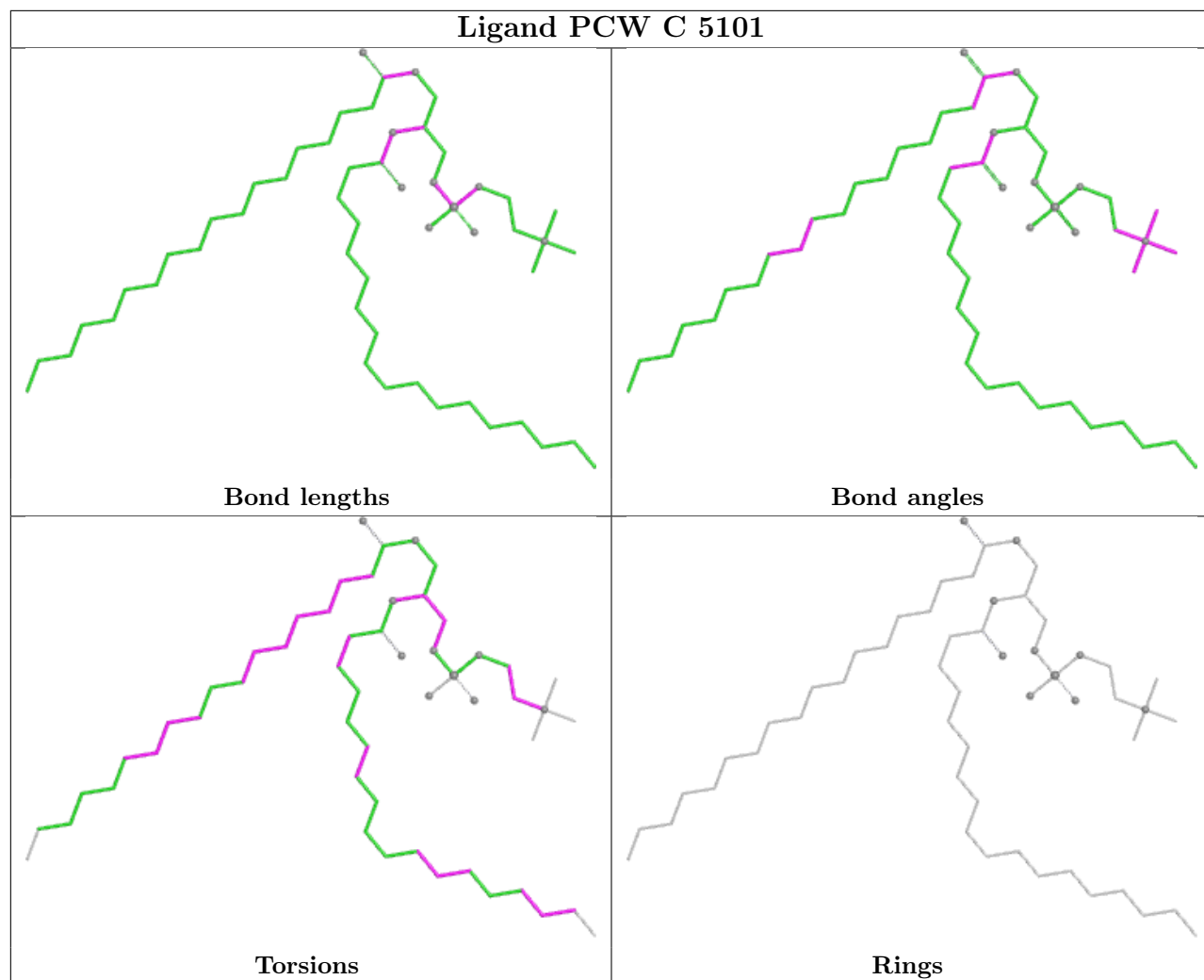
No monomer is involved in short contacts.

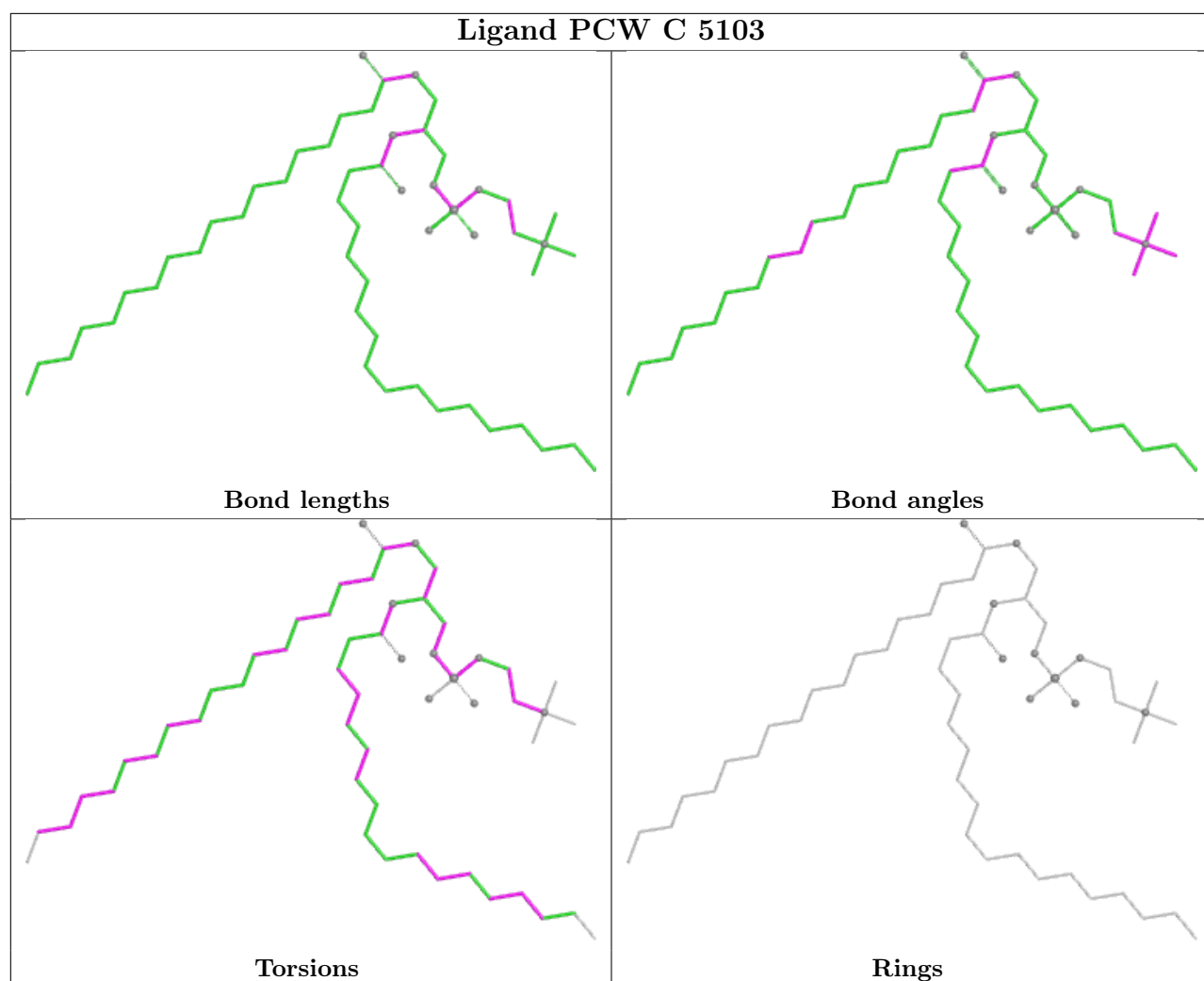
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

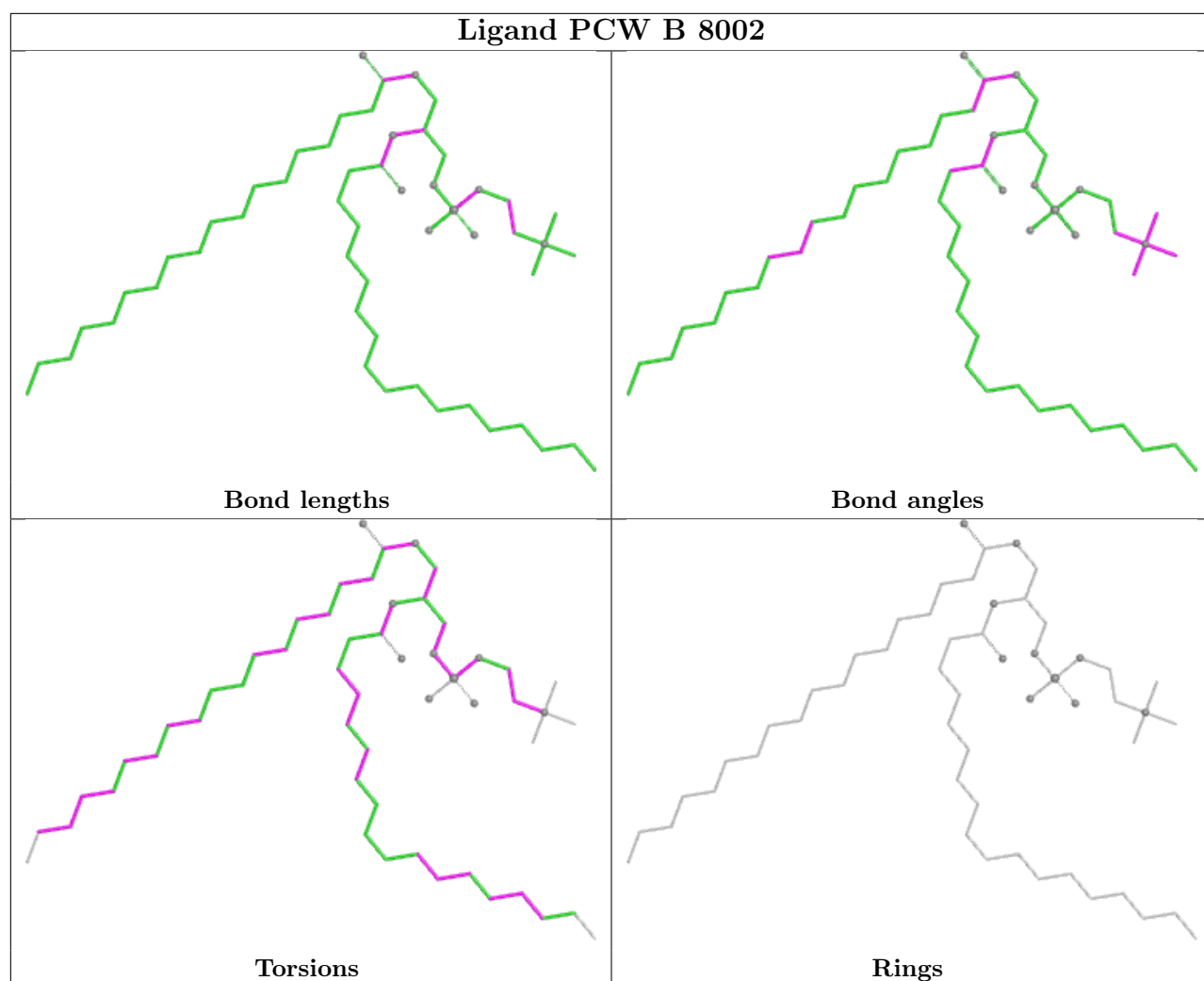


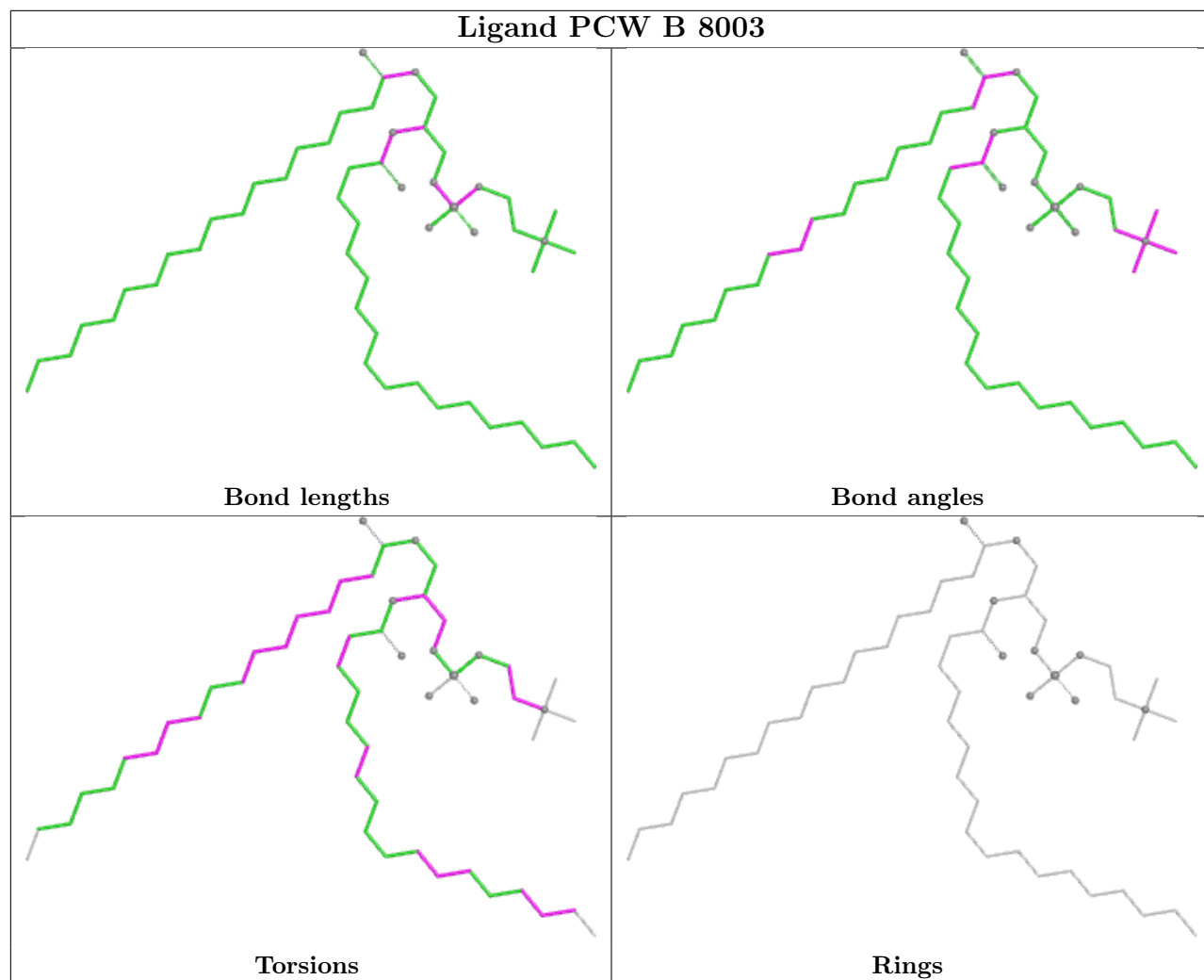


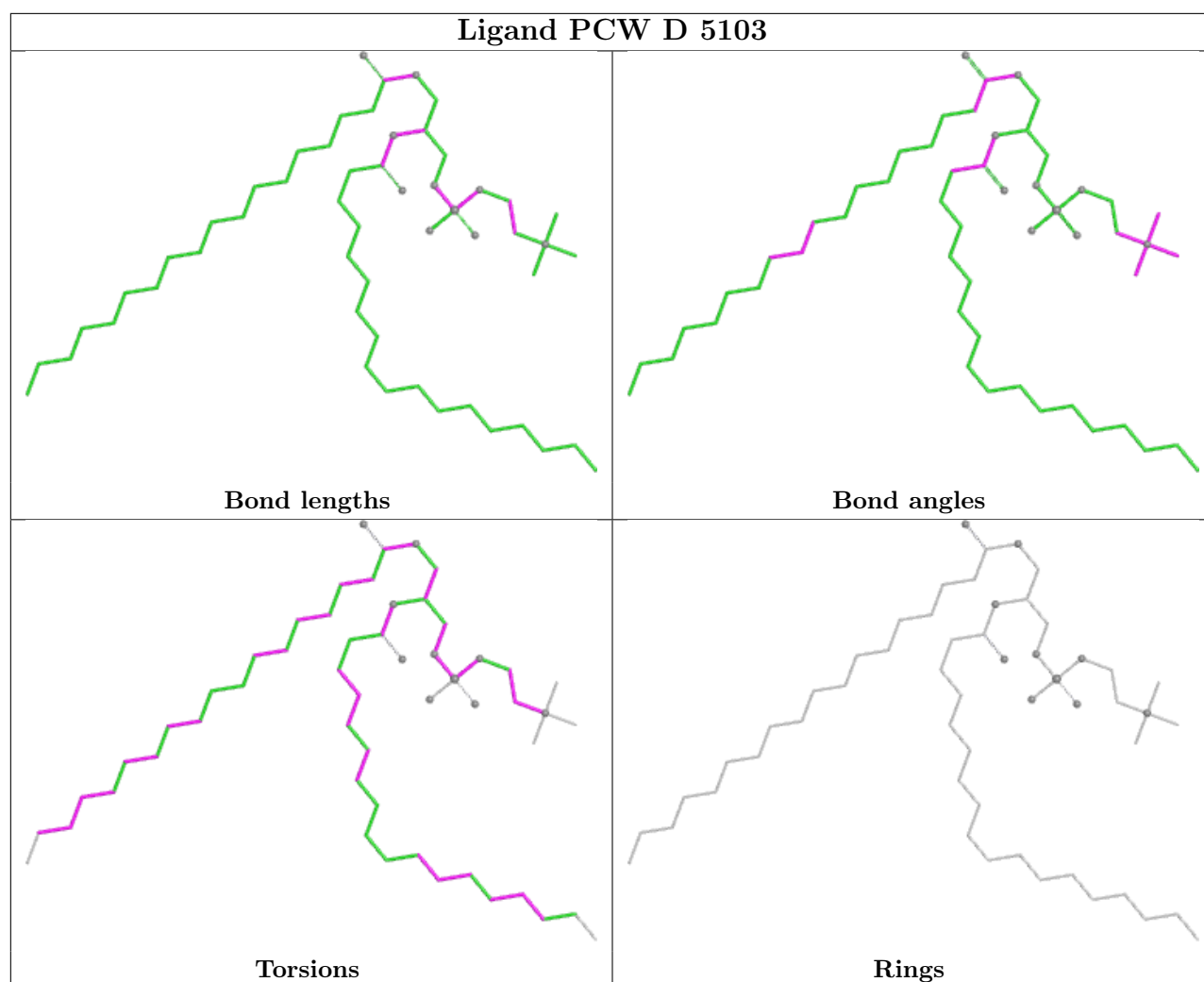












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

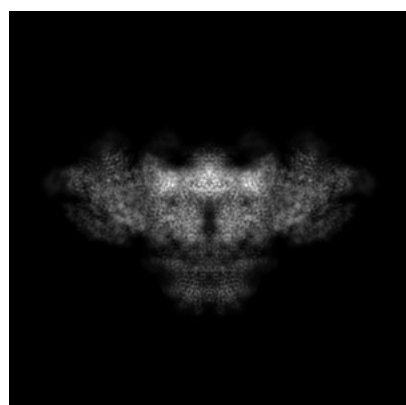
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43299. These allow visual inspection of the internal detail of the map and identification of artifacts.

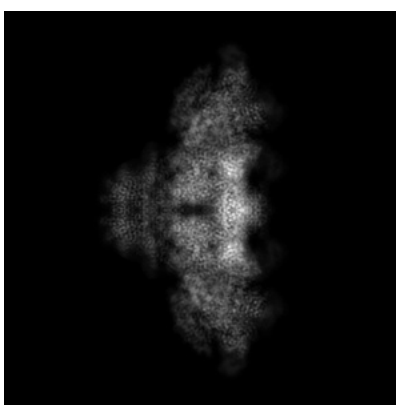
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

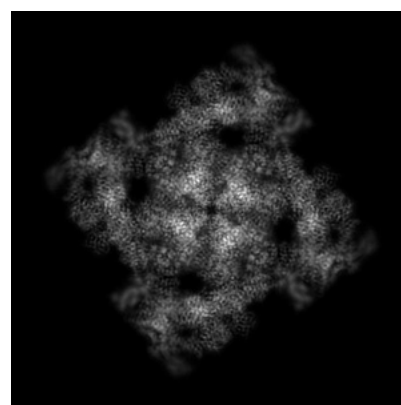
6.1.1 Primary map



X



Y



Z

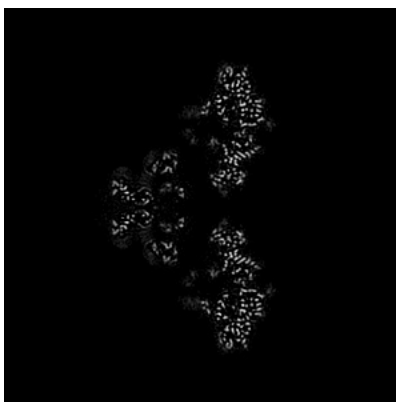
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

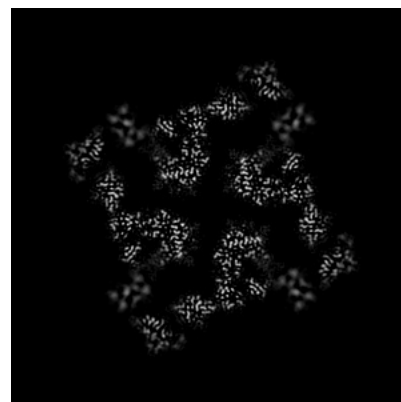
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

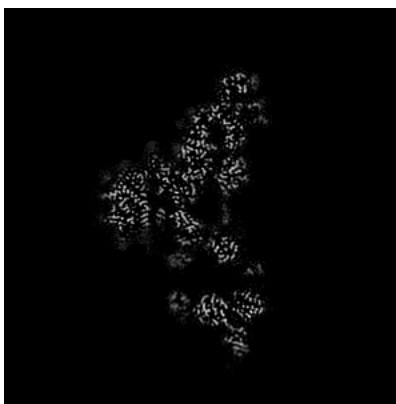
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

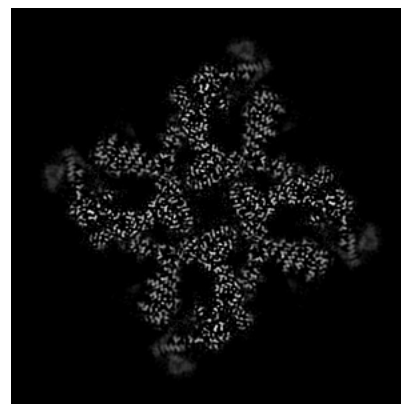
6.3.1 Primary map



X Index: 238



Y Index: 274

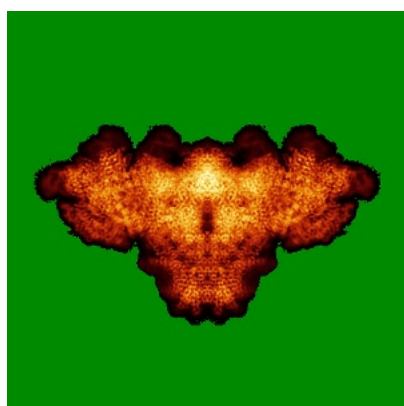


Z Index: 289

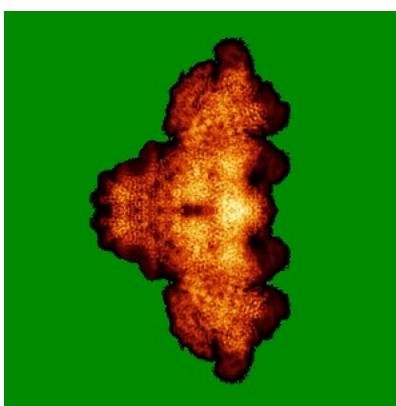
The images above show the largest variance slices of the map in three orthogonal directions.

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

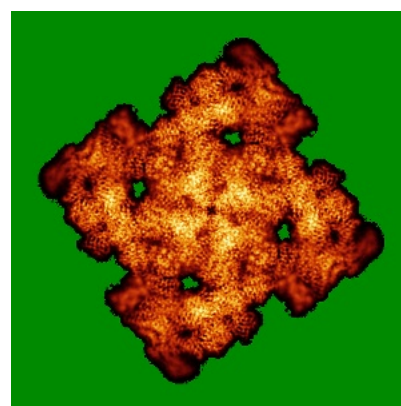
6.4.1 Primary map



X



Y

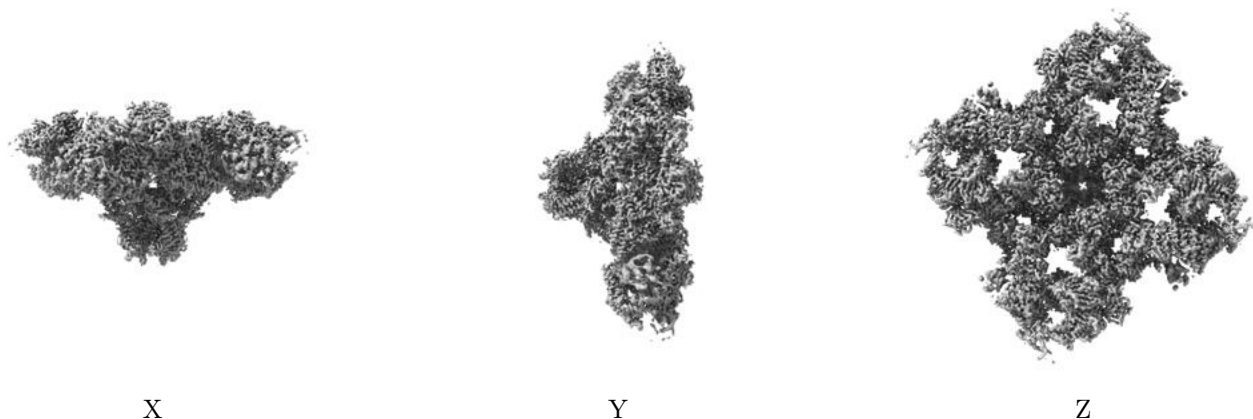


Z

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

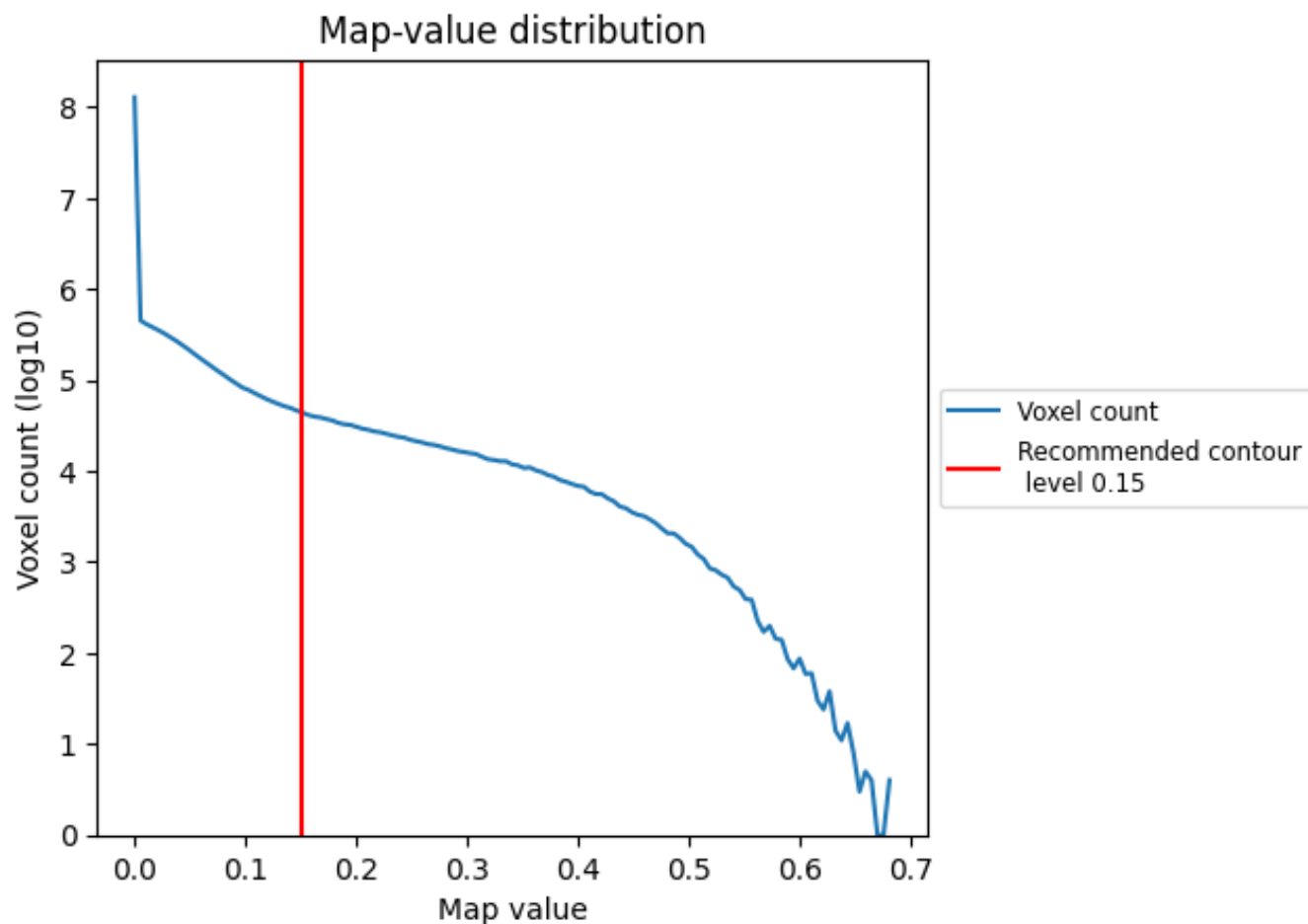
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

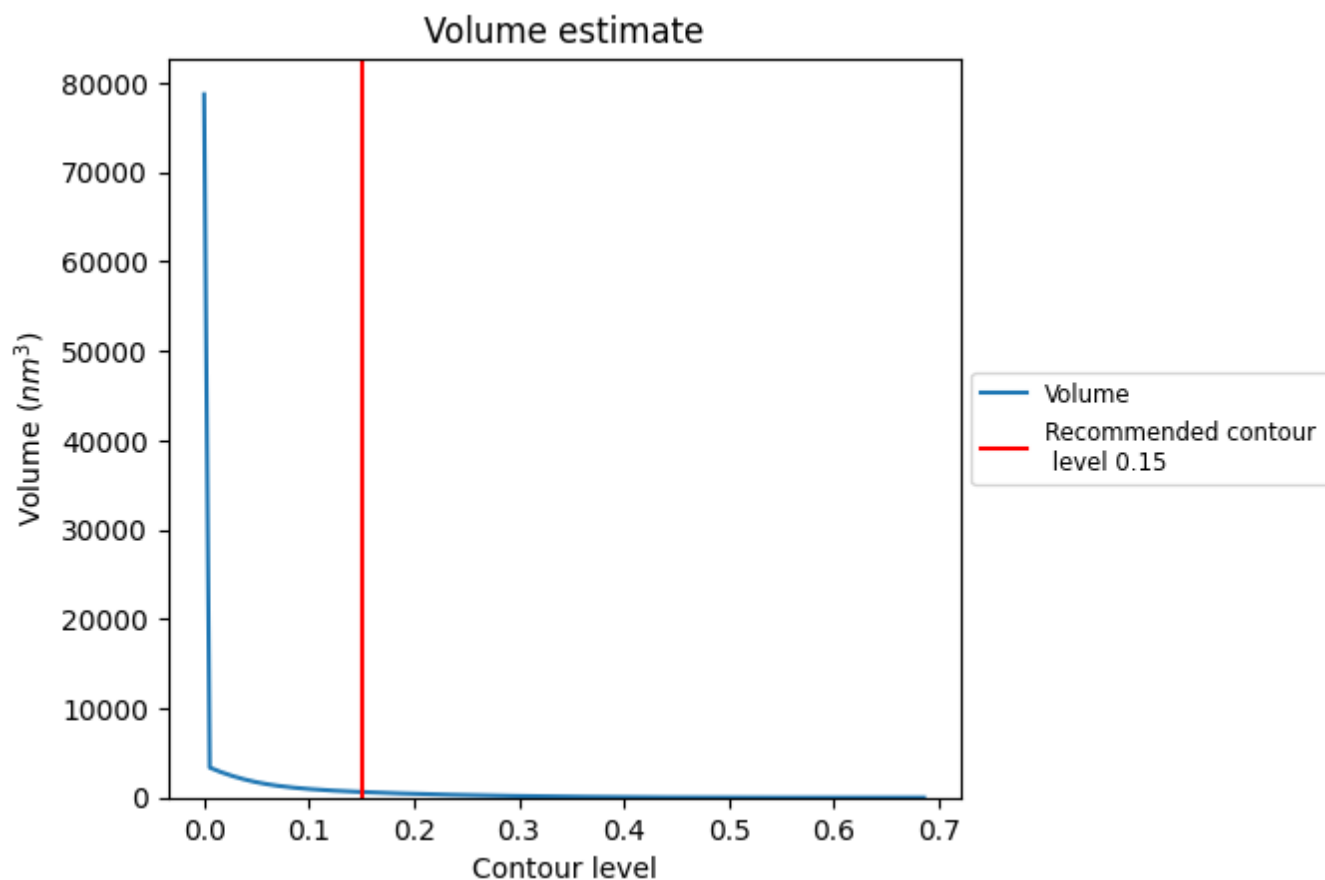
This section contains the results of statistical analysis of the map.

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.

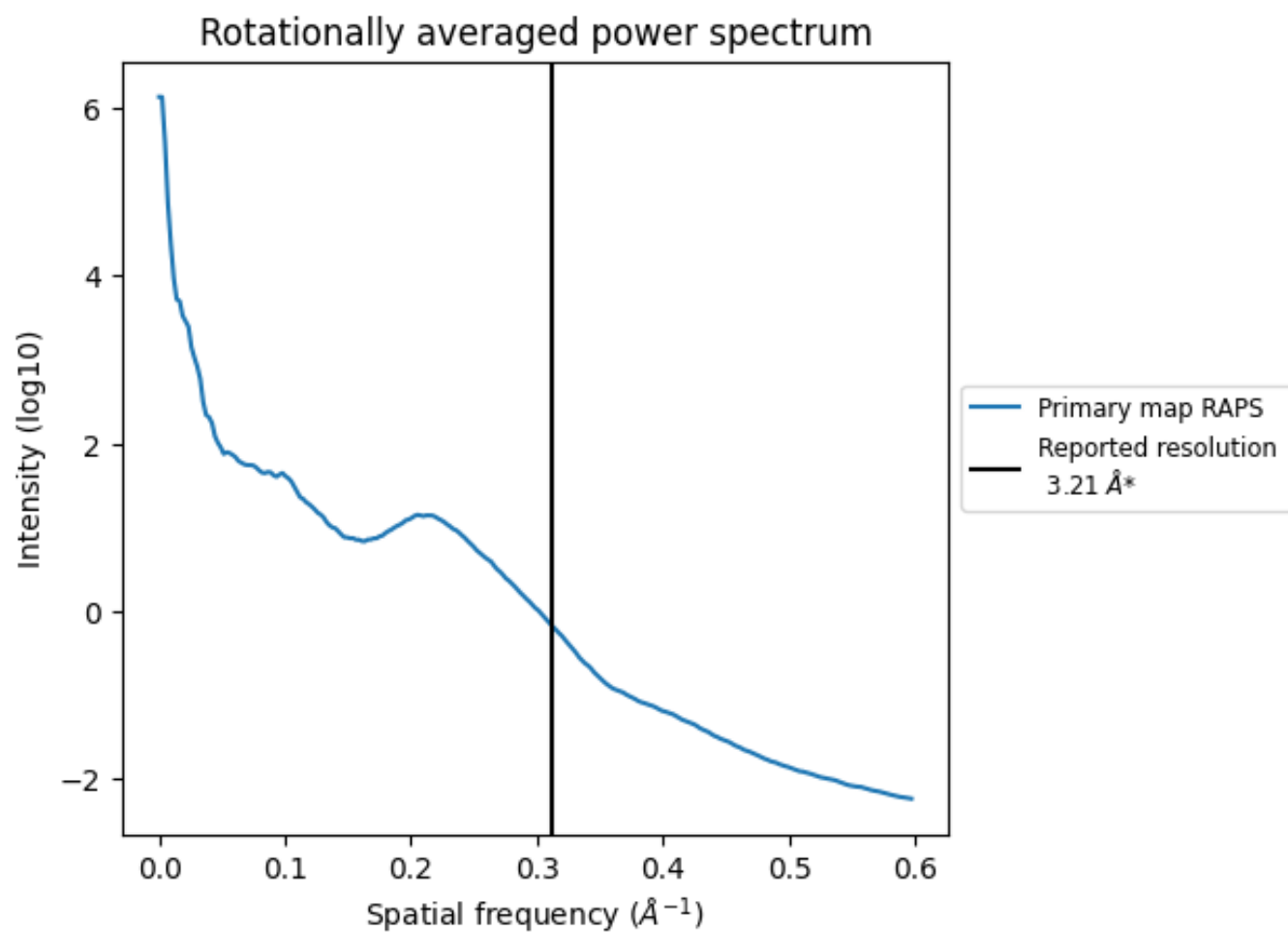
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 624 nm^3 ; this corresponds to an approximate mass of 564 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 0.312 Å⁻¹

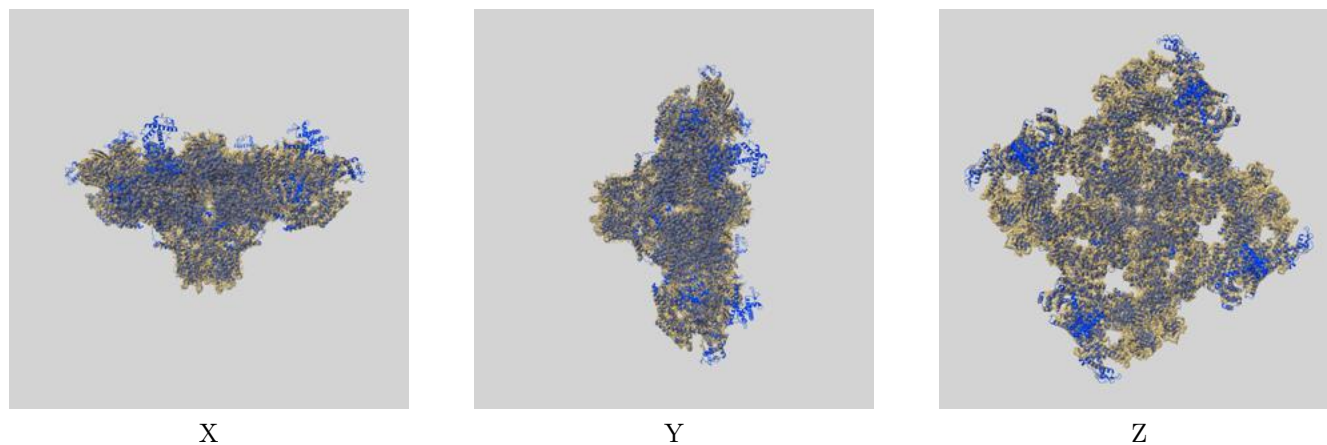
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

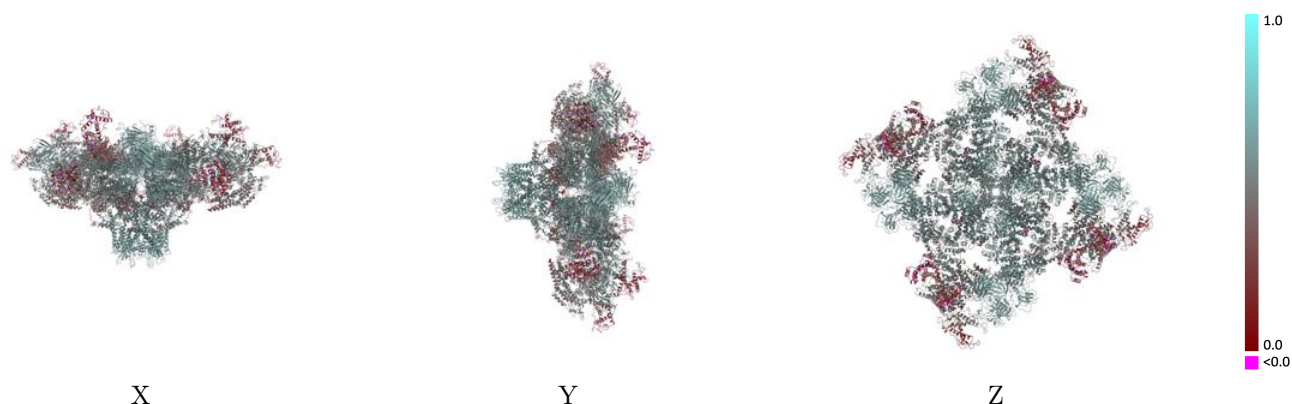
This section contains information regarding the fit between EMDB map EMD-43299 and PDB model 8VK3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

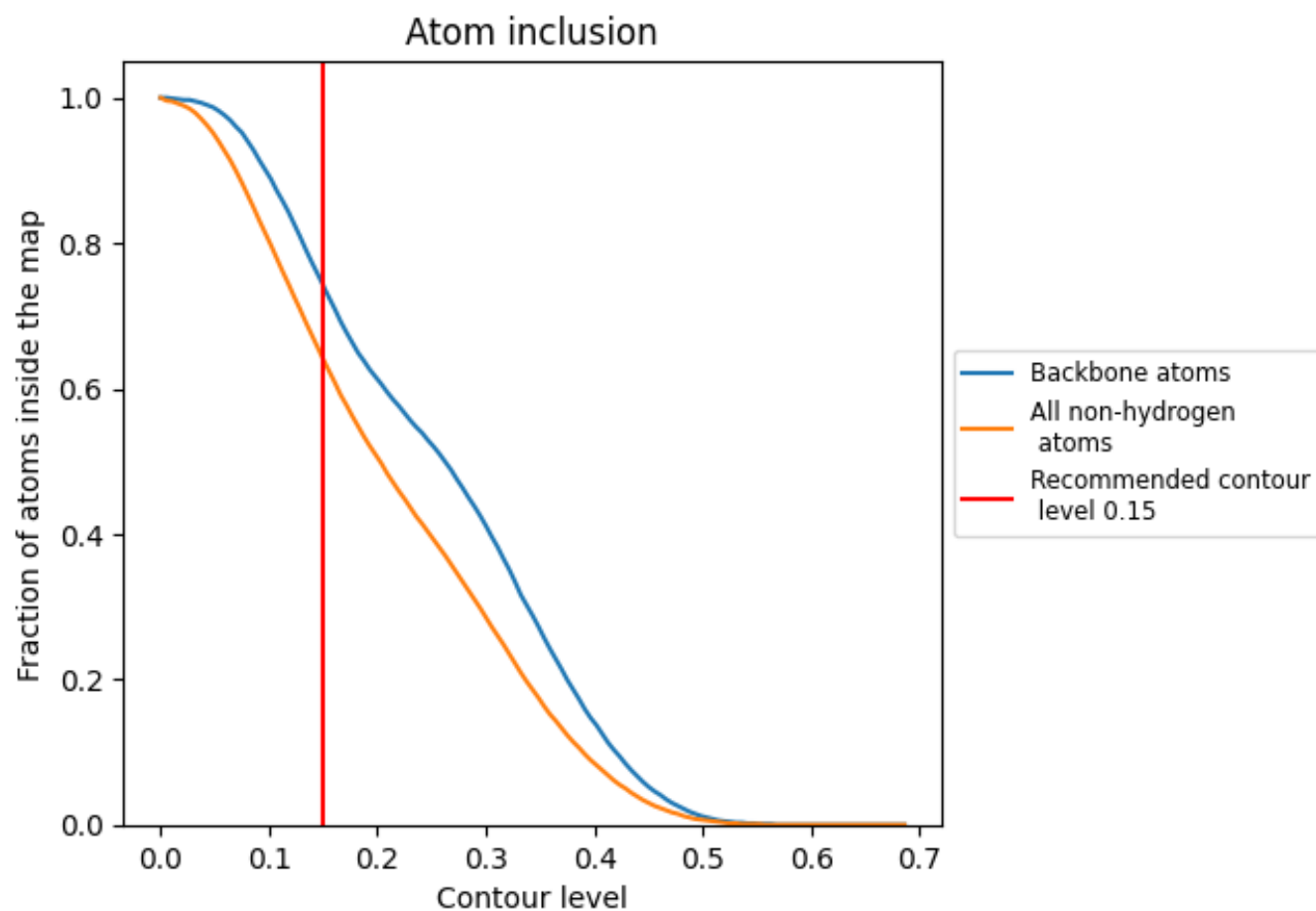


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6400	 0.4910
A	 0.6520	 0.5030
B	 0.6530	 0.5020
C	 0.6530	 0.5020
D	 0.6520	 0.5030
E	 0.7290	 0.5660
F	 0.7340	 0.5630
G	 0.7320	 0.5630
H	 0.7360	 0.5630
I	 0.3090	 0.1620
J	 0.2960	 0.1670
K	 0.3040	 0.1620
L	 0.2910	 0.1640
M	 0.3010	 0.1640
N	 0.2960	 0.1680
O	 0.3060	 0.1590
P	 0.2930	 0.1660

