



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:13 AM UTC

PDB ID : 9OL4 / pdb_00009ol4
EMDB ID : EMD-70589
Title : Cryo-EM Structure of Ryanodine Receptor 1: Drug Bound Open Conformation
Authors : Molinarolo, S.M.; Van Petegem, F.
Deposited on : 2025-05-12
Resolution : 3.37 Å(reported)
Based on initial model : 7TZC

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

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

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:

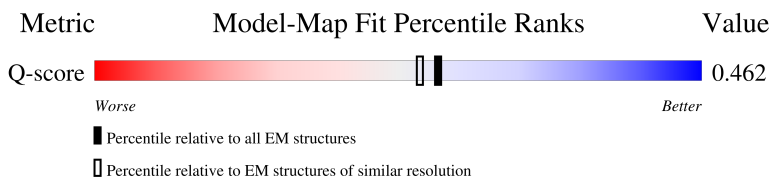
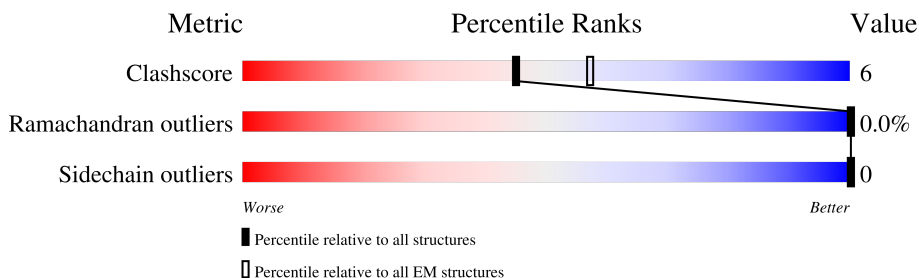
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.37 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	14287 (2.87 - 3.87)

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

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

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Mol	Chain	Length	Quality of chain
2	B	111	 86% 11% •
2	H	111	 86% 11% •
2	N	111	 86% 11% •
2	T	111	 86% 11% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 131292 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	4064	Total	C	N	O	S	0	0
			31873	20385	5494	5773	221		
1	G	4064	Total	C	N	O	S	0	0
			31873	20385	5494	5773	221		
1	M	4064	Total	C	N	O	S	0	0
			31873	20385	5494	5773	221		
1	S	4064	Total	C	N	O	S	0	0
			31873	20385	5494	5773	221		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			811	510	143	154	4		
2	H	107	Total	C	N	O	S	0	0
			811	510	143	154	4		
2	N	107	Total	C	N	O	S	0	0
			811	510	143	154	4		
2	T	107	Total	C	N	O	S	0	0
			811	510	143	154	4		

There are 12 discrepancies between the modelled and reference sequences:

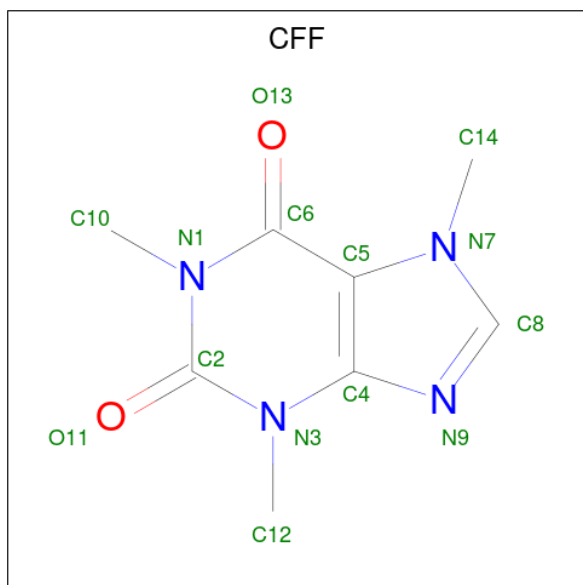
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P68106
B	-1	ASN	-	expression tag	UNP P68106
B	0	ALA	-	expression tag	UNP P68106
H	-2	SER	-	expression tag	UNP P68106
H	-1	ASN	-	expression tag	UNP P68106
H	0	ALA	-	expression tag	UNP P68106
N	-2	SER	-	expression tag	UNP P68106
N	-1	ASN	-	expression tag	UNP P68106
N	0	ALA	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-2	SER	-	expression tag	UNP P68106
T	-1	ASN	-	expression tag	UNP P68106
T	0	ALA	-	expression tag	UNP P68106

- Molecule 3 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).

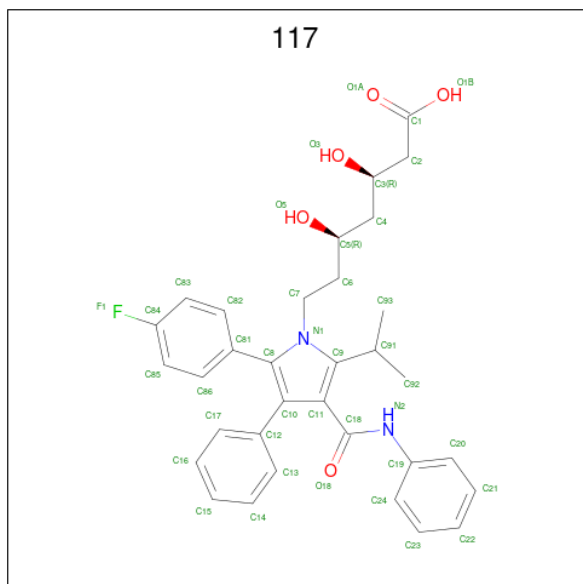


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	4	2	
3	G	1	Total	C	N	O	0
			14	8	4	2	
3	M	1	Total	C	N	O	0
			14	8	4	2	
3	S	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is 7-[2-(4-FLUORO-PHENYL)-5-ISOPROPYL-3-PHENYL-4-PHENYLCARBAMOYL-PYRROL-1-YL]- 3,5-DIHYDROXY-HEPTANOIC ACID (CCD ID: 117) (formula: $C_{33}H_{35}FN_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	A	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	A	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	G	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	G	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	G	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	M	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	M	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	M	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	S	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	S	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	S	1	Total	C	F	N	O	0
			41	33	1	2	5	

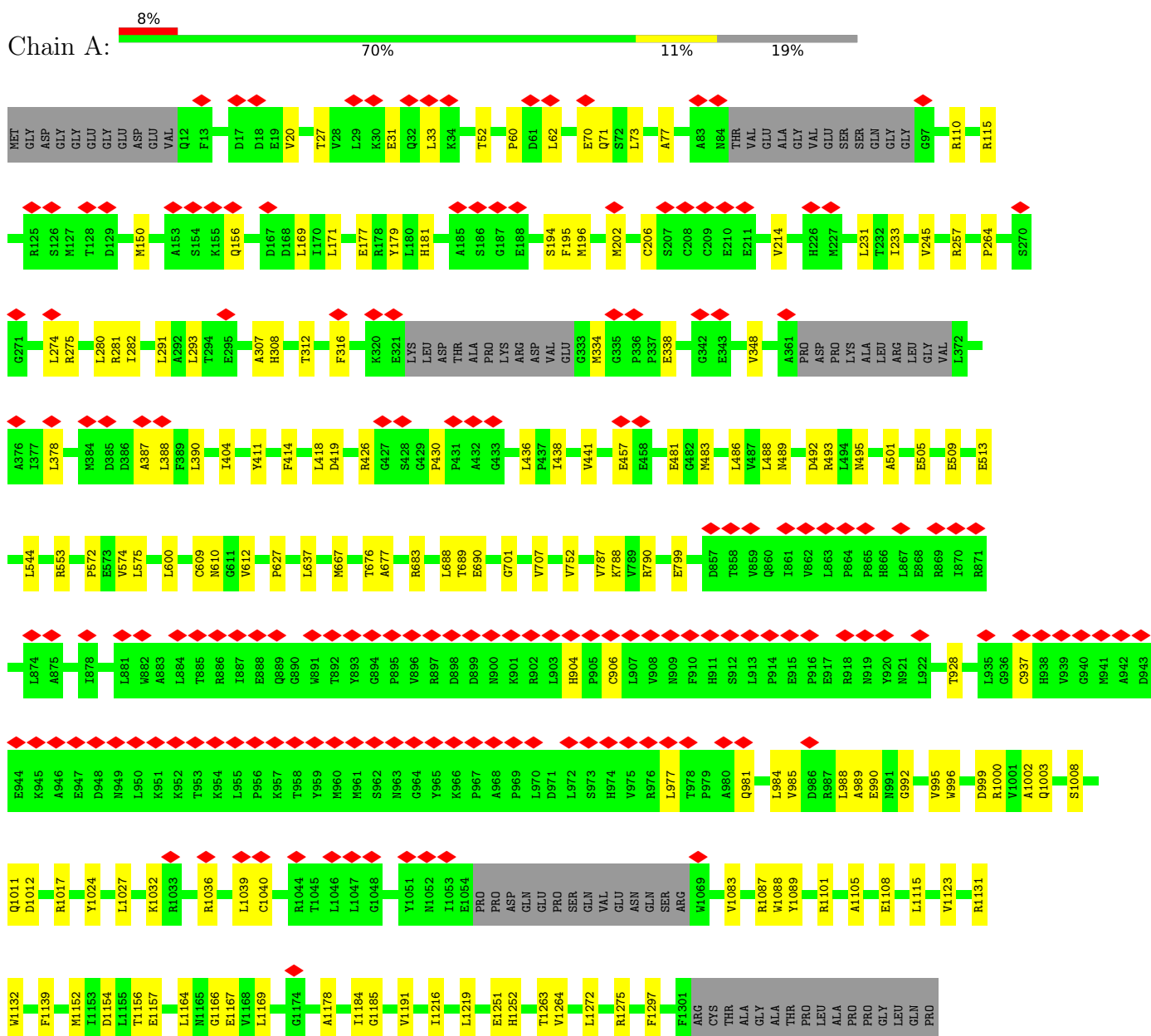
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots [i](#)

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

• Molecule 1: Ryanodine receptor 1



PRO	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LYS	GLU	ALA	GLU	ASP	LY
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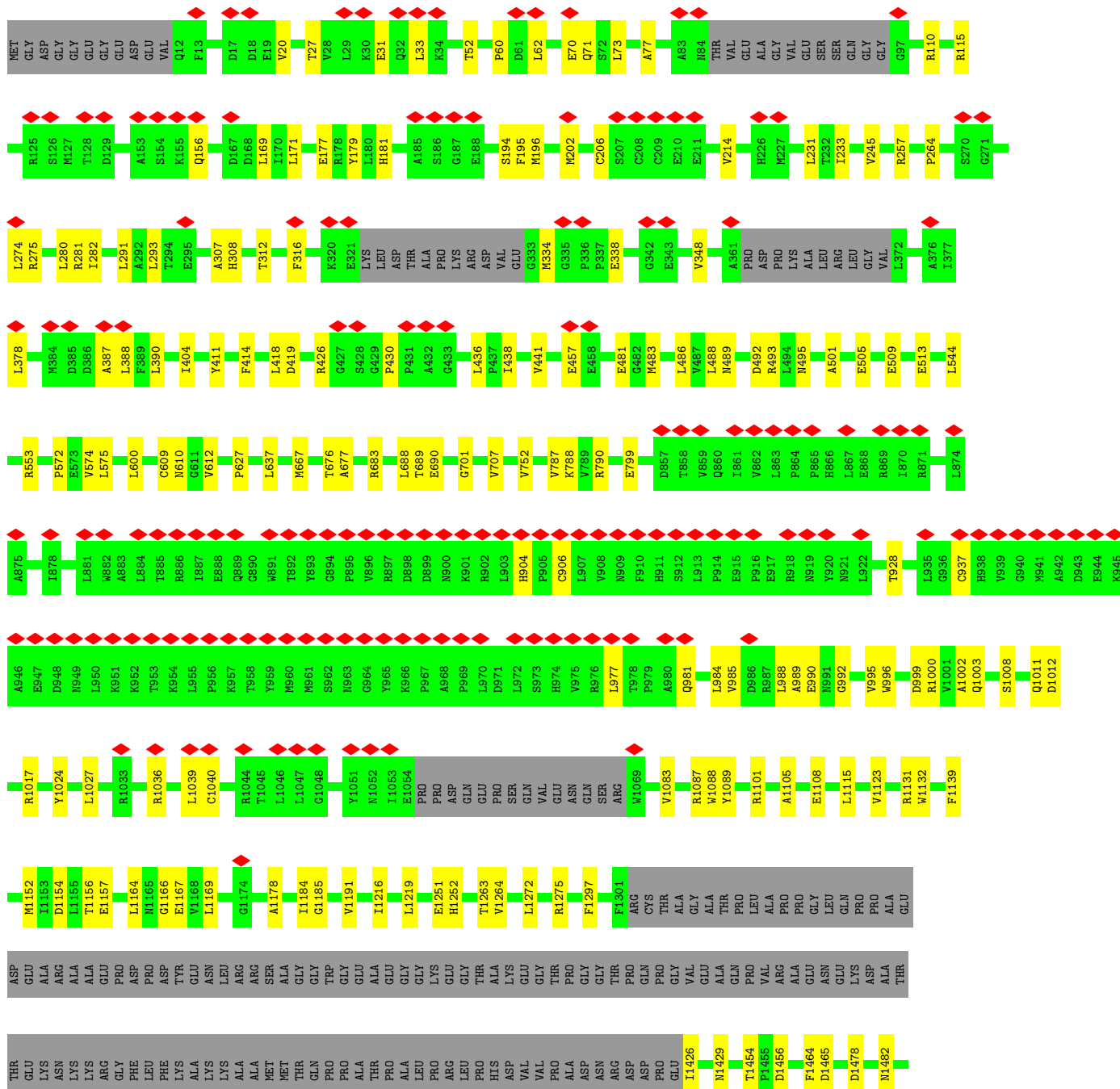
Chain G:







- Molecule 1: Ryanodine receptor 1

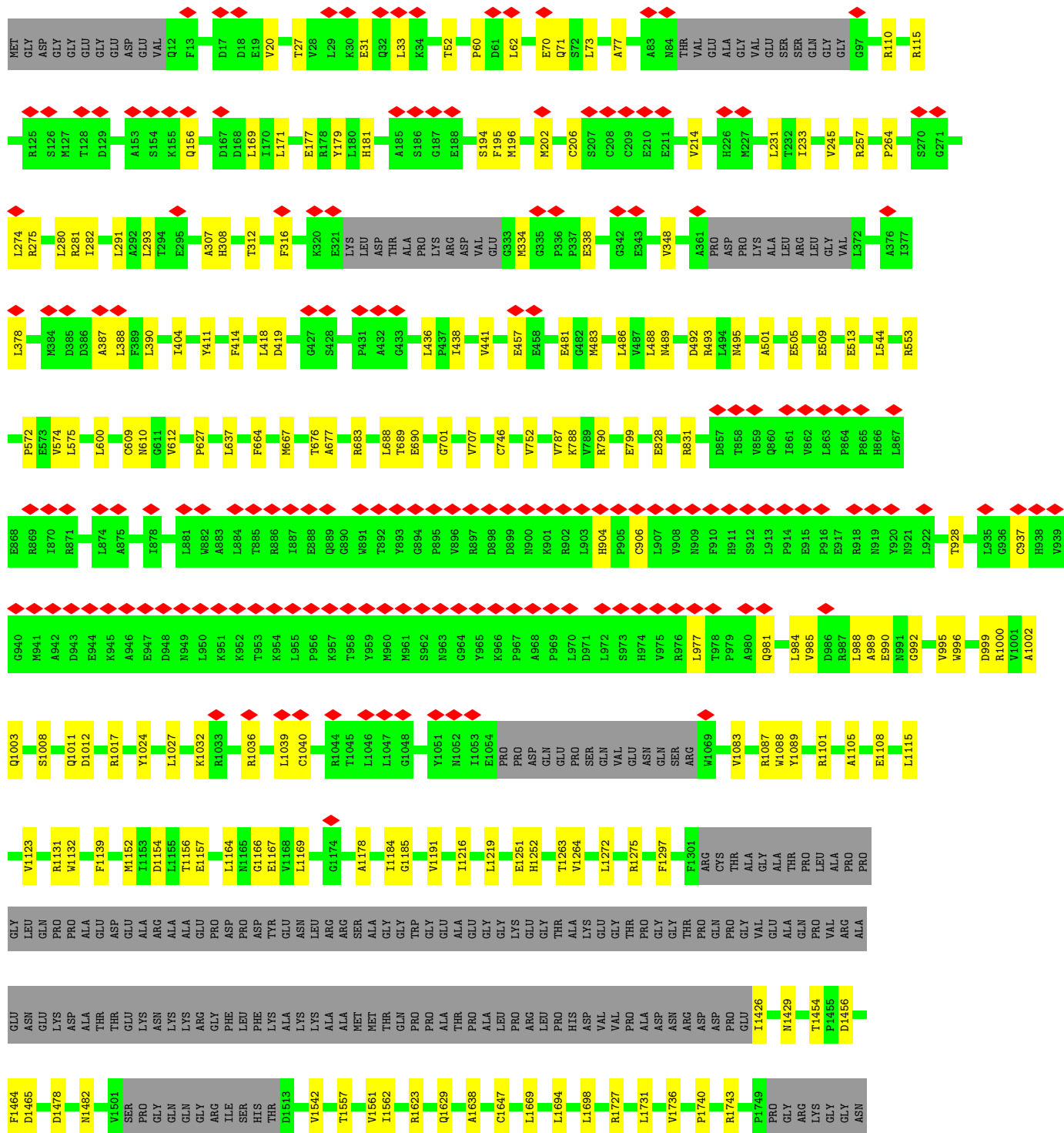






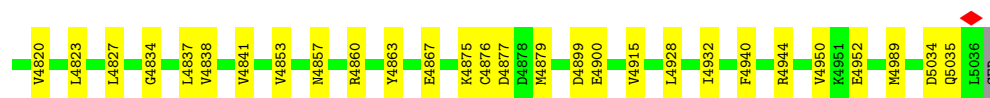


• Molecule 1: Ryanodine receptor 1



T3130	T3133	V3134	F3144	D3154	D3155	L3169	T3177	T3182	V3183	L3186	R3187	L3194	L3197	M3201	P3202	V3203	D3060	A3061	P3062	M3066	A3077	R3078	T3079	V3080	G3084	P3085	V3088	M3106	N3109	L3110	R3111	LEU	GLY	PRO	ASN	VAL	SER	V3236	V3245	L3246	D3247	R3248	L3249	L3253	L3256	A3257	GLU												
I3006	M3007	F3010	T3011	F3017	T3020	P3021	K3036	E3037	M3038	L3046	V3050	F3051	H3052	F3057	D3060	A3061	P3062	M3066	A3077	R3078	T3079	V3080	G3084	P3085	V3088	M3106	N3109	L3110	R3111	LEU	GLY	PRO	ASN	VAL	SER	V3236	V3245	L3246	D3247	R3248	L3249	L3253	L3256	A3257	GLU														
E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	Q2934	Y2935	A2936	V2937	T2938	R2939	GLY	LEU	LYS	ASP	MET	GLU	LEU	ASP	THR	SER	S2950	L2960	R2965	M2967	D2968	L2969	S2970	Q2971	E2972	F2973	L2974	E2978	ALA	VAL	VAL	SER	SER	GLN	ALA	ARG	VAL	GLU	LYS	S2989	E2992	T2995	L3003	P3004	L3005						
V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924
Y2805	R2806	W2807	P2808	I2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827	E2828	K2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864		
V2745	I2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	T2761	Y2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	Q2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	I2804
V2602	I2603	Q2620	R2624	H2625	L2626	F2628	V2630	P2631	E2635	M2639	P2640	L2643	L2644	R2650	C2651	E2670	L2678	R2697	D2716	ALA	SER	TYR	SER	SER	LYS	ALA	GLU	LYS	LYS	ALA	ALA	THR	VAL	ASP	ALA	GLY	ASN	PHE	ASP	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744												
GLY	VAL	ARG	ASP	ASP	ARG	ARG	HIS	GLY	GLU	PRO	PRO	GLU	N2414	E2449	R2452	T2478	LEU	GLY	LYS	ASP	GLY	ALA	L2485	K2499	V2503	Q2515	L2519	H2520	D2523	V2524	L2527	M2530	F2541	T2544	A2547	R2575	A2598	Q2599																					
M2228	F2251	Y2256	L2257	L2258	G2262	ILE	GLY	LEU	GLY	MET	G2269	S2270	T2271	D2274	V2275	A2276	V2280	L2286	E2292	Q2293	D2294	L2295	E2296	V2298	V2299	N2324	F2325	C2326	D2333	F2334	E2348	H2349	A2350	W2351	V2352	V2353	R2355	L2368	D2389	F2395																			
GLU	GLU	LYS	P2091	V2098	M2101	D2109	S2113	L2116	V2117	M2120	F2121	S2122	L2123	L2124	H2125	Q2126	Q2127	Y2128	M2153	L2159	Q2160	Q2161	I2162	R2163	S2164	L2165	P2172	E2175	N2176	L2177	M2178	N2196	R2199	M2203	V2212	G2216	GLY	GLY	THR	GLU	ALA	LYS	PRO	GLU	ALA	ASP	GLU	GLU	ASP	R1994	S2000								
LYS	GLU	ASP	GLU	GLU	GLU	LYS	ASP	ALA	ALA	ASP	C2021	P2022	L2023	T2044	GLN	LEU	GLU	PRO	GLU	GLU	THR	SER	LEU	SER	SER	ARG	LEU	ARG	SER	LEU	GLU	THR	VAL	LEU	VAL	LYS	LYS	SER	ALA	LYS	PRO	GLU	ALA	ASP	GLU	GLU	ASP	R1994	S2000										
ALA	R1768	L1762	V1765	P1773	L1786	PRO	ALA	ALA	GLY	VAL	C2021	P2022	L2023	T2044	GLN	LEU	GLU	PRO	GLU	GLU	THR	SER	LEU	SER	SER	ARG	LEU	ARG	SER	LEU	GLU	THR	VAL	LEU	VAL	LYS	LYS	SER	ALA	LYS	PRO	GLU	ALA	ASP	GLU	GLU	ASP	R1994	S2000										





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

Chain B: 86% 11% .



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

Chain H: 86% 11% .



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

Chain N: 86% 11% .



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

Chain T: 86% 11% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	694588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.866	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.123	Depositor
Map size (Å)	491.52, 491.52, 491.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 117, CFF, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	2/32589 (0.0%)	0.55	7/44174 (0.0%)
1	G	0.37	2/32589 (0.0%)	0.55	7/44174 (0.0%)
1	M	0.37	2/32589 (0.0%)	0.55	7/44174 (0.0%)
1	S	0.37	2/32589 (0.0%)	0.55	7/44174 (0.0%)
2	B	0.18	0/827	0.38	0/1111
2	H	0.18	0/827	0.38	0/1111
2	N	0.18	0/827	0.38	0/1111
2	T	0.18	0/827	0.38	0/1111
All	All	0.36	8/133664 (0.0%)	0.54	28/181140 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4915	VAL	C-O	-5.97	1.17	1.24
1	G	4915	VAL	C-O	-5.97	1.17	1.24
1	M	4915	VAL	C-O	-5.97	1.17	1.24
1	S	4915	VAL	C-O	-5.97	1.17	1.24
1	A	4640	GLU	N-CA	5.53	1.50	1.46
1	G	4640	GLU	N-CA	5.53	1.50	1.46
1	M	4640	GLU	N-CA	5.53	1.50	1.46
1	S	4640	GLU	N-CA	5.53	1.50	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4697	VAL	N-CA-C	-7.50	104.00	113.22
1	G	4697	VAL	N-CA-C	-7.50	104.00	113.22
1	M	4697	VAL	N-CA-C	-7.50	104.00	113.22
1	S	4697	VAL	N-CA-C	-7.50	104.00	113.22
1	A	4164	LEU	N-CA-C	-5.56	105.23	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4164	LEU	N-CA-C	-5.56	105.23	112.23
1	M	4164	LEU	N-CA-C	-5.56	105.23	112.23
1	S	4164	LEU	N-CA-C	-5.56	105.23	112.23
1	A	1012	ASP	CA-C-N	5.48	123.69	120.24
1	A	1012	ASP	C-N-CA	5.48	123.69	120.24
1	G	1012	ASP	CA-C-N	5.48	123.69	120.24
1	G	1012	ASP	C-N-CA	5.48	123.69	120.24
1	M	1012	ASP	CA-C-N	5.48	123.69	120.24
1	M	1012	ASP	C-N-CA	5.48	123.69	120.24
1	S	1012	ASP	CA-C-N	5.48	123.69	120.24
1	S	1012	ASP	C-N-CA	5.48	123.69	120.24
1	A	4867	GLU	N-CA-C	-5.23	107.03	113.41
1	G	4867	GLU	N-CA-C	-5.23	107.03	113.41
1	M	4867	GLU	N-CA-C	-5.23	107.03	113.41
1	S	4867	GLU	N-CA-C	-5.23	107.03	113.41
1	A	1011	GLN	N-CA-C	5.21	117.65	110.35
1	G	1011	GLN	N-CA-C	5.21	117.65	110.35
1	M	1011	GLN	N-CA-C	5.21	117.65	110.35
1	S	1011	GLN	N-CA-C	5.21	117.65	110.35
1	A	4877	ASP	N-CA-C	-5.14	107.00	113.28
1	G	4877	ASP	N-CA-C	-5.14	107.00	113.28
1	M	4877	ASP	N-CA-C	-5.14	107.00	113.28
1	S	4877	ASP	N-CA-C	-5.14	107.00	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31873	0	31185	400	0
1	G	31873	0	31185	408	0
1	M	31873	0	31185	403	0
1	S	31873	0	31185	406	0
2	B	811	0	806	8	0
2	H	811	0	806	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	811	0	806	8	0
2	T	811	0	806	8	0
3	A	14	0	10	1	0
3	G	14	0	10	1	0
3	M	14	0	10	1	0
3	S	14	0	10	1	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
4	M	1	0	0	0	0
4	S	1	0	0	0	0
5	A	123	0	102	8	0
5	G	123	0	102	10	0
5	M	123	0	102	10	0
5	S	123	0	102	9	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
All	All	131292	0	128412	1642	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 6.

All (1642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4629:TYR:OH	1:S:4860:ARG:NH1	1.94	1.00
1:M:4860:ARG:NH1	1:S:4629:TYR:OH	1.94	0.99
1:G:4860:ARG:NH1	1:M:4629:TYR:OH	1.94	0.98
1:A:4860:ARG:NH1	1:G:4629:TYR:OH	1.94	0.98
1:A:2626:LEU:HD22	1:A:2640:PRO:HB3	1.47	0.96
1:M:2626:LEU:HD22	1:M:2640:PRO:HB3	1.47	0.96
1:G:2626:LEU:HD22	1:G:2640:PRO:HB3	1.47	0.96
1:S:2626:LEU:HD22	1:S:2640:PRO:HB3	1.47	0.96
1:A:4205:TRP:CZ3	1:A:4989:MET:HE1	2.05	0.91
1:S:4205:TRP:CZ3	1:S:4989:MET:HE1	2.05	0.91
1:G:2324:ASN:OD1	1:G:2326:CYS:SG	2.29	0.90
1:M:2324:ASN:OD1	1:M:2326:CYS:SG	2.29	0.90
1:G:4205:TRP:CZ3	1:G:4989:MET:HE1	2.05	0.90
1:A:1638:ALA:HB1	1:A:1647:CYS:SG	2.12	0.90
1:S:2324:ASN:OD1	1:S:2326:CYS:SG	2.29	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4205:TRP:CZ3	1:M:4989:MET:HE1	2.05	0.89
1:A:2324:ASN:OD1	1:A:2326:CYS:SG	2.29	0.89
1:G:1638:ALA:HB1	1:G:1647:CYS:SG	2.12	0.89
1:M:1638:ALA:HB1	1:M:1647:CYS:SG	2.12	0.89
1:S:1638:ALA:HB1	1:S:1647:CYS:SG	2.12	0.88
1:G:206:CYS:SG	1:G:334:MET:HE1	2.17	0.85
1:M:206:CYS:SG	1:M:334:MET:HE1	2.17	0.85
1:S:206:CYS:SG	1:S:334:MET:HE1	2.17	0.84
1:A:206:CYS:SG	1:A:334:MET:HE1	2.17	0.83
1:G:989:ALA:HB2	1:G:1039:LEU:HD12	1.60	0.83
1:G:1426:ILE:CG2	1:G:1429:ASN:HB2	2.09	0.83
1:M:989:ALA:HB2	1:M:1039:LEU:HD12	1.60	0.83
1:A:989:ALA:HB2	1:A:1039:LEU:HD12	1.60	0.83
1:A:1426:ILE:CG2	1:A:1429:ASN:HB2	2.09	0.83
1:M:1426:ILE:CG2	1:M:1429:ASN:HB2	2.09	0.83
1:S:1426:ILE:CG2	1:S:1429:ASN:HB2	2.09	0.82
1:S:989:ALA:HB2	1:S:1039:LEU:HD12	1.60	0.82
1:S:3324:VAL:HG21	1:S:3361:THR:HG22	1.61	0.82
1:A:3324:VAL:HG21	1:A:3361:THR:HG22	1.61	0.82
1:G:2670:GLU:OE2	1:G:2916:LYS:HE3	1.81	0.81
1:G:3324:VAL:HG21	1:G:3361:THR:HG22	1.61	0.81
1:A:2670:GLU:OE2	1:A:2916:LYS:HE3	1.81	0.81
1:G:1156:THR:OG1	1:G:1157:GLU:OE1	1.99	0.81
1:M:3324:VAL:HG21	1:M:3361:THR:HG22	1.61	0.81
1:S:1156:THR:OG1	1:S:1157:GLU:OE1	1.99	0.81
1:A:3575:LEU:HD13	1:S:1219:LEU:CD1	2.11	0.81
1:A:1219:LEU:CD1	1:G:3575:LEU:HD13	2.11	0.80
1:M:1219:LEU:CD1	1:S:3575:LEU:HD13	2.11	0.80
1:M:2670:GLU:OE2	1:M:2916:LYS:HE3	1.81	0.80
1:S:2670:GLU:OE2	1:S:2916:LYS:HE3	1.81	0.80
1:G:1219:LEU:CD1	1:M:3575:LEU:HD13	2.11	0.80
1:G:4205:TRP:CH2	1:G:4989:MET:HE1	2.17	0.80
1:M:4205:TRP:CH2	1:M:4989:MET:HE1	2.17	0.79
1:S:4205:TRP:CH2	1:S:4989:MET:HE1	2.17	0.79
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	1.99	0.79
1:M:1156:THR:OG1	1:M:1157:GLU:OE1	1.99	0.79
1:M:1272:LEU:HD23	1:M:1561:VAL:HG21	1.65	0.79
1:A:4205:TRP:CH2	1:A:4989:MET:HE1	2.17	0.79
1:G:1272:LEU:HD23	1:G:1561:VAL:HG21	1.65	0.78
1:S:1272:LEU:HD23	1:S:1561:VAL:HG21	1.65	0.78
1:A:1272:LEU:HD23	1:A:1561:VAL:HG21	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:HIS:ND1	1:G:196:MET:HB2	2.01	0.76
1:M:667:MET:SD	1:M:790:ARG:NH2	2.59	0.76
1:A:181:HIS:ND1	1:A:196:MET:HB2	2.01	0.76
1:G:667:MET:SD	1:G:790:ARG:NH2	2.59	0.76
1:A:667:MET:SD	1:A:790:ARG:NH2	2.59	0.76
1:S:181:HIS:ND1	1:S:196:MET:HB2	2.01	0.76
1:S:667:MET:SD	1:S:790:ARG:NH2	2.59	0.75
1:A:2172:PRO:O	1:A:2176:ASN:ND2	2.20	0.75
1:M:2172:PRO:O	1:M:2176:ASN:ND2	2.20	0.75
1:M:2196:ASN:OD1	1:M:2199:ARG:NH2	2.20	0.75
1:M:181:HIS:ND1	1:M:196:MET:HB2	2.01	0.75
1:A:110:ARG:NH2	1:A:115:ARG:NH2	2.36	0.74
1:G:2172:PRO:O	1:G:2176:ASN:ND2	2.20	0.74
1:G:2196:ASN:OD1	1:G:2199:ARG:NH2	2.20	0.74
1:A:788:LYS:HG2	1:A:1629:GLN:HG3	1.70	0.74
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.20	0.74
1:G:110:ARG:NH2	1:G:115:ARG:NH2	2.36	0.74
1:S:2196:ASN:OD1	1:S:2199:ARG:NH2	2.20	0.74
1:M:414:PHE:CE2	1:M:418:LEU:HD11	2.23	0.74
1:G:414:PHE:CE2	1:G:418:LEU:HD11	2.23	0.74
1:G:2523:ASP:OD2	1:G:2575:ARG:NH2	2.21	0.74
1:S:788:LYS:HG2	1:S:1629:GLN:HG3	1.70	0.74
1:S:2172:PRO:O	1:S:2176:ASN:ND2	2.20	0.74
1:S:3329:ILE:O	1:S:3403:ARG:NH2	2.21	0.74
1:M:110:ARG:NH2	1:M:115:ARG:NH2	2.36	0.73
1:S:414:PHE:CE2	1:S:418:LEU:HD11	2.23	0.73
1:G:3329:ILE:O	1:G:3403:ARG:NH2	2.21	0.73
1:S:110:ARG:NH2	1:S:115:ARG:NH2	2.36	0.73
5:S:5104:117:H83	5:S:5105:117:H931	1.70	0.73
5:G:5104:117:H83	5:G:5105:117:H931	1.70	0.73
1:M:2523:ASP:OD2	1:M:2575:ARG:NH2	2.21	0.73
5:M:5104:117:H83	5:M:5105:117:H931	1.70	0.73
1:S:2523:ASP:OD2	1:S:2575:ARG:NH2	2.21	0.73
1:A:2523:ASP:OD2	1:A:2575:ARG:NH2	2.21	0.73
1:A:3329:ILE:O	1:A:3403:ARG:NH2	2.21	0.73
5:A:5104:117:H83	5:A:5105:117:H931	1.70	0.73
1:M:3329:ILE:O	1:M:3403:ARG:NH2	2.21	0.73
1:G:4670:ILE:HB	1:G:4714:ASN:HD21	1.54	0.73
1:A:3182:TYR:O	1:A:3186:LEU:HD23	1.89	0.73
1:G:788:LYS:HG2	1:G:1629:GLN:HG3	1.70	0.72
1:M:788:LYS:HG2	1:M:1629:GLN:HG3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:PHE:CE2	1:A:418:LEU:HD11	2.23	0.72
1:S:4205:TRP:CZ3	1:S:4989:MET:CE	2.73	0.72
1:A:1108:GLU:N	1:A:1108:GLU:OE1	2.23	0.72
1:M:4670:ILE:HB	1:M:4714:ASN:HD21	1.54	0.72
1:S:4670:ILE:HB	1:S:4714:ASN:HD21	1.54	0.72
1:G:4205:TRP:CZ3	1:G:4989:MET:CE	2.73	0.72
1:S:1108:GLU:OE1	1:S:1108:GLU:N	2.23	0.72
1:A:4205:TRP:CZ3	1:A:4989:MET:CE	2.73	0.72
1:S:3182:TYR:O	1:S:3186:LEU:HD23	1.89	0.71
1:G:3182:TYR:O	1:G:3186:LEU:HD23	1.89	0.71
1:G:1108:GLU:N	1:G:1108:GLU:OE1	2.23	0.71
1:M:3182:TYR:O	1:M:3186:LEU:HD23	1.89	0.71
1:A:4670:ILE:HB	1:A:4714:ASN:ND2	2.06	0.71
1:M:20:VAL:HG21	1:M:202:MET:HG3	1.73	0.71
1:M:4205:TRP:CZ3	1:M:4989:MET:CE	2.73	0.71
1:A:20:VAL:HG21	1:A:202:MET:HG3	1.73	0.71
1:S:20:VAL:HG21	1:S:202:MET:HG3	1.73	0.71
1:G:20:VAL:HG21	1:G:202:MET:HG3	1.73	0.71
1:G:4670:ILE:HB	1:G:4714:ASN:ND2	2.06	0.71
1:A:4670:ILE:HB	1:A:4714:ASN:HD21	1.54	0.71
1:M:1108:GLU:OE1	1:M:1108:GLU:N	2.23	0.70
1:M:3017:PHE:O	1:M:3036:LYS:NZ	2.24	0.70
1:S:3017:PHE:O	1:S:3036:LYS:NZ	2.24	0.70
1:S:4670:ILE:HB	1:S:4714:ASN:ND2	2.06	0.70
1:G:3017:PHE:O	1:G:3036:LYS:NZ	2.24	0.70
1:M:3534:MET:HA	1:M:3534:MET:HE3	1.72	0.70
1:M:52:THR:O	1:M:52:THR:HG22	1.91	0.70
1:M:4670:ILE:HB	1:M:4714:ASN:ND2	2.06	0.70
1:A:52:THR:HG22	1:A:52:THR:O	1.91	0.70
1:S:52:THR:HG22	1:S:52:THR:O	1.91	0.69
1:S:3534:MET:HA	1:S:3534:MET:HE3	1.72	0.69
1:A:3534:MET:HA	1:A:3534:MET:HE3	1.72	0.69
1:G:52:THR:O	1:G:52:THR:HG22	1.91	0.69
1:A:4205:TRP:CZ3	1:A:4989:MET:SD	2.86	0.69
1:G:4205:TRP:CZ3	1:G:4989:MET:SD	2.86	0.69
1:M:4205:TRP:CZ3	1:M:4989:MET:SD	2.86	0.69
1:A:3017:PHE:O	1:A:3036:LYS:NZ	2.24	0.69
1:G:3534:MET:HA	1:G:3534:MET:HE3	1.72	0.69
1:S:3144:PHE:CE2	1:S:3197:LEU:HD12	2.28	0.69
1:S:4205:TRP:CZ3	1:S:4989:MET:SD	2.86	0.69
1:M:4820:VAL:HG23	5:M:5103:117:C83	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:4820:VAL:HG23	5:S:5103:117:C83	2.23	0.68
2:T:106:ASN:OD1	2:T:107:LEU:N	2.27	0.68
1:M:4863:TYR:CD2	1:M:4876:CYS:SG	2.87	0.68
1:S:4581:LYS:HD2	1:S:4632:LEU:HD22	1.76	0.68
1:A:4863:TYR:CD2	1:A:4876:CYS:SG	2.87	0.68
1:M:4581:LYS:HD2	1:M:4632:LEU:HD22	1.76	0.68
1:S:4863:TYR:CD2	1:S:4876:CYS:SG	2.87	0.68
1:A:3144:PHE:CE2	1:A:3197:LEU:HD12	2.28	0.68
1:G:3144:PHE:CE2	1:G:3197:LEU:HD12	2.28	0.68
1:A:4581:LYS:HD2	1:A:4632:LEU:HD22	1.76	0.67
1:G:4581:LYS:HD2	1:G:4632:LEU:HD22	1.76	0.67
1:G:4820:VAL:HG23	5:G:5103:117:C83	2.23	0.67
1:M:3144:PHE:CE2	1:M:3197:LEU:HD12	2.28	0.67
1:A:4231:MET:HA	1:A:4231:MET:HE3	1.76	0.67
1:A:4820:VAL:HG23	5:A:5103:117:C83	2.23	0.67
2:H:106:ASN:OD1	2:H:107:LEU:N	2.27	0.67
1:G:4863:TYR:CD2	1:G:4876:CYS:SG	2.87	0.67
2:B:106:ASN:OD1	2:B:107:LEU:N	2.27	0.67
1:G:2212:VAL:HG22	1:G:2256:TYR:CE2	2.30	0.67
1:G:4231:MET:HA	1:G:4231:MET:HE3	1.76	0.67
1:S:4231:MET:HA	1:S:4231:MET:HE3	1.76	0.67
1:A:2212:VAL:HG22	1:A:2256:TYR:CE2	2.30	0.67
1:M:4231:MET:HA	1:M:4231:MET:HE3	1.76	0.67
2:N:106:ASN:OD1	2:N:107:LEU:N	2.27	0.67
1:A:2449:GLU:OE1	1:A:2452:ARG:NH2	2.29	0.67
1:M:2212:VAL:HG22	1:M:2256:TYR:CE2	2.30	0.67
1:M:3062:PRO:O	1:M:3066:ASN:ND2	2.28	0.66
1:A:3062:PRO:O	1:A:3066:ASN:ND2	2.28	0.66
1:S:2212:VAL:HG22	1:S:2256:TYR:CE2	2.30	0.66
1:G:3062:PRO:O	1:G:3066:ASN:ND2	2.28	0.66
1:S:3062:PRO:O	1:S:3066:ASN:ND2	2.28	0.66
1:M:2449:GLU:OE1	1:M:2452:ARG:NH2	2.29	0.66
1:G:2449:GLU:OE1	1:G:2452:ARG:NH2	2.29	0.66
1:G:2620:GLN:NE2	1:G:2912:THR:HG22	2.11	0.65
1:S:2620:GLN:NE2	1:S:2912:THR:HG22	2.11	0.65
1:S:2449:GLU:OE1	1:S:2452:ARG:NH2	2.29	0.65
1:G:1105:ALA:HB3	1:G:1191:VAL:HG11	1.78	0.65
1:S:1105:ALA:HB3	1:S:1191:VAL:HG11	1.78	0.64
1:M:1105:ALA:HB3	1:M:1191:VAL:HG11	1.78	0.64
1:A:1105:ALA:HB3	1:A:1191:VAL:HG11	1.78	0.64
1:M:2620:GLN:NE2	1:M:2912:THR:HG22	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2620:GLN:NE2	1:A:2912:THR:HG22	2.11	0.64
1:G:988:LEU:HD23	1:G:1039:LEU:HD22	1.80	0.64
1:A:1426:ILE:HG23	1:A:1429:ASN:HB2	1.79	0.64
1:M:3969:ILE:HG21	1:M:3980:LEU:HD12	1.80	0.64
1:S:988:LEU:HD23	1:S:1039:LEU:HD22	1.80	0.64
1:G:2967:MET:HA	1:G:2967:MET:HE3	1.80	0.64
1:M:1263:THR:HG22	1:M:1264:VAL:H	1.63	0.64
1:M:988:LEU:HD23	1:M:1039:LEU:HD22	1.80	0.64
1:S:977:LEU:HD22	1:S:981:GLN:HB3	1.80	0.64
1:S:1263:THR:HG22	1:S:1264:VAL:H	1.63	0.64
1:A:977:LEU:HA	1:A:981:GLN:OE1	1.98	0.64
1:M:977:LEU:HA	1:M:981:GLN:OE1	1.98	0.64
1:S:937:CYS:SG	1:S:984:LEU:HD13	2.38	0.64
1:S:3969:ILE:HG21	1:S:3980:LEU:HD12	1.80	0.64
1:A:988:LEU:HD23	1:A:1039:LEU:HD22	1.80	0.63
1:M:4215:ARG:HG2	1:M:4219:PHE:CZ	2.33	0.63
1:S:4205:TRP:HZ3	1:S:4989:MET:HE1	1.62	0.63
1:M:1426:ILE:HG23	1:M:1429:ASN:HB2	1.79	0.63
1:A:4586:PRO:HA	1:A:4628:VAL:HG11	1.80	0.63
1:G:4215:ARG:HG2	1:G:4219:PHE:CZ	2.33	0.63
1:A:977:LEU:HD22	1:A:981:GLN:HB3	1.80	0.63
1:A:2967:MET:HE3	1:A:2967:MET:HA	1.80	0.63
1:S:1426:ILE:HG23	1:S:1429:ASN:HB2	1.79	0.63
1:G:308:HIS:O	1:G:312:THR:HG22	1.98	0.63
1:S:308:HIS:O	1:S:312:THR:HG22	1.98	0.63
1:S:4586:PRO:HA	1:S:4628:VAL:HG11	1.80	0.63
1:A:3969:ILE:HG21	1:A:3980:LEU:HD12	1.80	0.63
1:A:937:CYS:SG	1:A:984:LEU:HD13	2.38	0.63
1:G:3969:ILE:HG21	1:G:3980:LEU:HD12	1.80	0.63
1:M:977:LEU:HD22	1:M:981:GLN:HB3	1.80	0.63
1:M:2967:MET:HA	1:M:2967:MET:HE3	1.80	0.63
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.32	0.63
1:A:4222:VAL:HG12	1:A:4950:VAL:CG1	2.29	0.63
1:G:179:TYR:N	1:G:194:SER:O	2.32	0.63
1:M:937:CYS:SG	1:M:984:LEU:HD13	2.38	0.63
1:A:1263:THR:HG22	1:A:1264:VAL:H	1.63	0.63
1:M:4586:PRO:HA	1:M:4628:VAL:HG11	1.80	0.63
1:S:4215:ARG:HG2	1:S:4219:PHE:CZ	2.33	0.63
1:S:4222:VAL:HG12	1:S:4950:VAL:CG1	2.29	0.63
1:A:20:VAL:HG11	1:A:202:MET:SD	2.39	0.62
1:A:2520:HIS:O	1:A:2524:VAL:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2527:LEU:HD12	1:A:2530:MET:HE3	1.81	0.62
1:G:1131:ARG:NH1	1:G:1178:ALA:O	2.32	0.62
1:G:2527:LEU:HD12	1:G:2530:MET:HE3	1.81	0.62
1:G:4222:VAL:HG12	1:G:4950:VAL:CG1	2.29	0.62
1:M:20:VAL:HG11	1:M:202:MET:SD	2.39	0.62
1:M:4222:VAL:HG12	1:M:4950:VAL:CG1	2.29	0.62
1:A:308:HIS:O	1:A:312:THR:HG22	1.98	0.62
1:G:2520:HIS:O	1:G:2524:VAL:HG22	1.99	0.62
1:S:2967:MET:HA	1:S:2967:MET:HE3	1.80	0.62
1:G:20:VAL:HG11	1:G:202:MET:SD	2.39	0.62
1:G:937:CYS:SG	1:G:984:LEU:HD13	2.38	0.62
1:S:977:LEU:HA	1:S:981:GLN:OE1	1.98	0.62
1:A:179:TYR:N	1:A:194:SER:O	2.32	0.62
1:A:701:GLY:O	1:A:1647:CYS:HB2	2.00	0.62
1:G:1426:ILE:HG23	1:G:1429:ASN:HB2	1.79	0.62
1:G:977:LEU:HD22	1:G:981:GLN:HB3	1.80	0.62
1:G:977:LEU:HA	1:G:981:GLN:OE1	1.98	0.62
1:M:2520:HIS:O	1:M:2524:VAL:HG22	1.99	0.62
1:S:2520:HIS:O	1:S:2524:VAL:HG22	1.99	0.62
1:M:308:HIS:O	1:M:312:THR:HG22	1.98	0.62
1:M:1131:ARG:NH1	1:M:1178:ALA:O	2.32	0.62
1:S:20:VAL:HG11	1:S:202:MET:SD	2.39	0.62
1:S:1131:ARG:NH1	1:S:1178:ALA:O	2.32	0.62
1:A:4215:ARG:HG2	1:A:4219:PHE:CZ	2.33	0.62
1:G:1263:THR:HG22	1:G:1264:VAL:H	1.63	0.62
1:G:2862:LEU:CD1	1:G:2932:MET:HE1	2.30	0.62
1:M:179:TYR:N	1:M:194:SER:O	2.32	0.61
1:A:2862:LEU:CD1	1:A:2932:MET:HE1	2.30	0.61
1:G:701:GLY:O	1:G:1647:CYS:HB2	2.00	0.61
1:M:3110:LEU:O	1:M:3110:LEU:HD23	2.00	0.61
1:S:179:TYR:N	1:S:194:SER:O	2.32	0.61
1:S:676:THR:HG22	1:S:677:ALA:H	1.65	0.61
1:M:2626:LEU:CD2	1:M:2640:PRO:HB3	2.27	0.61
1:S:206:CYS:SG	1:S:334:MET:CE	2.88	0.61
1:S:701:GLY:O	1:S:1647:CYS:HB2	2.00	0.61
1:S:2527:LEU:HD12	1:S:2530:MET:HE3	1.81	0.61
1:A:676:THR:HG22	1:A:677:ALA:H	1.65	0.61
1:G:3110:LEU:O	1:G:3110:LEU:HD23	2.00	0.61
1:G:4586:PRO:HA	1:G:4628:VAL:HG11	1.80	0.61
1:G:4820:VAL:HG23	5:G:5103:117:H83	1.83	0.61
1:S:2626:LEU:CD2	1:S:2640:PRO:HB3	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2485:LEU:HD22	1:A:2541:PHE:HE1	1.65	0.61
1:M:206:CYS:SG	1:M:334:MET:CE	2.88	0.61
1:M:2527:LEU:HD12	1:M:2530:MET:HE3	1.81	0.61
1:G:676:THR:HG22	1:G:677:ALA:H	1.65	0.61
1:G:2161:GLN:O	1:G:2165:LEU:HD22	2.01	0.61
1:G:2485:LEU:HD22	1:G:2541:PHE:HE1	1.65	0.61
1:M:701:GLY:O	1:M:1647:CYS:HB2	2.00	0.61
1:A:4820:VAL:HG23	5:A:5103:117:H83	1.83	0.61
1:G:206:CYS:SG	1:G:334:MET:CE	2.88	0.61
1:A:206:CYS:SG	1:A:334:MET:CE	2.88	0.60
1:G:989:ALA:HB2	1:G:1039:LEU:CD1	2.31	0.60
1:M:2862:LEU:CD1	1:M:2932:MET:HE1	2.30	0.60
1:M:4059:LEU:HD22	1:M:4170:ILE:CD1	2.31	0.60
1:S:4059:LEU:HD22	1:S:4170:ILE:CD1	2.31	0.60
1:A:2626:LEU:CD2	1:A:2640:PRO:HB3	2.27	0.60
1:M:676:THR:HG22	1:M:677:ALA:H	1.65	0.60
1:M:4820:VAL:HG23	5:M:5103:117:H83	1.83	0.60
1:A:989:ALA:HB2	1:A:1039:LEU:CD1	2.31	0.60
1:M:2485:LEU:HD22	1:M:2541:PHE:HE1	1.65	0.60
1:S:2485:LEU:HD22	1:S:2541:PHE:HE1	1.65	0.60
1:A:2116:LEU:O	1:A:2120:MET:HG2	2.02	0.60
1:G:2175:GLU:HA	1:G:2228:MET:HE1	1.83	0.60
1:S:2862:LEU:CD1	1:S:2932:MET:HE1	2.30	0.60
1:S:4820:VAL:HG23	5:S:5103:117:H83	1.83	0.60
1:A:799:GLU:OE1	1:A:1623:ARG:NH1	2.35	0.60
1:A:4059:LEU:HD22	1:A:4170:ILE:CD1	2.31	0.60
1:G:1272:LEU:HD23	1:G:1561:VAL:CG2	2.32	0.60
1:S:2161:GLN:O	1:S:2165:LEU:HD22	2.01	0.60
1:A:2161:GLN:O	1:A:2165:LEU:HD22	2.01	0.60
1:A:3110:LEU:HD23	1:A:3110:LEU:O	2.00	0.60
1:G:2116:LEU:O	1:G:2120:MET:HG2	2.02	0.60
1:G:4059:LEU:HD22	1:G:4170:ILE:CD1	2.31	0.60
1:M:2161:GLN:O	1:M:2165:LEU:HD22	2.01	0.60
1:S:3110:LEU:O	1:S:3110:LEU:HD23	2.00	0.60
1:M:2175:GLU:HA	1:M:2228:MET:HE1	1.83	0.59
1:A:2175:GLU:HA	1:A:2228:MET:HE1	1.83	0.59
1:S:2116:LEU:O	1:S:2120:MET:HG2	2.02	0.59
1:A:457:GLU:OE1	1:A:457:GLU:N	2.35	0.59
1:G:457:GLU:OE1	1:G:457:GLU:N	2.35	0.59
1:G:2598:ALA:O	1:G:2602:VAL:HG23	2.03	0.59
1:M:937:CYS:SG	1:M:984:LEU:CD1	2.91	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:LEU:HD23	1:A:1561:VAL:CG2	2.32	0.59
1:A:4215:ARG:O	1:A:4218:ILE:HG22	2.03	0.59
1:S:457:GLU:N	1:S:457:GLU:OE1	2.35	0.59
1:G:4083:ASP:OD2	1:G:4085:ARG:NH2	2.36	0.59
1:M:4083:ASP:OD2	1:M:4085:ARG:NH2	2.36	0.59
1:M:4205:TRP:HZ3	1:M:4989:MET:HE1	1.62	0.59
1:S:156:GLN:OE1	1:S:156:GLN:N	2.36	0.59
1:S:937:CYS:SG	1:S:984:LEU:CD1	2.91	0.59
1:S:2175:GLU:HA	1:S:2228:MET:HE1	1.83	0.59
1:G:4205:TRP:HZ3	1:G:4989:MET:HE1	1.62	0.59
1:G:4215:ARG:O	1:G:4218:ILE:HG22	2.03	0.59
1:S:4059:LEU:HD22	1:S:4170:ILE:HD12	1.85	0.59
1:G:156:GLN:OE1	1:G:156:GLN:N	2.36	0.59
1:M:156:GLN:N	1:M:156:GLN:OE1	2.36	0.59
1:M:2598:ALA:O	1:M:2602:VAL:HG23	2.03	0.59
1:G:281:ARG:NH2	1:G:307:ALA:O	2.36	0.58
1:G:799:GLU:OE1	1:G:1623:ARG:NH1	2.35	0.58
1:G:937:CYS:SG	1:G:984:LEU:CD1	2.91	0.58
1:M:281:ARG:NH2	1:M:307:ALA:O	2.36	0.58
1:M:2116:LEU:O	1:M:2120:MET:HG2	2.02	0.58
1:S:281:ARG:NH2	1:S:307:ALA:O	2.36	0.58
1:S:799:GLU:OE1	1:S:1623:ARG:NH1	2.35	0.58
1:S:3020:THR:HG22	1:S:3021:PRO:HD2	1.85	0.58
1:A:281:ARG:NH2	1:A:307:ALA:O	2.36	0.58
1:A:937:CYS:SG	1:A:984:LEU:CD1	2.91	0.58
1:A:4083:ASP:OD2	1:A:4085:ARG:NH2	2.36	0.58
1:M:457:GLU:OE1	1:M:457:GLU:N	2.35	0.58
1:M:989:ALA:HB2	1:M:1039:LEU:CD1	2.31	0.58
1:M:2544:THR:HG23	1:M:2547:ALA:H	1.68	0.58
1:S:195:PHE:C	1:S:196:MET:HE2	2.29	0.58
1:A:156:GLN:OE1	1:A:156:GLN:N	2.36	0.58
1:M:1272:LEU:HD23	1:M:1561:VAL:CG2	2.32	0.58
1:M:4059:LEU:HD22	1:M:4170:ILE:HD12	1.85	0.58
1:S:4215:ARG:O	1:S:4218:ILE:HG22	2.03	0.58
1:S:4820:VAL:CG2	5:S:5103:117:C83	2.81	0.58
1:A:2598:ALA:O	1:A:2602:VAL:HG23	2.03	0.58
1:G:4059:LEU:HD22	1:G:4170:ILE:HD12	1.85	0.58
1:S:2544:THR:HG23	1:S:2547:ALA:H	1.68	0.58
1:A:3944:GLU:OE1	1:A:3944:GLU:N	2.37	0.58
1:A:169:LEU:HD23	1:A:169:LEU:H	1.69	0.58
1:A:3020:THR:HG22	1:A:3021:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4820:VAL:CG2	5:A:5103:117:C83	2.81	0.58
1:G:2165:LEU:HB2	1:G:2178:MET:HE2	1.86	0.58
1:M:195:PHE:C	1:M:196:MET:HE2	2.29	0.58
1:M:3944:GLU:OE1	1:M:3944:GLU:N	2.37	0.58
1:G:2544:THR:HG23	1:G:2547:ALA:H	1.68	0.58
1:M:799:GLU:OE1	1:M:1623:ARG:NH1	2.35	0.58
1:M:4215:ARG:O	1:M:4218:ILE:HG22	2.03	0.58
1:S:989:ALA:HB2	1:S:1039:LEU:CD1	2.31	0.58
1:G:195:PHE:C	1:G:196:MET:HE2	2.29	0.58
1:G:3201:MET:HE3	1:G:3203:VAL:HG12	1.86	0.58
1:A:2544:THR:HG23	1:A:2547:ALA:H	1.68	0.58
1:G:3944:GLU:N	1:G:3944:GLU:OE1	2.37	0.58
1:M:4820:VAL:CG2	5:M:5103:117:C83	2.81	0.58
1:A:181:HIS:CE1	1:A:196:MET:HB2	2.39	0.57
1:A:195:PHE:C	1:A:196:MET:HE2	2.29	0.57
1:G:169:LEU:HD23	1:G:169:LEU:H	1.69	0.57
1:S:2598:ALA:O	1:S:2602:VAL:HG23	2.03	0.57
1:S:4573:ILE:HG23	1:S:4643:LEU:HD11	1.86	0.57
1:G:4820:VAL:CG2	5:G:5103:117:C83	2.81	0.57
1:S:4083:ASP:OD2	1:S:4085:ARG:NH2	2.36	0.57
1:A:2165:LEU:HB2	1:A:2178:MET:HE2	1.86	0.57
1:A:2635:GLU:OE1	1:A:2635:GLU:N	2.37	0.57
1:M:3169:LEU:HD13	1:M:3194:LEU:HD11	1.87	0.57
1:M:4573:ILE:HG23	1:M:4643:LEU:HD11	1.86	0.57
1:S:4217:PHE:CE1	1:S:4237:PHE:HB2	2.40	0.57
1:A:4059:LEU:HD22	1:A:4170:ILE:HD12	1.85	0.57
1:G:1157:GLU:OE1	1:G:1157:GLU:N	2.37	0.57
1:G:4576:ILE:HG23	1:G:4639:MET:HE2	1.86	0.57
1:M:3020:THR:HG22	1:M:3021:PRO:HD2	1.85	0.57
1:M:3201:MET:HE3	1:M:3203:VAL:HG12	1.86	0.57
1:G:2635:GLU:OE1	1:G:2635:GLU:N	2.37	0.57
1:M:1219:LEU:HD13	1:S:3575:LEU:HD13	1.86	0.57
1:S:169:LEU:HD23	1:S:169:LEU:H	1.69	0.57
1:S:3169:LEU:HD13	1:S:3194:LEU:HD11	1.87	0.57
1:S:3944:GLU:OE1	1:S:3944:GLU:N	2.37	0.57
1:G:414:PHE:CD1	1:G:436:LEU:HD22	2.40	0.57
1:M:2635:GLU:N	1:M:2635:GLU:OE1	2.37	0.57
1:M:4217:PHE:CE1	1:M:4237:PHE:HB2	2.40	0.57
1:M:181:HIS:CE1	1:M:196:MET:HB2	2.39	0.57
1:S:4576:ILE:HG23	1:S:4639:MET:HE2	1.86	0.57
1:A:1157:GLU:OE1	1:A:1157:GLU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3201:MET:HE3	1:A:3203:VAL:HG12	1.86	0.57
1:G:3020:THR:HG22	1:G:3021:PRO:HD2	1.85	0.57
1:M:414:PHE:CD1	1:M:436:LEU:HD22	2.40	0.57
1:A:4217:PHE:CE1	1:A:4237:PHE:HB2	2.40	0.57
1:A:4576:ILE:HG23	1:A:4639:MET:HE2	1.86	0.57
1:M:1157:GLU:OE1	1:M:1157:GLU:N	2.37	0.57
1:S:1157:GLU:OE1	1:S:1157:GLU:N	2.37	0.57
1:S:2165:LEU:HB2	1:S:2178:MET:HE2	1.86	0.57
1:G:2626:LEU:CD2	1:G:2640:PRO:HB3	2.27	0.56
1:S:1272:LEU:HD23	1:S:1561:VAL:CG2	2.32	0.56
1:M:2165:LEU:HB2	1:M:2178:MET:HE2	1.86	0.56
1:S:181:HIS:CE1	1:S:196:MET:HB2	2.39	0.56
1:S:3201:MET:HE3	1:S:3203:VAL:HG12	1.86	0.56
1:A:414:PHE:CD1	1:A:436:LEU:HD22	2.40	0.56
1:G:181:HIS:CE1	1:G:196:MET:HB2	2.39	0.56
1:M:4670:ILE:CG2	1:M:4714:ASN:ND2	2.69	0.56
1:S:414:PHE:CD1	1:S:436:LEU:HD22	2.40	0.56
1:A:3575:LEU:HD13	1:S:1219:LEU:HD13	1.86	0.56
1:G:3169:LEU:HD13	1:G:3194:LEU:HD11	1.87	0.56
1:G:4217:PHE:CE1	1:G:4237:PHE:HB2	2.40	0.56
1:A:3057:PHE:O	1:A:3060:ASP:OD1	2.24	0.56
1:M:3057:PHE:O	1:M:3060:ASP:OD1	2.24	0.56
1:A:4573:ILE:HG23	1:A:4643:LEU:HD11	1.86	0.56
1:G:2807:TRP:HB3	1:G:2808:PRO:HD3	1.88	0.56
1:G:4670:ILE:CG2	1:G:4714:ASN:ND2	2.69	0.56
1:M:4101:LYS:O	1:M:4101:LYS:HG2	2.06	0.56
1:S:2635:GLU:OE1	1:S:2635:GLU:N	2.37	0.56
1:S:3057:PHE:O	1:S:3060:ASP:OD1	2.24	0.56
1:A:4101:LYS:HG2	1:A:4101:LYS:O	2.06	0.56
1:A:4670:ILE:CG2	1:A:4714:ASN:ND2	2.69	0.56
1:G:4205:TRP:CH2	1:G:4989:MET:CE	2.89	0.56
1:M:169:LEU:H	1:M:169:LEU:HD23	1.69	0.56
1:S:3007:ASN:O	1:S:3011:THR:OG1	2.16	0.56
1:M:4576:ILE:HG23	1:M:4639:MET:HE2	1.86	0.56
1:A:3169:LEU:HD13	1:A:3194:LEU:HD11	1.87	0.56
1:M:3007:ASN:O	1:M:3011:THR:OG1	2.16	0.56
1:S:2807:TRP:HB3	1:S:2808:PRO:HD3	1.88	0.55
1:S:4101:LYS:O	1:S:4101:LYS:HG2	2.06	0.55
1:S:4670:ILE:CG2	1:S:4714:ASN:ND2	2.69	0.55
1:G:3057:PHE:O	1:G:3060:ASP:OD1	2.24	0.55
1:M:2807:TRP:HB3	1:M:2808:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:4670:ILE:CB	1:S:4714:ASN:ND2	2.70	0.55
1:G:4101:LYS:O	1:G:4101:LYS:HG2	2.06	0.55
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.88	0.55
1:A:4837:LEU:HD11	1:A:4932:ILE:HG23	1.88	0.55
1:G:4573:ILE:HG23	1:G:4643:LEU:HD11	1.86	0.55
1:G:4670:ILE:CB	1:G:4714:ASN:ND2	2.70	0.55
1:M:2778:GLY:HA3	1:M:2787:THR:HB	1.89	0.55
1:M:20:VAL:HG21	1:M:202:MET:SD	2.47	0.55
1:A:293:LEU:HD12	1:A:378:LEU:HD12	1.89	0.55
1:G:20:VAL:HG21	1:G:202:MET:SD	2.47	0.55
1:G:989:ALA:CB	1:G:1039:LEU:HD12	2.35	0.55
1:G:1219:LEU:HD13	1:M:3575:LEU:HD13	1.86	0.55
1:G:1943:LEU:HD13	1:G:2098:VAL:HG22	1.88	0.55
1:S:293:LEU:HD12	1:S:378:LEU:HD12	1.89	0.55
1:A:2212:VAL:HG22	1:A:2256:TYR:HE2	1.72	0.55
1:A:4670:ILE:CB	1:A:4714:ASN:ND2	2.70	0.55
1:G:177:GLU:O	1:G:177:GLU:HG2	2.07	0.55
1:G:3078:ARG:NH1	1:G:3155:ASP:OD2	2.40	0.55
1:M:4940:PHE:O	1:M:4944:ARG:HG3	2.07	0.55
1:S:4837:LEU:HD11	1:S:4932:ILE:HG23	1.88	0.55
1:S:4940:PHE:O	1:S:4944:ARG:HG3	2.07	0.55
1:A:20:VAL:HG21	1:A:202:MET:SD	2.47	0.55
1:A:4217:PHE:CD1	1:A:4237:PHE:HB2	2.42	0.55
1:M:4217:PHE:CD1	1:M:4237:PHE:HB2	2.42	0.55
1:M:4670:ILE:CB	1:M:4714:ASN:ND2	2.70	0.55
1:M:2212:VAL:HG22	1:M:2256:TYR:HE2	1.72	0.54
1:S:110:ARG:HH22	1:S:115:ARG:HH21	1.55	0.54
1:S:2212:VAL:HG22	1:S:2256:TYR:HE2	1.72	0.54
2:B:80:ASP:OD1	2:B:81:VAL:N	2.41	0.54
1:M:177:GLU:O	1:M:177:GLU:HG2	2.07	0.54
1:S:177:GLU:O	1:S:177:GLU:HG2	2.07	0.54
1:S:4205:TRP:CH2	1:S:4989:MET:CE	2.89	0.54
1:G:3607:GLU:HA	1:G:3610:GLU:HG3	1.89	0.54
1:G:4940:PHE:O	1:G:4944:ARG:HG3	2.07	0.54
1:M:110:ARG:HH22	1:M:115:ARG:HH21	1.55	0.54
1:M:2280:VAL:HG22	1:M:2280:VAL:O	2.08	0.54
2:N:80:ASP:OD1	2:N:81:VAL:N	2.41	0.54
1:A:316:PHE:CE1	1:A:348:VAL:HG22	2.43	0.54
1:A:989:ALA:CB	1:A:1039:LEU:HD12	2.35	0.54
1:A:4205:TRP:HZ3	1:A:4989:MET:HE1	1.62	0.54
1:M:1943:LEU:HD13	1:M:2098:VAL:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2280:VAL:O	1:S:2280:VAL:HG22	2.08	0.54
1:A:2807:TRP:HB3	1:A:2808:PRO:HD3	1.88	0.54
1:G:2778:GLY:HA3	1:G:2787:THR:HB	1.89	0.54
1:M:3078:ARG:NH1	1:M:3155:ASP:OD2	2.40	0.54
1:M:3607:GLU:HA	1:M:3610:GLU:HG3	1.89	0.54
1:S:20:VAL:HG21	1:S:202:MET:SD	2.47	0.54
1:S:2778:GLY:HA3	1:S:2787:THR:HB	1.89	0.54
1:S:4217:PHE:CD1	1:S:4237:PHE:HB2	2.42	0.54
1:A:2280:VAL:O	1:A:2280:VAL:HG22	2.08	0.54
1:A:4940:PHE:O	1:A:4944:ARG:HG3	2.07	0.54
1:G:1736:VAL:HG23	1:G:1736:VAL:O	2.08	0.54
1:G:4837:LEU:HD11	1:G:4932:ILE:HG23	1.88	0.54
1:S:4899:ASP:OD1	1:S:4900:GLU:HG3	2.08	0.54
1:A:1219:LEU:HD13	1:G:3575:LEU:HD13	1.86	0.54
1:A:2670:GLU:OE2	1:A:2916:LYS:CE	2.55	0.54
1:G:316:PHE:CE1	1:G:348:VAL:HG22	2.43	0.54
1:G:4217:PHE:CD1	1:G:4237:PHE:HB2	2.42	0.54
1:M:4899:ASP:OD1	1:M:4900:GLU:HG3	2.08	0.54
1:S:20:VAL:HG21	1:S:202:MET:CG	2.38	0.54
1:S:1943:LEU:HD13	1:S:2098:VAL:HG22	1.88	0.54
1:S:3078:ARG:NH1	1:S:3155:ASP:OD2	2.40	0.54
1:G:4682:GLU:OE1	1:G:4683:PHE:CD1	2.61	0.54
1:S:1736:VAL:O	1:S:1736:VAL:HG23	2.08	0.54
1:A:3607:GLU:HA	1:A:3610:GLU:HG3	1.89	0.54
1:M:20:VAL:HG21	1:M:202:MET:CG	2.38	0.54
1:M:4837:LEU:HD11	1:M:4932:ILE:HG23	1.88	0.54
1:A:177:GLU:HG2	1:A:177:GLU:O	2.07	0.54
1:G:4670:ILE:HG22	1:G:4714:ASN:ND2	2.23	0.54
1:M:60:PRO:HG2	1:M:62:LEU:HD11	1.90	0.54
1:S:1454:THR:OG1	1:S:1456:ASP:OD1	2.24	0.54
1:G:3130:THR:HA	1:G:3133:THR:HG22	1.90	0.53
1:G:4837:LEU:CD1	1:G:4932:ILE:HG23	2.38	0.53
1:M:293:LEU:HD12	1:M:378:LEU:HD12	1.89	0.53
1:M:4837:LEU:CD1	1:M:4932:ILE:HG23	2.38	0.53
1:S:60:PRO:HG2	1:S:62:LEU:HD11	1.90	0.53
1:A:4579:PHE:CD2	1:A:4639:MET:HE1	2.44	0.53
1:A:4682:GLU:OE1	1:A:4683:PHE:CD1	2.61	0.53
1:G:293:LEU:HD12	1:G:378:LEU:HD12	1.89	0.53
1:G:4899:ASP:OD1	1:G:4900:GLU:HG3	2.08	0.53
5:M:5104:117:H83	5:M:5105:117:C93	2.39	0.53
1:S:4682:GLU:OE1	1:S:4683:PHE:CD1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:110:ARG:HH22	1:M:115:ARG:NH2	2.05	0.53
1:M:3130:THR:HA	1:M:3133:THR:HG22	1.90	0.53
1:M:4670:ILE:HG22	1:M:4714:ASN:ND2	2.23	0.53
2:T:80:ASP:OD1	2:T:81:VAL:N	2.41	0.53
1:A:1561:VAL:HG23	1:A:1562:ILE:H	1.74	0.53
1:A:4670:ILE:HG22	1:A:4714:ASN:ND2	2.23	0.53
1:G:2280:VAL:HG22	1:G:2280:VAL:O	2.08	0.53
1:G:4579:PHE:CD2	1:G:4639:MET:HE1	2.44	0.53
2:H:80:ASP:OD1	2:H:81:VAL:N	2.41	0.53
1:S:4093:PHE:CZ	1:S:4097:MET:HE2	2.44	0.53
1:G:110:ARG:HH22	1:G:115:ARG:HH21	1.55	0.53
1:G:483:MET:HE2	1:G:483:MET:HA	1.90	0.53
1:G:3996:PHE:HD1	1:G:4016:LEU:HD11	1.73	0.53
1:M:4682:GLU:OE1	1:M:4683:PHE:CD1	2.61	0.53
1:S:2670:GLU:OE2	1:S:2916:LYS:CE	2.55	0.53
1:S:3607:GLU:HA	1:S:3610:GLU:HG3	1.89	0.53
1:A:1164:LEU:HB2	1:A:1169:LEU:HD21	1.91	0.53
1:G:1561:VAL:HG23	1:G:1562:ILE:H	1.74	0.53
1:M:1736:VAL:HG23	1:M:1736:VAL:O	2.08	0.53
1:S:3996:PHE:HD1	1:S:4016:LEU:HD11	1.73	0.53
1:A:20:VAL:HG21	1:A:202:MET:CG	2.38	0.53
1:A:2778:GLY:HA3	1:A:2787:THR:HB	1.89	0.53
1:A:3130:THR:HA	1:A:3133:THR:HG22	1.90	0.53
1:G:419:ASP:OD1	1:G:419:ASP:O	2.27	0.53
1:M:316:PHE:CE1	1:M:348:VAL:HG22	2.43	0.53
1:S:4579:PHE:CD2	1:S:4639:MET:HE1	2.44	0.53
1:S:4670:ILE:HG22	1:S:4714:ASN:ND2	2.23	0.53
1:G:110:ARG:HH22	1:G:115:ARG:NH2	2.05	0.53
1:M:4093:PHE:CZ	1:M:4097:MET:HE2	2.44	0.53
1:A:52:THR:O	1:A:52:THR:CG2	2.57	0.53
1:A:627:PRO:HG3	2:B:90:GLY:HA2	1.91	0.53
1:M:52:THR:O	1:M:52:THR:CG2	2.57	0.53
1:M:4205:TRP:CH2	1:M:4989:MET:CE	2.89	0.53
1:M:4579:PHE:CD2	1:M:4639:MET:HE1	2.44	0.53
1:G:627:PRO:HG3	2:H:90:GLY:HA2	1.91	0.53
1:G:1164:LEU:HB2	1:G:1169:LEU:HD21	1.91	0.53
1:M:483:MET:HE2	1:M:483:MET:HA	1.90	0.53
1:M:1008:SER:HB3	1:M:1017:ARG:HB3	1.91	0.53
1:M:3996:PHE:HD1	1:M:4016:LEU:HD11	1.73	0.53
1:S:316:PHE:CE1	1:S:348:VAL:HG22	2.43	0.53
1:S:1164:LEU:HB2	1:S:1169:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4207:MET:HA	1:A:4207:MET:HE2	1.91	0.52
1:A:4899:ASP:OD1	1:A:4900:GLU:HG3	2.08	0.52
1:G:60:PRO:HG2	1:G:62:LEU:HD11	1.90	0.52
1:G:989:ALA:HA	1:G:1039:LEU:CD1	2.39	0.52
1:G:4093:PHE:CZ	1:G:4097:MET:HE2	2.44	0.52
1:M:627:PRO:HG3	2:N:90:GLY:HA2	1.91	0.52
1:M:1815:LEU:HD22	1:M:1845:VAL:HG21	1.91	0.52
1:S:627:PRO:HG3	2:T:90:GLY:HA2	1.91	0.52
1:S:1561:VAL:HG23	1:S:1562:ILE:H	1.74	0.52
5:S:5104:117:H83	5:S:5105:117:C93	2.39	0.52
1:A:110:ARG:HH22	1:A:115:ARG:HH21	1.55	0.52
1:A:989:ALA:HA	1:A:1039:LEU:CD1	2.39	0.52
1:A:1736:VAL:HG23	1:A:1736:VAL:O	2.08	0.52
1:A:3996:PHE:HD1	1:A:4016:LEU:HD11	1.73	0.52
1:M:169:LEU:HD12	1:M:171:LEU:HD11	1.92	0.52
1:S:1815:LEU:HD22	1:S:1845:VAL:HG21	1.91	0.52
1:A:60:PRO:HG2	1:A:62:LEU:HD11	1.90	0.52
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.24	0.52
1:G:52:THR:O	1:G:52:THR:CG2	2.57	0.52
1:G:110:ARG:NH2	1:G:115:ARG:CZ	2.73	0.52
1:S:419:ASP:OD1	1:S:419:ASP:O	2.27	0.52
1:S:483:MET:HA	1:S:483:MET:HE2	1.90	0.52
1:S:1008:SER:HB3	1:S:1017:ARG:HB3	1.91	0.52
1:A:169:LEU:HD12	1:A:171:LEU:HD11	1.92	0.52
1:A:233:ILE:O	1:A:257:ARG:NH1	2.42	0.52
1:G:2628:PHE:HZ	1:G:2907:PRO:HD3	1.74	0.52
1:G:4207:MET:HE2	1:G:4207:MET:HA	1.91	0.52
1:M:1561:VAL:HG23	1:M:1562:ILE:H	1.74	0.52
1:S:3130:THR:HA	1:S:3133:THR:HG22	1.90	0.52
1:A:110:ARG:NH2	1:A:115:ARG:CZ	2.73	0.52
1:G:1008:SER:HB3	1:G:1017:ARG:HB3	1.91	0.52
1:G:1561:VAL:HG23	1:G:1562:ILE:N	2.25	0.52
1:M:2628:PHE:HZ	1:M:2907:PRO:HD3	1.74	0.52
1:S:233:ILE:O	1:S:257:ARG:NH1	2.42	0.52
1:S:989:ALA:HA	1:S:1039:LEU:CD1	2.39	0.52
1:S:1561:VAL:HG23	1:S:1562:ILE:N	2.25	0.52
1:S:4837:LEU:CD1	1:S:4932:ILE:HG23	2.38	0.52
1:A:419:ASP:O	1:A:419:ASP:OD1	2.27	0.52
1:A:483:MET:HE2	1:A:483:MET:HA	1.90	0.52
1:A:4093:PHE:CZ	1:A:4097:MET:HE2	2.44	0.52
1:A:4837:LEU:CD1	1:A:4932:ILE:HG23	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3545:THR:O	1:M:3549:VAL:HG22	2.10	0.52
1:S:52:THR:O	1:S:52:THR:CG2	2.57	0.52
1:A:4205:TRP:CH2	1:A:4989:MET:CE	2.89	0.52
1:G:169:LEU:HD12	1:G:171:LEU:HD11	1.92	0.52
1:G:2670:GLU:OE2	1:G:2916:LYS:CE	2.55	0.52
1:G:4791:TYR:OH	1:G:4815:ASP:OD1	2.28	0.52
1:S:3545:THR:O	1:S:3549:VAL:HG22	2.10	0.52
1:A:1561:VAL:HG23	1:A:1562:ILE:N	2.25	0.52
1:M:1024:TYR:HA	1:M:1027:LEU:HD12	1.92	0.52
1:S:1024:TYR:HA	1:S:1027:LEU:HD12	1.92	0.52
1:G:4207:MET:O	1:G:4210:VAL:HG22	2.10	0.52
1:M:989:ALA:CB	1:M:1039:LEU:HD12	2.35	0.52
1:A:275:ARG:NH1	1:A:338:GLU:OE1	2.43	0.52
1:A:1008:SER:HB3	1:A:1017:ARG:HB3	1.91	0.52
1:A:1024:TYR:HA	1:A:1027:LEU:HD12	1.92	0.52
1:A:3545:THR:O	1:A:3549:VAL:HG22	2.10	0.52
1:G:1024:TYR:HA	1:G:1027:LEU:HD12	1.92	0.52
1:S:110:ARG:NH2	1:S:115:ARG:CZ	2.73	0.52
1:S:2628:PHE:HZ	1:S:2907:PRO:HD3	1.74	0.52
1:S:4220:ASP:C	1:S:4220:ASP:OD2	2.53	0.52
1:A:110:ARG:HH22	1:A:115:ARG:NH2	2.05	0.51
1:A:4834:GLY:O	1:A:4838:VAL:HG23	2.10	0.51
1:G:20:VAL:HG21	1:G:202:MET:CG	2.38	0.51
1:G:1815:LEU:HD22	1:G:1845:VAL:HG21	1.91	0.51
1:G:4220:ASP:OD2	1:G:4220:ASP:C	2.53	0.51
1:A:390:LEU:HD23	1:A:390:LEU:H	1.75	0.51
1:A:4207:MET:O	1:A:4210:VAL:HG22	2.10	0.51
1:G:1928:GLN:HG3	1:G:1928:GLN:O	2.10	0.51
1:G:2970:SER:HA	1:G:2973:PHE:CE2	2.46	0.51
1:M:390:LEU:HD23	1:M:390:LEU:H	1.75	0.51
1:M:419:ASP:OD1	1:M:419:ASP:O	2.27	0.51
1:M:1557:THR:O	1:M:1557:THR:HG22	2.11	0.51
1:M:1561:VAL:HG23	1:M:1562:ILE:N	2.25	0.51
1:M:3992:PHE:HB3	1:M:4023:MET:HE1	1.92	0.51
1:S:4834:GLY:O	1:S:4838:VAL:HG23	2.10	0.51
1:A:1815:LEU:HD22	1:A:1845:VAL:HG21	1.91	0.51
1:A:2970:SER:HA	1:A:2973:PHE:CE2	2.46	0.51
1:M:1164:LEU:HB2	1:M:1169:LEU:HD21	1.91	0.51
1:M:4207:MET:HE2	1:M:4207:MET:HA	1.91	0.51
1:S:169:LEU:HD12	1:S:171:LEU:HD11	1.92	0.51
1:A:2628:PHE:HZ	1:A:2907:PRO:HD3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:ARG:NH1	1:G:338:GLU:OE1	2.43	0.51
1:G:390:LEU:HD23	1:G:390:LEU:H	1.75	0.51
1:G:999:ASP:O	1:G:1002:ALA:HB3	2.11	0.51
1:M:110:ARG:NH2	1:M:115:ARG:CZ	2.73	0.51
1:M:999:ASP:O	1:M:1002:ALA:HB3	2.11	0.51
1:M:1426:ILE:HG21	1:M:1429:ASN:HD22	1.76	0.51
1:M:1928:GLN:O	1:M:1928:GLN:HG3	2.10	0.51
1:M:4791:TYR:OH	1:M:4815:ASP:OD1	2.28	0.51
1:S:3052:HIS:O	1:S:3127:GLN:NE2	2.44	0.51
1:A:1928:GLN:HG3	1:A:1928:GLN:O	2.10	0.51
1:A:3916:ILE:O	1:A:3920:VAL:HG23	2.11	0.51
1:M:989:ALA:HA	1:M:1039:LEU:CD1	2.39	0.51
1:S:989:ALA:CB	1:S:1039:LEU:HD12	2.35	0.51
1:A:1557:THR:O	1:A:1557:THR:HG22	2.11	0.51
1:G:233:ILE:O	1:G:257:ARG:NH1	2.42	0.51
1:G:1454:THR:OG1	1:G:1456:ASP:OD1	2.24	0.51
1:G:1557:THR:HG22	1:G:1557:THR:O	2.11	0.51
5:G:5104:117:H83	5:G:5105:117:C93	2.39	0.51
1:M:1773:PRO:HA	1:M:2153:MET:HE1	1.93	0.51
1:M:4834:GLY:O	1:M:4838:VAL:HG23	2.10	0.51
1:S:1557:THR:O	1:S:1557:THR:HG22	2.11	0.51
1:S:1773:PRO:HA	1:S:2153:MET:HE1	1.93	0.51
1:A:1426:ILE:HG21	1:A:1429:ASN:HD22	1.76	0.51
1:M:3916:ILE:O	1:M:3920:VAL:HG23	2.11	0.51
1:S:3916:ILE:O	1:S:3920:VAL:HG23	2.11	0.51
1:A:3052:HIS:O	1:A:3127:GLN:NE2	2.44	0.51
1:A:3078:ARG:NH1	1:A:3155:ASP:OD2	2.40	0.51
1:G:3545:THR:O	1:G:3549:VAL:HG22	2.10	0.51
1:G:3916:ILE:O	1:G:3920:VAL:HG23	2.11	0.51
2:H:106:ASN:OD1	2:H:106:ASN:C	2.54	0.51
1:M:3052:HIS:O	1:M:3127:GLN:NE2	2.44	0.51
1:S:275:ARG:NH1	1:S:338:GLU:OE1	2.43	0.51
1:A:3992:PHE:HB3	1:A:4023:MET:HE1	1.92	0.51
1:G:3951:PHE:O	1:G:3955:MET:HG3	2.11	0.51
1:M:985:VAL:HG12	1:M:1036:ARG:HG3	1.93	0.51
1:S:985:VAL:HG12	1:S:1036:ARG:HG3	1.93	0.51
1:A:2355:ARG:NH2	1:A:2449:GLU:OE2	2.44	0.51
1:A:4940:PHE:CE2	1:A:4944:ARG:HD2	2.46	0.51
1:G:4834:GLY:O	1:G:4838:VAL:HG23	2.10	0.51
1:M:233:ILE:O	1:M:257:ARG:NH1	2.42	0.51
1:M:275:ARG:NH1	1:M:338:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3245:VAL:HG12	1:M:3246:LEU:N	2.26	0.51
1:S:4207:MET:HE2	1:S:4207:MET:HA	1.91	0.51
1:S:4207:MET:O	1:S:4210:VAL:HG22	2.10	0.51
1:A:999:ASP:O	1:A:1002:ALA:HB3	2.11	0.50
1:S:1928:GLN:HG3	1:S:1928:GLN:O	2.10	0.50
2:T:106:ASN:OD1	2:T:106:ASN:C	2.54	0.50
1:G:985:VAL:HG12	1:G:1036:ARG:HG3	1.93	0.50
1:G:3052:HIS:O	1:G:3127:GLN:NE2	2.44	0.50
1:G:3992:PHE:HB3	1:G:4023:MET:HE1	1.92	0.50
1:M:2970:SER:HA	1:M:2973:PHE:CE2	2.46	0.50
1:A:4160:LEU:O	1:A:4164:LEU:HD23	2.12	0.50
1:M:3951:PHE:O	1:M:3955:MET:HG3	2.11	0.50
2:N:106:ASN:OD1	2:N:106:ASN:C	2.54	0.50
1:S:390:LEU:HD23	1:S:390:LEU:H	1.75	0.50
1:S:2970:SER:HA	1:S:2973:PHE:CE2	2.46	0.50
1:S:4940:PHE:CE2	1:S:4944:ARG:HD2	2.46	0.50
1:S:214:VAL:HG21	1:S:390:LEU:HD11	1.93	0.50
1:S:404:ILE:HG21	1:S:481:GLU:HG2	1.93	0.50
1:S:3245:VAL:HG12	1:S:3246:LEU:N	2.26	0.50
2:B:106:ASN:OD1	2:B:106:ASN:C	2.54	0.50
1:G:4160:LEU:O	1:G:4164:LEU:HD23	2.12	0.50
1:G:4217:PHE:CE1	1:G:4237:PHE:CB	2.95	0.50
1:M:2670:GLU:OE2	1:M:2916:LYS:CE	2.55	0.50
1:M:4217:PHE:CE1	1:M:4237:PHE:CB	2.95	0.50
1:S:999:ASP:O	1:S:1002:ALA:HB3	2.11	0.50
1:A:985:VAL:HG12	1:A:1036:ARG:HG3	1.93	0.50
1:A:4791:TYR:OH	1:A:4815:ASP:OD1	2.28	0.50
5:A:5104:117:H83	5:A:5105:117:C93	2.39	0.50
1:M:31:GLU:O	1:M:33:LEU:HD12	2.12	0.50
1:M:4207:MET:O	1:M:4210:VAL:HG22	2.10	0.50
1:S:3992:PHE:HB3	1:S:4023:MET:HE1	1.92	0.50
1:A:3951:PHE:O	1:A:3955:MET:HG3	2.11	0.50
1:A:3077:ALA:HA	1:A:3080:VAL:HG12	1.94	0.50
1:A:3245:VAL:HG12	1:A:3246:LEU:N	2.26	0.50
1:G:4940:PHE:CE2	1:G:4944:ARG:HD2	2.46	0.50
1:M:404:ILE:HG21	1:M:481:GLU:HG2	1.93	0.50
1:M:1166:GLY:HA3	1:M:1216:ILE:HG21	1.94	0.50
1:A:1773:PRO:HA	1:A:2153:MET:HE1	1.93	0.50
1:A:4220:ASP:C	1:A:4220:ASP:OD2	2.53	0.50
1:G:989:ALA:CA	1:G:1039:LEU:CD1	2.90	0.50
1:G:3007:ASN:O	1:G:3011:THR:OG1	2.16	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3245:VAL:HG12	1:G:3246:LEU:N	2.26	0.50
1:M:4160:LEU:O	1:M:4164:LEU:HD23	2.12	0.50
1:M:4940:PHE:CE2	1:M:4944:ARG:HD2	2.46	0.50
1:S:509:GLU:O	1:S:513:GLU:OE1	2.30	0.50
1:S:1166:GLY:HA3	1:S:1216:ILE:HG21	1.94	0.50
1:G:1426:ILE:HG21	1:G:1429:ASN:HD22	1.76	0.49
1:S:1426:ILE:HG21	1:S:1429:ASN:HD22	1.76	0.49
1:A:404:ILE:HG21	1:A:481:GLU:HG2	1.93	0.49
1:A:989:ALA:CA	1:A:1039:LEU:CD1	2.90	0.49
1:A:2350:ALA:O	1:A:2354:VAL:HG23	2.13	0.49
1:G:1773:PRO:HA	1:G:2153:MET:HE1	1.93	0.49
1:G:2355:ARG:NH2	1:G:2449:GLU:OE2	2.44	0.49
1:M:214:VAL:HG21	1:M:390:LEU:HD11	1.93	0.49
1:M:2355:ARG:NH2	1:M:2449:GLU:OE2	2.44	0.49
1:M:4220:ASP:OD2	1:M:4220:ASP:C	2.53	0.49
1:A:1166:GLY:HA3	1:A:1216:ILE:HG21	1.94	0.49
1:G:2212:VAL:HG22	1:G:2256:TYR:HE2	1.72	0.49
1:M:989:ALA:CA	1:M:1039:LEU:CD1	2.90	0.49
1:M:1740:PRO:HA	1:M:1743:ARG:HG2	1.95	0.49
1:M:4204:GLN:HB3	1:M:4245:MET:HE2	1.94	0.49
1:S:4791:TYR:OH	1:S:4815:ASP:OD1	2.28	0.49
1:G:3708:THR:O	1:G:3711:THR:HG22	2.13	0.49
1:S:3951:PHE:O	1:S:3955:MET:HG3	2.11	0.49
1:A:509:GLU:O	1:A:513:GLU:OE1	2.30	0.49
1:G:1166:GLY:HA3	1:G:1216:ILE:HG21	1.94	0.49
1:G:2123:LEU:O	1:G:2127:GLN:HG2	2.13	0.49
1:M:3708:THR:O	1:M:3711:THR:HG22	2.13	0.49
1:S:4217:PHE:CE1	1:S:4237:PHE:CB	2.95	0.49
1:A:3708:THR:O	1:A:3711:THR:HG22	2.13	0.49
1:M:1454:THR:OG1	1:M:1456:ASP:OD1	2.24	0.49
1:M:2159:LEU:HD21	1:M:2163:ARG:CZ	2.43	0.49
1:G:404:ILE:HG21	1:G:481:GLU:HG2	1.93	0.49
1:G:4823:LEU:O	1:G:4827:LEU:HD13	2.13	0.49
1:S:31:GLU:O	1:S:33:LEU:HD12	2.12	0.49
1:A:214:VAL:HG21	1:A:390:LEU:HD11	1.93	0.49
1:A:1105:ALA:HB2	1:A:1191:VAL:HG21	1.95	0.49
1:A:4217:PHE:CE1	1:A:4237:PHE:CB	2.95	0.49
1:G:3077:ALA:HA	1:G:3080:VAL:HG12	1.94	0.49
1:M:509:GLU:O	1:M:513:GLU:OE1	2.30	0.49
1:M:2123:LEU:O	1:M:2127:GLN:HG2	2.13	0.49
1:M:3322:ILE:O	1:M:3326:ASN:ND2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:5105:117:H922	5:M:5105:117:N2	2.28	0.49
1:S:989:ALA:CA	1:S:1039:LEU:CD1	2.90	0.49
1:S:1105:ALA:HB2	1:S:1191:VAL:HG21	1.95	0.49
1:S:2355:ARG:NH2	1:S:2449:GLU:OE2	2.44	0.49
1:G:1740:PRO:HA	1:G:1743:ARG:HG2	1.95	0.49
1:G:2350:ALA:O	1:G:2354:VAL:HG23	2.13	0.49
5:G:5105:117:N2	5:G:5105:117:H922	2.28	0.49
1:M:2292:GLU:O	1:M:2296:GLU:HG3	2.13	0.49
1:M:2628:PHE:CZ	1:M:2907:PRO:HD3	2.48	0.49
1:S:110:ARG:HH22	1:S:115:ARG:NH2	2.05	0.49
1:S:3077:ALA:HA	1:S:3080:VAL:HG12	1.94	0.49
1:S:4160:LEU:O	1:S:4164:LEU:HD23	2.12	0.49
1:G:214:VAL:HG21	1:G:390:LEU:HD11	1.93	0.49
1:G:4204:GLN:HB3	1:G:4245:MET:HE2	1.94	0.49
1:S:2350:ALA:O	1:S:2354:VAL:HG23	2.13	0.49
1:S:4204:GLN:HB3	1:S:4245:MET:HE2	1.94	0.49
1:A:31:GLU:O	1:A:33:LEU:HD12	2.12	0.48
1:A:2159:LEU:HD21	1:A:2163:ARG:CZ	2.43	0.48
1:G:282:ILE:HD11	1:G:291:LEU:HD23	1.95	0.48
1:M:990:GLU:HA	1:M:1024:TYR:CD1	2.48	0.48
1:S:2159:LEU:HD21	1:S:2163:ARG:CZ	2.43	0.48
1:S:3708:THR:O	1:S:3711:THR:HG22	2.13	0.48
2:T:53:LYS:C	2:T:54:GLN:OE1	2.56	0.48
1:A:495:ASN:OD1	1:A:553:ARG:CZ	2.61	0.48
1:A:2292:GLU:O	1:A:2296:GLU:HG3	2.13	0.48
1:G:31:GLU:O	1:G:33:LEU:HD12	2.12	0.48
1:G:509:GLU:O	1:G:513:GLU:OE1	2.30	0.48
1:G:2292:GLU:O	1:G:2296:GLU:HG3	2.13	0.48
2:H:53:LYS:C	2:H:54:GLN:OE1	2.56	0.48
1:M:1101:ARG:NH1	1:M:1115:LEU:O	2.46	0.48
1:M:2350:ALA:O	1:M:2354:VAL:HG23	2.13	0.48
1:M:4823:LEU:O	1:M:4827:LEU:HD13	2.13	0.48
5:S:5105:117:H922	5:S:5105:117:N2	2.28	0.48
1:A:274:LEU:HD22	1:A:280:LEU:HD11	1.96	0.48
1:A:4204:GLN:HB3	1:A:4245:MET:HE2	1.94	0.48
5:A:5105:117:H922	5:A:5105:117:N2	2.28	0.48
2:B:53:LYS:C	2:B:54:GLN:OE1	2.56	0.48
1:M:1105:ALA:HB2	1:M:1191:VAL:HG21	1.95	0.48
1:S:2628:PHE:CZ	1:S:2907:PRO:HD3	2.48	0.48
1:A:2124:LEU:HD11	1:A:2128:TYR:HE1	1.79	0.48
1:G:688:LEU:HD23	1:G:690:GLU:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1252:HIS:O	1:G:1275:ARG:NH1	2.47	0.48
1:G:3249:LEU:O	1:G:3253:ILE:HD12	2.14	0.48
1:G:3456:GLN:O	1:G:3460:VAL:HG22	2.14	0.48
1:M:2124:LEU:HD11	1:M:2128:TYR:HE1	1.79	0.48
1:M:3768:SER:HA	1:M:3771:HIS:CD2	2.49	0.48
1:S:495:ASN:OD1	1:S:553:ARG:CZ	2.61	0.48
1:S:990:GLU:HA	1:S:1024:TYR:CD1	2.48	0.48
1:S:2292:GLU:O	1:S:2296:GLU:HG3	2.13	0.48
1:G:274:LEU:HD22	1:G:280:LEU:HD11	1.96	0.48
1:G:3768:SER:HA	1:G:3771:HIS:CD2	2.49	0.48
2:B:6:GLU:N	2:B:6:GLU:OE2	2.47	0.48
1:G:2159:LEU:HD21	1:G:2163:ARG:CZ	2.43	0.48
1:M:3249:LEU:O	1:M:3253:ILE:HD12	2.14	0.48
1:M:3456:GLN:O	1:M:3460:VAL:HG22	2.14	0.48
1:M:4860:ARG:HH12	1:S:4629:TYR:HH	1.54	0.48
1:A:264:PRO:HA	1:A:280:LEU:HD23	1.96	0.48
1:A:282:ILE:HD11	1:A:291:LEU:HD23	1.95	0.48
1:A:2628:PHE:CZ	1:A:2907:PRO:HD3	2.48	0.48
1:A:3336:LYS:O	1:A:3340:VAL:HG13	2.13	0.48
1:G:264:PRO:HA	1:G:280:LEU:HD23	1.96	0.48
1:G:495:ASN:OD1	1:G:553:ARG:CZ	2.61	0.48
1:G:990:GLU:HA	1:G:1024:TYR:CD1	2.48	0.48
1:G:3336:LYS:O	1:G:3340:VAL:HG13	2.13	0.48
1:M:3077:ALA:HA	1:M:3080:VAL:HG12	1.94	0.48
1:S:2123:LEU:O	1:S:2127:GLN:HG2	2.13	0.48
1:A:2123:LEU:O	1:A:2127:GLN:HG2	2.13	0.48
2:N:6:GLU:N	2:N:6:GLU:OE2	2.47	0.48
2:N:53:LYS:C	2:N:54:GLN:OE1	2.56	0.48
1:S:3183:VAL:O	1:S:3187:ARG:HG3	2.14	0.48
1:S:3249:LEU:O	1:S:3253:ILE:HD12	2.14	0.48
1:A:1740:PRO:HA	1:A:1743:ARG:HG2	1.95	0.48
1:A:3183:VAL:O	1:A:3187:ARG:HG3	2.14	0.48
1:A:3456:GLN:O	1:A:3460:VAL:HG22	2.14	0.48
1:M:1252:HIS:O	1:M:1275:ARG:NH1	2.47	0.48
1:S:4823:LEU:O	1:S:4827:LEU:HD13	2.13	0.48
1:A:990:GLU:HA	1:A:1024:TYR:CD1	2.48	0.48
2:H:6:GLU:N	2:H:6:GLU:OE2	2.47	0.48
1:S:3546:ASP:O	1:S:3597:GLN:NE2	2.47	0.48
1:S:3768:SER:HA	1:S:3771:HIS:CD2	2.49	0.48
1:A:1251:GLU:N	1:A:1251:GLU:OE1	2.46	0.47
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4823:LEU:O	1:A:4827:LEU:HD13	2.13	0.47
1:G:3546:ASP:O	1:G:3597:GLN:NE2	2.47	0.47
1:M:282:ILE:HD11	1:M:291:LEU:HD23	1.95	0.47
1:M:1219:LEU:HD11	1:S:3575:LEU:HD13	1.96	0.47
1:M:3183:VAL:O	1:M:3187:ARG:HG3	2.14	0.47
1:A:688:LEU:HD23	1:A:690:GLU:H	1.79	0.47
1:G:1105:ALA:HB2	1:G:1191:VAL:HG21	1.95	0.47
1:G:1263:THR:HG22	1:G:1264:VAL:N	2.30	0.47
1:G:3440:GLU:HA	1:G:3443:ILE:HG12	1.96	0.47
1:M:495:ASN:OD1	1:M:553:ARG:CZ	2.61	0.47
1:M:688:LEU:HD23	1:M:690:GLU:H	1.79	0.47
1:S:274:LEU:HD22	1:S:280:LEU:HD11	1.96	0.47
1:S:3440:GLU:HA	1:S:3443:ILE:HG12	1.96	0.47
2:T:6:GLU:N	2:T:6:GLU:OE2	2.47	0.47
1:A:1727:ARG:NH2	1:A:1773:PRO:O	2.47	0.47
1:A:2294:ASP:O	1:A:2298:VAL:HG23	2.15	0.47
1:G:1251:GLU:OE1	1:G:1251:GLU:N	2.46	0.47
1:G:2628:PHE:CZ	1:G:2907:PRO:HD3	2.48	0.47
1:M:1251:GLU:OE1	1:M:1251:GLU:N	2.46	0.47
1:M:3440:GLU:HA	1:M:3443:ILE:HG12	1.96	0.47
1:S:688:LEU:HD23	1:S:690:GLU:H	1.79	0.47
1:G:977:LEU:HD11	1:G:1040:CYS:SG	2.55	0.47
1:M:2294:ASP:O	1:M:2298:VAL:HG23	2.15	0.47
1:M:3336:LYS:O	1:M:3340:VAL:HG13	2.13	0.47
1:S:1251:GLU:OE1	1:S:1251:GLU:N	2.46	0.47
1:S:2650:ARG:NH1	1:S:2651:CYS:SG	2.88	0.47
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.47	0.47
1:A:3440:GLU:HA	1:A:3443:ILE:HG12	1.96	0.47
1:G:2650:ARG:NH1	1:G:2651:CYS:SG	2.88	0.47
1:S:282:ILE:HD11	1:S:291:LEU:HD23	1.95	0.47
1:S:3336:LYS:O	1:S:3340:VAL:HG13	2.13	0.47
1:S:4740:LEU:HD23	1:S:4741:LEU:HD23	1.96	0.47
1:A:1727:ARG:O	1:A:1731:LEU:HG	2.15	0.47
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.44	0.47
1:G:1727:ARG:NH2	1:G:1773:PRO:O	2.47	0.47
1:G:2124:LEU:HD11	1:G:2128:TYR:HE1	1.79	0.47
1:M:274:LEU:HD22	1:M:280:LEU:HD11	1.96	0.47
1:M:977:LEU:HD11	1:M:1040:CYS:SG	2.55	0.47
1:M:2650:ARG:NH1	1:M:2651:CYS:SG	2.88	0.47
1:M:3169:LEU:HD21	1:M:3197:LEU:CD2	2.45	0.47
1:M:3546:ASP:O	1:M:3597:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1740:PRO:HA	1:S:1743:ARG:HG2	1.95	0.47
1:S:2294:ASP:O	1:S:2298:VAL:HG23	2.15	0.47
1:S:3106:MET:HA	1:S:3109:ASN:ND2	2.30	0.47
1:A:2650:ARG:NH1	1:A:2651:CYS:SG	2.88	0.47
1:A:3249:LEU:O	1:A:3253:ILE:HD12	2.14	0.47
1:A:3546:ASP:O	1:A:3597:GLN:NE2	2.47	0.47
1:G:1969:LEU:C	1:G:1969:LEU:HD23	2.40	0.47
1:G:3183:VAL:O	1:G:3187:ARG:HG3	2.14	0.47
1:G:3322:ILE:O	1:G:3326:ASN:ND2	2.44	0.47
1:M:264:PRO:HA	1:M:280:LEU:HD23	1.96	0.47
1:M:488:LEU:O	1:M:492:ASP:OD2	2.33	0.47
1:M:600:LEU:CD2	1:M:1669:LEU:HD22	2.45	0.47
1:M:1727:ARG:O	1:M:1731:LEU:HG	2.15	0.47
1:M:4740:LEU:HD23	1:M:4741:LEU:HD23	1.96	0.47
1:S:1252:HIS:O	1:S:1275:ARG:NH1	2.47	0.47
1:A:1263:THR:HG22	1:A:1264:VAL:N	2.30	0.47
1:A:2644:LEU:HD13	1:A:2678:LEU:HD21	1.96	0.47
1:A:3106:MET:HA	1:A:3109:ASN:ND2	2.30	0.47
1:G:488:LEU:O	1:G:492:ASP:OD2	2.33	0.47
1:S:600:LEU:CD2	1:S:1669:LEU:HD22	2.45	0.47
1:S:3456:GLN:O	1:S:3460:VAL:HG22	2.14	0.47
1:A:977:LEU:HD11	1:A:1040:CYS:SG	2.55	0.47
1:A:2251:PHE:CG	1:A:2286:LEU:HD23	2.50	0.47
1:G:3169:LEU:HD21	1:G:3197:LEU:CD2	2.45	0.47
1:M:1164:LEU:CB	1:M:1169:LEU:HD21	2.45	0.47
1:M:2644:LEU:HD13	1:M:2678:LEU:HD21	1.96	0.47
1:M:609:CYS:O	1:M:612:VAL:HG22	2.15	0.47
1:M:2862:LEU:HD11	1:M:2932:MET:HE1	1.97	0.47
1:S:264:PRO:HA	1:S:280:LEU:HD23	1.96	0.47
1:S:488:LEU:O	1:S:492:ASP:OD2	2.33	0.47
1:S:1727:ARG:O	1:S:1731:LEU:HG	2.15	0.47
1:S:2124:LEU:HD11	1:S:2128:TYR:HE1	1.79	0.47
1:A:1969:LEU:HD23	1:A:1969:LEU:C	2.40	0.46
1:A:2624:ARG:NH1	1:A:2906:VAL:HG11	2.31	0.46
1:G:609:CYS:O	1:G:612:VAL:HG22	2.15	0.46
1:G:1101:ARG:NH1	1:G:1115:LEU:O	2.46	0.46
1:G:1164:LEU:CB	1:G:1169:LEU:HD21	2.45	0.46
1:G:3106:MET:HA	1:G:3109:ASN:ND2	2.30	0.46
1:M:3106:MET:HA	1:M:3109:ASN:ND2	2.30	0.46
1:S:2644:LEU:HD13	1:S:2678:LEU:HD21	1.96	0.46
1:A:609:CYS:O	1:A:612:VAL:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2624:ARG:NH1	1:M:2906:VAL:HG11	2.31	0.46
1:M:3256:LEU:HB3	1:M:3266:MET:SD	2.56	0.46
1:S:489:ASN:O	1:S:493:ARG:HG2	2.15	0.46
1:S:3256:LEU:HB3	1:S:3266:MET:SD	2.56	0.46
1:S:3322:ILE:O	1:S:3326:ASN:ND2	2.44	0.46
1:A:3169:LEU:HD21	1:A:3197:LEU:CD2	2.45	0.46
1:A:3521:GLY:HA2	1:A:3524:MET:HE2	1.97	0.46
1:G:2251:PHE:CG	1:G:2286:LEU:HD23	2.50	0.46
1:G:2644:LEU:HD13	1:G:2678:LEU:HD21	1.96	0.46
1:S:1164:LEU:CB	1:S:1169:LEU:HD21	2.45	0.46
1:S:1969:LEU:HD23	1:S:1969:LEU:C	2.40	0.46
1:S:2251:PHE:CG	1:S:2286:LEU:HD23	2.50	0.46
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.46	0.46
1:A:4740:LEU:HD23	1:A:4741:LEU:HD23	1.96	0.46
1:M:1727:ARG:NH2	1:M:1773:PRO:O	2.47	0.46
1:M:2897:LYS:O	1:M:2897:LYS:HG2	2.16	0.46
1:S:609:CYS:O	1:S:612:VAL:HG22	2.15	0.46
1:S:992:GLY:O	1:S:995:VAL:HG12	2.16	0.46
1:S:3169:LEU:HD21	1:S:3197:LEU:CD2	2.45	0.46
1:A:3521:GLY:O	1:A:3524:MET:HG2	2.16	0.46
1:S:2624:ARG:NH1	1:S:2906:VAL:HG11	2.31	0.46
1:A:488:LEU:O	1:A:492:ASP:OD2	2.33	0.46
1:G:2330:ARG:O	1:G:2333:ASP:OD1	2.34	0.46
1:G:2624:ARG:NH1	1:G:2906:VAL:HG11	2.31	0.46
1:G:4838:VAL:O	5:M:5103:117:H20	2.16	0.46
1:M:489:ASN:O	1:M:493:ARG:HG2	2.15	0.46
1:M:683:ARG:NE	1:M:707:VAL:O	2.48	0.46
1:S:977:LEU:HD11	1:S:1040:CYS:SG	2.55	0.46
1:A:600:LEU:CD2	1:A:1669:LEU:HD22	2.45	0.46
1:A:992:GLY:O	1:A:995:VAL:HG12	2.16	0.46
1:A:1464:PHE:O	1:A:1465:ASP:OD1	2.34	0.46
1:A:2348:GLU:O	1:A:2352:VAL:HG23	2.16	0.46
1:A:2825:LYS:HE3	1:A:2827:ARG:O	2.16	0.46
1:A:3256:LEU:HB3	1:A:3266:MET:SD	2.56	0.46
1:A:4217:PHE:CZ	1:A:4234:PHE:HA	2.51	0.46
1:G:489:ASN:O	1:G:493:ARG:HG2	2.15	0.46
1:G:600:LEU:CD2	1:G:1669:LEU:HD22	2.45	0.46
1:G:2897:LYS:O	1:G:2897:LYS:HG2	2.16	0.46
1:M:3521:GLY:O	1:M:3524:MET:HG2	2.16	0.46
1:S:1727:ARG:NH2	1:S:1773:PRO:O	2.47	0.46
1:S:2330:ARG:O	1:S:2333:ASP:OD1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ASN:O	1:A:493:ARG:HG2	2.15	0.46
1:G:1464:PHE:O	1:G:1465:ASP:OD1	2.34	0.46
1:G:2294:ASP:O	1:G:2298:VAL:HG23	2.15	0.46
1:G:3256:LEU:HB3	1:G:3266:MET:SD	2.56	0.46
1:G:4740:LEU:HD23	1:G:4741:LEU:HD23	1.96	0.46
1:A:387:ALA:C	1:A:388:LEU:HD22	2.41	0.46
1:A:1164:LEU:CB	1:A:1169:LEU:HD21	2.45	0.46
1:A:4952:GLU:OE1	1:A:4952:GLU:HA	2.16	0.46
5:A:5103:117:H20	1:S:4838:VAL:O	2.16	0.46
1:G:1727:ARG:O	1:G:1731:LEU:HG	2.15	0.46
1:G:4222:VAL:HG12	1:G:4950:VAL:HG11	1.98	0.46
1:M:2330:ARG:O	1:M:2333:ASP:OD1	2.34	0.46
1:A:150:MET:SD	1:A:150:MET:N	2.81	0.46
1:A:4567:LEU:HD22	5:A:5104:117:C85	2.46	0.46
1:G:387:ALA:C	1:G:388:LEU:HD22	2.41	0.46
1:G:1087:ARG:HG2	1:G:1154:ASP:CG	2.41	0.46
1:G:2862:LEU:HD11	1:G:2932:MET:HE1	1.97	0.46
1:M:3521:GLY:HA2	1:M:3524:MET:HE2	1.97	0.46
1:M:4838:VAL:O	5:S:5103:117:H20	2.16	0.46
1:G:992:GLY:O	1:G:995:VAL:HG12	2.16	0.45
1:M:2825:LYS:HE3	1:M:2827:ARG:O	2.16	0.45
1:M:4217:PHE:CZ	1:M:4234:PHE:HA	2.51	0.45
1:M:4222:VAL:HG12	1:M:4950:VAL:HG11	1.98	0.45
1:S:62:LEU:HD12	1:S:62:LEU:N	2.31	0.45
1:S:4217:PHE:CZ	1:S:4234:PHE:HA	2.51	0.45
1:S:4567:LEU:HD22	5:S:5104:117:C85	2.46	0.45
1:S:4952:GLU:OE1	1:S:4952:GLU:HA	2.16	0.45
1:A:1087:ARG:HG2	1:A:1154:ASP:CG	2.41	0.45
1:A:4780:PHE:O	1:A:4784:PHE:HD1	1.99	0.45
1:G:4780:PHE:O	1:G:4784:PHE:HD1	1.99	0.45
1:M:62:LEU:N	1:M:62:LEU:HD12	2.31	0.45
1:M:387:ALA:C	1:M:388:LEU:HD22	2.41	0.45
1:M:1464:PHE:O	1:M:1465:ASP:OD1	2.34	0.45
1:S:387:ALA:C	1:S:388:LEU:HD22	2.41	0.45
1:S:989:ALA:HA	1:S:1039:LEU:HD11	1.99	0.45
1:S:1263:THR:HG22	1:S:1264:VAL:N	2.30	0.45
1:A:2330:ARG:O	1:A:2333:ASP:OD1	2.34	0.45
1:M:989:ALA:HA	1:M:1039:LEU:HD11	1.99	0.45
1:M:992:GLY:O	1:M:995:VAL:HG12	2.16	0.45
1:M:1087:ARG:HG2	1:M:1154:ASP:CG	2.41	0.45
1:M:1969:LEU:HD23	1:M:1969:LEU:C	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD12	1:A:62:LEU:N	2.31	0.45
1:A:989:ALA:HA	1:A:1039:LEU:HD11	1.99	0.45
1:A:2822:THR:OG1	1:A:2938:THR:OG1	2.35	0.45
1:G:572:PRO:HA	1:G:575:LEU:HD13	1.98	0.45
1:G:2348:GLU:O	1:G:2352:VAL:HG23	2.16	0.45
1:M:2251:PHE:CG	1:M:2286:LEU:HD23	2.50	0.45
1:M:2348:GLU:O	1:M:2352:VAL:HG23	2.16	0.45
1:M:2822:THR:OG1	1:M:2938:THR:OG1	2.35	0.45
1:G:4817:ALA:O	1:G:4823:LEU:HB3	2.17	0.45
1:M:2271:THR:OG1	1:M:2274:ASP:OD2	2.34	0.45
1:M:2624:ARG:HH11	1:M:2906:VAL:HG11	1.82	0.45
1:M:4952:GLU:OE1	1:M:4952:GLU:HA	2.16	0.45
1:S:414:PHE:CE1	1:S:436:LEU:HD22	2.52	0.45
1:S:1087:ARG:HG2	1:S:1154:ASP:CG	2.41	0.45
1:S:3957:VAL:O	1:S:3961:VAL:HG23	2.17	0.45
1:A:414:PHE:CE1	1:A:436:LEU:HD22	2.52	0.45
1:A:3957:VAL:O	1:A:3961:VAL:HG23	2.17	0.45
1:A:4134:GLU:HB2	1:A:4135:PRO:HD3	1.99	0.45
1:A:4716:TRP:CH2	3:A:5101:CFF:H142	2.52	0.45
1:G:414:PHE:CE1	1:G:436:LEU:HD22	2.52	0.45
1:G:4134:GLU:HB2	1:G:4135:PRO:HD3	1.99	0.45
1:G:4217:PHE:CZ	1:G:4234:PHE:HA	2.51	0.45
1:M:414:PHE:CE1	1:M:436:LEU:HD22	2.52	0.45
1:M:2009:LEU:HG	1:M:2023:LEU:HD21	1.99	0.45
1:M:2159:LEU:HD12	1:M:2203:MET:HE2	1.99	0.45
1:M:3080:VAL:O	1:M:3084:GLY:HA3	2.17	0.45
1:S:1464:PHE:O	1:S:1465:ASP:OD1	2.34	0.45
1:S:1819:VAL:HG22	1:S:1926:LEU:HD13	1.98	0.45
1:S:2271:THR:OG1	1:S:2274:ASP:OD2	2.34	0.45
1:A:928:THR:HG23	1:A:988:LEU:HD21	1.98	0.45
1:A:4838:VAL:O	5:G:5103:117:H20	2.16	0.45
1:G:1478:ASP:OD1	1:G:1482:ASN:N	2.50	0.45
1:G:3521:GLY:HA2	1:G:3524:MET:HE2	1.97	0.45
1:G:3521:GLY:O	1:G:3524:MET:HG2	2.16	0.45
1:M:4716:TRP:CH2	3:M:5101:CFF:H142	2.52	0.45
1:S:231:LEU:HD11	1:S:245:VAL:HG12	1.99	0.45
1:S:2009:LEU:HG	1:S:2023:LEU:HD21	1.99	0.45
1:S:2159:LEU:HD12	1:S:2203:MET:HE2	1.99	0.45
1:S:2348:GLU:O	1:S:2352:VAL:HG23	2.16	0.45
1:S:2825:LYS:HE3	1:S:2827:ARG:O	2.16	0.45
1:S:2897:LYS:O	1:S:2897:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3521:GLY:O	1:S:3524:MET:HG2	2.16	0.45
1:A:2897:LYS:HG2	1:A:2897:LYS:O	2.16	0.45
1:G:62:LEU:N	1:G:62:LEU:HD12	2.31	0.45
1:M:2151:ASP:OD2	1:M:2189:LYS:NZ	2.41	0.45
1:M:2630:VAL:N	1:M:2631:PRO:HD2	2.32	0.45
1:M:4567:LEU:HD22	5:M:5104:117:C85	2.46	0.45
1:M:4817:ALA:O	1:M:4823:LEU:HB3	2.17	0.45
1:S:2624:ARG:HH11	1:S:2906:VAL:HG11	1.82	0.45
1:S:2862:LEU:HD11	1:S:2932:MET:HE1	1.97	0.45
1:S:3085:PRO:HD2	1:S:3088:VAL:HG21	1.99	0.45
1:S:3569:LEU:HD22	1:S:3569:LEU:H	1.82	0.45
1:S:4716:TRP:CH2	3:S:5101:CFF:H142	2.52	0.45
1:A:990:GLU:HA	1:A:1024:TYR:CG	2.52	0.45
1:A:2630:VAL:N	1:A:2631:PRO:HD2	2.32	0.45
1:A:2862:LEU:HD11	1:A:2932:MET:HE1	1.97	0.45
1:G:1943:LEU:HB2	1:G:2123:LEU:HD21	1.99	0.45
1:G:2825:LYS:HE3	1:G:2827:ARG:O	2.16	0.45
1:G:4853:VAL:O	1:G:4857:ASN:ND2	2.50	0.45
1:M:169:LEU:HD23	1:M:169:LEU:N	2.32	0.45
1:M:2971:GLN:HA	1:M:2974:ILE:HG22	1.99	0.45
1:M:3085:PRO:HD2	1:M:3088:VAL:HG21	1.99	0.45
1:M:3569:LEU:HD22	1:M:3569:LEU:H	1.82	0.45
1:S:928:THR:HG23	1:S:988:LEU:HD21	1.98	0.45
1:S:1101:ARG:NH1	1:S:1115:LEU:O	2.46	0.45
1:S:1123:VAL:HG12	1:S:1132:TRP:HB2	1.99	0.45
1:S:2971:GLN:HA	1:S:2974:ILE:HG22	1.99	0.45
1:S:4569:LEU:CD2	1:S:4646:LEU:HD22	2.47	0.45
1:S:4780:PHE:O	1:S:4784:PHE:HD1	1.99	0.45
1:A:438:ILE:O	1:A:441:VAL:HG12	2.17	0.45
1:A:572:PRO:HA	1:A:575:LEU:HD13	1.98	0.45
1:A:2009:LEU:HG	1:A:2023:LEU:HD21	1.99	0.45
1:A:2971:GLN:HA	1:A:2974:ILE:HG22	1.99	0.45
1:G:990:GLU:HA	1:G:1024:TYR:CG	2.52	0.45
1:G:2009:LEU:HG	1:G:2023:LEU:HD21	1.99	0.45
1:G:4567:LEU:HD22	5:G:5104:117:C85	2.46	0.45
1:M:70:GLU:HG3	1:M:71:GLN:HG2	1.99	0.45
1:S:3521:GLY:HA2	1:S:3524:MET:HE2	1.97	0.45
1:S:3959:LYS:NZ	1:S:4022:ASP:OD2	2.50	0.45
1:S:4853:VAL:O	1:S:4857:ASN:ND2	2.50	0.45
1:A:3969:ILE:HD13	1:A:4030:LEU:HD23	2.00	0.44
1:M:3957:VAL:O	1:M:3961:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:70:GLU:HG3	1:S:71:GLN:HG2	1.99	0.44
1:S:169:LEU:HD23	1:S:169:LEU:N	2.32	0.44
1:S:990:GLU:HA	1:S:1024:TYR:CG	2.52	0.44
1:S:1083:VAL:HG11	1:S:1088:TRP:CD1	2.52	0.44
1:A:989:ALA:CB	1:A:1039:LEU:CD1	2.95	0.44
1:A:2624:ARG:HH11	1:A:2906:VAL:HG11	1.82	0.44
1:A:2763:HIS:HE1	1:A:2790:MET:O	2.01	0.44
1:G:2624:ARG:HH11	1:G:2906:VAL:HG11	1.82	0.44
1:G:2768:PHE:O	1:G:2772:GLN:HG2	2.18	0.44
1:G:3957:VAL:O	1:G:3961:VAL:HG23	2.17	0.44
1:G:4952:GLU:HA	1:G:4952:GLU:OE1	2.16	0.44
1:M:572:PRO:HA	1:M:575:LEU:HD13	1.98	0.44
1:M:600:LEU:HD22	1:M:1669:LEU:HD22	2.00	0.44
1:M:928:THR:HG23	1:M:988:LEU:HD21	1.98	0.44
1:M:1478:ASP:OD1	1:M:1482:ASN:N	2.50	0.44
1:M:1943:LEU:HB2	1:M:2123:LEU:HD21	1.99	0.44
1:M:2768:PHE:O	1:M:2772:GLN:HG2	2.18	0.44
1:M:3571:TRP:CE3	1:M:3575:LEU:HD12	2.53	0.44
1:A:1123:VAL:HG12	1:A:1132:TRP:HB2	1.99	0.44
1:A:1478:ASP:OD1	1:A:1482:ASN:N	2.50	0.44
1:A:3080:VAL:O	1:A:3084:GLY:HA3	2.17	0.44
1:A:4207:MET:HE2	1:A:4207:MET:CA	2.48	0.44
1:G:2763:HIS:HE1	1:G:2790:MET:O	2.01	0.44
1:G:4716:TRP:CH2	3:G:5101:CFF:H142	2.52	0.44
1:M:231:LEU:HD11	1:M:245:VAL:HG12	1.99	0.44
1:S:438:ILE:O	1:S:441:VAL:HG12	2.17	0.44
1:A:73:LEU:HG	1:A:77:ALA:HB3	2.00	0.44
1:A:231:LEU:HD11	1:A:245:VAL:HG12	1.99	0.44
1:A:1083:VAL:HG11	1:A:1088:TRP:CD1	2.52	0.44
1:A:1819:VAL:HG22	1:A:1926:LEU:HD13	1.98	0.44
1:A:2159:LEU:HD12	1:A:2203:MET:HE2	1.99	0.44
1:A:3571:TRP:CE3	1:A:3575:LEU:HD12	2.53	0.44
1:A:4569:LEU:CD2	1:A:4646:LEU:HD22	2.47	0.44
1:A:4817:ALA:O	1:A:4823:LEU:HB3	2.17	0.44
1:G:1123:VAL:HG12	1:G:1132:TRP:HB2	1.99	0.44
1:G:4207:MET:HE2	1:G:4207:MET:CA	2.48	0.44
1:G:4860:ARG:HH12	1:M:4629:TYR:HH	1.51	0.44
1:M:1123:VAL:HG12	1:M:1132:TRP:HB2	1.99	0.44
1:M:1263:THR:HG22	1:M:1264:VAL:N	2.30	0.44
1:M:4134:GLU:HB2	1:M:4135:PRO:HD3	1.99	0.44
1:M:4780:PHE:O	1:M:4784:PHE:HD1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:600:LEU:HD22	1:S:1669:LEU:HD22	2.00	0.44
1:S:683:ARG:NE	1:S:707:VAL:O	2.48	0.44
1:S:4207:MET:HE2	1:S:4207:MET:CA	2.48	0.44
1:A:2768:PHE:O	1:A:2772:GLN:HG2	2.18	0.44
1:G:169:LEU:HD23	1:G:169:LEU:N	2.32	0.44
1:G:438:ILE:O	1:G:441:VAL:HG12	2.17	0.44
1:G:2630:VAL:N	1:G:2631:PRO:HD2	2.32	0.44
1:M:3969:ILE:HD13	1:M:4030:LEU:HD23	2.00	0.44
1:S:1478:ASP:OD1	1:S:1482:ASN:N	2.50	0.44
1:S:1943:LEU:HB2	1:S:2123:LEU:HD21	1.99	0.44
1:S:3080:VAL:O	1:S:3084:GLY:HA3	2.17	0.44
1:S:4134:GLU:HB2	1:S:4135:PRO:HD3	1.99	0.44
1:A:4708:THR:HG21	1:A:4775:TYR:HB2	2.00	0.44
1:G:70:GLU:HG3	1:G:71:GLN:HG2	1.99	0.44
1:G:73:LEU:HG	1:G:77:ALA:HB3	2.00	0.44
1:G:231:LEU:HD11	1:G:245:VAL:HG12	1.99	0.44
1:M:1819:VAL:HG22	1:M:1926:LEU:HD13	1.98	0.44
1:S:2763:HIS:HE1	1:S:2790:MET:O	2.01	0.44
1:S:4640:GLU:HB3	1:S:4641:PRO:CD	2.48	0.44
1:A:70:GLU:HG3	1:A:71:GLN:HG2	1.99	0.44
1:A:688:LEU:HD23	1:A:689:THR:N	2.33	0.44
1:G:1002:ALA:O	1:G:1003:GLN:C	2.61	0.44
1:G:1819:VAL:HG22	1:G:1926:LEU:HD13	1.98	0.44
1:G:2159:LEU:HD12	1:G:2203:MET:HE2	1.99	0.44
1:G:4569:LEU:CD2	1:G:4646:LEU:HD22	2.47	0.44
1:G:4670:ILE:C	1:G:4714:ASN:HD22	2.26	0.44
1:M:990:GLU:HA	1:M:1024:TYR:CG	2.52	0.44
1:M:3571:TRP:HE3	1:M:3575:LEU:HD12	1.83	0.44
1:M:4207:MET:HE2	1:M:4207:MET:CA	2.48	0.44
1:S:2822:THR:OG1	1:S:2938:THR:OG1	2.35	0.44
1:A:683:ARG:NE	1:A:707:VAL:O	2.48	0.44
1:A:752:VAL:O	1:A:752:VAL:HG13	2.18	0.44
1:G:2295:LEU:O	1:G:2299:VAL:HG23	2.18	0.44
1:G:2822:THR:OG1	1:G:2938:THR:OG1	2.35	0.44
1:G:2874:MET:HE1	1:G:2937:VAL:HG12	2.00	0.44
1:G:2971:GLN:HA	1:G:2974:ILE:HG22	1.99	0.44
1:G:4875:LYS:C	1:G:4876:CYS:SG	3.01	0.44
1:M:438:ILE:O	1:M:441:VAL:HG12	2.17	0.44
1:M:1083:VAL:HG11	1:M:1088:TRP:CD1	2.52	0.44
1:S:4817:ALA:O	1:S:4823:LEU:HB3	2.17	0.44
1:A:2295:LEU:O	1:A:2299:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4853:VAL:O	1:A:4857:ASN:ND2	2.50	0.44
1:G:609:CYS:O	1:G:610:ASN:OD1	2.36	0.44
1:G:928:THR:HG23	1:G:988:LEU:HD21	1.98	0.44
1:G:2212:VAL:HG13	1:G:2256:TYR:OH	2.17	0.44
1:G:3080:VAL:O	1:G:3084:GLY:HA3	2.17	0.44
1:M:688:LEU:HD23	1:M:689:THR:N	2.33	0.44
1:M:2295:LEU:O	1:M:2299:VAL:HG23	2.18	0.44
1:M:4875:LYS:C	1:M:4876:CYS:SG	3.01	0.44
1:S:2630:VAL:N	1:S:2631:PRO:HD2	2.32	0.44
1:A:2258:LEU:CD1	1:A:2294:ASP:HB3	2.48	0.43
1:A:3007:ASN:O	1:A:3011:THR:OG1	2.16	0.43
1:A:3569:LEU:H	1:A:3569:LEU:HD22	1.82	0.43
1:G:3569:LEU:H	1:G:3569:LEU:HD22	1.82	0.43
1:M:609:CYS:O	1:M:610:ASN:OD1	2.36	0.43
1:M:4569:LEU:CD2	1:M:4646:LEU:HD22	2.47	0.43
1:M:4853:VAL:O	1:M:4857:ASN:ND2	2.50	0.43
1:M:4879:MET:HG2	1:S:4578:LEU:HA	2.00	0.43
1:S:73:LEU:HG	1:S:77:ALA:HB3	2.00	0.43
1:S:181:HIS:HD1	1:S:196:MET:HB2	1.80	0.43
1:S:688:LEU:HD23	1:S:689:THR:N	2.33	0.43
1:A:609:CYS:O	1:A:610:ASN:OD1	2.36	0.43
1:A:787:VAL:O	1:A:788:LYS:HG3	2.18	0.43
1:A:2271:THR:OG1	1:A:2274:ASP:OD2	2.34	0.43
1:A:3110:LEU:HD21	1:A:3183:VAL:HG22	2.01	0.43
1:A:3959:LYS:NZ	1:A:4022:ASP:OD2	2.50	0.43
1:A:4640:GLU:HB3	1:A:4641:PRO:CD	2.48	0.43
1:A:4875:LYS:C	1:A:4876:CYS:SG	3.01	0.43
1:G:600:LEU:HD22	1:G:1669:LEU:HD22	2.00	0.43
1:G:989:ALA:HA	1:G:1039:LEU:HD11	1.99	0.43
1:G:2151:ASP:OD2	1:G:2189:LYS:NZ	2.41	0.43
1:G:4879:MET:HG2	1:M:4578:LEU:HA	2.00	0.43
1:M:73:LEU:HG	1:M:77:ALA:HB3	2.00	0.43
1:M:752:VAL:HG13	1:M:752:VAL:O	2.18	0.43
1:M:2258:LEU:CD1	1:M:2294:ASP:HB3	2.48	0.43
1:M:4636:THR:C	1:M:4638:TYR:H	2.27	0.43
1:M:4640:GLU:HB3	1:M:4641:PRO:CD	2.48	0.43
1:M:4670:ILE:C	1:M:4714:ASN:HD22	2.26	0.43
2:N:38:ASP:OD1	2:N:39:SER:N	2.51	0.43
1:S:572:PRO:HA	1:S:575:LEU:HD13	1.98	0.43
1:S:3133:THR:HG23	1:S:3134:VAL:HG23	2.01	0.43
1:A:3874:VAL:HG13	1:A:3874:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.44	0.43
1:A:4222:VAL:HG12	1:A:4950:VAL:HG11	1.98	0.43
1:A:4838:VAL:O	1:A:4841:VAL:HG22	2.18	0.43
2:B:38:ASP:OD1	2:B:39:SER:N	2.51	0.43
1:G:752:VAL:O	1:G:752:VAL:HG13	2.18	0.43
1:G:1083:VAL:HG11	1:G:1088:TRP:CD1	2.52	0.43
1:G:2965:ARG:HA	1:G:2968:ASP:OD2	2.19	0.43
1:G:3571:TRP:CE3	1:G:3575:LEU:HD12	2.53	0.43
1:G:4640:GLU:HB3	1:G:4641:PRO:CD	2.48	0.43
1:G:4708:THR:HG21	1:G:4775:TYR:HB2	2.00	0.43
1:M:787:VAL:O	1:M:788:LYS:HG3	2.18	0.43
1:M:2212:VAL:HG13	1:M:2256:TYR:OH	2.17	0.43
1:M:3874:VAL:O	1:M:3874:VAL:HG13	2.18	0.43
1:S:2295:LEU:O	1:S:2299:VAL:HG23	2.18	0.43
1:S:3110:LEU:HD21	1:S:3183:VAL:HG22	2.01	0.43
1:S:3571:TRP:CE3	1:S:3575:LEU:HD12	2.53	0.43
1:S:4222:VAL:HG12	1:S:4950:VAL:HG11	1.98	0.43
2:T:38:ASP:OD1	2:T:39:SER:N	2.51	0.43
1:A:1943:LEU:HB2	1:A:2123:LEU:HD21	1.99	0.43
1:A:3400:VAL:HG13	1:A:3403:ARG:HH21	1.83	0.43
1:A:3779:VAL:HG13	1:A:3797:THR:HG22	2.00	0.43
1:A:4636:THR:C	1:A:4638:TYR:H	2.27	0.43
1:G:688:LEU:HD23	1:G:689:THR:N	2.33	0.43
1:G:787:VAL:O	1:G:788:LYS:HG3	2.18	0.43
1:G:2258:LEU:CD1	1:G:2294:ASP:HB3	2.48	0.43
1:G:2599:GLN:O	1:G:2603:ILE:HG13	2.19	0.43
1:G:3874:VAL:O	1:G:3874:VAL:HG13	2.18	0.43
1:G:4838:VAL:O	1:G:4841:VAL:HG22	2.18	0.43
1:M:1002:ALA:O	1:M:1003:GLN:C	2.61	0.43
1:M:2965:ARG:HA	1:M:2968:ASP:OD2	2.19	0.43
1:M:3110:LEU:HD21	1:M:3183:VAL:HG22	2.01	0.43
1:M:3133:THR:HG23	1:M:3134:VAL:HG23	2.01	0.43
1:S:2368:LEU:HD23	1:S:2368:LEU:O	2.19	0.43
1:S:3400:VAL:HG13	1:S:3403:ARG:HH21	1.83	0.43
1:S:3969:ILE:HD13	1:S:4030:LEU:HD23	2.00	0.43
1:S:4636:THR:C	1:S:4638:TYR:H	2.27	0.43
1:S:4838:VAL:O	1:S:4841:VAL:HG22	2.18	0.43
1:A:2368:LEU:HD23	1:A:2368:LEU:O	2.19	0.43
1:A:2599:GLN:O	1:A:2603:ILE:HG13	2.19	0.43
1:A:3060:ASP:OD1	1:A:3060:ASP:N	2.43	0.43
1:A:4041:ALA:O	1:A:4045:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3110:LEU:HD21	1:G:3183:VAL:HG22	2.01	0.43
1:G:3571:TRP:HE3	1:G:3575:LEU:HD12	1.83	0.43
1:S:2768:PHE:O	1:S:2772:GLN:HG2	2.18	0.43
1:S:4875:LYS:C	1:S:4876:CYS:SG	3.01	0.43
1:A:2122:SER:O	1:A:2126:ARG:HG3	2.19	0.43
1:A:2151:ASP:OD2	1:A:2189:LYS:NZ	2.41	0.43
1:A:2212:VAL:HG13	1:A:2256:TYR:OH	2.17	0.43
1:A:3085:PRO:HD2	1:A:3088:VAL:HG21	1.99	0.43
1:A:3758:MET:SD	1:A:3758:MET:C	3.02	0.43
1:G:2515:GLN:O	1:G:2519:LEU:HG	2.19	0.43
1:G:3085:PRO:HD2	1:G:3088:VAL:HG21	1.99	0.43
1:G:3969:ILE:HD13	1:G:4030:LEU:HD23	2.00	0.43
1:M:989:ALA:CB	1:M:1039:LEU:CD1	2.95	0.43
1:M:3400:VAL:HG13	1:M:3403:ARG:HH21	1.83	0.43
1:M:3838:THR:HG22	1:M:3838:THR:O	2.19	0.43
1:S:2109:ASP:N	1:S:2109:ASP:OD1	2.52	0.43
1:S:2122:SER:O	1:S:2126:ARG:HG3	2.19	0.43
1:S:3758:MET:SD	1:S:3758:MET:C	3.02	0.43
1:A:600:LEU:HD22	1:A:1669:LEU:HD22	2.00	0.43
1:A:2874:MET:HE1	1:A:2937:VAL:HG12	2.00	0.43
1:A:4670:ILE:C	1:A:4714:ASN:HD22	2.26	0.43
1:G:2109:ASP:OD1	1:G:2109:ASP:N	2.52	0.43
1:G:2368:LEU:O	1:G:2368:LEU:HD23	2.19	0.43
1:G:3363:GLY:O	1:G:3367:LYS:HG2	2.19	0.43
1:G:3838:THR:O	1:G:3838:THR:HG22	2.19	0.43
1:M:2599:GLN:O	1:M:2603:ILE:HG13	2.19	0.43
1:M:3261:ALA:HB3	1:M:3266:MET:SD	2.59	0.43
1:M:3959:LYS:NZ	1:M:4022:ASP:OD2	2.50	0.43
1:A:3133:THR:HG23	1:A:3134:VAL:HG23	2.01	0.43
1:A:3363:GLY:O	1:A:3367:LYS:HG2	2.19	0.43
1:G:544:LEU:HD22	1:G:574:VAL:HG13	2.01	0.43
1:G:3400:VAL:HG13	1:G:3403:ARG:HH21	1.83	0.43
1:G:4041:ALA:O	1:G:4045:VAL:HG23	2.19	0.43
1:M:2763:HIS:HE1	1:M:2790:MET:O	2.01	0.43
1:M:3779:VAL:HG13	1:M:3797:THR:HG22	2.00	0.43
1:S:2212:VAL:HG13	1:S:2256:TYR:OH	2.17	0.43
1:S:2258:LEU:CD1	1:S:2294:ASP:HB3	2.48	0.43
1:S:2965:ARG:HA	1:S:2968:ASP:OD2	2.19	0.43
1:S:3261:ALA:HB3	1:S:3266:MET:SD	2.59	0.43
1:S:4006:ASP:HB2	1:S:4009:GLN:OE1	2.19	0.43
1:S:4041:ALA:O	1:S:4045:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:4708:THR:HG21	1:S:4775:TYR:HB2	2.00	0.43
1:A:544:LEU:HD22	1:A:574:VAL:HG13	2.01	0.43
1:A:1219:LEU:HD11	1:G:3575:LEU:HD13	1.96	0.43
1:A:3085:PRO:O	1:A:3088:VAL:HG22	2.19	0.43
1:A:4006:ASP:HB2	1:A:4009:GLN:OE1	2.19	0.43
1:G:989:ALA:CB	1:G:1039:LEU:CD1	2.95	0.43
1:G:3085:PRO:O	1:G:3088:VAL:HG22	2.19	0.43
1:G:3959:LYS:NZ	1:G:4022:ASP:OD2	2.50	0.43
1:M:996:TRP:CE2	1:M:1000:ARG:HG3	2.54	0.43
1:S:1089:TYR:HD2	1:S:1152:MET:HG2	1.84	0.43
1:S:4670:ILE:C	1:S:4714:ASN:HD22	2.26	0.43
1:A:3550:ARG:CB	1:A:3597:GLN:OE1	2.67	0.43
1:A:4576:ILE:CG2	1:A:4643:LEU:HD13	2.49	0.43
2:H:38:ASP:OD1	2:H:39:SER:N	2.51	0.43
1:M:544:LEU:HD22	1:M:574:VAL:HG13	2.01	0.43
1:M:2515:GLN:O	1:M:2519:LEU:HG	2.19	0.43
1:M:3363:GLY:O	1:M:3367:LYS:HG2	2.19	0.43
1:M:4726:ASP:C	1:M:4726:ASP:OD1	2.62	0.43
1:S:752:VAL:O	1:S:752:VAL:HG13	2.18	0.43
1:S:3874:VAL:O	1:S:3874:VAL:HG13	2.18	0.43
1:A:501:ALA:O	1:A:505:GLU:HG3	2.19	0.42
1:A:1089:TYR:HD2	1:A:1152:MET:HG2	1.84	0.42
1:A:1164:LEU:O	1:A:1167:GLU:N	2.50	0.42
1:A:2499:LYS:O	1:A:2503:VAL:HG23	2.19	0.42
1:A:2750:LYS:HG2	1:A:2750:LYS:O	2.20	0.42
1:A:4091:LYS:O	1:A:4095:LYS:NZ	2.52	0.42
1:A:4879:MET:HG2	1:G:4578:LEU:HA	2.00	0.42
1:G:501:ALA:O	1:G:505:GLU:HG3	2.19	0.42
1:G:3261:ALA:HB3	1:G:3266:MET:SD	2.59	0.42
1:G:4636:THR:C	1:G:4638:TYR:H	2.27	0.42
1:M:575:LEU:HD12	1:M:575:LEU:N	2.35	0.42
1:M:2109:ASP:OD1	1:M:2109:ASP:N	2.52	0.42
1:M:2122:SER:O	1:M:2126:ARG:HG3	2.19	0.42
1:M:3550:ARG:CB	1:M:3597:GLN:OE1	2.67	0.42
1:M:3991:GLY:O	1:M:3995:VAL:HG23	2.19	0.42
1:M:4006:ASP:HB2	1:M:4009:GLN:OE1	2.19	0.42
1:M:4576:ILE:CG2	1:M:4643:LEU:HD13	2.49	0.42
1:S:2499:LYS:O	1:S:2503:VAL:HG23	2.19	0.42
1:S:3363:GLY:O	1:S:3367:LYS:HG2	2.19	0.42
1:A:2515:GLN:O	1:A:2519:LEU:HG	2.19	0.42
1:A:3838:THR:O	1:A:3838:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3991:GLY:O	1:A:3995:VAL:HG23	2.19	0.42
1:G:411:TYR:HB2	1:G:486:LEU:HD21	2.01	0.42
1:G:2499:LYS:O	1:G:2503:VAL:HG23	2.19	0.42
1:G:3133:THR:HG23	1:G:3134:VAL:HG23	2.01	0.42
1:G:3758:MET:SD	1:G:3758:MET:C	3.02	0.42
1:M:2161:GLN:O	1:M:2165:LEU:CD2	2.67	0.42
1:M:3758:MET:SD	1:M:3758:MET:C	3.02	0.42
1:S:996:TRP:CE2	1:S:1000:ARG:HG3	2.54	0.42
1:S:1164:LEU:O	1:S:1167:GLU:N	2.50	0.42
1:S:2874:MET:HE1	1:S:2937:VAL:HG12	2.00	0.42
1:S:3991:GLY:O	1:S:3995:VAL:HG23	2.19	0.42
1:A:169:LEU:HD23	1:A:169:LEU:N	2.32	0.42
1:A:411:TYR:HB2	1:A:486:LEU:HD21	2.01	0.42
1:A:2965:ARG:HA	1:A:2968:ASP:OD2	2.19	0.42
1:A:3391:GLU:HA	1:A:3394:VAL:HG22	2.01	0.42
1:G:3550:ARG:CB	1:G:3597:GLN:OE1	2.67	0.42
1:M:2499:LYS:O	1:M:2503:VAL:HG23	2.19	0.42
1:M:2639:MET:HB3	1:M:2640:PRO:HD3	2.01	0.42
1:M:3391:GLU:HA	1:M:3394:VAL:HG22	2.01	0.42
1:S:637:LEU:HD12	1:S:637:LEU:N	2.35	0.42
1:S:787:VAL:O	1:S:788:LYS:HG3	2.18	0.42
1:S:2515:GLN:O	1:S:2519:LEU:HG	2.19	0.42
1:S:3571:TRP:HE3	1:S:3575:LEU:HD12	1.83	0.42
1:S:4576:ILE:CG2	1:S:4643:LEU:HD13	2.49	0.42
1:A:2624:ARG:NH1	1:A:2906:VAL:HG21	2.35	0.42
1:G:3046:LEU:O	1:G:3050:VAL:HG23	2.19	0.42
1:G:4576:ILE:CG2	1:G:4643:LEU:HD13	2.49	0.42
1:M:2874:MET:HE1	1:M:2937:VAL:HG12	2.00	0.42
1:M:4682:GLU:OE1	1:M:4682:GLU:C	2.63	0.42
1:M:4708:THR:HG21	1:M:4775:TYR:HB2	2.00	0.42
1:S:501:ALA:O	1:S:505:GLU:HG3	2.19	0.42
1:S:609:CYS:O	1:S:610:ASN:OD1	2.36	0.42
1:S:989:ALA:CB	1:S:1039:LEU:CD1	2.95	0.42
1:S:1935:VAL:O	1:S:1939:MET:HG2	2.20	0.42
1:S:3550:ARG:CB	1:S:3597:GLN:OE1	2.67	0.42
1:A:1297:PHE:CZ	1:A:1542:VAL:HG21	2.55	0.42
1:A:1805:GLU:HA	1:A:1808:ARG:NE	2.35	0.42
1:A:3261:ALA:HB3	1:A:3266:MET:SD	2.59	0.42
1:G:1935:VAL:O	1:G:1939:MET:HG2	2.20	0.42
1:G:2750:LYS:O	1:G:2750:LYS:HG2	2.20	0.42
1:M:3085:PRO:O	1:M:3088:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4041:ALA:O	1:M:4045:VAL:HG23	2.19	0.42
1:S:1272:LEU:CD2	1:S:1561:VAL:HG21	2.44	0.42
1:A:2113:SER:O	1:A:2117:VAL:HG23	2.20	0.42
1:A:2639:MET:HB3	1:A:2640:PRO:HD3	2.01	0.42
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	2.01	0.42
1:A:4578:LEU:HA	1:S:4879:MET:HG2	2.00	0.42
1:A:4726:ASP:C	1:A:4726:ASP:OD1	2.62	0.42
1:G:1297:PHE:CZ	1:G:1542:VAL:HG21	2.55	0.42
1:G:2122:SER:O	1:G:2126:ARG:HG3	2.19	0.42
1:G:2271:THR:OG1	1:G:2274:ASP:OD2	2.34	0.42
1:G:3536:ALA:HB3	1:G:3600:SER:CB	2.50	0.42
1:G:3991:GLY:O	1:G:3995:VAL:HG23	2.19	0.42
1:M:4838:VAL:O	1:M:4841:VAL:HG22	2.18	0.42
1:M:4928:LEU:O	1:M:4932:ILE:HG13	2.20	0.42
1:S:1297:PHE:CZ	1:S:1542:VAL:HG21	2.55	0.42
1:S:2599:GLN:O	1:S:2603:ILE:HG13	2.19	0.42
1:A:3046:LEU:O	1:A:3050:VAL:HG23	2.19	0.42
1:G:3391:GLU:HA	1:G:3394:VAL:HG22	2.01	0.42
1:G:4006:ASP:HB2	1:G:4009:GLN:OE1	2.19	0.42
1:M:3536:ALA:HB3	1:M:3600:SER:CB	2.50	0.42
1:M:3698:LEU:O	1:M:3702:VAL:HG23	2.20	0.42
1:M:3946:GLN:HA	1:M:3949:ARG:HG2	2.02	0.42
1:S:3085:PRO:O	1:S:3088:VAL:HG22	2.19	0.42
1:S:3391:GLU:HA	1:S:3394:VAL:HG22	2.01	0.42
1:S:4180:ARG:HD3	1:S:4192:ARG:HD3	2.01	0.42
1:S:4726:ASP:C	1:S:4726:ASP:OD1	2.62	0.42
1:A:610:ASN:OD1	1:A:610:ASN:C	2.63	0.42
1:A:3536:ALA:HB3	1:A:3600:SER:CB	2.50	0.42
1:G:2624:ARG:NH1	1:G:2906:VAL:HG21	2.35	0.42
1:G:2639:MET:HB3	1:G:2640:PRO:HD3	2.01	0.42
1:G:4138:ASP:O	1:G:4142:ASN:ND2	2.44	0.42
5:G:5105:117:H71	5:G:5105:117:H91	1.93	0.42
1:M:1089:TYR:HD2	1:M:1152:MET:HG2	1.84	0.42
1:M:2368:LEU:O	1:M:2368:LEU:HD23	2.19	0.42
1:S:3060:ASP:OD1	1:S:3060:ASP:N	2.43	0.42
1:A:1002:ALA:O	1:A:1003:GLN:C	2.61	0.42
1:A:4180:ARG:HD3	1:A:4192:ARG:HD3	2.01	0.42
1:G:996:TRP:CE2	1:G:1000:ARG:HG3	2.54	0.42
1:G:1805:GLU:HA	1:G:1808:ARG:NE	2.35	0.42
1:M:1935:VAL:O	1:M:1939:MET:HG2	2.20	0.42
1:S:575:LEU:N	1:S:575:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2643:LEU:HD23	1:S:2643:LEU:C	2.45	0.42
1:S:3779:VAL:HG13	1:S:3797:THR:HG22	2.00	0.42
1:S:4682:GLU:OE1	1:S:4682:GLU:C	2.63	0.42
1:A:637:LEU:HD12	1:A:637:LEU:N	2.35	0.42
1:A:3571:TRP:HE3	1:A:3575:LEU:HD12	1.83	0.42
1:A:3946:GLN:HA	1:A:3949:ARG:HG2	2.02	0.42
1:G:610:ASN:OD1	1:G:610:ASN:C	2.63	0.42
1:G:2113:SER:O	1:G:2117:VAL:HG23	2.20	0.42
1:G:2643:LEU:HD23	1:G:2643:LEU:C	2.45	0.42
1:G:3006:ILE:HG23	1:G:3010:PHE:CE2	2.55	0.42
1:G:4726:ASP:C	1:G:4726:ASP:OD1	2.62	0.42
1:M:2113:SER:O	1:M:2117:VAL:HG23	2.20	0.42
1:M:2960:LEU:HB3	1:M:3038:MET:HE2	2.02	0.42
1:M:4708:THR:HG22	1:M:4710:SER:H	1.85	0.42
1:S:411:TYR:HB2	1:S:486:LEU:HD21	2.01	0.42
1:S:544:LEU:HD22	1:S:574:VAL:HG13	2.01	0.42
1:S:1805:GLU:HA	1:S:1808:ARG:NE	2.35	0.42
1:S:1805:GLU:HA	1:S:1808:ARG:HE	1.85	0.42
1:S:2750:LYS:O	1:S:2750:LYS:HG2	2.20	0.42
1:A:1935:VAL:O	1:A:1939:MET:HG2	2.20	0.41
1:A:3281:LEU:HB2	1:A:3282:PRO:HD3	2.02	0.41
1:A:4708:THR:HG22	1:A:4710:SER:H	1.85	0.41
1:G:978:THR:N	1:G:981:GLN:OE1	2.50	0.41
1:G:3281:LEU:HB2	1:G:3282:PRO:HD3	2.02	0.41
1:G:4222:VAL:CG1	1:G:4950:VAL:CG1	2.98	0.41
1:G:4928:LEU:O	1:G:4932:ILE:HG13	2.20	0.41
1:M:637:LEU:HD12	1:M:637:LEU:N	2.35	0.41
1:M:1805:GLU:HA	1:M:1808:ARG:HE	1.85	0.41
1:M:2643:LEU:HD23	1:M:2643:LEU:C	2.45	0.41
1:S:2624:ARG:NH1	1:S:2906:VAL:HG21	2.35	0.41
1:S:3536:ALA:HB3	1:S:3600:SER:CB	2.50	0.41
1:A:996:TRP:CE2	1:A:1000:ARG:HG3	2.54	0.41
1:A:2276:ALA:O	1:A:2280:VAL:HG12	2.20	0.41
1:G:390:LEU:H	1:G:390:LEU:CD2	2.32	0.41
1:G:3698:LEU:O	1:G:3702:VAL:HG23	2.20	0.41
1:G:3779:VAL:HG13	1:G:3797:THR:HG22	2.00	0.41
1:M:610:ASN:OD1	1:M:610:ASN:C	2.63	0.41
1:M:2276:ALA:O	1:M:2280:VAL:HG12	2.20	0.41
1:S:1002:ALA:O	1:S:1003:GLN:C	2.61	0.41
1:S:2960:LEU:HB3	1:S:3038:MET:HE2	2.02	0.41
1:S:3006:ILE:HG23	1:S:3010:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3838:THR:O	1:S:3838:THR:HG22	2.19	0.41
1:A:390:LEU:H	1:A:390:LEU:CD2	2.32	0.41
1:A:575:LEU:HD12	1:A:575:LEU:N	2.35	0.41
1:A:2109:ASP:N	1:A:2109:ASP:OD1	2.52	0.41
1:A:4682:GLU:OE1	1:A:4682:GLU:C	2.63	0.41
1:G:683:ARG:NE	1:G:707:VAL:O	2.48	0.41
1:G:2333:ASP:OD1	1:G:2334:PHE:N	2.54	0.41
1:G:4682:GLU:OE1	1:G:4682:GLU:C	2.63	0.41
1:M:3003:LEU:HB2	1:M:3004:PRO:HD3	2.01	0.41
1:S:2639:MET:HB3	1:S:2640:PRO:HD3	2.01	0.41
1:S:3046:LEU:O	1:S:3050:VAL:HG23	2.19	0.41
1:G:1089:TYR:HD2	1:G:1152:MET:HG2	1.84	0.41
1:G:1805:GLU:HA	1:G:1808:ARG:HE	1.85	0.41
1:G:2276:ALA:O	1:G:2280:VAL:HG12	2.20	0.41
1:M:501:ALA:O	1:M:505:GLU:HG3	2.19	0.41
1:M:1297:PHE:CZ	1:M:1542:VAL:HG21	2.55	0.41
1:M:1805:GLU:HA	1:M:1808:ARG:NE	2.35	0.41
1:M:3046:LEU:O	1:M:3050:VAL:HG23	2.19	0.41
1:S:610:ASN:OD1	1:S:610:ASN:C	2.63	0.41
1:A:27:THR:HA	1:A:31:GLU:O	2.21	0.41
1:A:2101:MET:HA	1:A:2101:MET:HE3	2.02	0.41
1:A:3316:LEU:HD23	1:A:3353:LEU:CD2	2.51	0.41
1:A:3593:VAL:HA	1:A:3596:VAL:HG22	2.03	0.41
1:G:575:LEU:HD12	1:G:575:LEU:N	2.35	0.41
1:G:1867:GLU:HB2	1:G:1927:LEU:HD12	2.03	0.41
1:G:2161:GLN:O	1:G:2165:LEU:CD2	2.67	0.41
1:G:4020:GLN:O	1:G:4024:VAL:HG23	2.21	0.41
1:M:390:LEU:H	1:M:390:LEU:CD2	2.32	0.41
1:M:411:TYR:HB2	1:M:486:LEU:HD21	2.01	0.41
1:S:1694:LEU:O	1:S:1698:LEU:HG	2.20	0.41
1:S:3003:LEU:HB2	1:S:3004:PRO:HD3	2.01	0.41
1:S:4779:LYS:O	1:S:4783:ILE:HG13	2.21	0.41
1:S:5034:ASP:O	1:S:5035:GLN:HB2	2.21	0.41
1:A:3006:ILE:HG23	1:A:3010:PHE:CE2	2.55	0.41
1:G:637:LEU:HD12	1:G:637:LEU:N	2.35	0.41
1:G:828:GLU:OE2	1:G:831:ARG:NH1	2.51	0.41
1:G:4708:THR:HG22	1:G:4710:SER:H	1.85	0.41
1:G:5034:ASP:O	1:G:5035:GLN:HB2	2.21	0.41
1:M:27:THR:HA	1:M:31:GLU:O	2.21	0.41
1:M:1139:PHE:HZ	1:M:1169:LEU:O	2.04	0.41
1:M:4180:ARG:HD3	1:M:4192:ARG:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:27:THR:HA	1:S:31:GLU:O	2.21	0.41
1:S:390:LEU:H	1:S:390:LEU:CD2	2.32	0.41
1:S:2333:ASP:OD1	1:S:2334:PHE:N	2.54	0.41
1:S:3316:LEU:HD23	1:S:3353:LEU:CD2	2.51	0.41
1:S:3698:LEU:O	1:S:3702:VAL:HG23	2.20	0.41
1:S:3946:GLN:HA	1:S:3949:ARG:HG2	2.02	0.41
1:S:4928:LEU:O	1:S:4932:ILE:HG13	2.20	0.41
1:A:1805:GLU:HA	1:A:1808:ARG:HE	1.85	0.41
1:A:2333:ASP:OD1	1:A:2334:PHE:N	2.54	0.41
1:A:2992:GLU:O	1:A:2995:ILE:HG22	2.21	0.41
1:G:4772:ASP:OD1	1:G:4775:TYR:N	2.46	0.41
2:H:24:VAL:HG22	2:H:48:LYS:HG2	2.02	0.41
1:M:495:ASN:OD1	1:M:553:ARG:NH1	2.54	0.41
1:M:1426:ILE:HG23	1:M:1429:ASN:H	1.85	0.41
1:M:2624:ARG:NH1	1:M:2906:VAL:HG21	2.35	0.41
1:S:1184:ILE:HG23	1:S:1185:GLY:N	2.36	0.41
1:A:1426:ILE:HG23	1:A:1429:ASN:H	1.85	0.41
1:A:2643:LEU:HD23	1:A:2643:LEU:C	2.45	0.41
1:A:3698:LEU:O	1:A:3702:VAL:HG23	2.20	0.41
1:G:3593:VAL:HA	1:G:3596:VAL:HG22	2.03	0.41
1:M:1867:GLU:HB2	1:M:1927:LEU:HD12	2.03	0.41
1:M:2750:LYS:O	1:M:2750:LYS:HG2	2.20	0.41
1:M:3281:LEU:HB2	1:M:3282:PRO:HD3	2.02	0.41
1:M:3409:TYR:N	1:M:3410:PRO:HD2	2.36	0.41
1:M:4020:GLN:O	1:M:4024:VAL:HG23	2.21	0.41
5:M:5105:117:H91	5:M:5105:117:H71	1.93	0.41
1:S:828:GLU:OE2	1:S:831:ARG:NH1	2.51	0.41
1:S:1762:LEU:O	1:S:1765:VAL:HG22	2.21	0.41
1:S:1773:PRO:CA	1:S:2153:MET:HE1	2.51	0.41
1:S:3593:VAL:HA	1:S:3596:VAL:HG22	2.03	0.41
1:S:4708:THR:HG22	1:S:4710:SER:H	1.85	0.41
1:A:426:ARG:HB3	1:A:430:PRO:HA	2.03	0.41
1:A:1543:GLU:HG2	1:A:1544:PRO:HD2	2.03	0.41
1:A:1694:LEU:O	1:A:1698:LEU:HG	2.20	0.41
1:A:3530:GLN:O	1:A:3534:MET:HG2	2.21	0.41
1:A:4671:PHE:N	1:A:4714:ASN:HD22	2.19	0.41
1:G:205:ILE:HG23	1:G:206:CYS:N	2.36	0.41
1:G:904:HIS:HE1	1:G:906:CYS:SG	2.43	0.41
1:G:1543:GLU:HG2	1:G:1544:PRO:HD2	2.03	0.41
1:G:2960:LEU:HB3	1:G:3038:MET:HE2	2.02	0.41
1:G:3003:LEU:HB2	1:G:3004:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3530:GLN:O	1:G:3534:MET:HG2	2.21	0.41
1:G:3946:GLN:HA	1:G:3949:ARG:HG2	2.02	0.41
1:G:4091:LYS:O	1:G:4095:LYS:NZ	2.52	0.41
1:G:4779:LYS:O	1:G:4782:VAL:HG12	2.21	0.41
1:M:196:MET:HE2	1:M:196:MET:N	2.36	0.41
1:M:426:ARG:HB3	1:M:430:PRO:HA	2.03	0.41
1:M:1164:LEU:O	1:M:1167:GLU:N	2.50	0.41
1:M:1773:PRO:CA	1:M:2153:MET:HE1	2.51	0.41
1:M:3006:ILE:HG23	1:M:3010:PHE:CE2	2.55	0.41
1:M:3593:VAL:HA	1:M:3596:VAL:HG22	2.03	0.41
1:S:664:PHE:CE1	1:S:746:CYS:HB2	2.56	0.41
1:S:2101:MET:HA	1:S:2101:MET:HE3	2.02	0.41
1:S:2113:SER:O	1:S:2117:VAL:HG23	2.20	0.41
1:S:3281:LEU:HB2	1:S:3282:PRO:HD3	2.02	0.41
1:S:3409:TYR:N	1:S:3410:PRO:HD2	2.36	0.41
1:S:4231:MET:O	1:S:4235:VAL:HG23	2.21	0.41
1:A:1024:TYR:CZ	1:A:1032:LYS:HG2	2.56	0.41
1:A:1184:ILE:HG23	1:A:1185:GLY:N	2.36	0.41
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.36	0.41
1:A:5034:ASP:O	1:A:5035:GLN:HB2	2.21	0.41
1:G:664:PHE:CE1	1:G:746:CYS:HB2	2.56	0.41
1:G:1828:ASP:N	1:G:1828:ASP:OD1	2.54	0.41
1:G:2101:MET:HA	1:G:2101:MET:HE3	2.02	0.41
1:G:3201:MET:HA	1:G:3202:PRO:HD3	1.98	0.41
1:M:1184:ILE:HG23	1:M:1185:GLY:N	2.36	0.41
1:M:1694:LEU:O	1:M:1698:LEU:HG	2.20	0.41
1:M:3812:VAL:O	1:M:3816:MET:HG3	2.21	0.41
2:N:24:VAL:HG22	2:N:48:LYS:HG2	2.02	0.41
1:S:196:MET:HE2	1:S:196:MET:N	2.36	0.41
1:S:1024:TYR:CZ	1:S:1032:LYS:HG2	2.56	0.41
1:S:1867:GLU:HB2	1:S:1927:LEU:HD12	2.03	0.41
2:T:24:VAL:HG22	2:T:48:LYS:HG2	2.02	0.41
1:A:495:ASN:OD1	1:A:553:ARG:NH1	2.54	0.40
1:A:1154:ASP:OD1	1:A:1156:THR:OG1	2.39	0.40
1:A:4020:GLN:O	1:A:4024:VAL:HG23	2.21	0.40
1:G:202:MET:HE2	1:G:202:MET:HB2	1.99	0.40
1:G:3409:TYR:N	1:G:3410:PRO:HD2	2.36	0.40
1:G:4662:ASN:O	1:G:4662:ASN:OD1	2.40	0.40
1:G:4671:PHE:N	1:G:4714:ASN:HD22	2.19	0.40
1:M:1272:LEU:CD2	1:M:1561:VAL:HG21	2.44	0.40
1:M:1762:LEU:O	1:M:1765:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2101:MET:HE3	1:M:2101:MET:HA	2.02	0.40
1:M:4231:MET:O	1:M:4235:VAL:HG23	2.21	0.40
1:S:495:ASN:OD1	1:S:553:ARG:NH1	2.54	0.40
1:S:904:HIS:HE1	1:S:906:CYS:SG	2.43	0.40
1:S:1154:ASP:OD1	1:S:1156:THR:OG1	2.39	0.40
1:S:2276:ALA:O	1:S:2280:VAL:HG12	2.20	0.40
1:S:3916:ILE:CG2	1:S:3980:LEU:HD21	2.51	0.40
1:S:4671:PHE:N	1:S:4714:ASN:HD22	2.19	0.40
1:S:4779:LYS:O	1:S:4782:VAL:HG12	2.21	0.40
1:A:904:HIS:HE1	1:A:906:CYS:SG	2.43	0.40
1:G:462:GLU:HG2	1:G:463:GLU:N	2.37	0.40
1:G:495:ASN:OD1	1:G:553:ARG:NH1	2.54	0.40
1:G:3316:LEU:HD23	1:G:3353:LEU:CD2	2.51	0.40
1:G:3812:VAL:O	1:G:3816:MET:HG3	2.21	0.40
1:G:3916:ILE:CG2	1:G:3980:LEU:HD21	2.51	0.40
1:M:904:HIS:HE1	1:M:906:CYS:SG	2.43	0.40
1:M:1154:ASP:OD1	1:M:1156:THR:OG1	2.39	0.40
1:M:3530:GLN:O	1:M:3534:MET:HG2	2.21	0.40
1:M:4779:LYS:O	1:M:4782:VAL:HG12	2.21	0.40
1:M:4779:LYS:O	1:M:4783:ILE:HG13	2.21	0.40
1:S:1841:VAL:O	1:S:1845:VAL:HG23	2.22	0.40
1:A:1272:LEU:CD2	1:A:1561:VAL:HG21	2.44	0.40
1:A:1846:SER:O	1:A:1850:VAL:HG23	2.22	0.40
1:A:2865:VAL:HG21	1:A:2932:MET:HE2	2.04	0.40
1:A:4779:LYS:O	1:A:4782:VAL:HG12	2.21	0.40
1:G:196:MET:HE2	1:G:196:MET:N	2.36	0.40
1:G:1024:TYR:CZ	1:G:1032:LYS:HG2	2.56	0.40
1:G:4180:ARG:HD3	1:G:4192:ARG:HD3	2.01	0.40
1:G:4779:LYS:O	1:G:4783:ILE:HG13	2.21	0.40
1:M:1543:GLU:HG2	1:M:1544:PRO:HD2	2.03	0.40
1:M:1846:SER:O	1:M:1850:VAL:HG23	2.22	0.40
1:M:2333:ASP:OD1	1:M:2334:PHE:N	2.54	0.40
1:M:3050:VAL:HG21	1:M:3068:LEU:HD11	2.03	0.40
1:M:3316:LEU:HD23	1:M:3353:LEU:CD2	2.51	0.40
1:S:2203:MET:HE2	1:S:2203:MET:HB3	1.97	0.40
1:S:2992:GLU:O	1:S:2995:ILE:HG22	2.21	0.40
1:S:3812:VAL:O	1:S:3816:MET:HG3	2.21	0.40
1:A:1139:PHE:HZ	1:A:1169:LEU:O	2.04	0.40
1:A:1867:GLU:HB2	1:A:1927:LEU:HD12	2.03	0.40
1:A:2527:LEU:HD12	1:A:2530:MET:CE	2.50	0.40
1:A:2960:LEU:HB3	1:A:3038:MET:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3812:VAL:O	1:A:3816:MET:HG3	2.21	0.40
1:G:1154:ASP:OD1	1:G:1156:THR:OG1	2.39	0.40
1:G:1694:LEU:O	1:G:1698:LEU:HG	2.20	0.40
5:G:5105:117:H62	5:G:5105:117:C81	2.52	0.40
1:M:5034:ASP:O	1:M:5035:GLN:HB2	2.21	0.40
5:M:5105:117:H62	5:M:5105:117:C81	2.52	0.40
1:S:1426:ILE:HG23	1:S:1429:ASN:H	1.85	0.40
1:S:1846:SER:O	1:S:1850:VAL:HG23	2.22	0.40
1:S:4222:VAL:CG1	1:S:4950:VAL:CG1	2.98	0.40
1:A:2161:GLN:O	1:A:2165:LEU:CD2	2.67	0.40
1:A:3916:ILE:CG2	1:A:3980:LEU:HD21	2.51	0.40
2:B:24:VAL:HG22	2:B:48:LYS:HG2	2.02	0.40
1:G:172:VAL:HG22	1:G:179:TYR:CD1	2.57	0.40
1:G:426:ARG:HB3	1:G:430:PRO:HA	2.03	0.40
1:G:1139:PHE:HZ	1:G:1169:LEU:O	2.04	0.40
1:G:1426:ILE:HG23	1:G:1429:ASN:H	1.85	0.40
1:G:1762:LEU:O	1:G:1765:VAL:HG22	2.21	0.40
1:G:2525:GLY:O	1:G:2528:PRO:HD2	2.22	0.40
1:M:1841:VAL:O	1:M:1845:VAL:HG23	2.22	0.40
1:M:2638:LYS:HD2	1:M:2698:MET:SD	2.62	0.40
1:M:3388:GLU:O	1:M:3392:LEU:CD2	2.70	0.40
1:M:4662:ASN:O	1:M:4662:ASN:OD1	2.40	0.40
1:S:752:VAL:O	1:S:752:VAL:CG1	2.69	0.40
1:S:1139:PHE:HZ	1:S:1169:LEU:O	2.04	0.40
1:S:2161:GLN:O	1:S:2165:LEU:CD2	2.67	0.40
1:S:2914:LYS:HA	1:S:2914:LYS:HD2	1.94	0.40
1:S:3530:GLN:O	1:S:3534:MET:HG2	2.21	0.40
5:S:5105:117:C81	5:S:5105:117:H62	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3992/5037 (79%)	3897 (98%)	94 (2%)	1 (0%)	100	100
1	G	3992/5037 (79%)	3897 (98%)	94 (2%)	1 (0%)	100	100
1	M	3992/5037 (79%)	3897 (98%)	94 (2%)	1 (0%)	100	100
1	S	3992/5037 (79%)	3897 (98%)	94 (2%)	1 (0%)	100	100
2	B	105/111 (95%)	100 (95%)	5 (5%)	0	100	100
2	H	105/111 (95%)	100 (95%)	5 (5%)	0	100	100
2	N	105/111 (95%)	100 (95%)	5 (5%)	0	100	100
2	T	105/111 (95%)	100 (95%)	5 (5%)	0	100	100
All	All	16388/20592 (80%)	15988 (98%)	396 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3971	GLY
1	G	3971	GLY
1	M	3971	GLY
1	S	3971	GLY

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	3379/4276 (79%)	3379 (100%)	0	100	100
1	G	3379/4276 (79%)	3379 (100%)	0	100	100
1	M	3379/4276 (79%)	3379 (100%)	0	100	100
1	S	3379/4276 (79%)	3379 (100%)	0	100	100
2	B	86/91 (94%)	86 (100%)	0	100	100
2	H	86/91 (94%)	86 (100%)	0	100	100
2	N	86/91 (94%)	86 (100%)	0	100	100
2	T	86/91 (94%)	86 (100%)	0	100	100
All	All	13860/17468 (79%)	13860 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
1	A	201	ASN
1	A	465	GLN
1	A	797	HIS
1	A	909	ASN
1	A	911	HIS
1	A	1429	ASN
1	A	1598	GLN
1	A	1629	GLN
1	A	1640	HIS
1	A	1660	GLN
1	A	1702	HIS
1	A	1928	GLN
1	A	1953	HIS
1	A	2035	HIS
1	A	2100	HIS
1	A	2125	HIS
1	A	2441	HIS
1	A	2515	GLN
1	A	2620	GLN
1	A	2773	ASN
1	A	2780	ASN
1	A	2877	GLN
1	A	2931	GLN
1	A	3146	HIS
1	A	3313	ASN
1	A	3523	ASN
1	A	3608	GLN
1	A	3667	HIS
1	A	3970	GLN
1	A	3976	ASN
1	A	4204	GLN
1	A	4574	ASN
1	A	4714	ASN
1	A	4776	GLN
1	A	4812	HIS
1	A	4947	GLN
1	A	4983	HIS
1	G	113	HIS

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Mol	Chain	Res	Type
1	G	201	ASN
1	G	379	HIS
1	G	465	GLN
1	G	797	HIS
1	G	909	ASN
1	G	911	HIS
1	G	1429	ASN
1	G	1598	GLN
1	G	1629	GLN
1	G	1640	HIS
1	G	1660	GLN
1	G	1702	HIS
1	G	1928	GLN
1	G	1953	HIS
1	G	2035	HIS
1	G	2100	HIS
1	G	2441	HIS
1	G	2515	GLN
1	G	2620	GLN
1	G	2773	ASN
1	G	2780	ASN
1	G	2856	ASN
1	G	2858	GLN
1	G	2877	GLN
1	G	2931	GLN
1	G	3146	HIS
1	G	3313	ASN
1	G	3523	ASN
1	G	3608	GLN
1	G	3667	HIS
1	G	3970	GLN
1	G	3976	ASN
1	G	4204	GLN
1	G	4209	GLN
1	G	4574	ASN
1	G	4714	ASN
1	G	4776	GLN
1	G	4812	HIS
1	G	4983	HIS
1	M	113	HIS
1	M	201	ASN
1	M	379	HIS

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Mol	Chain	Res	Type
1	M	465	GLN
1	M	797	HIS
1	M	909	ASN
1	M	911	HIS
1	M	1429	ASN
1	M	1598	GLN
1	M	1629	GLN
1	M	1640	HIS
1	M	1660	GLN
1	M	1702	HIS
1	M	1928	GLN
1	M	1953	HIS
1	M	2035	HIS
1	M	2100	HIS
1	M	2441	HIS
1	M	2515	GLN
1	M	2620	GLN
1	M	2773	ASN
1	M	2780	ASN
1	M	2877	GLN
1	M	3109	ASN
1	M	3146	HIS
1	M	3313	ASN
1	M	3523	ASN
1	M	3608	GLN
1	M	3667	HIS
1	M	3970	GLN
1	M	4204	GLN
1	M	4209	GLN
1	M	4714	ASN
1	M	4776	GLN
1	M	4812	HIS
1	S	113	HIS
1	S	201	ASN
1	S	465	GLN
1	S	797	HIS
1	S	909	ASN
1	S	911	HIS
1	S	1429	ASN
1	S	1598	GLN
1	S	1629	GLN
1	S	1640	HIS

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Mol	Chain	Res	Type
1	S	1660	GLN
1	S	1702	HIS
1	S	1928	GLN
1	S	1953	HIS
1	S	2035	HIS
1	S	2100	HIS
1	S	2125	HIS
1	S	2441	HIS
1	S	2515	GLN
1	S	2620	GLN
1	S	2773	ASN
1	S	2780	ASN
1	S	2877	GLN
1	S	2931	GLN
1	S	3109	ASN
1	S	3146	HIS
1	S	3313	ASN
1	S	3422	HIS
1	S	3523	ASN
1	S	3608	GLN
1	S	3667	HIS
1	S	3970	GLN
1	S	3976	ASN
1	S	4204	GLN
1	S	4209	GLN
1	S	4714	ASN
1	S	4776	GLN
1	S	4812	HIS
1	S	4947	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	117	S	5104	-	44,44,44	0.79	1 (2%)	55,61,61	0.90	2 (3%)
5	117	G	5105	-	44,44,44	0.78	0	55,61,61	0.95	2 (3%)
3	CFF	A	5101	-	15,15,15	1.07	3 (20%)	23,23,23	2.22	9 (39%)
5	117	G	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.31	5 (9%)
5	117	M	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.31	5 (9%)
5	117	M	5105	-	44,44,44	0.78	0	55,61,61	0.95	2 (3%)
5	117	S	5105	-	44,44,44	0.78	0	55,61,61	0.95	2 (3%)
3	CFF	S	5101	-	15,15,15	1.07	3 (20%)	23,23,23	2.22	9 (39%)
5	117	A	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.31	5 (9%)
5	117	G	5104	-	44,44,44	0.79	1 (2%)	55,61,61	0.90	2 (3%)
5	117	M	5104	-	44,44,44	0.79	1 (2%)	55,61,61	0.90	2 (3%)
5	117	A	5105	-	44,44,44	0.78	0	55,61,61	0.95	2 (3%)
5	117	A	5104	-	44,44,44	0.79	1 (2%)	55,61,61	0.90	2 (3%)
5	117	S	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.31	5 (9%)
3	CFF	G	5101	-	15,15,15	1.07	3 (20%)	23,23,23	2.22	9 (39%)
3	CFF	M	5101	-	15,15,15	1.07	3 (20%)	23,23,23	2.22	9 (39%)

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	117	S	5104	-	-	0/33/33/33	0/4/4/4
5	117	G	5105	-	-	9/33/33/33	0/4/4/4
5	117	G	5103	-	-	6/33/33/33	0/4/4/4
5	117	M	5103	-	-	6/33/33/33	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	117	M	5105	-	-	9/33/33/33	0/4/4/4
3	CFF	A	5101	-	-	-	0/2/2/2
5	117	S	5105	-	-	9/33/33/33	0/4/4/4
3	CFF	S	5101	-	-	-	0/2/2/2
5	117	A	5103	-	-	6/33/33/33	0/4/4/4
5	117	G	5104	-	-	0/33/33/33	0/4/4/4
5	117	M	5104	-	-	0/33/33/33	0/4/4/4
5	117	A	5105	-	-	9/33/33/33	0/4/4/4
5	117	A	5104	-	-	0/33/33/33	0/4/4/4
5	117	S	5103	-	-	6/33/33/33	0/4/4/4
3	CFF	G	5101	-	-	-	0/2/2/2
3	CFF	M	5101	-	-	-	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	CFF	C6-N1	-2.43	1.35	1.40
3	G	5101	CFF	C6-N1	-2.43	1.35	1.40
3	M	5101	CFF	C6-N1	-2.43	1.35	1.40
3	S	5101	CFF	C6-N1	-2.43	1.35	1.40
5	A	5103	117	C12-C10	-2.21	1.45	1.49
5	G	5103	117	C12-C10	-2.21	1.45	1.49
5	M	5103	117	C12-C10	-2.21	1.45	1.49
5	S	5103	117	C12-C10	-2.21	1.45	1.49
3	A	5101	CFF	C2-N1	-2.19	1.34	1.39
3	G	5101	CFF	C2-N1	-2.19	1.34	1.39
3	M	5101	CFF	C2-N1	-2.19	1.34	1.39
3	S	5101	CFF	C2-N1	-2.19	1.34	1.39
5	A	5104	117	C12-C10	-2.12	1.45	1.49
5	G	5104	117	C12-C10	-2.12	1.45	1.49
5	M	5104	117	C12-C10	-2.12	1.45	1.49
5	S	5104	117	C12-C10	-2.12	1.45	1.49
3	A	5101	CFF	C2-N3	-2.06	1.35	1.39
3	G	5101	CFF	C2-N3	-2.06	1.35	1.39
3	M	5101	CFF	C2-N3	-2.06	1.35	1.39
3	S	5101	CFF	C2-N3	-2.06	1.35	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5103	117	C19-N2-C18	-6.06	116.69	127.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5103	117	C19-N2-C18	-6.06	116.69	127.45
5	M	5103	117	C19-N2-C18	-6.06	116.69	127.45
5	S	5103	117	C19-N2-C18	-6.06	116.69	127.45
3	A	5101	CFF	N3-C4-N9	4.84	133.88	126.27
3	G	5101	CFF	N3-C4-N9	4.84	133.88	126.27
3	M	5101	CFF	N3-C4-N9	4.84	133.88	126.27
3	S	5101	CFF	N3-C4-N9	4.84	133.88	126.27
3	A	5101	CFF	C5-C6-N1	3.88	119.16	112.06
3	G	5101	CFF	C5-C6-N1	3.88	119.16	112.06
3	M	5101	CFF	C5-C6-N1	3.88	119.16	112.06
3	S	5101	CFF	C5-C6-N1	3.88	119.16	112.06
3	A	5101	CFF	N3-C2-N1	3.65	121.70	117.14
3	G	5101	CFF	N3-C2-N1	3.65	121.70	117.14
3	M	5101	CFF	N3-C2-N1	3.65	121.70	117.14
3	S	5101	CFF	N3-C2-N1	3.65	121.70	117.14
5	A	5105	117	C6-C7-N1	3.30	117.93	112.16
5	G	5105	117	C6-C7-N1	3.30	117.93	112.16
5	M	5105	117	C6-C7-N1	3.30	117.93	112.16
5	S	5105	117	C6-C7-N1	3.30	117.93	112.16
5	A	5104	117	C11-C10-C8	3.10	109.34	106.82
5	G	5104	117	C11-C10-C8	3.10	109.34	106.82
5	M	5104	117	C11-C10-C8	3.10	109.34	106.82
5	S	5104	117	C11-C10-C8	3.10	109.34	106.82
3	A	5101	CFF	C6-C5-C4	-2.98	119.16	122.92
3	G	5101	CFF	C6-C5-C4	-2.98	119.16	122.92
3	M	5101	CFF	C6-C5-C4	-2.98	119.16	122.92
3	S	5101	CFF	C6-C5-C4	-2.98	119.16	122.92
3	A	5101	CFF	O13-C6-C5	-2.89	120.46	126.38
3	G	5101	CFF	O13-C6-C5	-2.89	120.46	126.38
3	M	5101	CFF	O13-C6-C5	-2.89	120.46	126.38
3	S	5101	CFF	O13-C6-C5	-2.89	120.46	126.38
3	A	5101	CFF	C6-N1-C2	-2.86	121.01	125.66
3	G	5101	CFF	C6-N1-C2	-2.86	121.01	125.66
3	M	5101	CFF	C6-N1-C2	-2.86	121.01	125.66
3	S	5101	CFF	C6-N1-C2	-2.86	121.01	125.66
3	A	5101	CFF	C8-N9-C4	2.85	109.82	102.98
3	G	5101	CFF	C8-N9-C4	2.85	109.82	102.98
3	M	5101	CFF	C8-N9-C4	2.85	109.82	102.98
3	S	5101	CFF	C8-N9-C4	2.85	109.82	102.98
5	A	5104	117	C12-C10-C8	-2.78	121.61	127.01
5	G	5104	117	C12-C10-C8	-2.78	121.61	127.01
5	M	5104	117	C12-C10-C8	-2.78	121.61	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	5104	117	C12-C10-C8	-2.78	121.61	127.01
5	A	5103	117	C5-C4-C3	2.62	118.43	114.28
5	G	5103	117	C5-C4-C3	2.62	118.43	114.28
5	M	5103	117	C5-C4-C3	2.62	118.43	114.28
5	S	5103	117	C5-C4-C3	2.62	118.43	114.28
5	A	5105	117	C5-C4-C3	2.49	118.22	114.28
5	G	5105	117	C5-C4-C3	2.49	118.22	114.28
5	M	5105	117	C5-C4-C3	2.49	118.22	114.28
5	S	5105	117	C5-C4-C3	2.49	118.22	114.28
3	A	5101	CFF	C5-C4-N9	-2.46	107.22	112.10
3	G	5101	CFF	C5-C4-N9	-2.46	107.22	112.10
3	M	5101	CFF	C5-C4-N9	-2.46	107.22	112.10
3	S	5101	CFF	C5-C4-N9	-2.46	107.22	112.10
5	A	5103	117	C4-C5-C6	-2.27	107.62	112.42
5	G	5103	117	C4-C5-C6	-2.27	107.62	112.42
5	M	5103	117	C4-C5-C6	-2.27	107.62	112.42
5	S	5103	117	C4-C5-C6	-2.27	107.62	112.42
3	A	5101	CFF	N7-C8-N9	-2.08	109.71	113.48
3	G	5101	CFF	N7-C8-N9	-2.08	109.71	113.48
3	M	5101	CFF	N7-C8-N9	-2.08	109.71	113.48
3	S	5101	CFF	N7-C8-N9	-2.08	109.71	113.48
5	A	5103	117	O18-C18-C11	-2.06	118.45	121.53
5	G	5103	117	O18-C18-C11	-2.06	118.45	121.53
5	M	5103	117	O18-C18-C11	-2.06	118.45	121.53
5	S	5103	117	O18-C18-C11	-2.06	118.45	121.53
5	A	5103	117	O3-C3-C4	-2.05	104.71	109.25
5	G	5103	117	O3-C3-C4	-2.05	104.71	109.25
5	M	5103	117	O3-C3-C4	-2.05	104.71	109.25
5	S	5103	117	O3-C3-C4	-2.05	104.71	109.25

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5103	117	C9-C11-C18-O18
5	A	5105	117	O5-C5-C6-C7
5	A	5105	117	C9-C11-C18-N2
5	G	5103	117	C9-C11-C18-O18
5	G	5105	117	O5-C5-C6-C7
5	G	5105	117	C9-C11-C18-N2
5	M	5103	117	C9-C11-C18-O18
5	M	5105	117	O5-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	M	5105	117	C9-C11-C18-N2
5	S	5103	117	C9-C11-C18-O18
5	S	5105	117	O5-C5-C6-C7
5	S	5105	117	C9-C11-C18-N2
5	A	5103	117	C20-C19-N2-C18
5	G	5103	117	C20-C19-N2-C18
5	M	5103	117	C20-C19-N2-C18
5	S	5103	117	C20-C19-N2-C18
5	A	5103	117	C24-C19-N2-C18
5	G	5103	117	C24-C19-N2-C18
5	M	5103	117	C24-C19-N2-C18
5	S	5103	117	C24-C19-N2-C18
5	A	5105	117	C4-C5-C6-C7
5	G	5105	117	C4-C5-C6-C7
5	M	5105	117	C4-C5-C6-C7
5	S	5105	117	C4-C5-C6-C7
5	A	5103	117	C10-C11-C18-N2
5	A	5103	117	C10-C11-C18-O18
5	A	5105	117	C10-C11-C18-N2
5	A	5105	117	C10-C11-C18-O18
5	G	5103	117	C10-C11-C18-N2
5	G	5103	117	C10-C11-C18-O18
5	G	5105	117	C10-C11-C18-N2
5	G	5105	117	C10-C11-C18-O18
5	M	5103	117	C10-C11-C18-N2
5	M	5103	117	C10-C11-C18-O18
5	M	5105	117	C10-C11-C18-N2
5	M	5105	117	C10-C11-C18-O18
5	S	5103	117	C10-C11-C18-N2
5	S	5103	117	C10-C11-C18-O18
5	S	5105	117	C10-C11-C18-N2
5	S	5105	117	C10-C11-C18-O18
5	A	5105	117	C6-C7-N1-C9
5	G	5105	117	C6-C7-N1-C9
5	M	5105	117	C6-C7-N1-C9
5	S	5105	117	C6-C7-N1-C9
5	A	5105	117	C9-C11-C18-O18
5	G	5105	117	C9-C11-C18-O18
5	M	5105	117	C9-C11-C18-O18
5	S	5105	117	C9-C11-C18-O18
5	A	5103	117	C9-C11-C18-N2
5	G	5103	117	C9-C11-C18-N2

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Mol	Chain	Res	Type	Atoms
5	M	5103	117	C9-C11-C18-N2
5	S	5103	117	C9-C11-C18-N2
5	A	5105	117	C6-C7-N1-C8
5	G	5105	117	C6-C7-N1-C8
5	M	5105	117	C6-C7-N1-C8
5	S	5105	117	C6-C7-N1-C8
5	A	5105	117	O1A-C1-C2-C3
5	G	5105	117	O1A-C1-C2-C3
5	M	5105	117	O1A-C1-C2-C3
5	S	5105	117	O1A-C1-C2-C3

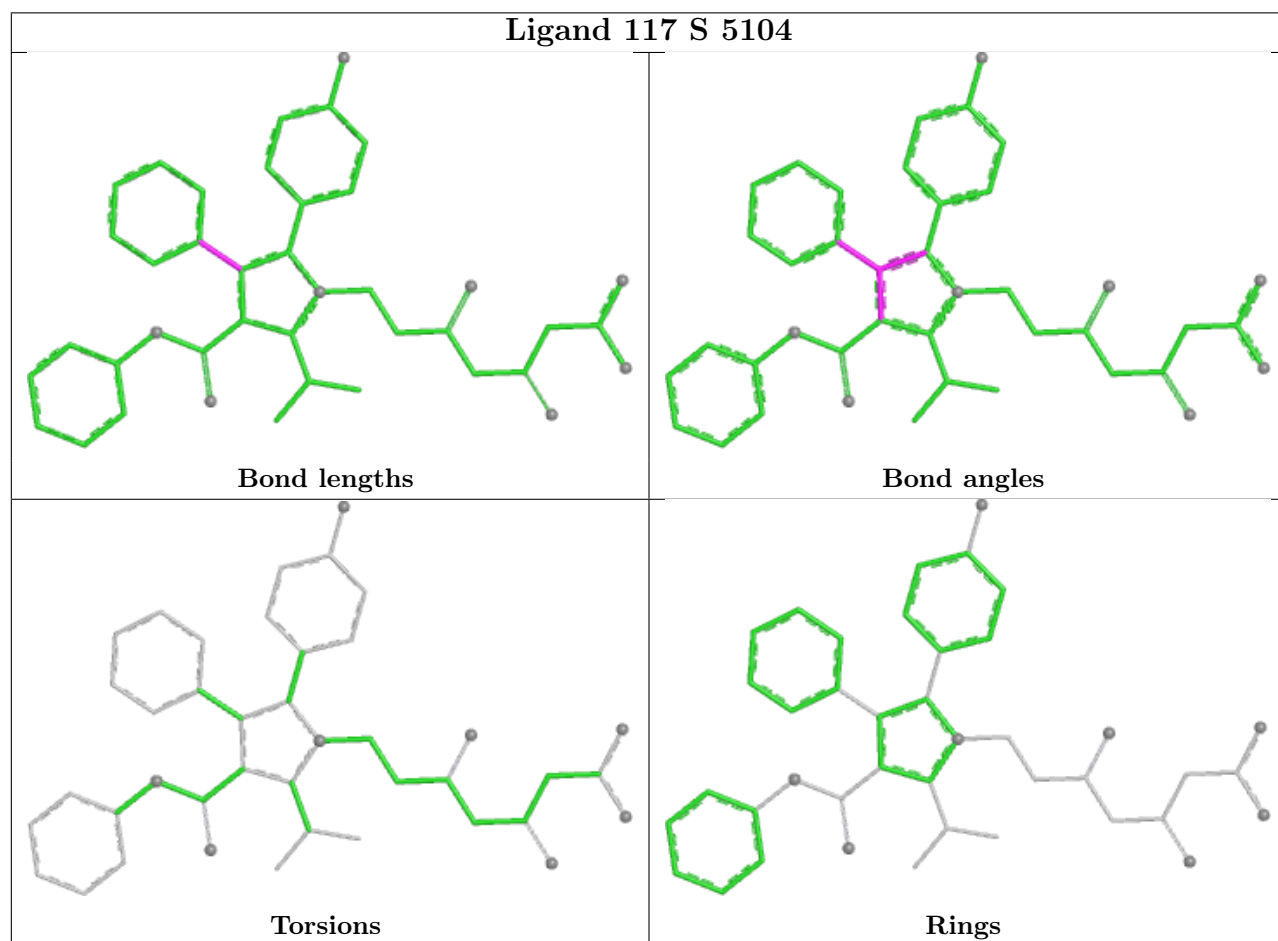
There are no ring outliers.

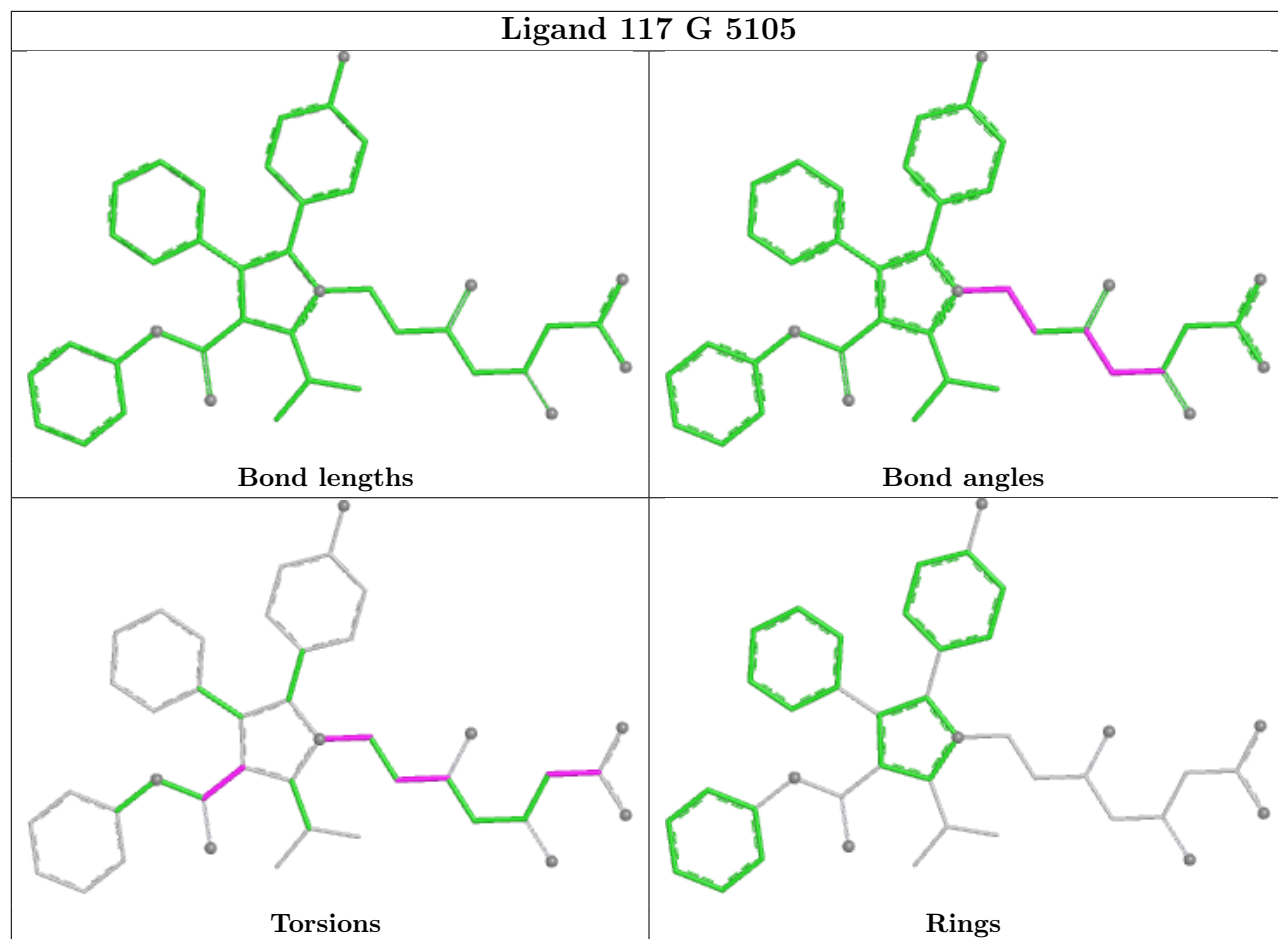
16 monomers are involved in 41 short contacts:

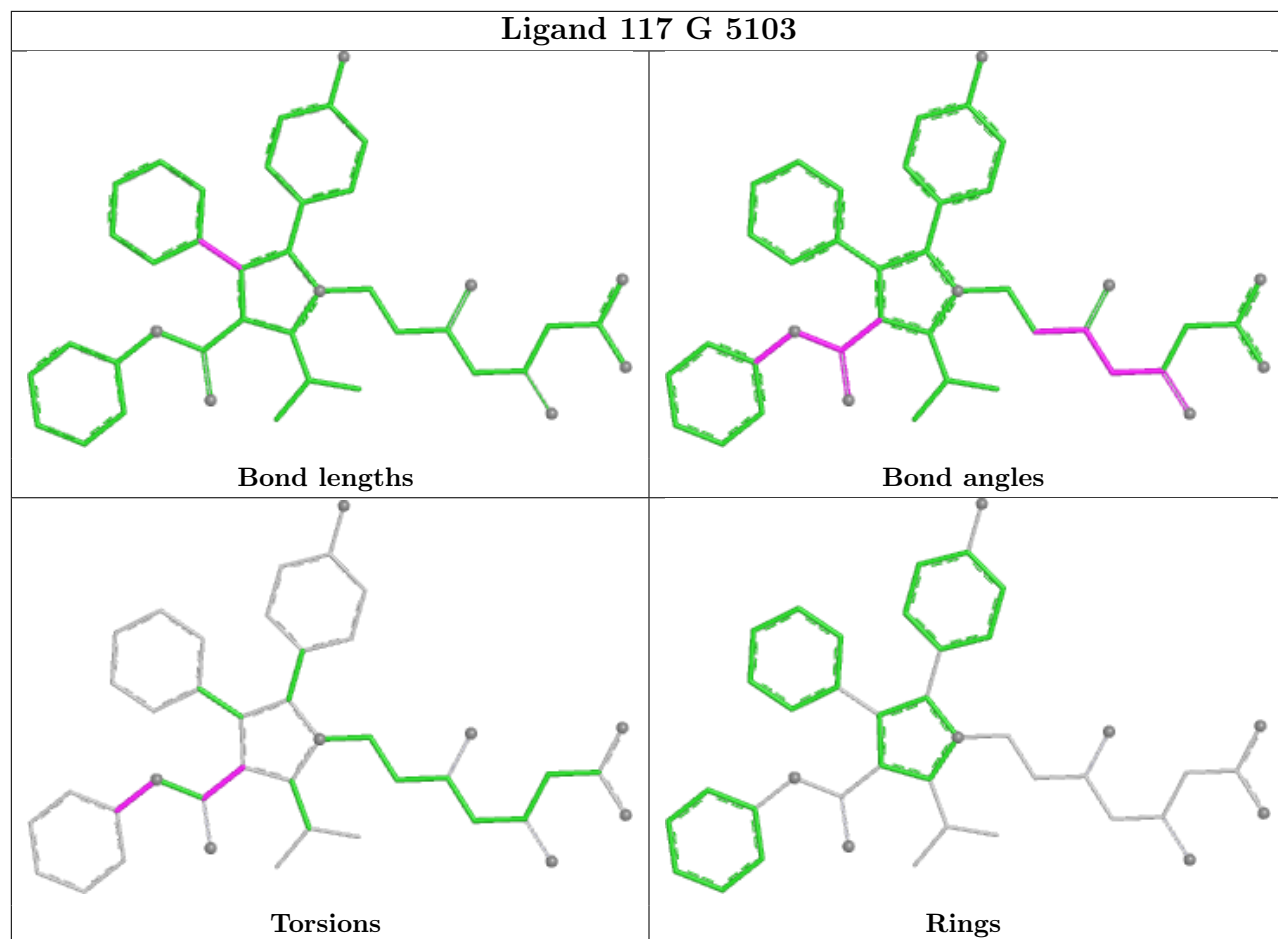
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	5104	117	3	0
5	G	5105	117	5	0
3	A	5101	CFF	1	0
5	G	5103	117	4	0
5	M	5103	117	4	0
5	M	5105	117	5	0
5	S	5105	117	4	0
3	S	5101	CFF	1	0
5	A	5103	117	4	0
5	G	5104	117	3	0
5	M	5104	117	3	0
5	A	5105	117	3	0
5	A	5104	117	3	0
5	S	5103	117	4	0
3	G	5101	CFF	1	0
3	M	5101	CFF	1	0

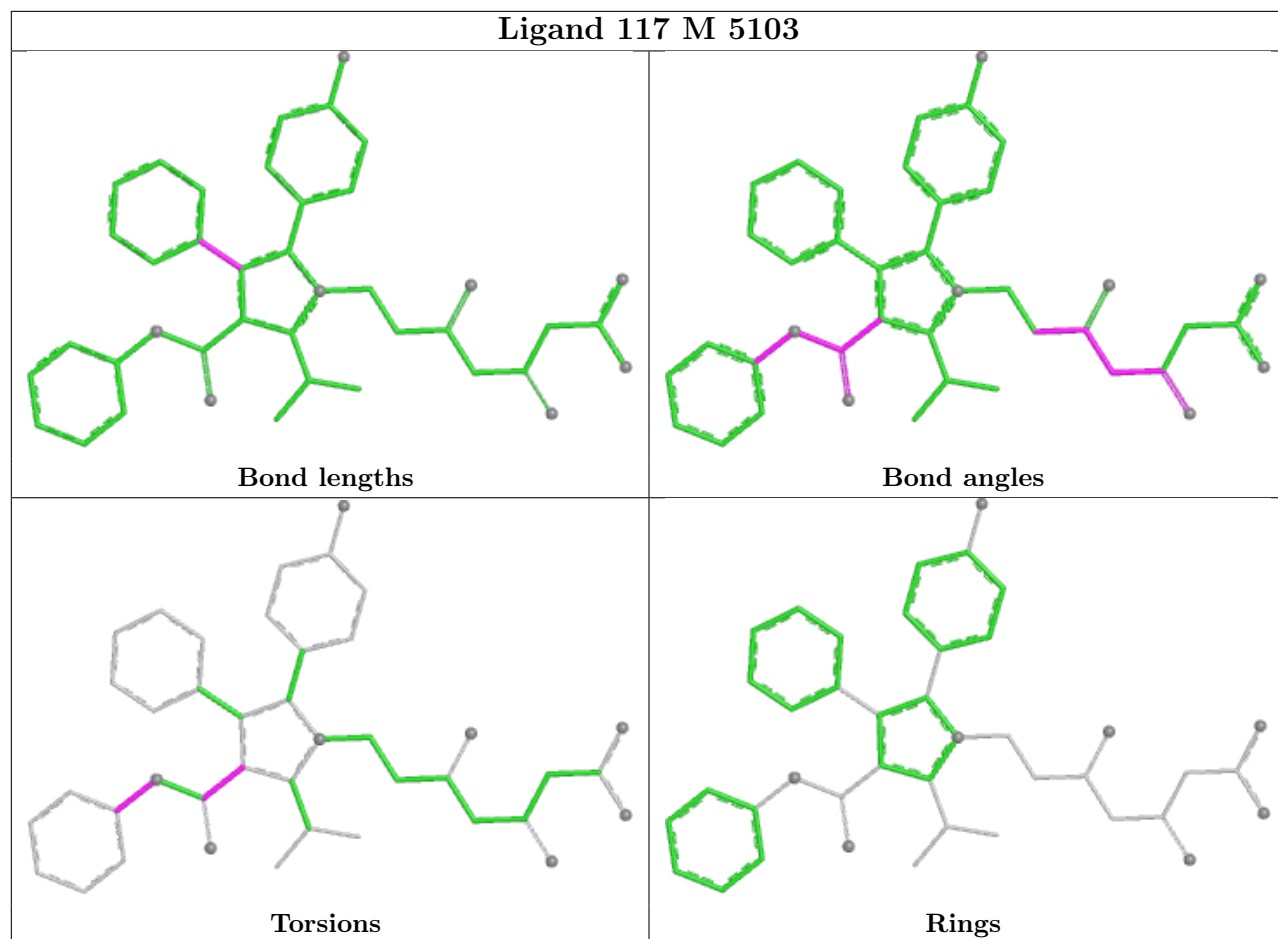
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

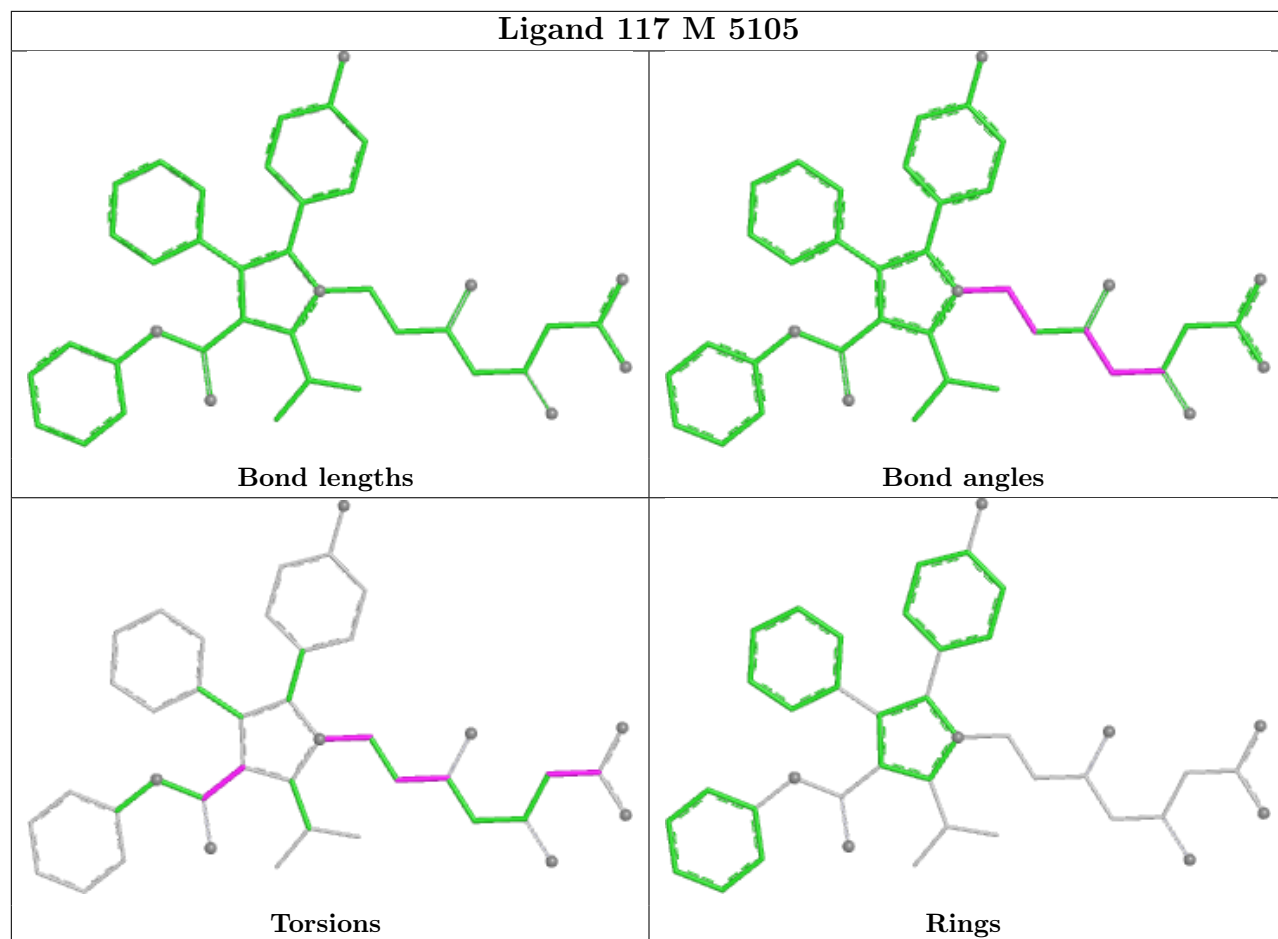
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

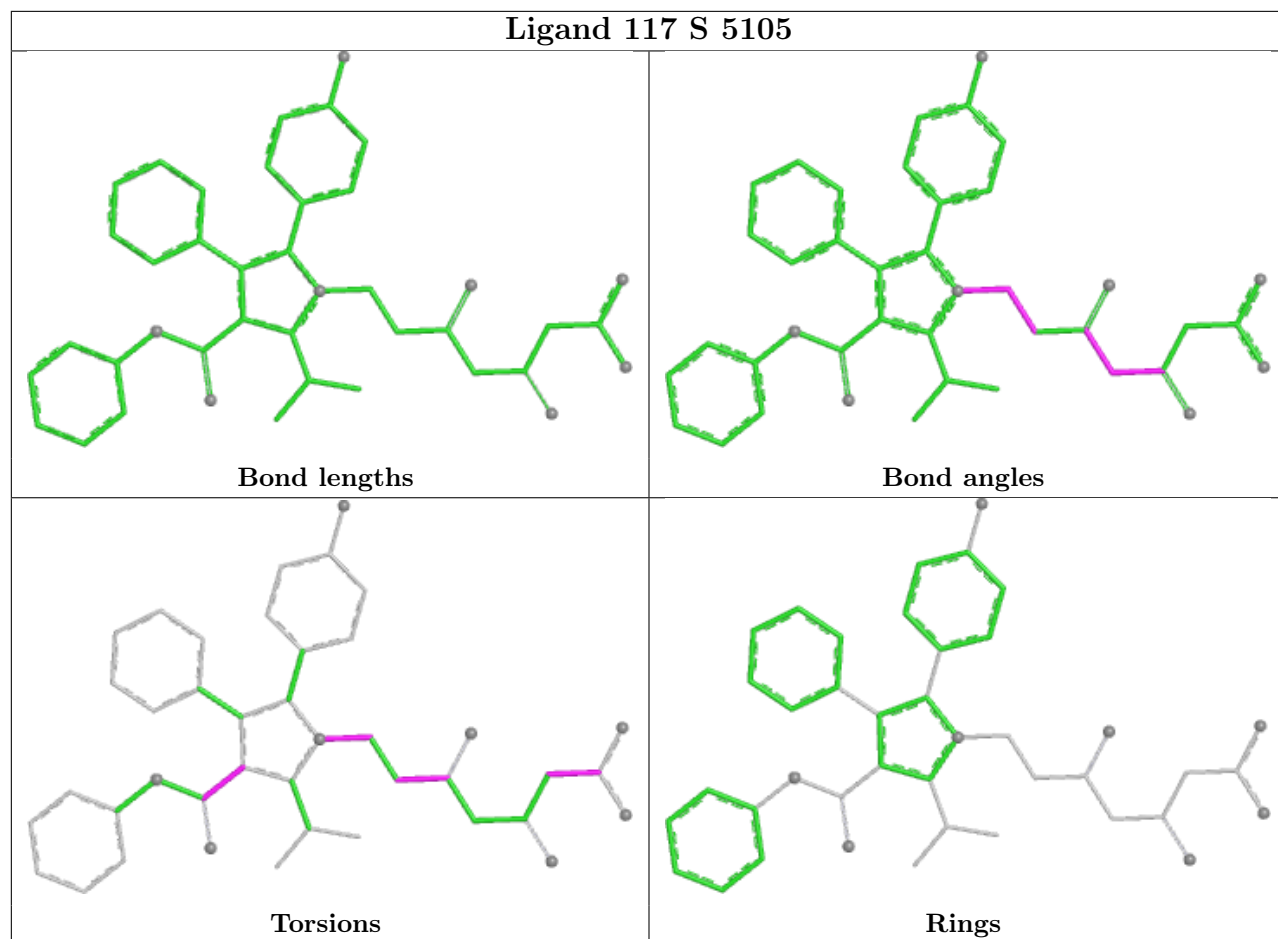


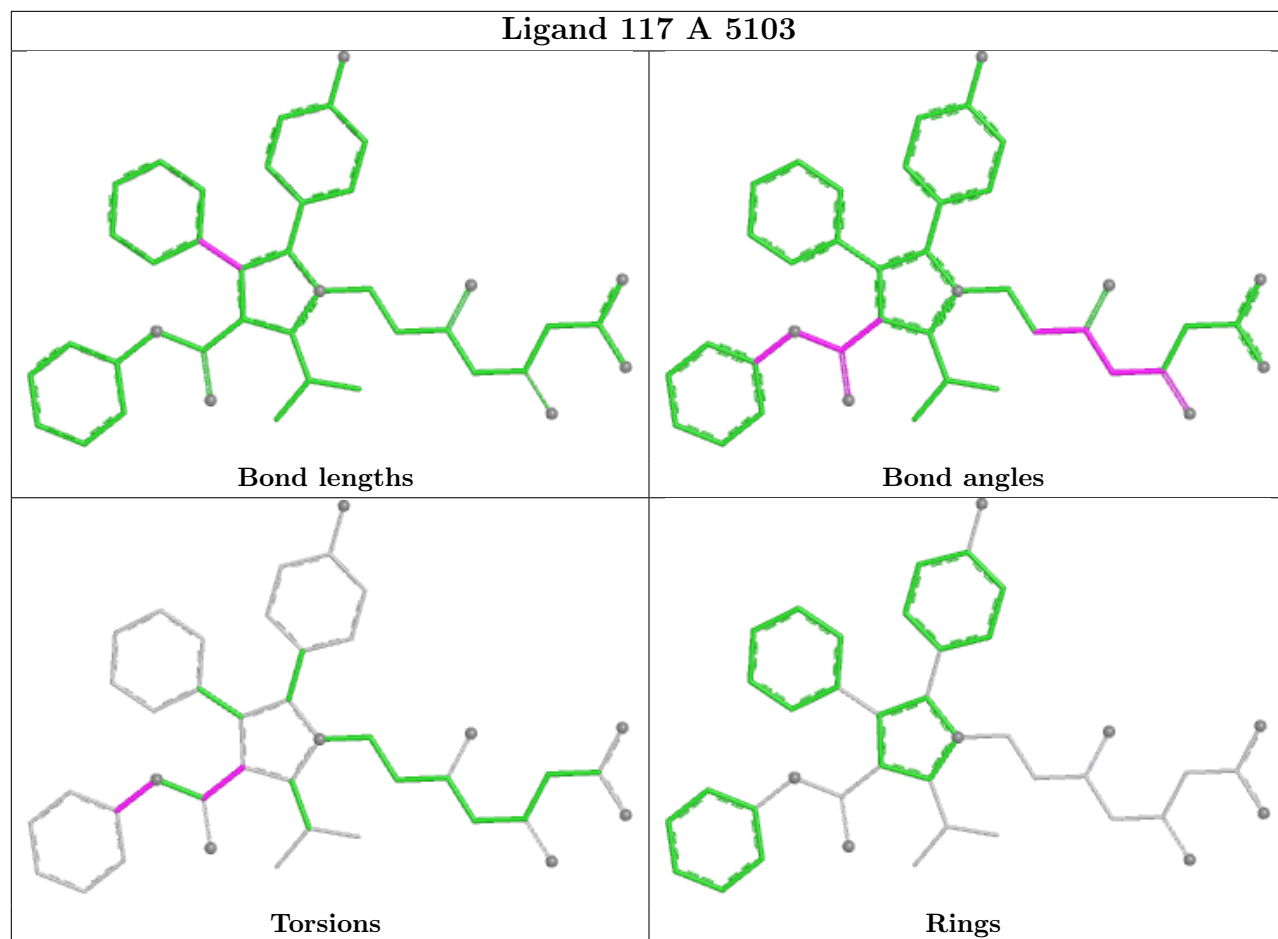


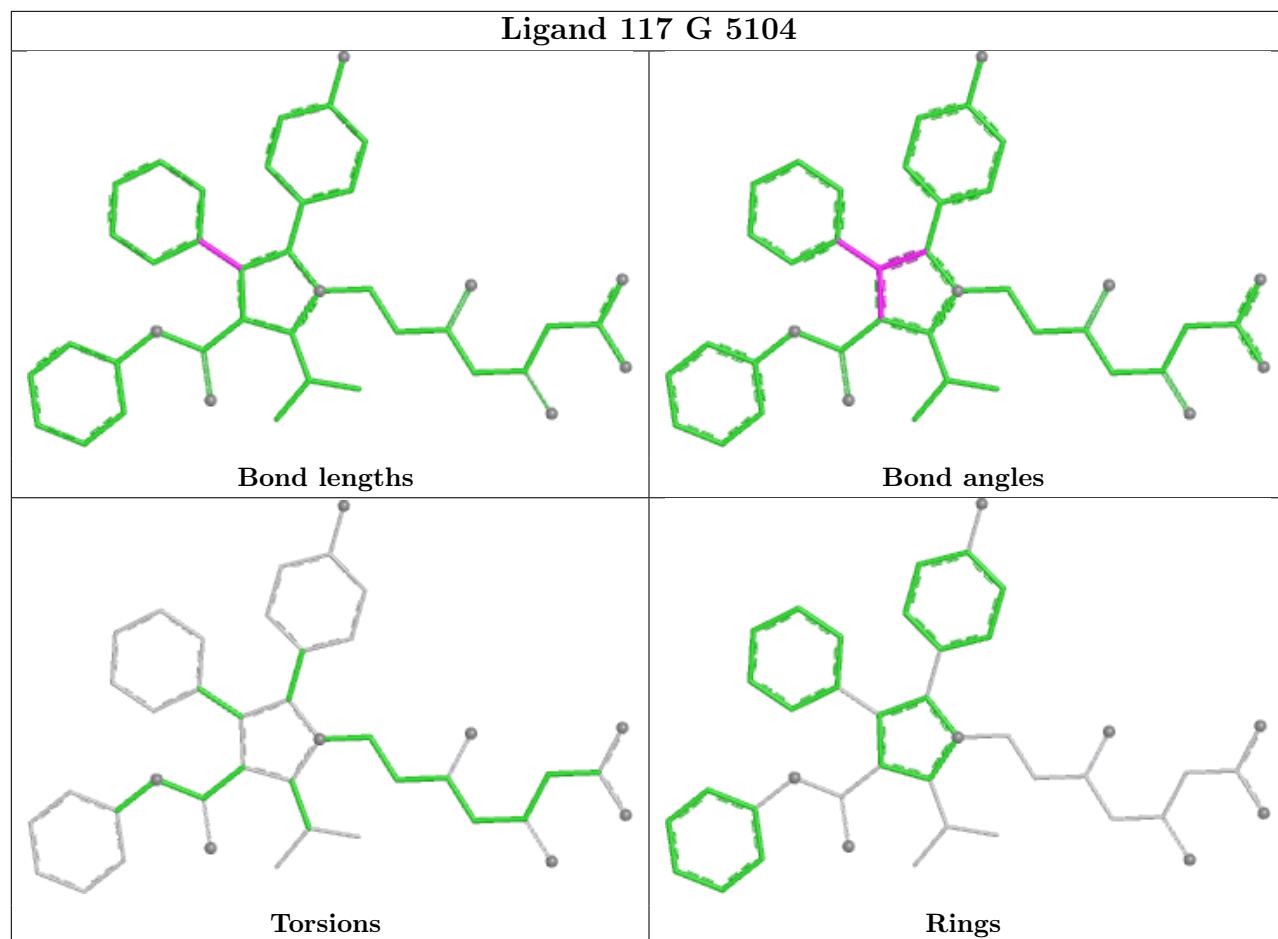


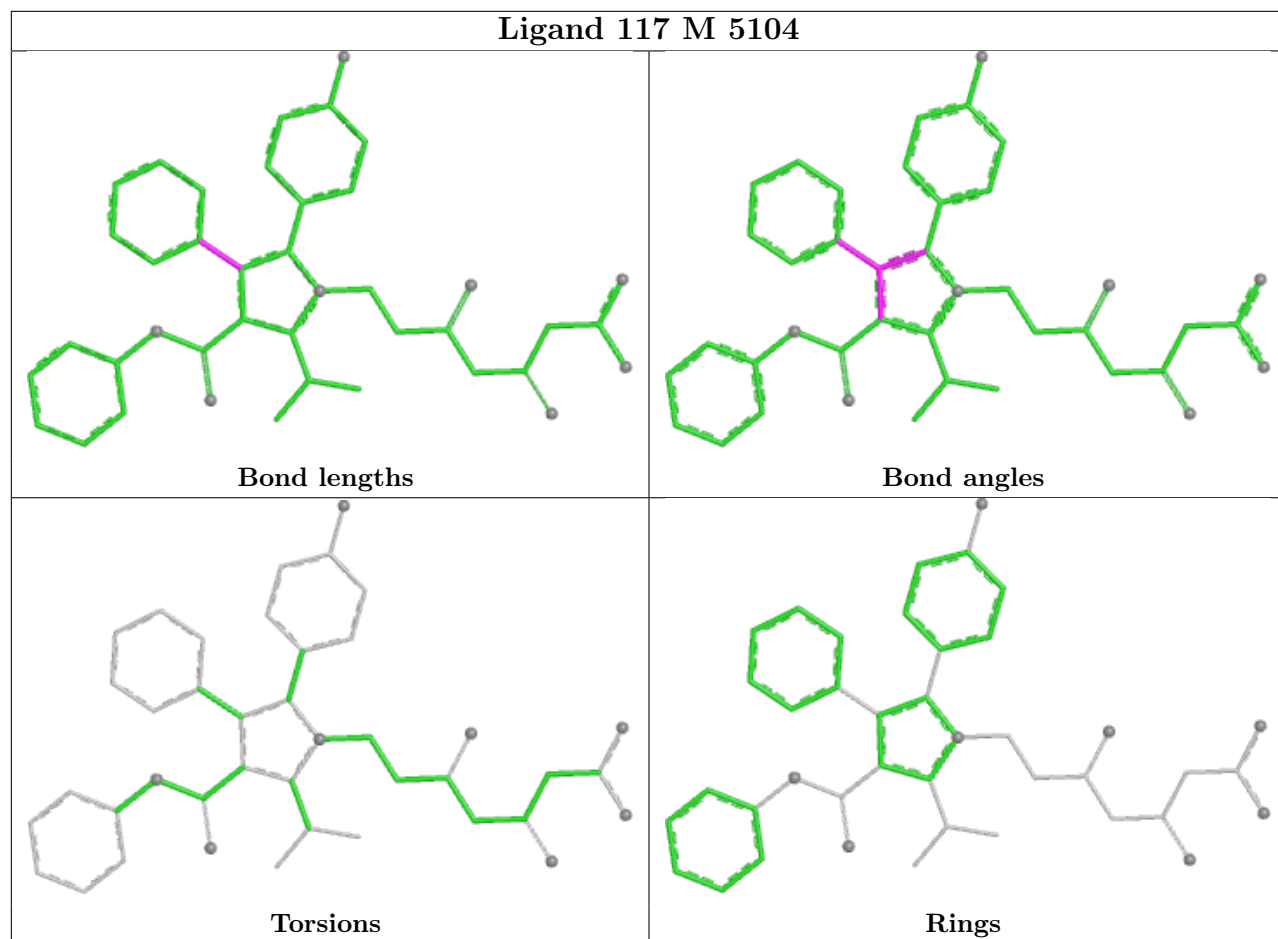


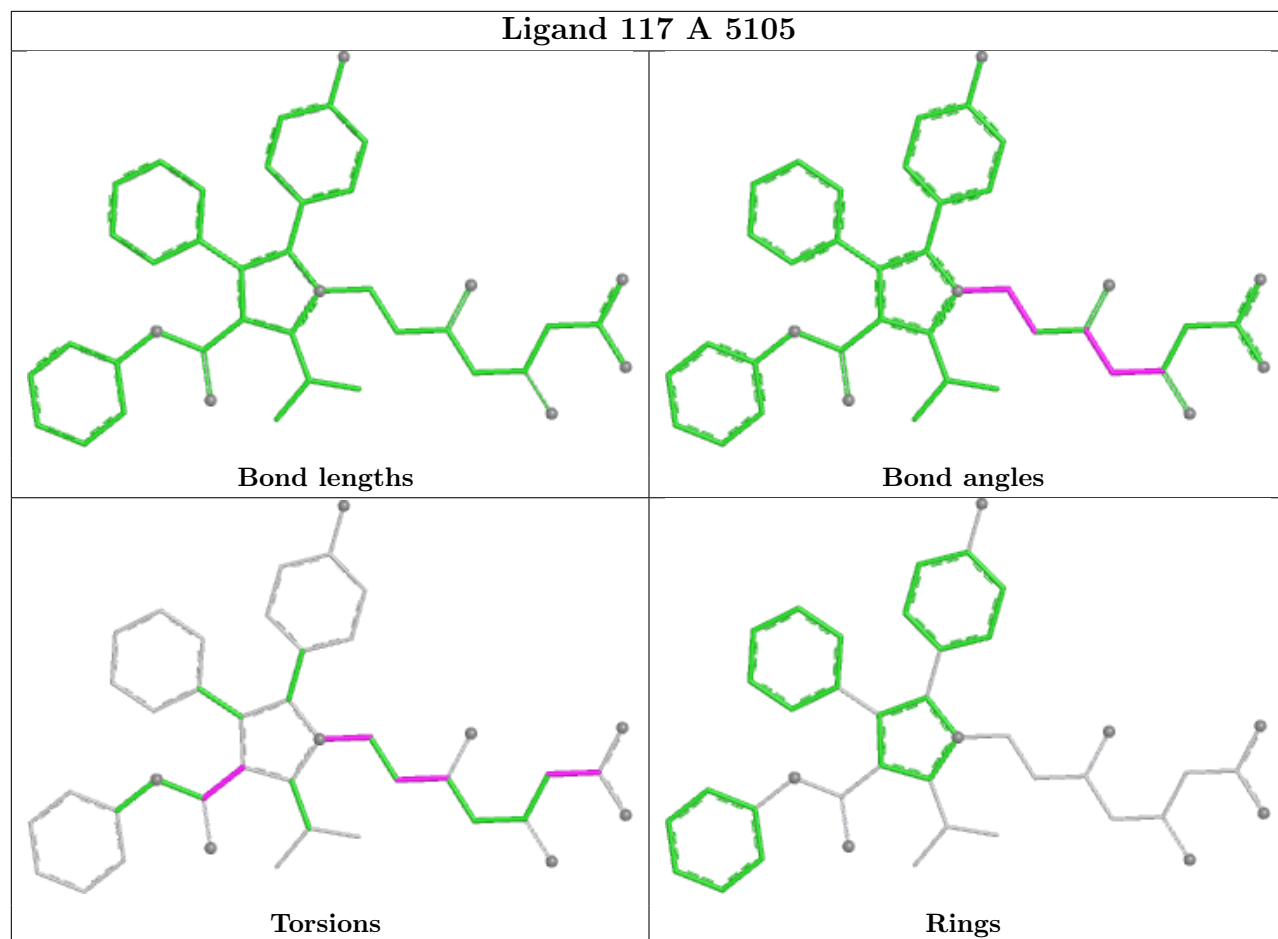


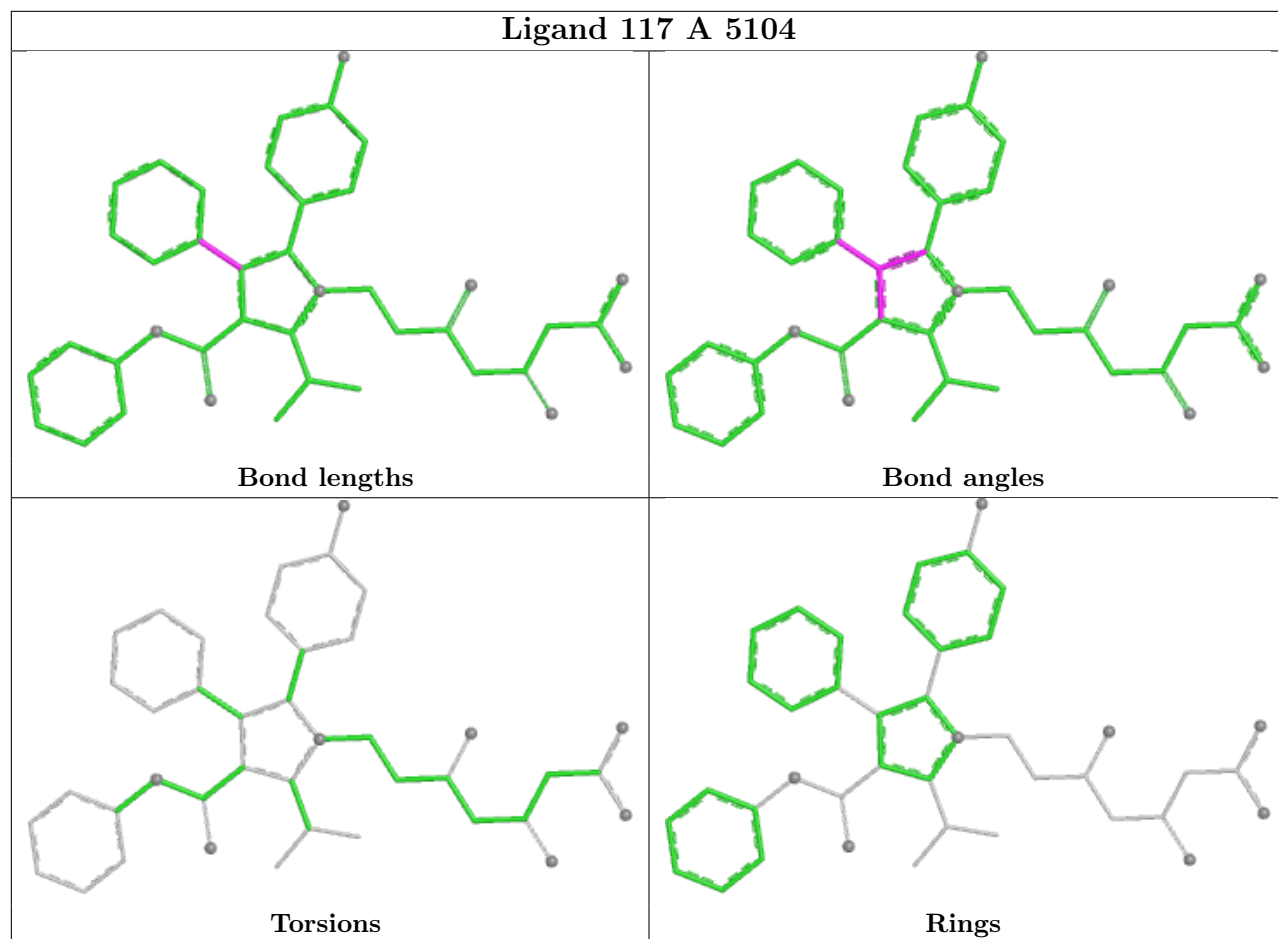


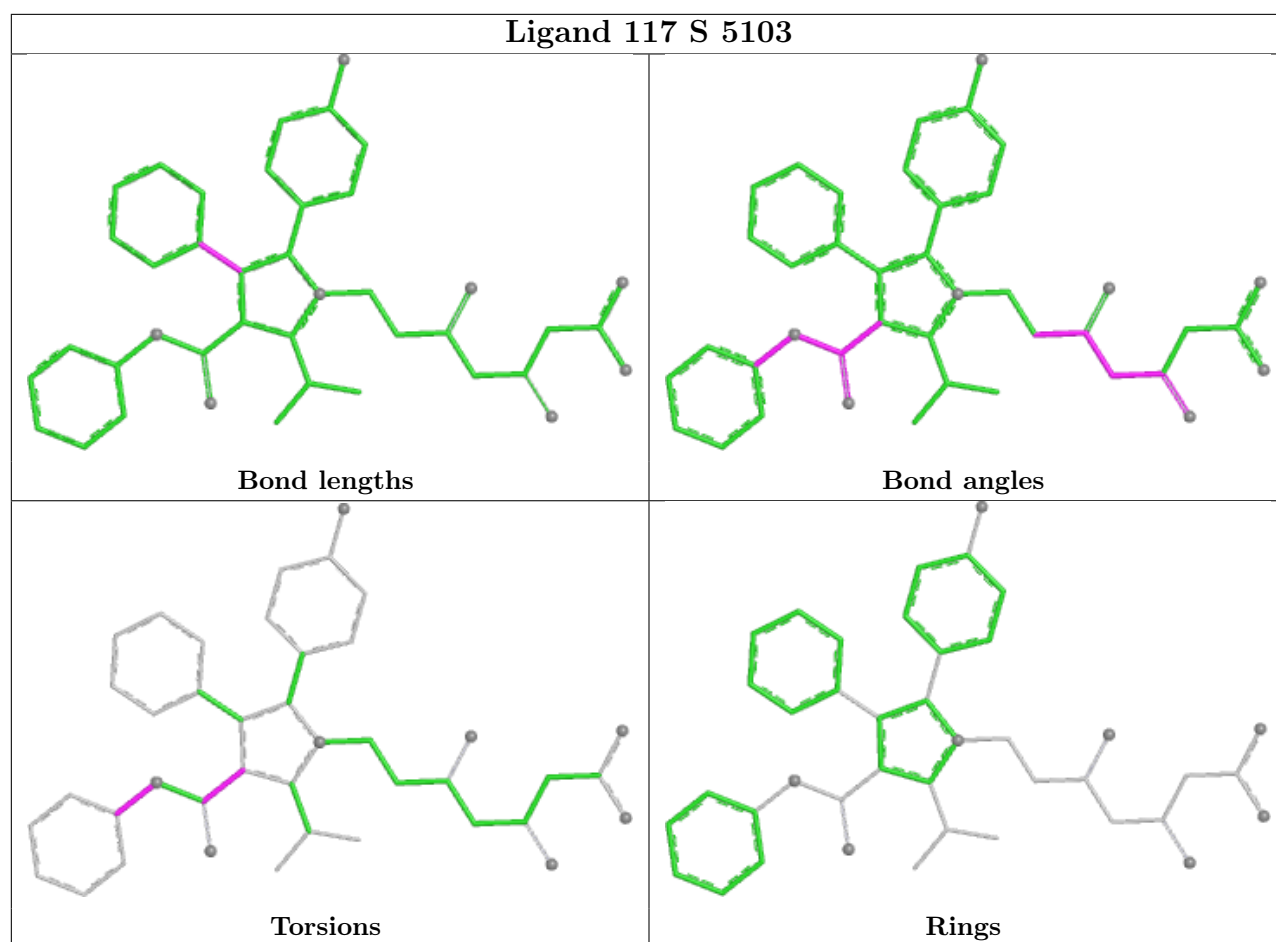












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

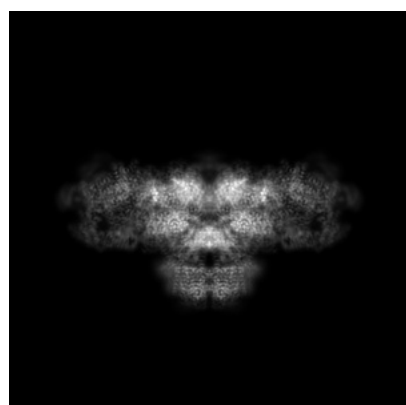
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70589. These allow visual inspection of the internal detail of the map and identification of artifacts.

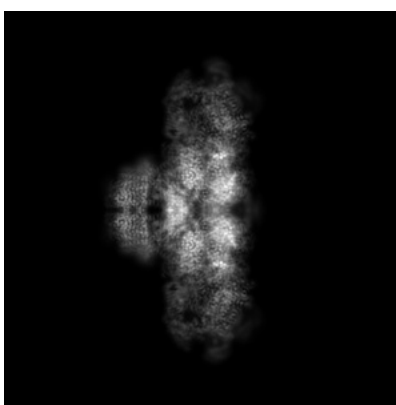
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

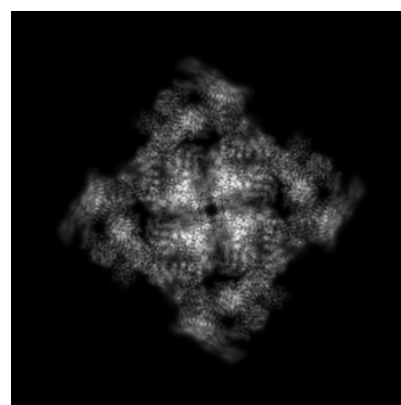
6.1.1 Primary map



X



Y



Z

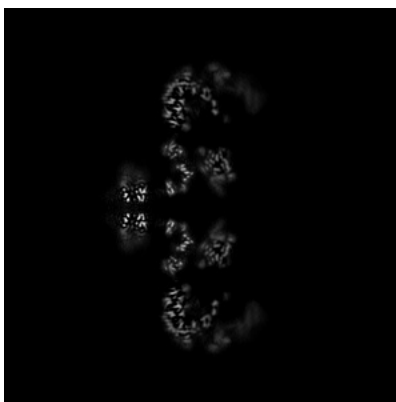
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

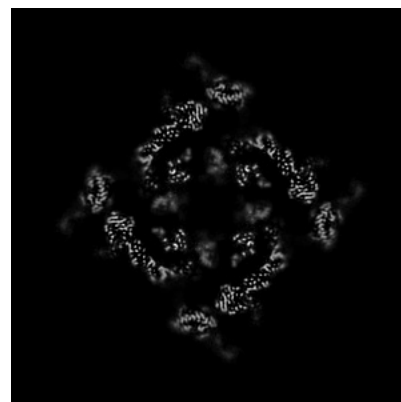
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

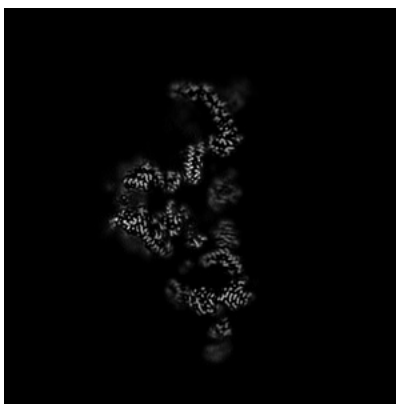
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

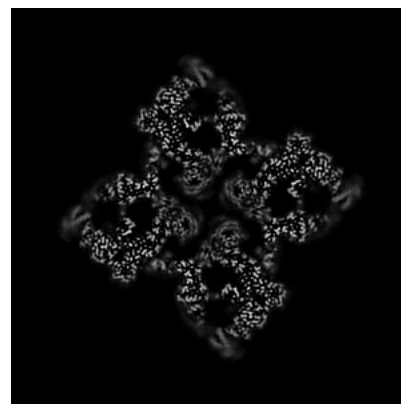
6.3.1 Primary map



X Index: 227



Y Index: 227

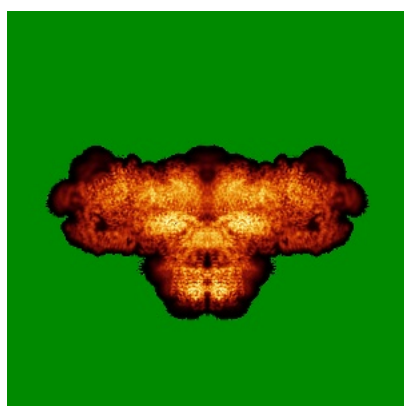


Z Index: 282

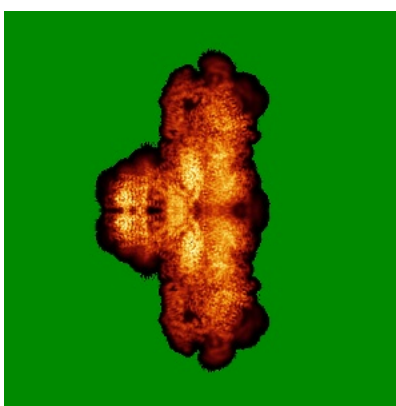
The images above show the largest variance slices of the map in three orthogonal directions.

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

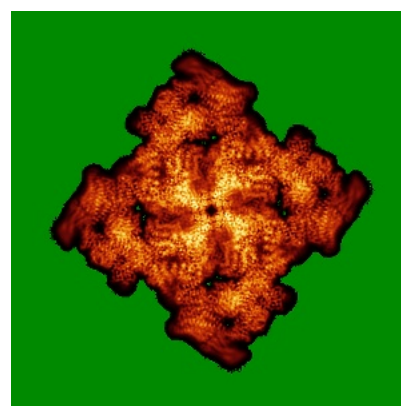
6.4.1 Primary map



X



Y

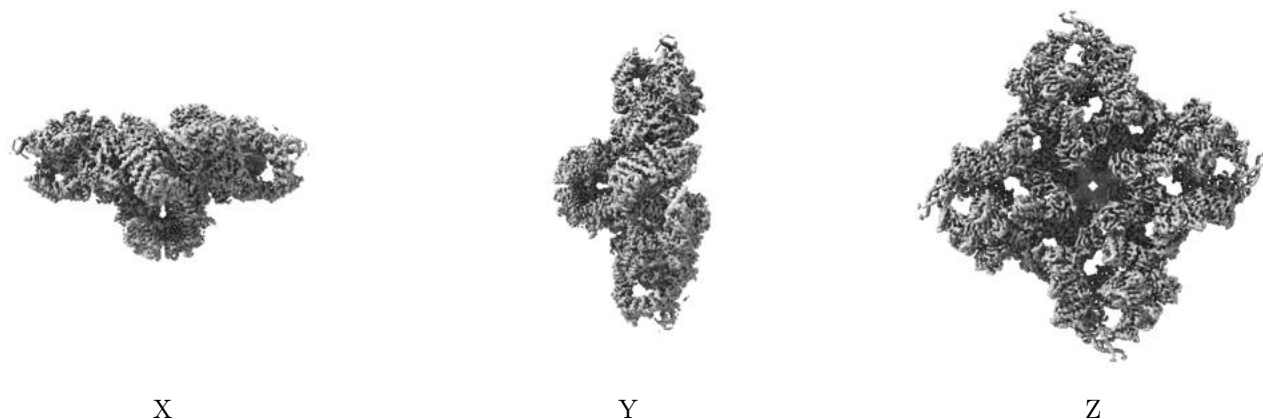


Z

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

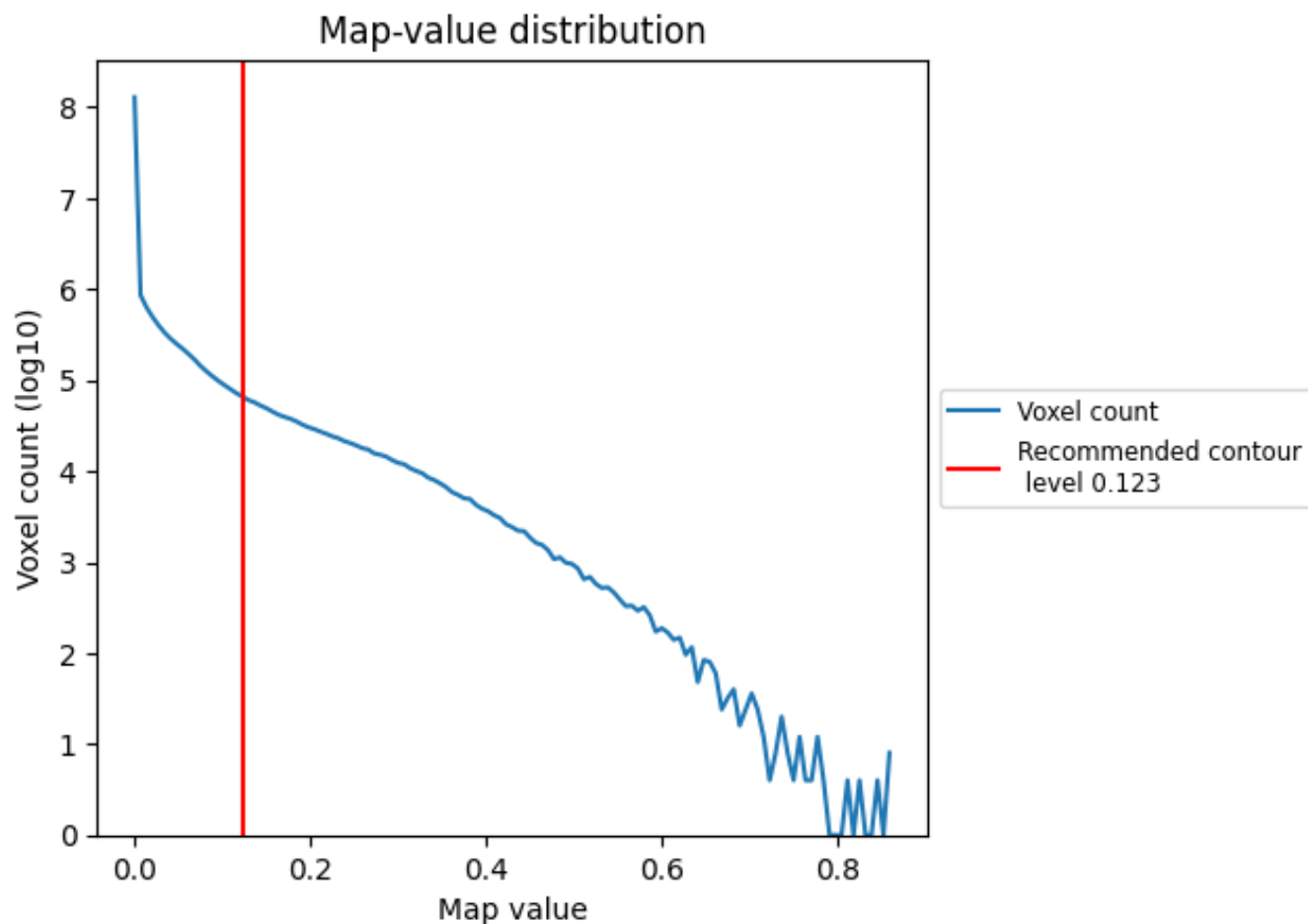
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

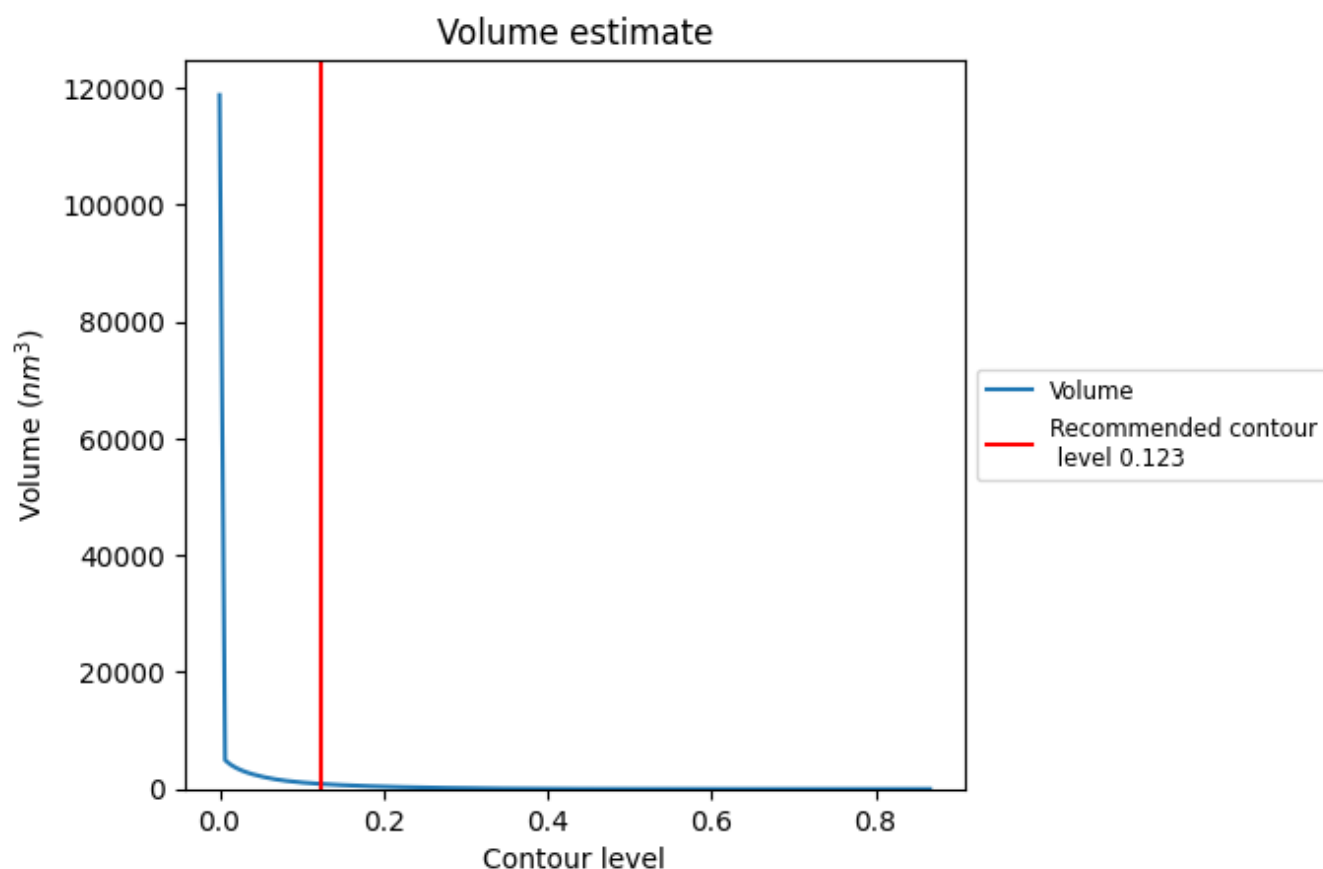
This section contains the results of statistical analysis of the map.

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.

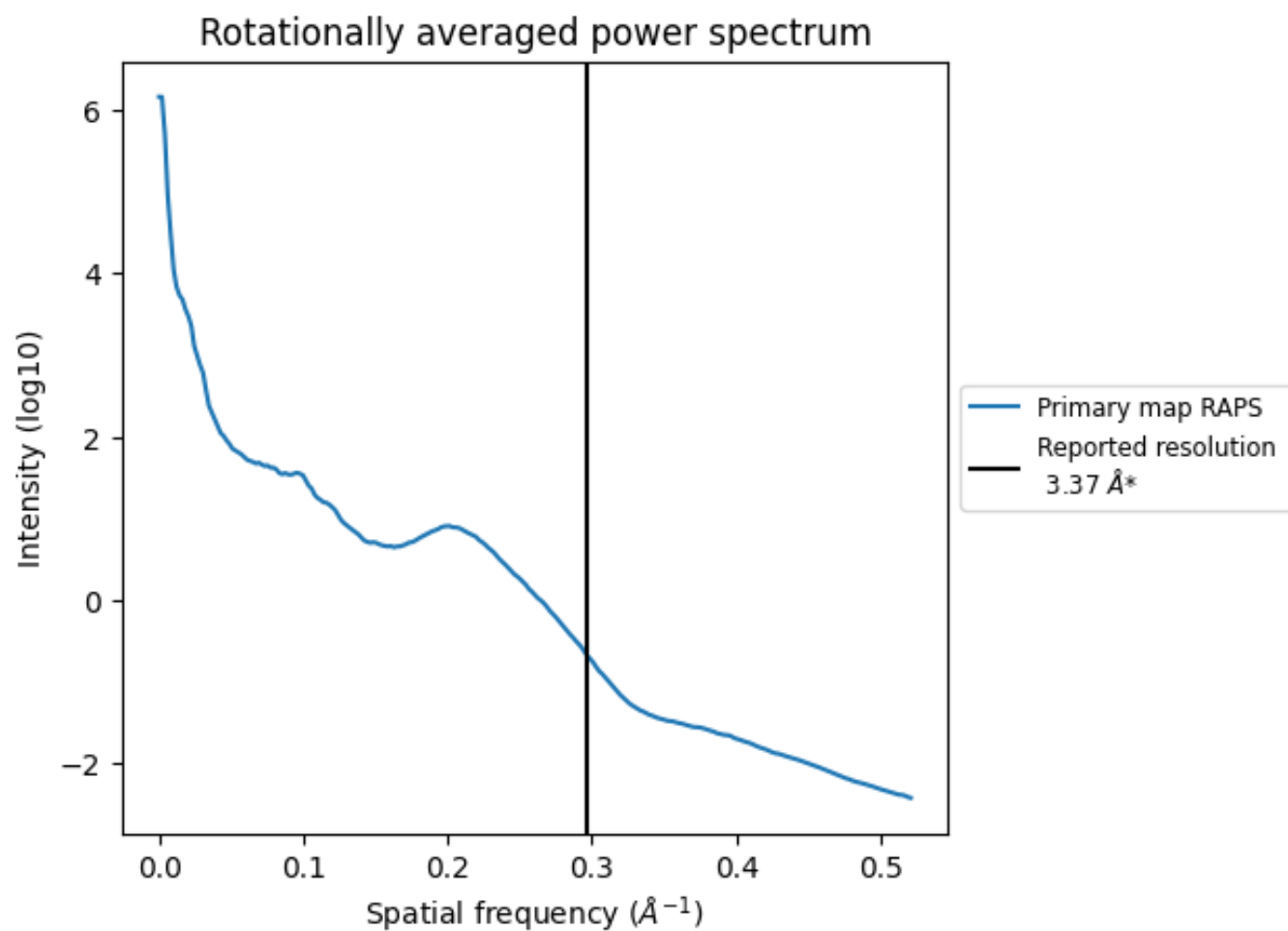
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 869 nm^3 ; this corresponds to an approximate mass of 785 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 0.297 Å⁻¹

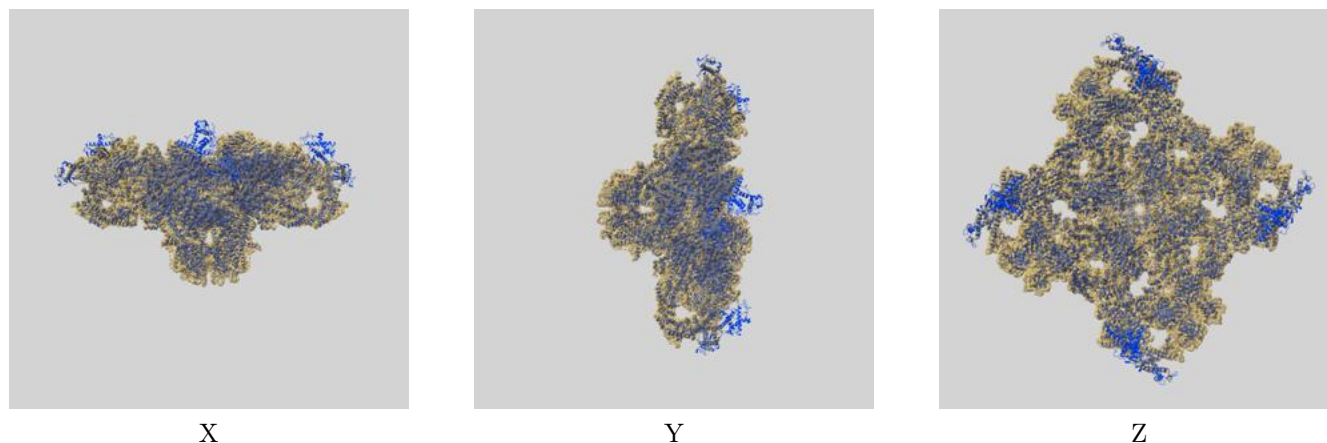
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

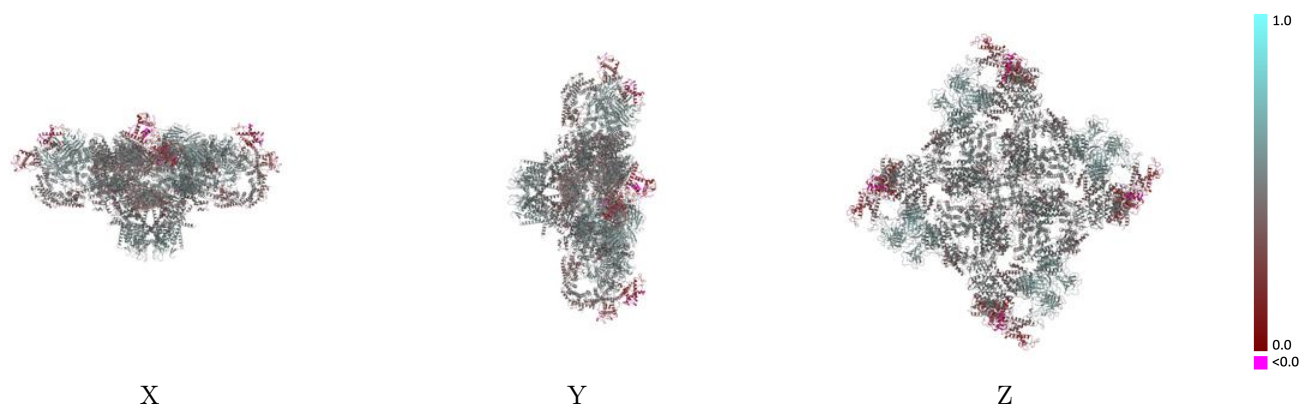
This section contains information regarding the fit between EMDB map EMD-70589 and PDB model 9OL4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



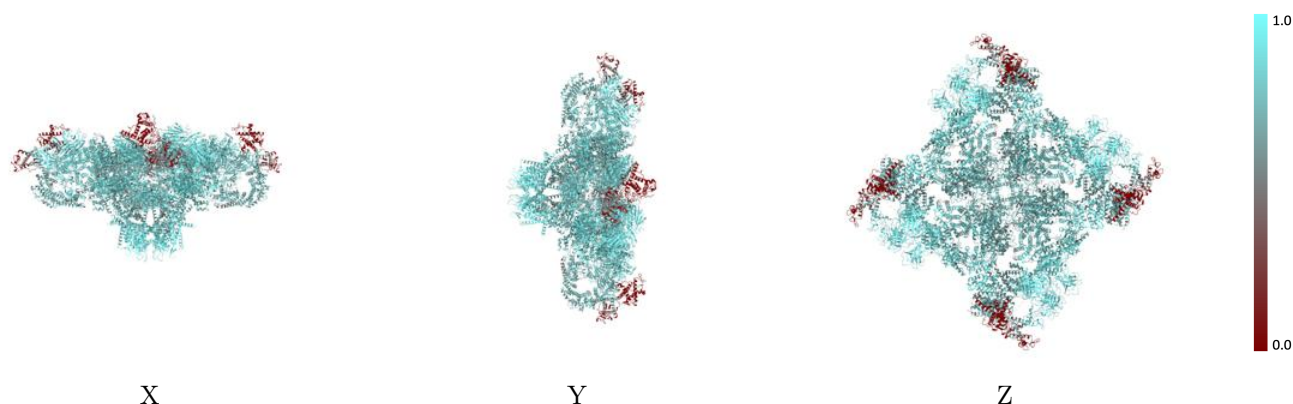
The images above show the 3D surface view of the map at the recommended contour level 0.123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



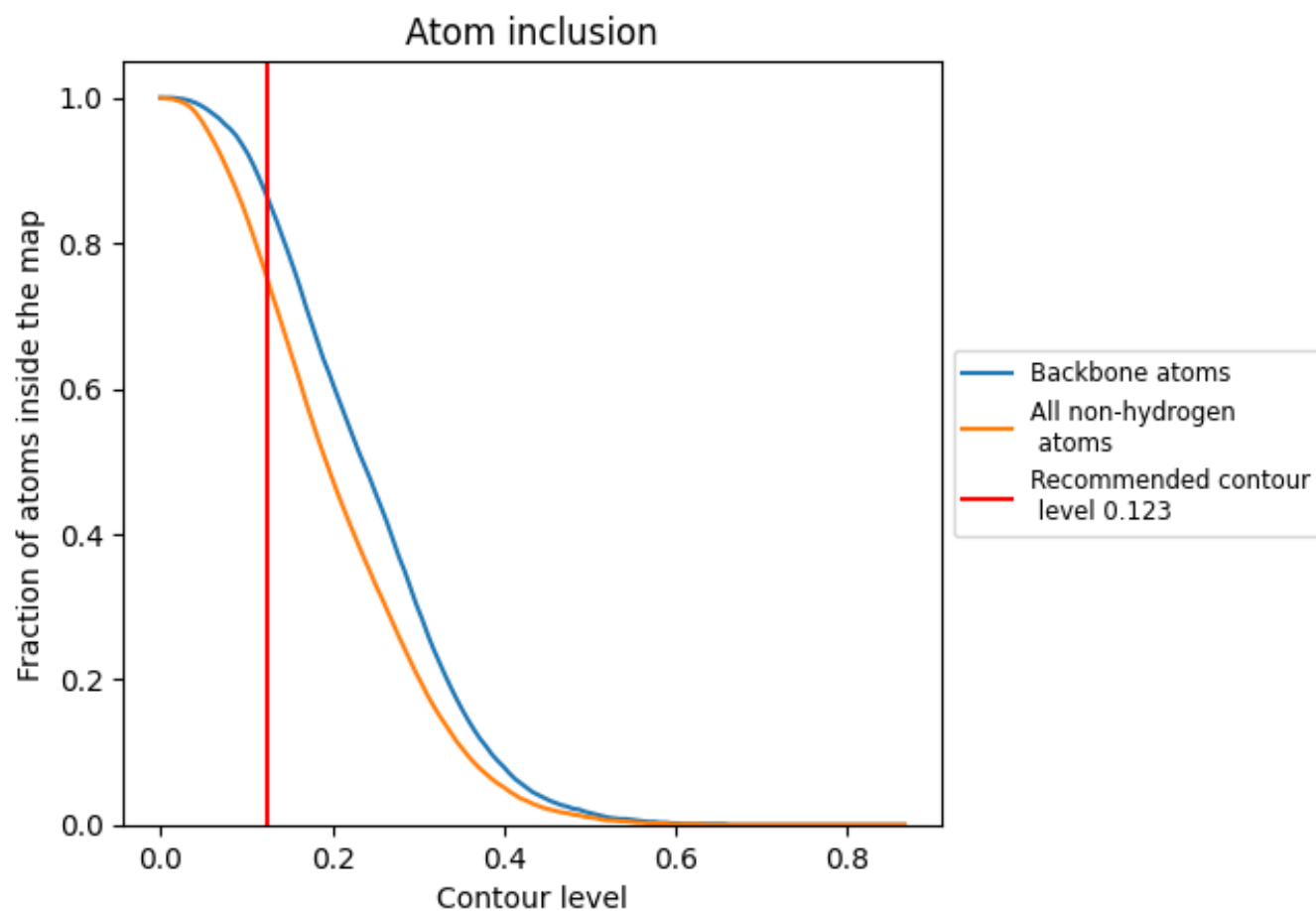
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.123).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 76% 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 (0.123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7560	0.4620
A	0.7530	0.4600
B	0.8570	0.5390
G	0.7530	0.4600
H	0.8570	0.5390
M	0.7530	0.4600
N	0.8570	0.5410
S	0.7530	0.4610
T	0.8570	0.5400

1.0

0.0

<0.0