



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:08 PM UTC

PDB ID : 8SEQ / pdb\_00008seq  
EMDB ID : EMD-40425  
Title : Cryo-EM Structure of RyR1 + AMP  
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.  
Deposited on : 2023-04-10  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

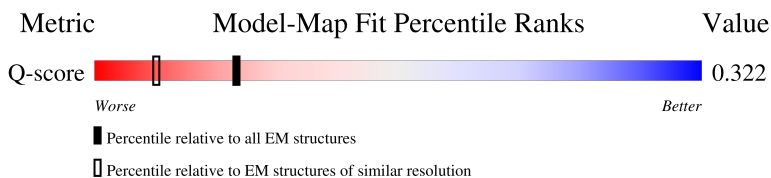
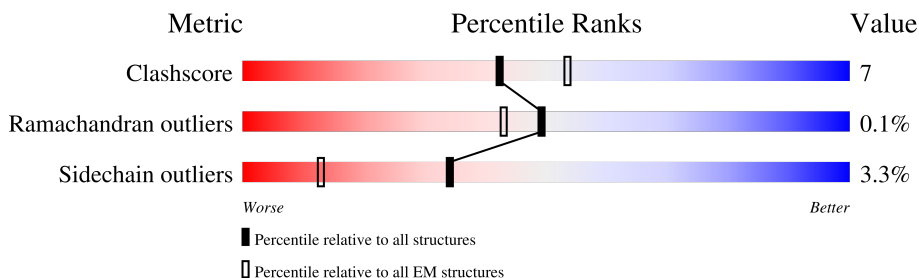
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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

The reported resolution of this entry is 3.40 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	14717 ( 2.90 - 3.90 )

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

Mol	Chain	Length	Quality of chain
1	A	5037	<p>18% (red), 69% (green), 17% (yellow), 13% (grey)</p>
1	B	5037	<p>18% (red), 69% (green), 17% (yellow), 13% (grey)</p>
1	C	5037	<p>18% (red), 69% (green), 17% (yellow), 13% (grey)</p>
1	D	5037	<p>18% (red), 69% (green), 17% (yellow), 13% (grey)</p>

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Mol	Chain	Length	Quality of chain
2	E	350	 26% 5% 69%
2	F	350	 26% 5% 69%
2	G	350	 26% 5% 69%
2	H	350	 26% 5% 69%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 142952 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
			Total	C	N	O	S		
1	A	4376	34896	22197	6022	6441	236	9	0
1	B	4376	34896	22197	6022	6441	236	9	0
1	C	4376	34896	22197	6022	6441	236	9	0
1	D	4376	34896	22197	6022	6441	236	9	0

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

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

There are 100 discrepancies between the modelled and reference sequences:

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

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

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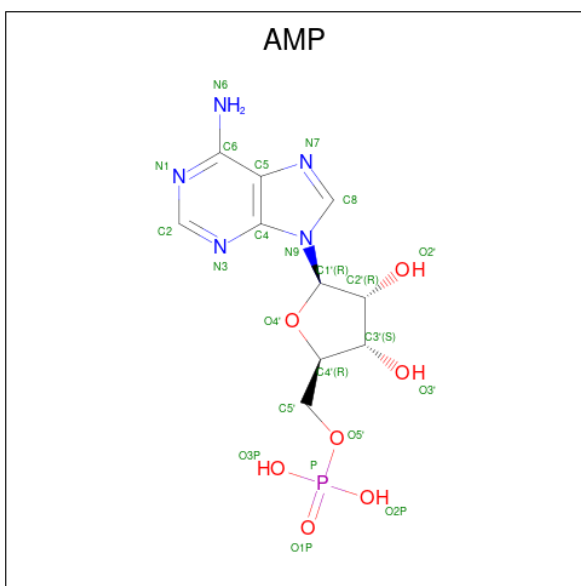
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression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

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

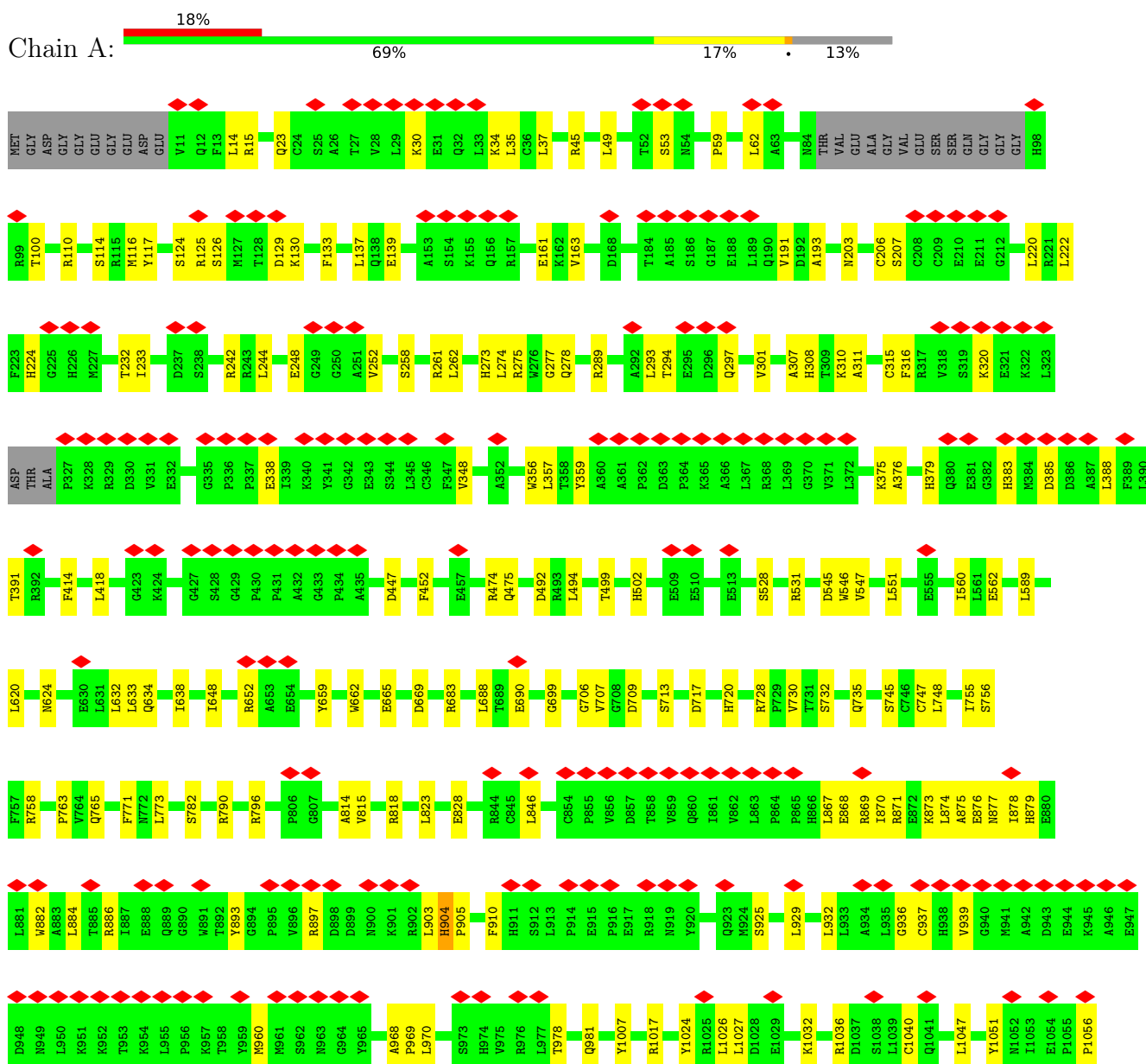
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

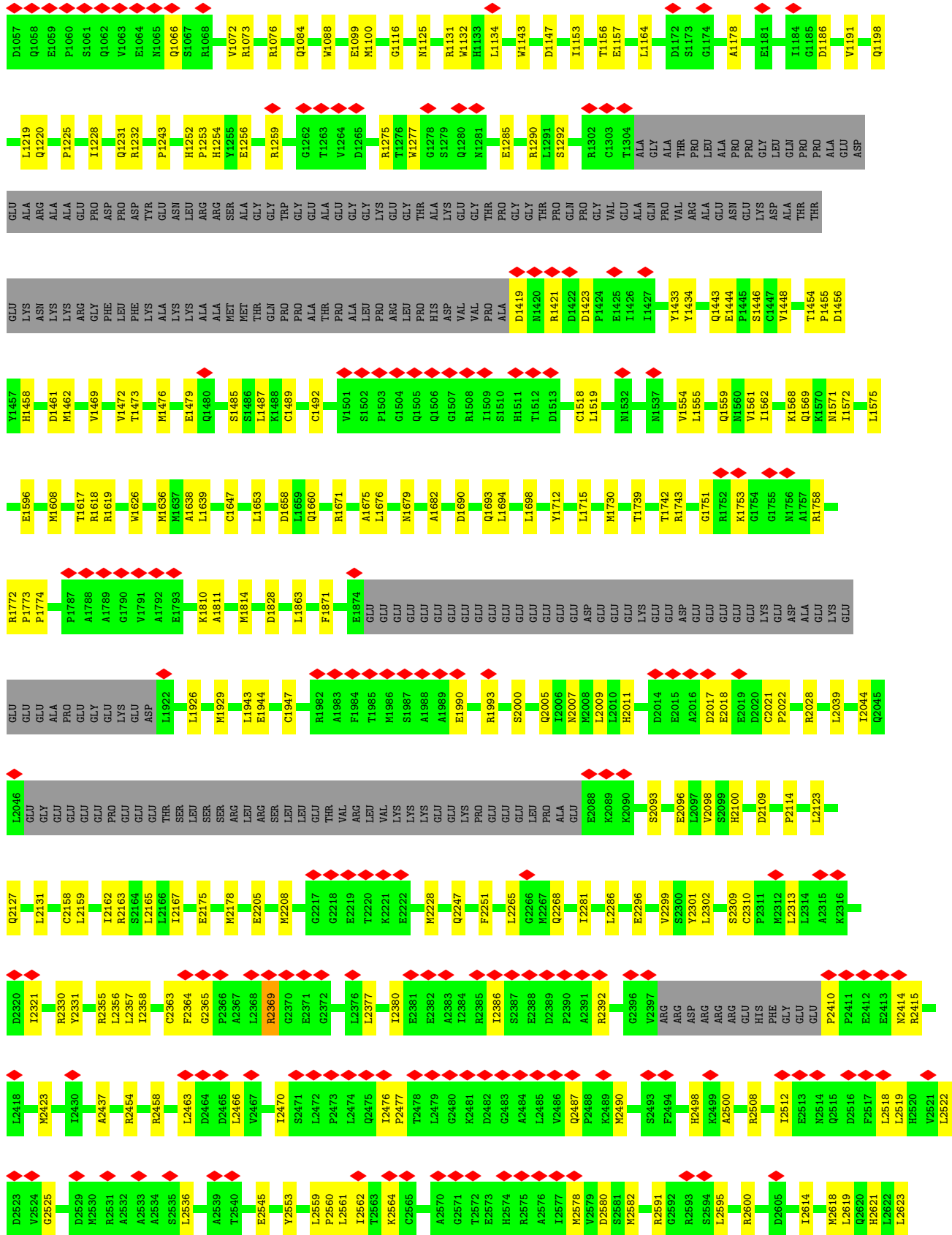
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0

### 3 Residue-property plots

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

- Molecule 1: Ryanodine receptor 1



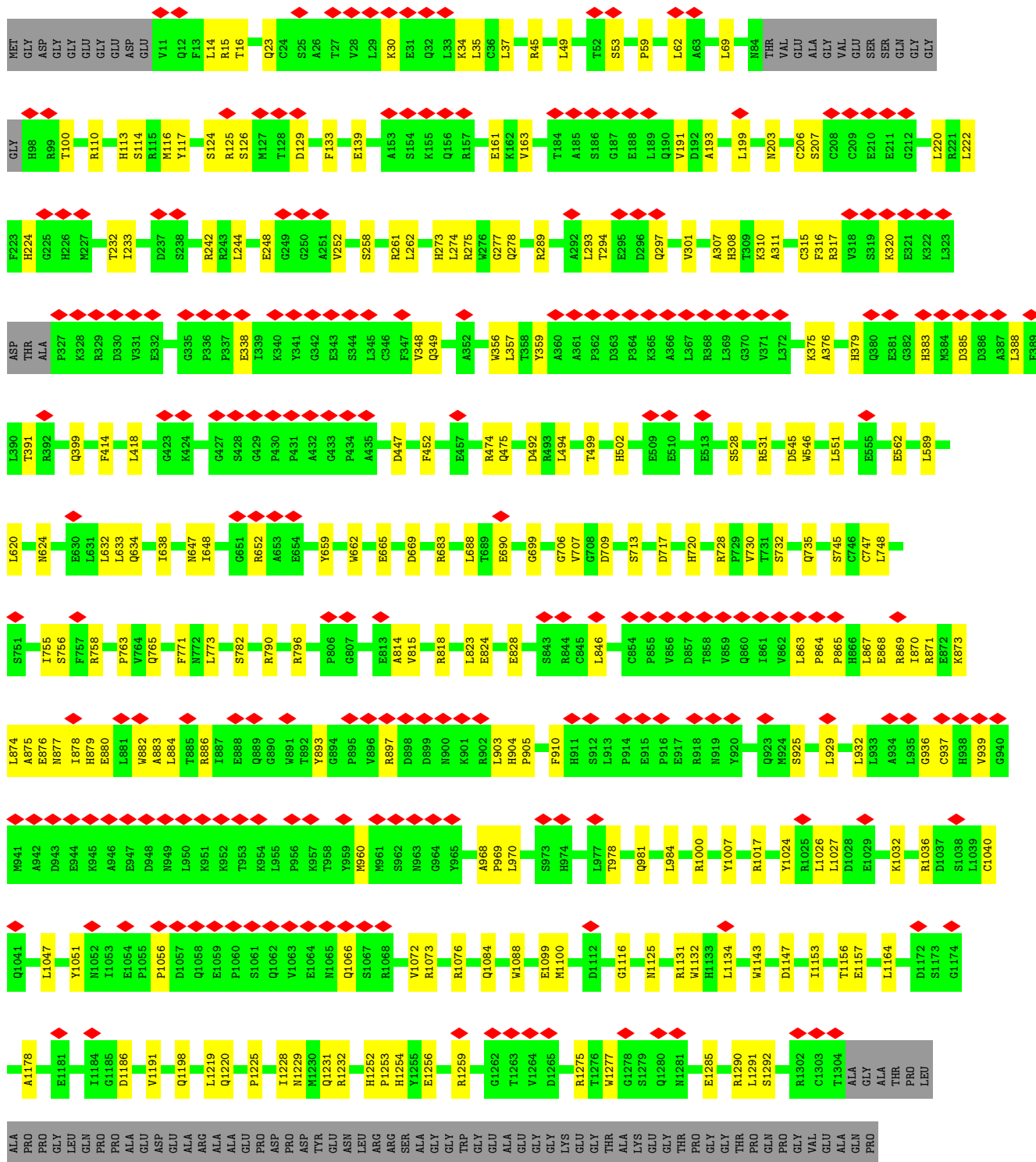


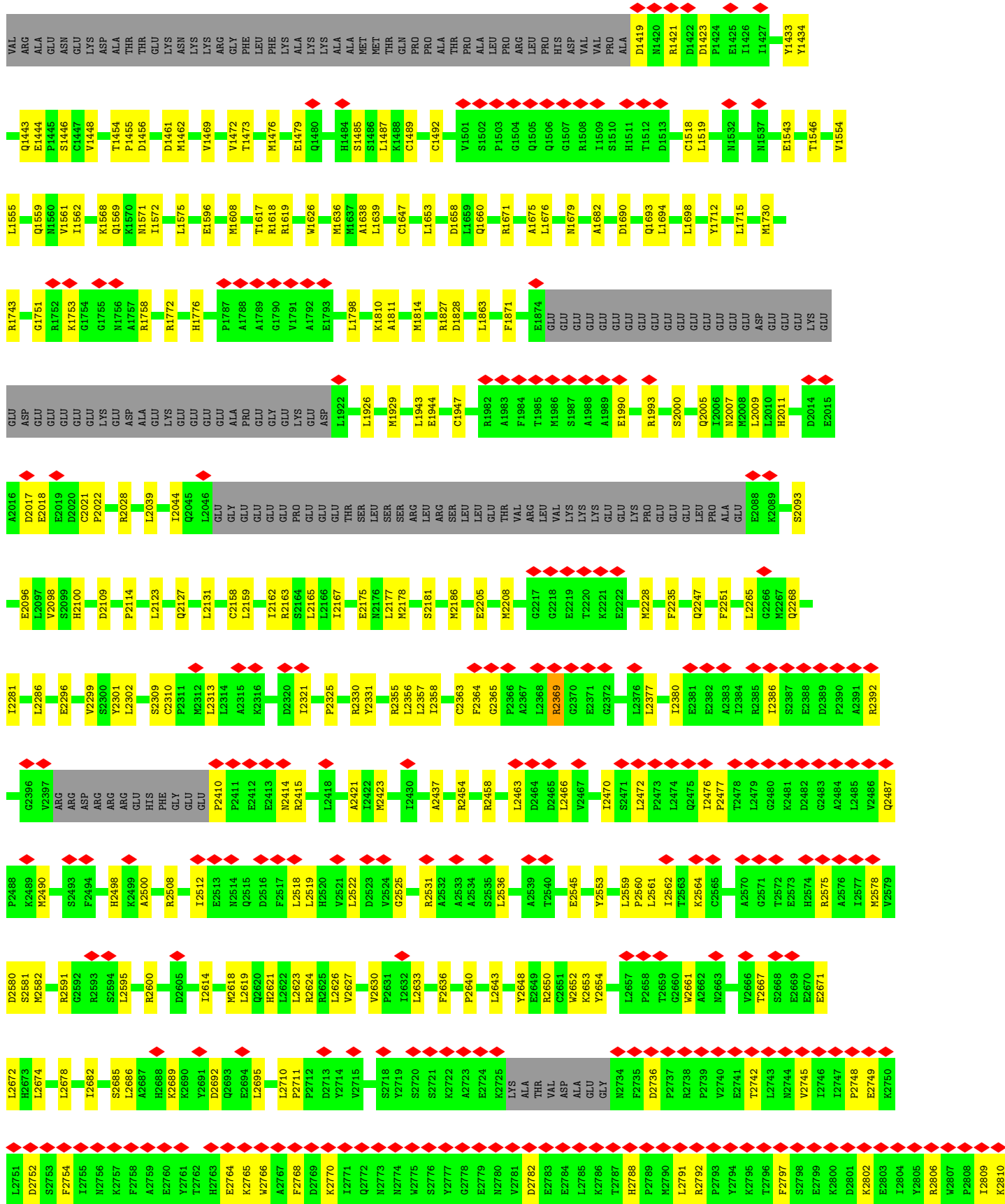
R3570	R3573	A3574	L3575	V3576	R3577	G3578	L3579	P3580	G3581	R3582	E3583	E3584	D3585	V35110	V35111	A3512	T35113	L35114	K35115	P3519	N3523	M3524	Q3530	D3531	M3534	L3535	A3536	K3537	T3538	R3539	Y3540	A3541	E3542	K3543	D3544	E3546	E3551	F3552	L3553	Q3554	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	V3563	E3564	G3565	S3566	P3567	V3632	V3633																																												
R3420	A3421	H3422	V3423	L3424	P3427	N3430	F3435	F3442	I3443	Y3444	H3449	N3450	R3453	F3458	V3459	V3460	Q3461	K3462	I3464	N3465	N3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	S3474	K3475	S3476	K3477	N3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	N3419																																															
E3331	A3332	W3333	M3335	K3336	R3337	V3340	F3341	A3342	Q3343	P3344	I3345	V3346	S3347	R3348	P3351	L3354	I3359	G3363	K3366	R3367	R3368	V3373	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	G3389	G3390	E3391	L3392	L3393	V3394	R3395	R3403	D3404	K3405	L3413	R3414	N3419																																																			
L3249	M3250	A3251	A3257	E3258	T3264	E3265	I3272	P3275	M3276	L3277	C3278	S3279	V3280	L3281	P3282	E3286	R3287	G3288	F3289	A3291	P3292	F3293	P3294	A3295	L3296	F3297	A3298	G3299	A3300	F3301	P3302	P3303	C3304	T3305	A3306	S3309	L3316	G3317	M3318	G3319	L3320	R3321	L3322	I3323	V3324	N3325	V3326	E3327	E3328	M3329	C3340	D3342	I3343	P3344	D3347	R3348																																											
D3160	S3171	L3175	T3178	K3179	N3180	T3181	Y3182	V3183	E3184	K3185	M3201	P3202	V3203	E3207	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	F3226	R3227	A3228	L3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	E3238	M3239	C3240	D3242	I3243	P3244	D3247	R3248																																																
L2974	L3075	E2977	A2978	V2980	M3081	K3082	S3083	G3084	P3085	E3086	I3087	L3092	R3093	S3094	F3095	A3099	D3102	M3106	V3107	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ARG	THR	GLN	VAL	K3123	G3124	N3128	E3037	M3038	I3039	L3042	L3046	A3047	A3048	Q3149	H3150	Q3151	D3154	V3156	I3157	L3158	D3159	V3065	W2966																																																
T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	LYS	ASP	MET	GLU	L2946	D2947	T2948	E2952	G2958	F2959	L2960	Q2961	Q2962	L2963	W2966																																													
L2674	L2675	L2676	L2677	L2678	L2682	L2685	L2686	L2687	L2688	L2689	L2690	L2692	L2693	L2694	L2695	L2696	L2697	L2698	L2699	L2701	L2702	L2703	L2704	L2705	L2706	L2707	L2708	L2709	L2710	L2711	L2712	L2713	L2714	L2715	L2716	L2717	L2718	L2719	L2720	L2721	L2722	L2723	L2724	L2725	L2726	L2727	L2728	L2729	L2730	L2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	L2740	L2741	L2742	L2743	L2744	L2745	L2746	L2747	L2748	L2749	L2750	L2751	L2752	L2753	L2754	L2755	L2756	L2757	L2758	L2759	L2760	L2761	L2762	L2763	L2764	L2765	L2766	L2767	L2768	L2769	L2770	L2771	L2772	L2773	L2774	L2775	L2776	L2777	L2778	L2779	L2780
R2624	R2625	L2626	V2627	V2630	P2631	L2632	L2633	F2636	Y2648	E2649	R2650	C2651	H2652	K2653	V2654	C2655	L2657	P2658	T2659	G2660	W2661	A2662	N2663	V2666	T2667	S2668	E2669	E2670	E2671	L2672	H2673	L2674	L2678	L2682	L2685	L2686	A2687	H2688	K2689	K2690	L2692	Q2693	E2694	L2695	W2715	Y2718	Y2719	S2720																																																			
LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	G2863	V2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	ALA	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	E2892	Q2893	E2894	L2894	E2895	A2896	K2897	L2898	G2899	C2900																																						
V2781	D2782	E2783	E2784	K2785	L2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	V2794	K2795	T2796	P2797	D2798	L2799	E2799	K2800	D2801	K2802	E2803	L2804	T2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	E2829	GLU	GLU	ARG	THR	LYS	LYS	G2899	N2780																																										





● Molecule 1: Ryanodine receptor 1

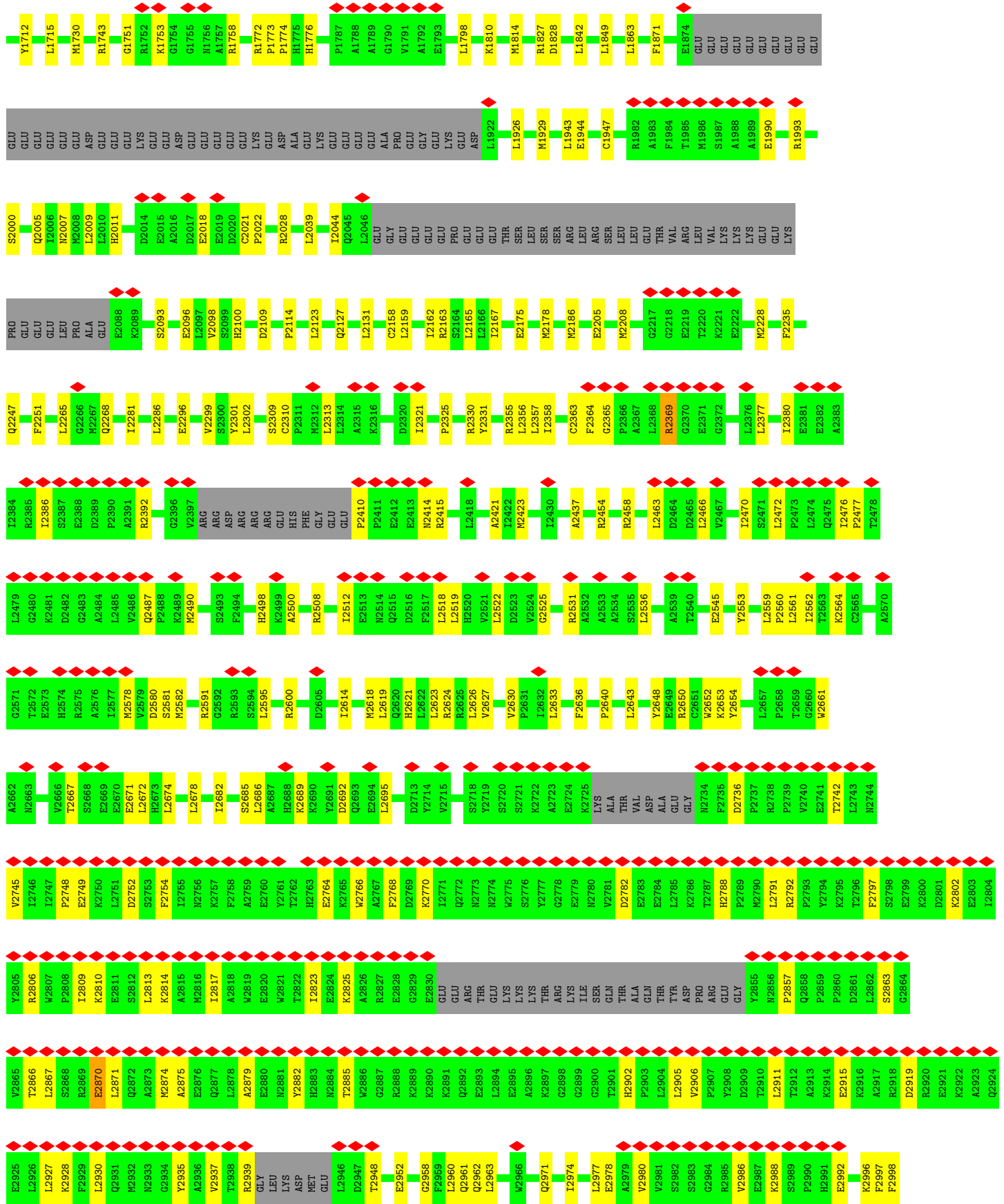




E2811	E2812	L2813	K2814	A2815	M2816	L2817	A2818	M2819	E2820	M2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	LYS	ARG	LYS	ILE	G2898	G2899	M3081	SER	GLN	THR	ALA	GLN	TVR	ASP	PRO	ARG	GLU	GLY	Y2855	M2856	F2857	Q2858	F2859	P2860	P2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870
L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	N2884	T2885	M2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	M3081	E28979	V2890	V2891	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	Q2923	E2925	L2927	K2928	F2929	L2930		
Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	GLY	M3038	LEU	LYS	ASP	MET	L2946	D2947	T2948	E2952	G2958	F2959	L2960	Q2961	Q2962	L2963	W2966	I2974	L2977	E2978	A2979	V2980	V2981	S2982	G2983	G2984	R2985	V2986	E2987	K2988	P2990	L2991	T2992	E2993	K2994	E2995	K2996	F2997	F2998	L3002	T3020	P3021	A3022	K3023	Y3024								
L3025	G3026	S3027	G3028	G3029	N3033	E3037	M3038	L3039	L3042	L3046	A3047	A3048	R3051	H3052	R3053	G3058	T3059	P3062	V3065	L3075	R3078	T3079	V3080	M3081	K3082	S3083	G3084	P3085	E3086	I3087	L3092	R3093	S3094	F3095	A3099	D3102	K3106	V3107	L3110	R3111	L3112	G3113	K3114	V3115																	
S3116	GLN	ALA	ARG	THR	GLN	VAL	K3123	G3124	N3128	V3134	A3135	L3136	H3146	Q3149	H3150	Q3151	D3154	D3155	V3156	I3157	L3158	D3159	D3160	S3171	L3175	T3178	K3179	N3180	T3181	V3182	V3183	E3184	K3185	M3201	P3202	V3203	E3207	Q3209	L3210	N3211	E3212	Y3213	M3214	A3215	G3216	S3217	V3218	Y3219													
T3220	T3221	K3222	S3223	P3224	L3225	E3226	R3227	A3228	L3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237	F3238	H3239	C3240	P3241	D3242	L3243	F3244	D3247	R3248	L3249	M3250	A3251	A3257	E3258	T3264	E3265	I3272	P3275	K3276	L3277	C3278	S3279	Y3280	L3281	P3282	E3286	G3288	P3289	E3290	A3291	P3292	P3293	A3295	L3296										
P3297	A3298	G3299	A3300	P3301	R3302	P3303	C3304	T3305	A3306	S3309	L3316	G3317	M3318	I3319	L3320	R3321	I3322	V3324	M3325	N3326	L3327	G3328	I3329	R3330	E3331	A3332	T3333	M3334	M3335	K3336	R3337	V3340	F3341	A3342	Q3343	P3344	V3346	I3348	S3347	R3348	P3351	I3359	G3363	R3364	L3365	R3366	K3367	R3368	V3373	E3376											
E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	R3394	R3395	R3403	D3404	I3413	R3414	N3419	R3420	A3421	H3422	V3423	L3424	T3425	E3426	F3427	M3430	F3435	F3442	H3449	N3450	R3453	F3458	V3459	V3460	Q3461	N3462	E3463	L3464	M3465	N3466	M3467	S3468	L3470												
T3471	A3472	D3473	S3474	K3475	S3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ALA	GLN	SER	GLY	GLY	SER	ASP	GLN	GLU	ARG	THR	LYS	LYS	R3498	R3499	G3500	D3501	R3502	V3503	S3504	V3505	Q3506	T3507	S3508	L3509	I3510	V3511	A3512	T3513	L3514	K3515	P3519	N3523	K3524	Q3530	D3531	M3534	L3535	M3536	K3537	R3538	T3539	E3540	E3541					
Y3540	A3541	L3542	K3543	D3544	E3547	E3548	E3551	F3552	L3553	Q3554	N3555	N3556	L3557	H3558	L3559	Q3560	G3561	K3562	V3563	E3564	G3565	S3566	P3567	R3570	M3573	A3574	L3575	Y3576	R3577	G3578	L3579	P3580	G3581	R3582	E3583	E3584	D3585	A3586	D3587	D3588	P3589	K3590	K3591	L3592	V3593	R3594	R3595	S3600	H3605	L3606	T3609	E3610									
H3611	P3612	Y3613	K3614	S3615	K3616	K3617	A3618	V3619	W3620	H3621	K3622	L3623	L3624	S3625	K3626	Q3627	R3628	R3629	R3630	A3631	V3632	V3633	A3634	C3635	F3636	R3637	K3638	R3648	M3652	L3662	G3661	E3662	Q3663	E3664	E3665	E3666	E3667	E3668	E3669	D3670	E3671	E3672	K3673	V3702	L3703	R3707	L3710	Y3722	M3723	E3736											
GLU	GLY	GLU	GLU	ASN	GLY	GLU	ALA	GLU	GLU	GLU	GLU	V3749	E3750	F3753	Q3766	Q3767	S3768	R3769	L3770	H3771	T3772	R3773	M3778	Q3781	T3786	G3788	M3793	V3794	N3809	K3815	Y3819	K3823	L3835	S3840	G3857	M3858	V3859	N3860	E3861	D3862	G3863	T3864	L3866	N3867	R3868	Q3869															
N3870	G3871	M3875	A3876	D3877	Q3882	Q3889	N3901	Y3902	L3903	R3904	S3905	Q3906	L3924	Q3927	I3930	D3941	V3957	L3965	T3966	E3967	R3984	V3990	M4000	L4016	M4044	V4049	E4050	S4051	M4064	L4068	R4069	D4070	L4071	V4072	G4073	S4074	E4075	A4076	D4079	Y4080																					







ASP	R4161	R4064	S3840	R3707	S3600	D3531	E3463	I3365	P3289	E3212	M3106	L3002
GLY	I4164	L4068	G3857	L3710	H3605	M3534	I3464	R3366	E3290	Y3213	V3107	T3020
MET	E4165	K4069	M3858	K3722	L3606	A3536	N3465	K3367	A3291	M3214	L3110	P3021
GLY	E4168	D4070	V3859	M3723	T3609	K3537	N3466	R3368	P3292	A3215	R3111	A3022
ALA	L4178	I4071	N3860	E3736	E3610	T3538	K3467	V3373	P3293	G3216	L3112	K3023
ALA	G4072	G4073	D3862	GLU	H3611	F3469	F3468	E3376	P3294	S3217	G3113	V3024
ALA	R4179	S4074	E3863	GLY	H3612	L3470	L3470	E3377	A3295	V3218	K3114	L3025
GLY	R4180	E4075	G3864	GLY	P3612	A3541	A3471	Q3378	L3296	Y3219	V3115	G3026
ALA	I4181	A4076	T3864	GLU	Y3613	A3542	A3472	L3379	P3297	T3220	S3116	S3027
ALA	E4182	A4076	V3865	ASN	K3614	K3543	A3473	R3380	A3298	T3221	GLN	G3028
GLY	I4183	D4079	I3866	GLY	R3615	K3544	D3473	L3381	G3299	K3222	ALA	ARG
GLY	M4184	V4080	V3867	GLU	S3615	S3474	S3474	E3382	A3300	S3223	ARG	THR
ALA	S4187	V4081	K3616	GLU	K3617	K3475	K3475	A3383	P3301	P3224	THR	GLN
ALA	R4188	V4081	K3617	GLU	K3617	K3475	K3475	A3384	P3302	P3224	VAL	GLN
ALA	R4189	T4082	Q3869	GLU	A3618	S3477	K3477	K3384	P3303	E3226	VAL	VAL
ALA	I4190	D4083	A3618	GLU	V3619	K3478	M3478	A3385	P3303	R3227	K3123	K3037
GLY	E4196	P4084	V3749	GLU	E3551	M3478	M3478	E3386	C3304	R3227	G3124	N3038
ALA	R4085	R4085	E3750	GLU	F3552	A3479	A3479	A3387	T3305	N3128	N3128	I3039
ALA	R4202	M3375	H3621	GLY	F3552	LYS	LYS	A3387	A3306	L3229	V3194	L3042
GLY	A4203	A3876	K3622	GLY	L3553	ALA	ALA	E3388	A3309	L3230	A3195	K3045
THR	Q4204	D3877	L3623	ASP	Q3554	ASP	ASP	E3389	S3309	G3231	L3136	L3046
VAL	M4205	F3753	L3624	ALA	N3555	ALA	ALA	G3390	S3309	G3231	A3136	L3046
ALA	E4206	Q3766	S3625	GLN	M3556	GLN	GLN	E3391	L3316	P3283	H3146	A3047
ALA	Q4209	S3767	K3626	SER	L3557	SER	SER	L3392	N3318	P3283	H3146	A3048
GLY	Q4209	R3769	Q3627	GLY	H3556	GLY	GLY	L3393	M3318	N3234	Q3149	H3052
ALA	E4212	L3770	Q3627	GLY	L3559	GLY	GLY	V3394	I3319	V3236	H3150	R3053
ALA	A4096	L3770	SER	SER	L3559	SER	SER	R3395	L3320	V3236	H3150	R3053
ALA	A4097	H3771	ASP	ASP	Q3560	ASP	ASP	R3395	R3321	E3237	Q3151	G3058
ARG	M4097	T3772	G3628	GLN	G3561	GLN	GLN	R3403	I3322	E3238	D3154	T3059
LEU	D4098	R3773	R3630	GLU	K3562	GLU	GLU	D3404	I3322	M3239	D3154	T3059
ALA	S4099	F3773	A3631	ARG	K3563	ARG	ARG	R3404	I3322	M3239	D3154	T3059
ALA	Q4100	M3778	V3632	THR	V3563	THR	THR	I3413	N3326	C3240	V3156	F3062
ALA	E4224	Q3781	V3632	LYS	E3564	LYS	LYS	R3414	R3327	P3241	I3157	F3062
ALA	G4225	G3788	G3565	LYS	G3565	LYS	LYS	R3414	L3327	D3242	L3156	V3065
ARG	G4226	G3788	S3566	LYS	S3566	LYS	LYS	R3414	L3327	D3242	L3156	V3065
ALA	E4227	G3788	P3567	R3498	P3567	R3498	R3498	N3419	L3327	P3244	D3159	V3065
LEU	K4230	M3793	R3570	R3499	R3570	R3499	R3499	R3420	D3330	D3247	S3171	L3075
GLY	M4231	V3794	M3638	G3500	G3500	G3500	G3500	R3421	D3330	D3247	S3171	L3075
LEU	I4242	L3798	M3638	D3501	D3501	D3501	D3501	H3422	A3332	R3248	L3175	R3078
SER	F4243	N3809	R3648	R3502	R3502	R3502	R3502	W3423	A3332	R3248	L3175	R3078
TYR	E4244	N3809	R3648	R3503	R3503	R3503	R3503	W3423	A3332	R3248	L3175	R3078
ARG	M4245	N3809	R3648	R3503	R3503	R3503	R3503	T3425	M3334	L3249	T3178	V3080
LEU	S4252	K3815	M3652	S3504	S3504	S3504	S3504	E3426	M3335	M3250	T3178	V3080
ARG	E4253	K3815	M3652	V3505	V3505	V3505	V3505	P3427	K3336	A3251	K3179	K3082
ARG	P4254	G3578	I3662	Q3506	Q3506	Q3506	Q3506	R3430	R3337	A3257	N3180	S3083
VAL	E4116	P3580	I3662	T3507	T3507	T3507	T3507	N3430	E3258	E3258	T3181	G3084
ARG	A4117	P3580	I3662	S3508	S3508	S3508	S3508	F3435	E3258	E3258	T3181	G3084
ARG	D4118	G3581	R3582	L3509	L3509	L3509	L3509	F3435	E3258	E3258	T3181	G3084
LEU	E4119	E3583	E3583	V3511	V3511	V3511	V3511	F3442	A3342	Q3343	T3181	G3084
LEU	M4120	E3584	E3584	T3513	T3513	T3513	T3513	H3449	F3344	P3275	M3201	R3093
ALA	E4121	E3585	E3585	L3514	L3514	L3514	L3514	N3450	F3344	P3275	P3202	S3094
ASP	M4121	E3586	E3586	K3515	K3515	K3515	K3515	N3450	F3344	P3275	P3202	S3094
GLU	M4122	E3688	E3688	R3519	R3519	R3519	R3519	R3463	S3347	C3278	E3207	A3099
GLU	M4123	E3688	E3688	P3519	P3519	P3519	P3519	F3468	S3347	C3278	E3207	A3099
PRO	M4124	E3689	E3689	N3523	N3523	N3523	N3523	V3469	R3348	Y3280	P3208	D3102
GLU	F4125	V3690	V3690	K3524	K3524	K3524	K3524	V3469	R3348	Y3280	P3208	D3102
ALA	H4156	E3692	E3692	R3524	R3524	R3524	R3524	V3469	R3348	Y3280	P3208	D3102
ALA	R4159	K3693	K3693	K3524	K3524	K3524	K3524	V3469	R3348	Y3280	P3208	D3102
LEU	L4160	K3694	K3694	R3524	R3524	R3524	R3524	V3469	R3348	Y3280	P3208	D3102
LEU	L4160	P3695	P3695	R3524	R3524	R3524	R3524	V3469	R3348	Y3280	P3208	D3102
LEU	V3702	R3594	R3594	R3524	R3524	R3524	R3524	V3469	R3348	Y3280	P3208	D3102
LEU	V3702	R3595	R3595	R3524	R3524	R3524	R3524	V3469	R3348	Y3280	P3208	D3102













## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.741	Depositor
Minimum map value	-0.326	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/35710	0.61	9/48359 (0.0%)
1	B	0.28	0/35710	0.61	8/48359 (0.0%)
1	C	0.28	0/35710	0.61	8/48359 (0.0%)
1	D	0.28	0/35710	0.61	8/48359 (0.0%)
2	E	0.21	0/834	0.54	0/1123
2	F	0.21	0/834	0.54	0/1123
2	G	0.21	0/834	0.54	0/1123
2	H	0.21	0/834	0.54	0/1123
All	All	0.28	0/146176	0.61	33/197928 (0.0%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4196	GLU	CA-CB-CG	6.92	127.95	114.10
1	C	4196	GLU	CA-CB-CG	6.92	127.95	114.10
1	D	4196	GLU	CA-CB-CG	6.92	127.95	114.10
1	A	4196	GLU	CA-CB-CG	6.91	127.92	114.10
1	B	3085	PRO	CA-N-CD	-6.27	103.23	112.00
1	C	3085	PRO	CA-N-CD	-6.27	103.23	112.00
1	D	3085	PRO	CA-N-CD	-6.27	103.23	112.00
1	A	3085	PRO	CA-N-CD	-6.24	103.26	112.00
1	A	4196	GLU	CB-CA-C	-6.05	99.88	109.80
1	B	4196	GLU	CB-CA-C	-6.05	99.88	109.80
1	C	4196	GLU	CB-CA-C	-6.05	99.88	109.80
1	D	4196	GLU	CB-CA-C	-5.96	99.91	109.75
1	D	5028	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	5028	PHE	CA-CB-CG	5.26	119.06	113.80
1	B	5028	PHE	CA-CB-CG	5.24	119.04	113.80
1	C	5028	PHE	CA-CB-CG	5.24	119.03	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4187	SER	CA-C-N	5.18	131.44	121.54
1	A	4187	SER	C-N-CA	5.18	131.44	121.54
1	B	905	PRO	N-CA-C	5.17	123.13	112.47
1	C	4187	SER	CA-C-N	5.17	131.42	121.54
1	C	4187	SER	C-N-CA	5.17	131.42	121.54
1	A	905	PRO	N-CA-C	5.17	123.12	112.47
1	D	4187	SER	CA-C-N	5.17	131.41	121.54
1	D	4187	SER	C-N-CA	5.17	131.41	121.54
1	B	4187	SER	CA-C-N	5.16	131.40	121.54
1	B	4187	SER	C-N-CA	5.16	131.40	121.54
1	C	905	PRO	N-CA-C	5.16	123.09	112.47
1	D	905	PRO	N-CA-C	5.16	123.09	112.47
1	A	3085	PRO	N-CD-CG	-5.15	95.48	103.20
1	B	3085	PRO	N-CD-CG	-5.13	95.50	103.20
1	C	3085	PRO	N-CD-CG	-5.13	95.50	103.20
1	D	3085	PRO	N-CD-CG	-5.13	95.51	103.20
1	A	904	HIS	N-CA-C	5.02	119.58	112.75

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34896	0	34522	478	0
1	B	34896	0	34522	469	0
1	C	34896	0	34522	472	0
1	D	34896	0	34522	479	0
2	E	818	0	824	8	0
2	F	818	0	824	8	0
2	G	818	0	824	8	0
2	H	818	0	824	8	0
3	A	23	0	12	1	0
3	B	23	0	12	1	0
3	C	23	0	12	1	0
3	D	23	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	142952	0	141432	1894	0

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

All (1894) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.71	0.73
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.71	0.72
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.71	0.72
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.71	0.71
1:D:233:ILE:HD12	1:D:242:ARG:HB3	1.73	0.71
1:C:1476:MET:HB3	1:C:1485:SER:HB3	1.73	0.71
1:A:233:ILE:HD12	1:A:242:ARG:HB3	1.73	0.71
1:B:1476:MET:HB3	1:B:1485:SER:HB3	1.73	0.70
1:C:233:ILE:HD12	1:C:242:ARG:HB3	1.73	0.70
1:C:3042:LEU:O	1:C:3046:LEU:HB2	1.91	0.70
1:A:1476:MET:HB3	1:A:1485:SER:HB3	1.73	0.70
1:B:3042:LEU:O	1:B:3046:LEU:HB2	1.91	0.70
1:D:3042:LEU:O	1:D:3046:LEU:HB2	1.91	0.69
1:B:233:ILE:HD12	1:B:242:ARG:HB3	1.73	0.69
1:D:1476:MET:HB3	1:D:1485:SER:HB3	1.73	0.69
1:A:3042:LEU:O	1:A:3046:LEU:HB2	1.91	0.69
1:B:745:SER:HB2	1:B:758:ARG:HB2	1.74	0.68
1:C:745:SER:HB2	1:C:758:ARG:HB2	1.74	0.68
1:D:745:SER:HB2	1:D:758:ARG:HB2	1.74	0.68
1:C:688:LEU:HD23	1:C:690:GLU:H	1.59	0.67
1:A:745:SER:HB2	1:A:758:ARG:HB2	1.74	0.67
1:D:688:LEU:HD23	1:D:690:GLU:H	1.59	0.67
1:D:3346:VAL:HG11	1:D:3414:ARG:HB3	1.77	0.67
1:A:4978:HIS:HA	1:A:4982:GLU:HG3	1.77	0.66
1:A:3257:ALA:HB1	1:A:3321:ARG:HD2	1.76	0.66
1:C:3257:ALA:HB1	1:C:3321:ARG:HD2	1.76	0.66
1:A:688:LEU:HD23	1:A:690:GLU:H	1.59	0.66
1:A:3346:VAL:HG11	1:A:3414:ARG:HB3	1.77	0.66
1:B:688:LEU:HD23	1:B:690:GLU:H	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3257:ALA:HB1	1:B:3321:ARG:HD2	1.76	0.66
1:D:3257:ALA:HB1	1:D:3321:ARG:HD2	1.76	0.66
1:B:4581:LYS:NZ	1:C:4877:ASP:O	2.28	0.66
1:C:4978:HIS:HA	1:C:4982:GLU:HG3	1.77	0.66
1:C:3346:VAL:HG11	1:C:3414:ARG:HB3	1.77	0.65
1:C:4581:LYS:NZ	1:D:4877:ASP:O	2.28	0.65
1:D:1116:GLY:HA3	1:D:1132:TRP:HB3	1.78	0.65
1:C:1116:GLY:HA3	1:C:1132:TRP:HB3	1.78	0.65
1:B:3346:VAL:HG11	1:B:3414:ARG:HB3	1.77	0.65
1:C:2007:ASN:O	1:C:2011:HIS:HB2	1.97	0.65
1:D:4978:HIS:HA	1:D:4982:GLU:HG3	1.77	0.65
1:A:4821:LYS:HG3	1:A:4824:ARG:HH21	1.62	0.65
1:B:1116:GLY:HA3	1:B:1132:TRP:HB3	1.78	0.65
1:B:4821:LYS:HG3	1:B:4824:ARG:HH21	1.62	0.65
1:B:4924:VAL:HA	1:B:4928:LEU:HD12	1.79	0.65
1:A:2961:GLN:NE2	1:A:3038:MET:SD	2.70	0.65
1:B:2007:ASN:O	1:B:2011:HIS:HB2	1.97	0.65
1:B:4978:HIS:HA	1:B:4982:GLU:HG3	1.77	0.64
1:A:4924:VAL:HA	1:A:4928:LEU:HD12	1.79	0.64
1:D:4821:LYS:HG3	1:D:4824:ARG:HH21	1.62	0.64
1:A:1116:GLY:HA3	1:A:1132:TRP:HB3	1.78	0.64
1:A:2007:ASN:O	1:A:2011:HIS:HB2	1.97	0.64
1:B:3332:ALA:HB3	1:B:3403:ARG:HD2	1.80	0.64
1:D:2007:ASN:O	1:D:2011:HIS:HB2	1.97	0.64
1:D:2961:GLN:NE2	1:D:3038:MET:SD	2.70	0.64
1:C:3332:ALA:HB3	1:C:3403:ARG:HD2	1.80	0.64
1:C:4924:VAL:HA	1:C:4928:LEU:HD12	1.79	0.64
1:A:3332:ALA:HB3	1:A:3403:ARG:HD2	1.80	0.64
1:A:1569:GLN:HB2	1:A:1572:ILE:HD12	1.80	0.64
1:B:2797:PHE:HE2	1:B:2802:LYS:HD3	1.63	0.64
1:D:4924:VAL:HA	1:D:4928:LEU:HD12	1.79	0.64
1:B:2958:GLY:O	1:B:2962:GLN:NE2	2.31	0.63
1:C:2797:PHE:HE2	1:C:2802:LYS:HD3	1.63	0.63
1:D:3332:ALA:HB3	1:D:3403:ARG:HD2	1.80	0.63
1:D:2958:GLY:O	1:D:2962:GLN:NE2	2.31	0.63
1:D:1569:GLN:HB2	1:D:1572:ILE:HD12	1.80	0.63
1:A:2958:GLY:O	1:A:2962:GLN:NE2	2.31	0.63
1:C:2958:GLY:O	1:C:2962:GLN:NE2	2.31	0.63
1:C:4821:LYS:HG3	1:C:4824:ARG:HH21	1.62	0.63
1:B:2961:GLN:NE2	1:B:3038:MET:SD	2.70	0.63
1:A:2797:PHE:HE2	1:A:2802:LYS:HD3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2797:PHE:HE2	1:D:2802:LYS:HD3	1.63	0.63
1:B:3075:LEU:O	1:B:3146:HIS:NE2	2.32	0.63
1:D:3075:LEU:O	1:D:3146:HIS:NE2	2.32	0.63
1:A:981:GLN:HG2	1:A:1047:LEU:HD11	1.81	0.62
1:B:659:TYR:O	1:B:662:TRP:NE1	2.33	0.62
1:B:1990:GLU:HB2	1:B:1993:ARG:HE	1.65	0.62
1:C:1024:TYR:O	1:C:1032:LYS:NZ	2.33	0.62
1:A:1990:GLU:HB2	1:A:1993:ARG:HE	1.64	0.62
1:A:3075:LEU:O	1:A:3146:HIS:NE2	2.32	0.62
1:C:1569:GLN:HB2	1:C:1572:ILE:HD12	1.80	0.62
1:C:659:TYR:O	1:C:662:TRP:NE1	2.32	0.62
1:D:659:TYR:O	1:D:662:TRP:NE1	2.32	0.62
1:A:659:TYR:O	1:A:662:TRP:NE1	2.32	0.62
1:A:3051:ARG:O	1:A:3053:ARG:NE	2.31	0.62
1:B:2978:GLU:OE2	1:B:3053:ARG:NH1	2.31	0.62
1:B:1569:GLN:HB2	1:B:1572:ILE:HD12	1.80	0.62
1:C:244:LEU:HD13	1:C:375:LYS:HD2	1.82	0.62
1:A:1024:TYR:O	1:A:1032:LYS:NZ	2.33	0.61
1:B:244:LEU:HD13	1:B:375:LYS:HD2	1.82	0.61
1:B:1024:TYR:O	1:B:1032:LYS:NZ	2.33	0.61
1:B:3051:ARG:O	1:B:3053:ARG:NE	2.31	0.61
1:C:1990:GLU:HB2	1:C:1993:ARG:HE	1.64	0.61
1:D:2978:GLU:OE2	1:D:3053:ARG:NH1	2.31	0.61
1:B:2630:VAL:HG12	1:B:2682:ILE:HD11	1.83	0.61
1:C:981:GLN:HG2	1:C:1047:LEU:HD11	1.81	0.61
1:D:981:GLN:HG2	1:D:1047:LEU:HD11	1.81	0.61
1:A:244:LEU:HD13	1:A:375:LYS:HD2	1.82	0.61
1:A:897:ARG:HB2	1:A:903:LEU:HD11	1.83	0.61
1:B:981:GLN:HG2	1:B:1047:LEU:HD11	1.81	0.61
1:C:3051:ARG:O	1:C:3053:ARG:NE	2.31	0.61
1:A:978:THR:OG1	1:A:981:GLN:OE1	2.19	0.61
1:A:3081:MET:HG3	1:A:3156:VAL:HA	1.83	0.61
1:D:1990:GLU:HB2	1:D:1993:ARG:HE	1.65	0.61
1:C:2630:VAL:HG12	1:C:2682:ILE:HD11	1.83	0.61
1:A:3368:ARG:NH2	1:A:3404:ASP:OD2	2.34	0.61
1:B:3236:VAL:HA	1:B:3239:MET:HG3	1.83	0.61
1:D:244:LEU:HD13	1:D:375:LYS:HD2	1.82	0.61
1:D:1024:TYR:O	1:D:1032:LYS:NZ	2.33	0.61
1:A:3236:VAL:HA	1:A:3239:MET:HG3	1.83	0.61
1:D:897:ARG:HB2	1:D:903:LEU:HD11	1.83	0.61
1:D:3236:VAL:HA	1:D:3239:MET:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3368:ARG:NH2	1:D:3404:ASP:OD2	2.34	0.60
1:A:2630:VAL:HG12	1:A:2682:ILE:HD11	1.83	0.60
1:B:897:ARG:HB2	1:B:903:LEU:HD11	1.83	0.60
1:C:897:ARG:HB2	1:C:903:LEU:HD11	1.83	0.60
1:D:3051:ARG:O	1:D:3053:ARG:NE	2.31	0.60
1:D:3081:MET:HG3	1:D:3156:VAL:HA	1.83	0.60
2:G:17:LYS:HG3	2:G:20:GLN:HE22	1.66	0.60
1:C:652:ARG:HB3	1:C:773:LEU:HD21	1.83	0.60
1:C:2961:GLN:NE2	1:C:3038:MET:SD	2.70	0.60
1:C:2978:GLU:OE2	1:C:3053:ARG:NH1	2.31	0.60
1:A:652:ARG:HB3	1:A:773:LEU:HD21	1.83	0.60
1:C:707:VAL:HG13	1:C:713:SER:HB2	1.83	0.60
1:A:2685:SER:O	1:A:2689:LYS:HB2	2.02	0.60
1:D:2630:VAL:HG12	1:D:2682:ILE:HD11	1.83	0.60
1:B:707:VAL:HG13	1:B:713:SER:HB2	1.83	0.60
1:B:2685:SER:O	1:B:2689:LYS:HB2	2.02	0.60
1:B:3081:MET:HG3	1:B:3156:VAL:HA	1.83	0.60
1:C:978:THR:OG1	1:C:981:GLN:OE1	2.19	0.60
1:C:3236:VAL:HA	1:C:3239:MET:HG3	1.83	0.60
1:B:978:THR:OG1	1:B:981:GLN:OE1	2.19	0.60
1:B:2992:GLU:OE2	1:B:2996:LYS:NZ	2.34	0.60
1:C:3075:LEU:O	1:C:3146:HIS:NE2	2.32	0.60
1:C:3368:ARG:NH2	1:C:3404:ASP:OD2	2.34	0.60
1:D:978:THR:OG1	1:D:981:GLN:OE1	2.19	0.60
1:A:707:VAL:HG13	1:A:713:SER:HB2	1.83	0.59
1:B:652:ARG:HB3	1:B:773:LEU:HD21	1.83	0.59
1:B:3368:ARG:NH2	1:B:3404:ASP:OD2	2.34	0.59
2:E:17:LYS:HG3	2:E:20:GLN:HE22	1.66	0.59
2:H:17:LYS:HG3	2:H:20:GLN:HE22	1.66	0.59
1:B:2619:LEU:HB3	1:B:2623:LEU:HD13	1.85	0.59
1:C:2992:GLU:OE2	1:C:2996:LYS:NZ	2.34	0.59
1:D:707:VAL:HG13	1:D:713:SER:HB2	1.84	0.59
2:F:17:LYS:HG3	2:F:20:GLN:HE22	1.66	0.59
1:A:475:GLN:NE2	1:A:528:SER:O	2.36	0.59
1:A:1232:ARG:NH2	1:A:1828:ASP:O	2.35	0.59
1:A:2992:GLU:OE2	1:A:2996:LYS:NZ	2.34	0.59
1:C:2619:LEU:HB3	1:C:2623:LEU:HD13	1.85	0.59
1:D:652:ARG:HB3	1:D:773:LEU:HD21	1.83	0.59
1:D:1232:ARG:NH2	1:D:1828:ASP:O	2.35	0.59
1:D:2992:GLU:OE2	1:D:2996:LYS:NZ	2.34	0.59
1:A:551:LEU:HB3	1:A:589:LEU:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1232:ARG:NH2	1:C:1828:ASP:O	2.35	0.59
1:C:3081:MET:HG3	1:C:3156:VAL:HA	1.83	0.59
1:D:551:LEU:HB3	1:D:589:LEU:HD11	1.85	0.59
1:D:2685:SER:O	1:D:2689:LYS:HB2	2.02	0.59
1:B:475:GLN:NE2	1:B:528:SER:O	2.36	0.58
1:C:551:LEU:HB3	1:C:589:LEU:HD11	1.85	0.58
1:D:2871:LEU:HG	1:D:2927:LEU:HD21	1.85	0.58
1:B:551:LEU:HB3	1:B:589:LEU:HD11	1.85	0.58
1:B:1252:HIS:O	1:B:1275:ARG:NH2	2.37	0.58
1:B:1810:LYS:HG2	1:B:1814:MET:HE2	1.85	0.58
1:D:475:GLN:NE2	1:D:528:SER:O	2.36	0.58
1:D:1943:LEU:HD13	1:D:2098:VAL:HG22	1.86	0.58
1:B:1232:ARG:NH2	1:B:1828:ASP:O	2.35	0.58
1:C:475:GLN:NE2	1:C:528:SER:O	2.36	0.58
1:C:4994:TYR:OH	1:C:4998:LYS:NZ	2.35	0.58
1:A:882:TRP:O	1:A:886:ARG:NH1	2.37	0.58
1:A:2871:LEU:HG	1:A:2927:LEU:HD21	1.85	0.58
1:C:1252:HIS:O	1:C:1275:ARG:NH2	2.36	0.58
1:D:1252:HIS:O	1:D:1275:ARG:NH2	2.37	0.58
1:C:763:PRO:O	1:C:765:GLN:NE2	2.37	0.58
1:D:2619:LEU:HB3	1:D:2623:LEU:HD13	1.85	0.58
1:A:161:GLU:HB3	1:D:3984:ARG:HH22	1.68	0.58
1:A:1252:HIS:O	1:A:1275:ARG:NH2	2.36	0.58
1:A:4581:LYS:NZ	1:B:4877:ASP:O	2.35	0.58
1:B:2960:LEU:HB2	1:B:3038:MET:HE3	1.86	0.58
1:C:1943:LEU:HD13	1:C:2098:VAL:HG22	1.86	0.58
1:C:2685:SER:O	1:C:2689:LYS:HB2	2.02	0.58
1:B:882:TRP:O	1:B:886:ARG:NH1	2.37	0.58
1:C:1810:LYS:HG2	1:C:1814:MET:HE2	1.85	0.58
1:D:289:ARG:HB3	1:D:301:VAL:HB	1.85	0.58
1:B:62:LEU:HD23	1:B:261:ARG:HH12	1.69	0.58
1:B:3990:VAL:HG13	1:B:4051:SER:HB3	1.86	0.58
1:C:289:ARG:HB3	1:C:301:VAL:HB	1.86	0.58
1:C:882:TRP:O	1:C:886:ARG:NH1	2.37	0.58
1:C:2823:ILE:HD11	1:C:2935:TYR:HB3	1.86	0.58
1:C:3990:VAL:HG13	1:C:4051:SER:HB3	1.86	0.58
1:D:882:TRP:O	1:D:886:ARG:NH1	2.37	0.58
1:A:2619:LEU:HB3	1:A:2623:LEU:HD13	1.85	0.57
1:D:638:ILE:HD12	1:D:1638:ALA:HB3	1.86	0.57
1:A:2960:LEU:HB2	1:A:3038:MET:HE3	1.86	0.57
1:C:2463:LEU:HA	1:C:2466:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2871:LEU:HG	1:C:2927:LEU:HD21	1.85	0.57
1:C:3524:MET:HA	1:C:3582:ARG:HH22	1.70	0.57
1:C:3702:VAL:HG13	1:C:3778:MET:HG2	1.86	0.57
1:D:763:PRO:O	1:D:765:GLN:NE2	2.37	0.57
1:D:3702:VAL:HG13	1:D:3778:MET:HG2	1.86	0.57
1:A:763:PRO:O	1:A:765:GLN:NE2	2.37	0.57
1:A:62:LEU:HD23	1:A:261:ARG:HH12	1.69	0.57
1:B:289:ARG:HB3	1:B:301:VAL:HB	1.86	0.57
1:B:1943:LEU:HD13	1:B:2098:VAL:HG22	1.86	0.57
1:B:2309:SER:OG	1:B:2321:ILE:O	2.22	0.57
1:D:3524:MET:HA	1:D:3582:ARG:HH22	1.70	0.57
1:A:638:ILE:HD12	1:A:1638:ALA:HB3	1.86	0.57
1:A:2309:SER:OG	1:A:2321:ILE:O	2.22	0.57
1:B:3524:MET:HA	1:B:3582:ARG:HH22	1.70	0.57
1:D:1810:LYS:HG2	1:D:1814:MET:HE2	1.85	0.57
1:A:1561:VAL:HG12	1:A:1562:ILE:HG13	1.87	0.57
1:A:1810:LYS:HG2	1:A:1814:MET:HE2	1.85	0.57
1:A:3635:CYS:HA	1:A:3638:MET:HG3	1.86	0.57
1:C:2595:LEU:O	1:C:2600:ARG:NH1	2.38	0.57
1:C:3052:HIS:NE2	1:C:3128:ASN:OD1	2.35	0.57
1:D:2309:SER:OG	1:D:2321:ILE:O	2.22	0.57
1:D:2960:LEU:HB2	1:D:3038:MET:HE3	1.86	0.57
1:B:2871:LEU:HG	1:B:2927:LEU:HD21	1.85	0.57
1:D:2823:ILE:HD11	1:D:2935:TYR:HB3	1.86	0.57
1:D:3990:VAL:HG13	1:D:4051:SER:HB3	1.86	0.57
1:A:1943:LEU:HD13	1:A:2098:VAL:HG22	1.86	0.57
1:A:2463:LEU:HA	1:A:2466:LEU:HD12	1.86	0.57
1:B:348:VAL:HB	1:B:357:LEU:HD22	1.87	0.57
1:C:62:LEU:HD23	1:C:261:ARG:HH12	1.69	0.57
1:C:2021:CYS:O	1:C:2028:ARG:NH2	2.38	0.57
1:D:2653:LYS:HB2	1:D:2661:TRP:HE3	1.70	0.57
1:D:3766:GLN:OE1	1:D:3769:ARG:NH2	2.38	0.57
1:B:747:CYS:HB2	1:B:756:SER:HB2	1.87	0.57
1:B:763:PRO:O	1:B:765:GLN:NE2	2.37	0.57
1:B:1653:LEU:O	1:B:1660:GLN:NE2	2.38	0.57
1:B:2595:LEU:O	1:B:2600:ARG:NH1	2.38	0.57
1:B:3635:CYS:HA	1:B:3638:MET:HG3	1.86	0.57
1:B:4994:TYR:OH	1:B:4998:LYS:NZ	2.35	0.57
1:C:728:ARG:NH2	1:C:1489:CYS:SG	2.78	0.57
1:C:5013:MET:HE1	1:C:5020:ASP:HB2	1.86	0.57
1:A:1653:LEU:O	1:A:1660:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2595:LEU:O	1:A:2600:ARG:NH1	2.38	0.57
1:A:2792:ARG:HB2	1:A:2797:PHE:HD1	1.70	0.57
1:A:3769:ARG:O	1:A:3773:ARG:NH1	2.38	0.57
1:A:3990:VAL:HG13	1:A:4051:SER:HB3	1.86	0.57
1:C:1454:THR:OG1	1:C:1456:ASP:OD1	2.23	0.57
1:D:62:LEU:HD23	1:D:261:ARG:HH12	1.69	0.57
1:D:1561:VAL:HG12	1:D:1562:ILE:HG13	1.87	0.57
1:D:2018:GLU:OE1	1:D:2028:ARG:NH1	2.38	0.57
1:D:2792:ARG:HB2	1:D:2797:PHE:HD1	1.70	0.57
1:A:289:ARG:HB3	1:A:301:VAL:HB	1.86	0.56
1:C:3766:GLN:OE1	1:C:3769:ARG:NH2	2.38	0.56
1:D:133:PHE:O	1:D:193:ALA:N	2.38	0.56
1:D:728:ARG:NH2	1:D:1489:CYS:SG	2.78	0.56
1:A:2823:ILE:HD11	1:A:2935:TYR:HB3	1.86	0.56
1:B:638:ILE:HD12	1:B:1638:ALA:HB3	1.86	0.56
1:B:2000:SER:O	1:B:2005:GLN:NE2	2.33	0.56
1:C:1561:VAL:HG12	1:C:1562:ILE:HG13	1.87	0.56
1:D:2021:CYS:O	1:D:2028:ARG:NH2	2.38	0.56
1:A:348:VAL:HB	1:A:357:LEU:HD22	1.87	0.56
1:A:3766:GLN:OE1	1:A:3769:ARG:NH2	2.38	0.56
1:B:2653:LYS:HB2	1:B:2661:TRP:HE3	1.70	0.56
1:B:3766:GLN:OE1	1:B:3769:ARG:NH2	2.38	0.56
1:B:5013:MET:HE1	1:B:5020:ASP:HB2	1.86	0.56
1:C:638:ILE:HD12	1:C:1638:ALA:HB3	1.86	0.56
1:C:3214:ASN:HB3	1:C:3217:SER:HB2	1.86	0.56
1:D:747:CYS:HB2	1:D:756:SER:HB2	1.87	0.56
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.78	0.56
1:A:2018:GLU:OE1	1:A:2028:ARG:NH1	2.38	0.56
1:B:2463:LEU:HA	1:B:2466:LEU:HD12	1.86	0.56
1:D:2463:LEU:HA	1:D:2466:LEU:HD12	1.86	0.56
1:D:2595:LEU:O	1:D:2600:ARG:NH1	2.38	0.56
1:A:2977:LEU:HA	1:A:2980:VAL:HG22	1.88	0.56
1:B:1454:THR:OG1	1:B:1456:ASP:OD1	2.23	0.56
1:B:1561:VAL:HG12	1:B:1562:ILE:HG13	1.87	0.56
1:B:2792:ARG:HB2	1:B:2797:PHE:HD1	1.70	0.56
1:B:3769:ARG:O	1:B:3773:ARG:NH1	2.38	0.56
1:C:2792:ARG:HB2	1:C:2797:PHE:HD1	1.70	0.56
1:D:3635:CYS:HA	1:D:3638:MET:HG3	1.86	0.56
1:D:4570:ALA:O	1:D:4574:ASN:ND2	2.39	0.56
1:A:3702:VAL:HG13	1:A:3778:MET:HG2	1.86	0.56
1:B:2021:CYS:O	1:B:2028:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3702:VAL:HG13	1:B:3778:MET:HG2	1.86	0.56
1:D:348:VAL:HB	1:D:357:LEU:HD22	1.87	0.56
1:D:1694:LEU:HB3	1:D:1715:LEU:HD12	1.88	0.56
1:D:2977:LEU:HA	1:D:2980:VAL:HG22	1.87	0.56
1:A:34:LYS:HB3	1:A:53:SER:HB3	1.87	0.56
1:A:133:PHE:O	1:A:193:ALA:N	2.38	0.56
1:A:683:ARG:NH1	1:A:707:VAL:O	2.34	0.56
1:A:2021:CYS:O	1:A:2028:ARG:NH2	2.38	0.56
1:B:3052:HIS:NE2	1:B:3128:ASN:OD1	2.35	0.56
1:D:3769:ARG:O	1:D:3773:ARG:NH1	2.38	0.56
1:D:5013:MET:HE1	1:D:5020:ASP:HB2	1.86	0.56
1:A:4938:ASP:OD1	1:D:4944:ARG:NH2	2.36	0.56
1:B:728:ARG:NH2	1:B:1489:CYS:SG	2.78	0.56
1:B:2823:ILE:HD11	1:B:2935:TYR:HB3	1.86	0.56
1:B:3214:ASN:HB3	1:B:3217:SER:HB2	1.86	0.56
1:B:4570:ALA:O	1:B:4574:ASN:ND2	2.39	0.56
1:C:2960:LEU:HB2	1:C:3038:MET:HE3	1.86	0.56
1:A:2653:LYS:HB2	1:A:2661:TRP:HE3	1.70	0.56
1:B:3048:ALA:O	1:B:3053:ARG:NH2	2.39	0.56
1:C:1694:LEU:HB3	1:C:1715:LEU:HD12	1.88	0.56
1:C:2018:GLU:OE1	1:C:2028:ARG:NH1	2.38	0.56
1:D:1653:LEU:O	1:D:1660:GLN:NE2	2.38	0.56
1:D:4994:TYR:OH	1:D:4998:LYS:NZ	2.35	0.56
1:C:2512:ILE:HG21	1:C:2518:LEU:HD13	1.88	0.56
1:D:3048:ALA:O	1:D:3053:ARG:NH2	2.39	0.56
1:A:747:CYS:HB2	1:A:756:SER:HB2	1.87	0.55
1:A:2000:SER:O	1:A:2005:GLN:NE2	2.32	0.55
1:A:3524:MET:HA	1:A:3582:ARG:HH22	1.70	0.55
1:B:1694:LEU:HB3	1:B:1715:LEU:HD12	1.88	0.55
1:B:2018:GLU:OE1	1:B:2028:ARG:NH1	2.38	0.55
1:B:2977:LEU:HA	1:B:2980:VAL:HG22	1.87	0.55
1:C:683:ARG:NH1	1:C:707:VAL:O	2.34	0.55
1:C:3459:VAL:HG13	1:C:3464:ILE:HB	1.89	0.55
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.88	0.55
1:A:3459:VAL:HG13	1:A:3464:ILE:HB	1.89	0.55
1:A:5013:MET:HE1	1:A:5020:ASP:HB2	1.86	0.55
1:B:707:VAL:HG23	1:B:782:SER:HB3	1.88	0.55
1:C:348:VAL:HB	1:C:357:LEU:HD22	1.87	0.55
1:C:2927:LEU:HD12	1:C:2930:LEU:HD12	1.88	0.55
1:C:4570:ALA:O	1:C:4574:ASN:ND2	2.39	0.55
1:D:3214:ASN:HB3	1:D:3217:SER:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4583:SER:HB2	1:D:4631:PHE:HE1	1.72	0.55
1:A:277:GLY:HA2	1:A:315:CYS:HB3	1.89	0.55
1:B:34:LYS:HB3	1:B:53:SER:HB3	1.87	0.55
1:C:2653:LYS:HB2	1:C:2661:TRP:HE3	1.70	0.55
1:C:3840:SER:OG	1:C:3877:ASP:OD1	2.24	0.55
1:D:277:GLY:HA2	1:D:315:CYS:HB3	1.89	0.55
1:D:2114:PRO:HB3	1:D:3707:ARG:HH12	1.72	0.55
1:D:3099:ALA:HA	1:D:3136:LEU:HD21	1.89	0.55
1:A:1694:LEU:HB3	1:A:1715:LEU:HD12	1.88	0.55
1:A:2512:ILE:HG21	1:A:2518:LEU:HD13	1.88	0.55
1:A:4583:SER:HB2	1:A:4631:PHE:HE1	1.72	0.55
1:C:3635:CYS:HA	1:C:3638:MET:HG3	1.86	0.55
1:A:3214:ASN:HB3	1:A:3217:SER:HB2	1.87	0.55
1:B:133:PHE:O	1:B:193:ALA:N	2.38	0.55
1:B:2512:ILE:HG21	1:B:2518:LEU:HD13	1.88	0.55
1:B:3459:VAL:HG13	1:B:3464:ILE:HB	1.89	0.55
1:C:633:LEU:HD13	1:C:1639:LEU:HD21	1.89	0.55
1:C:3769:ARG:O	1:C:3773:ARG:NH1	2.38	0.55
1:A:3048:ALA:O	1:A:3053:ARG:NH2	2.39	0.55
1:A:4570:ALA:O	1:A:4574:ASN:ND2	2.39	0.55
1:B:2265:LEU:O	1:B:2330:ARG:NH1	2.39	0.55
1:C:1653:LEU:O	1:C:1660:GLN:NE2	2.38	0.55
1:C:3048:ALA:O	1:C:3053:ARG:NH2	2.39	0.55
1:C:3419:ASN:OD1	1:C:3423:TRP:NE1	2.40	0.55
1:D:3459:VAL:HG13	1:D:3464:ILE:HB	1.89	0.55
1:D:23:GLN:NE2	1:D:203:ASN:OD1	2.40	0.55
1:A:1730:MET:O	1:A:1772:ARG:NH1	2.40	0.55
1:C:747:CYS:HB2	1:C:756:SER:HB2	1.87	0.55
1:C:2265:LEU:O	1:C:2330:ARG:NH1	2.39	0.55
1:C:2977:LEU:HA	1:C:2980:VAL:HG22	1.87	0.55
1:C:4583:SER:HB2	1:C:4631:PHE:HE1	1.72	0.55
1:D:1730:MET:O	1:D:1772:ARG:NH1	2.40	0.55
1:D:2000:SER:O	1:D:2005:GLN:NE2	2.33	0.55
1:A:2114:PRO:HB3	1:A:3707:ARG:HH12	1.72	0.55
1:B:633:LEU:HD13	1:B:1639:LEU:HD21	1.89	0.55
1:B:3419:ASN:OD1	1:B:3423:TRP:NE1	2.40	0.55
1:C:23:GLN:NE2	1:C:203:ASN:OD1	2.40	0.55
1:C:796:ARG:O	1:C:1619:ARG:NH2	2.40	0.55
1:B:796:ARG:O	1:B:1619:ARG:NH2	2.40	0.54
1:A:796:ARG:O	1:A:1619:ARG:NH2	2.40	0.54
1:A:2978:GLU:OE2	1:A:3053:ARG:NH1	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3419:ASN:OD1	1:A:3423:TRP:NE1	2.40	0.54
1:B:1730:MET:O	1:B:1772:ARG:NH1	2.40	0.54
1:B:2114:PRO:HB3	1:B:3707:ARG:HH12	1.72	0.54
1:B:4583:SER:HB2	1:B:4631:PHE:HE1	1.72	0.54
1:C:2114:PRO:HB3	1:C:3707:ARG:HH12	1.72	0.54
1:D:34:LYS:HB3	1:D:53:SER:HB3	1.87	0.54
1:A:2265:LEU:O	1:A:2330:ARG:NH1	2.40	0.54
1:B:23:GLN:NE2	1:B:203:ASN:OD1	2.40	0.54
1:C:3099:ALA:HA	1:C:3136:LEU:HD21	1.89	0.54
1:A:23:GLN:NE2	1:A:203:ASN:OD1	2.40	0.54
1:A:2927:LEU:HD12	1:A:2930:LEU:HD12	1.88	0.54
1:D:2265:LEU:O	1:D:2330:ARG:NH1	2.39	0.54
1:C:707:VAL:HG23	1:C:782:SER:HB3	1.88	0.54
1:D:707:VAL:HG23	1:D:782:SER:HB3	1.88	0.54
1:D:4886:HIS:HD2	1:D:4920:PHE:HE2	1.56	0.54
1:A:1944:GLU:HB3	1:A:2123:LEU:HD21	1.90	0.54
1:A:2131:LEU:HD12	1:A:3662:ILE:HG23	1.90	0.54
1:C:34:LYS:HB3	1:C:53:SER:HB3	1.87	0.54
1:A:867:LEU:HD13	1:A:929:LEU:HB3	1.90	0.54
1:B:3099:ALA:HA	1:B:3136:LEU:HD21	1.89	0.54
1:B:4112:LEU:O	1:B:4115:SER:OG	2.25	0.54
1:B:4886:HIS:HD2	1:B:4920:PHE:HE2	1.56	0.54
1:C:1730:MET:O	1:C:1772:ARG:NH1	2.40	0.54
1:C:1944:GLU:HB3	1:C:2123:LEU:HD21	1.90	0.54
1:C:2309:SER:OG	1:C:2321:ILE:O	2.22	0.54
1:D:669:ASP:OD1	1:D:790:ARG:NH1	2.40	0.54
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.23	0.54
1:A:2247:GLN:NE2	1:A:2281:ILE:O	2.41	0.54
1:A:3099:ALA:HA	1:A:3136:LEU:HD21	1.88	0.54
1:A:4886:HIS:HD2	1:A:4920:PHE:HE2	1.56	0.54
1:B:632:LEU:O	1:B:634:GLN:NE2	2.40	0.54
1:B:669:ASP:OD1	1:B:790:ARG:NH1	2.40	0.54
1:B:1944:GLU:HB3	1:B:2123:LEU:HD21	1.90	0.54
1:B:2247:GLN:NE2	1:B:2281:ILE:O	2.41	0.54
1:C:669:ASP:OD1	1:C:790:ARG:NH1	2.40	0.54
1:C:867:LEU:HD13	1:C:929:LEU:HB3	1.90	0.54
1:C:4112:LEU:O	1:C:4115:SER:OG	2.25	0.54
1:D:633:LEU:HD13	1:D:1639:LEU:HD21	1.89	0.54
1:D:2512:ILE:HG21	1:D:2518:LEU:HD13	1.88	0.54
1:D:3380:ARG:NH2	1:D:3450:ASN:OD1	2.41	0.54
1:A:4112:LEU:O	1:A:4115:SER:OG	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2927:LEU:HD12	1:B:2930:LEU:HD12	1.89	0.54
1:C:277:GLY:HA2	1:C:315:CYS:HB3	1.89	0.54
1:C:1277:TRP:O	1:C:1559:GLN:NE2	2.41	0.54
1:C:3380:ARG:NH2	1:C:3450:ASN:OD1	2.40	0.54
1:D:632:LEU:O	1:D:634:GLN:NE2	2.40	0.54
1:D:1277:TRP:O	1:D:1559:GLN:NE2	2.41	0.54
1:B:3380:ARG:NH2	1:B:3450:ASN:OD1	2.41	0.54
1:A:632:LEU:O	1:A:634:GLN:NE2	2.40	0.53
1:A:669:ASP:OD1	1:A:790:ARG:NH1	2.40	0.53
1:B:277:GLY:HA2	1:B:315:CYS:HB3	1.89	0.53
1:B:867:LEU:HD13	1:B:929:LEU:HB3	1.90	0.53
1:B:2131:LEU:HD12	1:B:3662:ILE:HG23	1.90	0.53
1:D:1454:THR:OG1	1:D:1456:ASP:OD1	2.23	0.53
1:D:4112:LEU:O	1:D:4115:SER:OG	2.25	0.53
1:A:633:LEU:HD13	1:A:1639:LEU:HD21	1.89	0.53
1:A:4994:TYR:OH	1:A:4998:LYS:NZ	2.35	0.53
1:B:3322:ILE:O	1:B:3326:ASN:ND2	2.41	0.53
1:D:796:ARG:O	1:D:1619:ARG:NH2	2.40	0.53
1:D:1944:GLU:HB3	1:D:2123:LEU:HD21	1.90	0.53
1:D:2927:LEU:HD12	1:D:2930:LEU:HD12	1.88	0.53
1:D:3322:ILE:O	1:D:3326:ASN:ND2	2.41	0.53
1:D:3419:ASN:OD1	1:D:3423:TRP:NE1	2.40	0.53
1:C:3882:GLN:HG3	1:C:3957:VAL:HG22	1.91	0.53
1:D:867:LEU:HD13	1:D:929:LEU:HB3	1.90	0.53
1:A:1277:TRP:O	1:A:1559:GLN:NE2	2.41	0.53
1:A:3380:ARG:NH2	1:A:3450:ASN:OD1	2.41	0.53
1:B:1277:TRP:O	1:B:1559:GLN:NE2	2.41	0.53
1:C:2000:SER:O	1:C:2005:GLN:NE2	2.33	0.53
1:D:3107:VAL:HG11	1:D:3171:SER:HB2	1.91	0.53
1:A:3322:ILE:O	1:A:3326:ASN:ND2	2.41	0.53
1:A:3924:LEU:HD21	1:A:3984:ARG:HH21	1.73	0.53
1:C:632:LEU:O	1:C:634:GLN:NE2	2.40	0.53
1:D:3524:MET:O	1:D:3595:ARG:NH1	2.42	0.53
1:D:3882:GLN:HG3	1:D:3957:VAL:HG22	1.91	0.53
1:A:2960:LEU:HD23	1:A:2963:LEU:HD12	1.91	0.53
1:A:3882:GLN:HG3	1:A:3957:VAL:HG22	1.91	0.53
1:B:2960:LEU:HD23	1:B:2963:LEU:HD12	1.91	0.53
1:D:125:ARG:NH1	1:D:126:SER:OG	2.42	0.53
1:D:1066:GLN:NE2	1:D:1461:ASP:OD1	2.39	0.53
1:B:3767:GLN:OE1	1:B:3809:ASN:ND2	2.38	0.53
1:C:4886:HIS:HD2	1:C:4920:PHE:HE2	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3208:PRO:HA	1:D:3211:ASN:HB2	1.91	0.53
1:B:3020:THR:HG23	1:B:3023:LYS:H	1.74	0.53
1:B:3524:MET:O	1:B:3595:ARG:NH1	2.42	0.53
1:C:3524:MET:O	1:C:3595:ARG:NH1	2.42	0.53
1:D:683:ARG:NH1	1:D:707:VAL:O	2.34	0.53
1:D:1099:GLU:OE2	1:D:1125:ASN:ND2	2.40	0.53
1:D:2131:LEU:HD12	1:D:3662:ILE:HG23	1.90	0.53
1:A:3984:ARG:HH22	1:B:161:GLU:HB3	1.74	0.53
1:B:3984:ARG:HH22	1:C:161:GLU:HB3	1.74	0.53
1:C:3573:MET:HB3	1:C:3577:ARG:HH21	1.73	0.53
1:D:3573:MET:HB3	1:D:3577:ARG:HH21	1.73	0.53
1:A:818:ARG:NH2	1:A:1027:LEU:O	2.42	0.53
1:A:4161:ARG:HA	1:A:4164:LEU:HD13	1.91	0.53
1:C:133:PHE:O	1:C:193:ALA:N	2.38	0.53
1:C:3020:THR:HG23	1:C:3023:LYS:H	1.74	0.53
1:B:3573:MET:HB3	1:B:3577:ARG:HH21	1.73	0.52
1:C:1066:GLN:NE2	1:C:1461:ASP:OD1	2.39	0.52
1:C:3984:ARG:HH22	1:D:161:GLU:HB3	1.74	0.52
1:B:224:HIS:NE2	1:B:385:ASP:O	2.42	0.52
1:C:3107:VAL:HG11	1:C:3171:SER:HB2	1.91	0.52
1:C:3924:LEU:HD21	1:C:3984:ARG:HH21	1.74	0.52
1:B:818:ARG:NH2	1:B:1027:LEU:O	2.42	0.52
1:B:3208:PRO:HA	1:B:3211:ASN:HB2	1.91	0.52
1:B:4866:SER:HB3	1:B:4873:ASP:HB2	1.92	0.52
1:C:222:LEU:HD23	1:C:388:LEU:HD13	1.92	0.52
1:C:224:HIS:NE2	1:C:385:ASP:O	2.42	0.52
1:C:1443:GLN:NE2	1:C:1555:LEU:O	2.40	0.52
1:C:2131:LEU:HD12	1:C:3662:ILE:HG23	1.90	0.52
1:D:222:LEU:HD23	1:D:388:LEU:HD13	1.92	0.52
1:A:1443:GLN:NE2	1:A:1555:LEU:O	2.41	0.52
1:A:2268[A]:GLN:OE1	1:A:2414:ASN:ND2	2.43	0.52
1:A:2268[B]:GLN:OE1	1:A:2414:ASN:ND2	2.43	0.52
1:A:3524:MET:O	1:A:3595:ARG:NH1	2.42	0.52
1:A:3573:MET:HB3	1:A:3577:ARG:HH21	1.73	0.52
1:A:4107:GLU:HA	1:A:4110:PHE:HB3	1.92	0.52
1:B:3107:VAL:HG11	1:B:3171:SER:HB2	1.91	0.52
1:C:818:ARG:NH2	1:C:1027:LEU:O	2.42	0.52
1:D:1100:MET:HE3	1:D:1198:GLN:HB3	1.91	0.52
1:D:1636:MET:HE3	1:D:1638:ALA:HB2	1.92	0.52
1:D:2268[A]:GLN:OE1	1:D:2414:ASN:ND2	2.43	0.52
1:D:3052:HIS:NE2	1:D:3128:ASN:OD1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3924:LEU:HD21	1:D:3984:ARG:HH21	1.74	0.52
1:D:4161:ARG:HA	1:D:4164:LEU:HD13	1.91	0.52
1:B:125:ARG:NH1	1:B:126:SER:OG	2.42	0.52
1:B:1636:MET:HE3	1:B:1638:ALA:HB2	1.92	0.52
1:B:3882:GLN:HG3	1:B:3957:VAL:HG22	1.90	0.52
1:C:125:ARG:NH1	1:C:126:SER:OG	2.42	0.52
1:C:4866:SER:HB3	1:C:4873:ASP:HB2	1.92	0.52
1:D:2423:MET:HE2	1:D:2498:HIS:HD2	1.75	0.52
1:D:3767:GLN:OE1	1:D:3809:ASN:ND2	2.38	0.52
1:A:3208:PRO:HA	1:A:3211:ASN:HB2	1.91	0.52
1:A:3556:ASN:HA	1:A:3559:LEU:HD23	1.92	0.52
1:B:222:LEU:HD23	1:B:388:LEU:HD13	1.92	0.52
1:C:2247:GLN:NE2	1:C:2281:ILE:O	2.41	0.52
1:D:4064:MET:HE1	1:D:4111:LEU:HB2	1.92	0.52
1:A:125:ARG:NH1	1:A:126:SER:OG	2.42	0.52
1:A:1100:MET:HE3	1:A:1198:GLN:HB3	1.91	0.52
1:B:2365:GLY:O	1:B:2369[B]:ARG:NE	2.39	0.52
1:B:3840:SER:OG	1:B:3877:ASP:OD1	2.24	0.52
1:B:3924:LEU:HD21	1:B:3984:ARG:HH21	1.73	0.52
1:D:818:ARG:NH2	1:D:1027:LEU:O	2.42	0.52
1:D:4107:GLU:HA	1:D:4110:PHE:HB3	1.92	0.52
1:A:3318:ASN:OD1	1:A:3321:ARG:NH1	2.43	0.52
1:A:4866:SER:HB3	1:A:4873:ASP:HB2	1.92	0.52
1:A:4877:ASP:O	1:D:4581:LYS:NZ	2.42	0.52
1:B:3318:ASN:OD1	1:B:3321:ARG:NH1	2.43	0.52
1:C:2879:ALA:HB1	1:C:2919:ASP:HB3	1.92	0.52
1:C:3318:ASN:OD1	1:C:3321:ARG:NH1	2.43	0.52
1:C:4064:MET:HE1	1:C:4111:LEU:HB2	1.92	0.52
1:D:3020:THR:HG23	1:D:3023:LYS:H	1.74	0.52
1:D:3556:ASN:HA	1:D:3559:LEU:HD23	1.92	0.52
1:D:4866:SER:HB3	1:D:4873:ASP:HB2	1.92	0.52
1:A:2879:ALA:HB1	1:A:2919:ASP:HB3	1.92	0.52
1:B:1443:GLN:NE2	1:B:1555:LEU:O	2.41	0.52
1:D:2247:GLN:NE2	1:D:2281:ILE:O	2.41	0.52
1:D:2960:LEU:HD23	1:D:2963:LEU:HD12	1.91	0.52
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.74	0.52
1:B:2268[A]:GLN:OE1	1:B:2414:ASN:ND2	2.43	0.52
1:B:2879:ALA:HB1	1:B:2919:ASP:HB3	1.92	0.52
1:C:2268[A]:GLN:OE1	1:C:2414:ASN:ND2	2.43	0.52
1:D:2268[B]:GLN:OE1	1:D:2414:ASN:ND2	2.43	0.52
1:A:4914:VAL:HG11	1:D:4884:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2268[B]:GLN:OE1	1:B:2414:ASN:ND2	2.43	0.51
1:B:4068:LEU:HA	1:B:4071:ILE:HB	1.92	0.51
1:B:4161:ARG:HA	1:B:4164:LEU:HD13	1.91	0.51
1:B:4823:LEU:HD22	1:C:4843:LEU:HD22	1.91	0.51
1:C:2423:MET:HE2	1:C:2498:HIS:HD2	1.75	0.51
1:C:3322:ILE:O	1:C:3326:ASN:ND2	2.41	0.51
1:C:4708:THR:HG21	1:C:4775:TYR:HB2	1.93	0.51
1:D:224:HIS:NE2	1:D:385:ASP:O	2.42	0.51
1:D:1443:GLN:NE2	1:D:1555:LEU:O	2.40	0.51
1:A:4068:LEU:HA	1:A:4071:ILE:HB	1.92	0.51
1:B:1084:GLN:NE2	1:B:1186:ASP:O	2.43	0.51
1:C:2749:GLU:HG3	1:C:2752:ASP:HB2	1.93	0.51
1:D:3458:PHE:O	1:D:3462:ASN:ND2	2.36	0.51
1:D:3596:VAL:O	1:D:3600:SER:OG	2.23	0.51
1:A:224:HIS:NE2	1:A:385:ASP:O	2.42	0.51
1:B:45:ARG:NH2	1:B:447:ASP:OD1	2.42	0.51
1:B:1100:MET:HE3	1:B:1198:GLN:HB3	1.91	0.51
1:C:2806:ARG:HD2	1:C:2810:LYS:HZ3	1.75	0.51
1:D:2437:ALA:O	1:D:2508:ARG:NH2	2.44	0.51
1:D:2749:GLU:HG3	1:D:2752:ASP:HB2	1.93	0.51
1:D:4708:THR:HG21	1:D:4775:TYR:HB2	1.93	0.51
1:A:222:LEU:HD23	1:A:388:LEU:HD13	1.92	0.51
1:A:796:ARG:HG3	1:A:1619:ARG:HH22	1.74	0.51
1:A:1099:GLU:OE2	1:A:1125:ASN:ND2	2.40	0.51
1:C:2960:LEU:HD23	1:C:2963:LEU:HD12	1.91	0.51
1:D:3318:ASN:OD1	1:D:3321:ARG:NH1	2.43	0.51
1:A:2423:MET:HE2	1:A:2498:HIS:HD2	1.75	0.51
1:B:356:TRP:O	1:B:379:HIS:N	2.43	0.51
1:B:2749:GLU:HG3	1:B:2752:ASP:HB2	1.93	0.51
1:C:1100:MET:HE3	1:C:1198:GLN:HB3	1.91	0.51
1:C:3556:ASN:HA	1:C:3559:LEU:HD23	1.92	0.51
1:B:3781:GLN:NE2	1:B:3819:TYR:OH	2.40	0.51
1:C:4161:ARG:HA	1:C:4164:LEU:HD13	1.91	0.51
1:C:4823:LEU:HD22	1:D:4843:LEU:HD22	1.91	0.51
1:D:1947:CYS:SG	1:D:2127:GLN:NE2	2.79	0.51
1:D:2365:GLY:O	1:D:2369[B]:ARG:NE	2.39	0.51
1:D:2879:ALA:HB1	1:D:2919:ASP:HB3	1.92	0.51
1:A:818:ARG:HH12	1:A:1026:LEU:HA	1.76	0.51
1:A:3052:HIS:NE2	1:A:3128:ASN:OD1	2.35	0.51
1:B:1947:CYS:SG	1:B:2127:GLN:NE2	2.79	0.51
1:B:2437:ALA:O	1:B:2508:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:TRP:O	1:C:379:HIS:N	2.43	0.51
1:C:2268[B]:GLN:OE1	1:C:2414:ASN:ND2	2.43	0.51
1:D:45:ARG:NH2	1:D:447:ASP:OD1	2.42	0.51
1:D:4068:LEU:HA	1:D:4071:ILE:HB	1.93	0.51
1:A:4064:MET:HE1	1:A:4111:LEU:HB2	1.92	0.51
1:B:818:ARG:HH12	1:B:1026:LEU:HA	1.76	0.51
1:B:1225:PRO:HG2	1:B:1228:ILE:HD13	1.93	0.51
1:B:1618:ARG:NH2	1:B:1619:ARG:O	2.44	0.51
1:B:3107:VAL:O	1:B:3111:ARG:HB2	2.11	0.51
1:B:4107:GLU:HA	1:B:4110:PHE:HB3	1.92	0.51
1:C:320:LYS:NZ	1:C:383:HIS:O	2.44	0.51
1:C:4107:GLU:HA	1:C:4110:PHE:HB3	1.92	0.51
1:A:1636:MET:HE3	1:A:1638:ALA:HB2	1.92	0.51
1:A:2437:ALA:O	1:A:2508:ARG:NH2	2.44	0.51
1:A:2749:GLU:HG3	1:A:2752:ASP:HB2	1.93	0.51
1:B:796:ARG:HG3	1:B:1619:ARG:HH22	1.74	0.51
1:B:3556:ASN:HA	1:B:3559:LEU:HD23	1.92	0.51
1:C:3537:LYS:NZ	1:C:3600:SER:O	2.44	0.51
1:A:356:TRP:O	1:A:379:HIS:N	2.43	0.51
1:A:1225:PRO:HG2	1:A:1228:ILE:HD13	1.93	0.51
1:B:4708:THR:HG21	1:B:4775:TYR:HB2	1.93	0.51
1:C:796:ARG:HG3	1:C:1619:ARG:HH22	1.74	0.51
1:C:1084:GLN:NE2	1:C:1186:ASP:O	2.43	0.51
1:C:3771:HIS:O	1:C:3815:LYS:NZ	2.44	0.51
1:A:45:ARG:NH2	1:A:447:ASP:OD1	2.42	0.50
1:A:320:LYS:NZ	1:A:383:HIS:O	2.44	0.50
1:A:3107:VAL:HG11	1:A:3171:SER:HB2	1.91	0.50
1:B:2423:MET:HE2	1:B:2498:HIS:HD2	1.75	0.50
1:C:3458:PHE:O	1:C:3462:ASN:ND2	2.36	0.50
1:A:2788:HIS:HB3	1:A:2791:LEU:HD23	1.93	0.50
1:B:273:HIS:CE1	1:B:338:GLU:H	2.30	0.50
1:B:4064:MET:HE1	1:B:4111:LEU:HB2	1.92	0.50
1:C:1618:ARG:NH2	1:C:1619:ARG:O	2.44	0.50
1:C:3208:PRO:HA	1:C:3211:ASN:HB2	1.91	0.50
1:A:545:ASP:N	1:A:545:ASP:OD1	2.44	0.50
1:A:2754:PHE:HE2	1:A:2813:LEU:HD11	1.76	0.50
1:B:1676:LEU:HD22	1:B:2167:ILE:HD12	1.93	0.50
1:B:2745:VAL:HG13	1:B:2814:LYS:HD2	1.94	0.50
1:C:273:HIS:CE1	1:C:338:GLU:H	2.29	0.50
1:C:1225:PRO:HG2	1:C:1228:ILE:HD13	1.93	0.50
1:D:273:HIS:CE1	1:D:338:GLU:H	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLY:N	1:A:709:ASP:OD2	2.39	0.50
1:A:1066:GLN:NE2	1:A:1461:ASP:OD1	2.39	0.50
1:B:2754:PHE:HE2	1:B:2813:LEU:HD11	1.76	0.50
1:B:2788:HIS:HB3	1:B:2791:LEU:HD23	1.93	0.50
1:C:1751:GLY:HA3	1:C:1758:ARG:HE	1.77	0.50
1:C:2745:VAL:HG13	1:C:2814:LYS:HD2	1.94	0.50
1:C:3107:VAL:O	1:C:3111:ARG:HB2	2.11	0.50
1:C:4068:LEU:HA	1:C:4071:ILE:HB	1.93	0.50
1:D:3107:VAL:O	1:D:3111:ARG:HB2	2.11	0.50
1:D:3771:HIS:O	1:D:3815:LYS:NZ	2.44	0.50
1:A:273:HIS:CE1	1:A:338:GLU:H	2.29	0.50
1:A:1084:GLN:NE2	1:A:1186:ASP:O	2.43	0.50
1:A:1679:ASN:HA	1:A:1682:ALA:HB3	1.93	0.50
1:A:1947:CYS:SG	1:A:2127:GLN:NE2	2.79	0.50
1:A:2299:VAL:HG11	1:A:2356:LEU:HB3	1.93	0.50
1:C:3781:GLN:NE2	1:C:3819:TYR:OH	2.40	0.50
1:C:3868:ARG:HH11	1:C:3870:ASN:HB3	1.76	0.50
1:D:3840:SER:OG	1:D:3877:ASP:OD1	2.24	0.50
1:A:932:LEU:HB3	1:A:937:CYS:HB3	1.93	0.50
1:A:1618:ARG:NH2	1:A:1619:ARG:O	2.44	0.50
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.24	0.50
1:A:3868:ARG:HH11	1:A:3870:ASN:HB3	1.76	0.50
1:A:4204:GLN:HG2	1:A:4245:MET:HG2	1.94	0.50
1:B:2764:GLU:HG3	1:B:2857:PRO:HB3	1.94	0.50
1:C:1636:MET:HE3	1:C:1638:ALA:HB2	1.92	0.50
1:C:2437:ALA:O	1:C:2508:ARG:NH2	2.44	0.50
1:D:2745:VAL:HG13	1:D:2814:LYS:HD2	1.94	0.50
1:A:3107:VAL:O	1:A:3111:ARG:HB2	2.11	0.50
1:A:3458:PHE:O	1:A:3462:ASN:ND2	2.36	0.50
1:A:3767:GLN:OE1	1:A:3809:ASN:ND2	2.38	0.50
1:A:4708:THR:HG21	1:A:4775:TYR:HB2	1.93	0.50
1:A:4892:ARG:NH1	1:B:4895:GLY:O	2.37	0.50
1:B:932:LEU:HB3	1:B:937:CYS:HB3	1.94	0.50
1:B:2310:CYS:HB3	1:B:2313:LEU:HB2	1.94	0.50
1:C:648:ILE:HG23	1:C:814:ALA:HB3	1.94	0.50
1:C:2299:VAL:HG11	1:C:2356:LEU:HB3	1.93	0.50
1:C:2764:GLU:HG3	1:C:2857:PRO:HB3	1.94	0.50
1:B:4204:GLN:HG2	1:B:4245:MET:HG2	1.94	0.50
1:D:796:ARG:HG3	1:D:1619:ARG:HH22	1.74	0.50
1:A:1676:LEU:HD22	1:A:2167:ILE:HD12	1.93	0.50
1:A:4917:ASP:HB2	1:D:4888:TYR:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1679:ASN:HA	1:B:1682:ALA:HB3	1.93	0.50
1:B:2882:TYR:O	1:B:2885:THR:OG1	2.28	0.50
1:C:2882:TYR:O	1:C:2885:THR:OG1	2.28	0.50
1:C:3227:ARG:NH1	1:C:3234:ASN:OD1	2.37	0.50
1:C:3767:GLN:OE1	1:C:3809:ASN:ND2	2.38	0.50
1:D:356:TRP:O	1:D:379:HIS:N	2.43	0.50
1:D:2764:GLU:HG3	1:D:2857:PRO:HB3	1.94	0.50
1:A:2764:GLU:HG3	1:A:2857:PRO:HB3	1.94	0.49
1:C:758:ARG:HA	1:C:763:PRO:HA	1.94	0.49
1:C:2867:LEU:HD12	1:C:2928:LYS:HZ3	1.77	0.49
1:C:4204:GLN:HG2	1:C:4245:MET:HG2	1.94	0.49
1:D:758:ARG:HA	1:D:763:PRO:HA	1.94	0.49
1:D:1618:ARG:NH2	1:D:1619:ARG:O	2.44	0.49
1:D:1676:LEU:HD22	1:D:2167:ILE:HD12	1.93	0.49
1:D:3244:PRO:HA	1:D:3248:ARG:HH21	1.76	0.49
1:D:3868:ARG:HH11	1:D:3870:ASN:HB3	1.76	0.49
1:B:320:LYS:NZ	1:B:383:HIS:O	2.44	0.49
1:B:3244:PRO:HA	1:B:3248:ARG:HH21	1.76	0.49
1:C:45:ARG:NH2	1:C:447:ASP:OD1	2.42	0.49
1:C:2310:CYS:HB3	1:C:2313:LEU:HB2	1.94	0.49
1:D:932:LEU:HB3	1:D:937:CYS:HB3	1.94	0.49
1:D:1225:PRO:HG2	1:D:1228:ILE:HD13	1.93	0.49
1:D:1423:ASP:N	1:D:1571:ASN:OD1	2.45	0.49
1:D:2648:TYR:O	1:D:2652:TRP:HB3	2.12	0.49
1:D:3781:GLN:NE2	1:D:3819:TYR:OH	2.40	0.49
2:E:21:THR:HA	2:E:49:ARG:HA	1.94	0.49
1:C:818:ARG:HH12	1:C:1026:LEU:HA	1.76	0.49
1:C:932:LEU:HB3	1:C:937:CYS:HB3	1.94	0.49
1:D:2788:HIS:HB3	1:D:2791:LEU:HD23	1.93	0.49
1:A:2648:TYR:O	1:A:2652:TRP:HB3	2.12	0.49
1:A:3244:PRO:HA	1:A:3248:ARG:HH21	1.76	0.49
1:B:683:ARG:NH1	1:B:707:VAL:O	2.34	0.49
1:B:1131:ARG:NH1	1:B:1178:ALA:O	2.46	0.49
1:B:2299:VAL:HG11	1:B:2356:LEU:HB3	1.93	0.49
1:C:1676:LEU:HD22	1:C:2167:ILE:HD12	1.93	0.49
1:C:2648:TYR:O	1:C:2652:TRP:HB3	2.13	0.49
1:C:3244:PRO:HA	1:C:3248:ARG:HH21	1.76	0.49
1:D:648:ILE:HG23	1:D:814:ALA:HB3	1.94	0.49
1:D:818:ARG:HH12	1:D:1026:LEU:HA	1.76	0.49
1:D:4204:GLN:HG2	1:D:4245:MET:HG2	1.94	0.49
1:A:2768:PHE:HD1	1:A:2857:PRO:HG2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4090:LYS:HG2	1:A:4123:ILE:HD11	1.95	0.49
1:A:4828:SER:O	1:A:4832:HIS:HB2	2.12	0.49
1:B:1066:GLN:NE2	1:B:1461:ASP:OD1	2.39	0.49
1:B:3391:GLU:HA	1:B:3394:VAL:HG22	1.95	0.49
1:B:3868:ARG:HH11	1:B:3870:ASN:HB3	1.76	0.49
1:B:4828:SER:O	1:B:4832:HIS:HB2	2.13	0.49
1:D:320:LYS:NZ	1:D:383:HIS:O	2.44	0.49
1:D:1256:GLU:HB3	1:D:1275:ARG:HE	1.77	0.49
1:D:2754:PHE:HE2	1:D:2813:LEU:HD11	1.76	0.49
1:A:2745:VAL:HG13	1:A:2814:LYS:HD2	1.94	0.49
1:A:3202:PRO:O	1:A:3214:ASN:ND2	2.45	0.49
1:B:1256:GLU:HB3	1:B:1275:ARG:HE	1.77	0.49
1:B:1751:GLY:HA3	1:B:1758:ARG:HE	1.77	0.49
1:B:4090:LYS:HG2	1:B:4123:ILE:HD11	1.95	0.49
1:C:262:LEU:HD13	1:C:274:LEU:HD11	1.94	0.49
1:C:1099:GLU:OE2	1:C:1125:ASN:ND2	2.40	0.49
1:C:1679:ASN:HA	1:C:1682:ALA:HB3	1.94	0.49
1:D:2299:VAL:HG11	1:D:2356:LEU:HB3	1.93	0.49
1:D:2742:THR:O	1:D:2814:LYS:NZ	2.46	0.49
1:D:4999:ASP:OD1	1:D:4999:ASP:N	2.46	0.49
1:A:939:VAL:HB	1:A:1051:TYR:HB3	1.95	0.49
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.46	0.49
1:A:2867:LEU:HD12	1:A:2928:LYS:HZ3	1.78	0.49
1:A:3180:ASN:HB2	1:A:3183:VAL:HG23	1.95	0.49
1:A:3391:GLU:HA	1:A:3394:VAL:HG22	1.95	0.49
1:A:4928:LEU:HD23	1:A:4931:ILE:HD12	1.95	0.49
1:A:4938:ASP:CG	1:D:4944:ARG:HH21	2.20	0.49
1:B:3180:ASN:HB2	1:B:3183:VAL:HG23	1.95	0.49
1:C:936:GLY:HA3	1:C:1056:PRO:HB3	1.95	0.49
1:C:2998:PHE:HA	1:C:3002:LEU:HD13	1.95	0.49
1:C:3575:LEU:HD23	1:D:1219:LEU:HD22	1.95	0.49
1:C:4828:SER:O	1:C:4832:HIS:HB2	2.13	0.49
1:D:1679:ASN:HA	1:D:1682:ALA:HB3	1.93	0.49
1:D:1751:GLY:HA3	1:D:1758:ARG:HE	1.77	0.49
2:F:21:THR:HA	2:F:49:ARG:HA	1.94	0.49
2:H:21:THR:HA	2:H:49:ARG:HA	1.94	0.49
1:A:1423:ASP:N	1:A:1571:ASN:OD1	2.45	0.49
1:A:3051:ARG:NH2	1:A:3102:ASP:OD1	2.46	0.49
1:B:3771:HIS:O	1:B:3815:LYS:NZ	2.44	0.49
1:C:2788:HIS:HB3	1:C:2791:LEU:HD23	1.93	0.49
1:C:3051:ARG:NH2	1:C:3102:ASP:OD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3523:ASN:O	1:C:3582:ARG:NH2	2.46	0.49
1:D:717:ASP:OD1	1:D:720:HIS:N	2.41	0.49
1:D:3227:ARG:NH1	1:D:3234:ASN:OD1	2.37	0.49
2:G:21:THR:HA	2:G:49:ARG:HA	1.94	0.49
1:A:870:ILE:HG13	1:A:874:LEU:HD23	1.95	0.49
1:A:2093:SER:OG	1:A:2096:GLU:OE1	2.31	0.49
1:B:2768:PHE:HD1	1:B:2857:PRO:HG2	1.78	0.49
1:B:2867:LEU:HD12	1:B:2928:LYS:HZ3	1.77	0.49
1:C:2093:SER:OG	1:C:2096:GLU:OE1	2.31	0.49
1:D:939:VAL:HB	1:D:1051:TYR:HB3	1.95	0.49
1:D:2310:CYS:HB3	1:D:2313:LEU:HB2	1.94	0.49
1:A:262:LEU:HD13	1:A:274:LEU:HD11	1.95	0.49
1:B:5012:LYS:HD3	1:B:5012:LYS:HA	1.64	0.49
1:C:870:ILE:HG13	1:C:874:LEU:HD23	1.95	0.49
1:D:1131:ARG:NH1	1:D:1178:ALA:O	2.46	0.49
1:D:3391:GLU:HA	1:D:3394:VAL:HG22	1.95	0.49
1:A:648:ILE:HG23	1:A:814:ALA:HB3	1.94	0.48
1:A:758:ARG:HA	1:A:763:PRO:HA	1.94	0.48
1:A:2365:GLY:O	1:A:2369[B]:ARG:NE	2.39	0.48
1:A:2806:ARG:HD2	1:A:2810:LYS:HZ3	1.78	0.48
1:A:3902:TYR:O	1:A:3906:GLN:NE2	2.45	0.48
1:B:717:ASP:OD1	1:B:720:HIS:N	2.41	0.48
1:B:870:ILE:HG13	1:B:874:LEU:HD23	1.95	0.48
1:C:4944:ARG:NH2	1:D:4938:ASP:OD1	2.43	0.48
1:D:2093:SER:OG	1:D:2096:GLU:OE1	2.31	0.48
1:D:2386:ILE:HG23	1:D:2392:ARG:HG3	1.95	0.48
1:B:939:VAL:HB	1:B:1051:TYR:HB3	1.95	0.48
1:C:2754:PHE:HE2	1:C:2813:LEU:HD11	1.76	0.48
1:C:3391:GLU:HA	1:C:3394:VAL:HG22	1.95	0.48
1:C:3442:PHE:HE1	1:C:3511:VAL:HG12	1.78	0.48
1:D:4821:LYS:HE2	1:D:4821:LYS:HB2	1.54	0.48
1:D:4828:SER:O	1:D:4832:HIS:HB2	2.12	0.48
1:A:1256:GLU:HB3	1:A:1275:ARG:HE	1.77	0.48
1:A:2874:MET:HE3	1:A:2937:VAL:HG12	1.96	0.48
1:A:4227:GLU:H	1:A:4227:GLU:HG3	1.43	0.48
1:B:758:ARG:HA	1:B:763:PRO:HA	1.94	0.48
1:B:2093:SER:OG	1:B:2096:GLU:OE1	2.31	0.48
1:B:2736:ASP:OD1	1:B:2736:ASP:N	2.47	0.48
1:C:1256:GLU:HB3	1:C:1275:ARG:HE	1.77	0.48
1:C:1423:ASP:N	1:C:1571:ASN:OD1	2.45	0.48
1:C:2512:ILE:HD13	1:C:2561:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2806:ARG:HD2	1:D:2810:LYS:HZ3	1.77	0.48
1:A:1751:GLY:HA3	1:A:1758:ARG:HE	1.77	0.48
1:A:3781:GLN:NE2	1:A:3819:TYR:OH	2.40	0.48
1:B:545:ASP:N	1:B:545:ASP:OD1	2.44	0.48
1:B:648:ILE:HG23	1:B:814:ALA:HB3	1.94	0.48
1:C:1131:ARG:NH1	1:C:1178:ALA:O	2.46	0.48
1:C:2742:THR:O	1:C:2814:LYS:NZ	2.46	0.48
1:D:3180:ASN:HB2	1:D:3183:VAL:HG23	1.95	0.48
1:D:4928:LEU:HD23	1:D:4931:ILE:HD12	1.95	0.48
1:A:936:GLY:HA3	1:A:1056:PRO:HB3	1.95	0.48
1:B:1099:GLU:OE2	1:B:1125:ASN:ND2	2.40	0.48
1:B:2512:ILE:HD13	1:B:2561:LEU:HD11	1.95	0.48
1:B:4928:LEU:HD23	1:B:4931:ILE:HD12	1.95	0.48
1:B:4999:ASP:OD1	1:B:4999:ASP:N	2.46	0.48
1:D:545:ASP:N	1:D:545:ASP:OD1	2.44	0.48
1:D:3442:PHE:HE1	1:D:3511:VAL:HG12	1.78	0.48
1:D:4090:LYS:HG2	1:D:4123:ILE:HD11	1.95	0.48
1:A:356:TRP:N	1:A:379:HIS:O	2.38	0.48
1:A:359:TYR:HA	1:A:376:ALA:HA	1.96	0.48
1:A:3442:PHE:HE1	1:A:3511:VAL:HG12	1.78	0.48
1:A:3523:ASN:O	1:A:3582:ARG:NH2	2.46	0.48
1:A:3788:GLY:HA2	1:A:3835:LEU:HD12	1.96	0.48
1:B:2648:TYR:O	1:B:2652:TRP:HB3	2.13	0.48
1:C:886:ARG:HE	1:C:904:HIS:HB2	1.79	0.48
1:C:2377:LEU:HA	1:C:2380:ILE:HG22	1.96	0.48
1:C:3794:VAL:HG11	1:C:3835:LEU:HD21	1.96	0.48
1:D:870:ILE:HG13	1:D:874:LEU:HD23	1.95	0.48
1:D:886:ARG:HE	1:D:904:HIS:HB2	1.79	0.48
1:D:936:GLY:HA3	1:D:1056:PRO:HB3	1.95	0.48
1:D:2768:PHE:HD1	1:D:2857:PRO:HG2	1.78	0.48
1:A:1253:PRO:O	1:A:1275:ARG:NH1	2.46	0.48
1:A:4165:GLU:HA	1:A:4168:GLU:HG2	1.95	0.48
1:B:359:TYR:HA	1:B:376:ALA:HA	1.96	0.48
1:B:936:GLY:HA3	1:B:1056:PRO:HB3	1.95	0.48
1:B:1698:LEU:HD21	1:B:1715:LEU:HD13	1.95	0.48
1:B:2165:LEU:HD12	1:B:2178:MET:HB3	1.95	0.48
1:B:3051:ARG:NH2	1:B:3102:ASP:OD1	2.46	0.48
1:B:3363:GLY:HA2	1:B:3366:ARG:HG2	1.96	0.48
1:B:4835:LYS:HB3	1:B:4835:LYS:HE2	1.56	0.48
1:C:3180:ASN:HB2	1:C:3183:VAL:HG23	1.95	0.48
1:C:4165:GLU:HA	1:C:4168:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4928:LEU:HD23	1:C:4931:ILE:HD12	1.95	0.48
1:D:2165:LEU:HD12	1:D:2178:MET:HB3	1.95	0.48
1:B:3575:LEU:HD23	1:C:1219:LEU:HD22	1.95	0.48
1:B:3794:VAL:HG11	1:B:3835:LEU:HD21	1.96	0.48
1:C:875:ALA:O	1:C:879:HIS:ND1	2.47	0.48
1:C:2165:LEU:HD12	1:C:2178:MET:HB3	1.95	0.48
1:C:4090:LYS:HG2	1:C:4123:ILE:HD11	1.95	0.48
1:D:748:LEU:HD13	1:D:755:ILE:HG12	1.96	0.48
1:A:886:ARG:HE	1:A:904:HIS:HB2	1.79	0.48
1:A:2998:PHE:HA	1:A:3002:LEU:HD13	1.95	0.48
1:B:706:GLY:N	1:B:709:ASP:OD2	2.39	0.48
1:B:875:ALA:O	1:B:879:HIS:ND1	2.47	0.48
1:B:1253:PRO:O	1:B:1275:ARG:NH1	2.46	0.48
1:C:939:VAL:HB	1:C:1051:TYR:HB3	1.95	0.48
1:C:1253:PRO:O	1:C:1275:ARG:NH1	2.46	0.48
1:C:2768:PHE:HD1	1:C:2857:PRO:HG2	1.78	0.48
1:D:262:LEU:HD13	1:D:274:LEU:HD11	1.94	0.48
1:D:1448:VAL:HG22	1:D:1554:VAL:HG23	1.96	0.48
1:D:2512:ILE:HD13	1:D:2561:LEU:HD11	1.95	0.48
1:A:110:ARG:NH2	1:A:117:TYR:OH	2.47	0.48
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.96	0.48
1:A:2310:CYS:HB3	1:A:2313:LEU:HB2	1.94	0.48
1:A:2386:ILE:HG23	1:A:2392:ARG:HG3	1.95	0.48
1:A:2863:SER:HA	1:A:2928:LYS:HG3	1.96	0.48
1:B:262:LEU:HD13	1:B:274:LEU:HD11	1.94	0.48
1:B:2742:THR:O	1:B:2814:LYS:NZ	2.46	0.48
1:B:3537:LYS:NZ	1:B:3600:SER:O	2.44	0.48
1:C:110:ARG:NH2	1:C:117:TYR:OH	2.47	0.48
1:C:248:GLU:HG2	1:C:252:VAL:HG21	1.96	0.48
1:C:359:TYR:HA	1:C:376:ALA:HA	1.96	0.48
1:C:1100:MET:HB2	1:C:1143:TRP:HZ2	1.79	0.48
1:C:2736:ASP:OD1	1:C:2736:ASP:N	2.47	0.48
1:C:2874:MET:HE3	1:C:2937:VAL:HG12	1.95	0.48
1:C:3723:MET:HE1	1:C:3793:MET:HA	1.96	0.48
1:A:877:ASN:HA	1:A:970:LEU:H	1.79	0.47
1:B:886:ARG:HE	1:B:904:HIS:HB2	1.79	0.47
1:B:2874:MET:HE3	1:B:2937:VAL:HG12	1.95	0.47
1:C:748:LEU:HD13	1:C:755:ILE:HG12	1.96	0.47
1:C:2365:GLY:O	1:C:2369[B]:ARG:NE	2.39	0.47
1:C:2870[A]:GLU:OE1	1:C:2939:ARG:NH2	2.47	0.47
1:C:3902:TYR:O	1:C:3906:GLN:NE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:875:ALA:O	1:D:879:HIS:ND1	2.47	0.47
1:D:1100:MET:HB2	1:D:1143:TRP:HZ2	1.79	0.47
1:D:2863:SER:HA	1:D:2928:LYS:HG3	1.96	0.47
1:D:2998:PHE:HA	1:D:3002:LEU:HD13	1.95	0.47
1:D:3523:ASN:O	1:D:3582:ARG:NH2	2.46	0.47
1:A:1292:SER:OG	1:A:1596:GLU:N	2.44	0.47
1:A:2165:LEU:HD12	1:A:2178:MET:HB3	1.95	0.47
1:A:3159:ASP:OD1	1:A:3159:ASP:N	2.46	0.47
1:A:3227:ARG:NH1	1:A:3234:ASN:OD1	2.37	0.47
1:A:3363:GLY:HA2	1:A:3366:ARG:HG2	1.96	0.47
1:B:2377:LEU:HA	1:B:2380:ILE:HG22	1.96	0.47
1:B:2998:PHE:HA	1:B:3002:LEU:HD13	1.95	0.47
1:C:877:ASN:HA	1:C:970:LEU:H	1.79	0.47
1:D:110:ARG:NH2	1:D:117:TYR:OH	2.47	0.47
1:D:359:TYR:HA	1:D:376:ALA:HA	1.96	0.47
1:D:1253:PRO:O	1:D:1275:ARG:NH1	2.46	0.47
1:D:2377:LEU:HA	1:D:2380:ILE:HG22	1.96	0.47
1:D:3233:PRO:HG2	1:D:3239:MET:HA	1.96	0.47
1:D:4835:LYS:HB3	1:D:4835:LYS:HE2	1.56	0.47
1:A:875:ALA:O	1:A:879:HIS:ND1	2.47	0.47
1:A:2490:MET:HE2	1:A:2545:GLU:HG2	1.96	0.47
1:A:2736:ASP:OD1	1:A:2736:ASP:N	2.47	0.47
1:B:3442:PHE:HE1	1:B:3511:VAL:HG12	1.78	0.47
1:C:1653:LEU:HD23	1:C:1660:GLN:HA	1.96	0.47
1:C:2477:PRO:HB3	1:C:2487:GLN:HG2	1.97	0.47
1:C:3875:MET:HE3	1:C:3875:MET:HB3	1.81	0.47
1:D:15:ARG:HG3	1:D:100:THR:HA	1.96	0.47
1:D:1712:TYR:OH	1:D:1814:MET:SD	2.72	0.47
1:D:2874:MET:HE3	1:D:2937:VAL:HG12	1.96	0.47
1:A:2742:THR:O	1:A:2814:LYS:NZ	2.46	0.47
1:B:14:LEU:HB2	1:B:163:VAL:HG13	1.97	0.47
1:B:15:ARG:HG3	1:B:100:THR:HA	1.96	0.47
1:B:3523:ASN:O	1:B:3582:ARG:NH2	2.46	0.47
1:B:3723:MET:HE1	1:B:3793:MET:HA	1.96	0.47
1:B:4049:VAL:HG11	1:B:4159:ARG:HH11	1.80	0.47
1:C:545:ASP:OD1	1:C:545:ASP:N	2.44	0.47
1:D:2736:ASP:N	1:D:2736:ASP:OD1	2.47	0.47
1:D:4165:GLU:HA	1:D:4168:GLU:HG2	1.95	0.47
1:A:868:GLU:HA	1:A:871:ARG:HB2	1.97	0.47
1:A:2748:PRO:HG2	1:A:2817:ILE:HD13	1.97	0.47
1:B:3233:PRO:HG2	1:B:3239:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:TRP:N	1:C:379:HIS:O	2.38	0.47
1:D:868:GLU:HA	1:D:871:ARG:HB2	1.97	0.47
1:D:1469:VAL:HG13	1:D:1492:CYS:HB3	1.96	0.47
1:D:2875:ALA:HB2	1:D:2927:LEU:HD22	1.97	0.47
1:A:1698:LEU:HD21	1:A:1715:LEU:HD13	1.95	0.47
1:C:15:ARG:HG3	1:C:100:THR:HA	1.96	0.47
1:D:37:LEU:HD21	1:D:191:VAL:HG21	1.97	0.47
1:D:2870[A]:GLU:OE1	1:D:2939:ARG:NH2	2.47	0.47
1:D:3567:PRO:HA	1:D:3570:ARG:HD3	1.96	0.47
1:D:3902:TYR:O	1:D:3906:GLN:NE2	2.45	0.47
1:A:15:ARG:HG3	1:A:100:THR:HA	1.96	0.47
1:A:1469:VAL:HG13	1:A:1492:CYS:HB3	1.96	0.47
1:A:1653:LEU:HD23	1:A:1660:GLN:HA	1.96	0.47
1:A:2870[A]:GLU:OE1	1:A:2939:ARG:NH2	2.47	0.47
1:A:3233:PRO:HG2	1:A:3239:MET:HA	1.96	0.47
1:A:3537:LYS:NZ	1:A:3600:SER:O	2.44	0.47
1:A:4895:GLY:O	1:D:4892:ARG:NH1	2.45	0.47
1:A:4999:ASP:N	1:A:4999:ASP:OD1	2.46	0.47
1:B:35:LEU:HD13	1:B:49:LEU:HD13	1.97	0.47
1:B:877:ASN:HA	1:B:970:LEU:H	1.79	0.47
1:B:1100:MET:HB2	1:B:1143:TRP:HZ2	1.79	0.47
1:B:1469:VAL:HG13	1:B:1492:CYS:HB3	1.96	0.47
1:B:2386:ILE:HG23	1:B:2392:ARG:HG3	1.95	0.47
1:B:2748:PRO:HG2	1:B:2817:ILE:HD13	1.97	0.47
1:B:3567:PRO:HA	1:B:3570:ARG:HD3	1.96	0.47
1:B:4944:ARG:NH2	1:C:4938:ASP:OD1	2.43	0.47
1:C:37:LEU:HD21	1:C:191:VAL:HG21	1.97	0.47
1:C:1698:LEU:HD21	1:C:1715:LEU:HD13	1.95	0.47
1:C:2875:ALA:HB2	1:C:2927:LEU:HD22	1.97	0.47
1:C:3363:GLY:HA2	1:C:3366:ARG:HG2	1.96	0.47
1:C:4227:GLU:H	1:C:4227:GLU:HG3	1.43	0.47
1:D:35:LEU:HD13	1:D:49:LEU:HD13	1.97	0.47
1:D:877:ASN:HA	1:D:970:LEU:H	1.79	0.47
1:D:1698:LEU:HD21	1:D:1715:LEU:HD13	1.95	0.47
1:D:1753:LYS:HB3	1:D:1758:ARG:HD2	1.96	0.47
1:D:2477:PRO:HB3	1:D:2487:GLN:HG2	1.97	0.47
1:D:2490:MET:HE2	1:D:2545:GLU:HG2	1.96	0.47
1:D:2692:ASP:HB3	1:D:2695:LEU:HB3	1.96	0.47
1:D:2748:PRO:HG2	1:D:2817:ILE:HD13	1.97	0.47
1:D:2882:TYR:O	1:D:2885:THR:OG1	2.28	0.47
1:D:3875:MET:HE3	1:D:3875:MET:HB3	1.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD21	1:A:191:VAL:HG21	1.97	0.47
1:A:1100:MET:HB2	1:A:1143:TRP:HZ2	1.79	0.47
1:A:2512:ILE:HD13	1:A:2561:LEU:HD11	1.95	0.47
1:A:2692:ASP:HB3	1:A:2695:LEU:HB3	1.96	0.47
1:B:356:TRP:N	1:B:379:HIS:O	2.38	0.47
1:B:1292:SER:OG	1:B:1596:GLU:N	2.44	0.47
1:B:1653:LEU:HD23	1:B:1660:GLN:HA	1.96	0.47
1:B:1712:TYR:OH	1:B:1814:MET:SD	2.72	0.47
1:C:35:LEU:HD13	1:C:49:LEU:HD13	1.97	0.47
1:C:1469:VAL:HG13	1:C:1492:CYS:HB3	1.96	0.47
1:C:2863:SER:HA	1:C:2928:LYS:HG3	1.96	0.47
1:D:1292:SER:OG	1:D:1596:GLU:N	2.44	0.47
1:D:2614:ILE:O	1:D:2650:ARG:NH2	2.43	0.47
1:A:248:GLU:HG2	1:A:252:VAL:HG21	1.96	0.47
1:B:248:GLU:HG2	1:B:252:VAL:HG21	1.96	0.47
1:B:2870[A]:GLU:OE1	1:B:2939:ARG:NH2	2.47	0.47
1:B:3788:GLY:HA2	1:B:3835:LEU:HD12	1.96	0.47
1:C:3316:LEU:HD11	1:C:3346:VAL:HA	1.97	0.47
1:C:4694:ASP:HA	1:C:4700:GLN:HE21	1.80	0.47
1:D:706:GLY:N	1:D:709:ASP:OD2	2.39	0.47
1:D:3051:ARG:NH2	1:D:3102:ASP:OD1	2.46	0.47
2:F:23:VAL:HG22	2:F:47:LYS:HG2	1.97	0.47
1:A:14:LEU:HB2	1:A:163:VAL:HG13	1.97	0.47
1:B:748:LEU:HD13	1:B:755:ILE:HG12	1.96	0.47
1:B:1753:LYS:HB3	1:B:1758:ARG:HD2	1.96	0.47
1:B:2490:MET:HE2	1:B:2545:GLU:HG2	1.96	0.47
1:C:3567:PRO:HA	1:C:3570:ARG:HD3	1.96	0.47
1:C:4993:MET:HE2	1:C:4993:MET:HB3	1.75	0.47
1:C:4999:ASP:N	1:C:4999:ASP:OD1	2.46	0.47
1:D:3333:THR:O	1:D:3337:ARG:NH1	2.48	0.47
1:D:3788:GLY:HA2	1:D:3835:LEU:HD12	1.96	0.47
1:D:4694:ASP:HA	1:D:4700:GLN:HE21	1.80	0.47
2:F:27:THR:HB	2:F:100:ASP:HB3	1.97	0.47
2:G:27:THR:HB	2:G:100:ASP:HB3	1.97	0.47
1:A:893:TYR:HB3	1:A:960:MET:HE2	1.98	0.46
1:A:2377:LEU:HA	1:A:2380:ILE:HG22	1.96	0.46
1:A:3536:ALA:HA	1:A:3539:ARG:HG2	1.97	0.46
1:A:3567:PRO:HA	1:A:3570:ARG:HD3	1.97	0.46
1:A:3794:VAL:HG11	1:A:3835:LEU:HD21	1.96	0.46
1:B:2863:SER:HA	1:B:2928:LYS:HG3	1.96	0.46
1:B:3333:THR:O	1:B:3337:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1292:SER:OG	1:C:1596:GLU:N	2.44	0.46
1:D:248:GLU:HG2	1:D:252:VAL:HG21	1.96	0.46
1:D:1653:LEU:HD23	1:D:1660:GLN:HA	1.96	0.46
1:D:3794:VAL:HG11	1:D:3835:LEU:HD21	1.96	0.46
2:E:23:VAL:HG22	2:E:47:LYS:HG2	1.97	0.46
2:F:8:SER:HB2	2:F:71:ARG:HB2	1.97	0.46
2:G:23:VAL:HG22	2:G:47:LYS:HG2	1.97	0.46
1:A:1712:TYR:OH	1:A:1814:MET:SD	2.72	0.46
1:A:1753:LYS:HB3	1:A:1758:ARG:HD2	1.97	0.46
1:B:37:LEU:HD21	1:B:191:VAL:HG21	1.97	0.46
1:C:14:LEU:HB2	1:C:163:VAL:HG13	1.97	0.46
1:C:3788:GLY:HA2	1:C:3835:LEU:HD12	1.96	0.46
1:D:294:THR:HG23	1:D:297:GLN:H	1.81	0.46
1:D:3202:PRO:O	1:D:3214:ASN:ND2	2.45	0.46
2:E:8:SER:HB2	2:E:71:ARG:HB2	1.97	0.46
2:H:23:VAL:HG22	2:H:47:LYS:HG2	1.97	0.46
1:A:717:ASP:OD1	1:A:720:HIS:N	2.41	0.46
1:A:4835:LYS:HB3	1:A:4835:LYS:HE2	1.56	0.46
1:B:110:ARG:NH2	1:B:117:TYR:OH	2.47	0.46
1:C:1285:GLU:HB2	1:C:1462:MET:HE1	1.98	0.46
1:C:1947:CYS:SG	1:C:2127:GLN:NE2	2.79	0.46
1:C:2386:ILE:HG23	1:C:2392:ARG:HG3	1.95	0.46
1:C:2623:LEU:HD12	1:C:2626:LEU:HD12	1.97	0.46
1:A:294:THR:HG23	1:A:297:GLN:H	1.81	0.46
1:A:3316:LEU:HD11	1:A:3346:VAL:HA	1.97	0.46
1:A:3333:THR:O	1:A:3337:ARG:NH1	2.48	0.46
1:A:3723:MET:HE1	1:A:3793:MET:HA	1.96	0.46
1:B:3316:LEU:HD11	1:B:3346:VAL:HA	1.97	0.46
1:C:1753:LYS:HB3	1:C:1758:ARG:HD2	1.96	0.46
1:C:4049:VAL:HG11	1:C:4159:ARG:HH11	1.80	0.46
1:D:492:ASP:OD1	1:D:546:TRP:NE1	2.42	0.46
1:D:3723:MET:HE1	1:D:3793:MET:HA	1.96	0.46
1:A:748:LEU:HD13	1:A:755:ILE:HG12	1.96	0.46
1:A:2882:TYR:O	1:A:2885:THR:OG1	2.28	0.46
1:B:277:GLY:N	1:B:316:PHE:O	2.48	0.46
1:B:884:LEU:HB2	1:B:969:PRO:HD3	1.98	0.46
1:B:893:TYR:HB3	1:B:960:MET:HE2	1.98	0.46
1:B:1285:GLU:HB2	1:B:1462:MET:HE1	1.98	0.46
1:B:3902:TYR:O	1:B:3906:GLN:NE2	2.45	0.46
1:C:868:GLU:HA	1:C:871:ARG:HB2	1.97	0.46
1:C:1448:VAL:HG22	1:C:1554:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2748:PRO:HG2	1:C:2817:ILE:HD13	1.97	0.46
1:C:3233:PRO:HG2	1:C:3239:MET:HA	1.96	0.46
1:D:815:VAL:O	1:D:1007:TYR:OH	2.34	0.46
1:D:1243:PRO:O	1:D:1458:HIS:ND1	2.34	0.46
1:D:3363:GLY:HA2	1:D:3366:ARG:HG2	1.96	0.46
1:A:161:GLU:OE1	1:D:3984:ARG:NH1	2.49	0.46
1:A:4049:VAL:HG11	1:A:4159:ARG:HH11	1.80	0.46
1:A:4694:ASP:HA	1:A:4700:GLN:HE21	1.80	0.46
1:B:232:THR:HG22	1:B:258:SER:HB3	1.98	0.46
1:B:1448:VAL:HG22	1:B:1554:VAL:HG23	1.96	0.46
1:B:2477:PRO:HB3	1:B:2487:GLN:HG2	1.97	0.46
1:B:2623:LEU:HD12	1:B:2626:LEU:HD12	1.97	0.46
1:B:4165:GLU:HA	1:B:4168:GLU:HG2	1.95	0.46
1:B:4865:LYS:HA	1:B:4865:LYS:HD2	1.49	0.46
1:C:5012:LYS:HD3	1:C:5012:LYS:HA	1.64	0.46
1:D:14:LEU:HB2	1:D:163:VAL:HG13	1.97	0.46
1:D:2623:LEU:HD12	1:D:2626:LEU:HD12	1.97	0.46
2:H:8:SER:HB2	2:H:71:ARG:HB2	1.97	0.46
1:B:275:ARG:NH1	1:B:278:GLN:OE1	2.49	0.46
1:B:492:ASP:OD1	1:B:546:TRP:NE1	2.42	0.46
1:B:868:GLU:HA	1:B:871:ARG:HB2	1.97	0.46
1:B:2410:PRO:HB3	1:B:2415:ARG:HB3	1.97	0.46
1:B:2692:ASP:HB3	1:B:2695:LEU:HB3	1.96	0.46
1:C:4989:MET:HE3	1:C:4989:MET:HB3	1.68	0.46
1:D:3275:PRO:HA	1:D:3278:CYS:HB2	1.98	0.46
1:D:4049:VAL:HG11	1:D:4159:ARG:HH11	1.80	0.46
1:A:1476:MET:HE3	1:A:1476:MET:HB2	1.81	0.46
1:A:2109:ASP:N	1:A:2109:ASP:OD1	2.49	0.46
1:A:2627:VAL:HG22	1:A:2678:LEU:HG	1.98	0.46
1:A:3771:HIS:O	1:A:3815:LYS:NZ	2.44	0.46
1:B:620:LEU:O	1:B:624:ASN:ND2	2.49	0.46
1:B:2742:THR:HB	1:B:2814:LYS:HG2	1.98	0.46
1:B:2875:ALA:HB2	1:B:2927:LEU:HD22	1.97	0.46
1:B:3536:ALA:HA	1:B:3539:ARG:HG2	1.97	0.46
1:B:4694:ASP:HA	1:B:4700:GLN:HE21	1.80	0.46
1:C:294:THR:HG23	1:C:297:GLN:H	1.81	0.46
1:C:2490:MET:HE2	1:C:2545:GLU:HG2	1.96	0.46
1:C:3175:LEU:O	1:C:3178:THR:OG1	2.33	0.46
1:C:3202:PRO:O	1:C:3214:ASN:ND2	2.45	0.46
1:C:3536:ALA:HA	1:C:3539:ARG:HG2	1.97	0.46
1:D:277:GLY:N	1:D:316:PHE:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1084:GLN:NE2	1:D:1186:ASP:O	2.43	0.46
2:H:27:THR:HB	2:H:100:ASP:HB3	1.97	0.46
1:A:35:LEU:HD13	1:A:49:LEU:HD13	1.97	0.46
1:A:1473:THR:HA	1:A:1487:LEU:O	2.16	0.46
1:A:2470:ILE:HG22	1:A:2525:GLY:HA3	1.98	0.46
1:A:2477:PRO:HB3	1:A:2487:GLN:HG2	1.97	0.46
1:B:1423:ASP:N	1:B:1571:ASN:OD1	2.45	0.46
1:C:732:SER:HB2	1:C:735:GLN:HB3	1.98	0.46
1:C:1712:TYR:OH	1:C:1814:MET:SD	2.72	0.46
1:C:2208:MET:HE2	1:C:2208:MET:HB2	1.88	0.46
1:C:2410:PRO:HB3	1:C:2415:ARG:HB3	1.97	0.46
1:C:2500:ALA:HB2	1:C:2553:TYR:HD1	1.81	0.46
1:C:3275:PRO:HA	1:C:3278:CYS:HB2	1.98	0.46
1:D:732:SER:HB2	1:D:735:GLN:HB3	1.98	0.46
1:D:1285:GLU:HB2	1:D:1462:MET:HE1	1.98	0.46
1:D:2410:PRO:HB3	1:D:2415:ARG:HB3	1.97	0.46
1:D:3316:LEU:HD11	1:D:3346:VAL:HA	1.97	0.46
1:D:4631:PHE:HE2	1:D:4633:GLU:HG2	1.81	0.46
1:A:531:ARG:NH2	1:A:562:GLU:OE2	2.37	0.46
1:A:620:LEU:O	1:A:624:ASN:ND2	2.49	0.46
1:A:815:VAL:O	1:A:1007:TYR:OH	2.34	0.46
1:B:3159:ASP:OD1	1:B:3159:ASP:N	2.46	0.46
1:B:3275:PRO:HA	1:B:3278:CYS:HB2	1.98	0.46
1:C:2692:ASP:HB3	1:C:2695:LEU:HB3	1.96	0.46
1:C:3333:THR:O	1:C:3337:ARG:NH1	2.48	0.46
1:D:2522:LEU:HB3	1:D:2582:MET:HE1	1.98	0.46
2:G:8:SER:HB2	2:G:71:ARG:HB2	1.97	0.46
1:A:3275:PRO:HA	1:A:3278:CYS:HB2	1.98	0.45
1:B:2519:LEU:HD12	1:B:2578:MET:HE1	1.99	0.45
1:B:4989:MET:HE3	1:B:4989:MET:HB3	1.68	0.45
1:C:277:GLY:N	1:C:316:PHE:O	2.48	0.45
1:D:275:ARG:NH1	1:D:278:GLN:OE1	2.49	0.45
1:D:665:GLU:HG2	1:D:745:SER:HA	1.98	0.45
1:D:893:TYR:HB3	1:D:960:MET:HE2	1.98	0.45
1:D:2109:ASP:OD1	1:D:2109:ASP:N	2.49	0.45
1:A:232:THR:HG22	1:A:258:SER:HB3	1.98	0.45
1:A:277:GLY:N	1:A:316:PHE:O	2.48	0.45
1:A:1285:GLU:HB2	1:A:1462:MET:HE1	1.98	0.45
1:B:2806:ARG:HD2	1:B:2810:LYS:HZ3	1.81	0.45
1:C:275:ARG:NH1	1:C:278:GLN:OE1	2.49	0.45
1:C:2519:LEU:HD12	1:C:2578:MET:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2522:LEU:HB3	1:C:2582:MET:HE1	1.98	0.45
1:D:1473:THR:HA	1:D:1487:LEU:O	2.16	0.45
1:D:2500:ALA:HB2	1:D:2553:TYR:HD1	1.81	0.45
1:D:3536:ALA:HA	1:D:3539:ARG:HG2	1.97	0.45
1:A:2500:ALA:HB2	1:A:2553:TYR:HD1	1.81	0.45
1:B:2559:LEU:HA	1:B:2562:ILE:HD12	1.99	0.45
1:C:815:VAL:O	1:C:1007:TYR:OH	2.34	0.45
1:C:893:TYR:HB3	1:C:960:MET:HE2	1.98	0.45
1:C:2109:ASP:N	1:C:2109:ASP:OD1	2.49	0.45
1:A:884:LEU:HB2	1:A:969:PRO:HD3	1.98	0.45
1:A:2522:LEU:HB3	1:A:2582:MET:HE1	1.98	0.45
1:A:2623:LEU:HD12	1:A:2626:LEU:HD12	1.97	0.45
1:B:1473:THR:HA	1:B:1487:LEU:O	2.16	0.45
1:C:620:LEU:O	1:C:624:ASN:ND2	2.49	0.45
1:C:4631:PHE:HE2	1:C:4633:GLU:HG2	1.81	0.45
1:D:2627:VAL:HG22	1:D:2678:LEU:HG	1.98	0.45
1:A:665:GLU:HG2	1:A:745:SER:HA	1.98	0.45
1:A:2875:ALA:HB2	1:A:2927:LEU:HD22	1.97	0.45
1:A:3175:LEU:O	1:A:3178:THR:OG1	2.33	0.45
1:A:4576:ILE:HG23	1:A:4639:MET:HG2	1.99	0.45
1:B:815:VAL:O	1:B:1007:TYR:OH	2.34	0.45
1:B:4631:PHE:HE2	1:B:4633:GLU:HG2	1.81	0.45
1:B:4821:LYS:HE2	1:B:4821:LYS:HB2	1.54	0.45
1:C:2559:LEU:HA	1:C:2562:ILE:HD12	1.99	0.45
1:D:620:LEU:O	1:D:624:ASN:ND2	2.49	0.45
1:D:5030:LYS:HE2	1:D:5030:LYS:HB2	1.76	0.45
1:A:232:THR:HG21	1:A:252:VAL:HG12	1.99	0.45
1:A:699:GLY:N	1:A:1647:CYS:O	2.50	0.45
1:A:2742:THR:HB	1:A:2814:LYS:HG2	1.98	0.45
1:A:4049:VAL:HG21	1:A:4159:ARG:HG2	1.99	0.45
1:B:2109:ASP:OD1	1:B:2109:ASP:N	2.49	0.45
1:B:2580:ASP:HB2	1:B:2618:MET:HE1	1.99	0.45
1:C:699:GLY:N	1:C:1647:CYS:O	2.50	0.45
1:C:876:GLU:HG2	1:C:910:PHE:CE2	2.52	0.45
1:C:2667:THR:HG21	1:C:2672:LEU:HD21	1.99	0.45
1:C:4581:LYS:HE3	1:C:4581:LYS:HB3	1.82	0.45
1:D:771:PHE:HB3	1:D:1472:VAL:HG23	1.99	0.45
1:D:884:LEU:HB2	1:D:969:PRO:HD3	1.98	0.45
1:D:1671:ARG:O	1:D:1675:ALA:HB2	2.17	0.45
1:D:2742:THR:HB	1:D:2814:LYS:HG2	1.98	0.45
1:D:3537:LYS:NZ	1:D:3600:SER:O	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:NH1	1:A:278:GLN:OE1	2.49	0.45
1:B:732:SER:HB2	1:B:735:GLN:HB3	1.98	0.45
1:B:2500:ALA:HB2	1:B:2553:TYR:HD1	1.81	0.45
1:C:884:LEU:HB2	1:C:969:PRO:HD3	1.98	0.45
1:C:1519:LEU:HD21	1:C:1572:ILE:HD13	1.99	0.45
1:D:232:THR:HG21	1:D:252:VAL:HG12	1.99	0.45
2:E:27:THR:HB	2:E:100:ASP:HB3	1.97	0.45
1:A:1116:GLY:O	1:A:1134:LEU:N	2.50	0.45
1:A:2519:LEU:HD12	1:A:2578:MET:HE1	1.98	0.45
1:A:2986:VAL:HG22	1:A:2988:LYS:H	1.82	0.45
1:A:3519:PRO:HB3	1:B:1220:GLN:HB2	1.99	0.45
1:A:4184:MET:N	1:A:5021:PHE:O	2.50	0.45
1:B:294:THR:HG23	1:B:297:GLN:H	1.81	0.45
1:B:665:GLU:HG2	1:B:745:SER:HA	1.98	0.45
1:B:2039:LEU:HB3	1:B:2044:ILE:HB	1.99	0.45
1:C:30:LYS:HA	1:C:30:LYS:HD2	1.79	0.45
1:C:206:CYS:SG	1:C:207:SER:N	2.90	0.45
1:C:1000:ARG:HD3	1:C:1000:ARG:HA	1.82	0.45
1:C:1473:THR:HA	1:C:1487:LEU:O	2.16	0.45
1:D:585:SER:O	1:D:588:SER:OG	2.28	0.45
1:D:1636:MET:HE2	1:D:1636:MET:HB3	1.88	0.45
1:D:2519:LEU:HD12	1:D:2578:MET:HE1	1.99	0.45
2:G:38:SER:OG	2:G:39:SER:N	2.50	0.45
1:A:2410:PRO:HB3	1:A:2415:ARG:HB3	1.97	0.45
1:B:2470:ILE:HG22	1:B:2525:GLY:HA3	1.98	0.45
1:B:2614:ILE:O	1:B:2650:ARG:NH2	2.43	0.45
1:B:2667:THR:HG21	1:B:2672:LEU:HD21	1.99	0.45
1:B:4576:ILE:HG23	1:B:4639:MET:HG2	1.99	0.45
1:C:2470:ILE:HG22	1:C:2525:GLY:HA3	1.98	0.45
1:C:2742:THR:HB	1:C:2814:LYS:HG2	1.98	0.45
1:D:232:THR:HG22	1:D:258:SER:HB3	1.98	0.45
1:D:876:GLU:HG2	1:D:910:PHE:CE2	2.52	0.45
1:D:1658:ASP:N	1:D:1658:ASP:OD1	2.50	0.45
1:D:1690:ASP:HB2	1:D:1693:GLN:HG3	1.99	0.45
1:A:1671:ARG:O	1:A:1675:ALA:HB2	2.17	0.45
1:A:3693:LYS:HD2	1:A:3693:LYS:HA	1.78	0.45
1:A:4202:ARG:O	1:A:4206:GLU:HG2	2.17	0.45
1:A:4631:PHE:HE2	1:A:4633:GLU:HG2	1.81	0.45
1:B:1671:ARG:O	1:B:1675:ALA:HB2	2.17	0.45
1:C:1419:ASP:OD1	1:C:1421:ARG:NH1	2.50	0.45
1:D:4202:ARG:O	1:D:4206:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4745:LEU:H	1:D:4745:LEU:HG	1.55	0.45
1:A:732:SER:HB2	1:A:735:GLN:HB3	1.98	0.44
1:B:876:GLU:HG2	1:B:910:PHE:CE2	2.52	0.44
1:B:1658:ASP:OD1	1:B:1658:ASP:N	2.50	0.44
1:B:2208:MET:HE2	1:B:2208:MET:HB2	1.88	0.44
1:C:771:PHE:HB3	1:C:1472:VAL:HG23	1.99	0.44
1:C:1690:ASP:HB2	1:C:1693:GLN:HG3	1.99	0.44
1:C:2580:ASP:HB2	1:C:2618:MET:HE1	1.99	0.44
1:C:2627:VAL:HG22	1:C:2678:LEU:HG	1.98	0.44
1:C:4049:VAL:HG21	1:C:4159:ARG:HG2	1.99	0.44
1:D:356:TRP:N	1:D:379:HIS:O	2.38	0.44
1:D:2296:GLU:HA	1:D:2299:VAL:HG12	1.99	0.44
1:D:3420:ARG:HH22	1:D:3519:PRO:HG2	1.82	0.44
1:A:206:CYS:SG	1:A:207:SER:N	2.90	0.44
1:A:876:GLU:HG2	1:A:910:PHE:CE2	2.52	0.44
1:A:1156:THR:OG1	1:A:1157:GLU:OE1	2.36	0.44
1:A:4821:LYS:HE2	1:A:4821:LYS:HB2	1.54	0.44
1:B:206:CYS:SG	1:B:207:SER:N	2.90	0.44
1:B:531:ARG:NH2	1:B:562:GLU:OE2	2.37	0.44
1:B:1116:GLY:O	1:B:1134:LEU:N	2.50	0.44
1:B:1147:ASP:HB3	1:B:1164:LEU:HD11	2.00	0.44
1:B:3202:PRO:O	1:B:3214:ASN:ND2	2.45	0.44
1:C:232:THR:HG22	1:C:258:SER:HB3	1.98	0.44
1:C:823:LEU:HD12	1:C:823:LEU:HA	1.89	0.44
1:D:206:CYS:SG	1:D:207:SER:N	2.90	0.44
1:D:1116:GLY:O	1:D:1134:LEU:N	2.50	0.44
1:D:2470:ILE:HG22	1:D:2525:GLY:HA3	1.98	0.44
1:D:2559:LEU:HA	1:D:2562:ILE:HD12	1.99	0.44
1:D:2770:LYS:HD2	1:D:2788:HIS:H	1.82	0.44
2:H:38:SER:OG	2:H:39:SER:N	2.50	0.44
1:A:2559:LEU:HA	1:A:2562:ILE:HD12	1.99	0.44
1:C:499:THR:HG23	1:C:502:HIS:H	1.83	0.44
1:C:1147:ASP:HB3	1:C:1164:LEU:HD11	2.00	0.44
1:A:499:THR:HG23	1:A:502:HIS:H	1.83	0.44
1:A:1658:ASP:N	1:A:1658:ASP:OD1	2.50	0.44
1:A:2039:LEU:HB3	1:A:2044:ILE:HB	1.99	0.44
1:B:499:THR:HG23	1:B:502:HIS:H	1.83	0.44
1:B:2986:VAL:HG22	1:B:2988:LYS:H	1.82	0.44
1:C:4913:ARG:NH2	1:C:4917:ASP:OD2	2.51	0.44
1:D:30:LYS:HA	1:D:30:LYS:HD2	1.79	0.44
1:D:3159:ASP:OD1	1:D:3159:ASP:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:ASP:HB3	1:A:1164:LEU:HD11	2.00	0.44
1:A:1220:GLN:HB2	1:D:3519:PRO:HB3	1.99	0.44
1:A:1243:PRO:O	1:A:1458:HIS:ND1	2.33	0.44
1:A:2355:ARG:HA	1:A:2358:ILE:HG12	1.99	0.44
1:A:2580:ASP:HB2	1:A:2618:MET:HE1	1.99	0.44
1:A:2654:TYR:HA	1:A:2661:TRP:H	1.83	0.44
1:A:2770:LYS:HD2	1:A:2788:HIS:H	1.83	0.44
1:A:4865:LYS:HA	1:A:4865:LYS:HD2	1.49	0.44
1:B:863:LEU:HA	1:B:864:PRO:HD3	1.85	0.44
1:C:717:ASP:OD1	1:C:720:HIS:N	2.41	0.44
1:C:4865:LYS:HD2	1:C:4865:LYS:HA	1.49	0.44
1:D:4576:ILE:HG23	1:D:4639:MET:HG2	1.99	0.44
1:A:161:GLU:HB3	1:D:3984:ARG:NH2	2.32	0.44
1:A:1690:ASP:HB2	1:A:1693:GLN:HG3	1.99	0.44
1:A:5012:LYS:HD3	1:A:5012:LYS:HA	1.64	0.44
1:B:2355:ARG:HA	1:B:2358:ILE:HG12	1.99	0.44
1:B:4202:ARG:O	1:B:4206:GLU:HG2	2.17	0.44
1:C:232:THR:HG21	1:C:252:VAL:HG12	1.99	0.44
1:C:665:GLU:HG2	1:C:745:SER:HA	1.98	0.44
1:C:2355:ARG:HA	1:C:2358:ILE:HG12	1.99	0.44
1:C:2614:ILE:O	1:C:2650:ARG:NH2	2.43	0.44
1:C:2770:LYS:HD2	1:C:2788:HIS:H	1.83	0.44
1:D:1519:LEU:HD21	1:D:1572:ILE:HD13	1.99	0.44
1:D:2251:PHE:HB2	1:D:2286:LEU:HD13	2.00	0.44
1:D:2560:PRO:O	1:D:2564:LYS:HD2	2.18	0.44
1:D:2654:TYR:HA	1:D:2661:TRP:H	1.83	0.44
1:D:2667:THR:HG21	1:D:2672:LEU:HD21	1.99	0.44
1:D:2986:VAL:HG22	1:D:2988:LYS:H	1.82	0.44
2:E:38:SER:OG	2:E:39:SER:N	2.50	0.44
1:A:308:HIS:HD2	1:A:310:LYS:HB3	1.83	0.44
1:A:771:PHE:HB3	1:A:1472:VAL:HG23	1.99	0.44
1:A:1739:THR:OG1	1:A:1742:THR:OG1	2.25	0.44
1:A:2671:GLU:HA	1:A:2674:LEU:HB2	2.00	0.44
1:A:3420:ARG:HH22	1:A:3519:PRO:HG2	1.82	0.44
1:A:4983:HIS:O	3:A:5101:AMP:N6	2.51	0.44
1:B:771:PHE:HB3	1:B:1472:VAL:HG23	1.99	0.44
1:B:1476:MET:HE3	1:B:1476:MET:HB2	1.81	0.44
1:B:1519:LEU:HD21	1:B:1572:ILE:HD13	1.99	0.44
1:B:2560:PRO:O	1:B:2564:LYS:HD2	2.18	0.44
1:B:2806:ARG:HA	1:B:2809:ILE:HD13	2.00	0.44
1:B:3321:ARG:HA	1:B:3324:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:PHE:O	1:C:418:LEU:HB2	2.18	0.44
1:C:730:VAL:HG12	1:C:1476:MET:HE2	2.00	0.44
1:C:2039:LEU:HB3	1:C:2044:ILE:HB	1.99	0.44
1:C:2251:PHE:HB2	1:C:2286:LEU:HD13	2.00	0.44
1:D:1147:ASP:HB3	1:D:1164:LEU:HD11	2.00	0.44
1:D:3092:LEU:HD12	1:D:3093:ARG:HG3	2.00	0.44
1:A:414:PHE:O	1:A:418:LEU:HB2	2.18	0.44
1:A:2806:ARG:HA	1:A:2809:ILE:HD13	2.00	0.44
1:B:1156:THR:OG1	1:B:1157:GLU:OE1	2.35	0.44
1:B:2770:LYS:HD2	1:B:2788:HIS:H	1.83	0.44
1:B:4993:MET:HE2	1:B:4993:MET:HB3	1.75	0.44
1:C:308:HIS:HD2	1:C:310:LYS:HB3	1.83	0.44
1:C:1671:ARG:O	1:C:1675:ALA:HB2	2.17	0.44
1:D:2633:LEU:HG	1:D:2695:LEU:HD21	2.00	0.44
1:D:4913:ARG:NH2	1:D:4917:ASP:OD2	2.51	0.44
2:F:38:SER:OG	2:F:39:SER:N	2.50	0.44
1:A:452:PHE:HE1	1:A:474:ARG:HB3	1.83	0.44
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.42	0.44
1:A:2621:HIS:HB3	1:A:2624:ARG:HH21	1.83	0.44
1:A:3321:ARG:HA	1:A:3324:VAL:HG12	2.00	0.44
1:B:699:GLY:N	1:B:1647:CYS:O	2.50	0.44
1:B:3218:VAL:O	1:B:3222:LYS:HB2	2.18	0.44
1:C:1156:THR:OG1	1:C:1157:GLU:OE1	2.36	0.44
1:C:1652:GLU:OE1	1:C:1656:ARG:NH2	2.46	0.44
1:C:2296:GLU:HA	1:C:2299:VAL:HG12	1.99	0.44
1:C:4202:ARG:O	1:C:4206:GLU:HG2	2.17	0.44
1:D:1739:THR:OG1	1:D:1742:THR:OG1	2.25	0.44
1:D:3218:VAL:O	1:D:3222:LYS:HB2	2.18	0.44
1:D:3694:LYS:HA	1:D:3695:PRO:HD3	1.90	0.44
1:D:4049:VAL:HG21	1:D:4159:ARG:HG2	1.99	0.44
1:A:683:ARG:HG2	1:A:717:ASP:HB3	2.00	0.43
1:B:2522:LEU:HB3	1:B:2582:MET:HE1	1.98	0.43
1:B:3264:THR:OG1	1:B:3265:GLU:OE1	2.36	0.43
1:C:2472:LEU:HD23	1:C:2472:LEU:HA	1.87	0.43
1:C:2560:PRO:O	1:C:2564:LYS:HD2	2.18	0.43
1:C:2633:LEU:HG	1:C:2695:LEU:HD21	2.00	0.43
1:C:2825:LYS:NZ	1:C:2935:TYR:OH	2.45	0.43
1:C:3420:ARG:HH22	1:C:3519:PRO:HG2	1.82	0.43
1:C:4576:ILE:HG23	1:C:4639:MET:HG2	1.99	0.43
1:C:4983:HIS:O	3:C:5101:AMP:N6	2.51	0.43
1:D:1419:ASP:OD1	1:D:1421:ARG:NH1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2580:ASP:HB2	1:D:2618:MET:HE1	1.99	0.43
1:D:4184:MET:N	1:D:5021:PHE:O	2.50	0.43
2:E:76:CYS:HB3	2:E:97:LEU:HB2	2.00	0.43
2:H:76:CYS:HB3	2:H:97:LEU:HB2	2.00	0.43
1:A:2357:LEU:HB3	1:A:2364:PHE:HE1	1.83	0.43
1:A:2667:THR:HG21	1:A:2672:LEU:HD21	1.99	0.43
1:A:4823:LEU:HD23	1:A:4823:LEU:HA	1.79	0.43
1:A:4965:SER:O	1:A:4969:ASP:HB2	2.18	0.43
1:A:4993:MET:HE2	1:A:4993:MET:HB3	1.75	0.43
1:B:232:THR:HG21	1:B:252:VAL:HG12	1.99	0.43
1:B:452:PHE:HE1	1:B:474:ARG:HB3	1.83	0.43
1:B:683:ARG:HG2	1:B:717:ASP:HB3	2.00	0.43
1:B:1036:ARG:O	1:B:1040:CYS:HB2	2.18	0.43
1:B:2686:LEU:HB3	1:B:2997:PHE:HE1	1.83	0.43
1:B:3592:ILE:HG22	1:B:3595:ARG:HH21	1.83	0.43
1:B:4049:VAL:HG21	1:B:4159:ARG:HG2	1.99	0.43
1:B:4823:LEU:HA	1:B:4823:LEU:HD23	1.79	0.43
1:C:2357:LEU:HB3	1:C:2364:PHE:HE1	1.83	0.43
1:C:3798:LEU:HD23	1:C:3798:LEU:HA	1.89	0.43
1:D:2621:HIS:HB3	1:D:2624:ARG:HH21	1.83	0.43
1:D:2806:ARG:HA	1:D:2809:ILE:HD13	2.00	0.43
1:A:2175:GLU:HG3	1:A:2228:MET:HB2	2.00	0.43
1:A:2633:LEU:HG	1:A:2695:LEU:HD21	2.00	0.43
1:A:2766:TRP:HE1	1:A:2788:HIS:HB2	1.84	0.43
1:A:3092:LEU:HD12	1:A:3093:ARG:HG3	1.99	0.43
1:A:4823:LEU:HD22	1:B:4843:LEU:HD22	1.99	0.43
1:B:1690:ASP:HB2	1:B:1693:GLN:HG3	1.99	0.43
1:B:4184:MET:N	1:B:5021:PHE:O	2.50	0.43
1:B:4913:ARG:NH2	1:B:4917:ASP:OD2	2.51	0.43
1:C:1116:GLY:O	1:C:1134:LEU:N	2.50	0.43
1:C:1658:ASP:N	1:C:1658:ASP:OD1	2.50	0.43
1:C:2591:ARG:HG2	1:C:2636:PHE:HB3	2.01	0.43
1:C:2986:VAL:HG22	1:C:2988:LYS:H	1.82	0.43
1:C:4965:SER:O	1:C:4969:ASP:HB2	2.18	0.43
1:D:452:PHE:HE1	1:D:474:ARG:HB3	1.83	0.43
1:D:1036:ARG:O	1:D:1040:CYS:HB2	2.18	0.43
1:D:3227:ARG:HA	1:D:3232:LEU:HD12	2.01	0.43
1:D:3264:THR:OG1	1:D:3265:GLU:OE1	2.36	0.43
1:D:4227:GLU:H	1:D:4227:GLU:HG3	1.43	0.43
1:D:4823:LEU:HD23	1:D:4823:LEU:HA	1.79	0.43
2:E:2:VAL:HG23	2:E:80:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2782:ASP:N	1:A:2782:ASP:OD1	2.52	0.43
1:A:4934:GLY:HA2	1:D:4937:ILE:HG12	2.00	0.43
1:B:124:SER:HB2	1:B:133:PHE:HA	2.01	0.43
1:B:414:PHE:O	1:B:418:LEU:HB2	2.18	0.43
1:B:1543:GLU:O	1:B:1546:THR:OG1	2.35	0.43
1:B:2159:LEU:HG	1:B:2163:ARG:HE	1.84	0.43
1:B:2627:VAL:HG22	1:B:2678:LEU:HG	1.98	0.43
1:B:2654:TYR:HA	1:B:2661:TRP:H	1.83	0.43
1:B:2825:LYS:NZ	1:B:2935:TYR:OH	2.45	0.43
1:B:3092:LEU:HD12	1:B:3093:ARG:HG3	2.00	0.43
1:C:1036:ARG:O	1:C:1040:CYS:HB2	2.18	0.43
1:C:2930:LEU:O	1:C:2935:TYR:N	2.49	0.43
1:C:3694:LYS:HA	1:C:3695:PRO:HD3	1.90	0.43
1:D:414:PHE:O	1:D:418:LEU:HB2	2.18	0.43
1:A:2560:PRO:O	1:A:2564:LYS:HD2	2.18	0.43
1:A:2686:LEU:HB3	1:A:2997:PHE:HE1	1.83	0.43
1:B:308:HIS:HD2	1:B:310:LYS:HB3	1.83	0.43
1:B:730:VAL:HG12	1:B:1476:MET:HE2	2.00	0.43
1:B:2591:ARG:HG2	1:B:2636:PHE:HB3	2.01	0.43
1:B:3458:PHE:O	1:B:3462:ASN:ND2	2.36	0.43
1:B:4965:SER:O	1:B:4969:ASP:HB2	2.18	0.43
1:B:4983:HIS:O	3:B:5101:AMP:N6	2.51	0.43
1:C:2621:HIS:HB3	1:C:2624:ARG:HH21	1.83	0.43
1:C:2806:ARG:HA	1:C:2809:ILE:HD13	2.00	0.43
1:C:3092:LEU:HD12	1:C:3093:ARG:HG3	2.00	0.43
1:C:3227:ARG:HA	1:C:3232:LEU:HD12	2.01	0.43
1:C:3535:LEU:O	1:C:3538:THR:OG1	2.32	0.43
1:D:2039:LEU:HB3	1:D:2044:ILE:HB	1.99	0.43
1:D:3157:ILE:HB	1:D:3202:PRO:HG3	2.01	0.43
1:D:4965:SER:O	1:D:4969:ASP:HB2	2.18	0.43
1:A:1519:LEU:HD21	1:A:1572:ILE:HD13	1.99	0.43
1:A:2158:CYS:O	1:A:2162:ILE:HG12	2.19	0.43
1:A:2251:PHE:HB2	1:A:2286:LEU:HD13	2.00	0.43
1:A:3323:ILE:HG12	1:A:3335:MET:HE1	2.01	0.43
1:A:4670:ILE:HB	1:A:4714:ASN:HD22	1.84	0.43
1:B:2621:HIS:HB3	1:B:2624:ARG:HH21	1.83	0.43
1:B:2633:LEU:HG	1:B:2695:LEU:HD21	2.00	0.43
1:C:492:ASP:OD1	1:C:546:TRP:NE1	2.42	0.43
1:C:2654:TYR:HA	1:C:2661:TRP:H	1.83	0.43
1:C:3592:ILE:HG22	1:C:3595:ARG:HH21	1.83	0.43
1:C:3693:LYS:HD2	1:C:3693:LYS:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:HIS:HD2	1:D:310:LYS:HB3	1.83	0.43
1:D:499:THR:HG23	1:D:502:HIS:H	1.83	0.43
1:D:3592:ILE:HG22	1:D:3595:ARG:HH21	1.83	0.43
1:D:4983:HIS:O	3:D:5101:AMP:N6	2.51	0.43
1:A:1036:ARG:O	1:A:1040:CYS:HB2	2.18	0.43
1:A:2296:GLU:HA	1:A:2299:VAL:HG12	1.99	0.43
1:A:4913:ARG:NH2	1:A:4917:ASP:OD2	2.51	0.43
1:A:5030:LYS:HB2	1:A:5030:LYS:HE2	1.76	0.43
1:B:823:LEU:HD23	1:B:1617:THR:HB	2.01	0.43
1:B:1419:ASP:OD1	1:B:1421:ARG:NH1	2.50	0.43
1:B:2205:GLU:O	1:B:2208:MET:N	2.52	0.43
1:C:2009:LEU:HD23	1:C:2022:PRO:HD2	2.01	0.43
1:C:2686:LEU:HB3	1:C:2997:PHE:HE1	1.83	0.43
1:C:3218:VAL:O	1:C:3222:LYS:HB2	2.18	0.43
1:C:3321:ARG:HA	1:C:3324:VAL:HG12	2.00	0.43
1:C:4670:ILE:HB	1:C:4714:ASN:HD22	1.84	0.43
1:D:2671:GLU:HA	1:D:2674:LEU:HB2	2.00	0.43
1:D:4670:ILE:HB	1:D:4714:ASN:HD22	1.84	0.43
1:A:1007:TYR:O	1:A:1017:ARG:NH2	2.51	0.43
1:A:3227:ARG:HA	1:A:3232:LEU:HD12	2.01	0.43
1:A:4884:LEU:HD11	1:B:4914:VAL:HG11	2.01	0.43
1:B:2296:GLU:HA	1:B:2299:VAL:HG12	1.99	0.43
1:B:2476:ILE:HG23	1:B:2536:LEU:HD21	2.01	0.43
1:B:2575:ARG:HA	1:B:2575:ARG:HD2	1.79	0.43
1:B:2766:TRP:HE1	1:B:2788:HIS:HB2	1.84	0.43
1:B:2911:LEU:HD13	1:B:2915:GLU:HG3	2.00	0.43
1:B:3420:ARG:HH22	1:B:3519:PRO:HG2	1.82	0.43
1:C:823:LEU:HD23	1:C:1617:THR:HB	2.01	0.43
1:D:1156:THR:OG1	1:D:1157:GLU:OE1	2.36	0.43
1:D:1674:CYS:SG	1:D:1717:SER:OG	2.71	0.43
1:D:2205:GLU:O	1:D:2208:MET:N	2.52	0.43
1:D:2357:LEU:HB3	1:D:2364:PHE:HE1	1.83	0.43
1:D:2782:ASP:OD1	1:D:2782:ASP:N	2.52	0.43
1:A:2301:TYR:HB3	1:A:2331:TYR:CE2	2.54	0.43
1:A:3575:LEU:HD23	1:B:1219:LEU:HD22	2.00	0.43
1:A:4745:LEU:H	1:A:4745:LEU:HG	1.55	0.43
1:B:113:HIS:NE2	1:B:399:GLN:O	2.51	0.43
1:B:2177:LEU:O	1:B:2181:SER:OG	2.36	0.43
1:C:1444:GLU:HG2	1:C:1446:SER:H	1.84	0.43
1:C:2766:TRP:HE1	1:C:2788:HIS:HB2	1.84	0.43
1:C:3264:THR:OG1	1:C:3265:GLU:OE1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4892:ARG:NH1	1:D:4895:GLY:O	2.48	0.43
1:D:113:HIS:NE2	1:D:399:GLN:O	2.51	0.43
1:D:683:ARG:HG2	1:D:717:ASP:HB3	2.00	0.43
1:D:2765:LYS:HA	1:D:2765:LYS:HD3	1.87	0.43
2:G:76:CYS:HB3	2:G:97:LEU:HB2	2.00	0.43
2:H:2:VAL:HG23	2:H:80:VAL:HG21	2.01	0.43
1:A:293:LEU:H	1:A:311:ALA:HB1	1.84	0.43
1:A:2591:ARG:HG2	1:A:2636:PHE:HB3	2.01	0.43
1:A:4977:THR:O	1:A:4981:GLU:HB2	2.19	0.43
1:B:765:GLN:NE2	1:B:1479:GLU:OE1	2.52	0.43
1:B:1000:ARG:HA	1:B:1000:ARG:HD3	1.82	0.43
1:B:1444:GLU:HG2	1:B:1446:SER:H	1.84	0.43
1:B:2009:LEU:HD23	1:B:2022:PRO:HD2	2.01	0.43
1:B:2301:TYR:HB3	1:B:2331:TYR:CE2	2.54	0.43
1:B:4686:LEU:O	1:B:4691:GLN:N	2.49	0.43
1:C:706:GLY:N	1:C:709:ASP:OD2	2.39	0.43
1:C:1007:TYR:O	1:C:1017:ARG:NH2	2.51	0.43
1:C:2911:LEU:HD13	1:C:2915:GLU:HG3	2.00	0.43
1:C:3901:ASN:OD1	1:C:3904:ARG:NH1	2.34	0.43
1:D:765:GLN:NE2	1:D:1479:GLU:OE1	2.52	0.43
1:D:2971:GLN:HG2	1:D:3045:LYS:HZ1	1.84	0.43
1:D:4991:PHE:HE2	1:D:5010:VAL:HG11	1.84	0.43
1:A:2948:THR:HG23	1:A:2952:GLU:HB2	2.01	0.42
1:A:3218:VAL:O	1:A:3222:LYS:HB2	2.18	0.42
1:A:3424:LEU:HD23	1:A:3424:LEU:HA	1.88	0.42
1:B:2251:PHE:HB2	1:B:2286:LEU:HD13	2.00	0.42
1:B:3106:MET:HG3	1:B:3110:LEU:HD13	2.01	0.42
1:B:3889:GLN:HG3	1:B:3967:GLU:HG3	2.02	0.42
1:C:452:PHE:HE1	1:C:474:ARG:HB3	1.83	0.42
1:C:1231[B]:GLN:H	1:C:1231[B]:GLN:HG3	1.61	0.42
1:C:2671:GLU:HA	1:C:2674:LEU:HB2	2.00	0.42
1:C:3218:VAL:HG22	1:C:3227:ARG:HD3	2.00	0.42
1:D:3207:GLU:OE1	1:D:3280:TYR:OH	2.33	0.42
1:D:3218:VAL:HG22	1:D:3227:ARG:HD3	2.00	0.42
1:D:3927:GLN:HA	1:D:3930:ILE:HG22	2.01	0.42
1:D:4977:THR:O	1:D:4981:GLU:HB2	2.19	0.42
1:A:1219:LEU:HD22	1:D:3575:LEU:HD23	2.01	0.42
1:A:1444:GLU:HG2	1:A:1446:SER:H	1.84	0.42
1:A:2205:GLU:O	1:A:2208:MET:N	2.52	0.42
1:A:3106:MET:HG3	1:A:3110:LEU:HD13	2.01	0.42
1:B:1076:ARG:HB3	1:B:1191:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1291:LEU:HD23	1:B:1291:LEU:HA	1.91	0.42
1:B:2671:GLU:HA	1:B:2674:LEU:HB2	2.00	0.42
1:B:2974:ILE:HD12	1:B:3053:ARG:HH12	1.84	0.42
1:B:4581:LYS:HE3	1:B:4581:LYS:HB3	1.82	0.42
1:B:4977:THR:O	1:B:4981:GLU:HB2	2.20	0.42
1:C:1066:GLN:HG3	1:C:1462:MET:HG2	2.01	0.42
1:C:2205:GLU:O	1:C:2208:MET:N	2.52	0.42
1:C:2301:TYR:HB3	1:C:2331:TYR:CE2	2.54	0.42
1:C:2476:ILE:HG23	1:C:2536:LEU:HD21	2.01	0.42
1:C:4821:LYS:HB2	1:C:4821:LYS:HE2	1.54	0.42
1:C:4977:THR:O	1:C:4981:GLU:HB2	2.20	0.42
1:D:114:SER:HB2	1:D:116:MET:HG3	2.02	0.42
1:D:2355:ARG:HA	1:D:2358:ILE:HG12	1.99	0.42
1:D:3768:SER:HA	1:D:3771:HIS:CD2	2.54	0.42
1:A:823:LEU:HD23	1:A:1617:THR:HB	2.01	0.42
1:A:823:LEU:HD22	1:A:1626:TRP:HB3	2.01	0.42
1:A:1419:ASP:OD1	1:A:1421:ARG:NH1	2.50	0.42
1:A:2302:LEU:HD23	1:A:2363:CYS:HB3	2.02	0.42
1:A:2974:ILE:HD12	1:A:3053:ARG:HH12	1.84	0.42
1:A:3207:GLU:OE1	1:A:3280:TYR:OH	2.33	0.42
1:A:3554:GLN:HA	1:A:3557:LEU:HG	2.02	0.42
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.54	0.42
1:B:1007:TYR:O	1:B:1017:ARG:NH2	2.51	0.42
1:B:3157:ILE:HB	1:B:3202:PRO:HG3	2.00	0.42
1:B:3218:VAL:HG22	1:B:3227:ARG:HD3	2.01	0.42
1:B:4016:LEU:HD12	1:B:4016:LEU:HA	1.84	0.42
1:C:114:SER:HB2	1:C:116:MET:HG3	2.02	0.42
1:C:683:ARG:HG2	1:C:717:ASP:HB3	2.00	0.42
1:C:2159:LEU:HG	1:C:2163:ARG:HE	1.84	0.42
1:C:2175:GLU:HG3	1:C:2228:MET:HB2	2.00	0.42
1:C:3159:ASP:OD1	1:C:3159:ASP:N	2.46	0.42
1:C:3768:SER:HA	1:C:3771:HIS:CD2	2.54	0.42
1:C:4092:ASP:HA	1:C:4095:LYS:HG2	2.02	0.42
1:D:730:VAL:HG12	1:D:1476:MET:HE2	2.00	0.42
1:D:823:LEU:HD23	1:D:1617:THR:HB	2.01	0.42
1:D:1444:GLU:HG2	1:D:1446:SER:H	1.84	0.42
1:D:2009:LEU:HD23	1:D:2022:PRO:HD2	2.01	0.42
1:D:2302:LEU:HD23	1:D:2363:CYS:HB3	2.02	0.42
1:D:2591:ARG:HG2	1:D:2636:PHE:HB3	2.00	0.42
1:D:2948:THR:HG23	1:D:2952:GLU:HB2	2.01	0.42
1:D:3321:ARG:HA	1:D:3324:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:VAL:HG23	2:F:80:VAL:HG21	2.01	0.42
1:A:730:VAL:HG12	1:A:1476:MET:HE2	2.00	0.42
1:A:1636:MET:HE2	1:A:1636:MET:HB3	1.88	0.42
1:A:2624:ARG:HD2	1:A:2906:VAL:HG11	2.02	0.42
1:A:3592:ILE:HG22	1:A:3595:ARG:HH21	1.83	0.42
1:B:293:LEU:H	1:B:311:ALA:HB1	1.84	0.42
1:B:869:ARG:CZ	1:B:870:ILE:HB	2.50	0.42
1:B:884:LEU:HD13	1:B:968:ALA:H	1.84	0.42
1:C:765:GLN:NE2	1:C:1479:GLU:OE1	2.52	0.42
1:C:884:LEU:HD13	1:C:968:ALA:H	1.84	0.42
1:C:2974:ILE:HD12	1:C:3053:ARG:HH12	1.84	0.42
1:C:3889:GLN:HG3	1:C:3967:GLU:HG3	2.01	0.42
1:C:4814:LEU:HD23	1:C:4814:LEU:HA	1.89	0.42
1:C:4991:PHE:HE2	1:C:5010:VAL:HG11	1.84	0.42
1:D:2159:LEU:HG	1:D:2163:ARG:HE	1.84	0.42
1:D:2175:GLU:HG3	1:D:2228:MET:HB2	2.00	0.42
2:F:76:CYS:HB3	2:F:97:LEU:HB2	2.00	0.42
1:A:130:LYS:NZ	1:D:2373:GLY:O	2.40	0.42
1:A:1076:ARG:HB3	1:A:1191:VAL:HG23	2.01	0.42
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.36	0.42
1:B:30:LYS:HA	1:B:30:LYS:HD2	1.80	0.42
1:B:1066:GLN:HG3	1:B:1462:MET:HG2	2.01	0.42
1:B:2158:CYS:O	1:B:2162:ILE:HG12	2.19	0.42
1:B:2302:LEU:HD23	1:B:2363:CYS:HB3	2.02	0.42
1:B:3227:ARG:HA	1:B:3232:LEU:HD12	2.01	0.42
1:C:2302:LEU:HD23	1:C:2363:CYS:HB3	2.02	0.42
1:C:4184:MET:N	1:C:5021:PHE:O	2.50	0.42
1:C:5030:LYS:HE2	1:C:5030:LYS:HB2	1.76	0.42
1:D:828:GLU:O	1:D:1073:ARG:NH1	2.53	0.42
1:D:878:ILE:HD11	1:D:925:SER:HB2	2.02	0.42
1:D:3323:ILE:HG12	1:D:3335:MET:HE1	2.01	0.42
1:A:30:LYS:HD2	1:A:30:LYS:HA	1.79	0.42
1:A:878:ILE:HD11	1:A:925:SER:HB2	2.02	0.42
1:A:884:LEU:HD13	1:A:968:ALA:H	1.84	0.42
1:A:3927:GLN:HA	1:A:3930:ILE:HG22	2.01	0.42
1:A:4991:PHE:HE2	1:A:5010:VAL:HG11	1.84	0.42
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.90	0.42
1:B:3175:LEU:O	1:B:3178:THR:OG1	2.33	0.42
1:C:863:LEU:HA	1:C:864:PRO:HD3	1.85	0.42
1:C:3157:ILE:HB	1:C:3202:PRO:HG3	2.00	0.42
1:C:3288:GLY:HA2	1:C:3303:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1007:TYR:O	1:D:1017:ARG:NH2	2.51	0.42
1:D:2686:LEU:HB3	1:D:2997:PHE:HE1	1.83	0.42
1:D:4989:MET:HE3	1:D:4989:MET:HB3	1.68	0.42
1:A:1066:GLN:HG3	1:A:1462:MET:HG2	2.01	0.42
1:A:2009:LEU:HD23	1:A:2022:PRO:HD2	2.01	0.42
1:A:2911:LEU:HD13	1:A:2915:GLU:HG3	2.00	0.42
1:A:2930:LEU:O	1:A:2935:TYR:N	2.49	0.42
1:A:3218:VAL:HG22	1:A:3227:ARG:HD3	2.00	0.42
1:A:3288:GLY:HA2	1:A:3303:PRO:HB3	2.01	0.42
1:A:3582:ARG:HD3	1:A:3582:ARG:HA	1.88	0.42
1:A:4044:MET:HE2	1:A:4044:MET:HB2	1.95	0.42
1:B:114:SER:HB2	1:B:116:MET:HG3	2.02	0.42
1:B:2039:LEU:HD22	1:B:2044:ILE:HG13	2.02	0.42
1:B:2175:GLU:HG3	1:B:2228:MET:HB2	2.00	0.42
1:B:2472:LEU:HA	1:B:2472:LEU:HD23	1.87	0.42
1:C:3207:GLU:OE1	1:C:3280:TYR:OH	2.33	0.42
1:C:3927:GLN:HA	1:C:3930:ILE:HG22	2.01	0.42
1:C:4827:LEU:HD23	1:C:4827:LEU:HA	1.89	0.42
1:C:4976:GLU:H	1:C:4976:GLU:HG2	1.59	0.42
1:D:124:SER:HB2	1:D:133:PHE:HA	2.01	0.42
1:D:1434:TYR:HA	1:D:1518:CYS:O	2.20	0.42
1:D:2158:CYS:O	1:D:2162:ILE:HG12	2.19	0.42
1:D:2301:TYR:HB3	1:D:2331:TYR:CE2	2.54	0.42
1:D:2624:ARG:HD2	1:D:2906:VAL:HG11	2.02	0.42
1:D:3175:LEU:O	1:D:3178:THR:OG1	2.33	0.42
1:D:4092:ASP:HA	1:D:4095:LYS:HG2	2.02	0.42
2:G:2:VAL:HG23	2:G:80:VAL:HG21	2.01	0.42
1:A:765:GLN:NE2	1:A:1479:GLU:OE1	2.52	0.42
1:A:2039:LEU:HD22	1:A:2044:ILE:HG13	2.02	0.42
1:A:2159:LEU:HG	1:A:2163:ARG:HE	1.84	0.42
1:A:3157:ILE:HB	1:A:3202:PRO:HG3	2.00	0.42
1:A:3889:GLN:HG3	1:A:3967:GLU:HG3	2.01	0.42
1:B:2357:LEU:HB3	1:B:2364:PHE:HE1	1.83	0.42
1:B:2902:HIS:HB3	1:B:2905:LEU:HG	2.02	0.42
1:B:3554:GLN:HA	1:B:3557:LEU:HG	2.01	0.42
1:B:3710:LEU:HD21	1:B:3781:GLN:HG2	2.02	0.42
1:B:4092:ASP:HA	1:B:4095:LYS:HG2	2.02	0.42
1:C:124:SER:HB2	1:C:133:PHE:HA	2.01	0.42
1:C:293:LEU:H	1:C:311:ALA:HB1	1.84	0.42
1:C:1636:MET:HE2	1:C:1636:MET:HB3	1.88	0.42
1:D:699:GLY:N	1:D:1647:CYS:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2766:TRP:HE1	1:D:2788:HIS:HB2	1.84	0.42
1:A:1773:PRO:HA	1:A:1774:PRO:HD3	1.94	0.42
1:A:3875:MET:HE3	1:A:3875:MET:HB3	1.81	0.42
1:B:1608:MET:HE3	1:B:1608:MET:HB2	1.84	0.42
1:C:1253:PRO:HG2	1:C:1254:HIS:CD2	2.55	0.42
1:C:3648:ARG:O	1:C:3652:MET:HG2	2.20	0.42
1:D:59:PRO:HD3	1:D:307:ALA:HB3	2.02	0.42
1:D:823:LEU:HD22	1:D:1626:TRP:HB3	2.01	0.42
1:D:1066:GLN:HG3	1:D:1462:MET:HG2	2.01	0.42
1:D:1253:PRO:HG2	1:D:1254:HIS:CD2	2.55	0.42
1:D:1608:MET:HE3	1:D:1608:MET:HB2	1.84	0.42
1:D:1773:PRO:HA	1:D:1774:PRO:HD3	1.94	0.42
1:D:2911:LEU:HD13	1:D:2915:GLU:HG3	2.00	0.42
1:D:4865:LYS:HA	1:D:4865:LYS:HD2	1.49	0.42
1:A:1926:LEU:HD23	1:A:1929:MET:HE2	2.02	0.42
1:A:3575:LEU:HD12	1:A:3575:LEU:HA	1.93	0.42
1:A:4645:CYS:SG	1:A:4646:LEU:N	2.93	0.42
1:B:418:LEU:HD11	1:B:494:LEU:HD22	2.02	0.42
1:B:2948:THR:HG23	1:B:2952:GLU:HB2	2.01	0.42
1:B:3376:GLU:O	1:B:3380:ARG:HG2	2.20	0.42
1:B:3539:ARG:NH1	1:B:3553:LEU:HG	2.35	0.42
1:B:3648:ARG:O	1:B:3652:MET:HG2	2.20	0.42
1:B:4645:CYS:SG	1:B:4646:LEU:N	2.93	0.42
1:B:4670:ILE:HB	1:B:4714:ASN:HD22	1.84	0.42
1:B:4991:PHE:HE2	1:B:5010:VAL:HG11	1.84	0.42
1:C:869:ARG:CZ	1:C:870:ILE:HB	2.50	0.42
1:C:878:ILE:HD11	1:C:925:SER:HB2	2.02	0.42
1:C:1773:PRO:HA	1:C:1774:PRO:HD3	1.94	0.42
1:C:2782:ASP:OD1	1:C:2782:ASP:N	2.52	0.42
1:C:3323:ILE:HG12	1:C:3335:MET:HE1	2.01	0.42
1:C:3965:LEU:HD23	1:C:3965:LEU:HA	1.94	0.42
1:D:3106:MET:HG3	1:D:3110:LEU:HD13	2.01	0.42
1:A:114:SER:HB2	1:A:116:MET:HG3	2.02	0.41
1:A:1253:PRO:HG2	1:A:1254:HIS:CD2	2.55	0.41
1:A:4989:MET:HE3	1:A:4989:MET:HB3	1.68	0.41
1:B:1290:ARG:HH12	1:B:1455:PRO:HA	1.85	0.41
1:B:1434:TYR:HA	1:B:1518:CYS:O	2.20	0.41
1:B:3033:ASN:O	1:B:3037:GLU:HG2	2.21	0.41
1:B:3823:LYS:HA	1:B:3823:LYS:HD3	1.83	0.41
1:C:1434:TYR:HA	1:C:1518:CYS:O	2.20	0.41
1:C:3106:MET:HG3	1:C:3110:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:LEU:H	1:D:311:ALA:HB1	1.84	0.41
1:D:869:ARG:CZ	1:D:870:ILE:HB	2.50	0.41
1:D:3889:GLN:HG3	1:D:3967:GLU:HG3	2.02	0.41
1:A:828:GLU:O	1:A:1073:ARG:NH1	2.53	0.41
1:A:1568:LYS:O	1:A:1569:GLN:NE2	2.53	0.41
1:A:2614:ILE:O	1:A:2650:ARG:NH2	2.43	0.41
1:B:878:ILE:HD11	1:B:925:SER:HB2	2.02	0.41
1:B:1926:LEU:HD23	1:B:1929:MET:HE2	2.02	0.41
1:B:2624:ARG:HD2	1:B:2906:VAL:HG11	2.02	0.41
1:B:3227:ARG:NH1	1:B:3234:ASN:OD1	2.37	0.41
1:B:3323:ILE:HG12	1:B:3335:MET:HE1	2.01	0.41
1:B:3768:SER:HA	1:B:3771:HIS:CD2	2.54	0.41
1:B:4044:MET:HE2	1:B:4044:MET:HB2	1.95	0.41
1:C:418:LEU:HD11	1:C:494:LEU:HD22	2.02	0.41
1:C:2624:ARG:HD2	1:C:2906:VAL:HG11	2.02	0.41
1:C:2948:THR:HG23	1:C:2952:GLU:HB2	2.01	0.41
1:C:3033:ASN:O	1:C:3037:GLU:HG2	2.21	0.41
1:C:4835:LYS:HE2	1:C:4835:LYS:HB3	1.56	0.41
1:D:1568:LYS:O	1:D:1569:GLN:NE2	2.53	0.41
1:D:1749:PRO:HA	1:D:1750:PRO:HD3	1.95	0.41
1:A:124:SER:HB2	1:A:133:PHE:HA	2.01	0.41
1:A:1608:MET:HE3	1:A:1608:MET:HB2	1.84	0.41
1:A:2454:ARG:CZ	1:A:2458:ARG:HH21	2.34	0.41
1:A:4686:LEU:O	1:A:4691:GLN:N	2.49	0.41
1:A:4995:LEU:HD23	1:A:4995:LEU:HA	1.93	0.41
1:B:116:MET:HE2	1:B:139:GLU:HA	2.02	0.41
1:B:2682:ILE:HD13	1:B:2682:ILE:HA	1.93	0.41
1:B:3160:ASP:OD1	1:B:3160:ASP:N	2.53	0.41
1:B:3288:GLY:HA2	1:B:3303:PRO:HB3	2.01	0.41
1:C:1849:LEU:HD23	1:C:1849:LEU:HA	1.87	0.41
1:C:2454:ARG:CZ	1:C:2458:ARG:HH21	2.34	0.41
1:C:3823:LYS:HD3	1:C:3823:LYS:HA	1.83	0.41
1:D:1076:ARG:HB3	1:D:1191:VAL:HG23	2.01	0.41
1:D:3288:GLY:HA2	1:D:3303:PRO:HB3	2.01	0.41
1:D:3554:GLN:HA	1:D:3557:LEU:HG	2.02	0.41
1:B:16:THR:OG1	1:B:69:LEU:O	2.36	0.41
1:B:823:LEU:HD22	1:B:1626:TRP:HB3	2.01	0.41
1:B:2454:ARG:CZ	1:B:2458:ARG:HH21	2.34	0.41
1:B:3628:ARG:NH2	1:B:3857:GLY:O	2.54	0.41
1:B:3693:LYS:HA	1:B:3693:LYS:HD2	1.78	0.41
1:C:59:PRO:HD3	1:C:307:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:MET:HE2	1:C:139:GLU:HA	2.02	0.41
1:C:129:ASP:OD1	1:C:129:ASP:N	2.54	0.41
1:C:823:LEU:HD22	1:C:1626:TRP:HB3	2.01	0.41
1:C:1076:ARG:HB3	1:C:1191:VAL:HG23	2.01	0.41
1:C:1290:ARG:HH12	1:C:1455:PRO:HA	1.85	0.41
1:C:2902:HIS:HB3	1:C:2905:LEU:HG	2.02	0.41
1:C:3272:ILE:O	1:C:3276:MET:HG2	2.20	0.41
1:D:531:ARG:NH2	1:D:562:GLU:OE2	2.37	0.41
1:D:2476:ILE:HG23	1:D:2536:LEU:HD21	2.01	0.41
1:D:2867:LEU:HD12	1:D:2928:LYS:HZ3	1.86	0.41
1:D:2974:ILE:HD12	1:D:3053:ARG:HH12	1.84	0.41
1:D:4995:LEU:HD23	1:D:4995:LEU:HA	1.94	0.41
1:A:59:PRO:HD3	1:A:307:ALA:HB3	2.02	0.41
1:A:1863:LEU:HB3	1:A:1871:PHE:HD2	1.86	0.41
1:A:4944:ARG:NH2	1:B:4938:ASP:O	2.54	0.41
1:B:220:LEU:HB2	1:B:391:THR:O	2.20	0.41
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.87	0.41
1:C:531:ARG:NH2	1:C:562:GLU:OE2	2.37	0.41
1:C:2186:MET:HE1	1:C:2235:PHE:HA	2.02	0.41
1:C:3376:GLU:O	1:C:3380:ARG:HG2	2.20	0.41
1:D:3272:ILE:O	1:D:3276:MET:HG2	2.20	0.41
1:D:3376:GLU:O	1:D:3380:ARG:HG2	2.20	0.41
1:D:3823:LYS:HD3	1:D:3823:LYS:HA	1.83	0.41
1:D:4843:LEU:O	1:D:4847:VAL:HG13	2.21	0.41
1:A:418:LEU:HD11	1:A:494:LEU:HD22	2.02	0.41
1:A:823:LEU:HD12	1:A:823:LEU:HA	1.89	0.41
1:A:3033:ASN:O	1:A:3037:GLU:HG2	2.20	0.41
1:A:3539:ARG:NH1	1:A:3553:LEU:HG	2.35	0.41
1:A:4092:ASP:HA	1:A:4095:LYS:HG2	2.02	0.41
1:A:4843:LEU:O	1:A:4847:VAL:HG13	2.21	0.41
1:B:828:GLU:O	1:B:1073:ARG:NH1	2.53	0.41
1:B:1229:ASN:HB2	1:B:1827:ARG:HG3	2.03	0.41
1:B:3875:MET:HE3	1:B:3875:MET:HB3	1.81	0.41
1:B:3927:GLN:HA	1:B:3930:ILE:HG22	2.01	0.41
1:C:1863:LEU:HB3	1:C:1871:PHE:HD2	1.86	0.41
1:C:4944:ARG:HH21	1:D:4938:ASP:CG	2.29	0.41
1:D:137:LEU:HA	1:D:137:LEU:HD23	1.88	0.41
1:D:418:LEU:HD11	1:D:494:LEU:HD22	2.02	0.41
1:D:873:LYS:HG2	1:D:970:LEU:HD13	2.02	0.41
1:D:884:LEU:HD13	1:D:968:ALA:H	1.84	0.41
1:D:1088:TRP:HB2	1:D:1153:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2825:LYS:NZ	1:D:2935:TYR:OH	2.45	0.41
1:A:220:LEU:HB2	1:A:391:THR:O	2.20	0.41
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	2.03	0.41
1:A:3373:VAL:HG11	1:A:3444:TYR:HB3	2.03	0.41
1:B:129:ASP:N	1:B:129:ASP:OD1	2.54	0.41
1:B:932:LEU:HD22	1:B:984:LEU:HD21	2.03	0.41
1:B:1636:MET:HE2	1:B:1636:MET:HB3	1.88	0.41
1:B:2186:MET:HE1	1:B:2235:PHE:HA	2.02	0.41
1:B:4944:ARG:HH21	1:C:4938:ASP:CG	2.29	0.41
1:C:49:LEU:HD23	1:C:49:LEU:HA	1.93	0.41
1:C:1243:PRO:O	1:C:1458:HIS:ND1	2.33	0.41
1:C:2158:CYS:O	1:C:2162:ILE:HG12	2.19	0.41
1:C:2866:THR:OG1	1:C:2867:LEU:N	2.54	0.41
1:C:3883:ASP:HA	1:C:3886:ARG:HB3	2.03	0.41
1:D:1476:MET:HE3	1:D:1476:MET:HB2	1.81	0.41
1:D:1926:LEU:HD23	1:D:1929:MET:HE2	2.02	0.41
1:D:2454:ARG:CZ	1:D:2458:ARG:HH21	2.34	0.41
1:D:3648:ARG:O	1:D:3652:MET:HG2	2.20	0.41
1:A:869:ARG:CZ	1:A:870:ILE:HB	2.50	0.41
1:A:1259:ARG:HH12	1:A:1596:GLU:HA	1.85	0.41
1:A:1434:TYR:HA	1:A:1518:CYS:O	2.20	0.41
1:A:2866:THR:OG1	1:A:2867:LEU:N	2.54	0.41
1:A:3659:ALA:HA	1:A:3663:LEU:HD12	2.03	0.41
1:A:3694:LYS:HA	1:A:3695:PRO:HD3	1.90	0.41
1:A:3937:TYR:O	1:A:4002:LYS:NZ	2.44	0.41
1:B:2930:LEU:O	1:B:2935:TYR:N	2.49	0.41
1:C:113:HIS:NE2	1:C:399:GLN:O	2.51	0.41
1:C:2039:LEU:HD22	1:C:2044:ILE:HG13	2.02	0.41
1:C:3582:ARG:HD3	1:C:3582:ARG:HA	1.87	0.41
1:D:129:ASP:OD1	1:D:129:ASP:N	2.54	0.41
1:D:2039:LEU:HD22	1:D:2044:ILE:HG13	2.02	0.41
1:D:2276:ALA:O	1:D:2279:SER:OG	2.36	0.41
1:D:2656:CYS:SG	1:D:3013:HIS:NE2	2.93	0.41
1:D:3033:ASN:O	1:D:3037:GLU:HG2	2.21	0.41
1:D:3659:ALA:HA	1:D:3663:LEU:HD12	2.03	0.41
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.87	0.41
1:A:873:LYS:HG2	1:A:970:LEU:HD13	2.02	0.41
1:A:1088:TRP:HB2	1:A:1153:ILE:HG22	2.01	0.41
1:A:2017:ASP:OD1	1:A:2017:ASP:N	2.54	0.41
1:A:2476:ILE:HG23	1:A:2536:LEU:HD21	2.01	0.41
1:A:2765:LYS:HA	1:A:2765:LYS:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3272:ILE:O	1:A:3276:MET:HG2	2.20	0.41
1:A:3376:GLU:O	1:A:3380:ARG:HG2	2.20	0.41
1:A:3628:ARG:NH2	1:A:3857:GLY:O	2.54	0.41
1:A:3710:LEU:HD21	1:A:3781:GLN:HG2	2.02	0.41
1:A:3883:ASP:HA	1:A:3886:ARG:HB3	2.03	0.41
1:A:3965:LEU:HD23	1:A:3965:LEU:HA	1.94	0.41
1:A:4850:LEU:HD23	1:A:4850:LEU:HA	1.93	0.41
1:B:1253:PRO:HG2	1:B:1254:HIS:CD2	2.55	0.41
1:B:1568:LYS:O	1:B:1569:GLN:NE2	2.53	0.41
1:B:1811:ALA:HA	1:B:1814:MET:HE3	2.03	0.41
1:B:2782:ASP:OD1	1:B:2782:ASP:N	2.52	0.41
1:B:3062:PRO:HA	1:B:3065:VAL:HG22	2.03	0.41
1:B:3207:GLU:OE1	1:B:3280:TYR:OH	2.33	0.41
1:B:3703:LEU:HD23	1:B:3703:LEU:HA	1.93	0.41
1:B:3722:TYR:HE1	1:B:3778:MET:HE1	1.86	0.41
1:B:3901:ASN:OD1	1:B:3904:ARG:NH1	2.34	0.41
1:C:547:VAL:HB	1:C:560:ILE:HD11	2.03	0.41
1:C:829:TYR:HB3	1:C:1073:ARG:HH11	1.86	0.41
1:C:1088:TRP:HB2	1:C:1153:ILE:HG22	2.02	0.41
1:C:1433:TYR:HB3	1:C:1575:LEU:HD23	2.03	0.41
1:C:1446:SER:O	1:C:1496:TRP:NE1	2.43	0.41
1:C:1842:LEU:HD23	1:C:1842:LEU:HA	1.95	0.41
1:C:2971:GLN:HG2	1:C:3045:LYS:NZ	2.36	0.41
1:C:3539:ARG:NH1	1:C:3553:LEU:HG	2.35	0.41
1:C:3554:GLN:HA	1:C:3557:LEU:HG	2.02	0.41
1:D:49:LEU:HD23	1:D:49:LEU:HA	1.93	0.41
1:D:2472:LEU:HD23	1:D:2472:LEU:HA	1.87	0.41
1:D:2902:HIS:HB3	1:D:2905:LEU:HG	2.02	0.41
1:D:4645:CYS:SG	1:D:4646:LEU:N	2.93	0.41
1:A:1811:ALA:HA	1:A:1814:MET:HE3	2.03	0.41
1:A:2208:MET:HE2	1:A:2208:MET:HB2	1.88	0.41
1:A:2902:HIS:HB3	1:A:2905:LEU:HG	2.02	0.41
1:A:3562:LYS:HE2	1:A:3562:LYS:HB2	1.92	0.41
1:B:865:PRO:HA	1:B:868:GLU:HG2	2.03	0.41
1:B:1433:TYR:HB3	1:B:1575:LEU:HD23	2.03	0.41
1:B:2531:ARG:HH22	1:B:2581:SER:HB2	1.85	0.41
1:B:2640:PRO:HA	1:B:2643:LEU:HB3	2.03	0.41
1:B:4813:LEU:O	1:B:4816:ILE:HG12	2.20	0.41
1:C:865:PRO:HA	1:C:868:GLU:HG2	2.03	0.41
1:C:1229:ASN:HB2	1:C:1827:ARG:HG3	2.03	0.41
1:C:1259:ARG:HH12	1:C:1596:GLU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3826:VAL:HG12	1:C:3830:GLN:HG3	2.03	0.41
1:C:4813:LEU:O	1:C:4816:ILE:HG12	2.20	0.41
1:D:547:VAL:HB	1:D:560:ILE:HD11	2.03	0.41
1:D:1126:GLY:HA3	1:D:1143:TRP:CZ3	2.56	0.41
1:D:2710:LEU:HA	1:D:2711:PRO:HD3	1.98	0.41
1:D:3201:MET:HG2	1:D:3203:VAL:H	1.86	0.41
1:D:3628:ARG:NH2	1:D:3857:GLY:O	2.54	0.41
1:D:3852:LYS:HE3	1:D:3852:LYS:HB3	1.94	0.41
1:A:1433:TYR:HB3	1:A:1575:LEU:HD23	2.03	0.40
1:A:2656:CYS:SG	1:A:3013:HIS:NE2	2.93	0.40
1:A:3201:MET:HG2	1:A:3203:VAL:H	1.86	0.40
1:A:3537:LYS:HZ1	1:A:3603:LEU:HB2	1.86	0.40
1:A:3648:ARG:O	1:A:3652:MET:HG2	2.20	0.40
1:A:3826:VAL:HG12	1:A:3830:GLN:HG3	2.03	0.40
1:A:4581:LYS:HE3	1:A:4581:LYS:HB3	1.82	0.40
1:A:4918:ILE:HD11	1:D:4888:TYR:HA	2.03	0.40
1:B:1863:LEU:HB3	1:B:1871:PHE:HD2	1.86	0.40
1:B:2159:LEU:HD21	1:B:2163:ARG:HH21	1.86	0.40
1:B:2710:LEU:HA	1:B:2711:PRO:HD3	1.98	0.40
1:B:3965:LEU:HD23	1:B:3965:LEU:HA	1.94	0.40
1:C:220:LEU:HB2	1:C:391:THR:O	2.20	0.40
1:C:2531:ARG:HH22	1:C:2581:SER:HB2	1.85	0.40
1:C:3062:PRO:HA	1:C:3065:VAL:HG22	2.03	0.40
1:C:3628:ARG:NH2	1:C:3857:GLY:O	2.54	0.40
1:C:4577:LEU:HD12	1:C:4577:LEU:HA	1.94	0.40
1:D:220:LEU:HB2	1:D:391:THR:O	2.20	0.40
1:D:1259:ARG:HH12	1:D:1596:GLU:HA	1.85	0.40
1:D:1488:LYS:HB2	1:D:1488:LYS:HE3	1.86	0.40
1:D:2531:ARG:HH22	1:D:2581:SER:HB2	1.85	0.40
1:D:3710:LEU:HD21	1:D:3781:GLN:HG2	2.02	0.40
1:D:4044:MET:HE2	1:D:4044:MET:HB2	1.95	0.40
1:A:116:MET:HE2	1:A:139:GLU:HA	2.02	0.40
1:A:1290:ARG:HH12	1:A:1455:PRO:HA	1.85	0.40
1:A:3390:GLY:HA2	1:A:3393:LEU:HD13	2.04	0.40
1:A:3601:ALA:O	1:A:3605:HIS:ND1	2.40	0.40
1:A:4555:LEU:HD12	1:A:4555:LEU:HA	1.94	0.40
1:A:4666:VAL:O	1:A:4670:ILE:HG12	2.21	0.40
1:A:4813:LEU:O	1:A:4816:ILE:HG12	2.20	0.40
1:B:1088:TRP:HB2	1:B:1153:ILE:HG22	2.02	0.40
1:B:1259:ARG:HH12	1:B:1596:GLU:HA	1.85	0.40
1:B:2866:THR:OG1	1:B:2867:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3201:MET:HG2	1:B:3203:VAL:H	1.86	0.40
1:B:3272:ILE:O	1:B:3276:MET:HG2	2.20	0.40
1:B:4745:LEU:H	1:B:4745:LEU:HG	1.55	0.40
1:C:1568:LYS:O	1:C:1569:GLN:NE2	2.53	0.40
1:C:1776:HIS:HB3	1:C:1798:LEU:HD13	2.04	0.40
1:C:3573:MET:HB3	1:C:3577:ARG:NH2	2.36	0.40
1:C:4686:LEU:O	1:C:4691:GLN:N	2.49	0.40
1:D:2159:LEU:HD21	1:D:2163:ARG:HH21	1.86	0.40
1:D:2640:PRO:HA	1:D:2643:LEU:HB3	2.03	0.40
1:D:4152:GLU:OE1	1:D:4192:ARG:NH1	2.51	0.40
1:D:4976:GLU:H	1:D:4976:GLU:HG2	1.59	0.40
1:A:3160:ASP:OD1	1:A:3160:ASP:N	2.53	0.40
1:A:4843:LEU:HD22	1:D:4823:LEU:HD22	2.03	0.40
1:B:59:PRO:HD3	1:B:307:ALA:HB3	2.02	0.40
1:B:873:LYS:HG2	1:B:970:LEU:HD13	2.02	0.40
1:B:2765:LYS:HA	1:B:2765:LYS:HD3	1.87	0.40
1:B:4000:MET:HG2	1:B:4016:LEU:HD23	2.04	0.40
1:C:1926:LEU:HD23	1:C:1929:MET:HE2	2.02	0.40
1:C:2640:PRO:HA	1:C:2643:LEU:HB3	2.04	0.40
1:C:3201:MET:HG2	1:C:3203:VAL:H	1.86	0.40
1:C:4016:LEU:HD12	1:C:4016:LEU:HA	1.84	0.40
1:D:179:TYR:N	1:D:194:SER:O	2.54	0.40
1:D:1776:HIS:HB3	1:D:1798:LEU:HD13	2.04	0.40
1:D:1849:LEU:HD23	1:D:1849:LEU:HA	1.87	0.40
1:D:2186:MET:HE1	1:D:2235:PHE:HA	2.02	0.40
1:D:3573:MET:HB3	1:D:3577:ARG:NH2	2.36	0.40
1:D:3826:VAL:HG12	1:D:3830:GLN:HG3	2.04	0.40
1:A:129:ASP:OD1	1:A:129:ASP:N	2.54	0.40
1:A:2825:LYS:NZ	1:A:2935:TYR:OH	2.45	0.40
1:A:3901:ASN:OD1	1:A:3904:ARG:NH1	2.34	0.40
1:B:647:ASN:ND2	1:B:824:GLU:OE2	2.54	0.40
1:B:1776:HIS:HB3	1:B:1798:LEU:HD13	2.04	0.40
1:B:2325:PRO:HB2	1:B:2421:ALA:HB1	2.04	0.40
1:C:484:LEU:HD21	1:C:540:PHE:HE1	1.87	0.40
1:C:873:LYS:HG2	1:C:970:LEU:HD13	2.02	0.40
1:C:932:LEU:HD22	1:C:984:LEU:HD21	2.03	0.40
1:D:144:GLU:HG3	1:D:175:SER:HB3	2.04	0.40
1:D:647:ASN:ND2	1:D:824:GLU:OE2	2.54	0.40
1:D:1229:ASN:HB2	1:D:1827:ARG:HG3	2.03	0.40
1:D:1863:LEU:HB3	1:D:1871:PHE:HD2	1.86	0.40
1:D:3390:GLY:HA2	1:D:3393:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3539:ARG:NH1	1:D:3553:LEU:HG	2.35	0.40
1:D:4000:MET:HG2	1:D:4016:LEU:HD23	2.04	0.40
1:D:4813:LEU:O	1:D:4816:ILE:HG12	2.20	0.40
1:D:4869:GLU:H	1:D:4869:GLU:HG2	1.74	0.40
1:D:5012:LYS:HD3	1:D:5012:LYS:HA	1.64	0.40
1:A:547:VAL:HB	1:A:560:ILE:HD11	2.03	0.40
1:A:2159:LEU:HD21	1:A:2163:ARG:HH21	1.86	0.40
1:A:3467:MET:O	1:A:3471:THR:OG1	2.37	0.40
1:B:317:ARG:HH12	1:B:349:GLN:N	2.20	0.40
1:B:880:GLU:HB3	1:B:883:ALA:HB3	2.03	0.40
1:B:2017:ASP:OD1	1:B:2017:ASP:N	2.54	0.40
1:C:266:ARG:NH2	1:C:331:VAL:O	2.51	0.40
1:C:2325:PRO:HB2	1:C:2421:ALA:HB1	2.04	0.40
1:C:3710:LEU:HD21	1:C:3781:GLN:HG2	2.02	0.40
1:C:3722:TYR:HE1	1:C:3778:MET:HE1	1.86	0.40
1:C:4801:LEU:HD23	1:C:4801:LEU:HA	1.87	0.40
1:D:116:MET:HE2	1:D:139:GLU:HA	2.02	0.40
1:D:1290:ARG:HH12	1:D:1455:PRO:HA	1.85	0.40
1:D:1445:PRO:HG2	1:D:1501:VAL:HG11	2.04	0.40
1:D:3062:PRO:HA	1:D:3065:VAL:HG22	2.03	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	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48 78
1	B	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48 78
1	C	4353/5037 (86%)	4200 (96%)	148 (3%)	5 (0%)	48 78
1	D	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	F	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	G	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	H	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
All	All	17832/21548 (83%)	17205 (96%)	607 (3%)	20 (0%)	49	78

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3692	GLU
1	A	4691	GLN
1	B	3692	GLU
1	B	4691	GLN
1	C	3692	GLU
1	C	4691	GLN
1	D	3692	GLU
1	D	4691	GLN
1	A	4712	PRO
1	B	4712	PRO
1	C	4712	PRO
1	D	4712	PRO
1	A	4819	GLY
1	B	4819	GLY
1	C	4819	GLY
1	D	4819	GLY
1	A	3292	PRO
1	B	3292	PRO
1	C	3292	PRO
1	D	3292	PRO

### 5.3.2 Protein sidechains [i](#)

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	3805/4276 (89%)	3673 (96%)	132 (4%)	32	56
1	B	3805/4276 (89%)	3673 (96%)	132 (4%)	32	56
1	C	3805/4276 (89%)	3674 (97%)	131 (3%)	32	57
1	D	3805/4276 (89%)	3673 (96%)	132 (4%)	32	56
2	E	88/304 (29%)	88 (100%)	0	100	100
2	F	88/304 (29%)	88 (100%)	0	100	100
2	G	88/304 (29%)	88 (100%)	0	100	100
2	H	88/304 (29%)	88 (100%)	0	100	100
All	All	15572/18320 (85%)	15045 (97%)	527 (3%)	34	57

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	LEU
1	A	1072	VAL
1	A	1231[A]	GLN
1	A	1231[B]	GLN
1	A	1743[A]	ARG
1	A	1743[B]	ARG
1	A	2100[A]	HIS
1	A	2100[B]	HIS
1	A	2369[A]	ARG
1	A	2369[B]	ARG
1	A	2870[A]	GLU
1	A	2870[B]	GLU
1	A	3039	ILE
1	A	3688	GLU
1	A	4178	LEU
1	A	4180	ARG
1	A	4181	ILE
1	A	4183	ILE
1	A	4188	ARG
1	A	4190	ILE
1	A	4196	GLU
1	A	4209	GLN
1	A	4212	GLU
1	A	4215	ARG
1	A	4221	VAL
1	A	4224	GLU
1	A	4227	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	4230	LYS
1	A	4231	MET
1	A	4244	GLU
1	A	4252	SER
1	A	4543	GLU
1	A	4544	LEU
1	A	4546	VAL
1	A	4549	VAL
1	A	4550	LYS
1	A	4555	LEU
1	A	4556	SER
1	A	4561	THR
1	A	4577	LEU
1	A	4578	LEU
1	A	4581	LYS
1	A	4583	SER
1	A	4584	ASP
1	A	4627	MET
1	A	4628	VAL
1	A	4633	GLU
1	A	4634	GLU
1	A	4635	SER
1	A	4639	MET
1	A	4645	CYS
1	A	4648	LEU
1	A	4649	LEU
1	A	4651	THR
1	A	4665	LYS
1	A	4666	VAL
1	A	4667	PRO
1	A	4680	LYS
1	A	4689	THR
1	A	4695	ASP
1	A	4697	VAL
1	A	4704	LEU
1	A	4706	LEU
1	A	4707	ASN
1	A	4708	THR
1	A	4710	SER
1	A	4713	SER
1	A	4716	TRP
1	A	4720	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	4721	LYS
1	A	4725	LEU
1	A	4727	LYS
1	A	4730	ASP
1	A	4731	ILE
1	A	4737	ILE
1	A	4743	MET
1	A	4745	LEU
1	A	4747	SER
1	A	4749	GLU
1	A	4772	ASP
1	A	4773	VAL
1	A	4774	LYS
1	A	4777	ILE
1	A	4779	LYS
1	A	4788	SER
1	A	4818	MET
1	A	4821	LYS
1	A	4822	THR
1	A	4824	ARG
1	A	4835	LYS
1	A	4837	LEU
1	A	4844	LEU
1	A	4861	LYS
1	A	4865	LYS
1	A	4867	GLU
1	A	4869	GLU
1	A	4871	GLU
1	A	4876	CYS
1	A	4887	MET
1	A	4889	VAL
1	A	4908	GLU
1	A	4911	LEU
1	A	4913	ARG
1	A	4920	PHE
1	A	4927	ILE
1	A	4932	ILE
1	A	4933	GLN
1	A	4945	ASP
1	A	4949	GLN
1	A	4951	LYS
1	A	4957	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	4965	SER
1	A	4966	ASP
1	A	4976	GLU
1	A	4980	LEU
1	A	4981	GLU
1	A	4985	LEU
1	A	4989	MET
1	A	4992	LEU
1	A	4995	LEU
1	A	4997	ASN
1	A	4998	LYS
1	A	5002	GLU
1	A	5004	THR
1	A	5006	GLN
1	A	5012	LYS
1	A	5015	GLN
1	A	5016	GLU
1	A	5028	PHE
1	A	5030	LYS
1	A	5031	GLN
1	A	5034	ASP
1	B	846	LEU
1	B	1072	VAL
1	B	1231[A]	GLN
1	B	1231[B]	GLN
1	B	1743[A]	ARG
1	B	1743[B]	ARG
1	B	2100[A]	HIS
1	B	2100[B]	HIS
1	B	2369[A]	ARG
1	B	2369[B]	ARG
1	B	2870[A]	GLU
1	B	2870[B]	GLU
1	B	3039	ILE
1	B	3688	GLU
1	B	4178	LEU
1	B	4180	ARG
1	B	4181	ILE
1	B	4183	ILE
1	B	4188	ARG
1	B	4190	ILE
1	B	4196	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	4209	GLN
1	B	4212	GLU
1	B	4215	ARG
1	B	4221	VAL
1	B	4224	GLU
1	B	4227	GLU
1	B	4230	LYS
1	B	4231	MET
1	B	4244	GLU
1	B	4252	SER
1	B	4543	GLU
1	B	4544	LEU
1	B	4546	VAL
1	B	4549	VAL
1	B	4550	LYS
1	B	4555	LEU
1	B	4556	SER
1	B	4561	THR
1	B	4577	LEU
1	B	4578	LEU
1	B	4581	LYS
1	B	4583	SER
1	B	4584	ASP
1	B	4627	MET
1	B	4628	VAL
1	B	4633	GLU
1	B	4634	GLU
1	B	4635	SER
1	B	4639	MET
1	B	4645	CYS
1	B	4648	LEU
1	B	4649	LEU
1	B	4651	THR
1	B	4665	LYS
1	B	4666	VAL
1	B	4667	PRO
1	B	4680	LYS
1	B	4689	THR
1	B	4695	ASP
1	B	4697	VAL
1	B	4704	LEU
1	B	4706	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	4707	ASN
1	B	4708	THR
1	B	4710	SER
1	B	4713	SER
1	B	4716	TRP
1	B	4720	VAL
1	B	4721	LYS
1	B	4725	LEU
1	B	4727	LYS
1	B	4730	ASP
1	B	4731	ILE
1	B	4737	ILE
1	B	4743	MET
1	B	4745	LEU
1	B	4747	SER
1	B	4749	GLU
1	B	4772	ASP
1	B	4773	VAL
1	B	4774	LYS
1	B	4777	ILE
1	B	4779	LYS
1	B	4788	SER
1	B	4818	MET
1	B	4821	LYS
1	B	4822	THR
1	B	4824	ARG
1	B	4835	LYS
1	B	4837	LEU
1	B	4844	LEU
1	B	4861	LYS
1	B	4865	LYS
1	B	4867	GLU
1	B	4869	GLU
1	B	4871	GLU
1	B	4876	CYS
1	B	4887	MET
1	B	4889	VAL
1	B	4908	GLU
1	B	4911	LEU
1	B	4913	ARG
1	B	4920	PHE
1	B	4927	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	4932	ILE
1	B	4933	GLN
1	B	4945	ASP
1	B	4949	GLN
1	B	4951	LYS
1	B	4957	LYS
1	B	4965	SER
1	B	4966	ASP
1	B	4976	GLU
1	B	4980	LEU
1	B	4981	GLU
1	B	4985	LEU
1	B	4989	MET
1	B	4992	LEU
1	B	4995	LEU
1	B	4997	ASN
1	B	4998	LYS
1	B	5002	GLU
1	B	5004	THR
1	B	5006	GLN
1	B	5012	LYS
1	B	5015	GLN
1	B	5016	GLU
1	B	5028	PHE
1	B	5030	LYS
1	B	5031	GLN
1	B	5034	ASP
1	C	846	LEU
1	C	1072	VAL
1	C	1231[A]	GLN
1	C	1231[B]	GLN
1	C	1743[A]	ARG
1	C	1743[B]	ARG
1	C	2100[A]	HIS
1	C	2100[B]	HIS
1	C	2369[A]	ARG
1	C	2369[B]	ARG
1	C	2870[A]	GLU
1	C	2870[B]	GLU
1	C	3039	ILE
1	C	3688	GLU
1	C	4178	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	4180	ARG
1	C	4181	ILE
1	C	4183	ILE
1	C	4188	ARG
1	C	4190	ILE
1	C	4196	GLU
1	C	4209	GLN
1	C	4212	GLU
1	C	4215	ARG
1	C	4221	VAL
1	C	4224	GLU
1	C	4227	GLU
1	C	4230	LYS
1	C	4231	MET
1	C	4244	GLU
1	C	4252	SER
1	C	4543	GLU
1	C	4544	LEU
1	C	4546	VAL
1	C	4549	VAL
1	C	4550	LYS
1	C	4555	LEU
1	C	4556	SER
1	C	4561	THR
1	C	4577	LEU
1	C	4578	LEU
1	C	4581	LYS
1	C	4583	SER
1	C	4584	ASP
1	C	4627	MET
1	C	4628	VAL
1	C	4633	GLU
1	C	4634	GLU
1	C	4635	SER
1	C	4639	MET
1	C	4645	CYS
1	C	4648	LEU
1	C	4651	THR
1	C	4665	LYS
1	C	4666	VAL
1	C	4667	PRO
1	C	4680	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	4689	THR
1	C	4695	ASP
1	C	4697	VAL
1	C	4704	LEU
1	C	4706	LEU
1	C	4707	ASN
1	C	4708	THR
1	C	4710	SER
1	C	4713	SER
1	C	4716	TRP
1	C	4720	VAL
1	C	4721	LYS
1	C	4725	LEU
1	C	4727	LYS
1	C	4730	ASP
1	C	4731	ILE
1	C	4737	ILE
1	C	4743	MET
1	C	4745	LEU
1	C	4747	SER
1	C	4749	GLU
1	C	4772	ASP
1	C	4773	VAL
1	C	4774	LYS
1	C	4777	ILE
1	C	4779	LYS
1	C	4788	SER
1	C	4818	MET
1	C	4821	LYS
1	C	4822	THR
1	C	4824	ARG
1	C	4835	LYS
1	C	4837	LEU
1	C	4844	LEU
1	C	4861	LYS
1	C	4865	LYS
1	C	4867	GLU
1	C	4869	GLU
1	C	4871	GLU
1	C	4876	CYS
1	C	4887	MET
1	C	4889	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	4908	GLU
1	C	4911	LEU
1	C	4913	ARG
1	C	4920	PHE
1	C	4927	ILE
1	C	4932	ILE
1	C	4933	GLN
1	C	4945	ASP
1	C	4949	GLN
1	C	4951	LYS
1	C	4957	LYS
1	C	4965	SER
1	C	4966	ASP
1	C	4976	GLU
1	C	4980	LEU
1	C	4981	GLU
1	C	4985	LEU
1	C	4989	MET
1	C	4992	LEU
1	C	4995	LEU
1	C	4997	ASN
1	C	4998	LYS
1	C	5002	GLU
1	C	5004	THR
1	C	5006	GLN
1	C	5012	LYS
1	C	5015	GLN
1	C	5016	GLU
1	C	5028	PHE
1	C	5030	LYS
1	C	5031	GLN
1	C	5034	ASP
1	D	846	LEU
1	D	1072	VAL
1	D	1231[A]	GLN
1	D	1231[B]	GLN
1	D	1743[A]	ARG
1	D	1743[B]	ARG
1	D	2100[A]	HIS
1	D	2100[B]	HIS
1	D	2369[A]	ARG
1	D	2369[B]	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	2870[A]	GLU
1	D	2870[B]	GLU
1	D	3039	ILE
1	D	3688	GLU
1	D	4178	LEU
1	D	4180	ARG
1	D	4181	ILE
1	D	4183	ILE
1	D	4188	ARG
1	D	4190	ILE
1	D	4196	GLU
1	D	4209	GLN
1	D	4212	GLU
1	D	4215	ARG
1	D	4221	VAL
1	D	4224	GLU
1	D	4227	GLU
1	D	4230	LYS
1	D	4231	MET
1	D	4244	GLU
1	D	4252	SER
1	D	4543	GLU
1	D	4544	LEU
1	D	4546	VAL
1	D	4549	VAL
1	D	4550	LYS
1	D	4555	LEU
1	D	4556	SER
1	D	4561	THR
1	D	4577	LEU
1	D	4578	LEU
1	D	4581	LYS
1	D	4583	SER
1	D	4584	ASP
1	D	4627	MET
1	D	4628	VAL
1	D	4633	GLU
1	D	4634	GLU
1	D	4635	SER
1	D	4639	MET
1	D	4645	CYS
1	D	4648	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	4649	LEU
1	D	4651	THR
1	D	4665	LYS
1	D	4666	VAL
1	D	4667	PRO
1	D	4680	LYS
1	D	4689	THR
1	D	4695	ASP
1	D	4697	VAL
1	D	4704	LEU
1	D	4706	LEU
1	D	4707	ASN
1	D	4708	THR
1	D	4710	SER
1	D	4713	SER
1	D	4716	TRP
1	D	4720	VAL
1	D	4721	LYS
1	D	4725	LEU
1	D	4727	LYS
1	D	4730	ASP
1	D	4731	ILE
1	D	4737	ILE
1	D	4743	MET
1	D	4745	LEU
1	D	4747	SER
1	D	4749	GLU
1	D	4772	ASP
1	D	4773	VAL
1	D	4774	LYS
1	D	4777	ILE
1	D	4779	LYS
1	D	4788	SER
1	D	4818	MET
1	D	4821	LYS
1	D	4822	THR
1	D	4824	ARG
1	D	4835	LYS
1	D	4837	LEU
1	D	4844	LEU
1	D	4861	LYS
1	D	4865	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	4867	GLU
1	D	4869	GLU
1	D	4871	GLU
1	D	4876	CYS
1	D	4887	MET
1	D	4889	VAL
1	D	4908	GLU
1	D	4911	LEU
1	D	4913	ARG
1	D	4920	PHE
1	D	4927	ILE
1	D	4932	ILE
1	D	4933	GLN
1	D	4945	ASP
1	D	4949	GLN
1	D	4951	LYS
1	D	4957	LYS
1	D	4965	SER
1	D	4966	ASP
1	D	4976	GLU
1	D	4980	LEU
1	D	4981	GLU
1	D	4985	LEU
1	D	4989	MET
1	D	4992	LEU
1	D	4995	LEU
1	D	4997	ASN
1	D	4998	LYS
1	D	5002	GLU
1	D	5004	THR
1	D	5006	GLN
1	D	5012	LYS
1	D	5015	GLN
1	D	5016	GLU
1	D	5028	PHE
1	D	5030	LYS
1	D	5031	GLN
1	D	5034	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	151	HIS
1	A	201	ASN
1	A	241	GLN
1	A	297	GLN
1	A	308	HIS
1	A	405	HIS
1	A	479	GLN
1	A	533	ASN
1	A	576	ASN
1	A	624	ASN
1	A	877	ASN
1	A	1058	GLN
1	A	1660	GLN
1	A	1719	HIS
1	A	1938	GLN
1	A	2095	GLN
1	A	2127	GLN
1	A	2260	ASN
1	A	2498	HIS
1	A	2515	GLN
1	A	2673	HIS
1	A	2877	GLN
1	A	2881	ASN
1	A	2931	GLN
1	A	2933	ASN
1	A	3180	ASN
1	A	3608	GLN
1	A	3851	ASN
1	A	3895	HIS
1	A	4120	ASN
1	A	4162	ASN
1	A	4216	GLN
1	A	4574	ASN
1	A	4700	GLN
1	A	4707	ASN
1	A	4728	HIS
1	A	4832	HIS
1	A	4886	HIS
1	A	4947	GLN
1	B	201	ASN
1	B	241	GLN
1	B	297	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	308	HIS
1	B	405	HIS
1	B	533	ASN
1	B	576	ASN
1	B	624	ASN
1	B	866	HIS
1	B	877	ASN
1	B	1058	GLN
1	B	1660	GLN
1	B	1719	HIS
1	B	1938	GLN
1	B	2095	GLN
1	B	2127	GLN
1	B	2260	ASN
1	B	2498	HIS
1	B	2515	GLN
1	B	2673	HIS
1	B	2877	GLN
1	B	2881	ASN
1	B	2924	GLN
1	B	2931	GLN
1	B	2933	ASN
1	B	3180	ASN
1	B	3608	GLN
1	B	3851	ASN
1	B	3895	HIS
1	B	4120	ASN
1	B	4162	ASN
1	B	4216	GLN
1	B	4574	ASN
1	B	4700	GLN
1	B	4707	ASN
1	B	4728	HIS
1	B	4832	HIS
1	B	4886	HIS
1	B	4947	GLN
1	C	98	HIS
1	C	151	HIS
1	C	201	ASN
1	C	241	GLN
1	C	255	HIS
1	C	297	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	308	HIS
1	C	405	HIS
1	C	533	ASN
1	C	576	ASN
1	C	866	HIS
1	C	877	ASN
1	C	1660	GLN
1	C	1719	HIS
1	C	2045	GLN
1	C	2095	GLN
1	C	2260	ASN
1	C	2498	HIS
1	C	2515	GLN
1	C	2673	HIS
1	C	2877	GLN
1	C	2881	ASN
1	C	2924	GLN
1	C	2931	GLN
1	C	2933	ASN
1	C	3180	ASN
1	C	3608	GLN
1	C	3851	ASN
1	C	3895	HIS
1	C	4102	GLN
1	C	4120	ASN
1	C	4162	ASN
1	C	4216	GLN
1	C	4574	ASN
1	C	4700	GLN
1	C	4707	ASN
1	C	4728	HIS
1	C	4886	HIS
1	C	4947	GLN
1	D	84	ASN
1	D	151	HIS
1	D	201	ASN
1	D	241	GLN
1	D	297	GLN
1	D	308	HIS
1	D	379	HIS
1	D	405	HIS
1	D	533	ASN

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Mol	Chain	Res	Type
1	D	576	ASN
1	D	624	ASN
1	D	866	HIS
1	D	877	ASN
1	D	1660	GLN
1	D	1719	HIS
1	D	2095	GLN
1	D	2260	ASN
1	D	2498	HIS
1	D	2515	GLN
1	D	2673	HIS
1	D	2877	GLN
1	D	2881	ASN
1	D	2924	GLN
1	D	2931	GLN
1	D	2962	GLN
1	D	3180	ASN
1	D	3608	GLN
1	D	3851	ASN
1	D	3895	HIS
1	D	4120	ASN
1	D	4162	ASN
1	D	4216	GLN
1	D	4574	ASN
1	D	4700	GLN
1	D	4707	ASN
1	D	4728	HIS
1	D	4832	HIS
1	D	4886	HIS
1	D	4947	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AMP	C	5101	-	25,25,25	1.36	5 (20%)	37,38,38	1.87	8 (21%)
3	AMP	B	5101	-	25,25,25	1.36	5 (20%)	37,38,38	1.87	8 (21%)
3	AMP	A	5101	-	25,25,25	1.36	5 (20%)	37,38,38	1.87	8 (21%)
3	AMP	D	5101	-	25,25,25	1.36	5 (20%)	37,38,38	1.87	8 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	C	5101	-	-	2/10/26/26	0/3/3/3
3	AMP	B	5101	-	-	2/10/26/26	0/3/3/3
3	AMP	A	5101	-	-	2/10/26/26	0/3/3/3
3	AMP	D	5101	-	-	2/10/26/26	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	5101	AMP	C5-C4	4.26	1.46	1.39
3	A	5101	AMP	C5-C4	4.26	1.46	1.39
3	C	5101	AMP	C5-C4	4.26	1.46	1.39
3	B	5101	AMP	C5-C4	4.25	1.46	1.39
3	C	5101	AMP	C5-N7	-2.51	1.34	1.39
3	D	5101	AMP	C5-N7	-2.51	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5101	AMP	C5-N7	-2.50	1.34	1.39
3	A	5101	AMP	C5-N7	-2.50	1.34	1.39
3	B	5101	AMP	C5-C6	2.38	1.47	1.41
3	D	5101	AMP	C5-C6	2.38	1.47	1.41
3	C	5101	AMP	C5-C6	2.38	1.47	1.41
3	A	5101	AMP	C5-C6	2.37	1.47	1.41
3	C	5101	AMP	C8-N7	2.17	1.35	1.31
3	A	5101	AMP	C8-N7	2.17	1.35	1.31
3	B	5101	AMP	C8-N7	2.17	1.35	1.31
3	D	5101	AMP	C8-N7	2.17	1.35	1.31
3	A	5101	AMP	C4-N9	-2.11	1.33	1.37
3	B	5101	AMP	C4-N9	-2.11	1.33	1.37
3	D	5101	AMP	C4-N9	-2.11	1.33	1.37
3	C	5101	AMP	C4-N9	-2.11	1.33	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5101	AMP	C5-C4-N3	-5.65	118.94	126.72
3	B	5101	AMP	C5-C4-N3	-5.64	118.95	126.72
3	D	5101	AMP	C5-C4-N3	-5.64	118.95	126.72
3	C	5101	AMP	C5-C4-N3	-5.64	118.95	126.72
3	A	5101	AMP	N3-C4-N9	4.60	134.98	127.17
3	D	5101	AMP	N3-C4-N9	4.60	134.98	127.17
3	C	5101	AMP	N3-C4-N9	4.59	134.98	127.17
3	B	5101	AMP	N3-C4-N9	4.59	134.98	127.17
3	A	5101	AMP	C2-N3-C4	3.69	120.85	111.83
3	B	5101	AMP	C2-N3-C4	3.69	120.85	111.83
3	D	5101	AMP	C2-N3-C4	3.69	120.85	111.83
3	C	5101	AMP	C2-N3-C4	3.69	120.85	111.83
3	D	5101	AMP	N3-C2-N1	-3.36	123.50	128.58
3	B	5101	AMP	N3-C2-N1	-3.36	123.50	128.58
3	A	5101	AMP	N3-C2-N1	-3.35	123.51	128.58
3	C	5101	AMP	N3-C2-N1	-3.35	123.51	128.58
3	A	5101	AMP	C4-C5-N7	-3.13	107.00	110.58
3	D	5101	AMP	C4-C5-N7	-3.12	107.02	110.58
3	B	5101	AMP	C4-C5-N7	-3.12	107.02	110.58
3	C	5101	AMP	C4-C5-N7	-3.12	107.02	110.58
3	A	5101	AMP	C4-N9-C8	2.84	108.72	105.74
3	C	5101	AMP	C4-N9-C8	2.84	108.72	105.74
3	D	5101	AMP	C4-N9-C8	2.84	108.72	105.74
3	B	5101	AMP	C4-N9-C8	2.83	108.71	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5101	AMP	C5-N7-C8	2.35	107.14	103.45
3	D	5101	AMP	C5-N7-C8	2.35	107.14	103.45
3	C	5101	AMP	C5-N7-C8	2.34	107.13	103.45
3	B	5101	AMP	C5-N7-C8	2.34	107.13	103.45
3	A	5101	AMP	N9-C8-N7	-2.03	111.06	113.94
3	C	5101	AMP	N9-C8-N7	-2.03	111.06	113.94
3	D	5101	AMP	N9-C8-N7	-2.02	111.06	113.94
3	B	5101	AMP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5101	AMP	O4'-C4'-C5'-O5'
3	B	5101	AMP	O4'-C4'-C5'-O5'
3	C	5101	AMP	O4'-C4'-C5'-O5'
3	D	5101	AMP	O4'-C4'-C5'-O5'
3	A	5101	AMP	C3'-C4'-C5'-O5'
3	B	5101	AMP	C3'-C4'-C5'-O5'
3	C	5101	AMP	C3'-C4'-C5'-O5'
3	D	5101	AMP	C3'-C4'-C5'-O5'

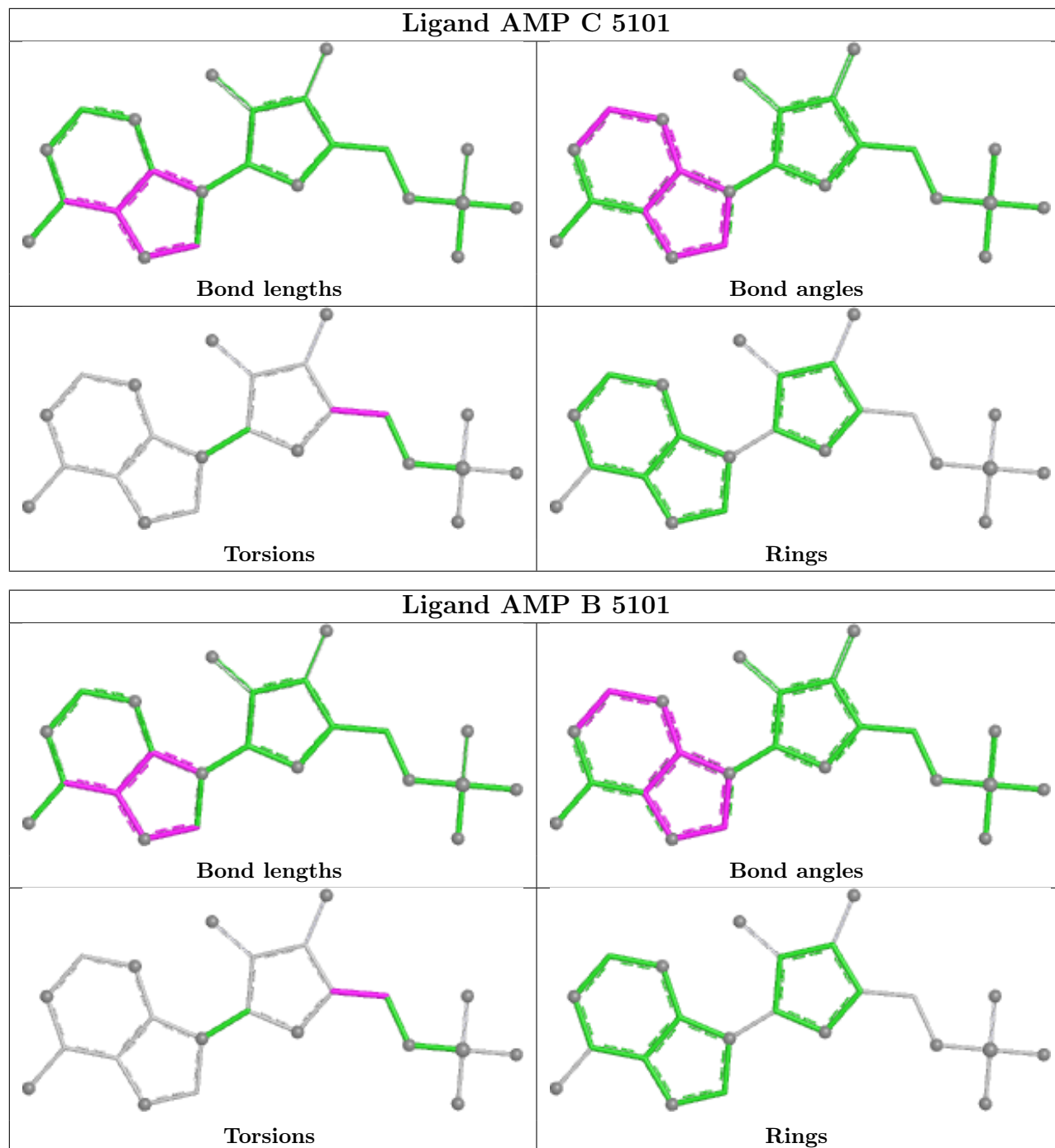
There are no ring outliers.

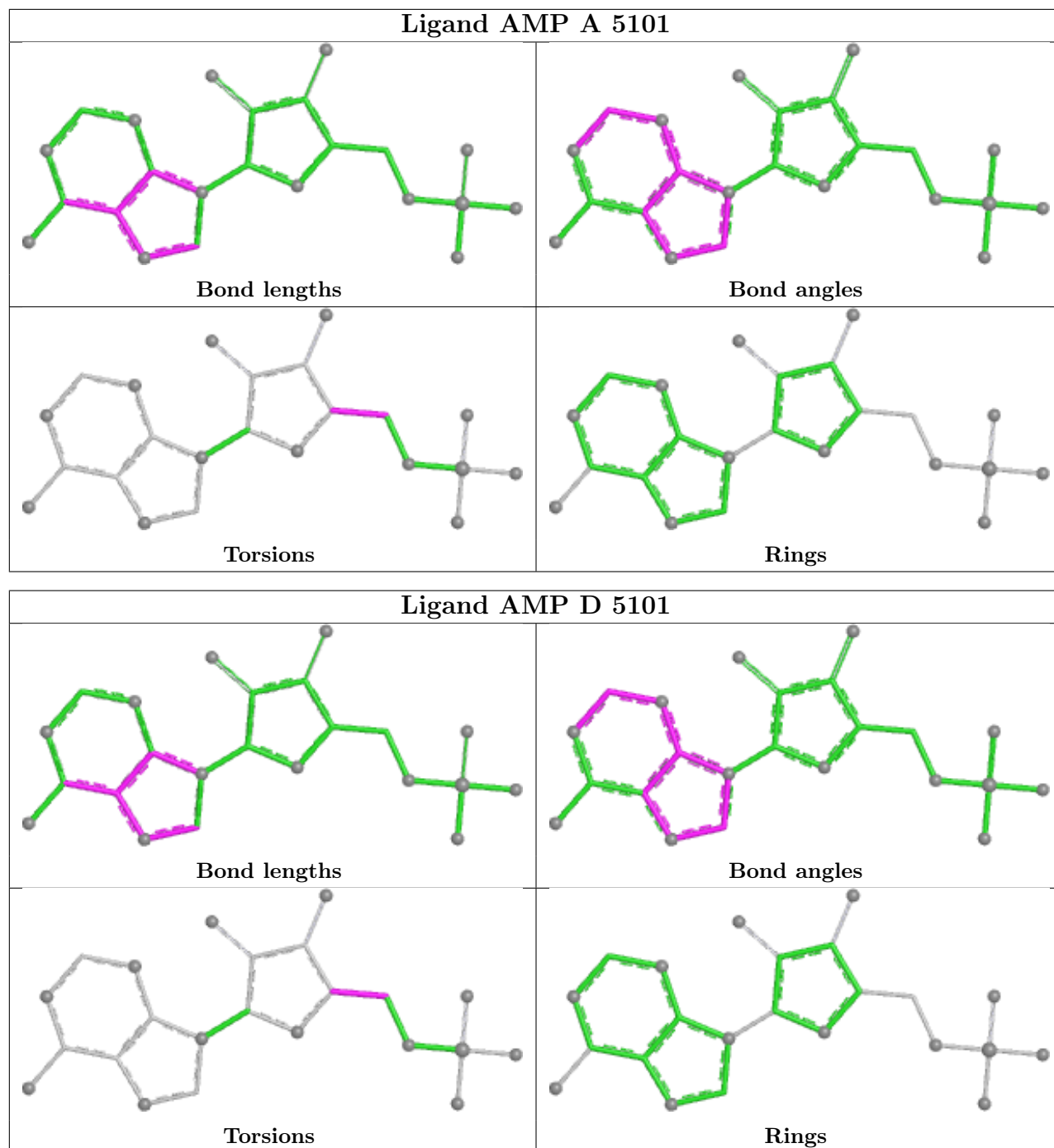
4 monomers are involved in 4 short contacts:

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

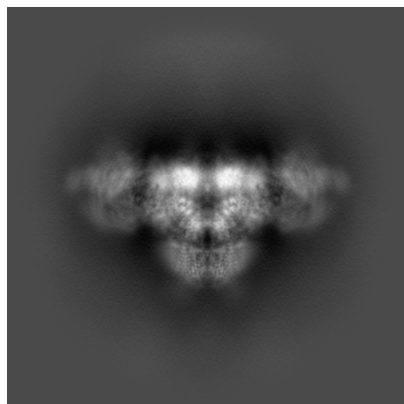
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40425. These allow visual inspection of the internal detail of the map and identification of artifacts.

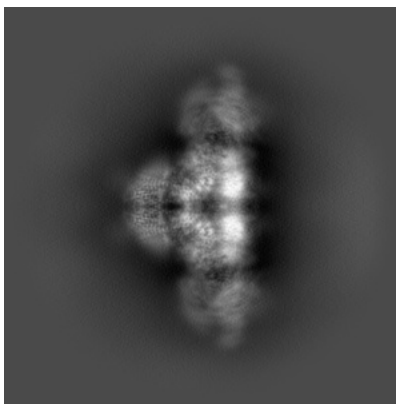
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

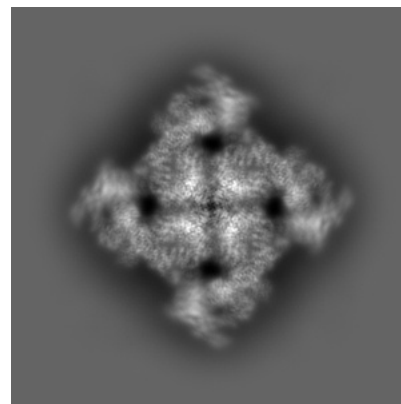
#### 6.1.1 Primary map



X

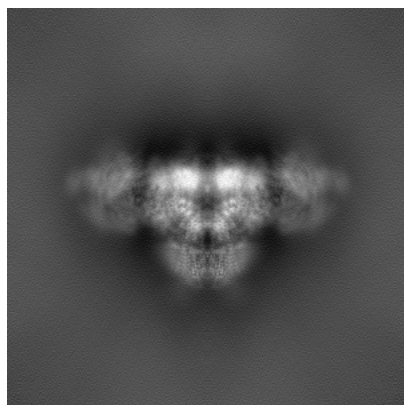


Y

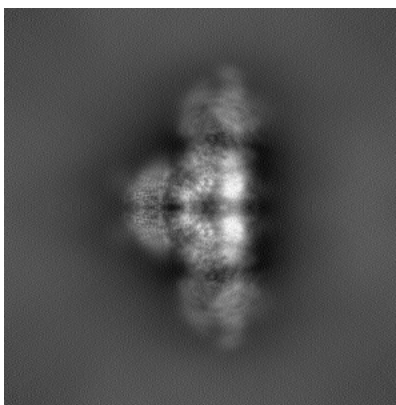


Z

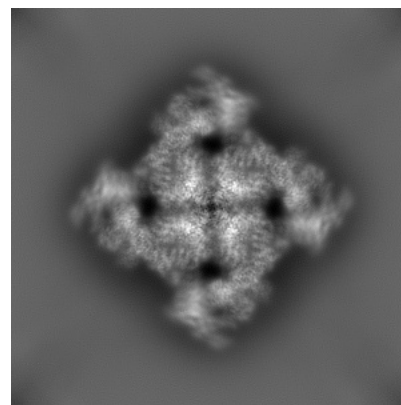
#### 6.1.2 Raw map



X



Y

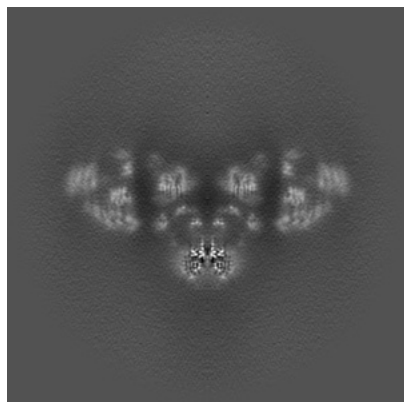


Z

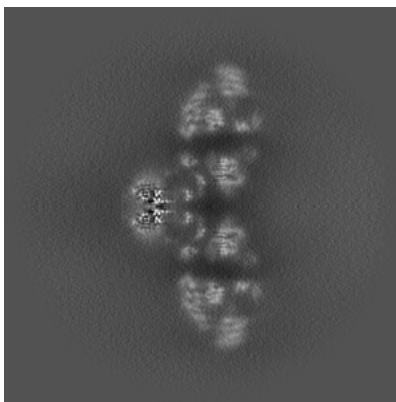
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

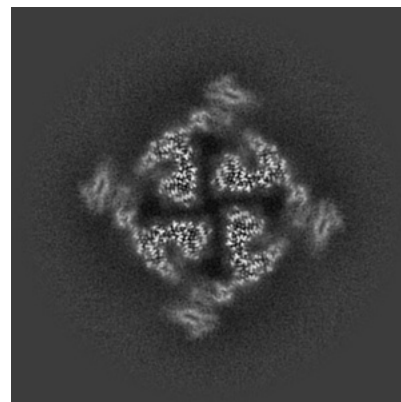
### 6.2.1 Primary map



X Index: 200

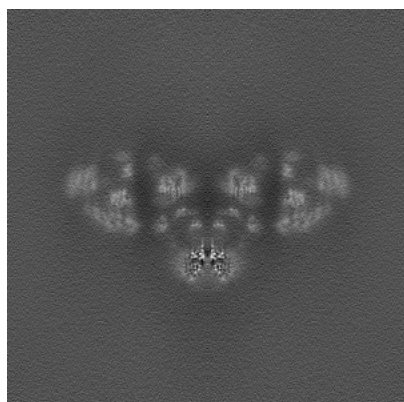


Y Index: 200

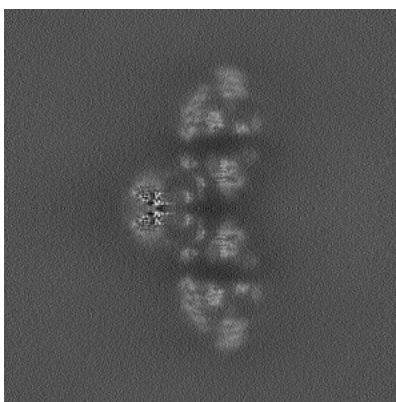


Z Index: 200

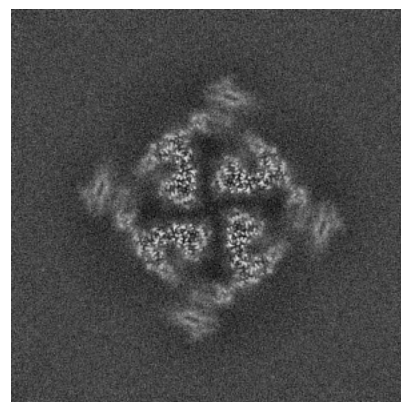
### 6.2.2 Raw map



X Index: 200



Y Index: 200

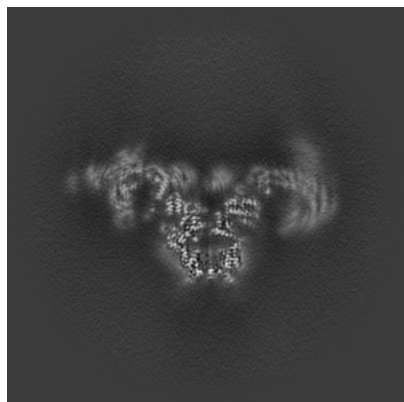


Z Index: 200

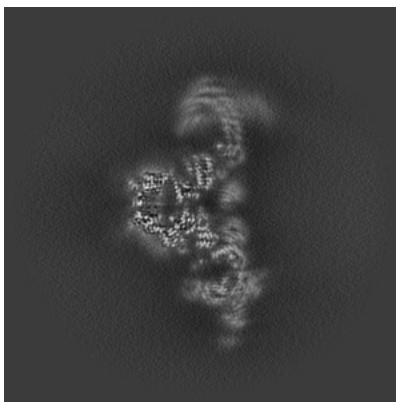
The images above show central slices of the map in three orthogonal directions.

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

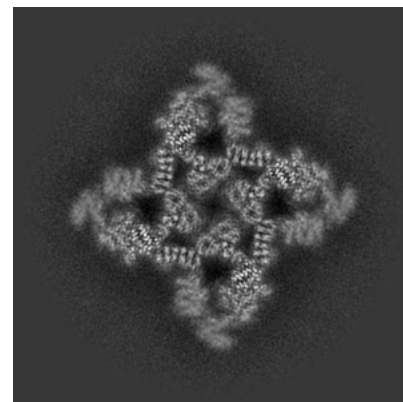
### 6.3.1 Primary map



X Index: 218

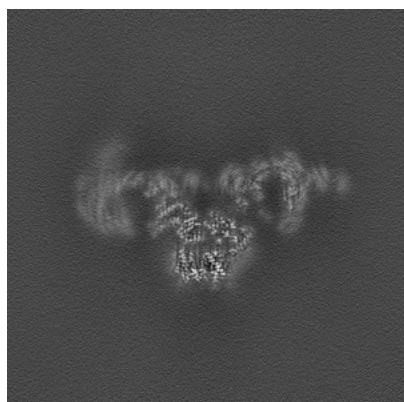


Y Index: 182

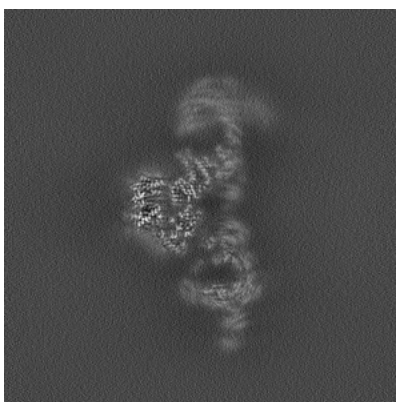


Z Index: 223

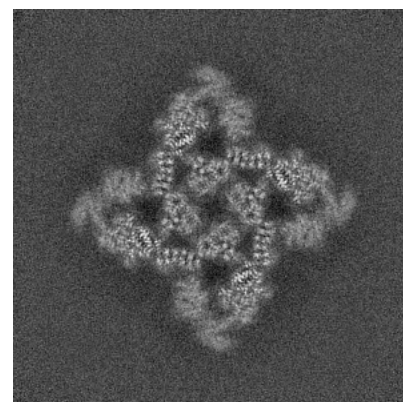
### 6.3.2 Raw map



X Index: 186



Y Index: 186

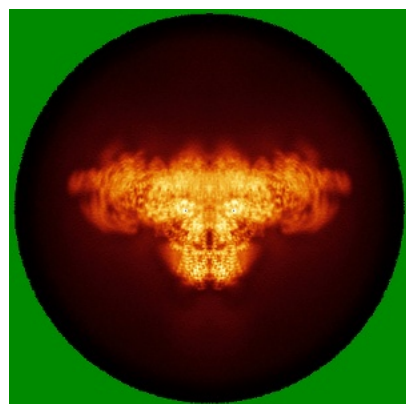


Z Index: 222

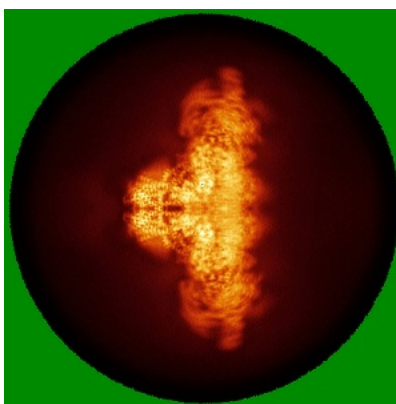
The images above show the largest variance slices of the map in three orthogonal directions.

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

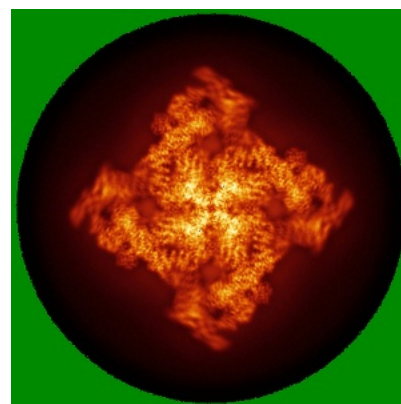
### 6.4.1 Primary map



X

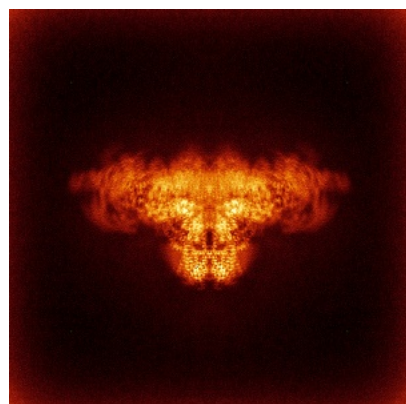


Y

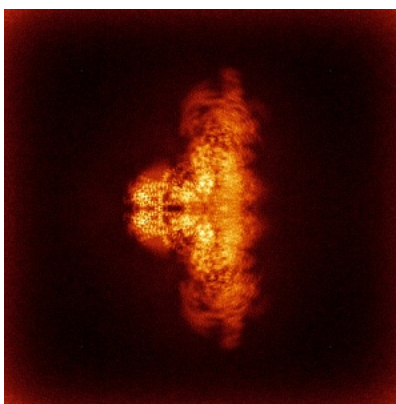


Z

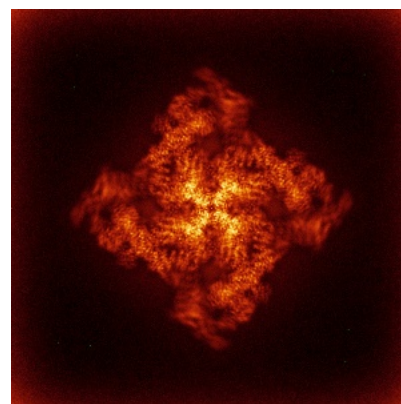
### 6.4.2 Raw map



X



Y

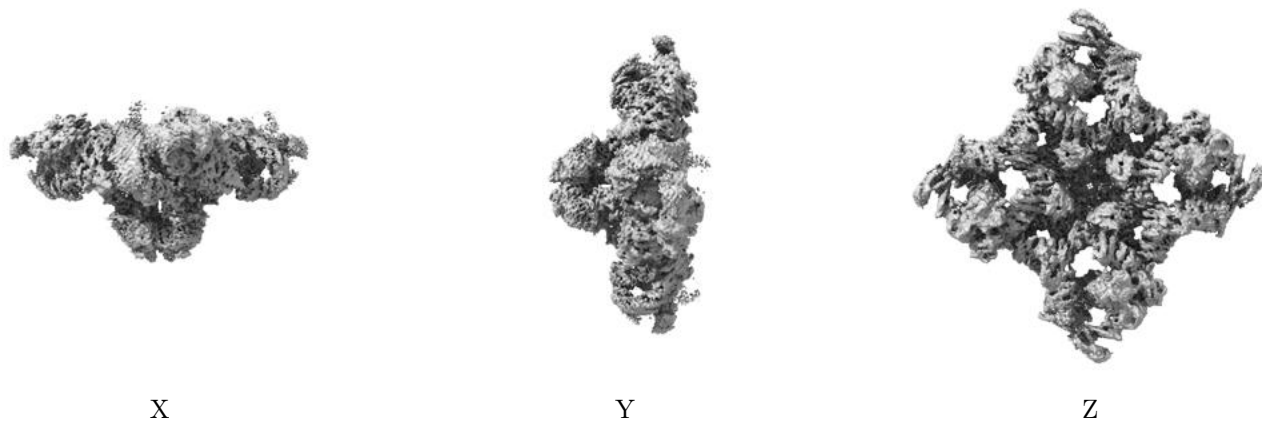


Z

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

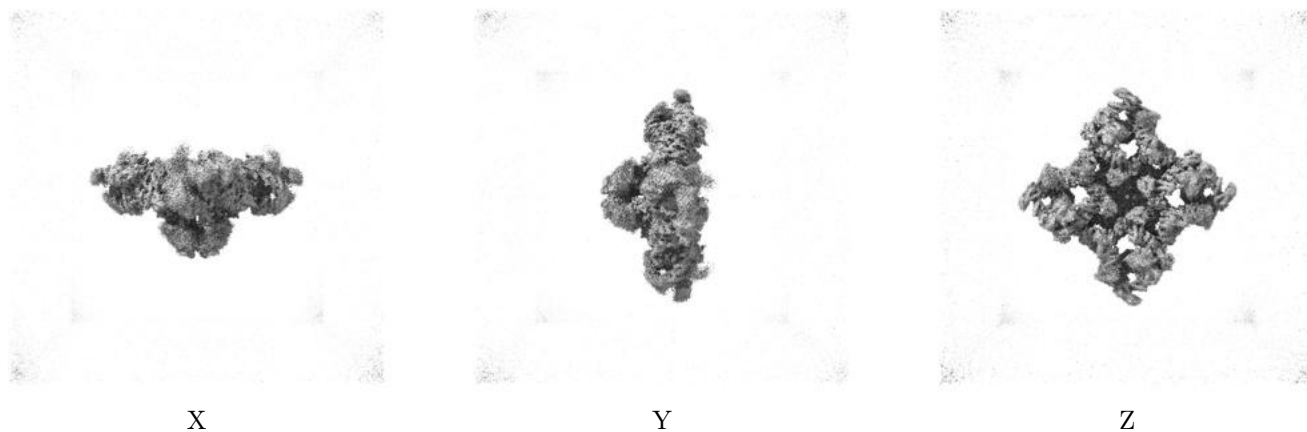
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

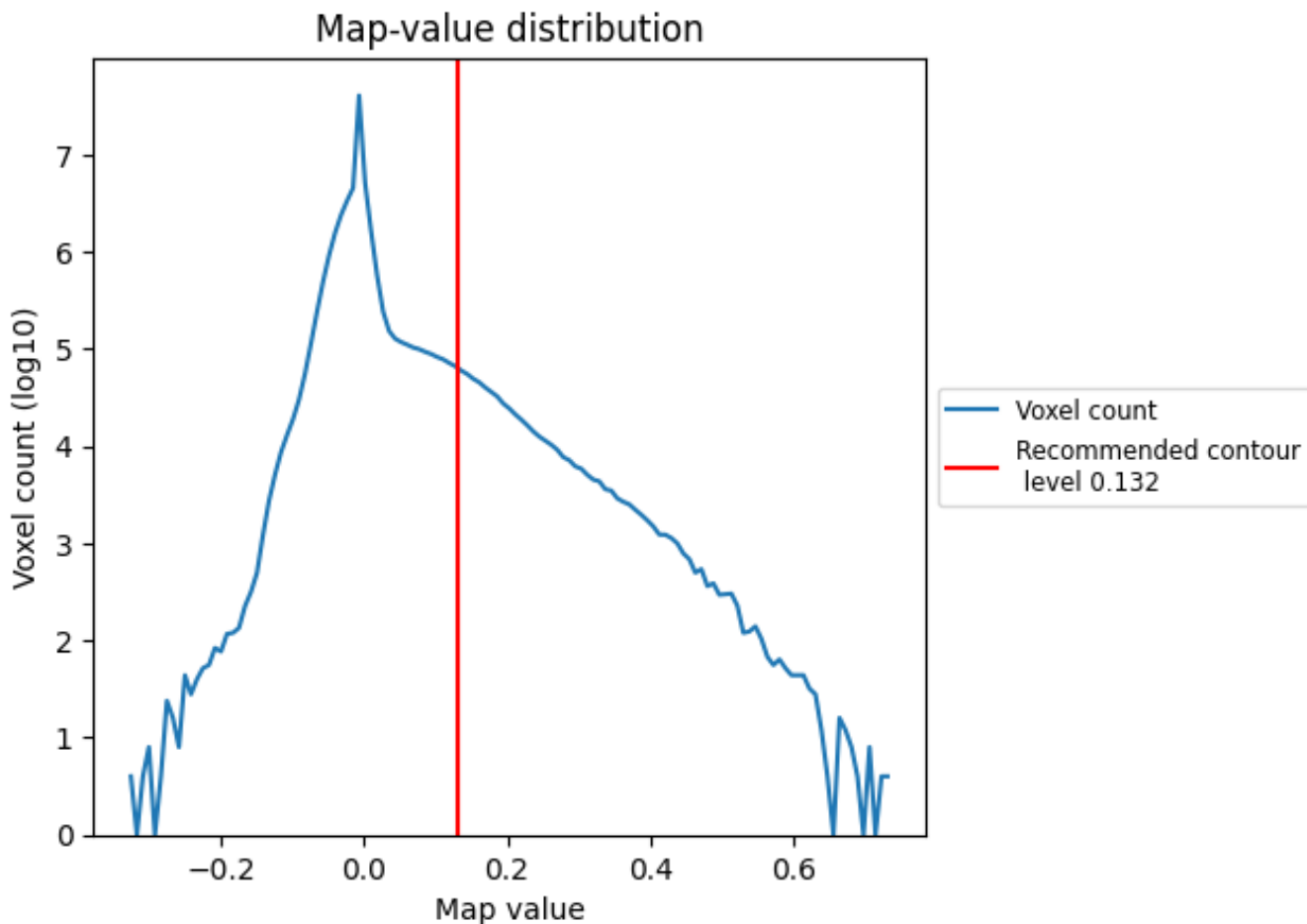
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

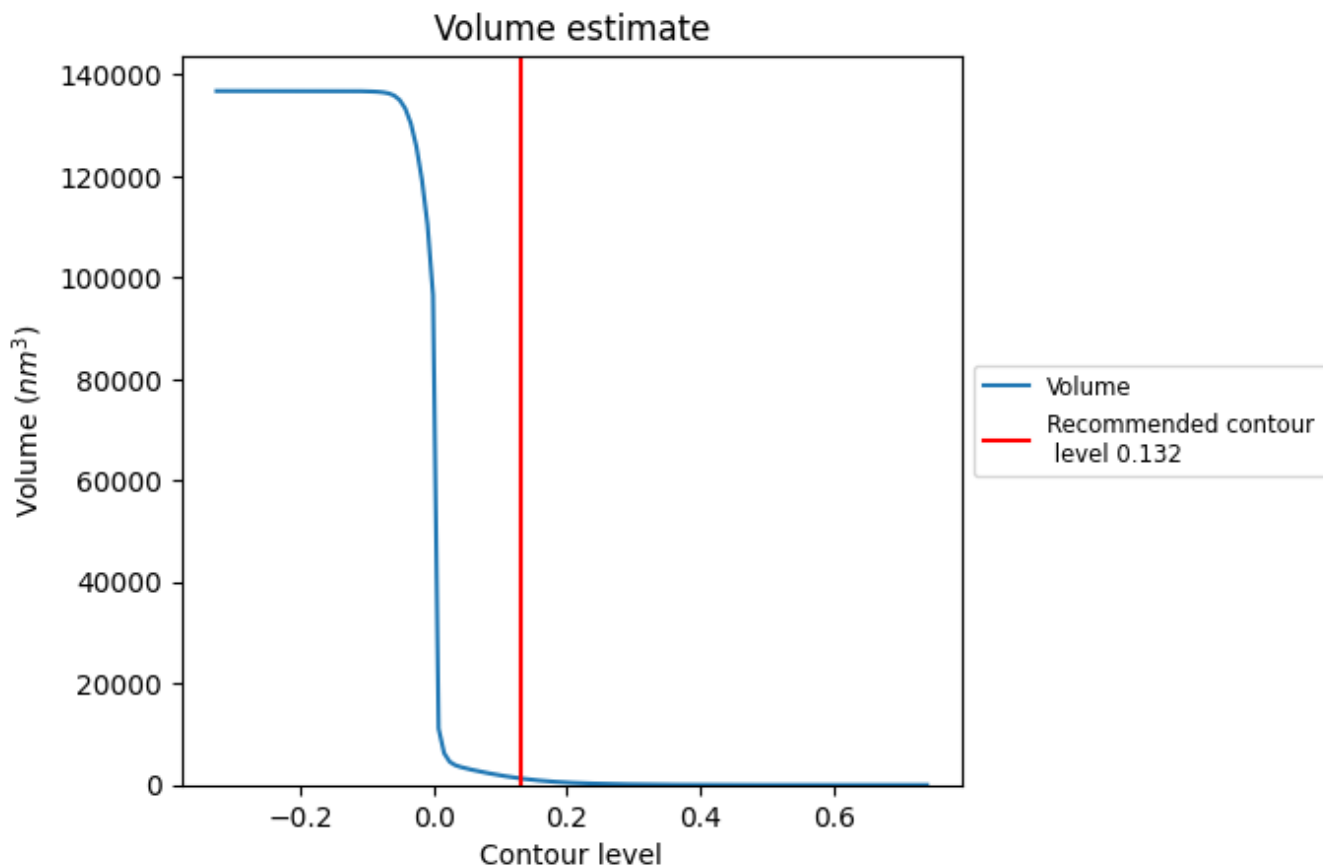
This section contains the results of statistical analysis of the map.

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



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

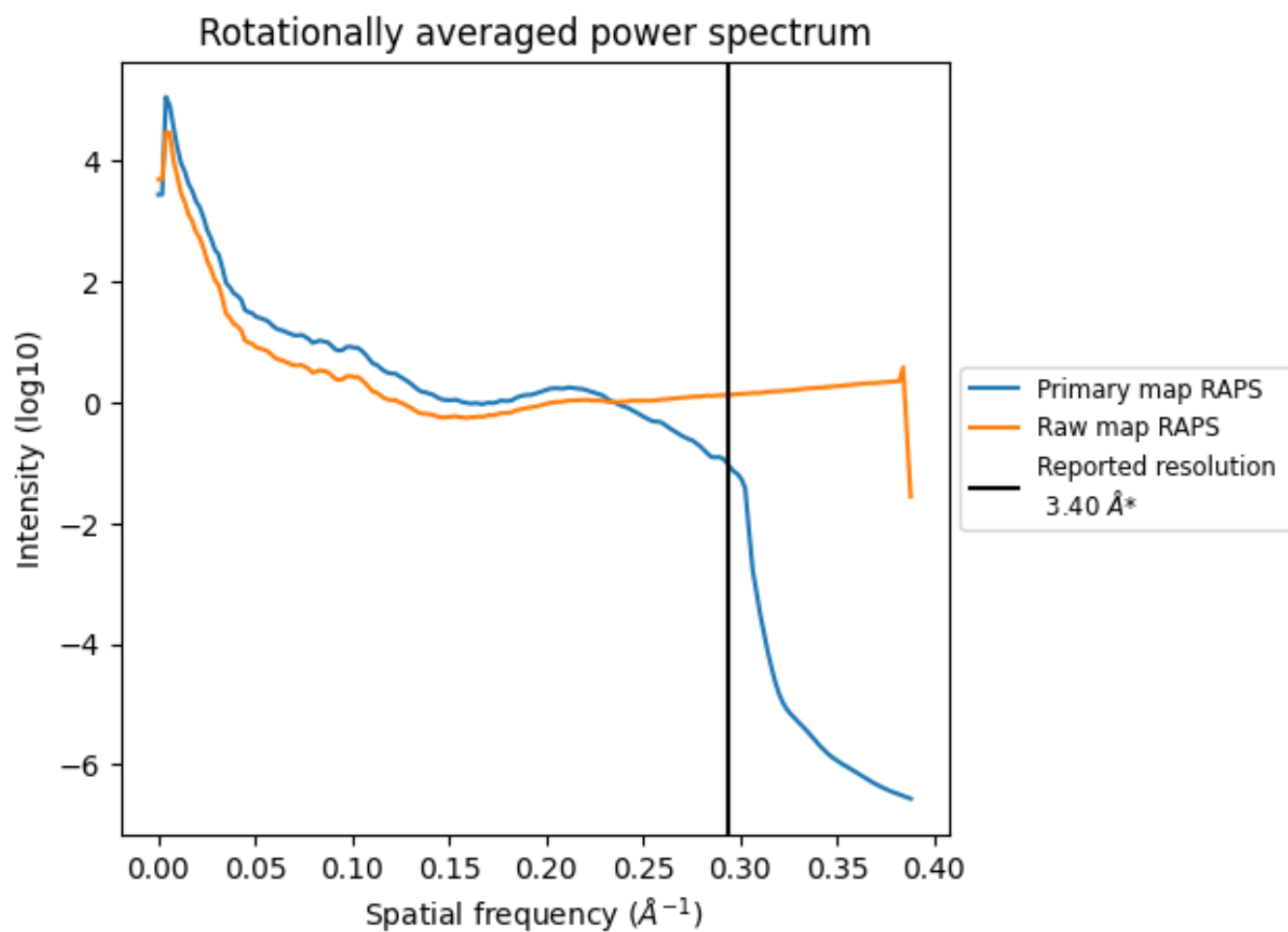
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1261  $\text{nm}^3$ ; this corresponds to an approximate mass of 1139 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 i

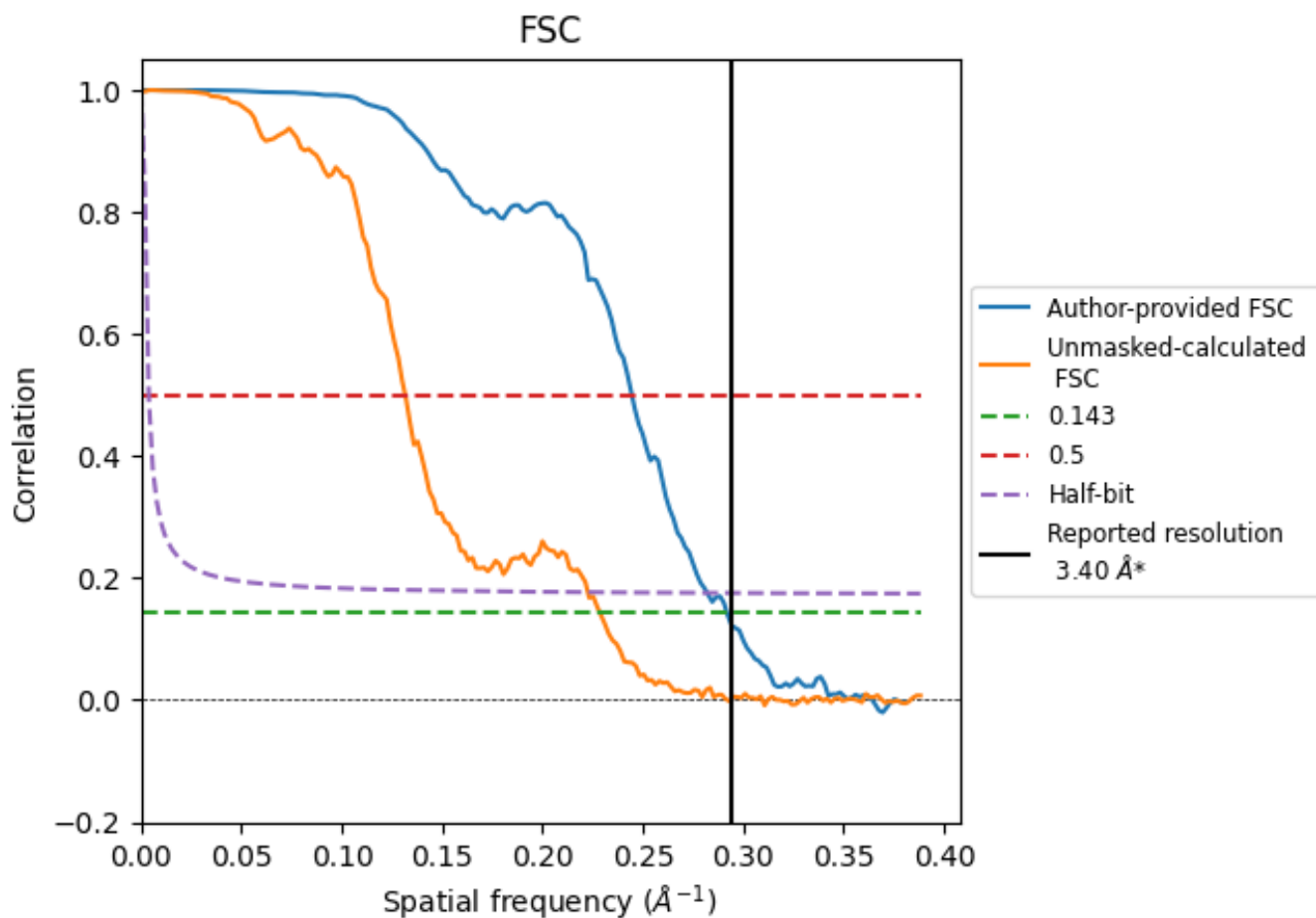


\*Reported resolution corresponds to spatial frequency of  $0.294 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

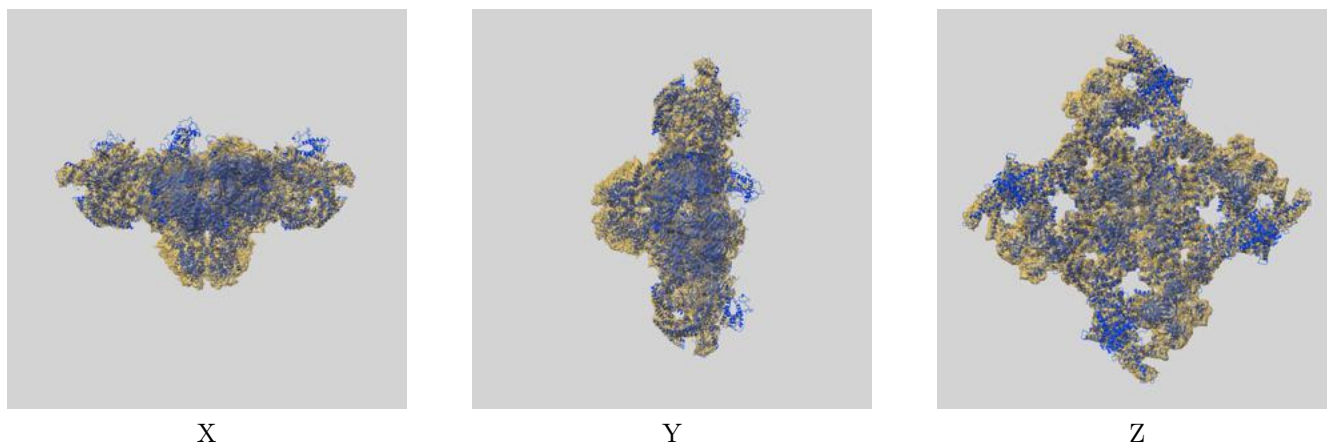
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.09	3.55
Unmasked-calculated*	4.37	7.60	4.49

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.37 differs from the reported value 3.4 by more than 10 %

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

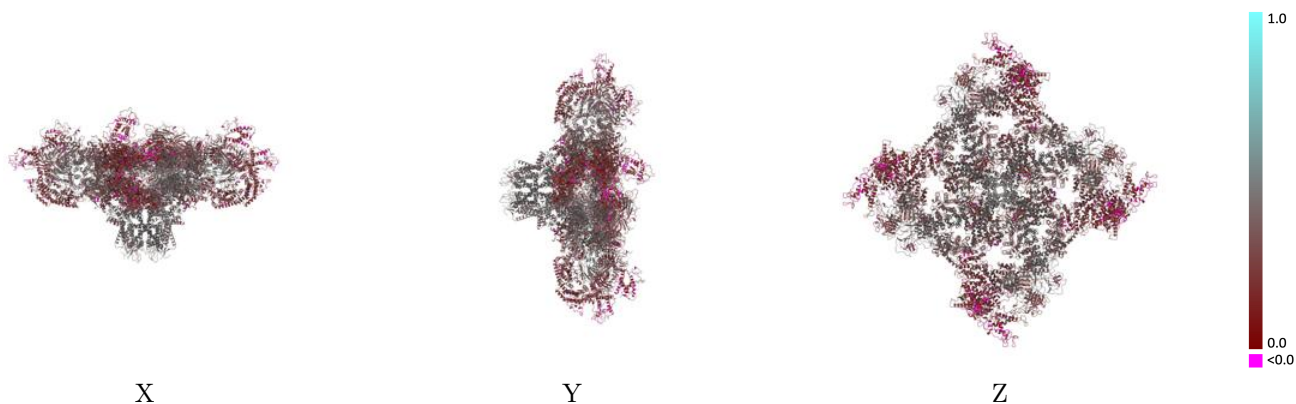
This section contains information regarding the fit between EMDB map EMD-40425 and PDB model 8SEQ. Per-residue inclusion information can be found in section 3 on page 9.

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



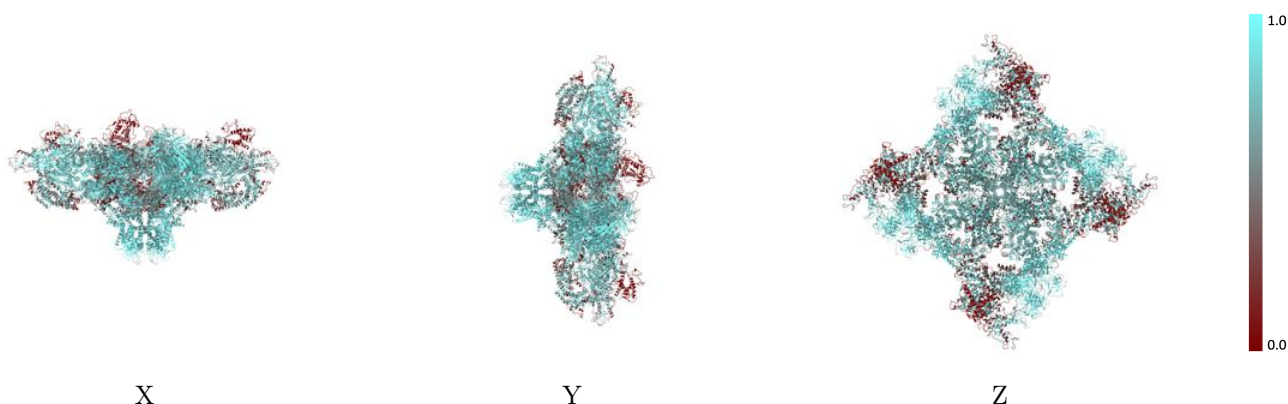
The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



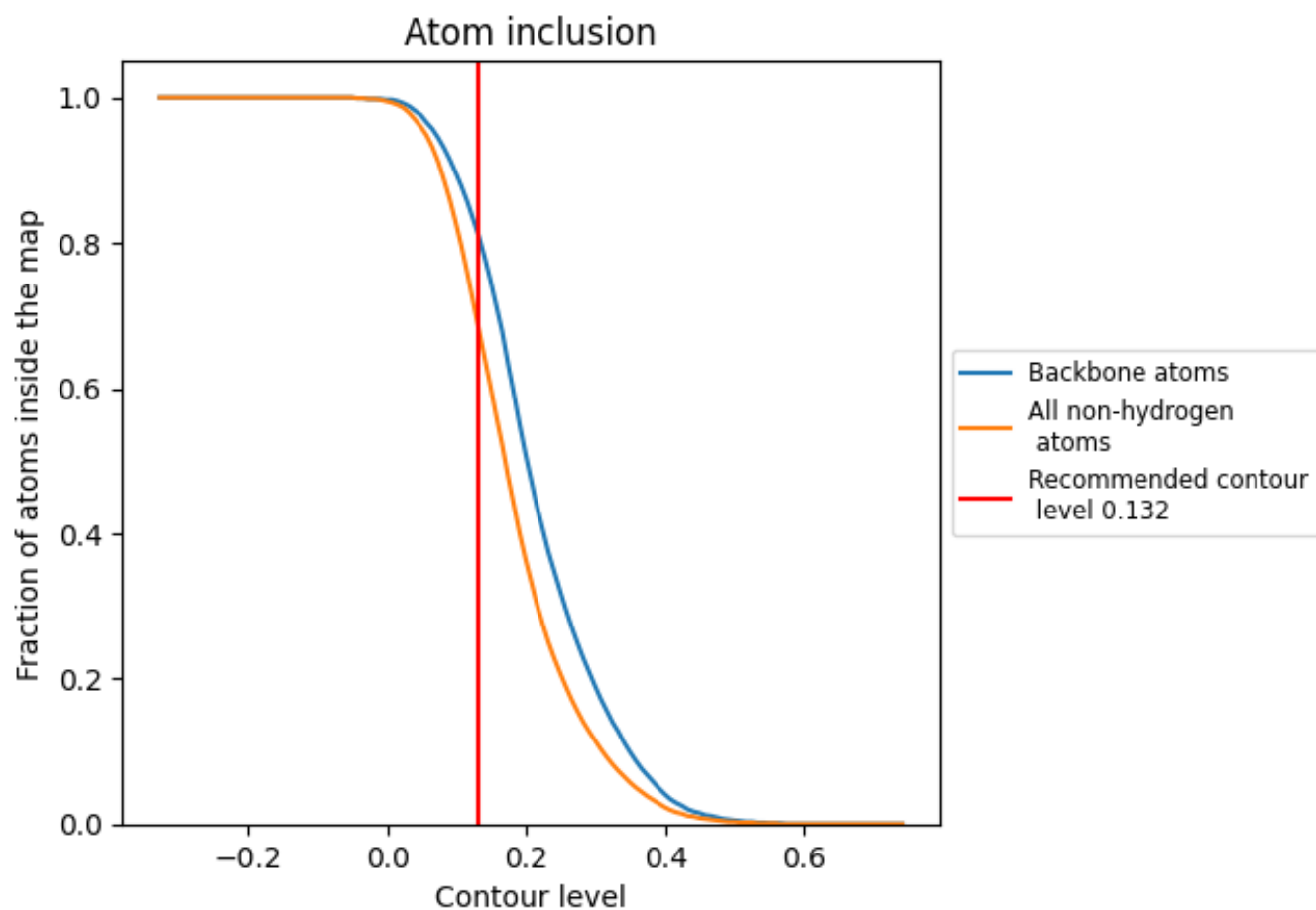
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.132).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6820	 0.3220
A	 0.6780	 0.3210
B	 0.6790	 0.3200
C	 0.6790	 0.3200
D	 0.6790	 0.3200
E	 0.8500	 0.3890
F	 0.8500	 0.3880
G	 0.8500	 0.3900
H	 0.8500	 0.3920

