



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:33 AM UTC

PDB ID : 5TAY / pdb_00005tay
EMDB ID : EMD-8389
Title : Structure of rabbit RyR1 (ryanodine dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 4.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

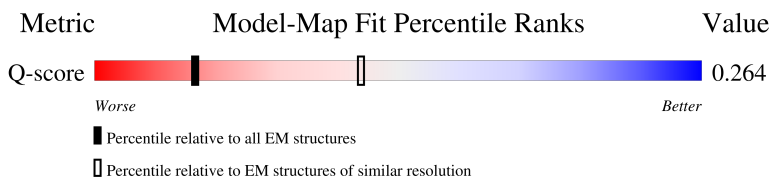
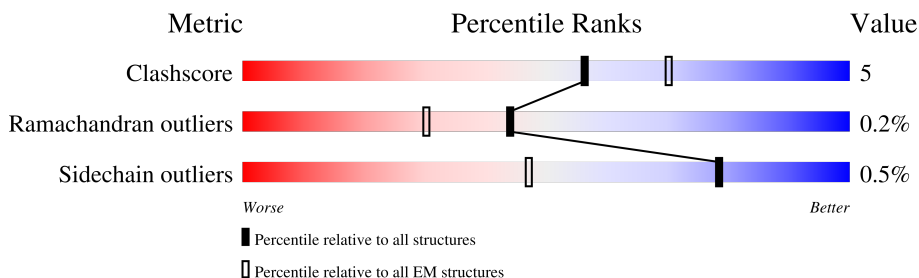
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 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.



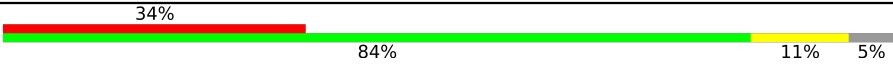
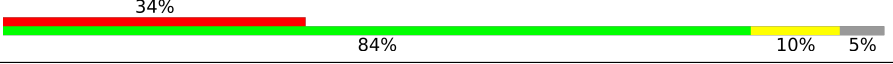
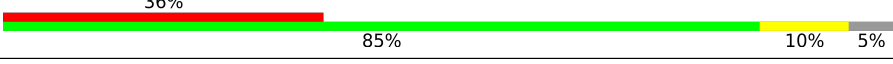
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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

Mol	Chain	Length	Quality of chain
1	A	108	
1	F	108	
1	H	108	
1	J	108	

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Mol	Chain	Length	Quality of chain
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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

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

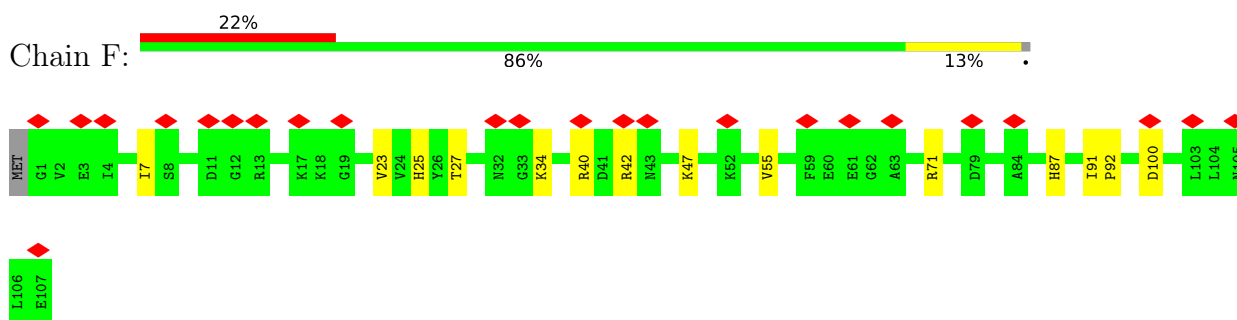
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

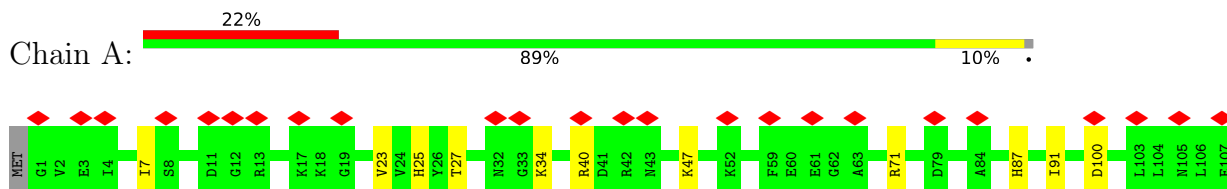
3 Residue-property plots [i](#)

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

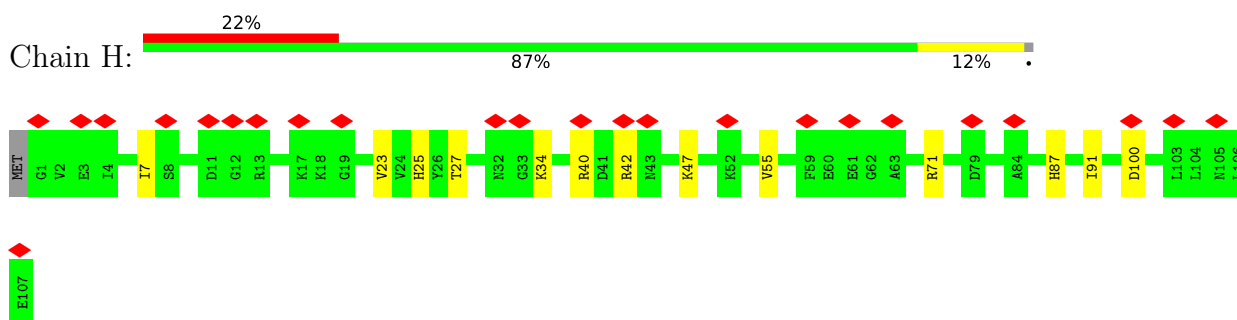
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



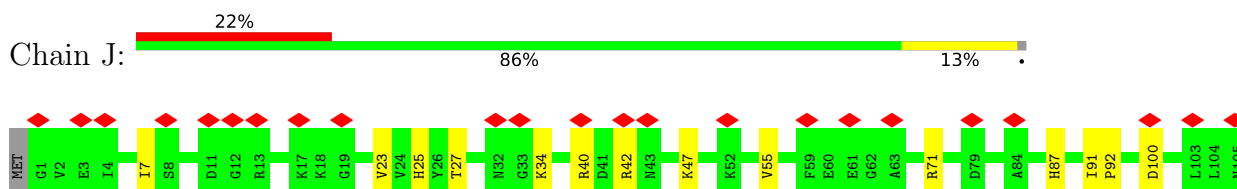
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



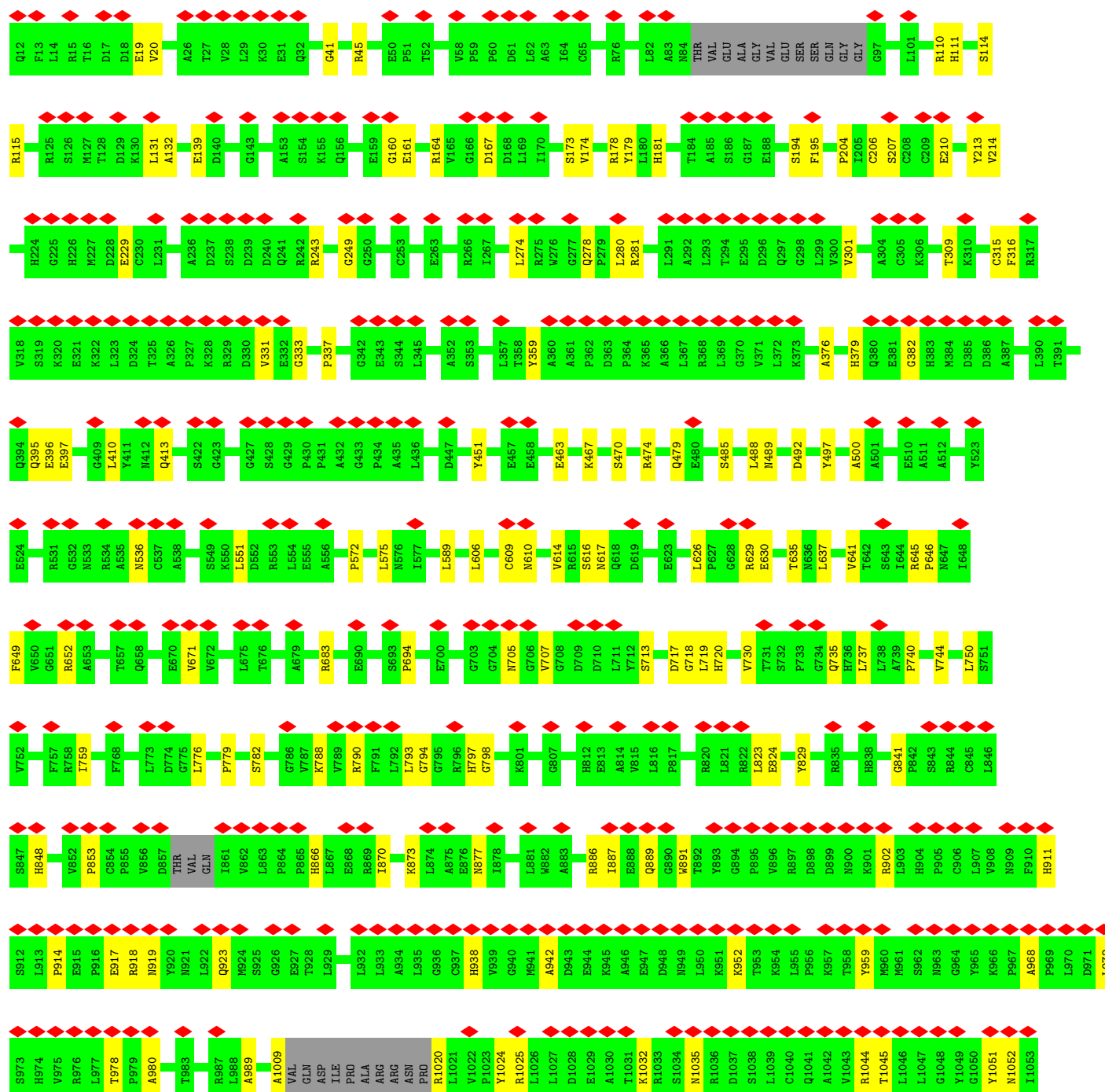
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



L106
E107

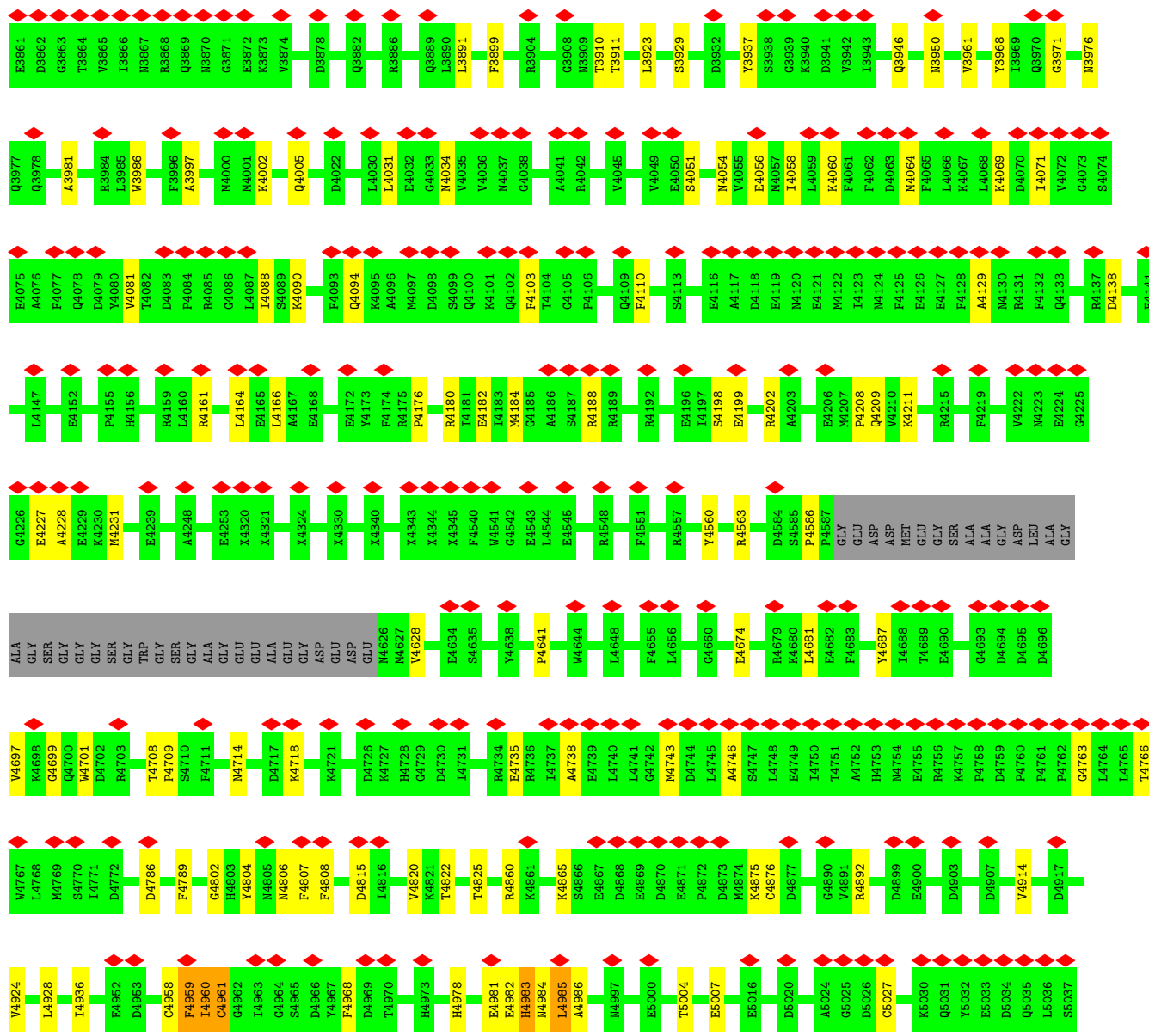
• Molecule 2: Ryanodine receptor 1

Chain B: 34% 84% 11% 5%

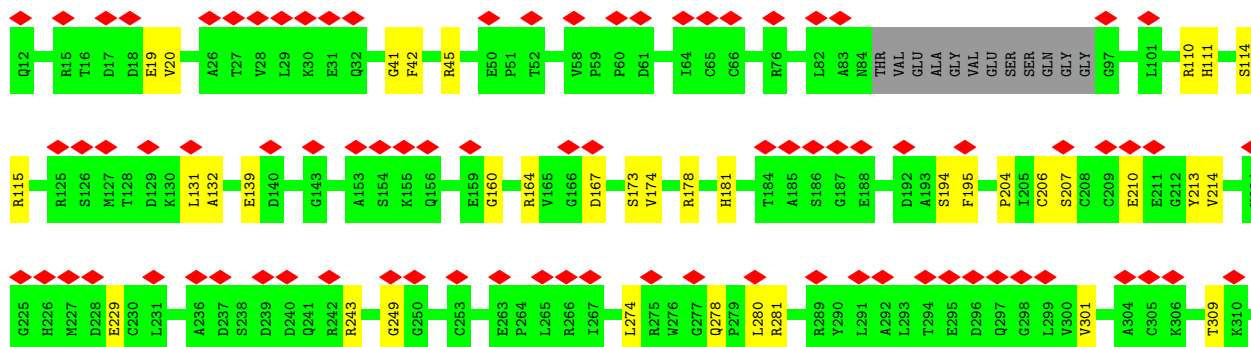
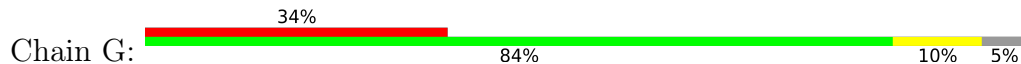


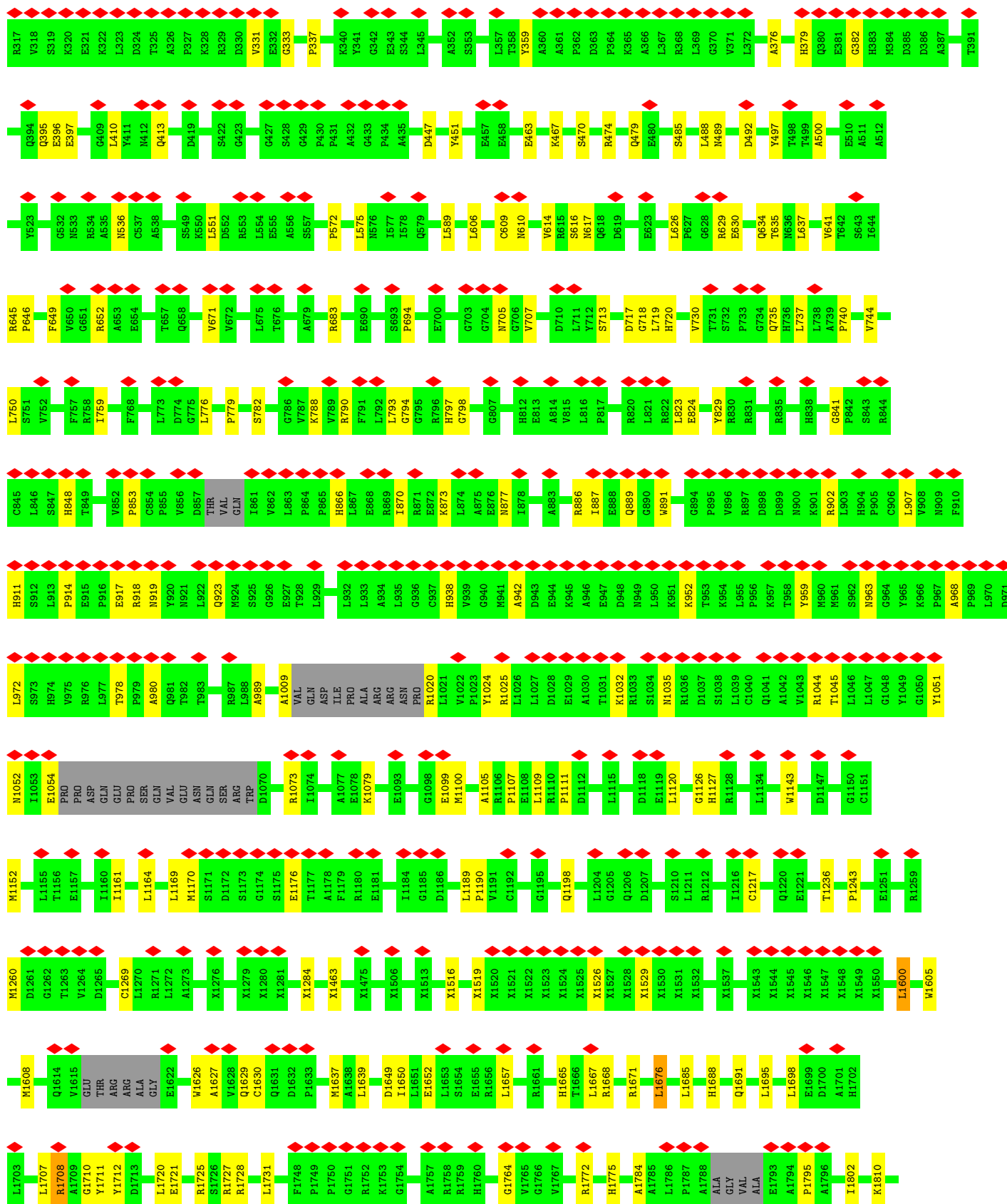


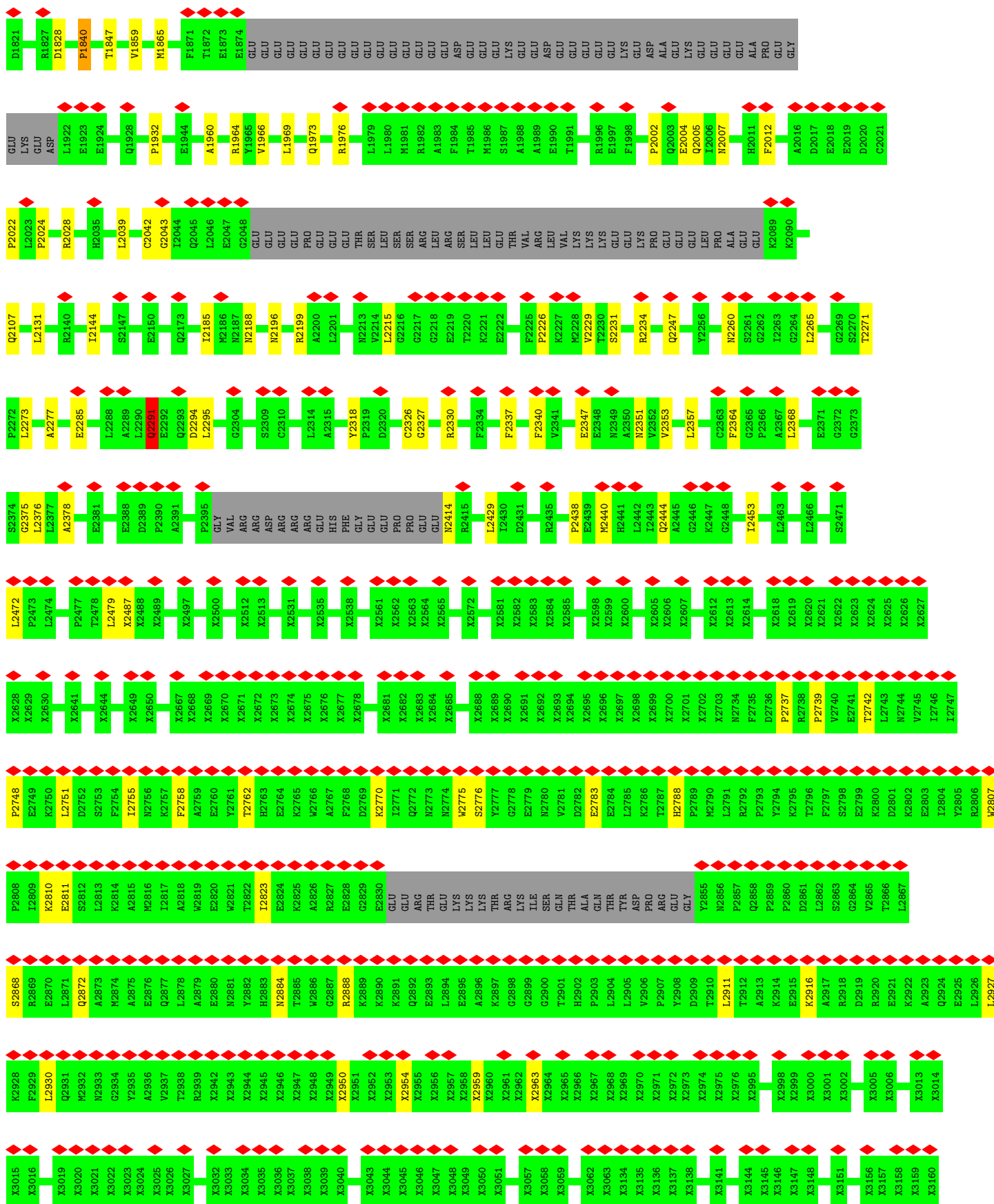
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W3661	I3662	L3663	T3664	E3665	D3666	H3667	S3668	M3673	I3674	D3675	D3676	L3677	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	K3694	P3695	L3698	R3707	L3710	T3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	I3728	G3733	H3734	L3735	E3736	E3737	Q3738	G3739	E3740	N3741	GLU	GLU	ALA							
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X3440	X3441	X3442	X3443	X3444	X3445	X3446	X3450	X3451	X3454	X3455	X3456	X3457	X3458	X3459	X3462	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3522	X3523	X3524	X3525	X3526	X3527	X3528	X3529	X3530	X3531	X3532	X3533	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3545	X3546	X3547	X3548	X3549					
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X3301	X3302	X3303	X3304	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365					
X3227	X3228	X3229	X3230	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3267	X3268	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3291	X3292	X3293	X3294	X3295	X3296	X3297	X3298		
X3135	X3136	X3137	X3138	X3142	X3143	X3144	X3145	X3146	X3147	X3148	X3153	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3170	X3171	X3172	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3199	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3225	X3226							
X2971	X2972	X2973	X2974	X2975	X2976	X2985	X2986	X2987	X2988	X2989	X3000	X3001	X3002	X3003	X3006	X3013	X3014	X3015	X3016	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3031	X3032	X3033	X3034	X3035	X3036	X3037	X3038	X3039	X3040	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3051	X3057	X3058	X3061	X3062	X3063	X3134							
D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	M2933	Q2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954	X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2965	X2966	X2967	X2968	X2969	X2970	
Tyr	ASP	PRO	ARG	GLU	Y2855	N2856	Q2857	Q2858	P2859	P2860	L2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	V2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	L2893	D2894	E2895	E2896	A2897	K2897	Q2898	G2899	L2899	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908
P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	Y2805	V2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLU	LVS	LVS	THR	ARG	LVS	ILE	SER	GLN	ALA	GLN	THR		



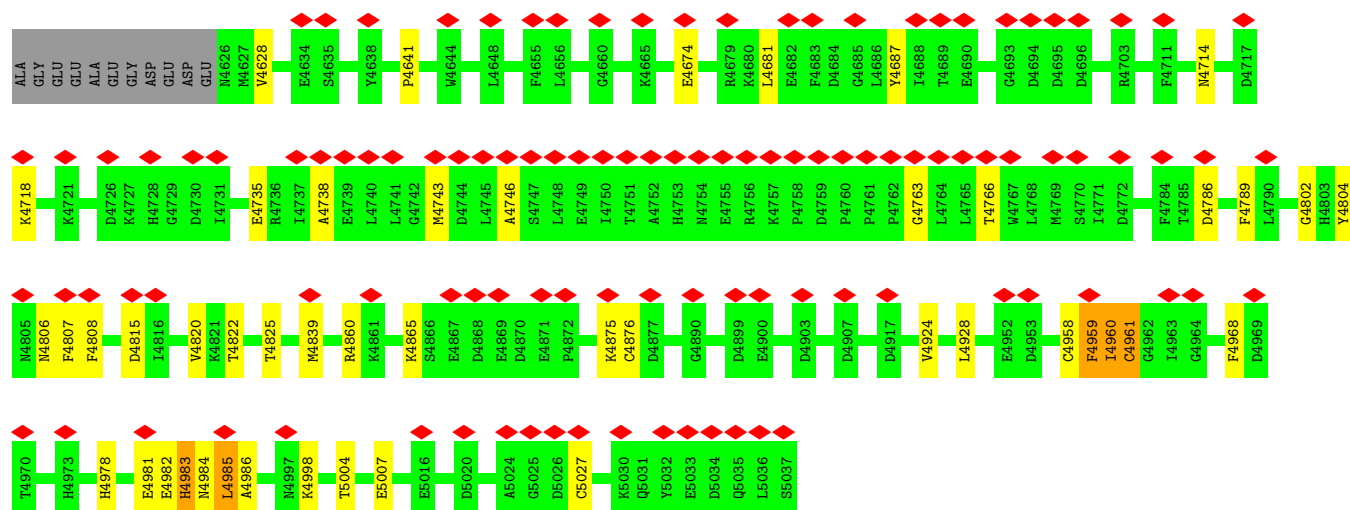
• Molecule 2: Ryanodine receptor 1



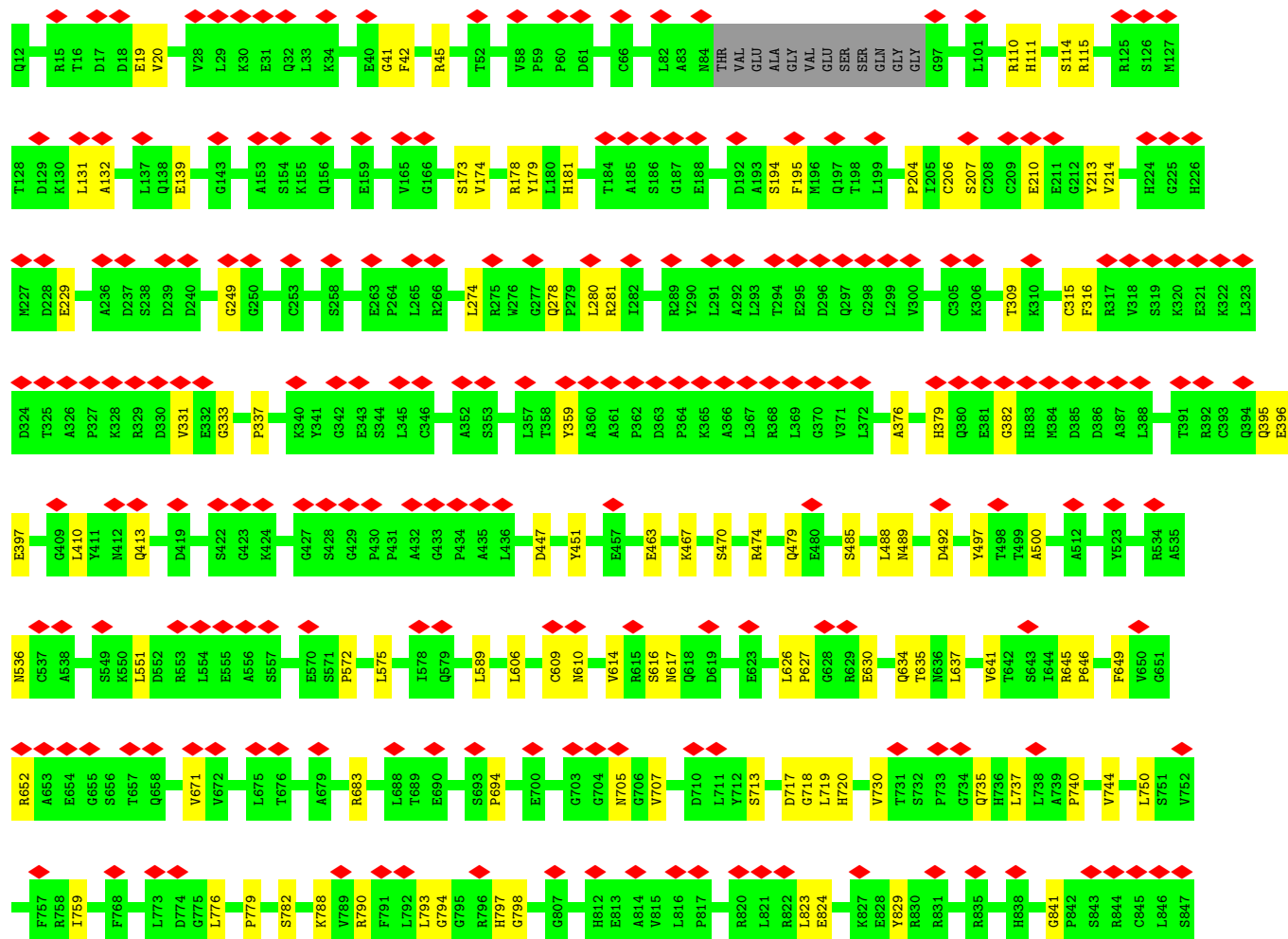
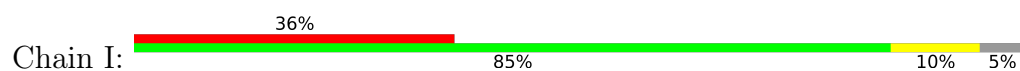








• Molecule 2: Ryanodine receptor 1



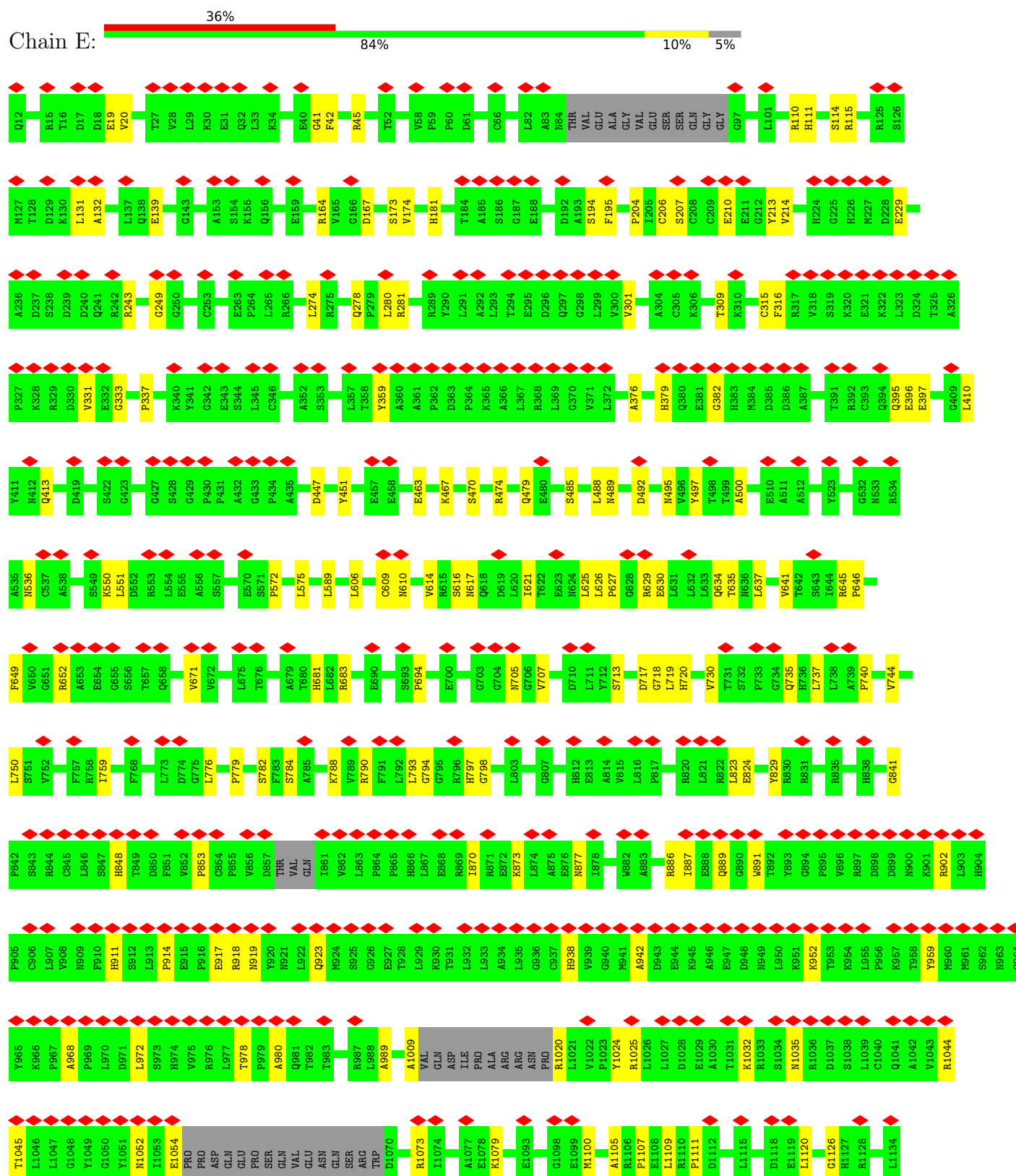


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X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3336	X3337	X3338	X3339	X3340	X3341	X3342	X3345										X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3367	X3368	X3369	X3370	X3371	X3374										X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390																							
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R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	T2910	L2911		T2912	A2913	K2914	E2915	K2916		A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927		K2928	F2929	L2930	Q2931	N2932	N2933	G2934	Y2935	A2936	Y2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949																																					
E2828	G2829	E2830	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	M2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868		R2869	E2870	L2871	Q2872		A2873	N2874	A2875	A2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	N2884		T2885	W2886	G2887																																						
F2768	D2769	K2770	L2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	L2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	L2796	F2797	S2798	E2799	D2800	L2801	K2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	I2823	E2824	K2825	A2826	R2827																																							
X2676	X2677	X2678	X2681		X2682	X2683	X2684	X2685		X2688										X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	N2766	A2767																															
X2591	X2595		X2598		X2599	X2600	X2603		X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2617		X2618	X2619	X2620	X2621	X2622	X2624	X2625	X2626	X2627	X2630		X2633		X2640		X2641	X2642	X2643	X2644	X2649		X2650	X2651	X2652	X2653	X2654	X2655	X2658		X2665		X2666	X2667	X2668	X2669	X2670	X2671	X2672	X2673	X2674	X2675	N2766	A2767																																		
Q2444	A2445	G2446	K2447		I2453		R2454		V2461		P2462	L2463	L2466	V2467	I2470		S2471	L2472	P2473	L2474	P2477		T2478	L2479	X2487	X2488	X2489	X2497		X2500		X2512		X2513	X2531		X2532	X2535		X2538		X2561		X2562	X2563	X2564	X2565	X2569		X2570	X2571	X2572	X2580		X2581	X2582	X2583	X2584	X2585																																							
L2357	C2363	F2364	G2365	P2366	A2367	L2368	E2371	G2372	G2373	S2374	G2375	L2376	L2377	A2378	E2381	E2388	D2389	P2390	A2391	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	GLU	PRO	GLU	GLU	R2414	R2415	V2416	L2429	I2430	D2431	R2435	P2438	E2439	M2440	H2441	L2442	L2443																																																



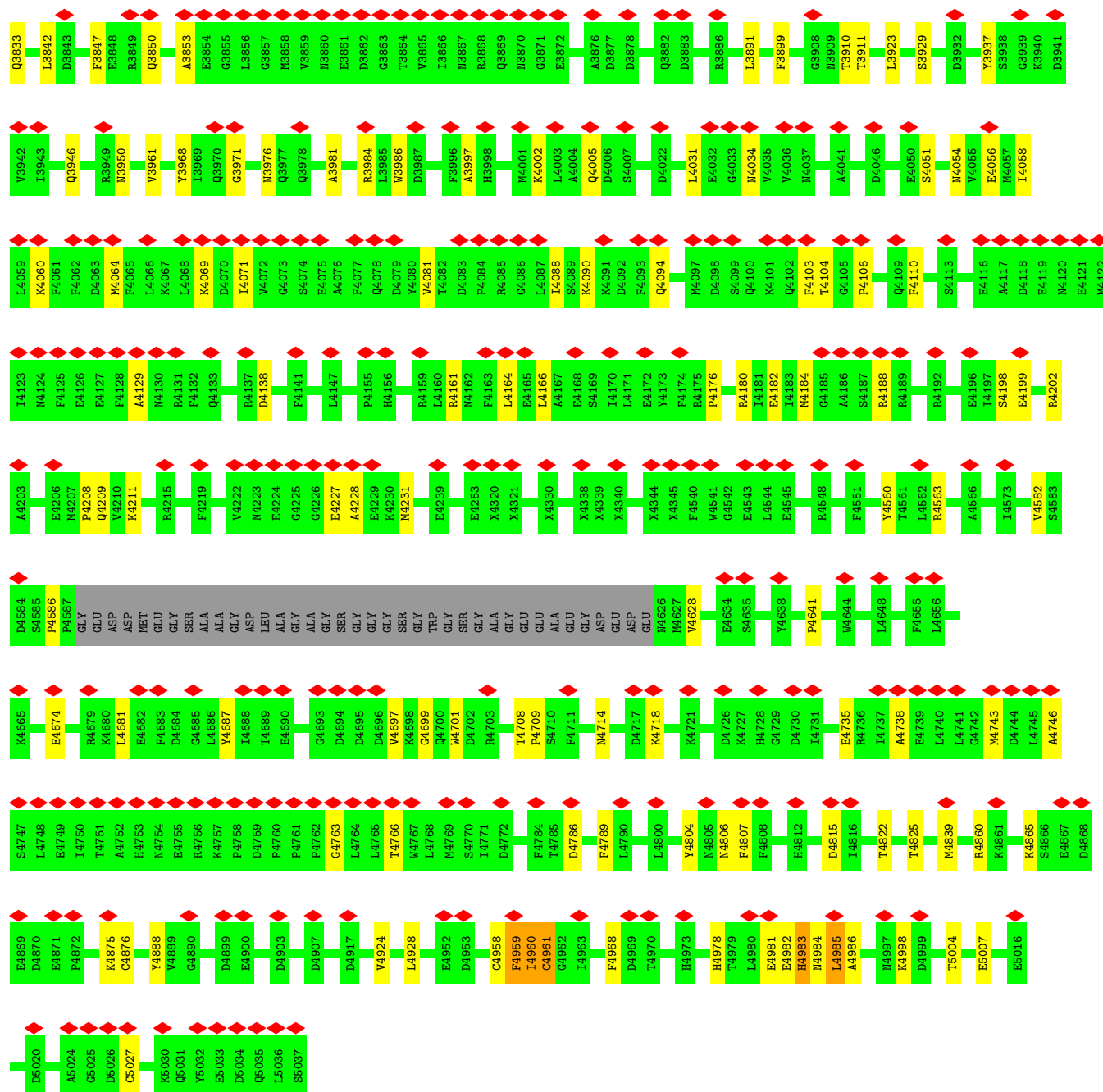
• Molecule 2: Ryanodine receptor 1

Chain E:





S3714	K3795	Y2855	E2915	X2997	X3140	X3218	X3290	X3354	X3415	X3527	X3590	X3690	S3714
K3715	T2796	N2856	K2916	X2998	X3141	X3219	X3291	X3355	X3416	X3528	X3591	X3600	K3715
L3716	F2797	P2857	A2917	X3002	X3144	X3220	X3292	X3356	X3417	X3529	X3592	X3601	L3716
D3717	S2798	Q2858	R2918	X3003	X3145	X3221	X3293	X3357	X3418	X3530	X3593	X3602	D3717
L3728	E2799	P2859	R2919	X3004	X3146	X3224	X3294	X3358	X3419	X3531	X3596	X3603	L3728
C3733	K2800	P2860	R2920	X3005	X3147	X3225	X3295	X3359	X3420	X3532	X3597	X3604	C3733
H3734	D2801	L2862	K2922	X3006	X3148	X3226	X3296	X3360	X3421	X3533	X3600	X3605	H3734
E3736	K2802	L2863	A2923	X3007	X3151	X3227	X3299	X3362	X3424	X3534	X3601	X3606	E3736
G3738	E2803	Q2864	Q2924	X3008	X3155	X3228	X3300	X3363	X3425	X3535	X3602	X3607	G3738
G3739	I2804	V2865	Q2925	X3009	X3156	X3231	X3301	X3364	X3426	X3536	X3603	X3608	G3739
E3740	Y2805	T2866	E2926	X3010	X3157	X3232	X3302	X3365	X3427	X3537	X3604	X3609	E3740
E3741	R2806	L2867	L2927	X3011	X3158	X3233	X3303	X3366	X3428	X3538	X3605	X3610	E3741
GLY	W2807	S2868	K2928	X3012	X3159	X3234	X3304	X3367	X3429	X3539	X3606	X3611	GLY
GLU	P2808	R2869	F2929	X3013	X3160	X3235	X3305	X3368	X3430	X3540	X3607	X3612	GLU
ALA	E2749	E2870	L2930	X3014	X3161	X3236	X3306	X3369	X3431	X3541	X3608	X3613	ALA
GLU	K2750	L2871	Q2932	X3015	X3162	X3237	X3309	X3370	X3432	X3542	X3609	X3614	GLU
E3747	D2751	Q2872	M2933	X3016	X3163	X3241	X3310	X3371	X3433	X3543	X3610	X3615	E3747
E3748	S2752	A2873	M2934	X3017	X3164	X3242	X3311	X3372	X3434	X3544	X3611	X3616	E3748
V3749	S2753	L2813	M2935	X3018	X3165	X3243	X3312	X3373	X3435	X3545	X3612	X3617	V3749
E3750	F2754	K2814	Q2936	X3019	X3166	X3244	X3313	X3374	X3436	X3546	X3613	X3618	E3750
E3751	I2755	A2815	Y2935	X3020	X3167	X3245	X3314	X3375	X3437	X3547	X3614	X3619	E3751
V3752	T2756	E2816	E2937	X3021	X3168	X3246	X3315	X3376	X3438	X3548	X3615	X3620	V3752
F3753	K2757	L2817	V2937	X3022	X3169	X3247	X3316	X3377	X3439	X3549	X3616	X3621	F3753
E3754	F2758	A2818	T2938	X3023	X3170	X3248	X3317	X3378	X3440	X3550	X3617	X3622	E3754
E3759	A2759	E2819	R2939	X3024	X3171	X3249	X3318	X3379	X3441	X3551	X3618	X3623	E3759
E2760	E2760	E2820	K2942	X3025	X3172	X3250	X3319	X3380	X3442	X3552	X3619	X3624	E2760
V2761	V2761	W2821	Q2943	X3026	X3173	X3251	X3320	X3381	X3443	X3553	X3620	X3625	V2761
T2762	T2762	Y2822	Y2882	X3027	X3174	X3252	X3321	X3382	X3444	X3554	X3621	X3626	T2762
E2763	E2763	L2823	N2883	X3028	X3175	X3253	X3322	X3383	X3445	X3555	X3622	X3627	E2763
E2764	E2764	E2824	T2884	X3029	X3176	X3254	X3323	X3384	X3446	X3556	X3623	X3628	E2764
K2765	K2765	K2825	T2885	X3030	X3177	X3255	X3324	X3385	X3447	X3557	X3624	X3629	K2765
W2766	W2766	A2826	W2886	X3031	X3178	X3256	X3325	X3386	X3448	X3558	X3625	X3630	W2766
A2767	A2767	E2827	E2887	X3032	X3179	X3257	X3326	X3387	X3449	X3559	X3626	X3631	A2767
F2768	F2768	E2828	K2888	X3033	X3180	X3258	X3327	X3388	X3450	X3560	X3627	X3632	F2768
D2769	D2769	G2829	K2889	X3034	X3181	X3259	X3328	X3389	X3451	X3561	X3628	X3633	D2769
K2770	K2770	E2830	K2890	X3035	X3182	X3260	X3329	X3390	X3452	X3562	X3629	X3634	K2770
I2771	I2771	GLU	K2891	X3036	X3183	X3261	X3330	X3391	X3453	X3563	X3630	X3635	I2771
Q2772	Q2772	ARG	Q2892	X3037	X3190	X3262	X3331	X3392	X3454	X3564	X3631	X3636	Q2772
N2773	N2773	THR	Q2893	X3038	X3191	X3263	X3332	X3393	X3455	X3565	X3632	X3637	N2773
W2774	W2774	GLU	L2894	X3039	X3192	X3264	X3333	X3394	X3456	X3566	X3633	X3638	W2774
K2775	K2775	LVS	E2895	X3040	X3193	X3265	X3334	X3395	X3457	X3567	X3634	X3639	K2775
S2776	S2776	LVS	A2896	X3041	X3194	X3266	X3335	X3396	X3458	X3568	X3635	X3640	S2776
Y2777	Y2777	THR	K2897	X3042	X3195	X3267	X3336	X3397	X3459	X3569	X3636	X3641	Y2777
G2778	G2778	ARG	Q2898	X3043	X3196	X3268	X3337	X3398	X3460	X3570	X3637	X3642	G2778
E2779	E2779	LVS	Q2899	X3044	X3197	X3269	X3338	X3399	X3461	X3571	X3638	X3643	E2779
N2780	N2780	ILE	Q2900	X3045	X3198	X3270	X3339	X3400	X3462	X3572	X3639	X3644	N2780
V2781	V2781	GLN	T2901	X3046	X3199	X3271	X3340	X3401	X3463	X3573	X3640	X3645	V2781
D2782	D2782	THR	H2902	X3047	X3200	X3272	X3341	X3402	X3464	X3574	X3641	X3646	D2782
E2783	E2783	GLN	P2903	X3048	X3201	X3273	X3342	X3403	X3465	X3575	X3642	X3647	E2783
E2784	E2784	THR	L2904	X3049	X3202	X3274	X3343	X3404	X3466	X3576	X3643	X3648	E2784
E2785	E2785	TVR	L2905	X3050	X3203	X3275	X3344	X3405	X3467	X3577	X3644	X3649	E2785
ASP	ASP	TVR	V2906	X3051	X3204	X3276	X3345	X3406	X3468	X3578	X3645	X3650	ASP
K2786	K2786	PRO	P2907	X3052	X3205	X3277	X3346	X3407	X3469	X3579	X3646	X3651	K2786
T2787	T2787	ARG	Y2908	X3053	X3206	X3278	X3347	X3408	X3470	X3580	X3647	X3652	T2787
H2788	H2788	GLY	L2909	X3054	X3207	X3279	X3348	X3409	X3471	X3581	X3648	X3653	H2788
P2789	P2789	GLY	D2909	X3055	X3208	X3280	X3349	X3410	X3472	X3582	X3649	X3654	P2789
W2790	W2790	GLY	T2910	X3056	X3209	X3281	X3350	X3411	X3473	X3583	X3650	X3655	W2790
L2791	L2791	GLY	T2911	X3057	X3210	X3282	X3351	X3412	X3474	X3584	X3651	X3656	L2791
P2792	P2792	GLY	T2912	X3058	X3211	X3283	X3352	X3413	X3475	X3585	X3652	X3657	P2792
F2793	F2793	GLY	A2913	X3059	X3212	X3284	X3353	X3414	X3476	X3586	X3653	X3658	F2793
Y2794	Y2794	K2914	K2914	X3060	X3213	X3285	X3354	X3415	X3477	X3587	X3654	X3659	Y2794
				X3061	X3214	X3286	X3355	X3416	X3478	X3588	X3655	X3660	
				X3062	X3215	X3287	X3356	X3417	X3479	X3589	X3656	X3661	
				X3063	X3216	X3288	X3357	X3418	X3480		X3657	X3662	
				X3064	X3217	X3289	X3358	X3419	X3481		X3658	X3663	
				X3065	X3218	X3290	X3359	X3420	X3482		X3659	X3664	
				X3066	X3219	X3291	X3360	X3421	X3483		X3660	X3665	
				X3067	X3220	X3292	X3361	X3422	X3484		X3661	X3666	
				X3068	X3221	X3293	X3362	X3423	X3485		X3662	X3667	
				X3069	X3222	X3294	X3363	X3424	X3486		X3663	X3668	
				X3070	X3223	X3295	X3364	X3425	X3487		X3664	X3669	
				X3071	X3224	X3296	X3365	X3426	X3488		X3665	X3670	
				X3072	X3225	X3297	X3366	X3427	X3489		X3666	X3671	
				X3073	X3226	X3298	X3367	X3428	X3490		X3667	X3672	
				X3074	X3227	X3299	X3368	X3429	X3491		X3668	X3673	
				X3075	X3228	X3300	X3369	X3430	X3492		X3669	X3674	
				X3076	X3229	X3301	X3370	X3431	X3493		X3670	X3675	
				X3077	X3230	X3302	X3371	X3432	X3494		X3671	X3676	
				X3078	X3231	X3303	X3372	X3433	X3495		X3672	X3677	
				X3079	X3232	X3304	X3373	X3434	X3496		X3673	X3678	
				X3080	X3233	X3305	X3374	X3435	X3497		X3674	X3679	
				X3081	X3234	X3306	X3375	X3436	X3498		X3675	X3680	
				X3082	X3235	X3307	X3376	X3437	X3499		X3676	X3681	
				X3083	X3236	X3308	X3377	X3438	X3500		X3677	X3682	
				X3084	X3237	X3309	X3378	X3439	X3501		X3678	X3683	
				X3085	X3238	X3310	X3379	X3440	X3502		X3679	X3684	
				X3086	X3239	X3311	X3380	X3441	X3503		X3680	X3685	
				X3087	X3240	X3312	X3381	X3442	X3504		X3681	X3686	
				X3088	X3241	X3313	X3382	X3443	X3505		X3682	X3687	
				X3089	X3242	X3314	X3383	X3444	X3506		X3683	X3688	
				X3090	X3243	X3315	X3384	X3445	X3507		X3684	X3689	
				X3091	X3244	X3316	X3385	X3446	X3508		X3685	X3690	
				X3092	X3245	X3317	X3386	X3447	X3509		X3686	X3691	
				X3093	X3246	X3318	X3387	X3448	X3510		X3687	X3692	
				X3094	X3247	X3319	X3388	X3449	X3511		X3688	X3693	
				X3095	X3248	X3320	X3389	X3450	X3512		X3689	X3694	
				X3096	X3249	X3321	X3390	X3451	X3513		X3690	X3695	
				X3097	X3250	X3322	X3391	X3452	X3514		X3691	X3696	
				X3098	X3251	X3323	X3392	X3453	X3515		X3692	X3697	
				X3099	X3252	X3324	X3393	X3454	X3516		X3693	X3698	
				X3100	X3253	X3325	X3394	X3455	X3517		X3694	X3699	
				X3101	X3254	X3326	X3395	X3456	X3518		X3695	X3700	
				X3102	X3255	X3327	X3396	X3457	X3519		X3696	X3701	
				X3103	X3256	X3328	X3397	X3458	X3520		X3697	X3702	
				X3104	X3257	X3329	X3398	X					



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.133	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.20	0/834	0.46	0/1123
1	F	0.20	0/834	0.46	0/1123
1	H	0.20	0/834	0.46	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.21	0/25428	0.52	0/34534
2	E	0.21	0/25428	0.52	0/34534
2	G	0.21	0/25428	0.52	0/34534
2	I	0.21	0/25428	0.52	0/34534
All	All	0.21	0/105048	0.51	0/142628

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide

Continued on next page...

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Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4807	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	I	694	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	6	0
1	F	818	0	824	10	0
1	H	818	0	824	9	0
1	J	818	0	824	9	0
2	B	29499	0	24750	275	0
2	E	29499	0	24750	275	0
2	G	29499	0	24750	266	0
2	I	29499	0	24750	268	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102296	1091	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1091) 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)
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.29	1.49
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	1.29	1.48
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	1.29	1.48
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	1.29	1.48
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.09	1.41
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.09	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.09	1.39
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.09	1.39
2:G:4968:PHE:CE2	2:G:4978:HIS:HE1	1.56	1.16
2:E:4968:PHE:CE2	2:E:4978:HIS:HE1	1.56	1.05
2:I:4968:PHE:CE2	2:I:4978:HIS:HE1	1.56	1.02
2:B:4968:PHE:CE2	2:B:4978:HIS:HE1	1.56	1.02
2:G:4968:PHE:CD2	2:G:4978:HIS:ND1	2.30	1.00
2:I:4968:PHE:CD2	2:I:4978:HIS:ND1	2.30	1.00
2:B:4968:PHE:CD2	2:B:4978:HIS:ND1	2.30	0.99
2:E:4968:PHE:CD2	2:E:4978:HIS:ND1	2.30	0.98
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.35	0.94
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.35	0.94
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.35	0.93
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.35	0.93
2:B:4231:MET:HE1	2:B:4960:ILE:HA	1.63	0.80
2:I:4231:MET:HE1	2:I:4960:ILE:HA	1.63	0.79
2:E:4231:MET:HE1	2:E:4960:ILE:HA	1.63	0.79
2:G:4231:MET:HE1	2:G:4960:ILE:HA	1.63	0.78
2:G:4968:PHE:CD2	2:G:4978:HIS:CE1	2.72	0.77
2:B:4231:MET:SD	2:B:4960:ILE:HD12	2.32	0.70
2:G:4231:MET:SD	2:G:4960:ILE:HD12	2.32	0.69
2:I:4231:MET:SD	2:I:4960:ILE:HD12	2.32	0.69
2:E:4231:MET:SD	2:E:4960:ILE:HD12	2.32	0.69
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.92	0.67
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.67
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.67
2:I:4968:PHE:CD2	2:I:4978:HIS:CE1	2.72	0.67
2:B:626:LEU:HD23	2:B:630:GLU:H	1.60	0.67
2:I:626:LEU:HD23	2:I:630:GLU:H	1.60	0.66
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.66
2:E:4968:PHE:HD2	2:E:4978:HIS:ND1	1.90	0.66
2:G:626:LEU:HD23	2:G:630:GLU:H	1.60	0.66
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.92	0.66
2:E:626:LEU:HD23	2:E:630:GLU:H	1.60	0.66
2:G:111:HIS:HD2	2:G:114:SER:H	1.42	0.66
2:B:111:HIS:HD2	2:B:114:SER:H	1.42	0.66
2:I:111:HIS:HD2	2:I:114:SER:H	1.42	0.66
2:G:4968:PHE:HD2	2:G:4978:HIS:ND1	1.90	0.65
2:E:3762:ARG:O	2:E:3766:GLN:NE2	2.30	0.65
2:I:4968:PHE:HD2	2:I:4978:HIS:ND1	1.90	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.93	0.65
2:G:1170:MET:HE1	2:G:1176:GLU:HG3	1.79	0.64
2:E:4968:PHE:CD2	2:E:4978:HIS:CE1	2.72	0.64
2:E:111:HIS:HD2	2:E:114:SER:H	1.42	0.64
2:E:1170:MET:HE1	2:E:1176:GLU:HG3	1.79	0.64
2:G:3762:ARG:O	2:G:3766:GLN:NE2	2.30	0.64
2:B:1170:MET:HE1	2:B:1176:GLU:HG3	1.79	0.63
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.31	0.63
2:I:3762:ARG:O	2:I:3766:GLN:NE2	2.30	0.63
2:B:3762:ARG:O	2:B:3766:GLN:NE2	2.30	0.63
2:I:1170:MET:HE1	2:I:1176:GLU:HG3	1.79	0.63
2:B:4968:PHE:HD2	2:B:4978:HIS:ND1	1.90	0.63
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.97	0.62
2:E:4968:PHE:HE2	2:E:4978:HIS:HE1	0.67	0.62
2:I:132:ALA:HA	2:I:194:SER:HB2	1.82	0.62
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.62
2:G:132:ALA:HA	2:G:194:SER:HB2	1.82	0.62
2:B:132:ALA:HA	2:B:194:SER:HB2	1.82	0.61
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.61
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.61
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.83	0.61
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.34	0.61
2:E:132:ALA:HA	2:E:194:SER:HB2	1.82	0.61
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.61
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.83	0.61
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.34	0.61
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.61
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.83	0.61
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.34	0.61
2:G:4182:GLU:OE2	2:G:4983:HIS:CE1	2.54	0.61
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.83	0.60
2:B:4182:GLU:OE2	2:B:4983:HIS:CE1	2.54	0.60
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.83	0.60
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.34	0.60
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.84	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:E:4982:GLU:HG3	2:E:5027:CYS:SG	2.42	0.60
2:E:4182:GLU:OE2	2:E:4983:HIS:CE1	2.54	0.60
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.83	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:B:1100:MET:HE2	2:B:1198:GLN:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.84	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.84	0.60
2:G:4982:GLU:HG3	2:G:5027:CYS:SG	2.42	0.60
2:I:4182:GLU:OE2	2:I:4983:HIS:CE1	2.54	0.60
2:E:1100:MET:HE2	2:E:1198:GLN:HB3	1.84	0.59
2:B:4820:VAL:HG21	2:I:4839:MET:HE2	1.82	0.59
2:B:4968:PHE:HE2	2:B:4978:HIS:HE1	0.67	0.59
2:B:4982:GLU:HG3	2:B:5027:CYS:SG	2.42	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.35	0.59
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.35	0.59
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.83	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.59
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.83	0.59
2:I:4982:GLU:HG3	2:I:5027:CYS:SG	2.42	0.59
1:F:34:LYS:HD3	2:E:629:ARG:HD2	1.85	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.58
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.35	0.58
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.84	0.58
2:B:4968:PHE:CD2	2:B:4978:HIS:CE1	2.72	0.58
2:G:1164:LEU:HB3	2:G:1169:LEU:HD21	1.86	0.58
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.36	0.58
2:I:4968:PHE:HE2	2:I:4978:HIS:HE1	0.67	0.58
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.58
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.21	0.58
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.58
2:I:1100:MET:HE2	2:I:1198:GLN:HB3	1.84	0.58
2:I:1164:LEU:HB3	2:I:1169:LEU:HD21	1.86	0.58
2:B:1164:LEU:HB3	2:B:1169:LEU:HD21	1.86	0.58
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.21	0.58
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.36	0.58
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.36	0.58
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.58
2:G:1100:MET:HE2	2:G:1198:GLN:HB3	1.84	0.57
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.86	0.57
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.36	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.57
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.36	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4056:GLU:HG3	2:B:4166:LEU:HD21	1.87	0.57
2:G:4056:GLU:HG3	2:G:4166:LEU:HD21	1.87	0.57
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.86	0.57
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.38	0.57
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.21	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.57
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.87	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.57
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.35	0.57
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:I:4056:GLU:HG3	2:I:4166:LEU:HD21	1.87	0.57
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.87	0.57
2:B:4184:MET:HE2	2:B:4188:ARG:HA	1.87	0.57
2:G:2107:GLN:HG3	2:G:3681:GLY:HA2	1.87	0.57
2:G:4968:PHE:HE2	2:G:4978:HIS:HE1	0.67	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.87	0.57
2:E:1164:LEU:HB3	2:E:1169:LEU:HD21	1.86	0.57
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.38	0.56
2:I:4180:ARG:HH22	2:I:4981:GLU:HA	1.70	0.56
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.88	0.56
2:E:4056:GLU:HG3	2:E:4166:LEU:HD21	1.87	0.56
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.38	0.56
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.38	0.56
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.87	0.56
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.87	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.86	0.56
2:G:4184:MET:HE2	2:G:4188:ARG:HA	1.87	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.69	0.56
2:I:2107:GLN:HG3	2:I:3681:GLY:HA2	1.87	0.56
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.38	0.56
2:E:3734:HIS:O	2:E:3738:GLY:N	2.39	0.56
2:E:4184:MET:HE2	2:E:4188:ARG:HA	1.87	0.56
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.56
2:B:4180:ARG:HH22	2:B:4981:GLU:HA	1.70	0.56
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.38	0.56
2:I:744:VAL:HG22	2:I:759:ILE:HG12	1.88	0.56
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.71	0.56
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3734:HIS:O	2:G:3738:GLY:N	2.39	0.56
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.87	0.56
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.38	0.56
2:G:4180:ARG:HH22	2:G:4981:GLU:HA	1.70	0.56
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.88	0.56
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.56
2:E:2107:GLN:HG3	2:E:3681:GLY:HA2	1.87	0.56
2:G:359:TYR:HA	2:G:376:ALA:HA	1.88	0.56
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.87	0.56
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.87	0.56
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.38	0.56
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.71	0.56
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.38	0.56
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.87	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.38	0.56
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.38	0.56
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.87	0.56
2:B:395:GLN:HG3	2:B:397:GLU:H	1.71	0.56
2:B:744:VAL:HG22	2:B:759:ILE:HG12	1.88	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.56
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.21	0.56
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.71	0.55
2:I:4184:MET:HE2	2:I:4188:ARG:HA	1.87	0.55
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.71	0.55
2:G:744:VAL:HG22	2:G:759:ILE:HG12	1.88	0.55
2:G:395:GLN:HG3	2:G:397:GLU:H	1.71	0.55
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.87	0.55
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.71	0.55
2:I:395:GLN:HG3	2:I:397:GLU:H	1.71	0.55
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.71	0.55
2:E:609:CYS:SG	2:E:610:ASN:N	2.80	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.87	0.55
2:B:1009:ALA:O	2:B:1020:ARG:N	2.40	0.55
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.55
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.87	0.55
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.55
2:B:2107:GLN:HG3	2:B:3681:GLY:HA2	1.87	0.55
2:E:744:VAL:HG22	2:E:759:ILE:HG12	1.88	0.55
2:G:4161:ARG:HD3	2:G:4164:LEU:HD12	1.89	0.55
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.89	0.55
2:B:4982:GLU:OE1	2:B:4982:GLU:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.87	0.55
2:I:359:TYR:HA	2:I:376:ALA:HA	1.88	0.55
2:I:609:CYS:SG	2:I:610:ASN:N	2.80	0.55
2:I:1009:ALA:O	2:I:1020:ARG:N	2.40	0.55
2:I:4982:GLU:OE1	2:I:4982:GLU:HA	2.07	0.55
2:E:4180:ARG:HH22	2:E:4981:GLU:HA	1.70	0.55
2:B:359:TYR:HA	2:B:376:ALA:HA	1.88	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:I:730:VAL:O	2:I:735:GLN:NE2	2.40	0.54
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.90	0.54
2:E:1009:ALA:O	2:E:1020:ARG:N	2.40	0.54
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.54
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.40	0.54
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.40	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.54
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.89	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.81	0.54
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.90	0.54
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.89	0.54
2:G:609:CYS:SG	2:G:610:ASN:N	2.80	0.54
2:I:4161:ARG:HD3	2:I:4164:LEU:HD12	1.89	0.54
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.90	0.54
2:B:609:CYS:SG	2:B:610:ASN:N	2.80	0.54
2:G:730:VAL:O	2:G:735:GLN:NE2	2.40	0.54
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.41	0.54
2:E:730:VAL:O	2:E:735:GLN:NE2	2.40	0.54
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.71	0.54
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.90	0.54
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.41	0.54
2:G:315:CYS:SG	2:G:316:PHE:N	2.81	0.54
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.41	0.54
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.90	0.54
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.41	0.54
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.90	0.54
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.89	0.54
2:E:4982:GLU:OE1	2:E:4982:GLU:HA	2.07	0.54
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.90	0.54
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.54
2:B:730:VAL:O	2:B:735:GLN:NE2	2.40	0.54
2:B:4161:ARG:HD3	2:B:4164:LEU:HD12	1.89	0.54
2:I:315:CYS:SG	2:I:316:PHE:N	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.90	0.54
2:E:395:GLN:HG3	2:E:397:GLU:H	1.71	0.54
2:E:2196:ASN:OD1	2:E:2199:ARG:NH1	2.37	0.54
2:B:614:VAL:HG22	2:B:616:SER:H	1.73	0.54
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.71	0.54
2:G:1009:ALA:O	2:G:1020:ARG:N	2.40	0.54
2:G:4982:GLU:OE1	2:G:4982:GLU:HA	2.07	0.54
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.41	0.54
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.72	0.54
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.72	0.54
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.90	0.54
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.72	0.54
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.89	0.54
2:E:2479:LEU:O	2:E:2487:UNK:N	2.41	0.54
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.41	0.53
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.90	0.53
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.37	0.53
2:I:2479:LEU:O	2:I:2487:UNK:N	2.41	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.53
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	1.90	0.53
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.90	0.53
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.73	0.53
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.81	0.53
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.90	0.53
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.89	0.53
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.40	0.53
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.40	0.53
2:E:614:VAL:HG22	2:E:616:SER:H	1.73	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.90	0.53
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.89	0.53
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.90	0.53
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.90	0.53
2:E:4161:ARG:HD3	2:E:4164:LEU:HD12	1.89	0.53
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	1.90	0.53
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	1.90	0.53
2:E:2347:GLU:O	2:E:2351:ASN:N	2.41	0.53
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	1.90	0.53
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.41	0.53
2:E:315:CYS:SG	2:E:316:PHE:N	2.81	0.53
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.41	0.53
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.74	0.53
2:B:2479:LEU:O	2:B:2487:UNK:N	2.41	0.53
2:I:3733:CYS:HA	2:I:3766:GLN:HG2	1.91	0.53
2:E:4738:ALA:HA	2:E:4743:MET:HE3	1.91	0.53
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.81	0.53
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.72	0.53
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.73	0.53
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.90	0.53
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.74	0.53
2:E:4865:LYS:HG3	2:E:4875:LYS:HZ3	1.74	0.53
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.73	0.52
2:B:3734:HIS:O	2:B:3738:GLY:N	2.39	0.52
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.52
2:I:614:VAL:HG22	2:I:616:SER:H	1.73	0.52
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.42	0.52
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.89	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.91	0.52
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.92	0.52
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.74	0.52
2:G:4738:ALA:HA	2:G:4743:MET:HE3	1.91	0.52
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.92	0.52
2:I:4738:ALA:HA	2:I:4743:MET:HE3	1.91	0.52
2:E:1516:UNK:N	2:E:1529:UNK:O	2.43	0.52
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.52
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.37	0.52
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.42	0.52
2:B:3733:CYS:HA	2:B:3766:GLN:HG2	1.91	0.52
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.92	0.52
2:G:1516:UNK:N	2:G:1529:UNK:O	2.42	0.52
2:I:1516:UNK:N	2:I:1529:UNK:O	2.42	0.52
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.92	0.52
2:B:1516:UNK:N	2:B:1529:UNK:O	2.42	0.52
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.52
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.73	0.52
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.92	0.52
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.91	0.52
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.91	0.52
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.92	0.52
2:G:2479:LEU:O	2:G:2487:UNK:N	2.41	0.52
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.92	0.52
2:E:3733:CYS:HA	2:E:3766:GLN:HG2	1.91	0.52
2:B:4738:ALA:HA	2:B:4743:MET:HE3	1.91	0.52
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.75	0.52
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.92	0.52
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.92	0.52
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.91	0.52
2:B:1152:MET:HE1	2:B:1217:CYS:HB3	1.92	0.52
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.92	0.52
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.52
2:I:1152:MET:HE1	2:I:1217:CYS:HB3	1.92	0.52
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.74	0.52
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.52
2:B:3968:TYR:O	2:B:3976:ASN:ND2	2.43	0.52
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.52
2:I:3734:HIS:O	2:I:3738:GLY:N	2.39	0.52
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.74	0.52
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.75	0.51
1:J:34:LYS:HE3	2:I:634:GLN:HB3	1.93	0.51
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.93	0.51
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.93	0.51
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.92	0.51
2:G:331:VAL:HG12	2:G:333:GLY:H	1.76	0.51
2:I:331:VAL:HG12	2:I:333:GLY:H	1.76	0.51
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.74	0.51
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.74	0.51
2:G:614:VAL:HG22	2:G:616:SER:H	1.73	0.51
2:G:3968:TYR:O	2:G:3976:ASN:ND2	2.43	0.51
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.93	0.51
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.93	0.51
2:G:3733:CYS:HA	2:G:3766:GLN:HG2	1.91	0.51
2:G:160:GLY:O	2:I:3984:ARG:NH2	2.39	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.81	0.51
2:I:3968:TYR:O	2:I:3976:ASN:ND2	2.43	0.51
2:B:3981:ALA:HA	2:B:3986:TRP:HE1	1.76	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.93	0.51
2:B:2353:VAL:O	2:B:2357:LEU:N	2.44	0.51
2:B:4865:LYS:HG3	2:B:4875:LYS:HZ3	1.76	0.51
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.75	0.51
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.75	0.51
2:I:2353:VAL:O	2:I:2357:LEU:N	2.44	0.51
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.44	0.51
1:A:27:THR:HB	1:A:100:ASP:HB3	1.94	0.51
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.81	0.51
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.44	0.51
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.93	0.51
2:E:331:VAL:HG12	2:E:333:GLY:H	1.76	0.51
2:E:2353:VAL:O	2:E:2357:LEU:N	2.44	0.51
2:E:3968:TYR:O	2:E:3976:ASN:ND2	2.43	0.51
2:B:331:VAL:HG12	2:B:333:GLY:H	1.76	0.50
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.37	0.50
2:G:2347:GLU:O	2:G:2351:ASN:N	2.41	0.50
2:G:2353:VAL:O	2:G:2357:LEU:N	2.44	0.50
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	1.93	0.50
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.44	0.50
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.93	0.50
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.50
2:I:3981:ALA:HA	2:I:3986:TRP:HE1	1.76	0.50
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.50
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.42	0.50
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.44	0.50
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	1.93	0.50
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.50
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.94	0.50
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.50
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.44	0.50
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.50
2:G:1152:MET:HE1	2:G:1217:CYS:HB3	1.92	0.50
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.94	0.50
2:E:1152:MET:HE1	2:E:1217:CYS:HB3	1.92	0.50
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.50
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.92	0.50
2:I:2347:GLU:O	2:I:2351:ASN:N	2.41	0.50
2:B:160:GLY:O	2:E:3984:ARG:NH2	2.43	0.50
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.50
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.77	0.50
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.94	0.50
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.77	0.50
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.49
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	1.93	0.49
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.77	0.49
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.94	0.49
2:E:3981:ALA:HA	2:E:3986:TRP:HE1	1.76	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.94	0.49
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.77	0.49
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.77	0.49
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.77	0.49
2:B:4090:LYS:O	2:B:4094:GLN:N	2.46	0.49
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.94	0.49
2:G:4865:LYS:HG3	2:G:4875:LYS:HZ3	1.76	0.49
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.49
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.78	0.49
2:B:4984:ASN:C	2:B:4986:ALA:H	2.21	0.49
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.78	0.49
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.77	0.49
2:I:1243:PRO:HB2	2:I:1600:LEU:HD22	1.95	0.49
2:E:1243:PRO:HB2	2:E:1600:LEU:HD22	1.95	0.49
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.49
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.95	0.49
2:B:1243:PRO:HB2	2:B:1600:LEU:HD22	1.95	0.49
2:G:1243:PRO:HB2	2:G:1600:LEU:HD22	1.95	0.49
2:G:3997:ALA:HA	2:G:4058:ILE:HD11	1.95	0.49
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.95	0.49
2:I:2868:SER:O	2:I:2872:GLN:N	2.45	0.49
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.77	0.49
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.49
2:B:4822:THR:O	2:B:4825:THR:OG1	2.30	0.49
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.95	0.49
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.95	0.49
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.78	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.41	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.78	0.49
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.95	0.49
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.95	0.48
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.94	0.48
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.78	0.48
2:I:4984:ASN:C	2:I:4986:ALA:H	2.21	0.48
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	1.93	0.48
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.95	0.48
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.96	0.48
2:I:794:GLY:H	2:I:798:GLY:HA3	1.78	0.48
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.96	0.48
2:B:794:GLY:H	2:B:798:GLY:HA3	1.78	0.48
2:B:3997:ALA:HA	2:B:4058:ILE:HD11	1.95	0.48
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.96	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.48
2:G:3981:ALA:HA	2:G:3986:TRP:HE1	1.76	0.48
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.44	0.48
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.94	0.48
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.42	0.48
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.96	0.48
2:I:866:HIS:O	2:I:1051:TYR:OH	2.28	0.48
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.48
2:I:3997:ALA:HA	2:I:4058:ILE:HD11	1.95	0.48
2:E:794:GLY:H	2:E:798:GLY:HA3	1.78	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.48
2:E:4090:LYS:O	2:E:4094:GLN:N	2.46	0.48
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.96	0.48
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.95	0.48
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.29	0.48
2:G:4090:LYS:O	2:G:4094:GLN:N	2.46	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.96	0.48
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.48
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.94	0.48
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.96	0.48
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.96	0.48
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.96	0.48
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.95	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.29	0.48
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.95	0.48
2:E:4822:THR:O	2:E:4825:THR:OG1	2.30	0.48
2:G:2911:LEU:HB2	2:G:2916:LYS:HE3	1.96	0.48
2:E:4984:ASN:C	2:E:4986:ALA:H	2.21	0.48
2:B:1650:ILE:HG13	2:B:1707:LEU:HD21	1.96	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.95	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.95	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.78	0.48
2:B:978:THR:HB	2:B:980:ALA:H	1.80	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4822:THR:O	2:G:4825:THR:OG1	2.30	0.47
2:G:4984:ASN:C	2:G:4986:ALA:H	2.21	0.47
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.94	0.47
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.95	0.47
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.95	0.47
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.96	0.47
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.29	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.95	0.47
2:E:3997:ALA:HA	2:E:4058:ILE:HD11	1.95	0.47
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.78	0.47
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.97	0.47
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.79	0.47
2:I:4090:LYS:O	2:I:4094:GLN:N	2.46	0.47
2:I:4786:ASP:OD2	2:I:4789:PHE:N	2.46	0.47
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.96	0.47
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.96	0.47
2:E:1650:ILE:HG13	2:E:1707:LEU:HD21	1.96	0.47
2:E:2375:GLY:HA3	2:E:2378:ALA:HB3	1.97	0.47
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.95	0.47
2:E:2911:LEU:HB2	2:E:2916:LYS:HE3	1.96	0.47
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.96	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.47
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.96	0.47
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.97	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.47
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.97	0.47
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.97	0.47
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.95	0.47
2:B:2375:GLY:HA3	2:B:2378:ALA:HB3	1.97	0.47
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.49	0.47
2:I:978:THR:HB	2:I:980:ALA:H	1.80	0.47
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.97	0.47
2:E:978:THR:HB	2:E:980:ALA:H	1.80	0.47
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.96	0.47
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.43	0.47
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.96	0.47
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.49	0.47
2:I:1650:ILE:HG13	2:I:1707:LEU:HD21	1.96	0.47
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.97	0.47
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.49	0.47
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2911:LEU:HB2	2:B:2916:LYS:HE3	1.96	0.47
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.79	0.47
2:E:645:ARG:N	2:E:824:GLU:O	2.42	0.47
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.97	0.47
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.49	0.47
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.47
2:B:111:HIS:CD2	2:B:114:SER:H	2.29	0.46
2:G:485:SER:HA	2:G:488:LEU:HB2	1.96	0.46
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.79	0.46
2:I:2375:GLY:HA3	2:I:2378:ALA:HB3	1.97	0.46
2:E:1865:MET:SD	2:E:1865:MET:N	2.89	0.46
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.98	0.46
2:B:1865:MET:SD	2:B:1865:MET:N	2.88	0.46
2:B:4786:ASP:OD2	2:B:4789:PHE:N	2.46	0.46
2:G:2375:GLY:HA3	2:G:2378:ALA:HB3	1.97	0.46
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.96	0.46
2:E:485:SER:HA	2:E:488:LEU:HB2	1.96	0.46
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.98	0.46
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.48	0.46
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.96	0.46
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.98	0.46
2:I:2364:PHE:HD1	2:I:2429:LEU:HD21	1.81	0.46
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.48	0.46
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.96	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.97	0.46
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.48	0.46
2:I:4822:THR:O	2:I:4825:THR:OG1	2.30	0.46
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.48	0.46
2:E:2364:PHE:HD1	2:E:2429:LEU:HD21	1.81	0.46
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.79	0.46
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.84	0.46
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.97	0.46
2:B:2868:SER:O	2:B:2872:GLN:N	2.45	0.46
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.46
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.84	0.46
2:G:1650:ILE:HG13	2:G:1707:LEU:HD21	1.96	0.46
2:G:1865:MET:SD	2:G:1865:MET:N	2.88	0.46
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.97	0.46
2:I:2911:LEU:HB2	2:I:2916:LYS:HE3	1.96	0.46
2:B:485:SER:HA	2:B:488:LEU:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2364:PHE:HD1	2:B:2429:LEU:HD21	1.81	0.46
2:G:978:THR:HB	2:G:980:ALA:H	1.79	0.46
2:G:2364:PHE:HD1	2:G:2429:LEU:HD21	1.80	0.46
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.84	0.46
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.34	0.46
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.97	0.46
2:I:485:SER:HA	2:I:488:LEU:HB2	1.96	0.46
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.97	0.45
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.98	0.45
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.34	0.45
2:I:1865:MET:SD	2:I:1865:MET:N	2.88	0.45
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.81	0.45
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.47	0.45
2:B:4958:CYS:HB2	2:B:4961:CYS:H	1.82	0.45
2:G:2291:GLN:HE21	2:G:2294:ASP:H	1.65	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.48	0.45
2:E:2291:GLN:HE21	2:E:2294:ASP:H	1.64	0.45
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.97	0.45
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.98	0.45
2:B:4069:LYS:HG3	2:B:4129:ALA:HB1	1.99	0.45
2:G:4069:LYS:HG3	2:G:4129:ALA:HB1	1.99	0.45
2:I:4231:MET:HE1	2:I:4960:ILE:HD12	1.99	0.45
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.14	0.45
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.99	0.45
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.34	0.45
2:I:4005:GLN:HE21	2:I:4110:PHE:HE1	1.63	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.97	0.45
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.97	0.45
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.99	0.45
2:G:4231:MET:HE1	2:G:4960:ILE:HD12	1.99	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:E:4005:GLN:HE21	2:E:4110:PHE:HE1	1.63	0.45
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.14	0.45
2:B:4005:GLN:HE21	2:B:4110:PHE:HE1	1.63	0.45
2:G:278:GLN:N	2:G:315:CYS:SG	2.90	0.45
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.75	0.45
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.81	0.45
2:G:4786:ASP:OD2	2:G:4789:PHE:N	2.46	0.45
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.52	0.45
2:I:4069:LYS:HG3	2:I:4129:ALA:HB1	1.99	0.45
2:I:4958:CYS:HB2	2:I:4961:CYS:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4069:LYS:HG3	2:E:4129:ALA:HB1	1.99	0.45
1:H:34:LYS:HD3	2:G:629:ARG:HD2	1.99	0.45
2:B:164:ARG:N	2:B:167:ASP:OD2	2.43	0.45
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.45
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	1.99	0.45
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.48	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.90	0.45
2:I:2291:GLN:HE21	2:I:2294:ASP:H	1.65	0.45
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.99	0.45
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.97	0.45
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.98	0.45
2:B:2291:GLN:HE21	2:B:2294:ASP:H	1.64	0.45
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.48	0.45
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.30	0.45
2:G:4820:VAL:HG21	2:E:4839:MET:HE2	1.99	0.45
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.97	0.45
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.47	0.45
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.99	0.45
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	1.99	0.45
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.84	0.45
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.97	0.45
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.46	0.45
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.75	0.45
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.81	0.45
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.52	0.45
2:G:4005:GLN:HE21	2:G:4110:PHE:HE1	1.63	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.99	0.45
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.30	0.45
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.52	0.45
2:B:4231:MET:HE1	2:B:4960:ILE:HD12	1.99	0.45
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.30	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.99	0.45
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.45
2:E:4958:CYS:HB2	2:E:4961:CYS:H	1.82	0.45
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.71	0.44
2:B:4960:ILE:HG12	2:B:4985:LEU:HD23	2.00	0.44
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.99	0.44
2:E:2959:UNK:O	2:E:2963:UNK:N	2.50	0.44
2:I:652:ARG:HB2	2:I:750:LEU:HD13	1.99	0.44
2:I:4960:ILE:HG12	2:I:4985:LEU:HD23	2.00	0.44
2:E:206:CYS:SG	2:E:207:SER:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.99	0.44
2:B:278:GLN:N	2:B:315:CYS:SG	2.90	0.44
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.34	0.44
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	1.99	0.44
2:G:2959:UNK:O	2:G:2963:UNK:N	2.50	0.44
2:G:3759:GLU:O	2:G:3763:LEU:N	2.48	0.44
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.44
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.14	0.44
2:B:645:ARG:N	2:B:824:GLU:O	2.42	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.99	0.44
2:G:206:CYS:SG	2:G:207:SER:N	2.90	0.44
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.14	0.44
2:G:652:ARG:HB2	2:G:750:LEU:HD13	2.00	0.44
2:G:4960:ILE:HG12	2:G:4985:LEU:HD23	2.00	0.44
2:I:278:GLN:N	2:I:315:CYS:SG	2.90	0.44
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.75	0.44
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.99	0.44
2:E:3759:GLU:O	2:E:3763:LEU:N	2.48	0.44
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.99	0.44
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.34	0.44
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.99	0.44
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.44
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.99	0.44
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.00	0.44
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.00	0.44
2:E:606:LEU:O	2:E:617:ASN:ND2	2.51	0.44
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	1.99	0.44
2:E:4959:PHE:CD1	2:E:4959:PHE:O	2.70	0.44
2:B:606:LEU:O	2:B:617:ASN:ND2	2.51	0.44
2:B:652:ARG:HB2	2:B:750:LEU:HD13	1.99	0.44
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.00	0.44
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.99	0.44
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.52	0.44
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.44
2:E:793:LEU:HB2	2:E:797:HIS:H	1.83	0.44
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.99	0.44
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.75	0.44
2:E:4231:MET:HE1	2:E:4960:ILE:HD12	1.99	0.44
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.30	0.44
2:B:2959:UNK:O	2:B:2963:UNK:N	2.50	0.44
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4959:PHE:O	2:G:4959:PHE:CD1	2.71	0.44
2:I:641:VAL:HG21	2:I:705:ASN:HA	2.00	0.44
2:I:911:HIS:O	2:I:918:ARG:NH2	2.48	0.44
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.48	0.44
2:I:2959:UNK:O	2:I:2963:UNK:N	2.50	0.44
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.99	0.44
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	2.00	0.44
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.00	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.51	0.44
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	2.00	0.44
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.51	0.44
2:E:4786:ASP:OD2	2:E:4789:PHE:N	2.46	0.44
2:E:4960:ILE:HG12	2:E:4985:LEU:HD23	2.00	0.44
1:F:34:LYS:HE3	2:E:634:GLN:HB3	2.00	0.43
2:I:606:LEU:O	2:I:617:ASN:ND2	2.51	0.43
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.43
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.82	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.43
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.00	0.43
2:G:606:LEU:O	2:G:617:ASN:ND2	2.51	0.43
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.48	0.43
2:I:2297:LYS:O	2:I:2300:SER:OG	2.34	0.43
2:B:243:ARG:NH1	2:B:301:VAL:O	2.49	0.43
2:B:793:LEU:HB2	2:B:797:HIS:H	1.83	0.43
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.99	0.43
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.66	0.43
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.43
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.66	0.43
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.66	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.01	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.90	0.43
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.00	0.43
2:B:4563:ARG:NH1	2:B:4815:ASP:OD1	2.52	0.43
2:B:4968:PHE:HD2	2:B:4978:HIS:HD1	1.47	0.43
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.99	0.43
2:G:1695:LEU:HB3	2:G:1810:LYS:HZ2	1.83	0.43
2:G:4958:CYS:HB2	2:G:4961:CYS:H	1.82	0.43
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.99	0.43
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	2.00	0.43
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:652:ARG:HB2	2:E:750:LEU:HD13	1.99	0.43
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	2.01	0.43
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.00	0.43
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.43
2:G:889:GLN:O	2:G:902:ARG:NH1	2.52	0.43
2:G:914:PRO:HD2	2:G:917:GLU:HB2	2.00	0.43
2:G:2775:TRP:HZ3	2:G:2783:GLU:HA	1.84	0.43
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.00	0.43
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.84	0.43
2:I:4563:ARG:NH1	2:I:4815:ASP:OD1	2.52	0.43
2:E:914:PRO:HD2	2:E:917:GLU:HB2	2.00	0.43
2:E:919:ASN:O	2:E:923:GLN:N	2.52	0.43
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.99	0.43
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.67	0.43
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.01	0.43
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.84	0.43
2:B:889:GLN:O	2:B:902:ARG:NH1	2.52	0.43
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.99	0.43
2:B:1695:LEU:HB3	2:B:1810:LYS:HZ2	1.83	0.43
2:G:641:VAL:HG21	2:G:705:ASN:HA	2.00	0.43
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.29	0.43
2:E:2775:TRP:HZ3	2:E:2783:GLU:HA	1.84	0.43
2:B:2297:LYS:O	2:B:2300:SER:OG	2.35	0.43
2:B:2440:MET:O	2:B:2444:GLN:N	2.51	0.43
2:G:4563:ARG:NH1	2:G:4815:ASP:OD1	2.52	0.43
2:E:889:GLN:O	2:E:902:ARG:NH1	2.52	0.43
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.51	0.43
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.34	0.43
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	2.00	0.43
2:G:4198:SER:OG	2:G:4199:GLU:N	2.52	0.43
2:I:4071:ILE:HG13	2:I:4103:PHE:HZ	1.84	0.43
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.84	0.43
1:J:55:VAL:HA	2:I:1784:ALA:HA	2.00	0.43
2:B:870:ILE:HD12	2:B:873:LYS:HB2	2.01	0.43
2:B:911:HIS:O	2:B:918:ARG:NH2	2.48	0.43
2:B:1966:VAL:HA	2:B:1969:LEU:HB3	2.01	0.43
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	2.00	0.43
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.84	0.43
2:G:1966:VAL:HA	2:G:1969:LEU:HB3	2.01	0.43
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	2.01	0.43
2:I:793:LEU:HB2	2:I:797:HIS:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2440:MET:O	2:I:2444:GLN:N	2.51	0.43
2:I:4198:SER:OG	2:I:4199:GLU:N	2.52	0.43
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.30	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.49	0.43
2:E:870:ILE:HD12	2:E:873:LYS:HB2	2.01	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	2.01	0.43
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.43
2:B:4936:ILE:HG21	2:I:4927:ILE:HG12	2.01	0.43
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.43
2:G:793:LEU:HB2	2:G:797:HIS:H	1.83	0.43
2:G:2440:MET:O	2:G:2444:GLN:N	2.51	0.43
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.54	0.43
2:E:1966:VAL:HA	2:E:1969:LEU:HB3	2.01	0.43
2:E:2368:LEU:HD13	2:E:2376:LEU:HD23	2.01	0.43
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	2.00	0.43
2:B:919:ASN:O	2:B:923:GLN:N	2.52	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.01	0.42
2:B:2368:LEU:HD13	2:B:2376:LEU:HD23	2.01	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.01	0.42
2:G:829:TYR:HE2	2:G:1608:MET:HE2	1.84	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.44	0.42
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.01	0.42
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.42
2:E:1708:ARG:HG2	2:E:1711:TYR:CD2	2.54	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.01	0.42
2:E:4563:ARG:NH1	2:E:4815:ASP:OD1	2.52	0.42
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.99	0.42
2:B:866:HIS:O	2:B:1051:TYR:OH	2.28	0.42
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.54	0.42
2:B:4071:ILE:HG13	2:B:4103:PHE:HZ	1.84	0.42
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.01	0.42
2:I:1966:VAL:HA	2:I:1969:LEU:HB3	2.01	0.42
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.01	0.42
2:E:649:PHE:HB3	2:E:776:LEU:HD13	2.01	0.42
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.00	0.42
2:E:4198:SER:OG	2:E:4199:GLU:N	2.52	0.42
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.29	0.42
2:B:914:PRO:HD2	2:B:917:GLU:HB2	2.00	0.42
2:G:20:VAL:HG12	2:G:204:PRO:HA	2.01	0.42
2:G:919:ASN:O	2:G:923:GLN:N	2.52	0.42
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4071:ILE:HG13	2:G:4103:PHE:HZ	1.84	0.42
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.84	0.42
2:I:919:ASN:O	2:I:923:GLN:N	2.52	0.42
2:I:1695:LEU:HB3	2:I:1810:LYS:HZ2	1.84	0.42
2:I:2775:TRP:HZ3	2:I:2783:GLU:HA	1.84	0.42
2:I:3754:GLU:HG3	2:I:4718:LYS:HD2	2.01	0.42
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.79	0.42
2:E:2742:THR:OG1	2:E:2811:GLU:OE1	2.34	0.42
2:E:3754:GLU:HG3	2:E:4718:LYS:HD2	2.01	0.42
2:B:489:ASN:HA	2:B:492:ASP:HB2	2.01	0.42
2:B:649:PHE:HB3	2:B:776:LEU:HD13	2.02	0.42
2:B:829:TYR:HE2	2:B:1608:MET:HE2	1.84	0.42
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.93	0.42
2:B:4051:SER:OG	2:B:4054:ASN:OD1	2.37	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.00	0.42
2:G:4051:SER:OG	2:G:4054:ASN:OD1	2.37	0.42
2:I:20:VAL:HG12	2:I:204:PRO:HA	2.01	0.42
2:I:889:GLN:O	2:I:902:ARG:NH1	2.52	0.42
2:I:914:PRO:HD2	2:I:917:GLU:HB2	2.00	0.42
2:I:4051:SER:OG	2:I:4054:ASN:OD1	2.37	0.42
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.47	0.42
2:E:2440:MET:O	2:E:2444:GLN:N	2.51	0.42
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.54	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.85	0.42
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.52	0.42
2:G:649:PHE:HB3	2:G:776:LEU:HD13	2.01	0.42
2:I:649:PHE:HB3	2:I:776:LEU:HD13	2.01	0.42
2:I:829:TYR:HE2	2:I:1608:MET:HE2	1.84	0.42
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.54	0.42
2:E:829:TYR:HE2	2:E:1608:MET:HE2	1.84	0.42
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.84	0.42
2:E:2776:SER:O	2:E:2788:HIS:N	2.52	0.42
2:E:4071:ILE:HG13	2:E:4103:PHE:HZ	1.84	0.42
1:H:34:LYS:HE3	2:G:634:GLN:HB3	2.02	0.42
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.42
2:B:3754:GLU:HG3	2:B:4718:LYS:HD2	2.01	0.42
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	2.01	0.42
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.84	0.42
2:G:645:ARG:N	2:G:824:GLU:O	2.42	0.42
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.93	0.42
2:E:280:LEU:HD21	2:E:316:PHE:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4984:ASN:C	2:E:4986:ALA:N	2.77	0.42
1:J:92:PRO:HD3	2:I:627:PRO:HB2	2.01	0.42
2:B:2215:LEU:HD23	2:B:2260:ASN:HB3	2.02	0.42
2:B:2775:TRP:HZ3	2:B:2783:GLU:HA	1.84	0.42
2:B:4198:SER:OG	2:B:4199:GLU:N	2.52	0.42
2:B:4708:THR:HA	2:B:4709:PRO:HD3	1.94	0.42
2:G:489:ASN:HA	2:G:492:ASP:HB2	2.01	0.42
2:G:2012:PHE:CG	2:G:2022:PRO:HD3	2.55	0.42
2:G:2776:SER:O	2:G:2788:HIS:N	2.52	0.42
2:I:181:HIS:CE1	2:I:195:PHE:HB2	2.55	0.42
2:E:181:HIS:CE1	2:E:195:PHE:HB2	2.55	0.42
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.00	0.42
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.93	0.42
2:E:1695:LEU:HB3	2:E:1810:LYS:HZ2	1.83	0.42
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.01	0.42
2:E:4998:LYS:NZ	2:E:5007:GLU:OE1	2.48	0.42
2:B:181:HIS:CE1	2:B:195:PHE:HB2	2.55	0.42
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.55	0.42
2:I:1708:ARG:HG2	2:I:1711:TYR:CD2	2.54	0.42
2:I:3842:LEU:O	2:I:3929:SER:OG	2.38	0.42
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	2.02	0.42
2:E:20:VAL:HG12	2:E:204:PRO:HA	2.01	0.42
2:E:788:LYS:HG2	2:E:1629:GLN:HA	2.02	0.42
2:E:2012:PHE:CG	2:E:2022:PRO:HD3	2.55	0.42
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.55	0.42
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.02	0.42
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.55	0.42
2:B:3842:LEU:O	2:B:3929:SER:OG	2.38	0.42
2:G:214:VAL:HG12	2:G:274:LEU:HD12	2.02	0.42
2:G:870:ILE:HD12	2:G:873:LYS:HB2	2.01	0.42
2:G:1708:ARG:HG2	2:G:1711:TYR:CD2	2.54	0.42
2:G:3754:GLU:HG3	2:G:4718:LYS:HD2	2.01	0.42
2:G:3842:LEU:O	2:G:3929:SER:OG	2.38	0.42
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.52	0.42
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.85	0.42
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	2.01	0.42
1:F:25:HIS:HB3	1:F:40:ARG:HD3	2.02	0.42
1:F:87:HIS:H	1:F:91:ILE:HB	1.85	0.42
2:B:20:VAL:HG12	2:B:204:PRO:HA	2.01	0.42
2:B:1189:LEU:HD12	2:B:1190:PRO:HD2	2.02	0.42
2:B:2950:UNK:O	2:B:2954:UNK:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4804:TYR:HB3	2:B:4806:ASN:HD22	1.85	0.42
2:G:243:ARG:NH1	2:G:301:VAL:O	2.49	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.85	0.42
2:G:3759:GLU:HA	2:G:3762:ARG:HB2	2.02	0.42
2:I:870:ILE:HD12	2:I:873:LYS:HB2	2.01	0.42
2:I:2012:PHE:CG	2:I:2022:PRO:HD3	2.55	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:E:2215:LEU:HD23	2:E:2260:ASN:HB3	2.02	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:E:4708:THR:HA	2:E:4709:PRO:HD3	1.94	0.42
1:H:25:HIS:HB3	1:H:40:ARG:HD3	2.02	0.41
1:J:25:HIS:HB3	1:J:40:ARG:HD3	2.02	0.41
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.84	0.41
2:B:1284:UNK:HA	2:B:1463:UNK:HA	2.02	0.41
2:G:181:HIS:CE1	2:G:195:PHE:HB2	2.55	0.41
2:G:788:LYS:HG2	2:G:1629:GLN:HA	2.02	0.41
2:G:2185:ILE:HA	2:G:2188:ASN:ND2	2.35	0.41
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.41
2:G:2950:UNK:O	2:G:2954:UNK:N	2.53	0.41
2:E:3759:GLU:HA	2:E:3762:ARG:HB2	2.02	0.41
2:E:4960:ILE:HA	2:E:4960:ILE:HD13	1.83	0.41
1:H:87:HIS:H	1:H:91:ILE:HB	1.85	0.41
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.41
2:B:4231:MET:CE	2:B:4960:ILE:HD12	2.51	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.41
2:I:214:VAL:HG12	2:I:274:LEU:HD12	2.02	0.41
2:I:2368:LEU:HD13	2:I:2376:LEU:HD23	2.01	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.01	0.41
2:I:4984:ASN:C	2:I:4986:ALA:N	2.77	0.41
2:E:278:GLN:N	2:E:315:CYS:SG	2.90	0.41
2:E:489:ASN:HA	2:E:492:ASP:HB2	2.01	0.41
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	2.02	0.41
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	2.02	0.41
2:G:4231:MET:CE	2:G:4960:ILE:HD12	2.50	0.41
2:I:2742:THR:OG1	2:I:2811:GLU:OE1	2.34	0.41
2:I:2950:UNK:O	2:I:2954:UNK:N	2.53	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:2185:ILE:HA	2:E:2188:ASN:HD21	1.85	0.41
2:B:2776:SER:O	2:B:2788:HIS:N	2.52	0.41
2:G:164:ARG:N	2:G:167:ASP:OD2	2.43	0.41
2:G:173:SER:HB3	2:G:178:ARG:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:280:LEU:HD21	2:G:316:PHE:HE2	1.85	0.41
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	2.03	0.41
2:G:4984:ASN:C	2:G:4986:ALA:N	2.77	0.41
2:G:5004:THR:H	2:G:5007:GLU:HB2	1.86	0.41
2:I:173:SER:HB3	2:I:178:ARG:H	1.85	0.41
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.93	0.41
2:I:2185:ILE:HA	2:I:2188:ASN:ND2	2.35	0.41
2:I:3759:GLU:HA	2:I:3762:ARG:HB2	2.02	0.41
2:E:173:SER:OG	2:E:174:VAL:N	2.54	0.41
2:E:2950:UNK:O	2:E:2954:UNK:N	2.53	0.41
2:E:4804:TYR:HB3	2:E:4806:ASN:HD22	1.85	0.41
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	2.03	0.41
2:B:3759:GLU:O	2:B:3763:LEU:N	2.48	0.41
2:B:5004:THR:H	2:B:5007:GLU:HB2	1.86	0.41
2:I:280:LEU:HD21	2:I:316:PHE:HE2	1.85	0.41
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.44	0.41
2:I:1189:LEU:HD12	2:I:1190:PRO:HD2	2.02	0.41
2:I:2215:LEU:HD23	2:I:2260:ASN:HB3	2.02	0.41
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.84	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.55	0.41
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	2.03	0.41
2:I:4804:TYR:HB3	2:I:4806:ASN:HD22	1.85	0.41
2:I:4928:LEU:HD13	2:I:4928:LEU:HA	1.91	0.41
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.52	0.41
2:B:173:SER:HB3	2:B:178:ARG:H	1.85	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CD2	2.54	0.41
2:B:4697:VAL:O	2:B:4701:TRP:N	2.52	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.55	0.41
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	2.01	0.41
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.41
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.52	0.41
2:I:4231:MET:CE	2:I:4960:ILE:HD12	2.51	0.41
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	2.03	0.41
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.84	0.41
2:E:3842:LEU:O	2:E:3929:SER:OG	2.38	0.41
2:E:4231:MET:CE	2:E:4960:ILE:HD12	2.51	0.41
1:F:92:PRO:HD3	2:E:627:PRO:HB2	2.02	0.41
2:B:173:SER:OG	2:B:174:VAL:N	2.54	0.41
2:B:788:LYS:HG2	2:B:1629:GLN:HA	2.02	0.41
2:B:4984:ASN:C	2:B:4986:ALA:N	2.77	0.41
2:G:911:HIS:O	2:G:918:ARG:NH2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2185:ILE:HA	2:I:2188:ASN:HD21	1.85	0.41
2:I:2776:SER:O	2:I:2788:HIS:N	2.52	0.41
2:I:3361:UNK:O	2:I:3365:UNK:N	2.54	0.41
2:E:2437:ALA:HA	2:E:2438:PRO:HD3	1.94	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.02	0.41
2:B:1817:GLU:O	2:B:1821:ASP:N	2.50	0.41
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.84	0.41
2:G:1189:LEU:HD12	2:G:1190:PRO:HD2	2.02	0.41
2:G:2039:LEU:HA	2:G:2042:CYS:HB3	2.03	0.41
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	2.02	0.41
2:G:3361:UNK:O	2:G:3365:UNK:N	2.54	0.41
2:G:4060:LYS:NZ	2:G:4064:MET:SD	2.94	0.41
2:I:173:SER:OG	2:I:174:VAL:N	2.54	0.41
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.85	0.41
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.52	0.41
1:A:25:HIS:HB3	1:A:40:ARG:HD3	2.02	0.41
1:A:87:HIS:H	1:A:91:ILE:HB	1.85	0.41
1:J:87:HIS:H	1:J:91:ILE:HB	1.85	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.03	0.41
2:B:2039:LEU:HA	2:B:2042:CYS:HB3	2.03	0.41
2:B:2185:ILE:HA	2:B:2188:ASN:HD21	1.85	0.41
2:B:3361:UNK:O	2:B:3365:UNK:N	2.54	0.41
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	2.02	0.41
2:G:173:SER:OG	2:G:174:VAL:N	2.54	0.41
2:G:1284:UNK:HA	2:G:1463:UNK:HA	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.03	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.93	0.41
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	2.03	0.41
2:G:4839:MET:HE2	2:I:4820:VAL:HG21	2.03	0.41
2:I:489:ASN:HA	2:I:492:ASP:HB2	2.01	0.41
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	2.03	0.41
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.54	0.41
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	2.02	0.41
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.52	0.41
2:I:4060:LYS:NZ	2:I:4064:MET:SD	2.94	0.41
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	2.03	0.41
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.30	0.41
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	2.02	0.41
2:E:2129:ASP:O	2:E:2133:GLU:N	2.49	0.41
2:E:4051:SER:OG	2:E:4054:ASN:OD1	2.37	0.41
2:E:4060:LYS:NZ	2:E:4064:MET:SD	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	2.02	0.41
2:E:4697:VAL:O	2:E:4701:TRP:N	2.52	0.41
2:E:5004:THR:H	2:E:5007:GLU:HB2	1.86	0.41
2:B:2012:PHE:CG	2:B:2022:PRO:HD3	2.55	0.41
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	2.02	0.41
2:B:3677:LEU:O	2:B:3698:LEU:N	2.54	0.41
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	2.03	0.41
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	2.03	0.41
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.02	0.41
2:G:2185:ILE:HA	2:G:2188:ASN:HD21	1.85	0.41
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	2.02	0.41
2:I:788:LYS:HG2	2:I:1629:GLN:HA	2.02	0.41
2:I:2144:ILE:H	2:I:2144:ILE:HG13	1.79	0.41
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.54	0.41
1:A:34:LYS:HD3	2:B:629:ARG:HD2	2.03	0.40
2:B:280:LEU:HD21	2:B:316:PHE:HE2	1.85	0.40
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.30	0.40
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.87	0.40
2:G:866:HIS:O	2:G:1051:TYR:OH	2.28	0.40
2:G:2215:LEU:HD23	2:G:2260:ASN:HB3	2.02	0.40
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.40
2:E:911:HIS:O	2:E:918:ARG:NH2	2.48	0.40
2:E:1189:LEU:HD12	2:E:1190:PRO:HD2	2.02	0.40
2:E:3658:LYS:HA	2:E:3661:TRP:CE2	2.56	0.40
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	2.02	0.40
2:B:3658:LYS:HA	2:B:3661:TRP:CE2	2.56	0.40
2:G:907:LEU:O	2:G:963:ASN:ND2	2.42	0.40
2:I:1284:UNK:HA	2:I:1463:UNK:HA	2.02	0.40
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.02	0.40
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.87	0.40
2:E:164:ARG:N	2:E:167:ASP:OD2	2.43	0.40
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.02	0.40
2:E:495:ASN:HD21	2:E:550:LYS:HE3	1.87	0.40
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.03	0.40
1:H:55:VAL:HA	2:G:1784:ALA:HA	2.04	0.40
2:B:3694:LYS:HA	2:B:3695:PRO:HD3	1.93	0.40
2:B:3847:PHE:HA	2:B:3850:GLN:HG2	2.04	0.40
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.55	0.40
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	2.02	0.40
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.03	0.40
2:E:2185:ILE:HA	2:E:2188:ASN:ND2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3361:UNK:O	2:E:3365:UNK:N	2.54	0.40
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.55	0.40
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	2.04	0.40
2:B:2185:ILE:HA	2:B:2188:ASN:ND2	2.35	0.40
2:B:3759:GLU:HA	2:B:3762:ARG:HB2	2.02	0.40
2:G:3676:ASP:N	2:G:3676:ASP:OD1	2.52	0.40
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.40	0.40
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.03	0.40
2:I:5004:THR:H	2:I:5007:GLU:HB2	1.86	0.40
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.04	0.40
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.02	0.40
2:E:3847:PHE:HA	2:E:3850:GLN:HG2	2.04	0.40
2:B:2467:VAL:HA	2:B:2470:ILE:HD12	2.03	0.40
2:B:4060:LYS:NZ	2:B:4064:MET:SD	2.94	0.40
2:G:4804:TYR:HB3	2:G:4806:ASN:HD22	1.85	0.40
2:I:645:ARG:N	2:I:824:GLU:O	2.42	0.40
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.40
2:E:621:ILE:O	2:E:625:LEU:N	2.52	0.40
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	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	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2892 (89%)	337 (10%)	6 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	43	77
2	G	3235/4416 (73%)	2895 (90%)	334 (10%)	6 (0%)	43	77
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	43	77
All	All	13360/18096 (74%)	11944 (89%)	1392 (10%)	24 (0%)	44	77

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU
2	B	1840	PRO
2	B	4985	LEU
2	G	1840	PRO
2	G	4985	LEU
2	I	1840	PRO
2	I	4985	LEU
2	E	1840	PRO
2	B	1932	PRO
2	B	2291	GLN
2	B	4641	PRO
2	G	1932	PRO
2	G	2291	GLN
2	G	4641	PRO
2	I	1932	PRO
2	I	2291	GLN
2	I	4641	PRO
2	E	1932	PRO
2	E	2291	GLN
2	E	4641	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	E	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	G	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
2	I	2493/3022 (82%)	2481 (100%)	12 (0%)	81	81
All	All	10324/12444 (83%)	10276 (100%)	48 (0%)	78	81

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	719	LEU
2	B	1600	LEU
2	B	1657	LEU
2	B	1676	LEU
2	B	2144	ILE
2	B	3663	LEU
2	B	3805	LEU
2	B	4959	PHE
2	B	4960	ILE
2	B	4961	CYS
2	B	4983	HIS
2	G	131	LEU
2	G	719	LEU
2	G	1600	LEU
2	G	1657	LEU
2	G	1676	LEU
2	G	2144	ILE
2	G	3663	LEU
2	G	3805	LEU
2	G	4959	PHE
2	G	4960	ILE
2	G	4961	CYS
2	G	4983	HIS
2	I	131	LEU
2	I	719	LEU
2	I	1600	LEU

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Mol	Chain	Res	Type
2	I	1657	LEU
2	I	1676	LEU
2	I	2144	ILE
2	I	3663	LEU
2	I	3805	LEU
2	I	4959	PHE
2	I	4960	ILE
2	I	4961	CYS
2	I	4983	HIS
2	E	131	LEU
2	E	719	LEU
2	E	1600	LEU
2	E	1657	LEU
2	E	1676	LEU
2	E	2144	ILE
2	E	3663	LEU
2	E	3805	LEU
2	E	4959	PHE
2	E	4960	ILE
2	E	4961	CYS
2	E	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (237) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	32	ASN
1	J	87	HIS
2	B	84	ASN
2	B	113	HIS
2	B	201	ASN
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	489	ASN
2	B	495	ASN
2	B	582	HIS
2	B	593	HIS

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Mol	Chain	Res	Type
2	B	725	HIS
2	B	797	HIS
2	B	838	HIS
2	B	1041	GLN
2	B	1206	GLN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1702	HIS
2	B	1719	HIS
2	B	1760	HIS
2	B	1775	HIS
2	B	1861	GLN
2	B	1953	HIS
2	B	1973	GLN
2	B	2007	ASN
2	B	2041	HIS
2	B	2100	HIS
2	B	2260	ASN
2	B	2291	GLN
2	B	3704	HIS
2	B	3809	ASN
2	B	3814	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	3982	HIS
2	B	4005	GLN
2	B	4034	ASN
2	B	4037	ASN
2	B	4120	ASN
2	B	4142	ASN
2	B	4209	GLN
2	B	4246	GLN
2	B	4553	ASN
2	B	4806	ASN
2	B	4832	HIS

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Mol	Chain	Res	Type
2	B	4949	GLN
2	B	4987	ASN
2	B	5006	GLN
2	G	84	ASN
2	G	113	HIS
2	G	201	ASN
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN
2	G	479	GLN
2	G	489	ASN
2	G	495	ASN
2	G	582	HIS
2	G	593	HIS
2	G	725	HIS
2	G	797	HIS
2	G	838	HIS
2	G	921	ASN
2	G	1041	GLN
2	G	1206	GLN
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1760	HIS
2	G	1775	HIS
2	G	1861	GLN
2	G	1953	HIS
2	G	2005	GLN
2	G	2007	ASN
2	G	2041	HIS
2	G	2100	HIS
2	G	2127	GLN
2	G	2188	ASN
2	G	2260	ASN
2	G	2291	GLN
2	G	3704	HIS
2	G	3809	ASN
2	G	3814	GLN

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Mol	Chain	Res	Type
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	3982	HIS
2	G	4005	GLN
2	G	4034	ASN
2	G	4037	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4209	GLN
2	G	4246	GLN
2	G	4553	ASN
2	G	4574	ASN
2	G	4806	ASN
2	G	4832	HIS
2	G	4949	GLN
2	G	4987	ASN
2	G	5006	GLN
2	I	84	ASN
2	I	113	HIS
2	I	201	ASN
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	479	GLN
2	I	489	ASN
2	I	495	ASN
2	I	593	HIS
2	I	725	HIS
2	I	797	HIS
2	I	838	HIS
2	I	921	ASN
2	I	1041	GLN
2	I	1206	GLN
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS

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Mol	Chain	Res	Type
2	I	1691	GLN
2	I	1693	GLN
2	I	1702	HIS
2	I	1719	HIS
2	I	1760	HIS
2	I	1775	HIS
2	I	1861	GLN
2	I	1953	HIS
2	I	2005	GLN
2	I	2041	HIS
2	I	2100	HIS
2	I	2127	GLN
2	I	2260	ASN
2	I	2291	GLN
2	I	3704	HIS
2	I	3809	ASN
2	I	3814	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	3982	HIS
2	I	4005	GLN
2	I	4034	ASN
2	I	4037	ASN
2	I	4120	ASN
2	I	4142	ASN
2	I	4209	GLN
2	I	4246	GLN
2	I	4553	ASN
2	I	4806	ASN
2	I	4832	HIS
2	I	4949	GLN
2	I	4987	ASN
2	I	5006	GLN
2	E	84	ASN
2	E	113	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS

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Mol	Chain	Res	Type
2	E	383	HIS
2	E	413	GLN
2	E	479	GLN
2	E	489	ASN
2	E	495	ASN
2	E	582	HIS
2	E	593	HIS
2	E	797	HIS
2	E	838	HIS
2	E	1041	GLN
2	E	1206	GLN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1702	HIS
2	E	1719	HIS
2	E	1760	HIS
2	E	1775	HIS
2	E	1861	GLN
2	E	1953	HIS
2	E	2005	GLN
2	E	2041	HIS
2	E	2100	HIS
2	E	2127	GLN
2	E	2188	ASN
2	E	2260	ASN
2	E	2291	GLN
2	E	3809	ASN
2	E	3814	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3976	ASN
2	E	3982	HIS
2	E	4005	GLN
2	E	4034	ASN
2	E	4037	ASN
2	E	4120	ASN

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Mol	Chain	Res	Type
2	E	4142	ASN
2	E	4209	GLN
2	E	4246	GLN
2	E	4553	ASN
2	E	4574	ASN
2	E	4806	ASN
2	E	4832	HIS
2	E	4949	GLN
2	E	4987	ASN
2	E	5006	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	G	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.85
1	G	4345:UNK	C	4540:PHE	N	73.85
1	I	4345:UNK	C	4540:PHE	N	73.85
1	E	4345:UNK	C	4540:PHE	N	73.85
1	B	3613:UNK	C	3639:THR	N	45.57
1	G	3613:UNK	C	3639:THR	N	45.57
1	I	3613:UNK	C	3639:THR	N	45.57
1	E	3613:UNK	C	3639:THR	N	45.57
1	B	4253:GLU	C	4320:UNK	N	29.50
1	G	4253:GLU	C	4320:UNK	N	29.50
1	I	4253:GLU	C	4320:UNK	N	29.50
1	E	4253:GLU	C	4320:UNK	N	29.50
1	B	3163:UNK	C	3170:UNK	N	15.85
1	G	3163:UNK	C	3170:UNK	N	15.85
1	I	3163:UNK	C	3170:UNK	N	15.85
1	E	3163:UNK	C	3170:UNK	N	15.85
1	B	3063:UNK	C	3134:UNK	N	15.15
1	G	3063:UNK	C	3134:UNK	N	15.15
1	I	3063:UNK	C	3134:UNK	N	15.15
1	E	3063:UNK	C	3134:UNK	N	15.15
1	B	3468:UNK	C	3511:UNK	N	14.46
1	G	3468:UNK	C	3511:UNK	N	14.46
1	I	3468:UNK	C	3511:UNK	N	14.46
1	E	3468:UNK	C	3511:UNK	N	14.46
1	B	2703:UNK	C	2734:ASN	N	13.26
1	G	2703:UNK	C	2734:ASN	N	13.26
1	I	2703:UNK	C	2734:ASN	N	13.26
1	E	2703:UNK	C	2734:ASN	N	13.26
1	B	3236:UNK	C	3241:UNK	N	13.11
1	G	3236:UNK	C	3241:UNK	N	13.11
1	I	3236:UNK	C	3241:UNK	N	13.11
1	E	3236:UNK	C	3241:UNK	N	13.11

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1564:UNK	C	1573:MET	N	12.51
1	G	1564:UNK	C	1573:MET	N	12.51
1	I	1564:UNK	C	1573:MET	N	12.51
1	E	1564:UNK	C	1573:MET	N	12.51
1	B	2976:UNK	C	2995:UNK	N	12.28
1	G	2976:UNK	C	2995:UNK	N	12.28
1	I	2976:UNK	C	2995:UNK	N	12.28
1	E	2976:UNK	C	2995:UNK	N	12.28
1	B	3254:UNK	C	3261:UNK	N	8.55
1	G	3254:UNK	C	3261:UNK	N	8.55
1	I	3254:UNK	C	3261:UNK	N	8.55
1	E	3254:UNK	C	3261:UNK	N	8.55
1	B	1297:UNK	C	1430:UNK	N	5.58
1	G	1297:UNK	C	1430:UNK	N	5.58
1	I	1297:UNK	C	1430:UNK	N	5.58
1	E	1297:UNK	C	1430:UNK	N	5.58
1	B	2479:LEU	C	2487:UNK	N	3.51
1	G	2479:LEU	C	2487:UNK	N	3.51
1	I	2479:LEU	C	2487:UNK	N	3.51
1	E	2479:LEU	C	2487:UNK	N	3.51
1	B	2939:ARG	C	2942:UNK	N	3.39
1	G	2939:ARG	C	2942:UNK	N	3.39
1	I	2939:ARG	C	2942:UNK	N	3.39
1	E	2939:ARG	C	2942:UNK	N	3.39

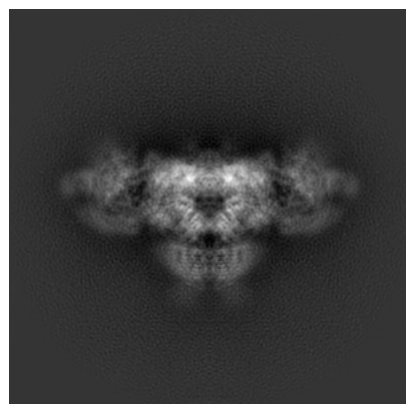
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8389. These allow visual inspection of the internal detail of the map and identification of artifacts.

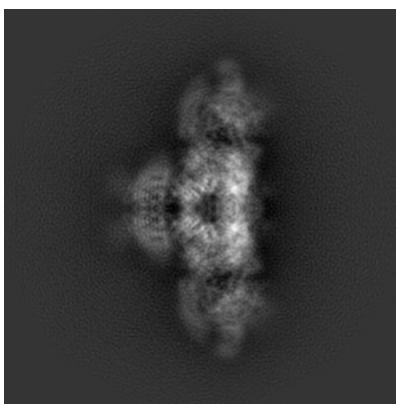
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

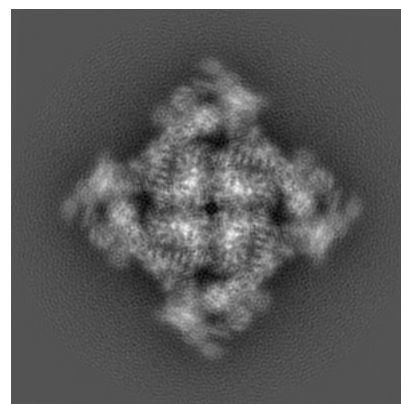
6.1.1 Primary map



X

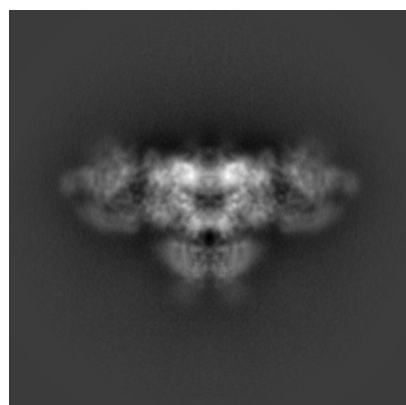


Y

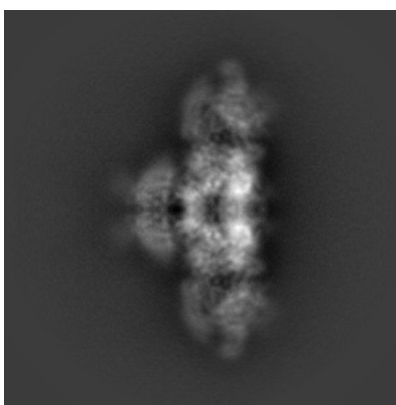


Z

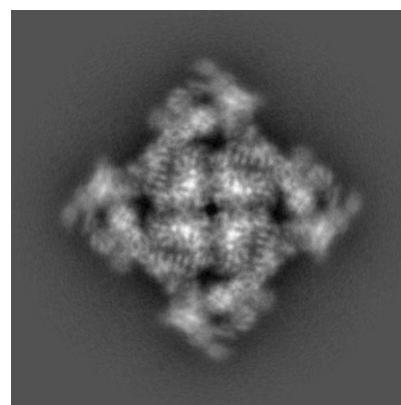
6.1.2 Raw map



X



Y

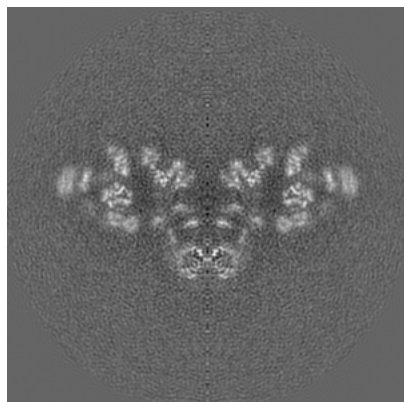


Z

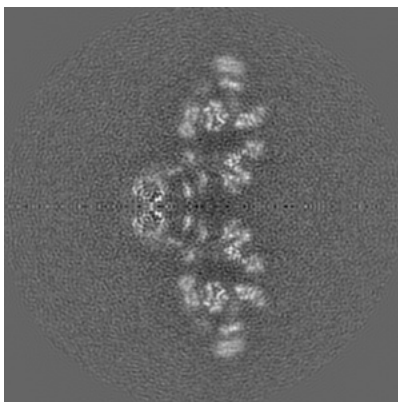
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

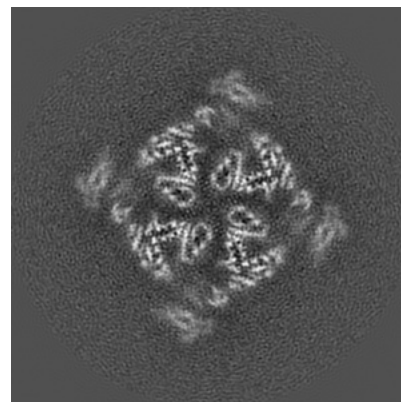
6.2.1 Primary map



X Index: 200

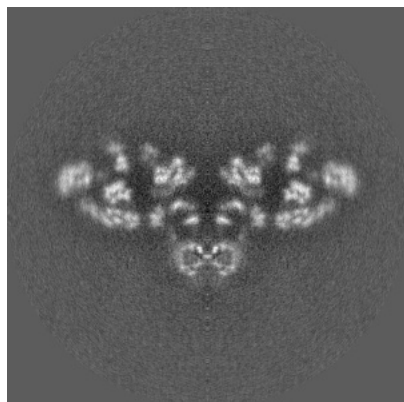


Y Index: 200

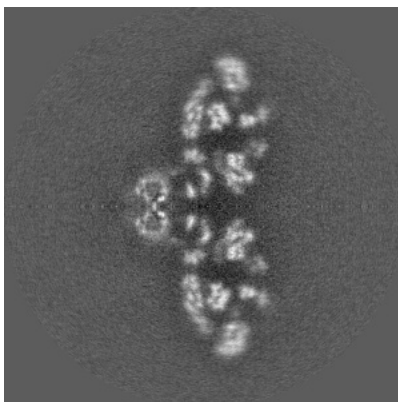


Z Index: 200

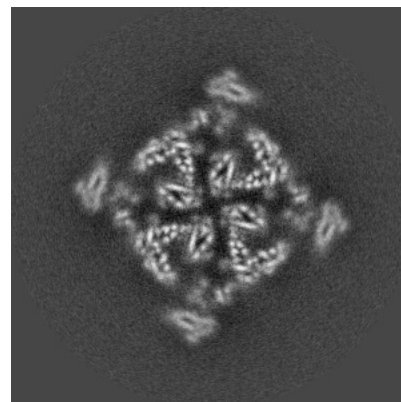
6.2.2 Raw map



X Index: 200



Y Index: 200

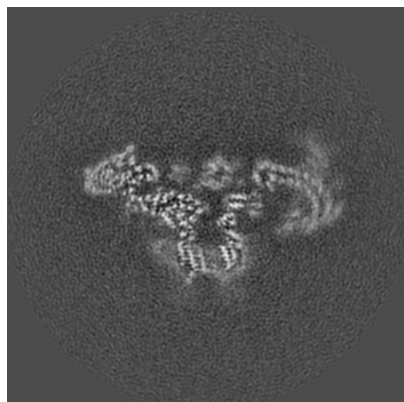


Z Index: 200

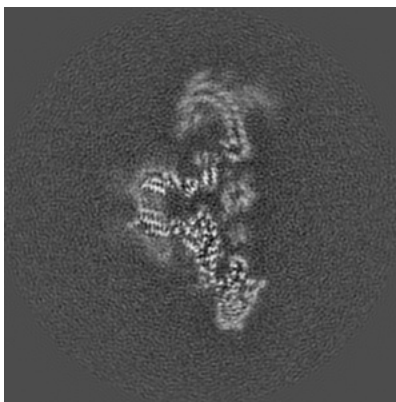
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

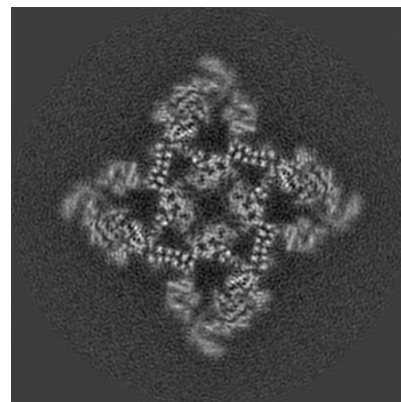
6.3.1 Primary map



X Index: 225

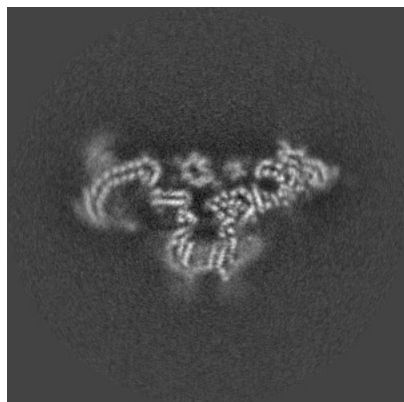


Y Index: 175

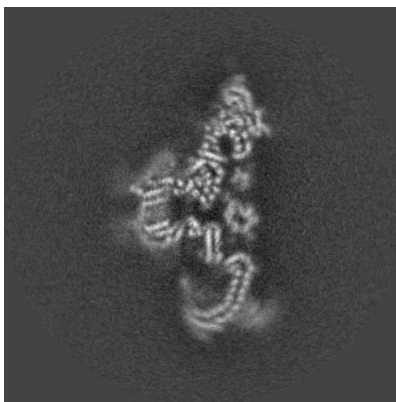


Z Index: 226

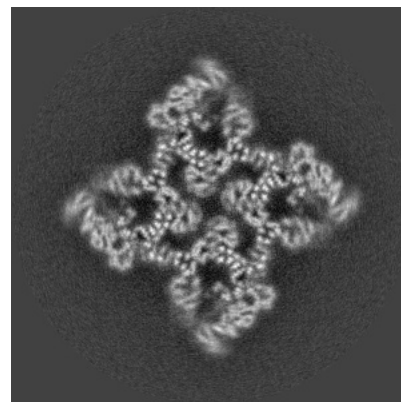
6.3.2 Raw map



X Index: 175



Y Index: 225

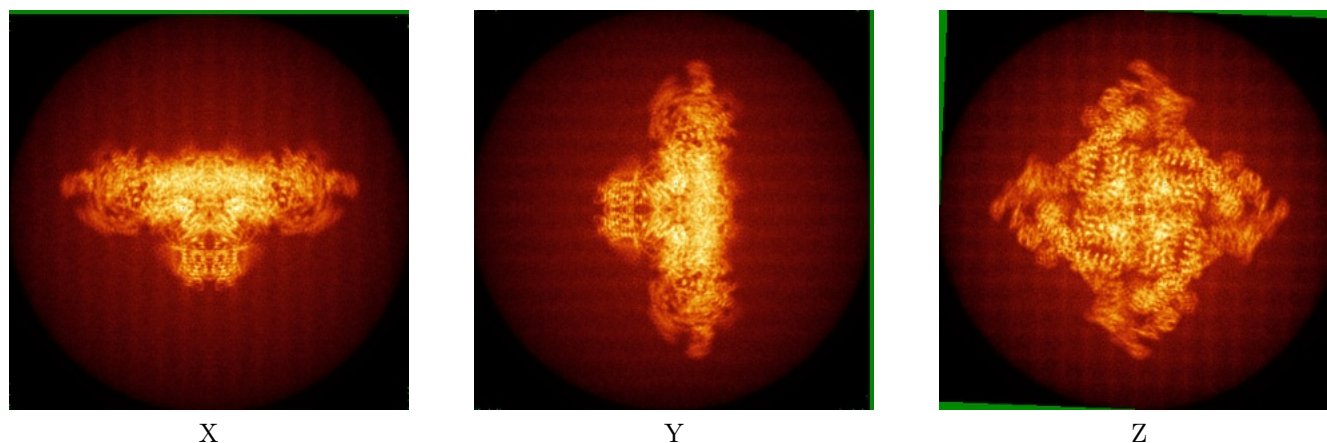


Z Index: 234

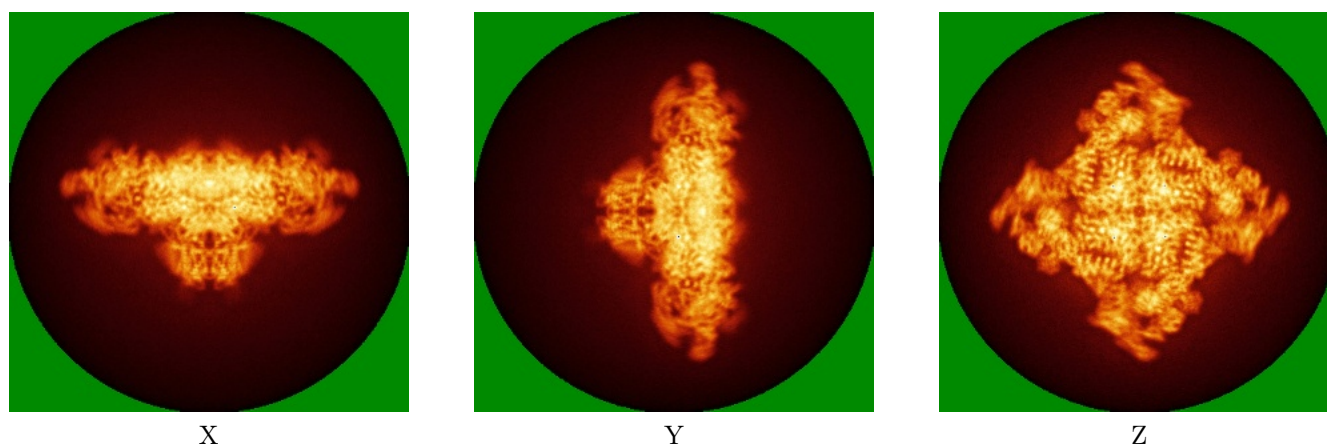
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

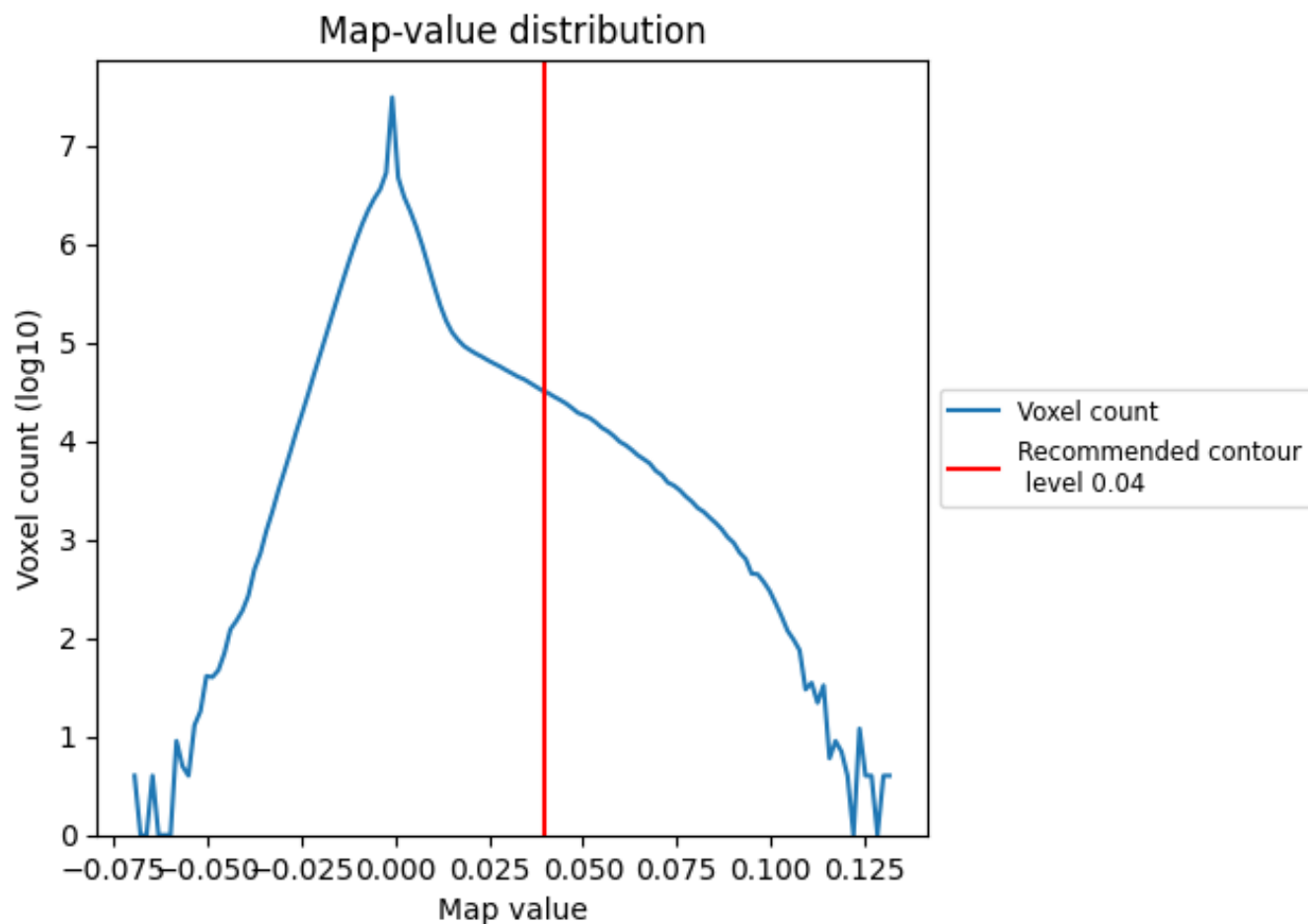
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

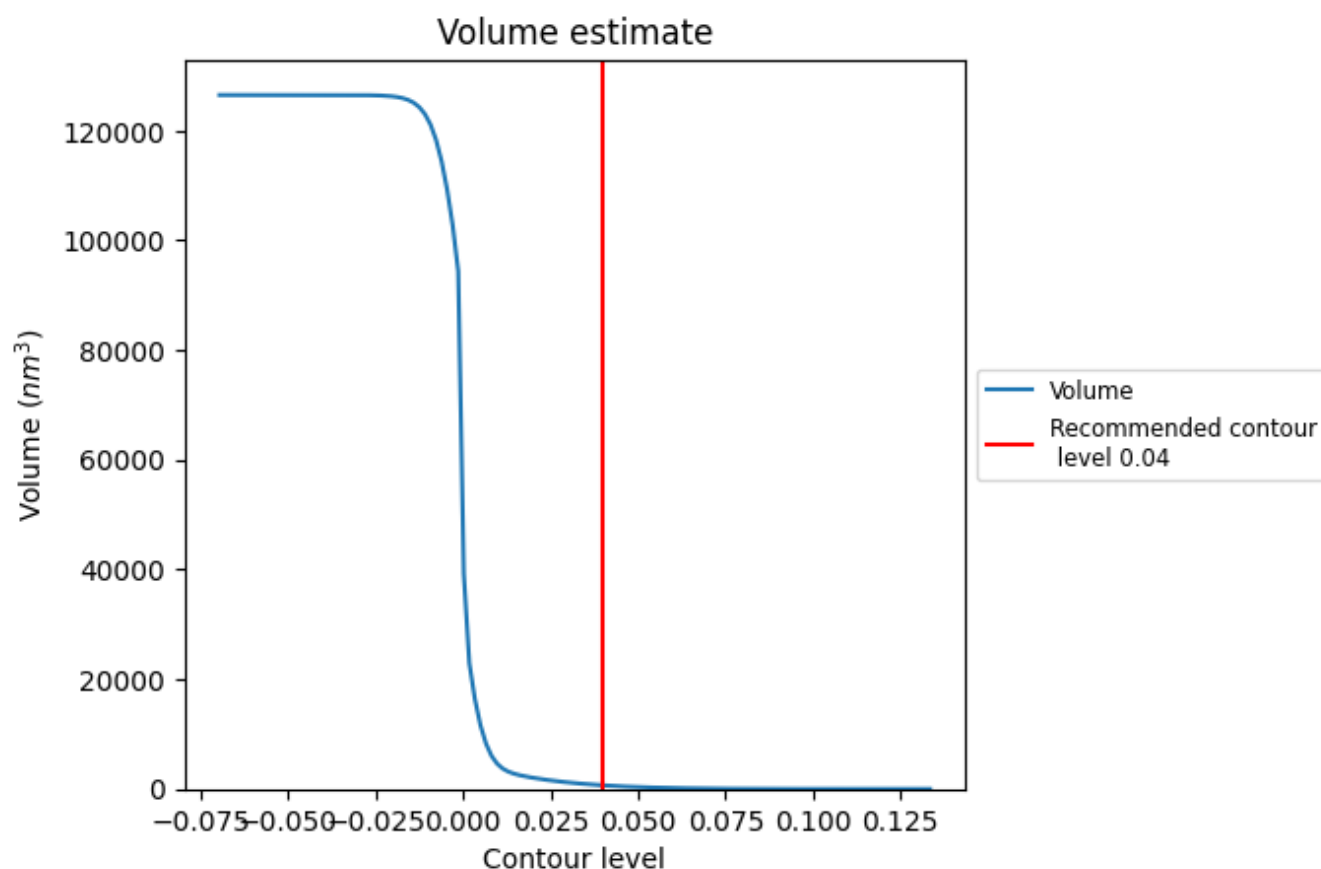
This section contains the results of statistical analysis of the map.

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.

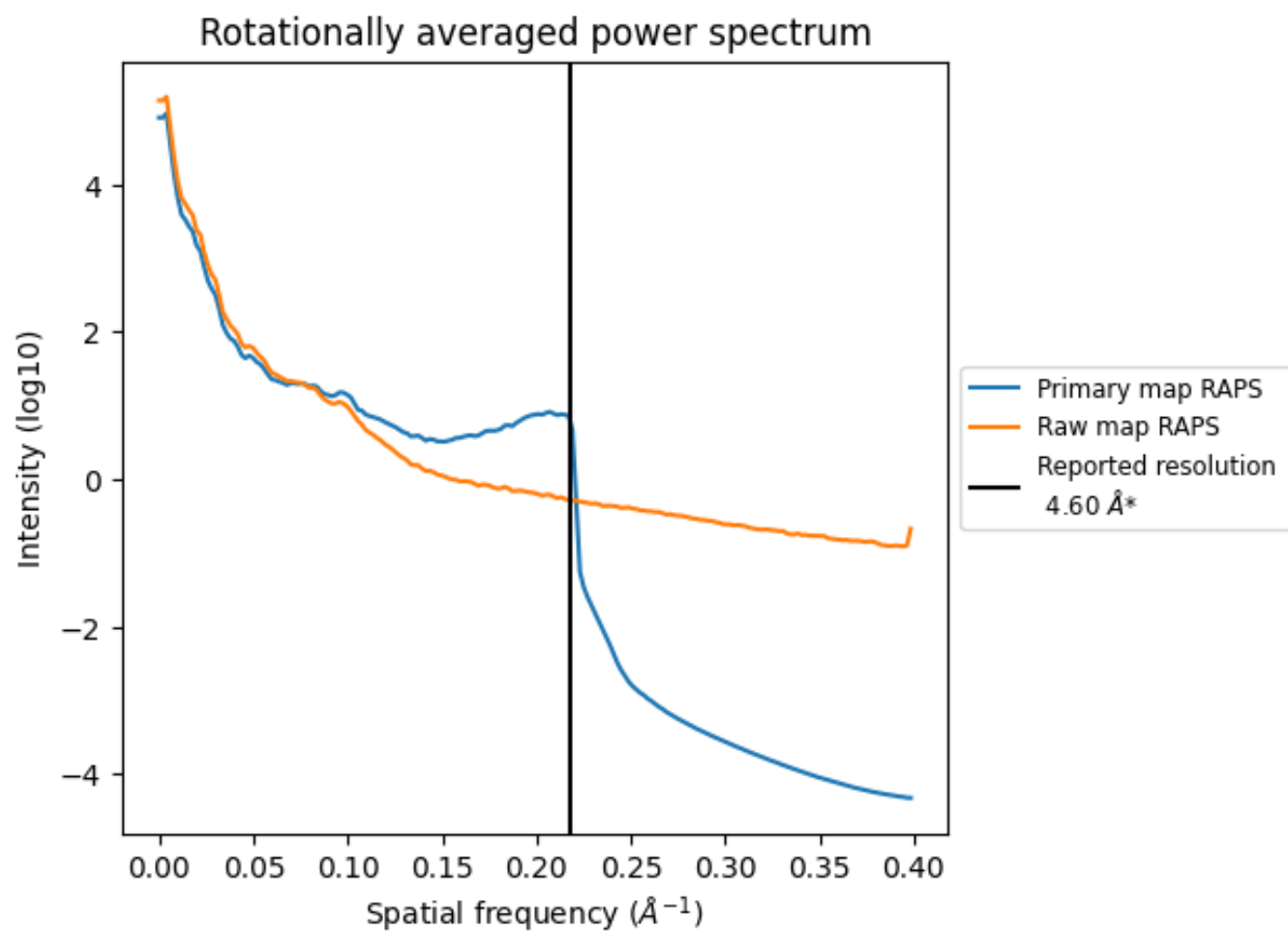
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 666 nm³; this corresponds to an approximate mass of 601 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

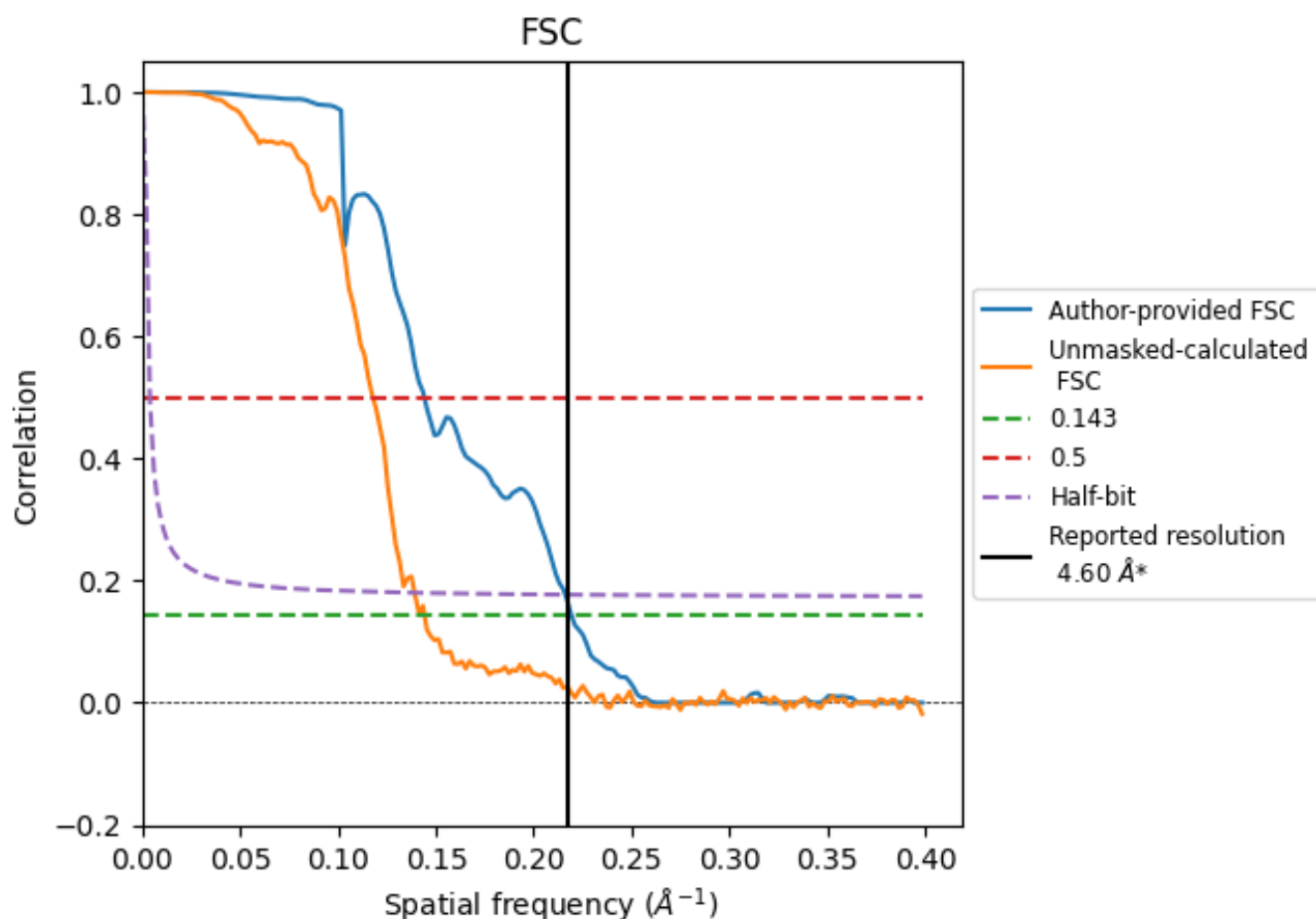


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.56	6.94	4.63
Unmasked-calculated*	6.93	8.49	7.18

*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 6.93 differs from the reported value 4.6 by more than 10 %

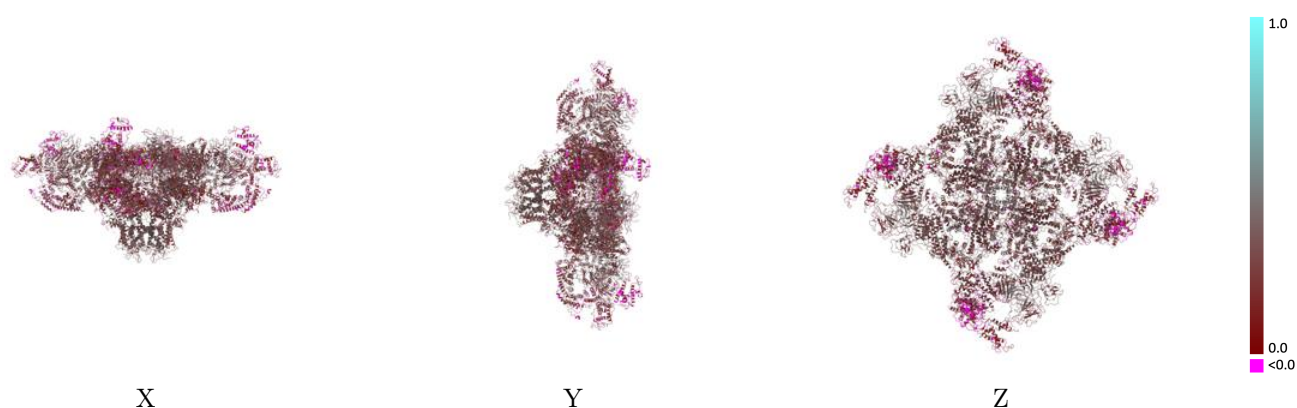
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8389 and PDB model 5TAY. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

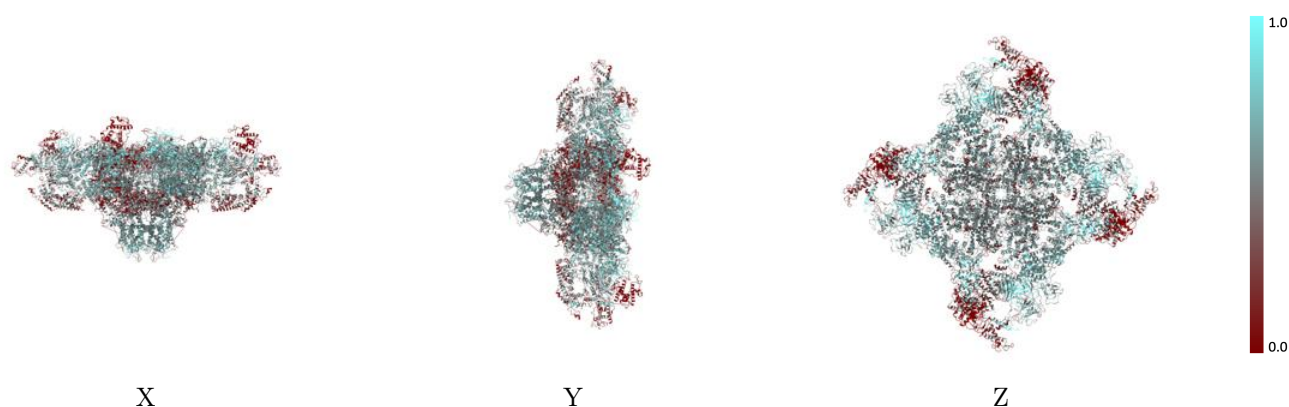
This section was not generated.

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



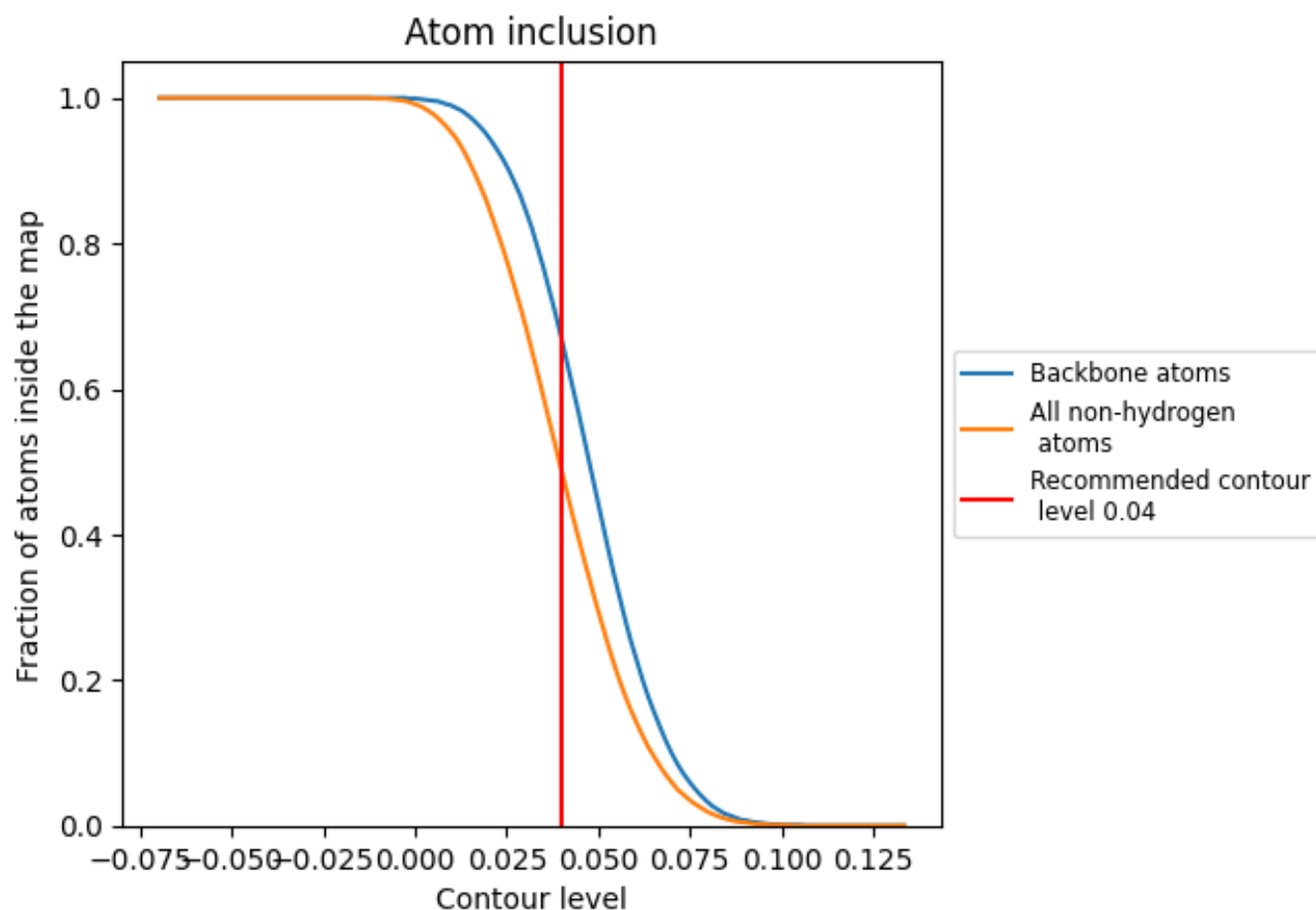
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 49% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4870	0.2640
A	0.5660	0.3270
B	0.4910	0.2670
E	0.4800	0.2570
F	0.5670	0.3310
G	0.4890	0.2650
H	0.5670	0.3300
I	0.4810	0.2590
J	0.5650	0.3280

1.0

0.0

<0.0