



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:32 PM UTC

PDB ID : 7JMF / pdb_00007jmf
EMDB ID : EMD-22392
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 42 - State 6 (S6)
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on : 2020-07-31
Resolution : 4.50 Å(reported)
Based on initial model : 5TB4

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

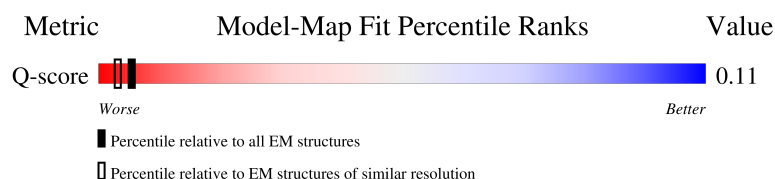
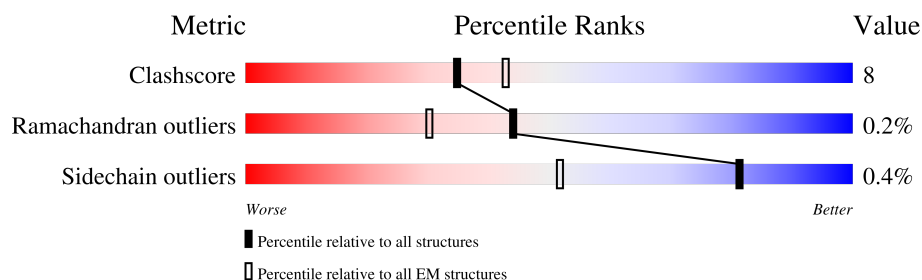
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	108	89% 67% 32%
1	F	108	84% 69% 31%
1	H	108	90% 69% 31%
1	J	108	87% 69% 31%

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Mol	Chain	Length	Quality of chain
2	B	4687	63% 73% 16% 11%
2	E	4687	64% 73% 16% 11%
2	G	4687	69% 73% 16% 11%
2	I	4687	70% 73% 16% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	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	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	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	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

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

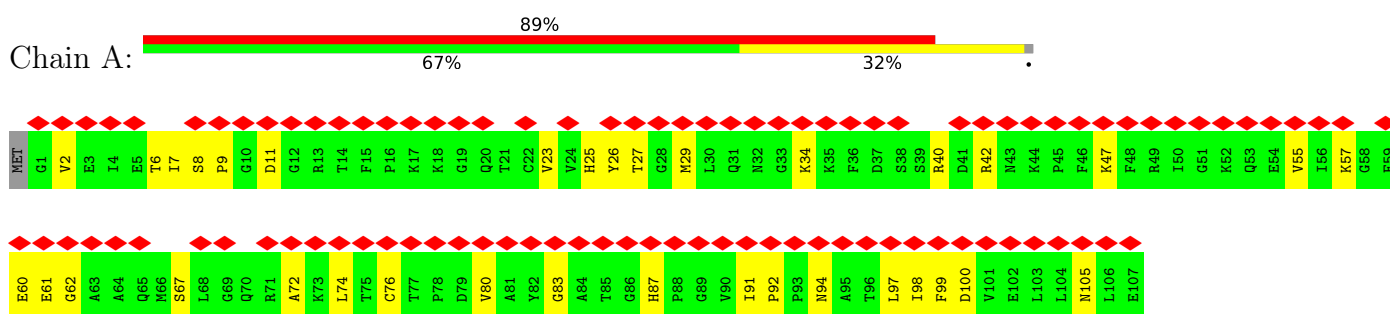
by depositor).

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

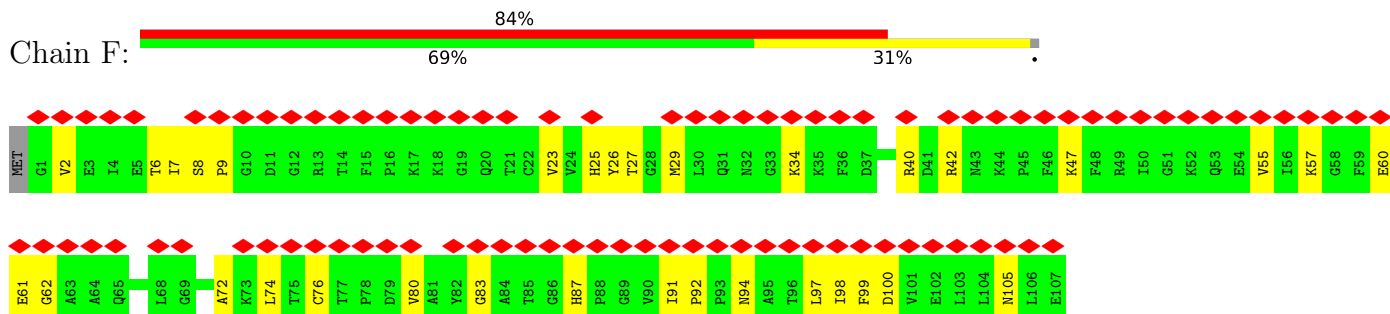
3 Residue-property plots [i](#)

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.

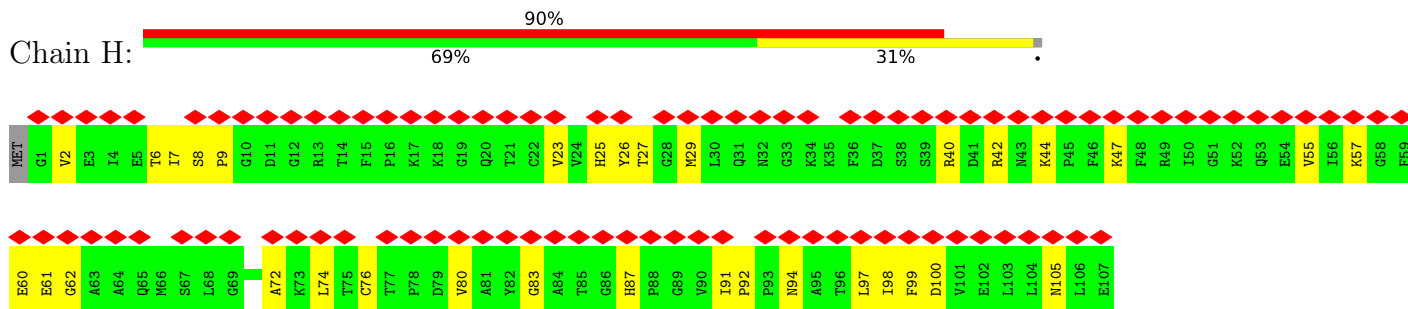
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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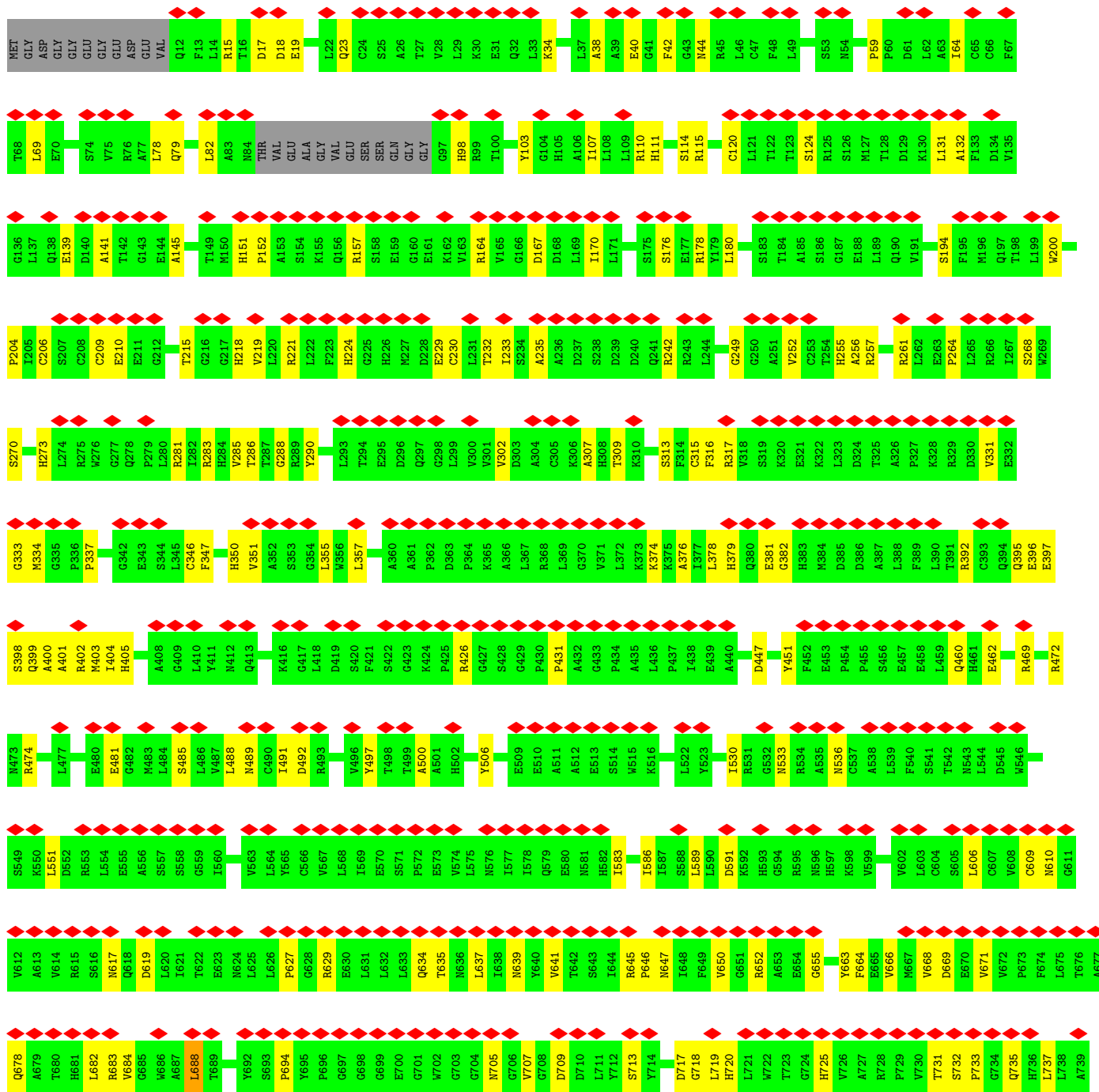
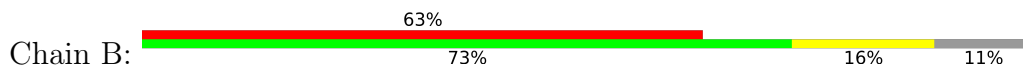


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



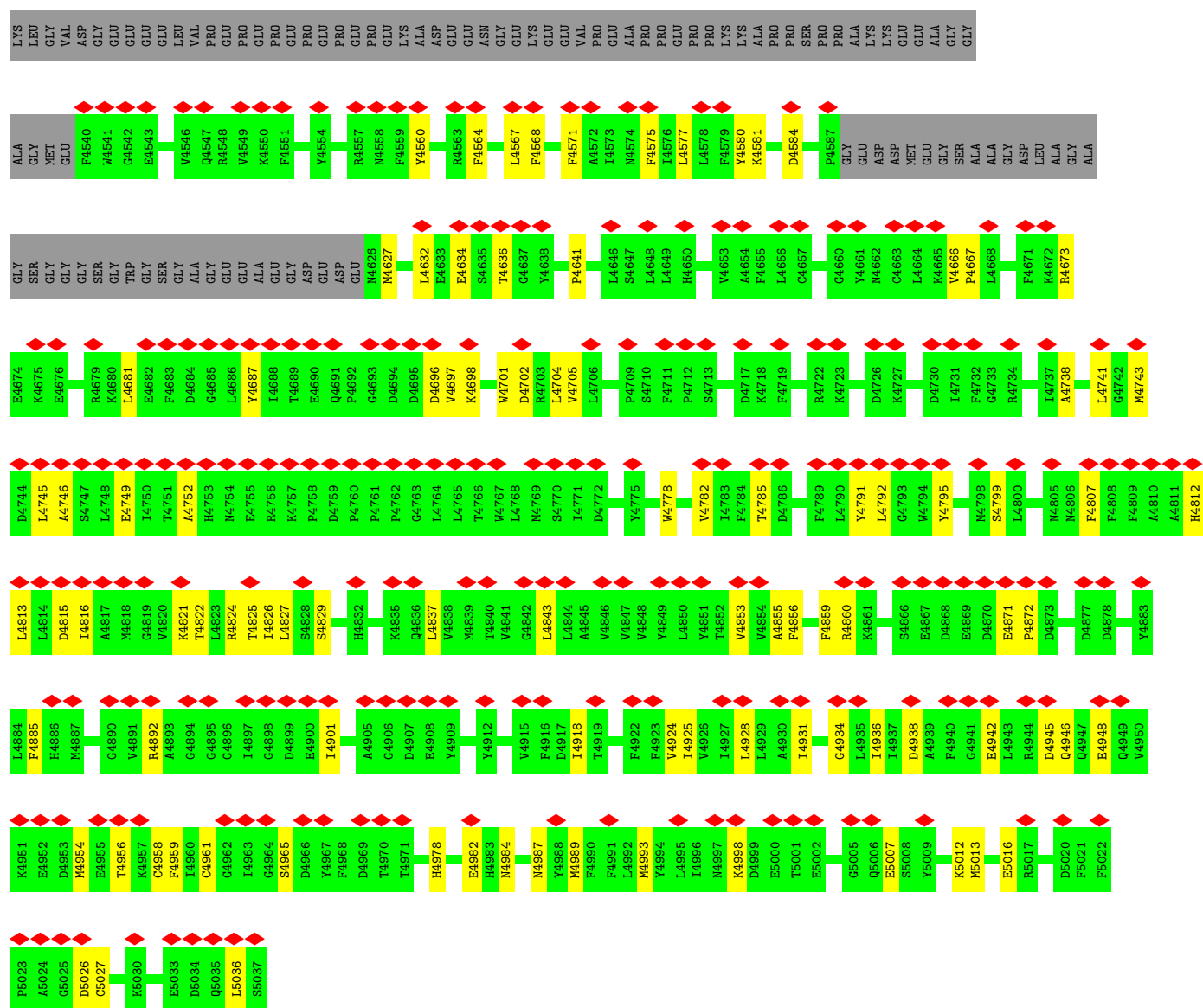


• Molecule 2: ryanodine receptor 1

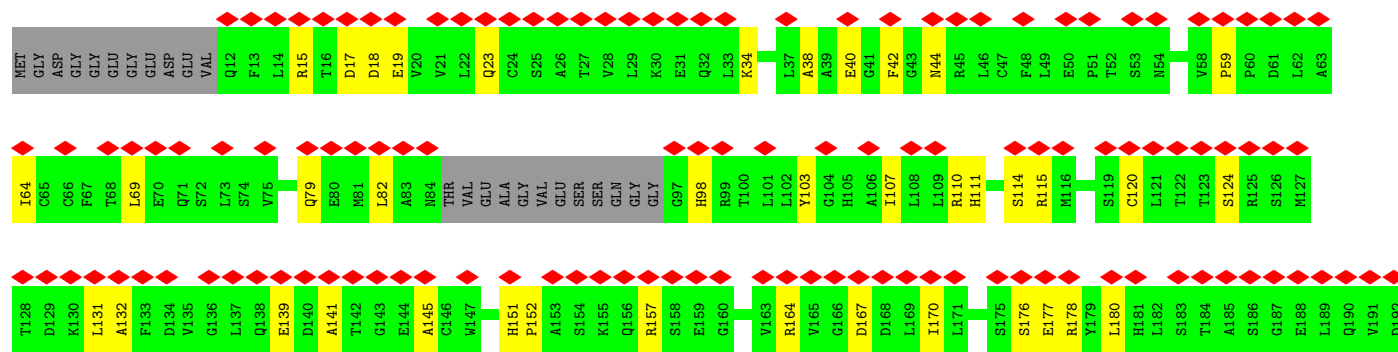
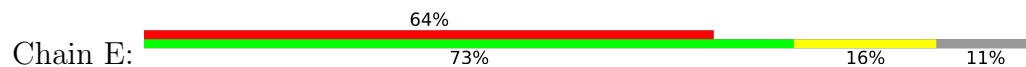


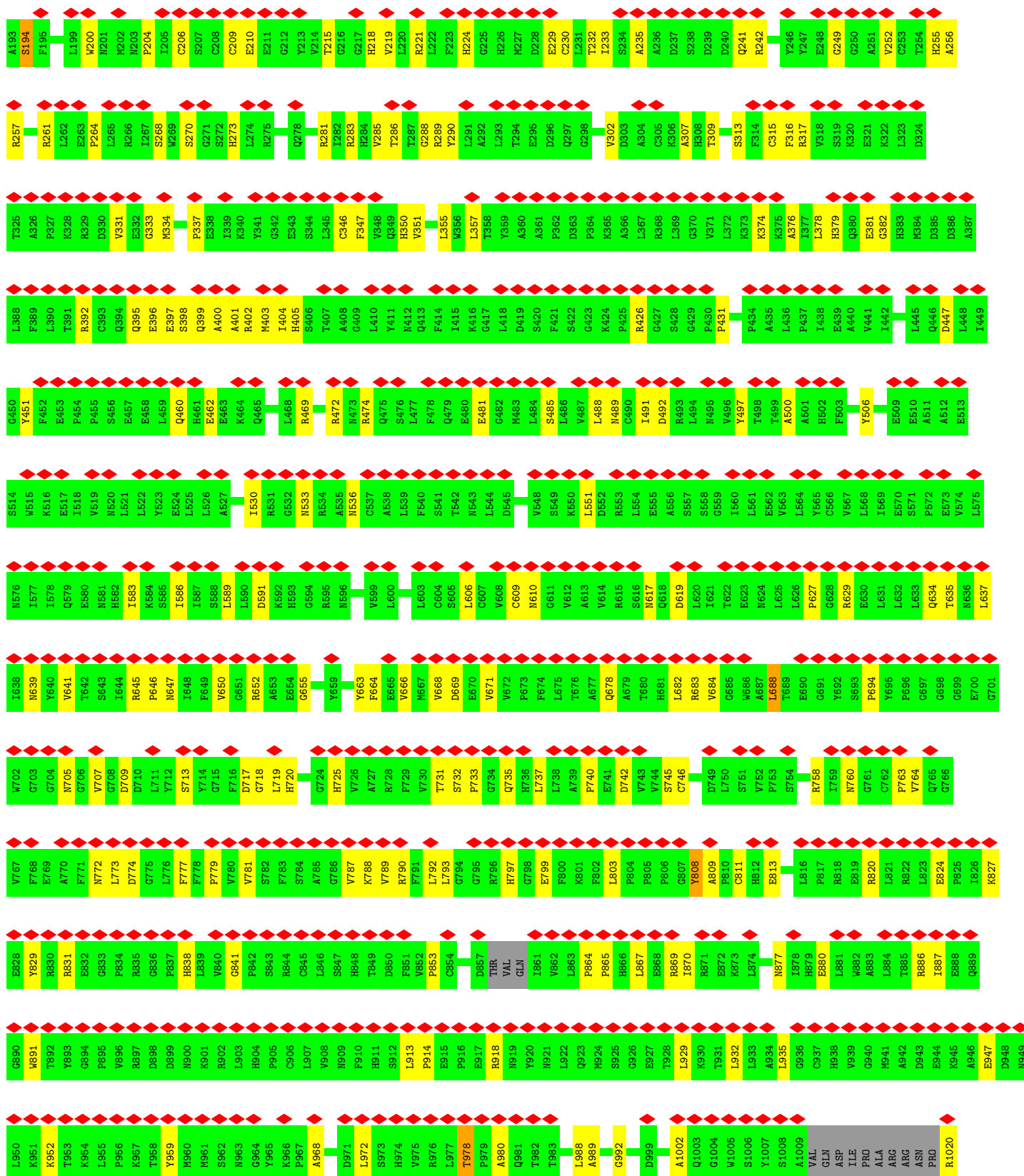
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X3371	X3372	X3373	X3374	X3375	X3376	X3377	X3378	X3379	X3380	X3381	X3382	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3395	X3396	X3397	X3398	X3399	X3400	X3401	X3402	X3403	X3404	X3405	X3406	X3407	X3408	X3409	X3410	X3411	X3412	X3413	X3414	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430																																				
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	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3289	X3290	X3293	X3294	X3295	X3296	X3297	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3309	X3310																																						
X3177	X3178	X3179	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3218	X3219	X3220	X3221	X3222	X3223	X3224	X3225	X3226	X3229	X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3241	X3242																																						
X3036	X3037	X3038	X3039	X3040	X3041	X3042	X3043	X3044	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3054	X3055	X3056	X3057	X3058	X3059	X3060	X3061	X3062	X3063	X3064	X3065	X3066	X3067	X3068	X3069	X3070	X3073	X3074	X3075	X3076	X3095	X3096	X3097	X3098	X3099	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3034	X3035																						
E2893	L2894	E2895	A2896	E2897	L2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	V2908	D2909	T2910	L2911	T2912	A2913	G2914	E2915	P2916	A2917	L2918	D2919	E2920	E2921	X2922	A2923	Q2924	E2925	L2926	L2927	X2928	F2929	L2930	Q2931	N2932	G2933	G2934	Y2935	A2936	P2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953	X2954																																				
X2955	X2956	X2957	X2958	X2959	X2960	X2961	X2962	X2963	X2964	X2965	X2966	X2968	X2969	X2970	X2973	X2974	X2975	X2976	X2995	X2996	X2997	X2998	X2999	X3000	X3001	X3002	X3003	X3004	X3005	X3006	X3009	X3010	X3011	X3012	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3026	X3027	X3028	X3029	X3030	X3031	X3034	X3035																																								
ARG	THR	GLU	LYS	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	L2878	A2879	E2880	N2881	P2882	H2883	N2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892																																					
N2773	N2774	W2775	S2776	L2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	N2790	L2791	R2792	P2793	V2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	L2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	K2810	E2811	S2812	L2813	L2814	A2815	N2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	Q2772																																			
X2641	X2642	X2643	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2662	X2663	X2664	X2665	X2666	X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	P2735	D2736	P2737	P2738	P2739	V2740	E2741	L2742	L2743	N2744	W2745	L2746	L2747	P2748	E2749	X2750	L2751	D2752	L2753	P2754	L2755	N2756	D2757	P2758	A2759	E2760	X2761	T2762	H2763	E2764	K2765	W2766	A2767	P2768	D2769	T2770	T2771	Q2772
X2541	X2544	X2550	X2551	X2552	X2553	X2554	X2555	X2556	X2557	X2558	X2559	X2560	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2589	X2590	X2591	X2592	X2593	X2594	X2595	X2596	X2597	X2598	X2599	X2600	X2601	X2602	X2603	X2604	X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615																																							

LEU	E4229	P4155	R4085	K4021	M9955	L3888	K3823	E3757	E3685	X3535
ALA	K4230	H4156	G4086	D4022	S9956	L3889	K3824	M3758	E3686	X3536
ALA	F4234	D4157	I4087	M4023	V9957	L3890	E3825	E3759	E3687	X3537
ALA	F4234	P4158	I4088	V4024	A9958	L3890	V3826	K3760	E3688	X3538
ALA	E4239	R4159	S4089	L4027	V9961	E3893	F3829	R3762	E3689	X3539
ARG	D4240	L4160	K4090	L4030	N9962	G3894	Q3830	L3763	V3690	X3540
ALA	T4241	R4161	K4091	L4031	N9963	H3895	Q3831	L3764	E3691	X3541
LEU	I4242	L4164	D4092	E4032	S9964	N3896	I3832	Y3765	E3692	X3542
GLY	I4242	E4165	F4093	G4033	S9964	N3897	Q3833	Q3766	K3693	X3543
LEU	M4245	E4168	Q4094	G4033	L3965	D3898	Q3833	Q3767	K3694	X3544
LEU	Q4246	E4168	K4095	N4034	F3899	F3899	M3836	S3768	X3605	X3545
TYR	A4249	E4168	A4096	V4035	Y9968	Q3900	Q3837	R3769	X3606	X3546
ARG	A4249	E4168	M4097	V4036	G9971	N3901	Q3837	L3770	X3607	X3547
SER	Q4250	L4171	D4098	M4037	P9972	R3904	S3840	H3771	A3709	X3548
LEU	Q4250	E4172	S4099	G4038	C9973	T3905	V3841	L3772	L3710	X3549
ARG	I4251	Y4173	Q4100	M4039	T3974	Q3906	L3842	R3773	T3711	X3550
ARG	S4252	F4174	K4101	M4039	G3975	T3907	D3843	E3712	K3611	X3551
VAL	E4253	R4175	Q4102	R4042	N3976	G3908	L3844	K3713	X3612	X3552
ARG	PR0	P4176	F4103	G4043	Q3977	G3909	N3845	S3714	X3613	X3553
GLY	GLY	Y4177	T4104	M4044	Q3978	N3909	N3846	K3715	T3639	X3554
GLY	GLY	L4178	G4105	V4045	S9979	T3910	A3846	L3716	Y3642	X3555
ARG	PR0	G4179	G4105	D4046	L3980	T3911	F3847	D3717	N3643	X3557
THR	ALA	R4180	P4106	M4047	A3981	T3912	E3848	E3718	L3644	X3558
ALA	ASP	I4181	E4107	L4048	H9982	T3916	R3849	D3719	P3645	X3559
ASP	ASP	E4182	Q4109	V4049	S9983	I3917	A3785	L3721	X3560	X3560
GLY	ASP	A4186	F4110	E4050	R3984	I3917	Q3850	Y3720	R3648	X3561
GLY	GLY	S4187	F4110	S4051	L3985	I3917	N3851	C3786	A3649	X3562
ALA	GLY	R4188	F4111	S4052	L3986	V3920	K3852	Y3722	C3650	X3563
ALA	ALA	R4189	S4113	M4054	A3988	D3921	A3853	M3723	M3652	X3564
ALA	ALA	R4192	E4116	V4055	V3990	L3924	G3857	A3792	F3653	X3565
ALA	ALA	R4192	E4117	E4056	G3991	R3925	M3858	D3727	L3654	X3566
LEU	ALA	S4198	A4117	L4059	G3992	Q3927	R3859	M3729	E3655	X3567
LEU	GLY	E4199	D4118	K4060	F9992	E3928	V3860	A3730	S3656	X3568
TRP	GLY	T4200	E4119	F4061	L3993	S3929	E3861	K3731	X3569	X3569
ALA	ALA	R4201	M4120	F4062	H3994	I3930	E3862	S3732	X3570	X3570
VAL	GLY	R4202	M4121	D4063	V3995	S3931	D3863	C3733	I3662	X3571
VAL	GLY	R4202	M4122	F4063	F3996	D3932	G3864	H3734	L3663	X3572
ALA	ALA	A4203	I4123	M4064	A3997	F3933	V3865	L3735	X3573	X3573
ALA	ALA	Q4204	M4124	F4065	H3998	Y3934	V3866	E3736	X3574	X3574
ALA	GLY	W4205	F4125	F4066	M3999	K3935	I3867	E3737	E3665	X3575
ALA	GLY	E4206	E4126	L4066	M4001	Y3937	N3867	E3737	E3666	X3576
ALA	GLY	W4207	E4127	K4067	K4002	Y3937	L3805	D3666	H3667	X3577
ALA	ALA	P4208	M4129	L4068	L4003	S3938	N3868	G3738	D3667	X3578
ALA	ALA	K4211	M4130	K4069	A4004	S3939	Q3869	G3739	E3668	X3579
THR	GLY	K4211	R4131	D4070	A4005	K3940	N3870	E3740	F3669	X3580
VAL	ALA	R4215	F4132	V4072	Q4005	D3941	G3871	N3741	E3670	X3581
ALA	ALA	R4215	Q4133	G4073	S4008	V3942	E3872	GLY	X3582	X3582
ALA	ALA	I4218	A4136	S4074	Q4009	I3943	K3873	ALA	M3673	X3583
THR	ALA	I4218	R4137	E4075	I4010	I3943	M3875	GLU	I3674	X3584
ALA	ALA	V4221	D4138	A4076	E4011	Q3946	A3876	GLU	D3676	X3585
ALA	ALA	V4222	T4139	F4077	L4012	G3947	D3877	E3748	D3676	X3586
ALA	ALA	M4223	G4140	Q4078	L4013	K3948	V3879	V3749	K3679	X3587
ALA	ALA	E4224	L4146	D4079	L4016	N3949	L3820	E3751	A3680	X3588
GLY	ALA	G4225	L4147	Y4080	N3950	N3950	E3879	V3751	G3681	X3589
ALA	ALA	G4226	L4147	V4081	F3951	F3951	T3881	S3752	E3682	X3590
LEU	ALA	E4227	E4152	T4082	Q4020	A3954	Q3882	F3753	Q3683	X3591
ALA	ALA	A4228	H4153	D4083	Q4020	A3954	L3884	E3754	E3684	X3592
ALA	ALA	A4228	V4154	P4084	Q4020	A3954	F3886	K3756	X3593	X3594



• Molecule 2: ryanodine receptor 1



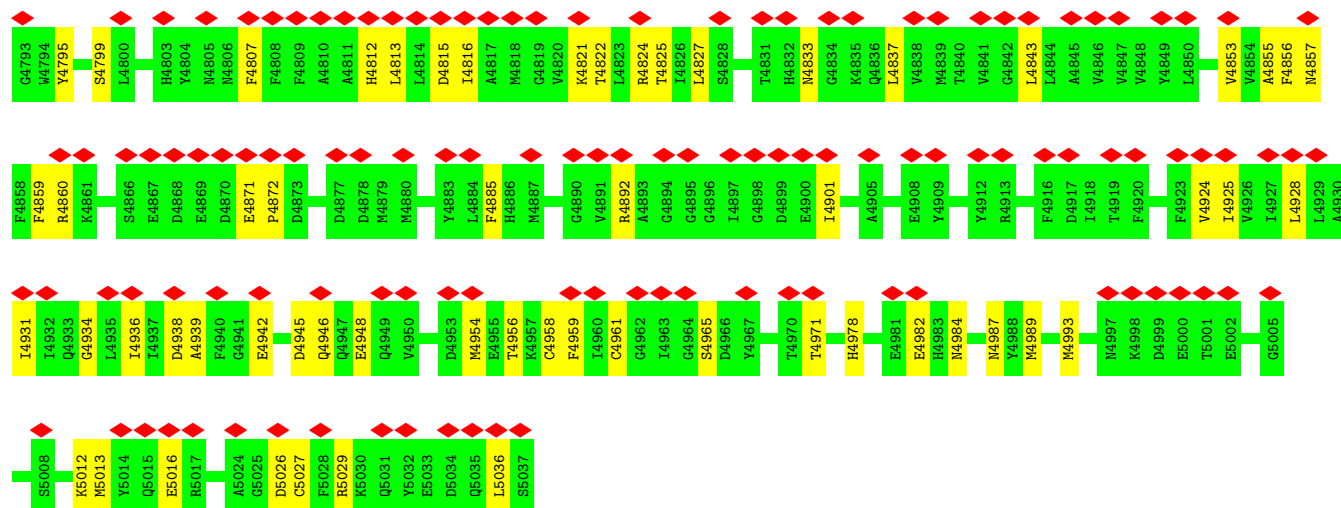




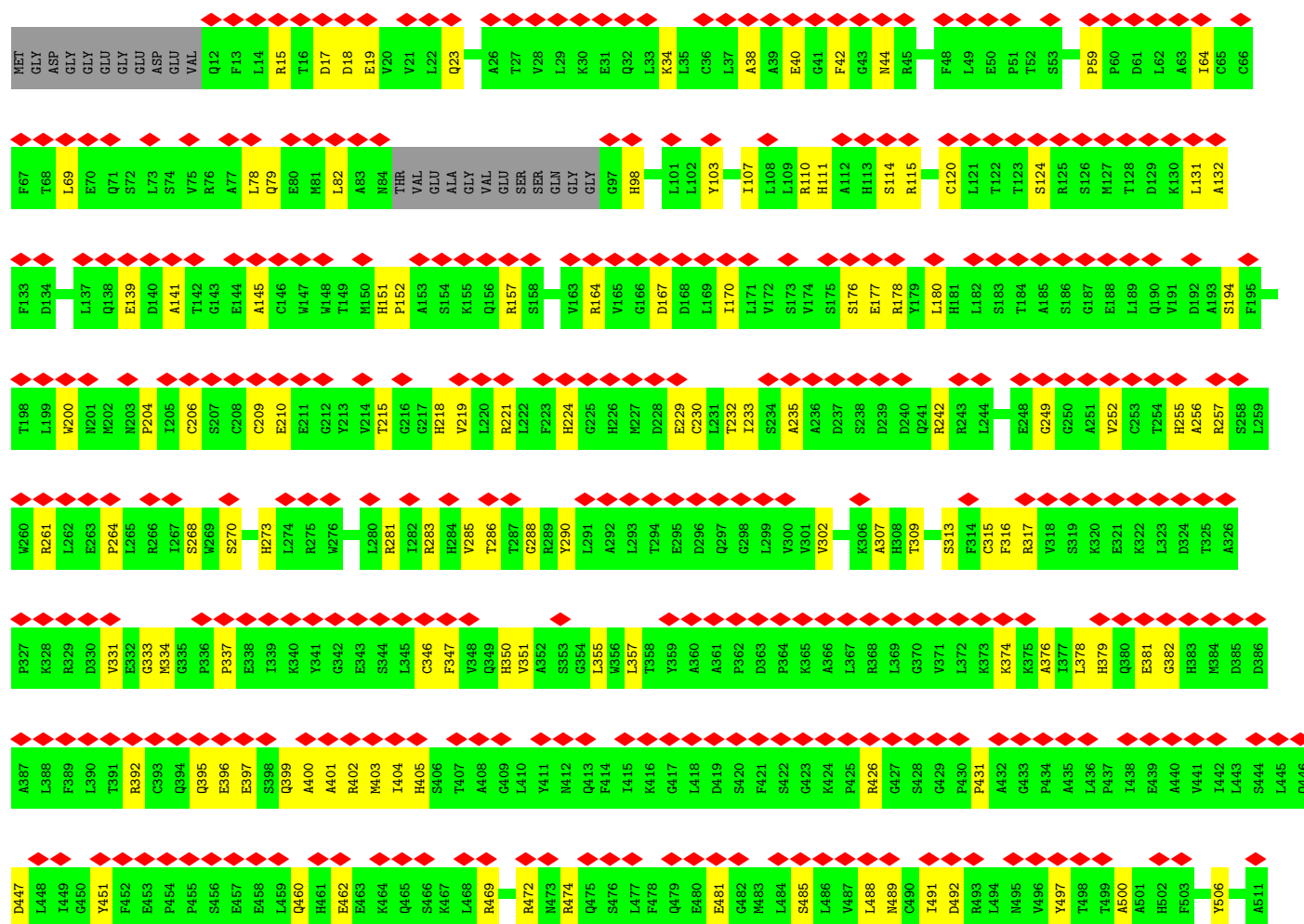
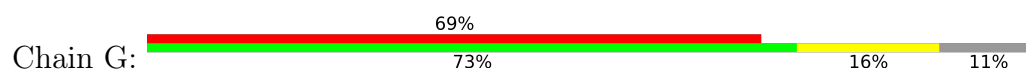
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• Molecule 2: ryanodine receptor 1

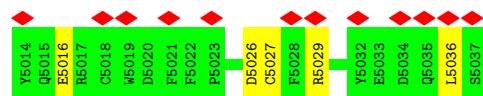




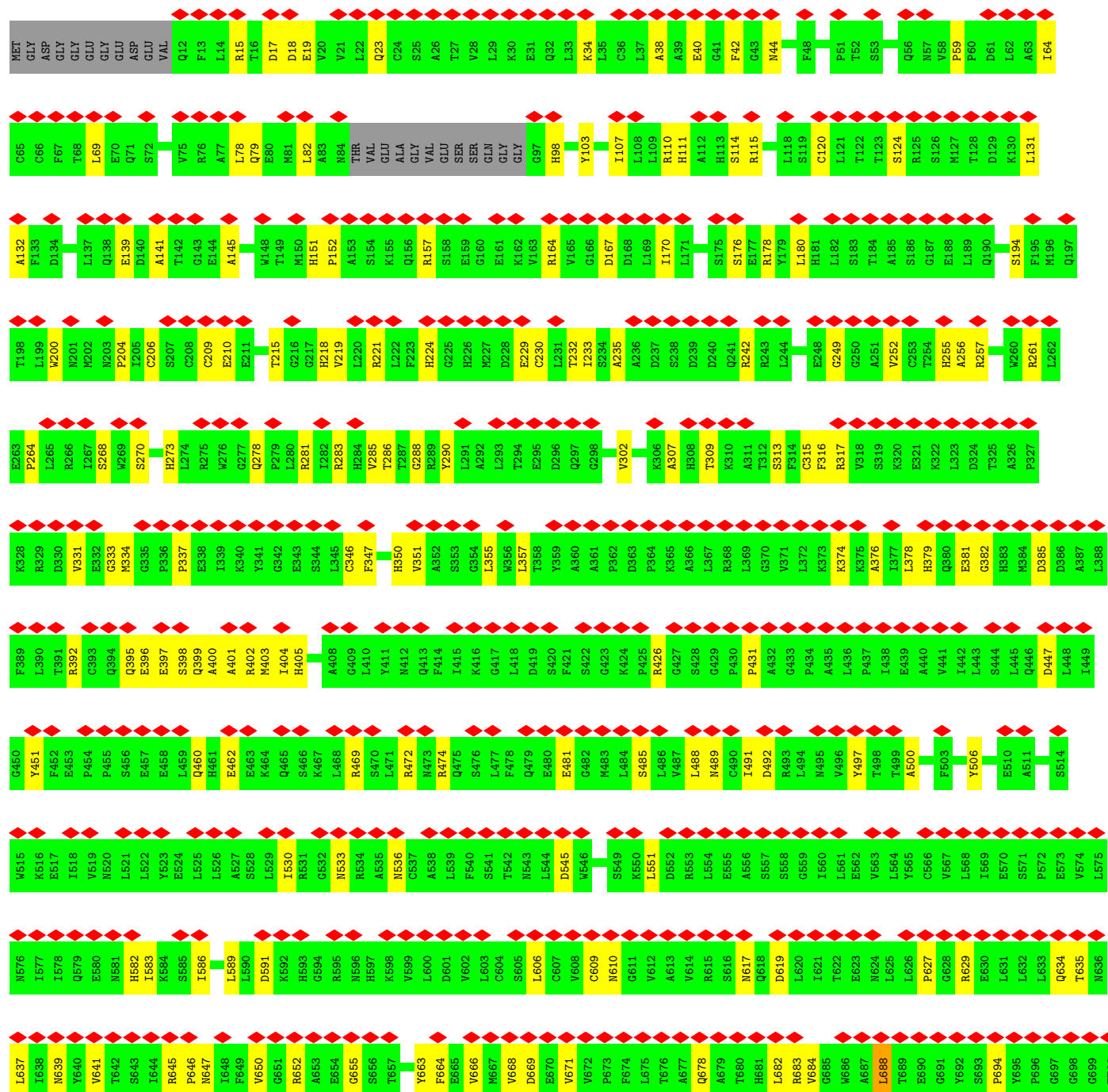
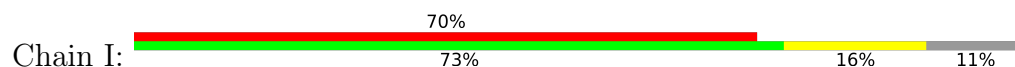
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W2819	E2820	W2821	T2822	T2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLY	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	ALA	GLN	THR	TVR	ASP	ARG	GLY	N2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	N2874	A2875	E2876	Q2877	L2878																				
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X2669	X2670	X2671	X2672	X2673	X2674	X2675	X2676	X2677	X2678	X2679	X2680	X2681	X2682	X2683	X2684	X2685	X2686	X2687	X2688	X2689	X2690	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2699	X2700	X2701	X2702	X2703	N2734	F2735	D2736	Y2737	R2738	Y2739	V2740	E2741	T2742	L2743	N2744	Y2745	L2746	I2747	Y2748	E2749	K2750	L2751	D2752	S2753	L2754	L2755	N2756	K2757	F2758																
X2605	X2606	X2607	X2608	X2609	X2610	X2611	X2612	X2613	X2614	X2615	X2616	X2617	X2618	X2619	X2620	X2621	X2622	X2623	X2624	X2625	X2626	X2627	X2628	X2629	X2632	X2633	X2636	X2637	X2640	X2641	X2644	X2645	X2646	X2647	X2648	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2656	X2657	X2658	X2659	X2660	X2661	X2662	X2663	X2664	X2665	X2666	X2668																					
X2541	X2542	X2543	X2544	X2545	X2548	X2549	X2550	X2551	X2552	X2555	X2556	X2557	X2558	X2559	X2560	X2561	X2562	X2563	X2564	X2565	X2566	X2567	X2568	X2569	X2570	X2571	X2572	X2573	X2574	X2575	X2576	X2577	X2578	X2579	X2580	X2581	X2582	X2583	X2584	X2585	X2586	X2587	X2588	X2591	X2592	X2593	X2594	X2595	X2598	X2599	X2602	X2603	X2604																						
L2472	P2473	L2474	Q2475	L2476	T2477	T2478	L2479	X2487	X2488	X2489	X2490	X2491	X2492	X2493	X2494	X2495	X2496	X2497	X2498	X2499	X2500	X2501	X2503	X2504	X2505	X2506	X2507	X2508	X2509	X2510	X2511	X2512	X2513	X2514	X2515	X2516	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2524	X2525	X2526	X2527	X2528	X2529	X2530	X2531	X2532	X2533	X2534	X2535	X2536	X2538																		
E2348	N2349	A2350	N2351	V2352	V2353	V2354	R2355	L2356	L2357	I2358	R2359	K2360	P2361	E2362	C2363	F2364	G2365	P2366	A2367	L2368	R2369	G2370	E2371	P2372	G2373	S2374	G2375	L2376	L2377	A2378	A2379	I2380	E2381	E2382	A2383	I2384	R2385	I2386	S2387	G2388	E2389	P2390	A2391	G2394	P2395	GLY	VAL	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	S2476																		
GLU	PRO	PRO	GLU	N2414	R2415	G2419	I2422	N2423	S2424	F2425	Y2426	A2427	A2428	L2429	I2430	D2431	L2432	L2433	G2434	R2435	C2436	A2437	P2438	E2439	M2440	H2441	L2442	L2443	Q2444	A2445	G2446	K2447	G2448	E2449	A2450	L2451	R2452	I2453	R2454	A2455	I2456	L2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466	G2467	E2468	I2469	L2470	S2471																			

E4050	S3983	I3916	E3854	G3788	I3728	H3667	X3581	X3520	X3413	X3353	X3291	X3221
S4051	R3984	I3917	Q3855	E3789	M3729	S3668	X3582	X3621	X3414	X3354	X3292	X3222
S4052	L3985	C3918	L3856	T3790	A3730	F3669	X3583	X3622	X3415	X3355	X3293	X3223
S4053	W3986	T3919	Q3857	G3791	K3731	E3670	X3584	X3623	X3416	X3356	X3294	X3224
N4054	D3987	V3920	S3732	G3792	S3732	D3671	X3585	X3624	X3417	X3357	X3295	X3225
E4056	A3988	L3924	C3733	M3793	C3733	R3672	X3586	X3625	X3418	X3358	X3296	X3226
E4056	V3989	R3925	M3793	V3794	H3734	M3673	X3587	X3626	X3419	X3359	X3297	X3227
N4057	V3990	L3926	S3795	V3795	L3735	I3674	X3588	X3627	X3420	X3360	X3298	X3228
	G3991	E3928	D3862	S3796	E3736	D3675	X3589	X3628	X3421	X3361	X3299	X3229
	F3992	S3929	T3797	T3797	E3737	D3676	X3590	X3629	X3422	X3362	X3300	X3230
	L3993	L3930	G3863	L3798	G3738	L3677	X3591	X3630	X3423	X3363	X3301	X3231
	H3994	I3931	T3864	K3799	G3739	S3678	X3592	X3631	X3424	X3364	X3302	X3232
	V3995	D3932	V3865	L3800	K3679	K3679	X3593	X3632	X3425	X3365	X3303	X3233
	F3996		L3866	G3801	A3680		X3594	X3633	X3426	X3366		X3234
	A3997	W3935	M3867	I3802	M3741		X3595	X3634	X3427	X3367	X3307	
	H3998	Y3936	R3868	S3803	GLY		X3596	X3635	X3428	X3368	X3308	
	M3999	Y3937	Q3869	I3804	ALA		X3597	X3636	X3429	X3369	X3309	
	M4000	Y3938	N3870	L3805	GLU		X3598	X3637	X3430	X3370	X3310	
	M4001	S3938	G3871	N3806	GLU		X3599	X3638	X3431	X3371	X3311	
	K4002	G3939	E3872	G3807	E3748		X3600	X3639	X3432	X3372	X3312	
	L4003	K3940	K3873	G3808	V3749		X3601	X3640	X3433	X3373	X3313	
	A4004	V3942	M3874	N3809	E3750		X3602	X3641	X3434	X3374	X3314	
	Q4005	I3943	M3875	V3812	E3751		X3603	X3642	X3435	X3375	X3315	
	D4006	A3876	A3876	Q3813	S3752		X3604	X3643	X3436	X3376	X3316	
	S4007	D3877	D3877	Q3814	F3753		X3605	X3644	X3437	X3377	X3317	
	S4008	E3945	K3878	K3815	E3754		X3606	X3645	X3438	X3378	X3318	
	Q4009	Q3946	E3879	M3816	E3755		X3607	X3646	X3439	X3379	X3319	
	I4010	G3947	F3880	L3817	K3756		X3608	X3647	X3440	X3380	X3320	
	E4011	K3948	I3881	D3818	E3757		X3609	X3648	X3441	X3381	X3321	
	L4012	R3949	Q3882	Y3819	M3758		X3610	X3649	X3442	X3382	X3322	
	L4013	N3950	D3883	L3820	K3759		X3611	X3650	X3443	X3383	X3323	
	K4014	F3951	L3884	K3821	K3760		X3612	X3651	X3444	X3384	X3324	
	E4015	S3952	F3885	D3822	Q3761		X3613	X3652	X3445	X3385	X3325	
	L4016	K3953	K3886	K3823	R3762		X3639	X3653	X3446	X3386	X3326	
	L4017	A3954			L3763		P3640	X3654	X3447	X3387	X3327	
	L4018	M3955			L3764		L3641	X3655	X3448	X3388	X3328	
	L4019	N3956	Q3889	F3829	H3704		N3642	X3656	X3449	X3389	X3329	
	L4020	V3957	L3890	Q3830	F3705		N3643	X3657	X3450	X3390	X3330	
	K4021	A3958	C3892	S3831	Q3765		L3644	X3658	X3451	X3391	X3331	
	D4022	K3959	E3893	I3832	Q3766		P3645	X3659	X3452	X3392	X3332	
	M4023	G3894	G3894	Q3833	S3768		H3647	X3660	X3453	X3393	X3333	
	V4024	H3895	M3836	M3836	R3707		R3648	X3661	X3454	X3394	X3334	
		N3963	Q3837	T3838	L3710		A3649	X3662	X3455	X3395	X3335	
	L4027	L3965	T3839	C3839	T3711		C3650	X3663	X3456	X3396	X3336	
	L4028	Y3968	V3841	V3841	E3712		N3651	X3664	X3457	X3397	X3337	
	S4029	Q3970	L3842	L3842	S3713		L3654	X3665	X3458	X3398	X3338	
	L4030	T3905	D3843	D3843	S3714		F3653	X3666	X3459	X3399	X3339	
		Q3973	L3844	L3844	K3715		L3654	X3667	X3460	X3400	X3340	
		F3972	N3845	N3845	L3716		E3655	X3668	X3461	X3401	X3341	
		T3974	F3846	F3846	D3717		S3656	X3669	X3462	X3402	X3342	
		Q3977	V3779	V3779	E3718		Y3657	X3670	X3463	X3403	X3343	
			L3780	L3780	G3719		K3658	X3671	X3464	X3404	X3344	
			K3781	K3781	Y3720		A3659	X3672	X3465	X3405	X3345	
			M3782	M3782	L3721		L3660	X3673	X3466	X3406	X3346	
			I3783	I3783	Y3722		L3663	X3674	X3467	X3407	X3347	
			S3784	S3784	M3723		E3664	X3675	X3468	X3408	X3348	
			A3785	A3785	A3724		E3665	X3676	X3469	X3409	X3349	
			C3786	C3786	Y3725		D3666	X3677	X3470	X3410	X3350	
			K3787	K3787	A3726			X3678	X3471	X3411	X3351	
					D3727			X3679	X3472	X3412	X3352	





• Molecule 2: ryanodine receptor 1



G701	G702	G703	G704	N705	G706	G707	G708	D709	D710	L711	L712	S713	Y714	D717	G718	L719	H720	L721	W722	L723	G724	H725	V726	A727	W728	P729	V730	L731	S732	P733	G734	G735	H736	L737	L738	A739	P740	E741	D742	V743	V744	S745	C746	D749	L750	S751	V752	P753	S754	I755	S756	F757	I759	N760	G761	C762																																																																																																																																							
P763	V764	Q765	G766	V767	F768	E769	A770	F771	N772	L773	D774	G775	L776	F777	F778	P779	V780	W781	S782	F783	S784	A785	G786	V787	K788	W789	P790	S791	L792	L793	G797	G798	E799	F800	K801	F802	L803	P804	P805	P806	G807	Y808	A809	P810	C811	H812	E813	A814	V815	L816	P817	R818	E819	R820	L821	R822	L823	E824																																																																																																																																					
P825	I826	K827	E828	Y829	R830	R831	E832	G833	P834	R835	G836	P837	H838	L839	V840	G841	P842	S843	R844	C845	L846	S847	H848	T849	D850	F851	V852	P853	C854	P855	V856	D857	THR	VAL	G861	V862	L863	P864	P865	H866	L867	E868	R869	I870	R871	E872	K873	L874	A875	E876	N877	I878	H879	E880	L881	W882	A883	L884																																																																																																																																					
T885	R886	I887	E888	Q889	G890	K891	T892	Y893	G894	P895	V896	R897	D898	D899	N900	K901	L902	L903	H904	P905	C906	L907	V908	N909	F910	H911	S912	L913	P914	E915	P916	E917	R918	N919	Y920	N921	L922	Q923	N924	S925	G926	E927	T928	L929	K930	E931	T931	L932	L933	A934	L935	G936	C937	H938	V939	G940	N941	A942	D943	E944																																																																																																																																			
K945	A946	E947	D948	N949	L950	K951	K952	T953	K954	L955	P956	K957	T958	Y959	N960	N961	S962	N963	G964	A968	P969	L970	D971	L972	S973	H974	V975	R976	L977	T978	P979	A980	Q981	T982	T983	L984	V985	D986	E987	L988	A989	G992	A997	R998	D999	K1000	V1001	A1002	Q1003	V1005	S1006	V1007	S1008	A1009	VAL																																																																																																																																								
GLN	ASP	ILE	PRO	ALA	ARG	ARG	ASN	PRO	R1020	L1021	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	E1029	A1030	T1031	K1032	R1033	S1034	N1035	R1036	D1037	S1038	L1039	C1040	Q1041	A1042	V1043	R1044	T1045	L1046	L1047	G1048	Y1049	G1050	Y1051	N1052	T1053	E1054	PRO	PRO	ASP	GLN	GLU	PRO	PRO	SER	GLN	VAL	GLU	ASN	GLN	SER	ARG	THR	D1070																																																																																																																																			
R1071	V1072	R1073	I1074	F1075	R1076	A1077	E1078	K1079	S1080	Y1081	T1082	V1083	Q1084	S1085	G1086	R1087	W1088	Y1089	K1090	E1091	F1092	E1093	A1094	V1095	T1096	E1099	M1100	V1102	G1103	W1104	A1105	R1106	P1107	E1108	L1109	R1110	P1111	D1112	V1113	E1114	L1115	G1116	A1117	D1118	E1119	L1120	A1121	Y1122	V1123	F1124	G1125	H1127	R1128	G1129	Q1130	R1131																																																																																																																																							
W1132	H1133	L1134	G1135	S1136	F1139	G1140	B1141	P1142	W1143	Q1144	S1145	G1146	D1147	V1148	V1149	G1150	C1151	M1152	I1153	D1154	L1155	T1156	E1157	N1158	T1159	I1160	I1161	F1162	L1164	N1165	G1166	E1167	V1168	L1169	M1170	S1171	D1172	S1173	G1174	S1175	E1176	T1177	A1178	F1179	R1180	E1181	I1182	E1183	I1184	G1185	D1186	G1187	F1188	L1189	P1190	V1191	C1192																																																																																																																																						
S1193	L1194	G1195	P1196	Q1197	Q1198	V1199	G1200	H1201	L1202	N1203	L1204	G1205	Q1206	D1207	V1208	S1209	S1210	L1211	R1212	F1213	F1214	A1215	I1216	C1217	G1218	L1219	Q1220	E1221	G1222	F1223	E1224	P1225	F1226	A1227	I1228	N1229	M1230	Q1231	P1232	V1233	T1234	T1235	T1236	W1237	F1238	S1239	K1240	S1241	L1242	P1243	Q1244	F1245	E1246	P1247	V1248	P1249	P1250	E1251	H1252																																																																																																																																				
P1253	H1254	Y1255	E1256	V1257	A1258	R1259	M1260	G1261	T1262	T1263	V1264	D1265	T1266	P1267	P1268	C1269	L1270	R1271	L1272	A1273	L1274	A1275	L1276	X1277	X1278	X1279	X1280	X1281	X1282	X1283	X1284	X1285	X1286	X1287	X1288	X1289	X1290	X1291	X1292	X1293	X1294	X1295	X1296	X1297	X1298	X1299	X1300	X1301	X1302	X1303	X1304	X1305	X1306	X1307	X1308	X1309	X1310	X1311	X1312	X1313	X1314	X1315	X1316	X1317	X1318	X1319	X1320	X1321	X1322	X1323	X1324	X1325	X1326	X1327	X1328	X1329	X1330	X1331	X1332	X1333	X1334	X1335	X1336	X1337	X1338	X1339	X1340	X1341	X1342	X1343	X1344	X1345	X1346	X1347	X1348	X1349	X1350	X1351	X1352	X1353	X1354	X1355	X1356	X1357	X1358	X1359	X1360	X1361	X1362	X1363	X1364	X1365	X1366	X1367	X1368	X1369	X1370	X1371	X1372	X1373	X1374	X1375	X1376	X1377	X1378	X1379	X1380	X1381	X1382	X1383	X1384	X1385	X1386	X1387	X1388	X1389	X1390	X1391	X1392	X1393	X1394	X1395	X1396	X1397	X1398	X1399	X1400	X1401	X1402	X1403	X1404	X1405	X1406	X1407	X1408	X1409	X1410	X1411	X1412	X1413	X1414	X1415	X1416	X1417	X1418	X1419	X1420	X1421	X1422	X1423	X1424	X1425	X1426	X1427	X1428	X1429	X1430	X1431	X1432	X1433	X1434	X1435	X1436	X1437	X1438	X1439	X1440	X1441	X1442	X1443	X1444
X1445	X1446	X1447	X1448	X1449	X1450	X1451	X1452	X1453	X1454	X1455	X1456	X1457	X1458	X1459	X1460	X1461	X1462	X1463	X1464	X1465	X1466	X1467	X1468	X1469	X1470	X1471	X1472	X1473	X1474	X1475	X1476	X1477	X1478	X1479	X1480	X1481	X1482	X1483	X1484	X1485	X1486	X1487	X1488	X1489	X1490	X1491	X1492	X1493	X1494	X1495	X1496	X1497	X1498	X1499	X1500	X1501	X1502	X1503	X1504	X1505	X1506	X1507	X1508	X1509	X1510	X1511	X1512	X1513	X1514	X1515	X1516	X1517	X1518	X1519	X1520	X1521	X1522	X1523	X1524	X1525	X1526	X1527	X1528	X1529	X1530	X1531	X1532	X1533	X1534	X1535	X1536	X1537	X1538	X1539	X1540	X1541	X1542	X1543	X1544	X1545	X1546	X1547	X1548	X1549	X1550	X1551	X1552	X1553	X1554	X1555	X1556	X1557	X1558	X1559	X1560	X1561	X1562	X1563	X1564	X1565	X1566	X1567	X1568	X1569	X1570	X1571	X1572	X1573	X1574	X1575	X1576	X1577	X1578	X1579	X1580	X1581	X1582	X1583																																																					
R1584	K1585	N1586	P1587	A1588	P1589	Q1590	C1591	P1592	P1593	R1594	L1595	E1596	V1597	Q1598	N1599	L1600	M1601	P1602	V1603	S1604	W1605	S1606	R1607	M1608	P1609	M1610	H1611	F1612	L1613	Q1614	V1615	GLU	THR	ARG	ARG	ALA	GLY	E1622	R1623	L1624	G1625	W1626	A1627	V1628	C1629	C1630	Q1631	D1632	P1633	L1634	T1635	M1636	M1637	A1638	L1639	H1640	I1641	P1642	E1643																																																																																																																																				

S5037	D4969	A4905	M4833	L4764	Q4700	T4636	A4572	GLU	GLY	ALA	GLY	VAL	GLU	THR	ALA	ALA
T4970	C4906	Q4836	Q4837	L4765	W4701	Q4637	I4573	GLU	ALA	ALA	GLY	VAL	GLU	ALA	ALA	ALA
P4972	D4907	L4837	V4838	T4766	R4702	Y4638	N4574	PRO	GLY	GLY	GLY	PRO	GLU	LEU	ALA	GLY
H4978	E4908	E4839	M4839	W4767	L4704	P4641	F4576	GLN	GLY	ALA	ASP	PRO	LEU	LEU	ALA	ALA
E4981	Y4909	T4840	T4840	L4768	W4705	L4706	L4577	PRO	ASP	GLY	GLY	TRP	LEU	LEU	GLY	GLY
E4982	E4910	V4841	S4770	M4769	P4709	C4645	F4578	PRO	GLY	GLY	GLY	ALA	TRP	GLY	GLY	GLY
H4983	L4911	D4842	L4771	S4770	S4710	L4646	F4579	PRO	GLY	GLY	GLY	ALA	VAL	VAL	ALA	ALA
N4984	Y4912	L4843	D4772	D4772	F4711	L4648	Y4580	PRO	THR	THR	THR	ASP	VAL	VAL	ALA	ALA
N4987	V4915	L4844	Y4775	Y4775	P4712	L4649	S4583	PRO	ALA	ALA	ALA	ASP	ARG	ARG	GLY	GLY
Y4988	F4916	A4845	W4778	W4778	P4712	H4650	D4584	PRO	ALA	ALA	ALA	ASP	ARG	ARG	GLY	GLY
M4989	T4919	V4846	R4779	R4779	S4713	T4651		PRO	GLY	GLY	GLY	ASP	VAL	VAL	ALA	ALA
F4990	F4922	Y4849	Y4782	Y4782	W4716	V4653	P4587	PRO	GLY	GLY	GLY	THR	ALA	ALA	THR	THR
F4991	F4923	L4850	L4783	L4783	D4717	L4654	GLY	PRO	GLY	GLY	GLY	THR	ALA	ALA	VAL	VAL
L4992	V4924	Y4851	F4784	F4784	K4718	F4655	ASP	PRO	GLY	GLY	GLY	ALA	ALA	ALA	ALA	ALA
M4993	L4925	T4852	T4785	T4785	F4719	L4656	MET	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
Y4994	V4926	V4853	D4786	D4786	W4720	C4657	GLY	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
L4995	V4927	A4855	F4789	F4789	K4721	L4658	GLY	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
L4996	L4928	F4856	L4790	L4790	R4722	T4659	ALA	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
N4997	L4929	M4857	Y4791	Y4791	K4723	M4662	GLY	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
K4998	A4930	F4858	L4792	L4792	D4726	C4663	ASP	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
D4999	I4931	F4859	L4792	L4792	K4727	L4664	GLY	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
E5002	Q4934	R4860	Y4795	Y4795	D4730	K4665	F4540	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
H5003	L4935	K4865	W4798	W4798	D4730	K4665	W4541	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
T5004	L4936	S4866	S4799	S4799	I4731	P4667	G4542	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
G5005	I4937	E4867	L4800	L4800	R4734	L4668	E4543	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
Q5006	D4938	D4868	E4871	E4871	E4735	F4671	V4546	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
E5007	S5008	E4869	F4807	F4807	R4736	K4672	Q4547	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
S5008	A4939	D4870	M4806	M4806	I4737	R4673	R4548	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
Y5009	F4940	E4871	F4808	F4808	A4738	E4674	V4549	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
W5010	G4941	E4872	F4809	F4809	L4740	K4675	K4550	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
W5011	E4942	D4873	A4810	A4810	L4741	L4677	F4551	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
K5012	L4943	D4873	A4811	A4811	G4742	A4678	Y4554	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
M5013	R4944	M4879	H4812	H4812	M4743	K4680	L4555	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
Y5014	D4945	D4879	L4813	L4813	D4744	L4681	S4556	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
Q5015	Q4946	M4879	D4815	D4815	L4745	E4682	R4557	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
E5016	Q4947	M4880	L4814	L4814	L4745	L4681	M4558	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
E5019	E4948	Y4883	L4814	L4814	L4745	L4681	F4559	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
D5020	K4951	V4891	D4884	D4884	T4751	Y4687	T4561	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
F5021	C4952	R4892	L4884	L4884	T4751	L4687	L4562	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
F5022	D4953	F4892	F4885	F4885	A4762	L4687	R4563	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
P5023	M4954	A4893	L4816	L4816	H4753	E4683	L4565	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
A5024	E4955	G4894	A4817	A4817	N4754	D4684	Y4560	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
G5025	T4956	M4887	M4818	M4818	E4749	Q4685	R4557	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
D5026	K4957	G4890	G4819	G4819	I4750	L4686	T4561	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
C5027	C4957	V4820	V4820	V4820	T4751	Y4687	L4626	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
F5028	C4958	V4891	K4821	K4821	T4751	L4687	L4632	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
R5029	F4959	R4892	T4822	T4822	A4762	L4687	L4565	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
K5030	T4960	A4893	L4823	L4823	H4753	E4683	L4566	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
Q5031	C4961	G4894	R4824	R4824	N4754	Q4691	E4634	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
Y5032	G4962	C4895	T4825	T4825	E4755	P4692	S4635	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
E5033	T4963	G4896	L4827	L4827	R4756	Q4692		PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
D5034	G4964	I4897	L4827	L4827	K4757	D4694	L4632	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
S5035	S4965	T4897	S4829	S4829	P4758	D4695	F4564	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
Q5036	D4966	G4898	L4827	L4827	D4759	D4696	L4567	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
L5036	Y4967	D4899	Y4830	Y4830	P4760	V4697	F4568	PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
	F4968	E4900	T4831	T4831	P4761	K4698		PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA
		I4901	H4832	H4832	P4762	G4699		PRO	GLY	GLY	GLY	ASP	ALA	ALA	ALA	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.404	Depositor
Minimum map value	-0.232	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.16	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	0.22	0/834	0.58	1/1123 (0.1%)
1	F	0.21	0/834	0.58	1/1123 (0.1%)
1	H	0.21	0/834	0.58	1/1123 (0.1%)
1	J	0.21	0/834	0.58	1/1123 (0.1%)
2	B	0.26	0/25428	0.61	2/34534 (0.0%)
2	E	0.26	0/25428	0.61	2/34534 (0.0%)
2	G	0.26	0/25428	0.61	2/34534 (0.0%)
2	I	0.26	0/25428	0.61	2/34534 (0.0%)
All	All	0.26	0/105048	0.61	12/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	17
2	E	0	18
2	G	0	17
2	I	0	17
All	All	0	69

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4872	PRO	N-CA-C	-6.25	105.22	113.65
2	I	4872	PRO	N-CA-C	-6.18	105.30	113.65
2	B	4872	PRO	N-CA-C	-6.17	105.32	113.65
2	G	4872	PRO	N-CA-C	-5.94	105.27	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4063	ASP	CA-CB-CG	5.77	118.37	112.60

There are no chirality outliers.

5 of 69 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	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	20	0
1	F	818	0	824	19	0
1	H	818	0	824	19	0
1	J	818	0	824	20	0
2	B	29369	0	24710	425	0
2	E	29369	0	24708	434	0
2	G	29369	0	24708	436	0
2	I	29369	0	24711	440	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	120756	0	102133	1793	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 8.

The worst 5 of 1793 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:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.65	0.78
2:G:177:GLU:HG3	2:I:2452:ARG:HH12	1.54	0.70
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.72	0.70
2:G:111:HIS:HD2	2:G:114:SER:H	1.38	0.70
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.72	0.70

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%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4687 (69%)	2862 (88%)	367 (11%)	6 (0%)	43	77
2	E	3235/4687 (69%)	2861 (88%)	367 (11%)	7 (0%)	43	77
2	G	3235/4687 (69%)	2863 (88%)	365 (11%)	7 (0%)	43	77
2	I	3235/4687 (69%)	2863 (88%)	365 (11%)	7 (0%)	43	77
All	All	13360/19180 (70%)	11833 (89%)	1500 (11%)	27 (0%)	44	77

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1829	PRO
2	B	1932	PRO
2	E	1829	PRO
2	G	1829	PRO

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Mol	Chain	Res	Type
2	I	1829	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	2493/3209 (78%)	2485 (100%)	8 (0%)	86	84
2	E	2493/3209 (78%)	2484 (100%)	9 (0%)	84	82
2	G	2493/3209 (78%)	2483 (100%)	10 (0%)	84	82
2	I	2493/3209 (78%)	2483 (100%)	10 (0%)	84	82
All	All	10324/13192 (78%)	10287 (100%)	37 (0%)	81	82

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	688	LEU
2	I	4154	VAL
2	I	815	VAL
2	I	3663	LEU
2	E	3663	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 220 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	113	HIS
2	G	2858	GLN
2	I	5031	GLN
2	I	3809	ASN

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Mol	Chain	Res	Type
2	G	203	ASN

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	12
2	B	12

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Mol	Chain	Number of breaks
2	G	12
2	E	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3613:UNK	C	3639:THR	N	43.91
1	B	3613:UNK	C	3639:THR	N	43.68
1	G	3613:UNK	C	3639:THR	N	43.62
1	E	3613:UNK	C	3639:THR	N	43.61
1	I	3163:UNK	C	3170:UNK	N	16.30

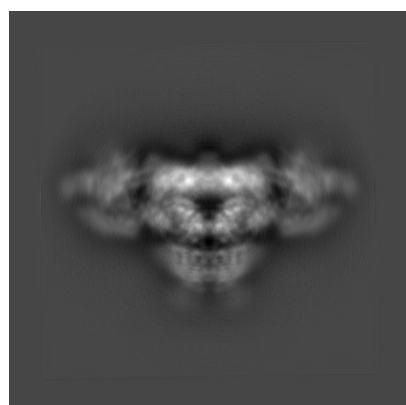
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22392. These allow visual inspection of the internal detail of the map and identification of artifacts.

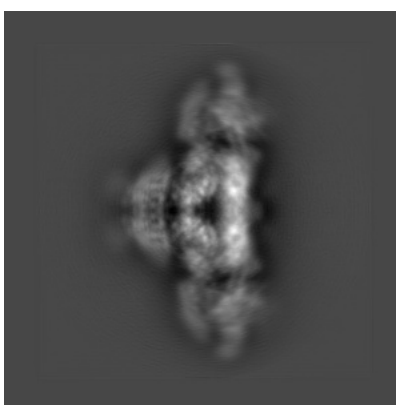
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

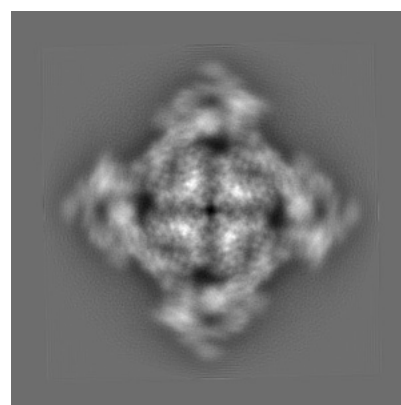
6.1.1 Primary map



X



Y

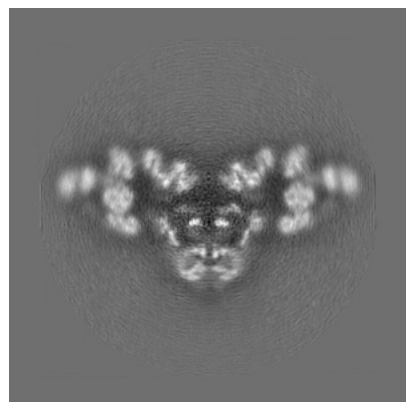


Z

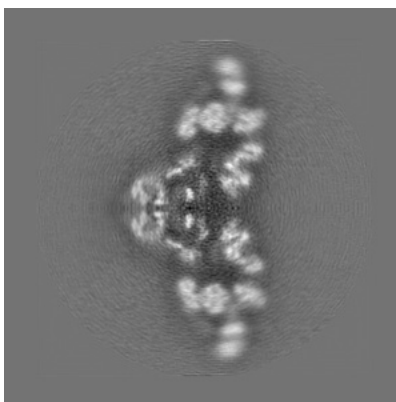
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

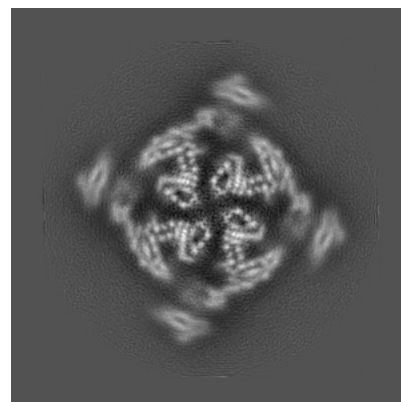
6.2.1 Primary map



X Index: 200



Y Index: 200

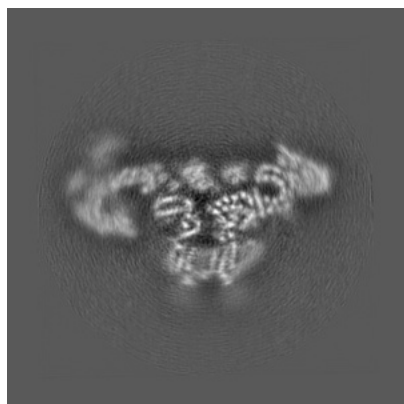


Z Index: 200

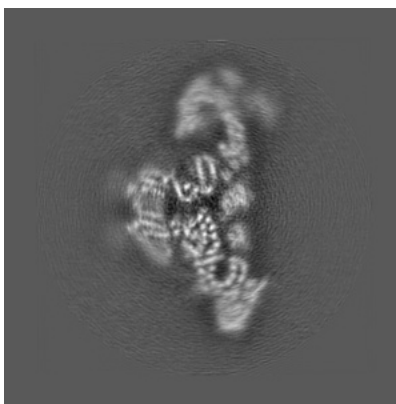
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

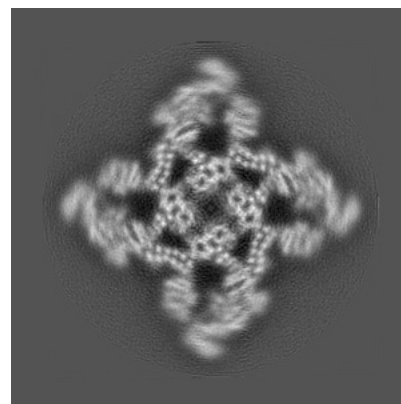
6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 226

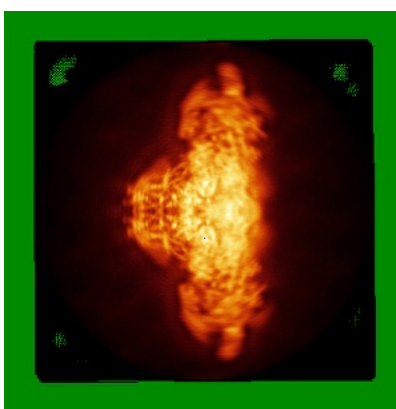
The images above show the largest variance slices of the map in three orthogonal directions.

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

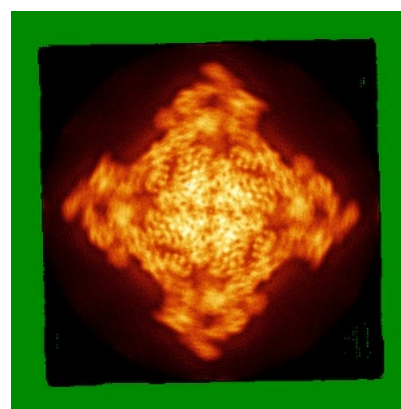
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

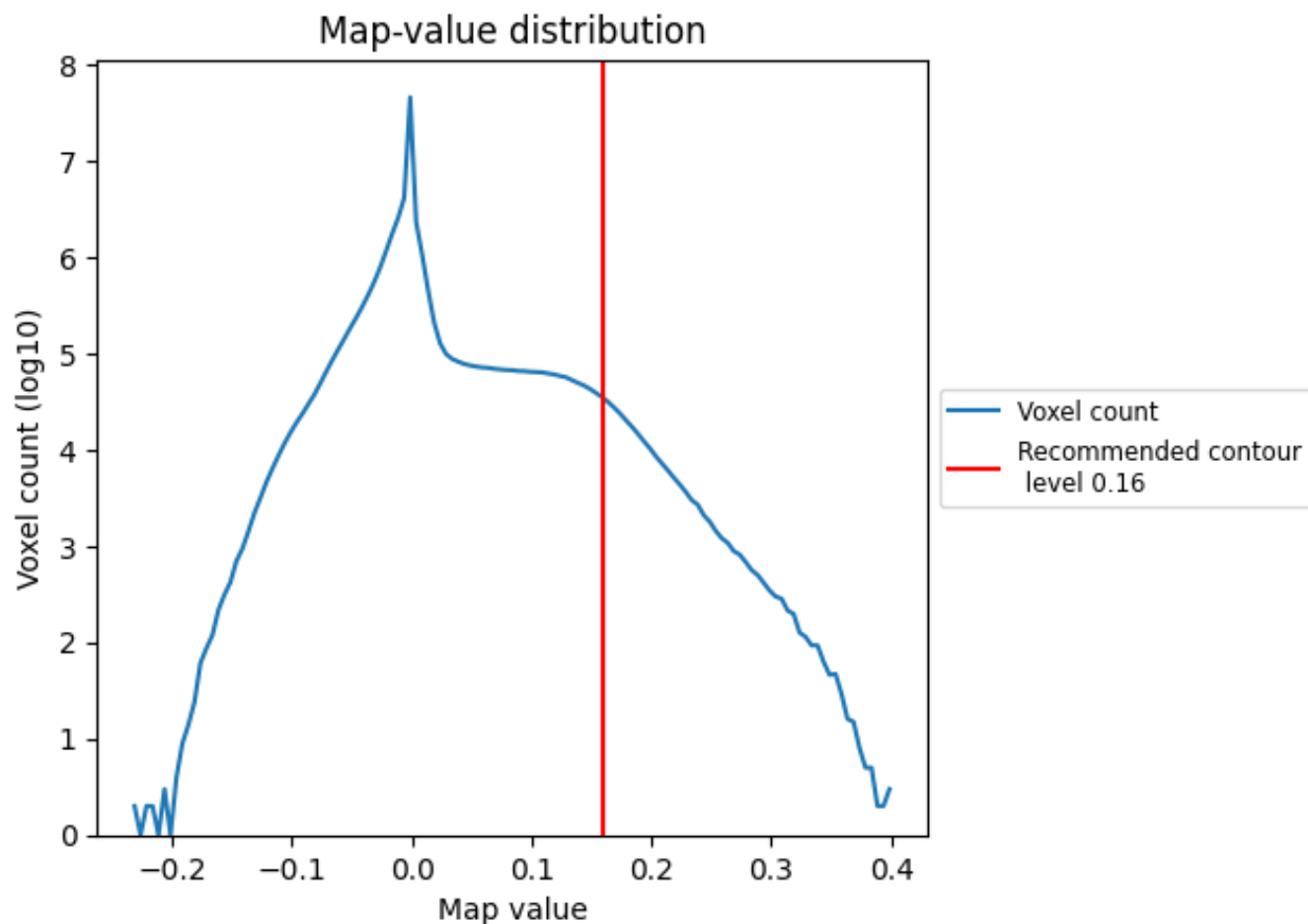
6.6 Mask visualisation

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

7 Map analysis [i](#)

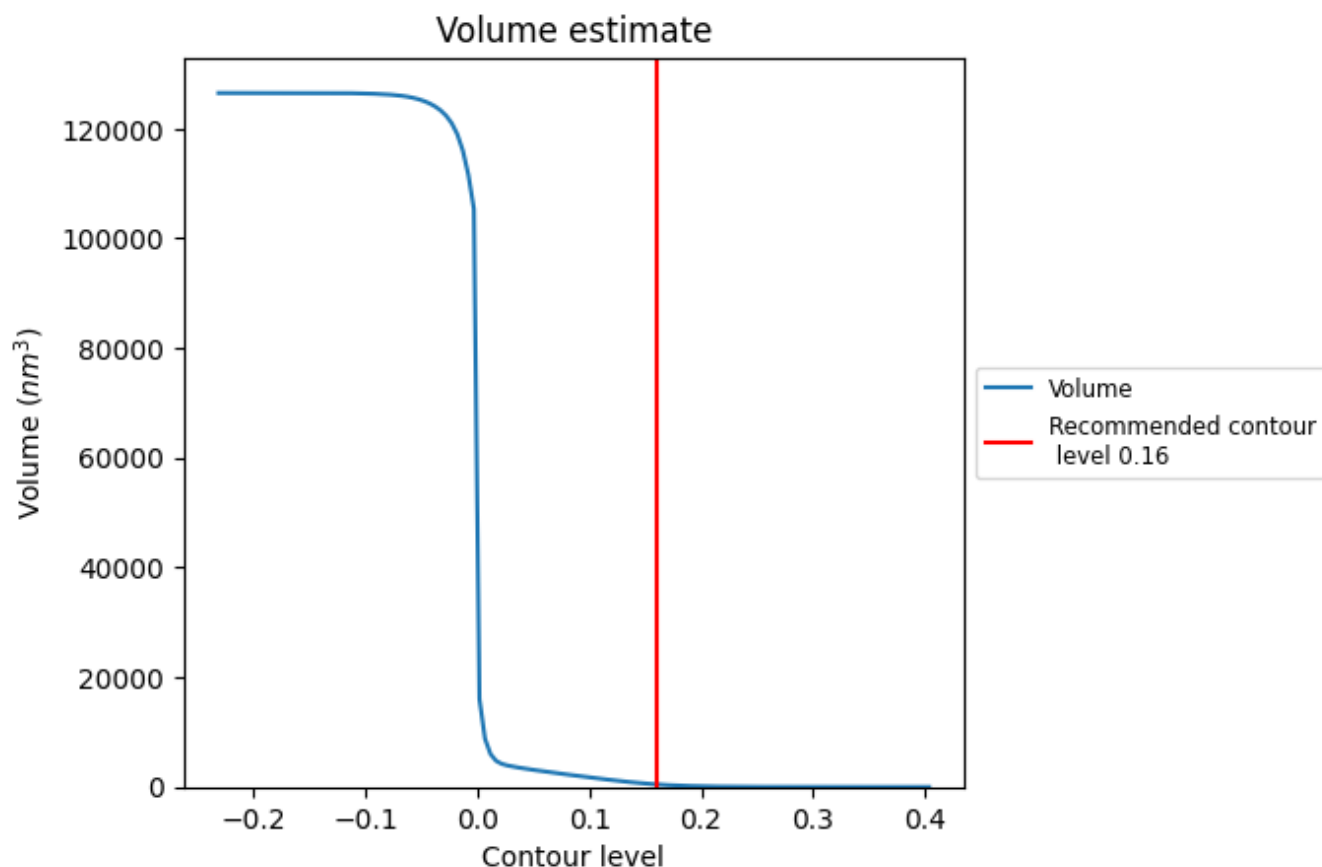
This section contains the results of statistical analysis of the map.

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.

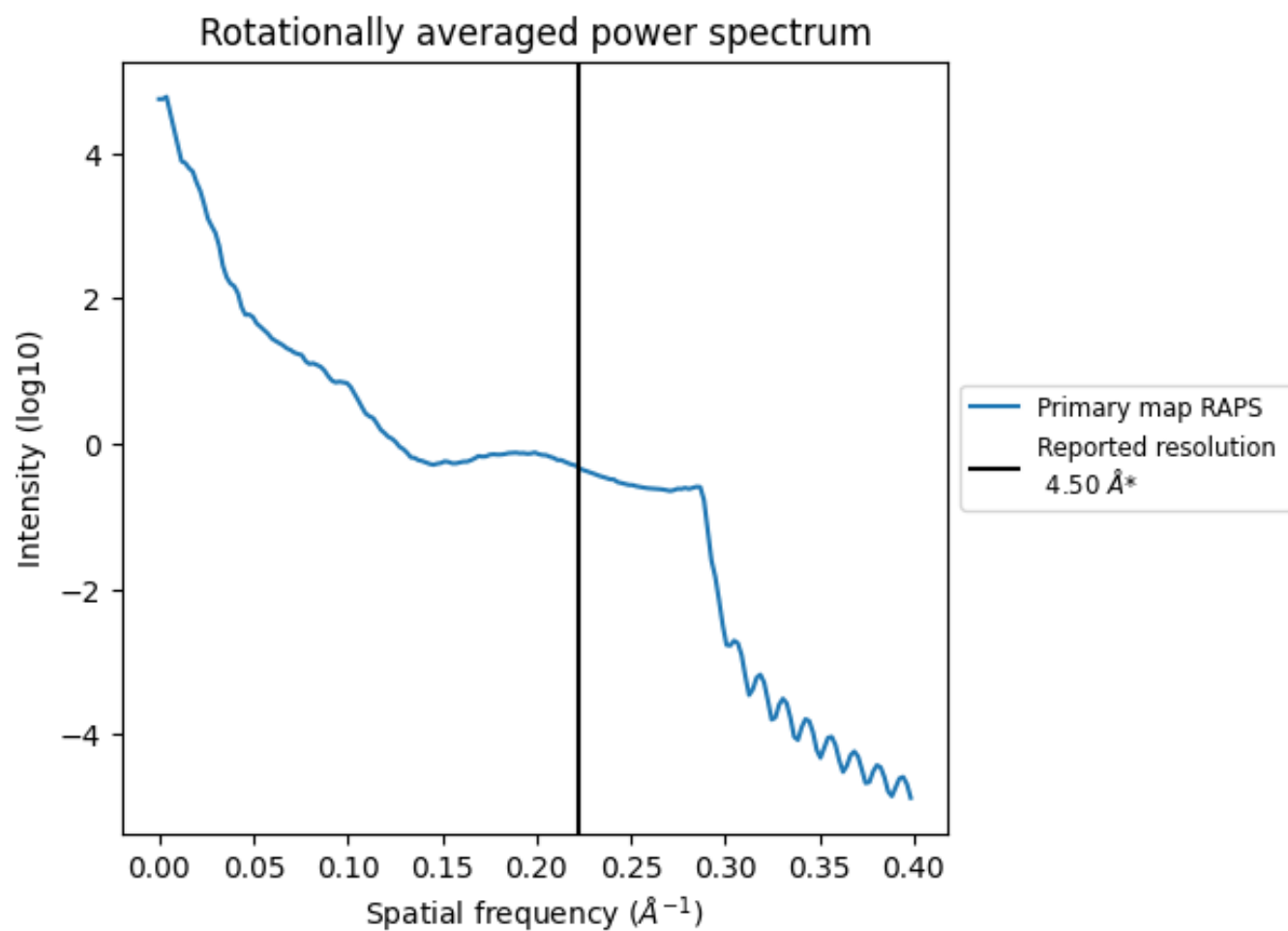
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 469 nm³; this corresponds to an approximate mass of 423 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8 Fourier-Shell correlation

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

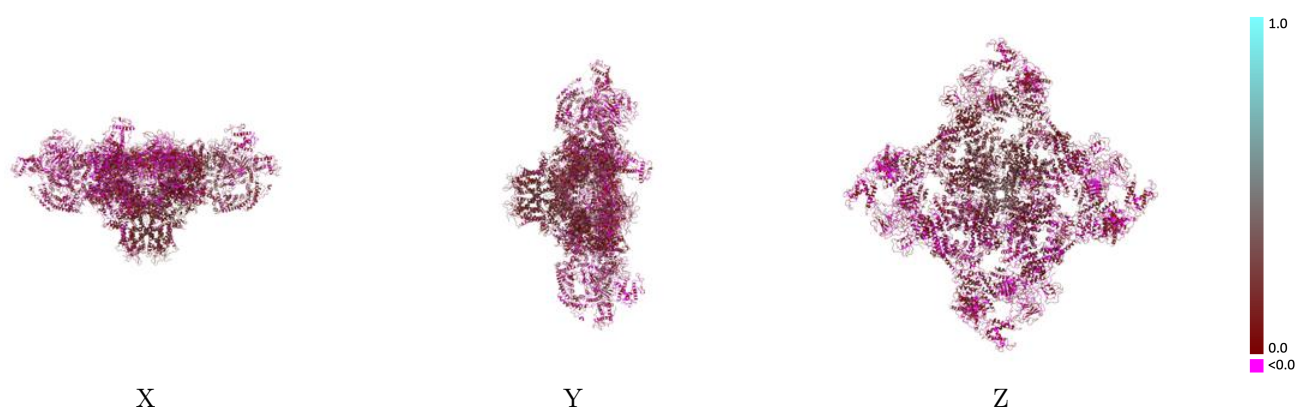
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22392 and PDB model 7JMF. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

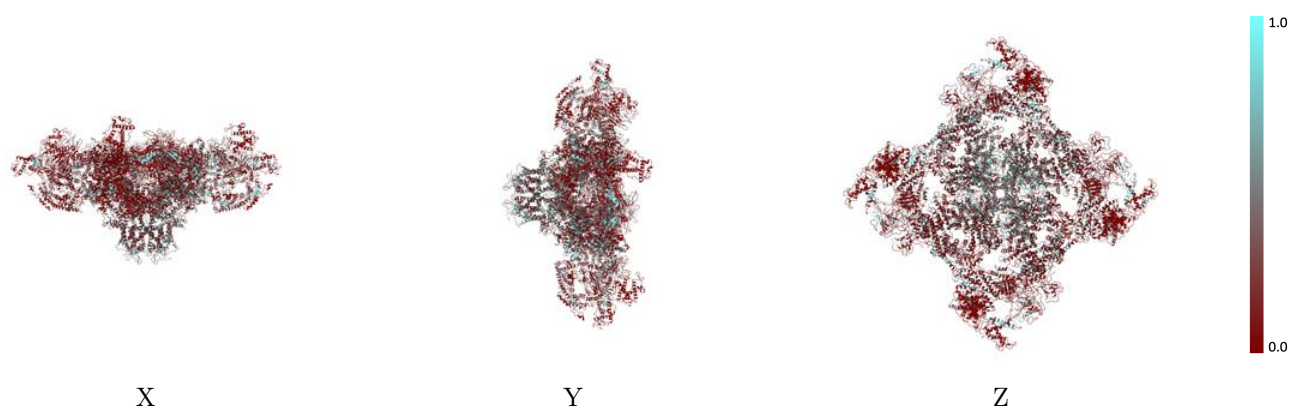
This section was not generated.

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



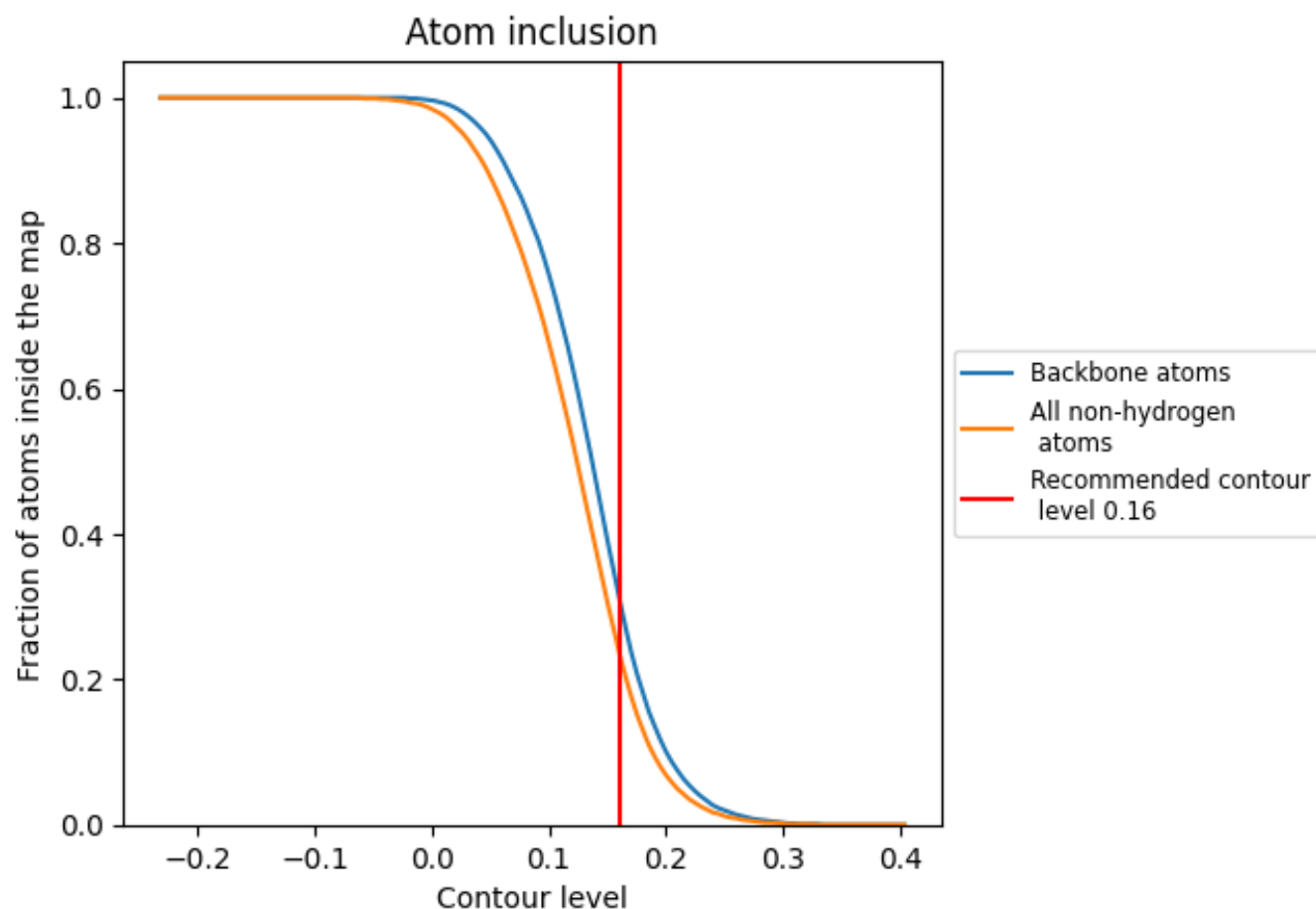
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 31% of all backbone atoms, 24% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2380	0.1100
A	0.1450	0.1330
B	0.2720	0.1490
E	0.2580	0.1200
F	0.1430	0.0750
G	0.2200	0.0820
H	0.1090	0.0850
I	0.2150	0.0890
J	0.1250	0.0820

