



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 07:11 PM EST

PDB ID : 7JMI
EMDB ID : EMD-22395
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 29 - State 3 (S3)
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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

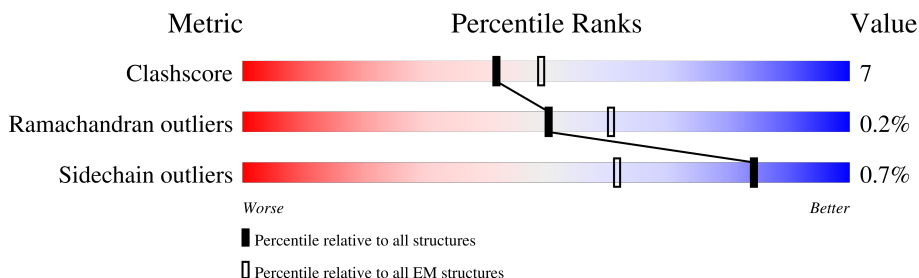
1 Overall quality at a glance

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	107	
1	F	107	
1	H	107	
1	J	107	
2	B	4687	
2	E	4687	
2	G	4687	
2	I	4687	

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 type 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 (three-letter code: 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 (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

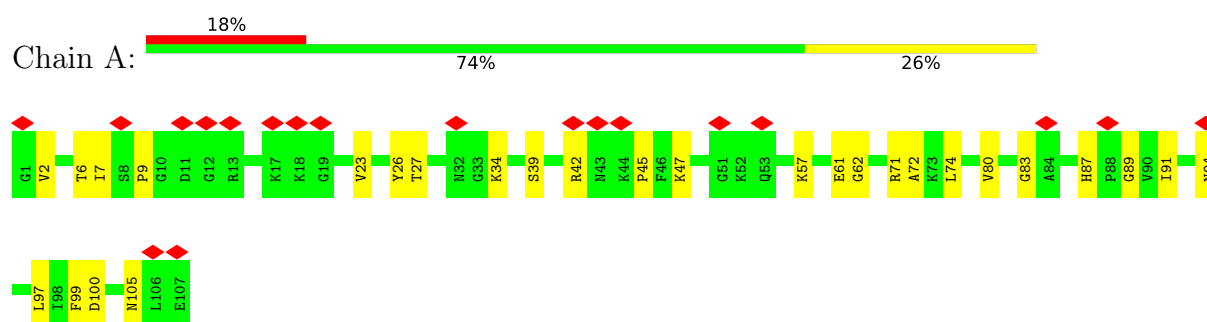
Interest" by depositor).

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

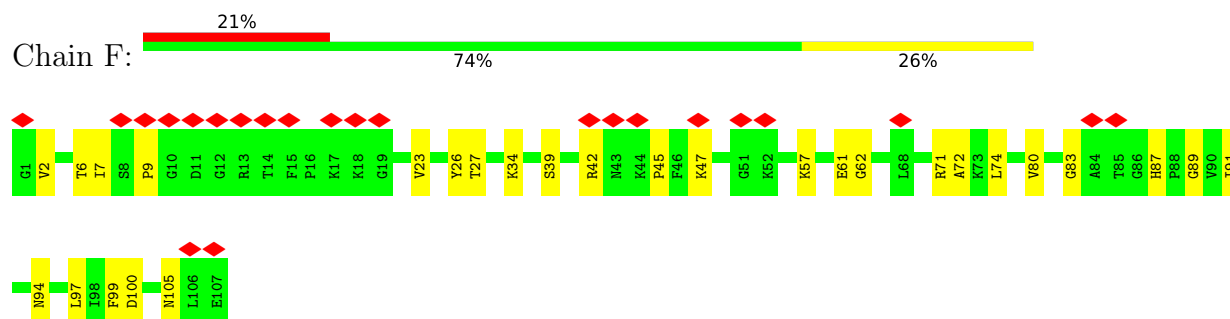
3 Residue-property plots [i](#)

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.

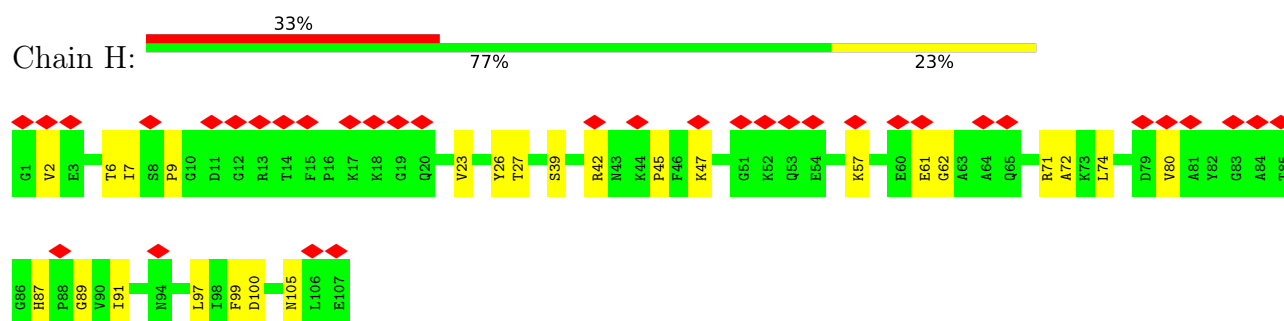
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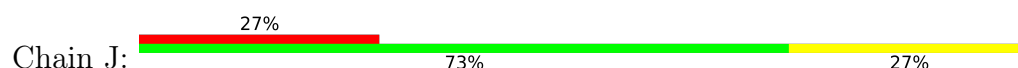
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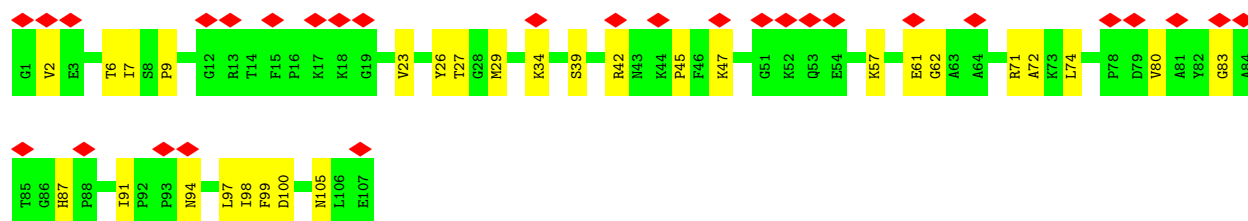


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

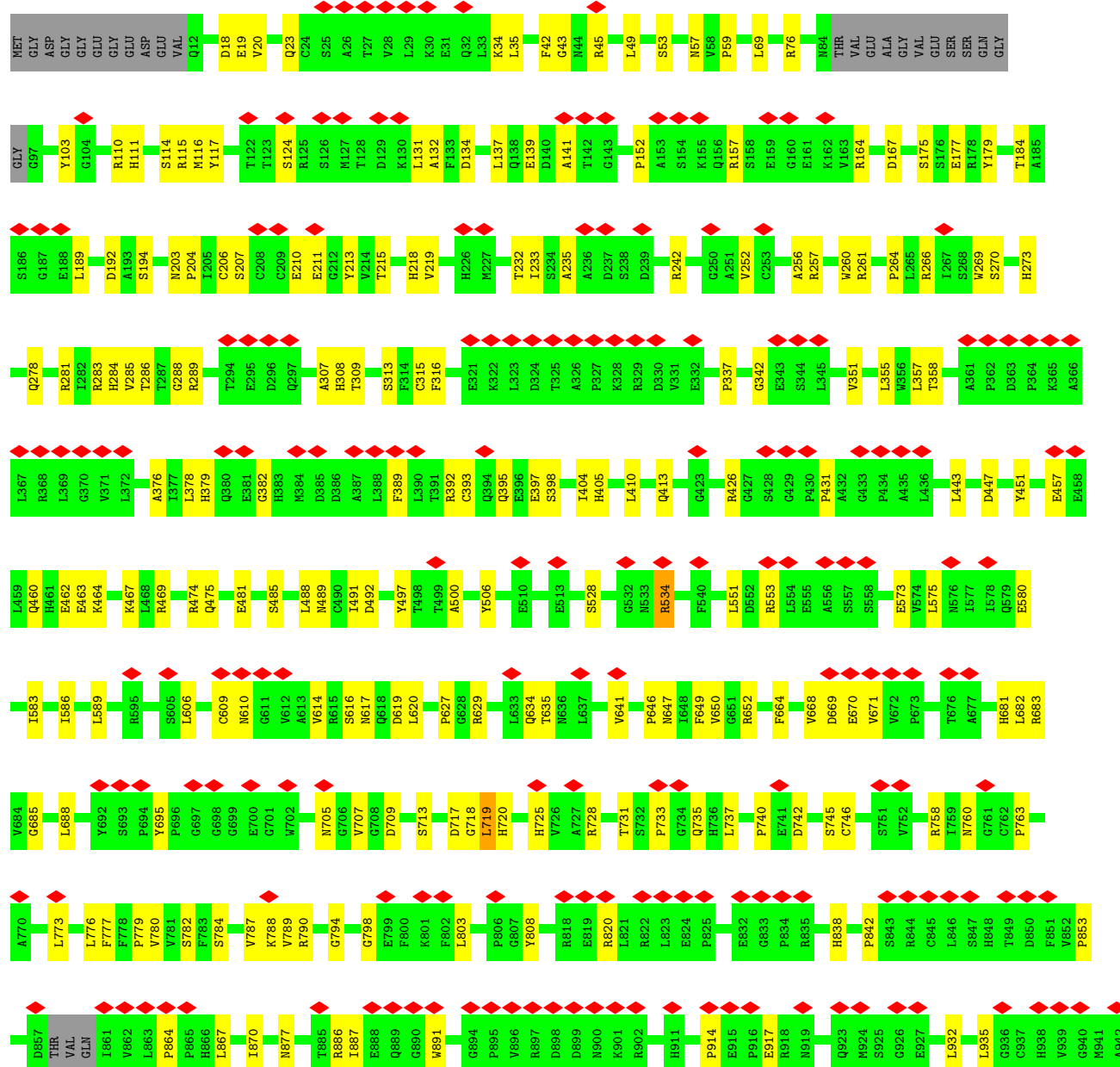
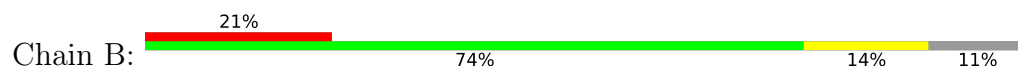


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



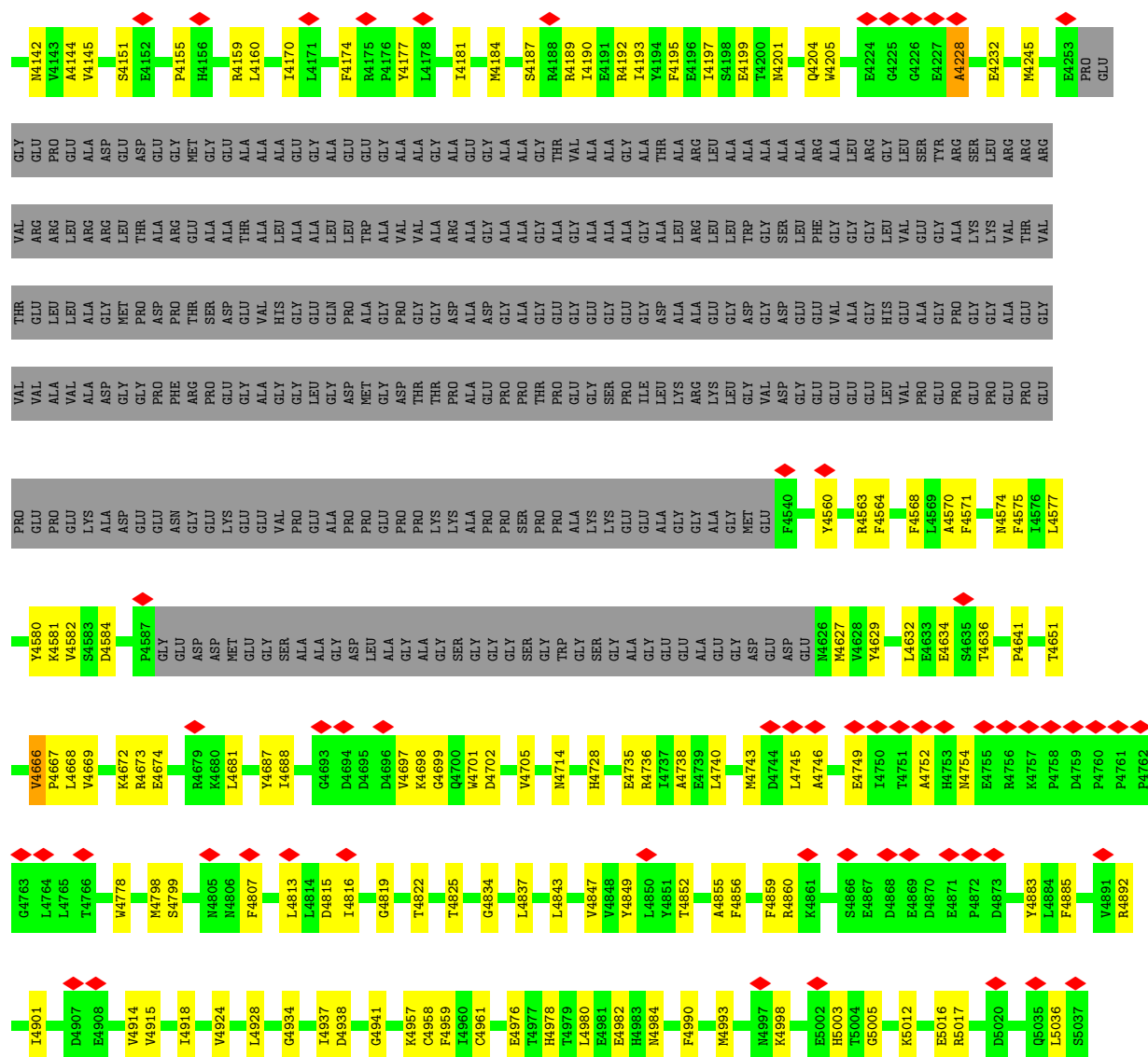


• Molecule 2: ryanodine receptor type 1

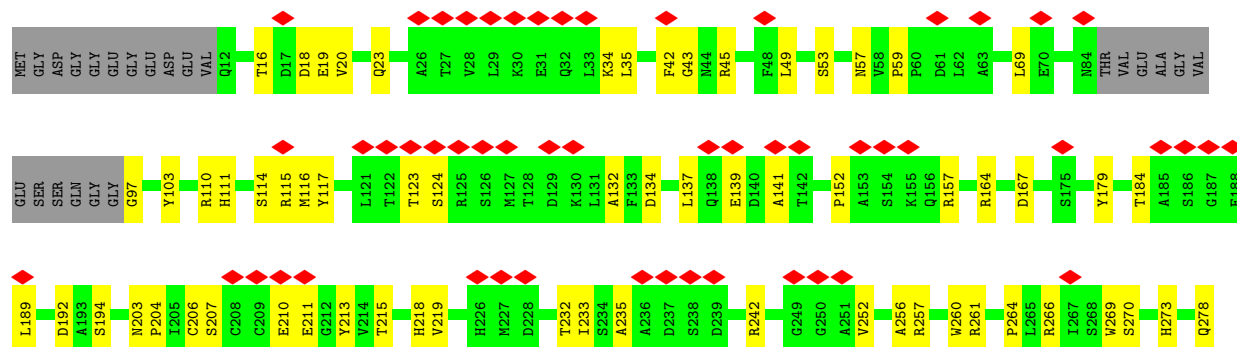
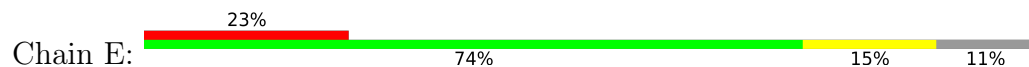


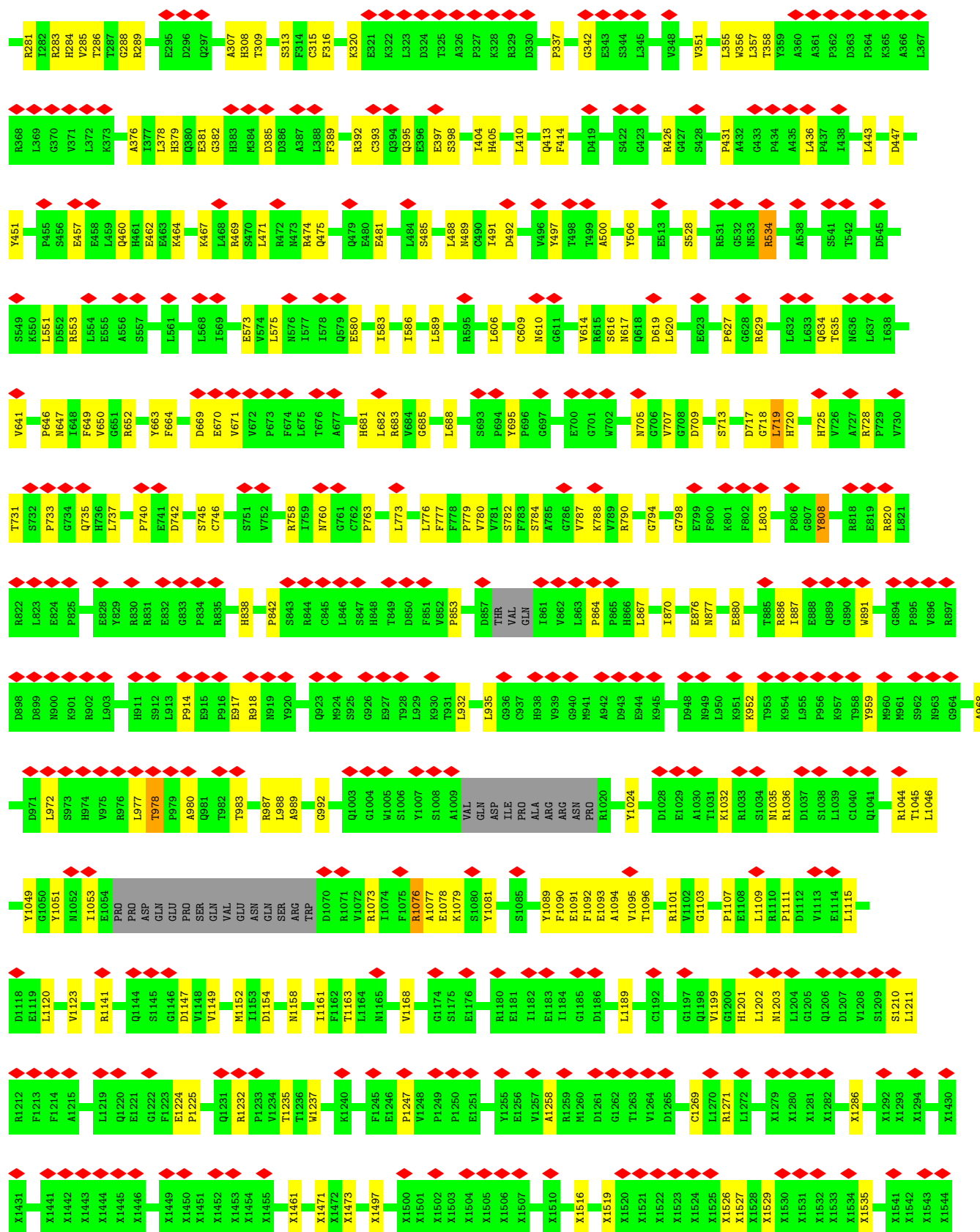


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V4049	S3931	K3715	K3716	X3424	X3248	X3016	G2899	THR	E2779	X2673	R2458
F4050	D3932	L3716	L3717	X3425	X3249	X3017	G2900	ARG	N2780		S2459
S4051		D3717		X3426	X3250		T2901	LYS	V2781		L2460
E4056	Y3935	Y3720		X3427	X3251	X3020	H2902	ILE	D2782	X2692	L2463
L4059	Y3936	L3735		X3430	X3252	X3021	P2903	GLN	X2693	X2694	L2464
F4062	S3938	E3736		X3431	X3253	X3022	L2904	ALA	E2783	X2695	D2465
D4063	Q3939	X3584		X3432	X3254	X3023	L2905	GLN	L2784	X2696	L2466
M4064	K3940	X3586		X3433	X3261	X3027	V2906	THR	L2785		
	D3941	X3587		X3435	X3262		P2907	ASP	T2787	X2697	I2469
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F3951	F3951	X3606		X3468	X3265	X3046	T2910	GLU	X2700		
M3955	M3955	X3607		X3511	X3273	X3047	L2911	GLY	L2791	Q2475	L2476
Q3960	Q3960	X3608		X3512	X3276	X3048	T2912		R2792	X2702	
N3963	N3963	X3609		X3516	X3280	X3049	A2913		P2793	X2703	L2479
T3966	T3966	X3610		X3517	X3283	X3053	A2914		Y2794	N2794	X2487
G3971	G3971	X3611		X3518	X3285	X3060	K2915		K2795	F2735	X2488
P3972	P3972	X3612		X3519	X3286		E2916		P2860	D2736	
C3973	C3973	X3613		X3520	X3287	X3067	K2917		P2861	P2737	X2493
N3976	N3976	Y3642		X3521	X3288	X3068	A2918		L2862	R2738	
R3984	R3984	K3658		X3522	X3289	X3069	D2919		S2863	P2739	X2502
V3990	V3990	A3659		X3523	X3290	X3070	R2920		G2864	V2740	X2510
L3993	L3993	A3660		X3524	X3291	X3071	E2921		V2865	E2741	X2511
F3996	F3996	K3661		X3527	X3292	X3072	K2922		L2866	T2742	X2512
K4002	K4002	L3663		X3534	X3293	X3073	A2923		S2867	L2743	X2513
L4012	L4012	T3664		X3539	X3294	X3074	Q2924		S2868	N2744	X2514
L4016	L4016	E3665		X3540	X3295	X3075	E2925		R2869	V2745	X2515
G4101	G4101	D3666		X3543	X3296	X3076	L2926		E2870	L2746	X2516
G4102	G4102	H3667		X3546	X3297	X3077	L2927		L2871	I2747	X2517
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F4107	F4107	E3682		X3556	X3314	X3080	L2930		M2874	L2751	
L4108	L4108	Q3683		X3560	X3343	X3081	Q2931		A2875	D2752	X2561
A4117	A4117	E3684		X3561	X3344	X3082	M2932		E2876	S2753	X2562
D4118	D4118	E3685		X3562	X3345	X3083	N2933		Q2877	L2813	X2563
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F4125	F4125	E3688		X3565	X3348	X3086	A2936		E2880	N2756	X2566
E4126	E4126	E3689		X3566	X3349	X3087	V2937		N2881	K2757	
F4128	F4128	E3690		X3567	X3351	X3088	T2938		L2817	F2758	X2586
E4134	E4134	E3691		X3568	X3352	X3089	R2939		A2818	A2759	
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A4136	A4136	K3693		X3570	X3354	X3091	X2941		E2820	Y2761	
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		L3698		X3573	X3357	X3094	X2944		E2823	E2764	
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				X3586	X3370	X3107	X2957			S2776	
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				X3592	X3376	X3113	X2963				
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				X3630	X3414	X3151	X3001				
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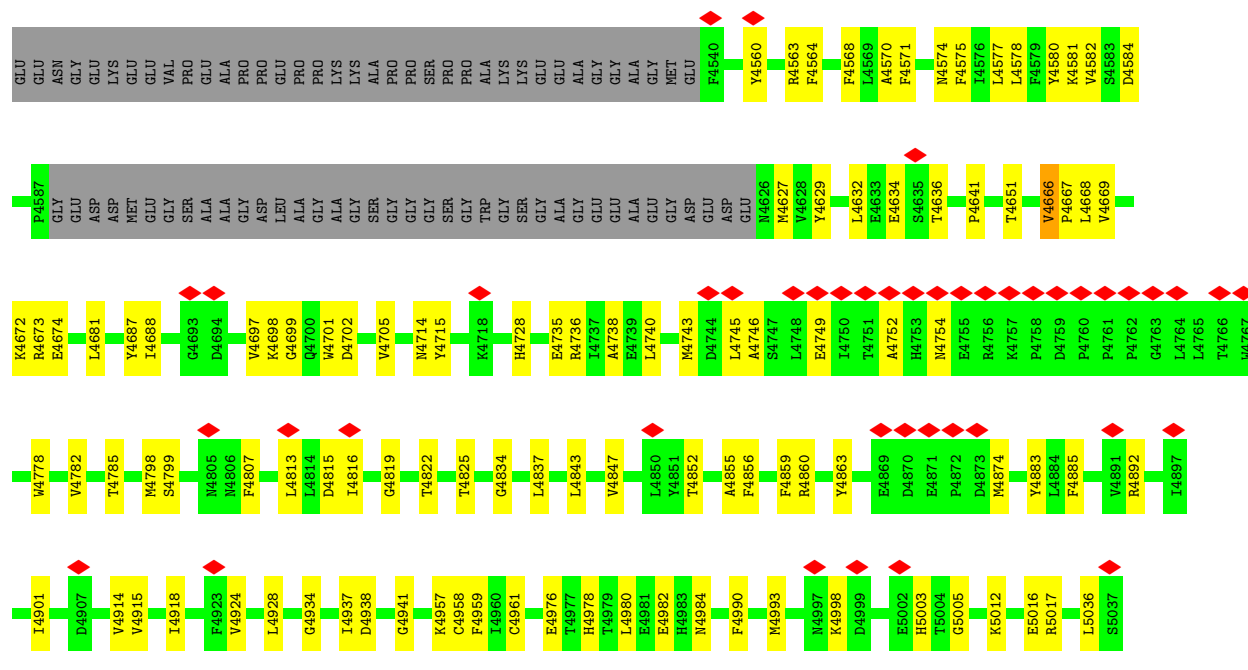
• Molecule 2: ryanodine receptor type 1



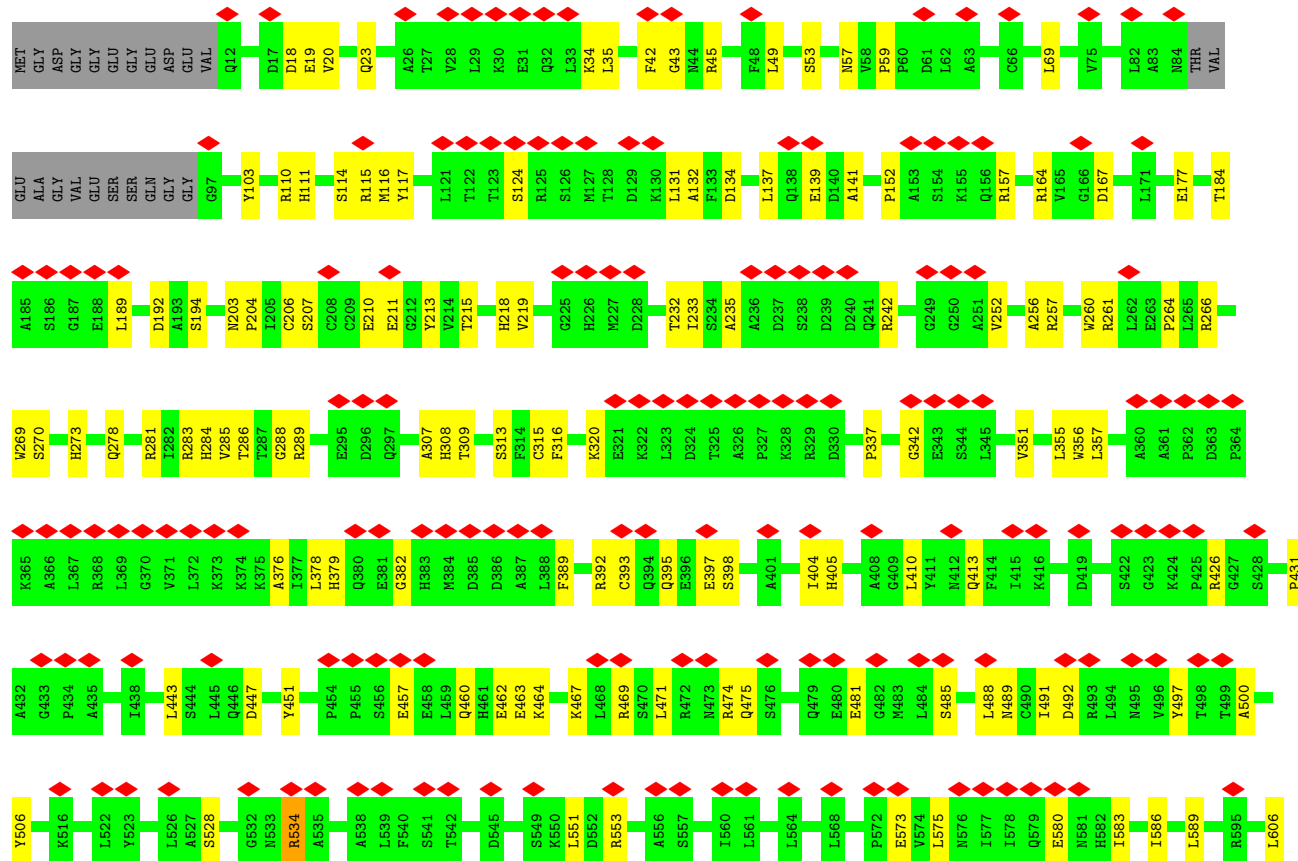
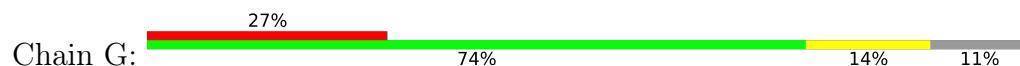








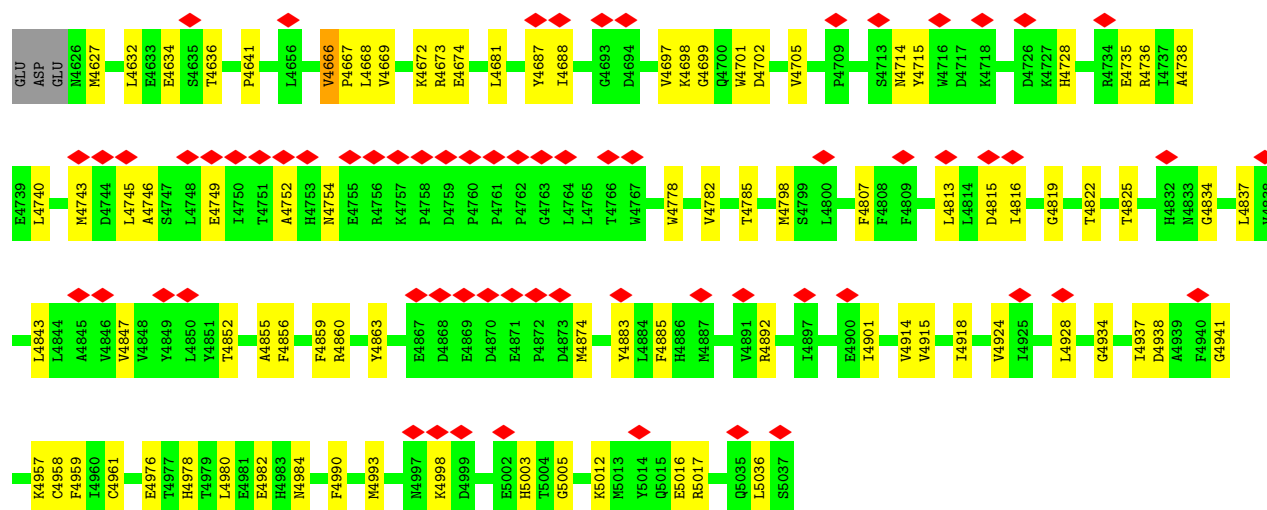
• Molecule 2: ryanodine receptor type 1



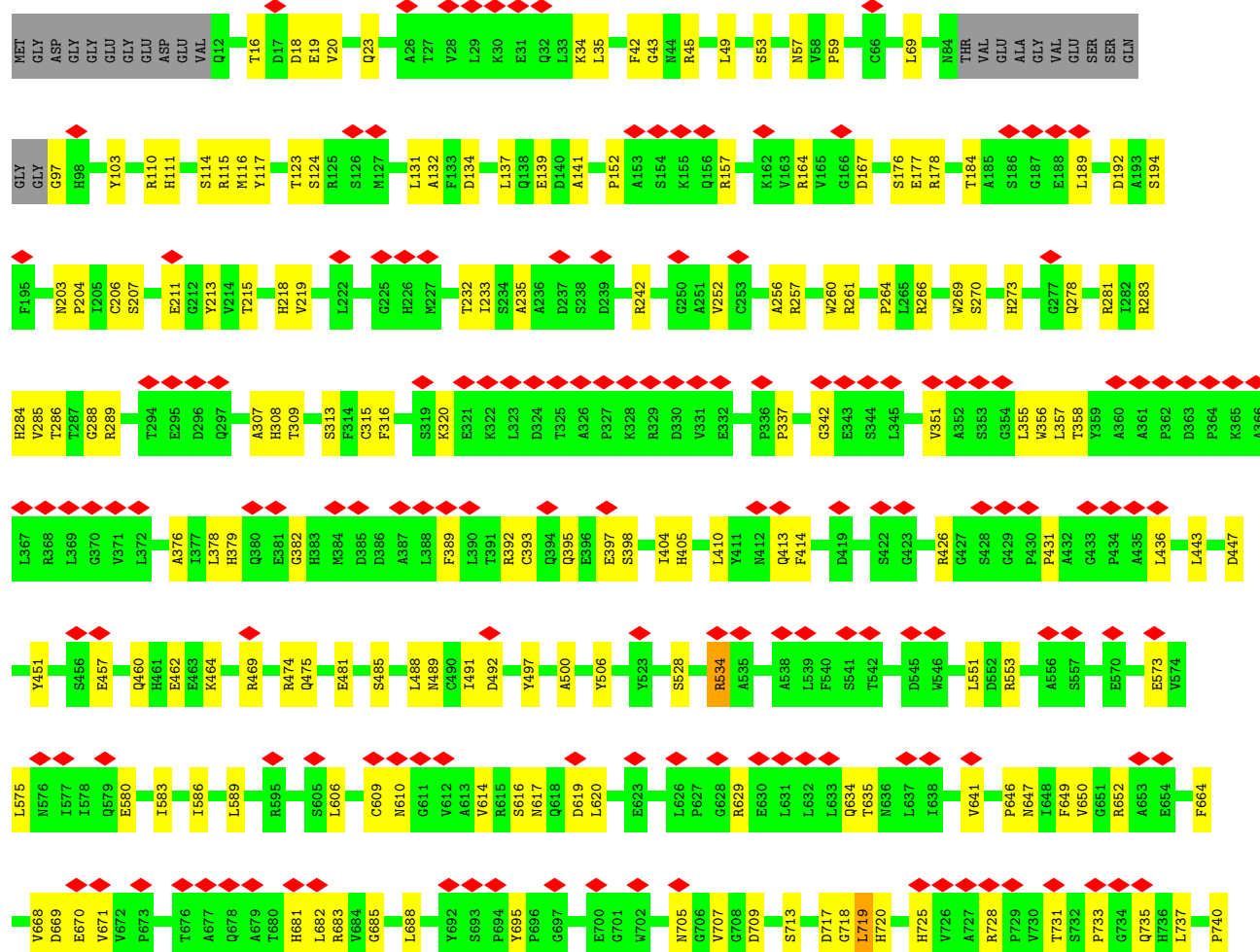
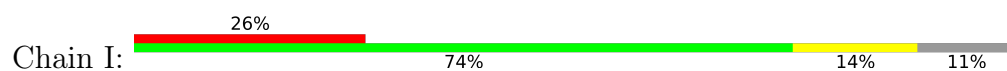








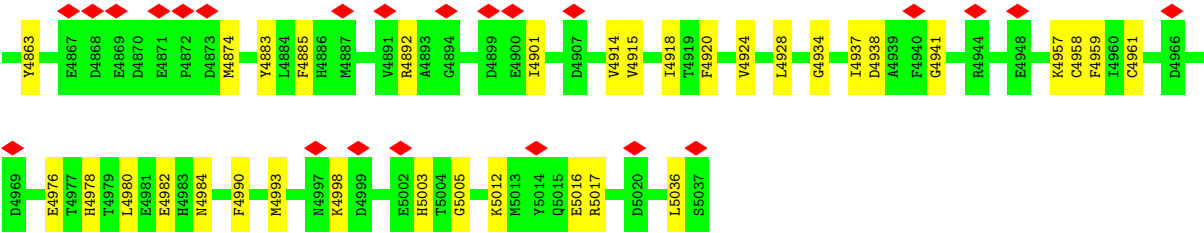
• Molecule 2: ryanodine receptor type 1





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X3392	X3393	X3394	X3412	X3419	X3423	X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3516	X3517	X3520	X3521	X3524	X3534	X3539	X3540	X3543	X3546	X3547	X3552	X3556	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567													
X3247	X3248	X3249	X3250	X3251	X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3273	X3274	X3275	X3276	X3279	X3283	X3284	X3285	X3286	X3311	X3312	X3313	X3314	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3366	X3387	X3390	X3391								
X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2995	X3013	X3014	X3015	X3016	X3017	X3020	X3021	X3022	X3023	X3045	X3046	X3047	X3050	X3060	X3134	X3135	X3136	X3137	X3138	X3139	X3142	X3143	X3189	X3190	X3191	X3192	X3193	X3194	X3195	X3196	X3197	X3221	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246										
M2881	Y2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	L2911	T2912	A2913	E2914	E2915	K2916	A2917	D2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	K2928	F2929	M2930	Q2931	M2932	T2933	G2934	Y2935	A2936	V2937	R2938	R2939	E2942
W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	LYS	LYS	THR	ARG	ILE	GLN	THR	ALA	GLN	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	G2864	V2865	T2866	L2867	S2868	L2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880				
Y2761	T2762	H2763	E2764	K2765	W2766	A2767	P2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	T2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	E2802	E2803	L2804	Y2805	R2806	W2807	P2808	L2809	L2751	D2752	S2753	F2754	L2755	K2756	F2758	A2759	W2819	E2820
X2611	X2614	X2618	X2645	X2646	X2649	X2650	X2651	X2652	X2653	X2654	X2655	X2673	X2674	X2691	X2692	X2693	X2694	X2695	X2696	X2697	X2698	X2700	X2701	X2702	X2703	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742	L2743	N2744	V2745	L2746	L2747	P2748	E2749	K2750	L2752	D2753	F2754	L2755	K2756	F2758	A2759	W2819	E2820							
V2467	G2468	L2469	L2470	S2471	L2472	L2474	Q2475	L2476	P2477	T2478	L2479	X2487	X2488	Y2502	X2510	X2511	X2512	X2513	X2514	X2515	X2516	X2517	X2518	X2519	X2520	X2521	X2522	X2523	X2526	X2529	X2530	X2531	X2532	X2533	X2536	X2537	X2554	X2561	X2562	X2563	X2564	X2565	X2566	X2586	X2598	X2604	X2610											
E2381	E2382	R2385	E2388	A2391	P2395	GLY	VAL	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	PRO	GLU	N2414	T2430	C2436	A2437	P2438	N2440	H2441	Q2444	A2445	G2446	K2447	G2448	L2451	R2452	A2455	T2456	L2457	R2458	S2459	L2460	V2461	P2462	L2463	D2464	D2465	L2466											
V2275	A2276	T2281	D2282	N2283	N2284	A2287	L2288	A2289	Q2291	E2292	L2295	E2296	A2303	L2307	L2314	A2315	Y2318	P2319	D2320	T2221	E2222	L2223	S2231	R2234	F2235	L2236	C2237	Y2238	R2241	R2248	F2251	L2254	S2255	Y2256	L2257	E2259	S2261	G2262	L2263	G2264	L2265	G2266	M2267	Q2268	G2269	D2274												
ARG	SER	LEU	THR	VAL	ARG	LEU	LYS	LYS	GLU	GLU	PRO	GLU	GLU	LEU	PRO	ALA	GLU	K2089	K2090	L2094	V2102	W2103	R2104	W2105	A2106	Q2107	E2115	R2118	L2124	H2125	G2132	L2135	R2136	L2137	L2138	P2139	R2140	A2141	V2142	S2147	E2150	L2159																

E4755	R4756	K4757	P4758	D4759	P4760	P4761	P4762	G4763	L4764	L4765	T4766	W4767	D4772	W4778	V4782	T4785	K4798	S4799	F4807	F4808	F4809	L4813	L4814	D4815	L4816	A4817	N4818	O4819	T4822	T4825	H4832	N4833	O4834	L4837	L4843	L4844	V4847	V4848	T4852	A4855	F4856	F4859	R4860				
L4656	L4664	L4665	V4666	P4667	L4668	V4669	K4672	R4673	E4674	R4679	K4680	L4681	Y4687	I4688	G4693	D4694	D4695	D4696	V4697	K4698	G4699	Q4700	W4701	D4702	Y4705	N4714	Y4715	D4726	K4727	H4728	R4734	E4735	R4736	L4737	A4738	E4739	L4740	N4743	D4744	L4745	A4746	E4749	I4750	T4751	A4752	H4753	N4754
V4582	S4583	D4584	P4587	GLY	ASP	ASP	ASP	MET	GLY	GLY	SER	ALA	ALA	ALA	ASP	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	ALA	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ALA	ARG	GLU	ALA	ALA	ALA	LEU	ALA	GLY	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	
ASP	PRO	SER	GLU	VAL	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		
PRO	PHE	ARG	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Y4582	S4583	D4584	P4587	GLY	ASP	ASP	ASP	MET	GLY	GLY	SER	ALA	ALA	ALA	ASP	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ALA	ARG	GLU	ALA	ALA	ALA	LEU	ALA	GLY	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	
ASP	PRO	SER	GLU	VAL	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
PRO	PHE	ARG	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Y4582	S4583	D4584	P4587	GLY	ASP	ASP	ASP	MET	GLY	GLY	SER	ALA	ALA	ALA	ASP	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ALA	ARG	GLU	ALA	ALA	ALA	LEU	ALA	GLY	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	
ASP	PRO	SER	GLU	VAL	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
PRO	PHE	ARG	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Y4582	S4583	D4584	P4587	GLY	ASP	ASP	ASP	MET	GLY	GLY	SER	ALA	ALA	ALA	ASP	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
ALA	ARG	GLU	ALA	ALA	ALA	LEU	ALA	GLY	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	
ASP	PRO	SER	GLU	VAL	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
PRO	PHE	ARG	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Y4582	S4583	D4584	P4587	GLY	ASP	ASP	ASP	MET	GLY	GLY	SER	ALA	ALA	ALA	ASP	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ARG	GLU	ALA	ALA	ALA	LEU	ALA	GLY	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	
ASP	PRO	SER	GLU	VAL	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
PRO	PHE	ARG	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
Y4582	S4583	D4584	P4587	GLY	ASP	ASP	ASP	MET	GLY	GLY	SER	ALA	ALA	ALA	ASP	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ALA	ARG	GLU	ALA	ALA	ALA	LEU	ALA	GLY	LEU	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	
ASP	PRO	SER	GLU	VAL	HIS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
PRO	PHE	ARG	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
GLU	ASN	GLY	GLY	LYS	GLU	VAL	PRO	GLU	ALA	ALA	PRO	PRO	PRO	PRO	PRO	SER	PRO	LYS	LYS	LEU	LEU	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY							



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	0.549	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	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: ZN, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/834	0.56	0/1123
1	F	0.31	0/834	0.56	0/1123
1	H	0.31	0/834	0.56	0/1123
1	J	0.31	0/834	0.56	0/1123
2	B	0.30	0/25428	0.55	5/34534 (0.0%)
2	E	0.30	0/25428	0.55	5/34534 (0.0%)
2	G	0.30	0/25428	0.55	5/34534 (0.0%)
2	I	0.30	0/25428	0.55	5/34534 (0.0%)
All	All	0.30	0/105048	0.55	20/142628 (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	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	64

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	719	LEU	CA-CB-CG	6.09	129.30	115.30
2	G	719	LEU	CA-CB-CG	6.08	129.29	115.30
2	E	719	LEU	CA-CB-CG	6.08	129.28	115.30
2	I	719	LEU	CA-CB-CG	6.07	129.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1667	LEU	CA-CB-CG	5.71	128.43	115.30

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	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	18	0
1	F	818	0	824	17	0
1	H	818	0	824	17	0
1	J	818	0	824	18	0
2	B	29369	0	24711	395	0
2	E	29369	0	24713	406	0
2	G	29369	0	24713	395	0
2	I	29369	0	24712	397	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	102145	1629	0

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

The worst 5 of 1629 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:I:2318:TYR:HH	2:I:2414:ASN:N	1.88	0.72
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.88	0.71
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.88	0.71
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.56	0.71
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.56	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	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
1	F	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
1	H	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
1	J	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4687 (69%)	2890 (89%)	339 (10%)	6 (0%)	47	81
2	E	3235/4687 (69%)	2887 (89%)	342 (11%)	6 (0%)	47	81
2	G	3235/4687 (69%)	2892 (89%)	337 (10%)	6 (0%)	47	81
2	I	3235/4687 (69%)	2889 (89%)	340 (10%)	6 (0%)	47	81
All	All	13360/19176 (70%)	11926 (89%)	1410 (11%)	24 (0%)	50	81

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	I	1708	ARG

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Mol	Chain	Res	Type
2	B	1932	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	88/88 (100%)	88 (100%)	0	100	100
1	F	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	J	88/88 (100%)	88 (100%)	0	100	100
2	B	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
All	All	10324/13188 (78%)	10256 (99%)	68 (1%)	84	90

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	1964	ARG
2	I	3787	LYS
2	I	4137	ARG
2	E	3663	LEU
2	E	1964	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	224	HIS
2	I	4142	ASN
2	I	395	GLN
2	I	1972	ASN

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Mol	Chain	Res	Type
2	E	479	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 monosaccharides 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	G	12
2	B	12

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Mol	Chain	Number of breaks
2	I	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	G	3613:UNK	C	3639:THR	N	44.80
1	B	3613:UNK	C	3639:THR	N	44.74
1	I	3613:UNK	C	3639:THR	N	44.65
1	E	3613:UNK	C	3639:THR	N	44.57
1	B	3163:UNK	C	3170:UNK	N	16.54

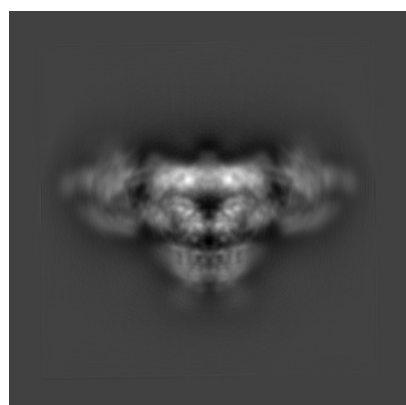
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22395. These allow visual inspection of the internal detail of the map and identification of artifacts.

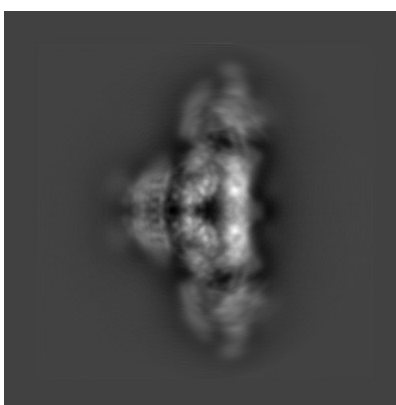
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

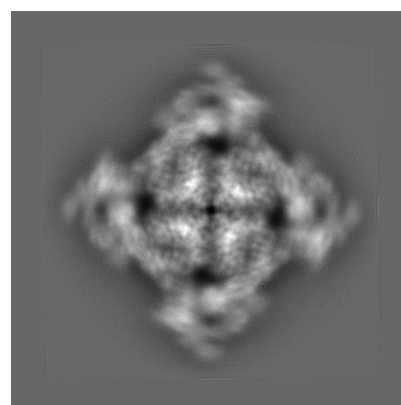
6.1.1 Primary map



X



Y

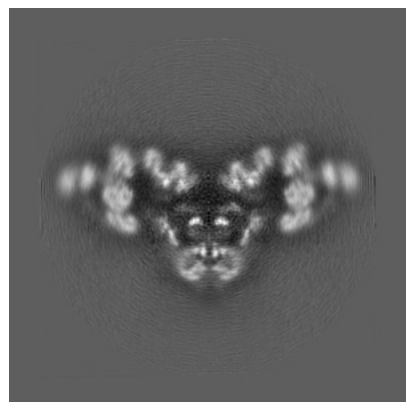


Z

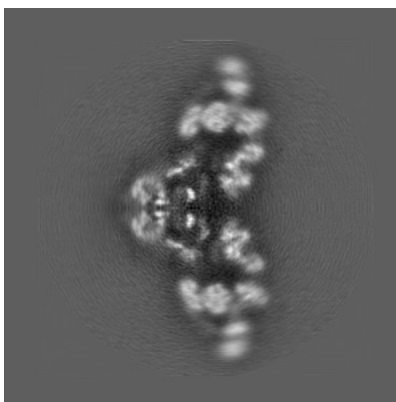
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

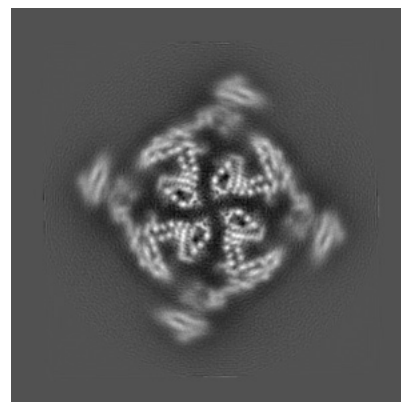
6.2.1 Primary map



X Index: 200



Y Index: 200

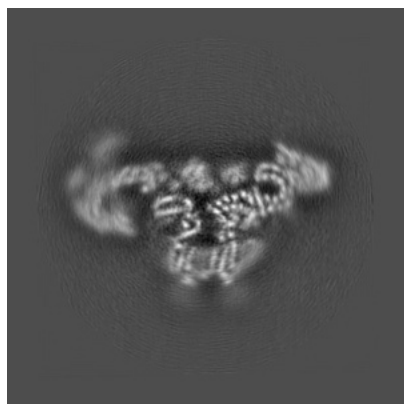


Z Index: 200

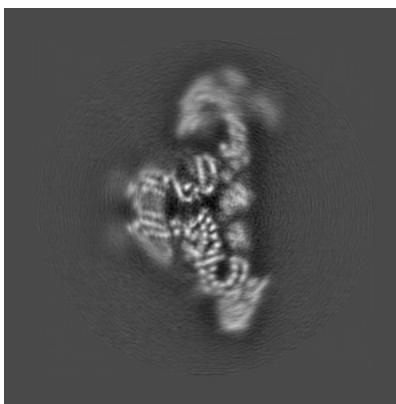
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

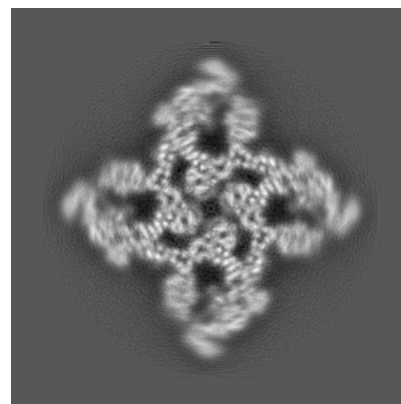
6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 230

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

6.4 Orthogonal surface views [i](#)

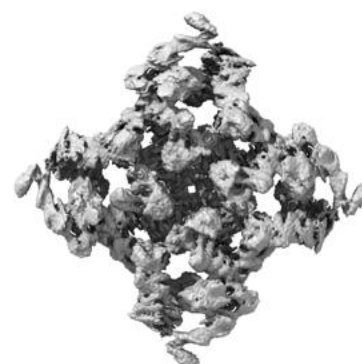
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

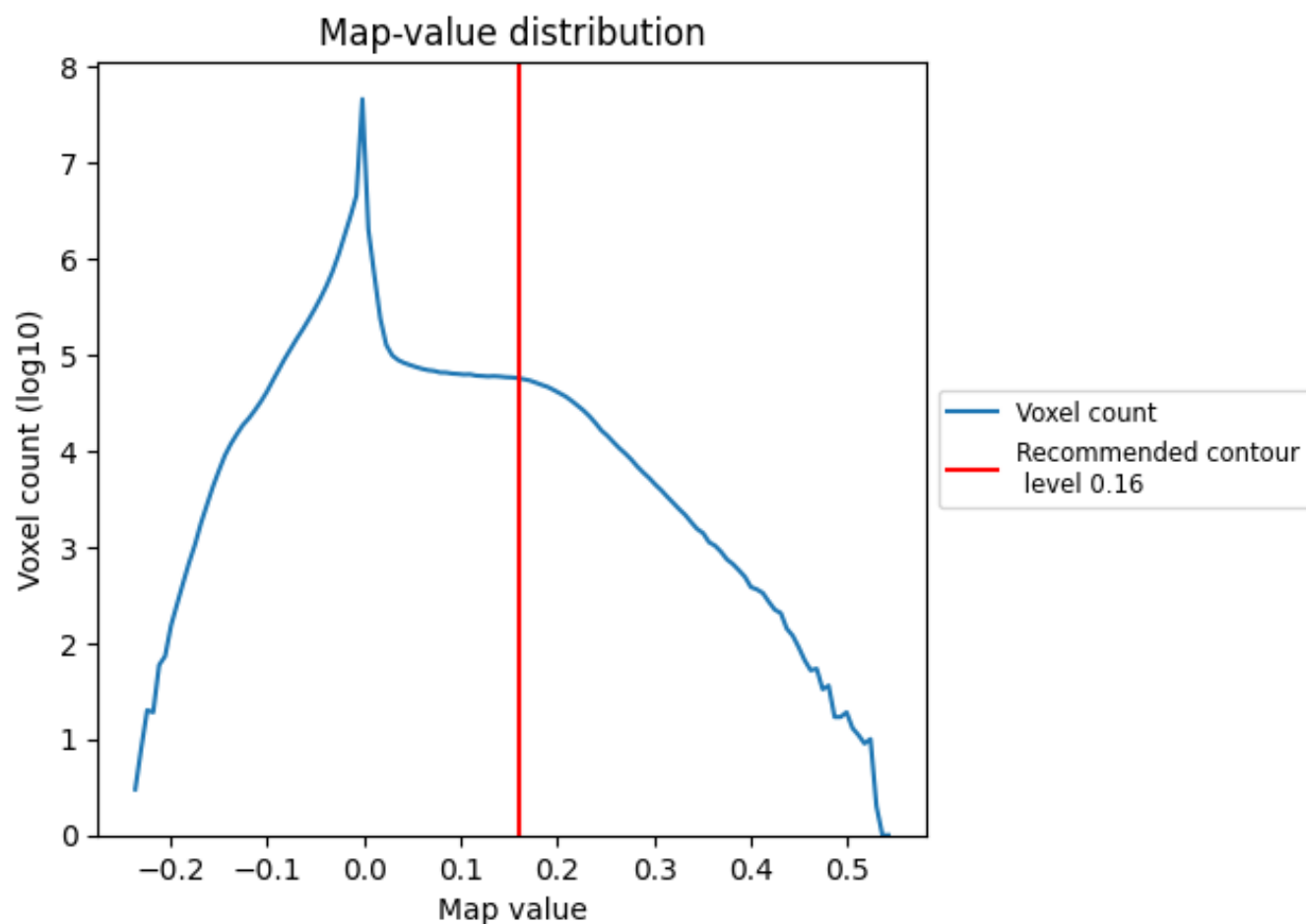
6.5 Mask visualisation

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

7 Map analysis [i](#)

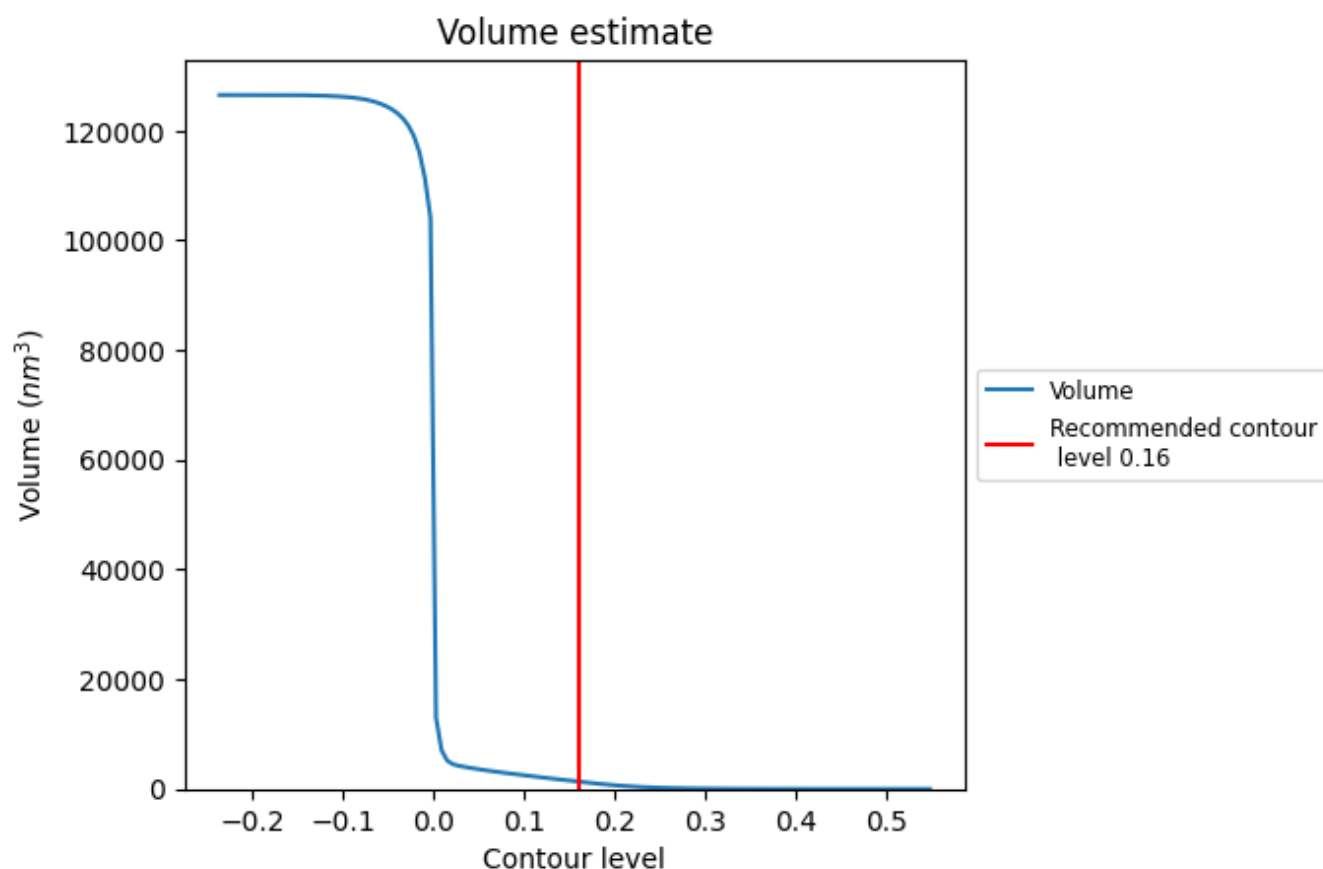
This section contains the results of statistical analysis of the map.

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.

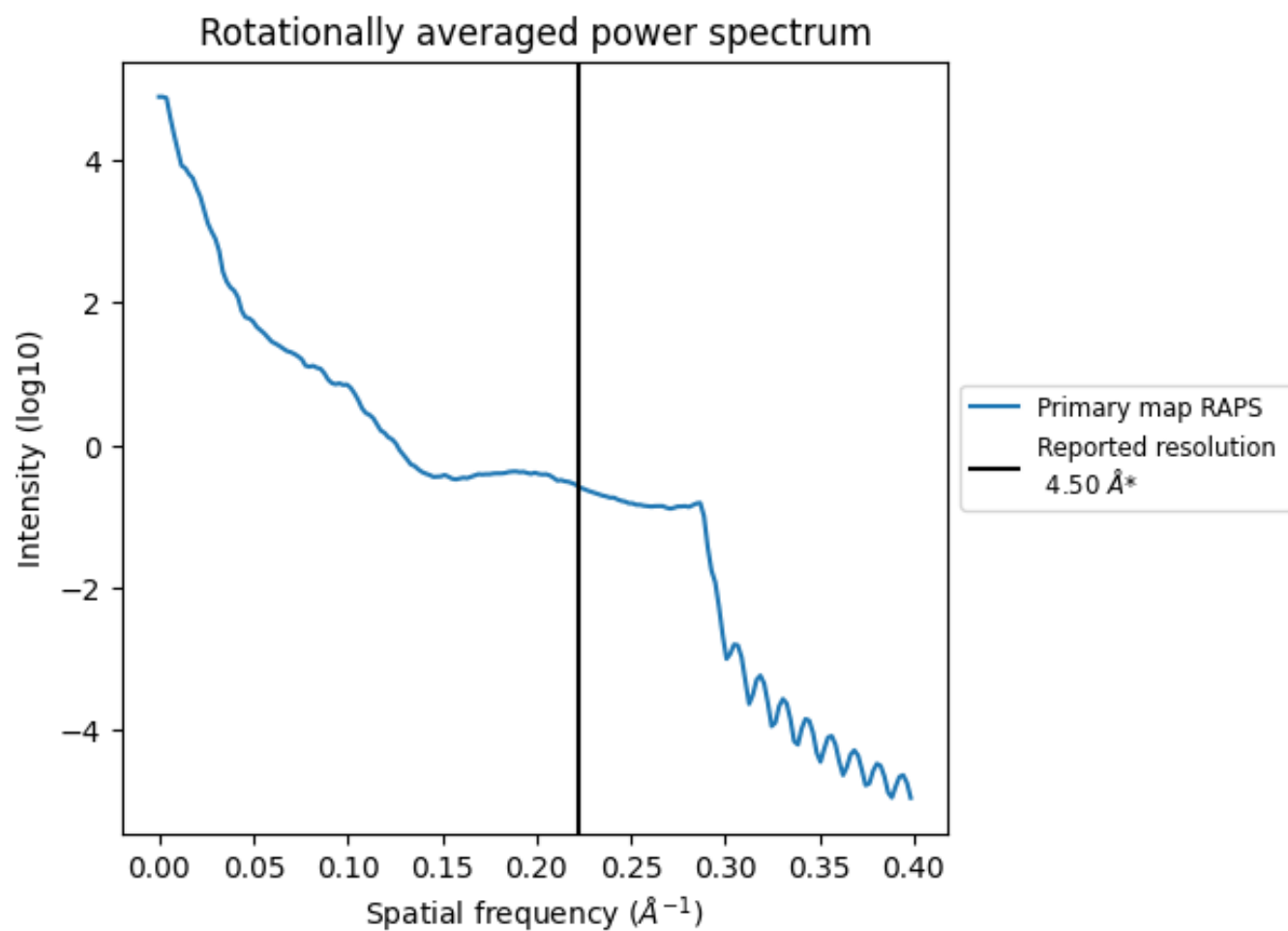
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1337 nm³; this corresponds to an approximate mass of 1208 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

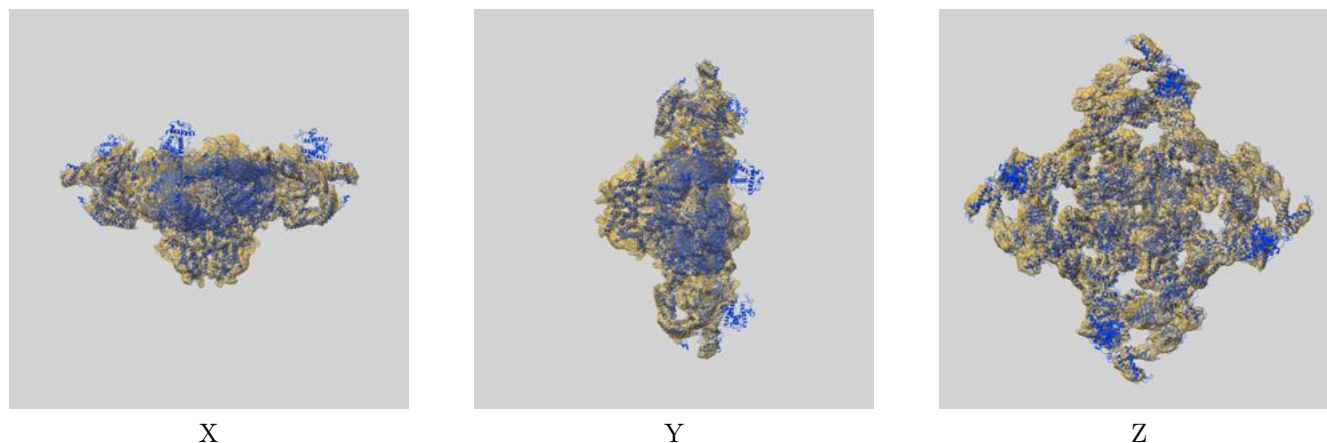
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

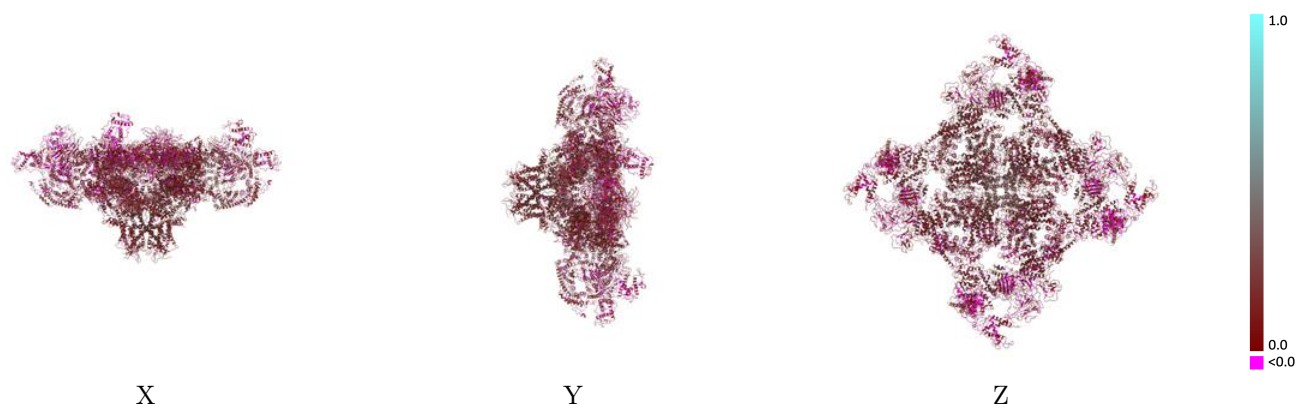
This section contains information regarding the fit between EMDB map EMD-22395 and PDB model 7JMI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



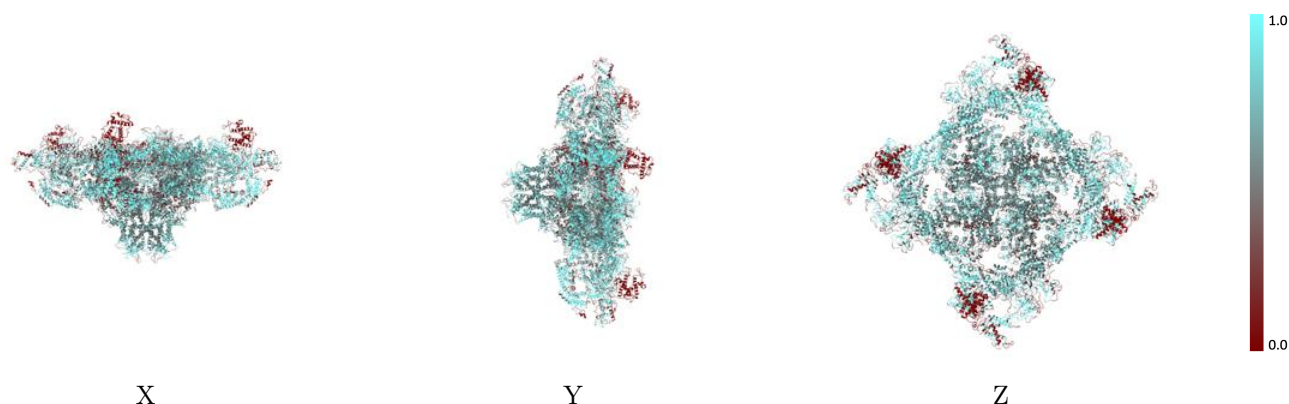
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



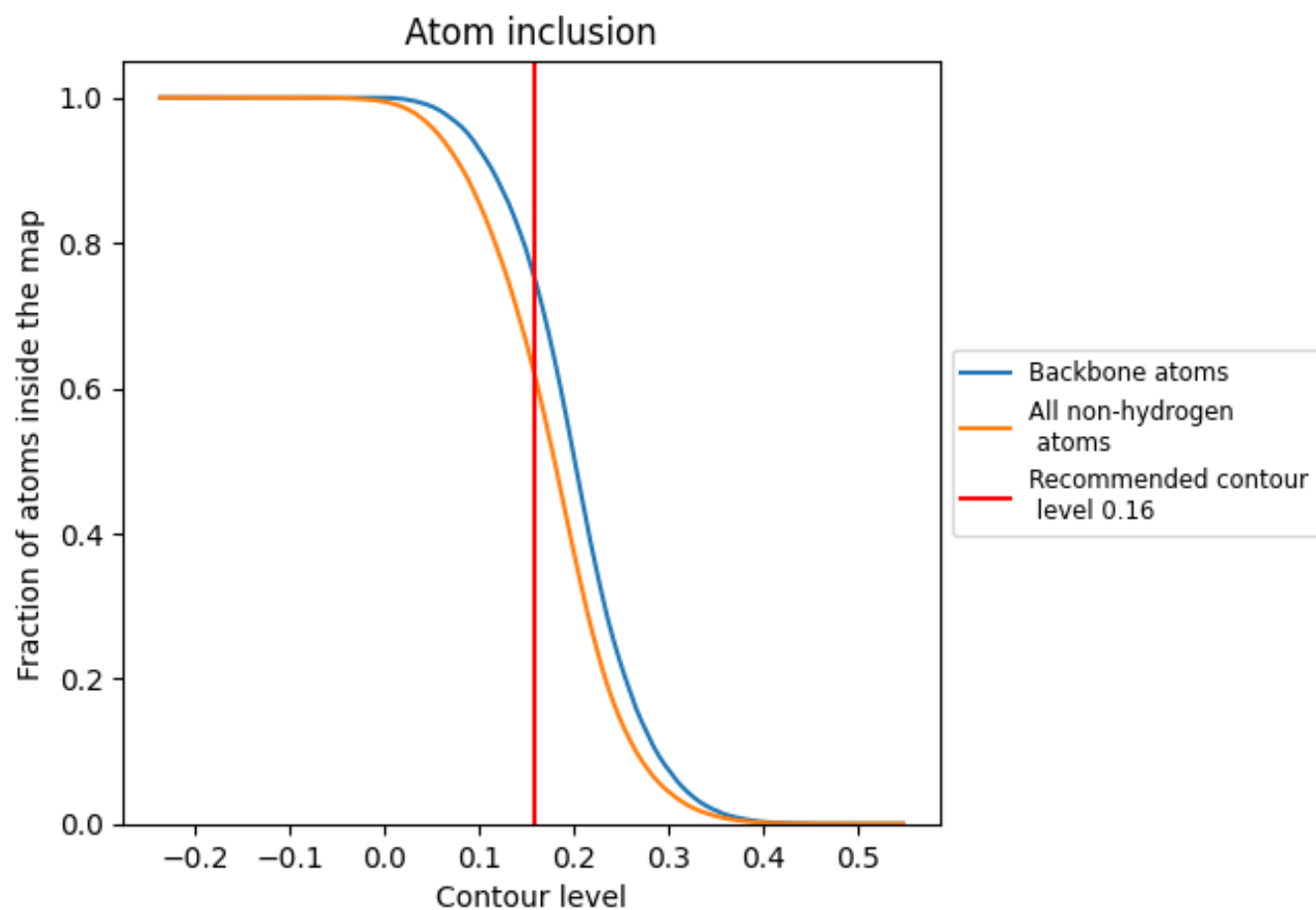
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 61% 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	<div></div> 0.6142	<div></div> 0.1530
A	<div></div> 0.7022	<div></div> 0.1430
B	<div></div> 0.6326	<div></div> 0.1730
E	<div></div> 0.6194	<div></div> 0.1580
F	<div></div> 0.6700	<div></div> 0.1150
G	<div></div> 0.5956	<div></div> 0.1340
H	<div></div> 0.6216	<div></div> 0.1130
I	<div></div> 0.6041	<div></div> 0.1490
J	<div></div> 0.6439	<div></div> 0.1220

1.0

0.0

<0.0