



wwPDB EM Validation Summary Report ⓘ

Jan 25, 2024 – 01:37 PM EST

PDB ID : 8DTY
EMDB ID : EMD-27711
Title : Recombinant mouse RyR2 triple phosphomimetic mutant S2807D/S2813D/S2030D in complex with FKBP12.6 and nanodisc under closed-state conditions
Authors : Iyer, K.A.; Hu, Y.; Murayama, T.; Samsó, M.
Deposited on : 2022-07-26
Resolution : 3.50 Å (reported)
Based on initial model : 6WOU

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.dev70
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) : 2.36

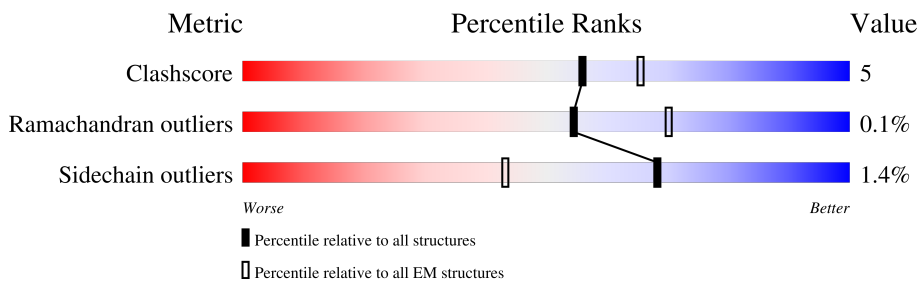
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	4966	
1	B	4966	
1	C	4966	
1	D	4966	
2	E	107	
2	F	107	
2	G	107	
2	H	107	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 128772 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4004	31374	19934	5355	5887	198	0	0
1	B	4004	31374	19934	5355	5887	198	0	0
1	C	4004	31374	19934	5355	5887	198	0	0
1	D	4004	31374	19934	5355	5887	198	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2030	ASP	SER	engineered mutation	UNP E9Q401
A	2807	ASP	SER	engineered mutation	UNP E9Q401
A	2813	ASP	SER	engineered mutation	UNP E9Q401
B	2030	ASP	SER	engineered mutation	UNP E9Q401
B	2807	ASP	SER	engineered mutation	UNP E9Q401
B	2813	ASP	SER	engineered mutation	UNP E9Q401
C	2030	ASP	SER	engineered mutation	UNP E9Q401
C	2807	ASP	SER	engineered mutation	UNP E9Q401
C	2813	ASP	SER	engineered mutation	UNP E9Q401
D	2030	ASP	SER	engineered mutation	UNP E9Q401
D	2807	ASP	SER	engineered mutation	UNP E9Q401
D	2813	ASP	SER	engineered mutation	UNP E9Q401

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

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

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

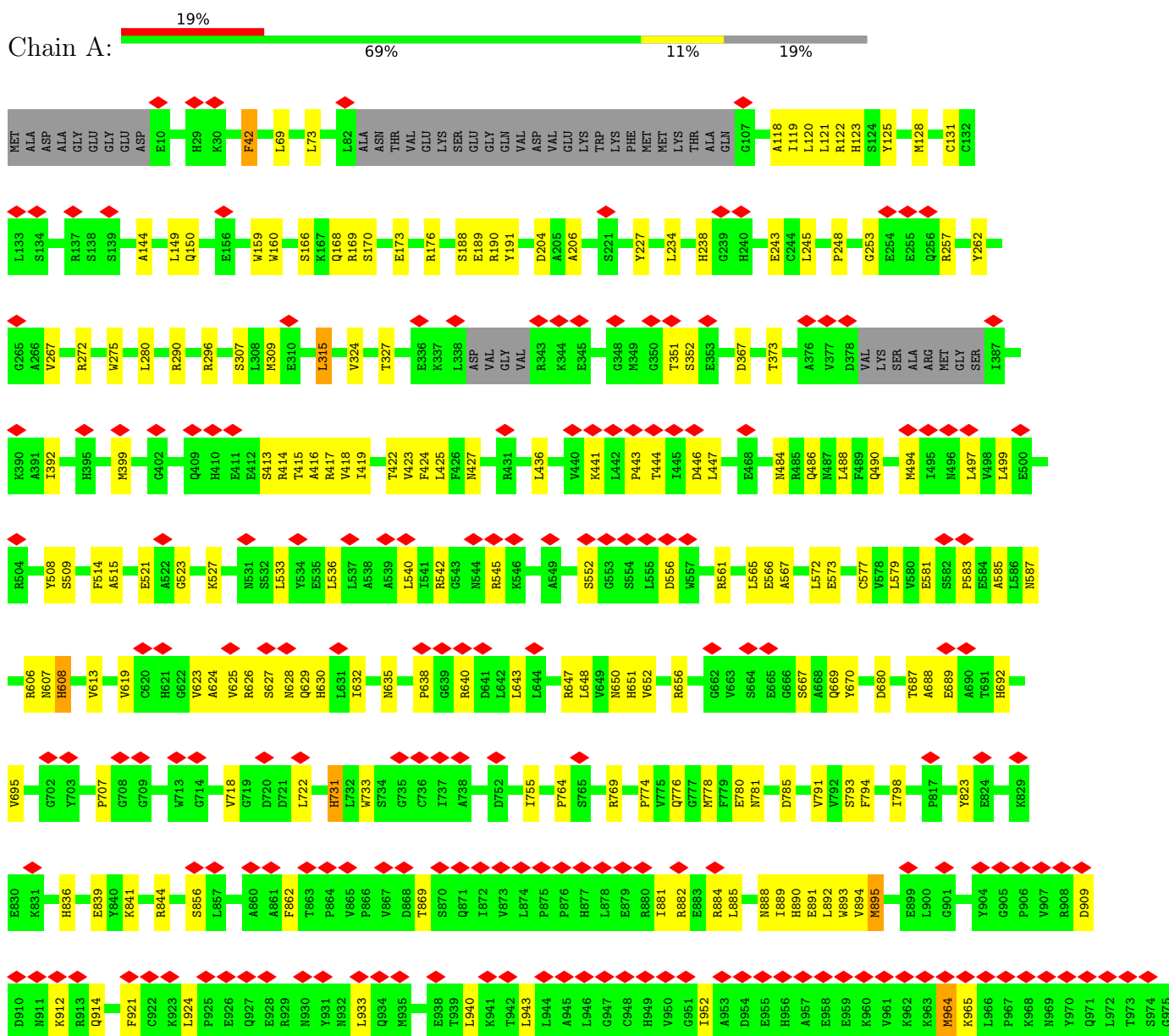
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

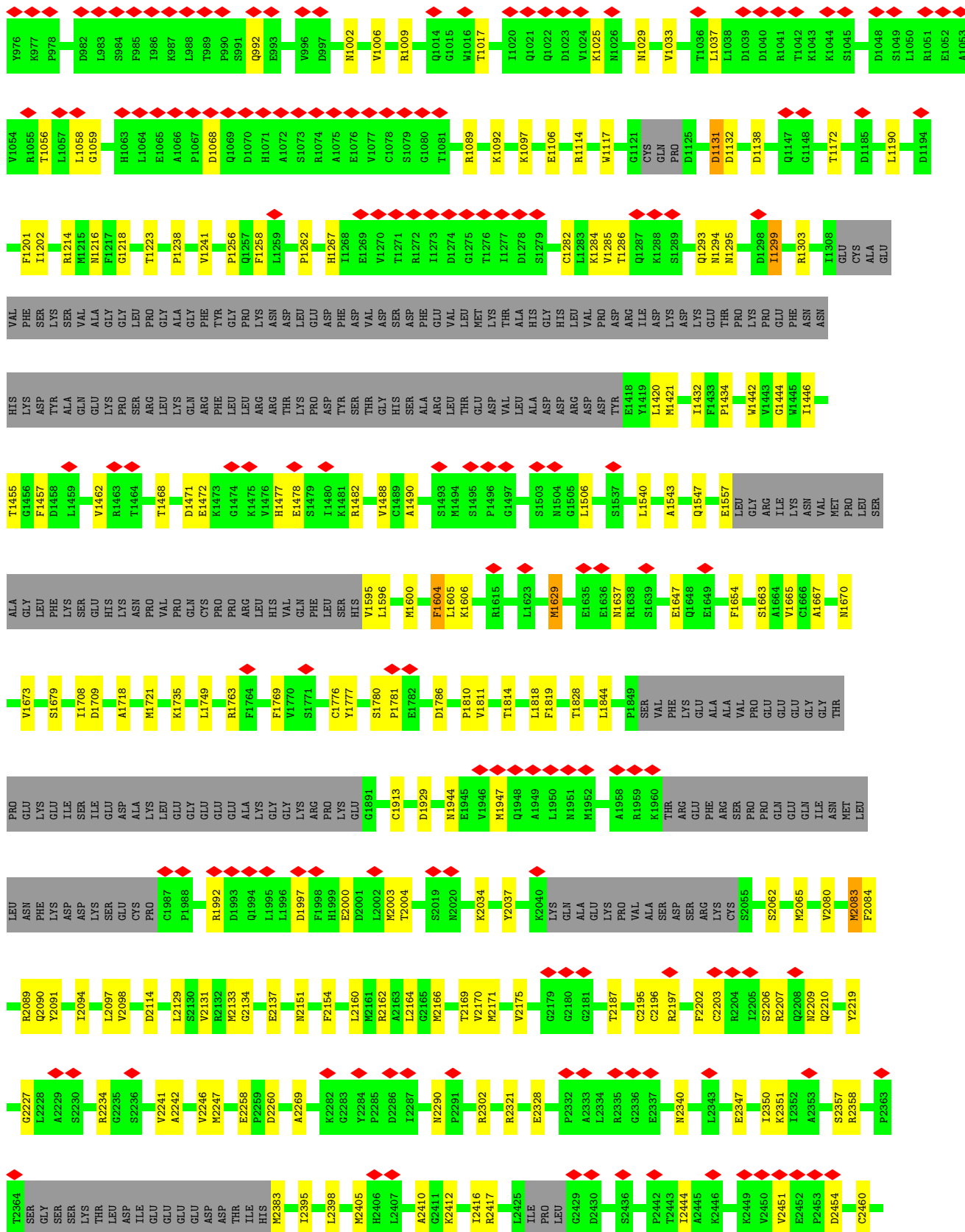
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

3 Residue-property plots [i](#)

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

• Molecule 1: Ryanodine receptor 2

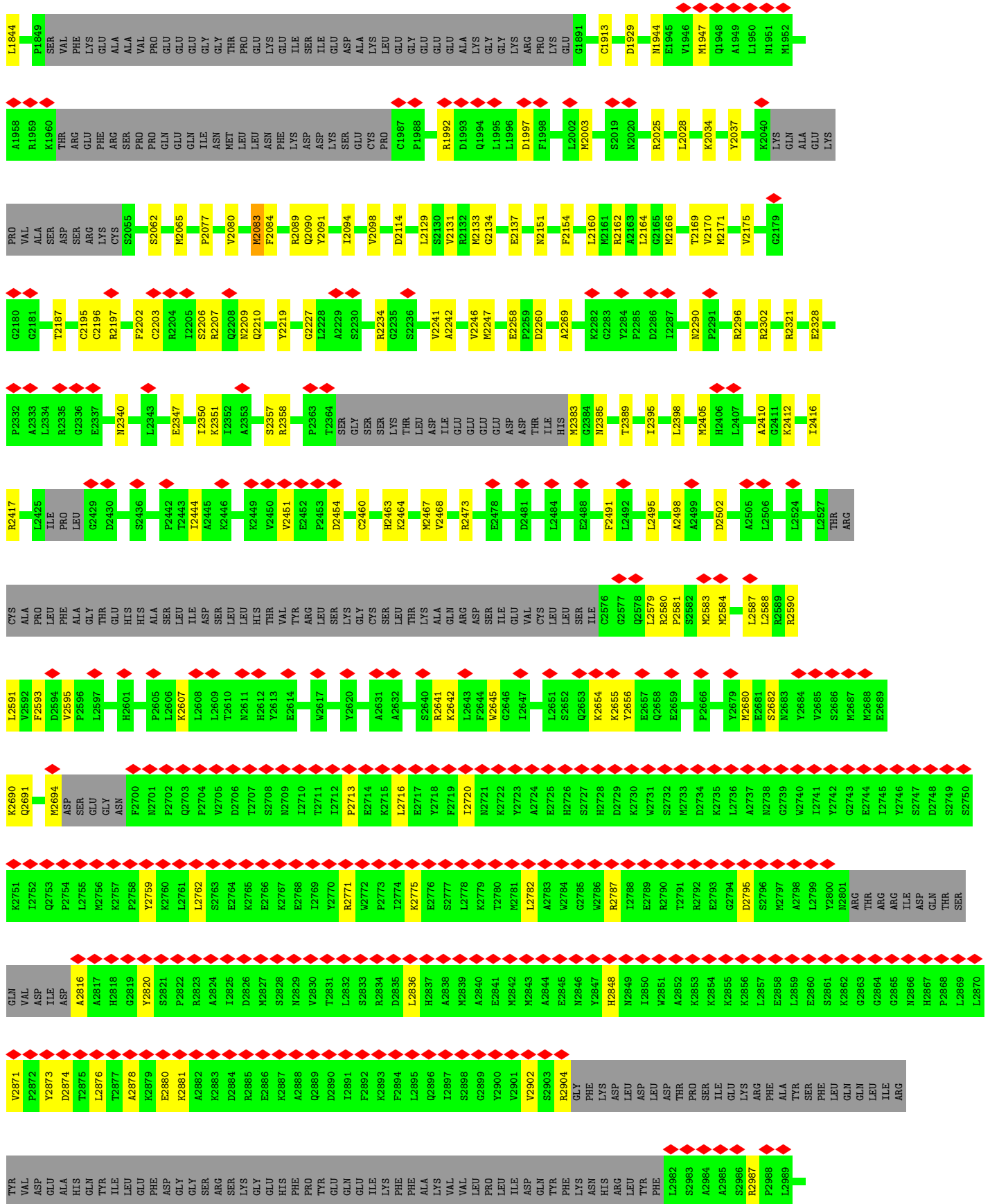


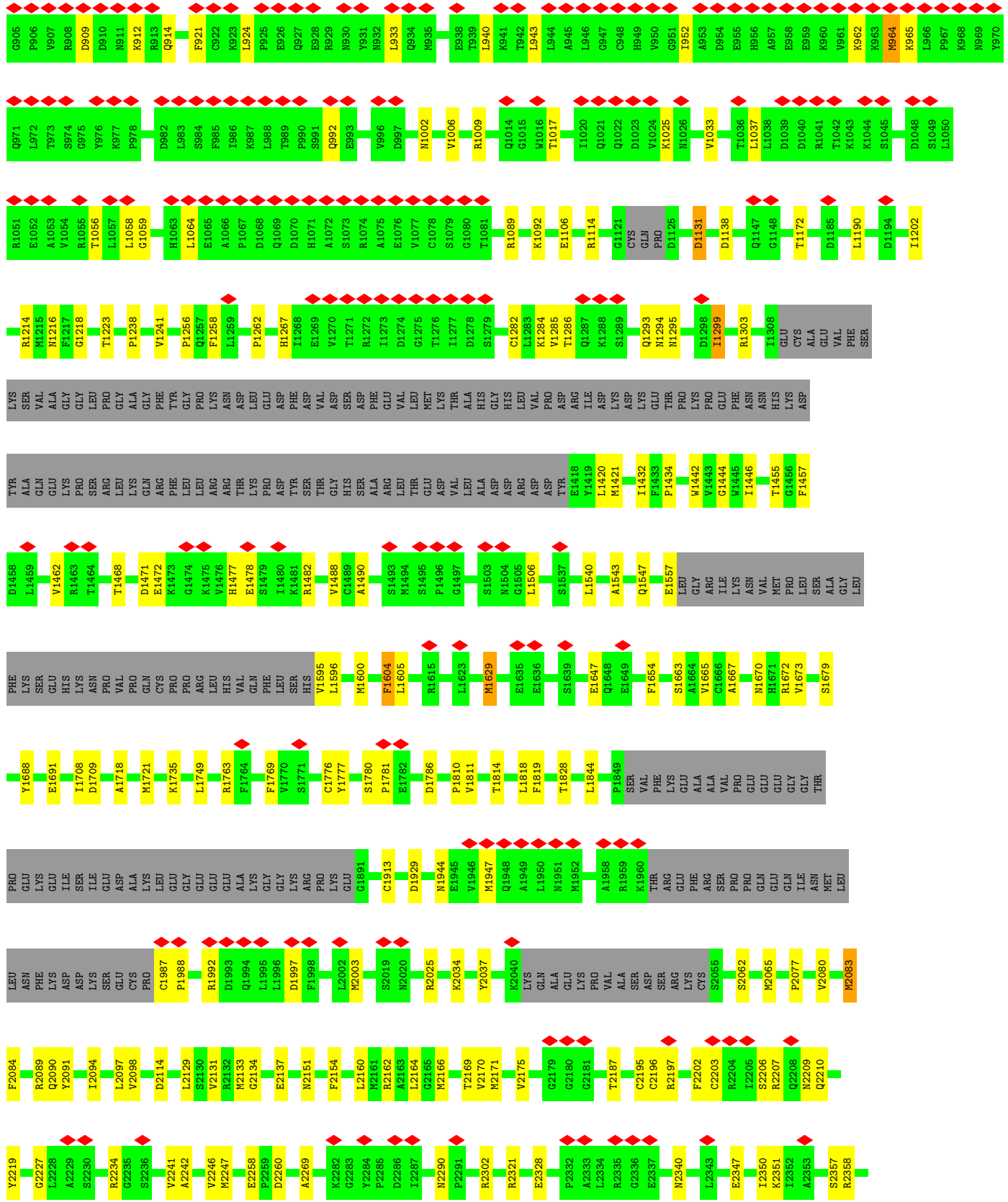


H2463	H2464	M2467	V2468	R2473	E2478	D2481	L2484	E2488	F2491	L2492	L2495	A2498	D2502	A2505	L2506	L2524	L2527	THR	ARG	CYS	PRO	LEU	PHE	ALA	GLY	THR	GLU	HIS	HIS	SER	LEU	ILE	ASP	LEU	LEU	HIS	VAL	THR	ARG	SER																				
LYS	GLY	SER	SER	THR	LYS	ALA	GLN	ARG	ASP	ILE	GLU	VAL	CYS	LEU	LEU	SER	ILE	C2576	G2577	Q2578	R2580	P2581	S2582	M2583	M2584	L2587	L2588	R2589	R2590	L2591	V2592	F2593	D2594	V2595	L2596	L2597	H2601	P2605	L2606	K2607	L2608	L2609	T2610	N2611	H2612	Y2613	E2614	H2617	Y2620	A2631										
A2632	S2640	R2641	K2642	L2643	M2644	W2645	G2646	L2647	L2651	S2652	Q2653	K2654	K2655	Y2656	E2657	Q2658	E2659	P2666	Y2679	M2680	E2681	S2682	M2683	Y2684	Y2684	V2685	S2686	M2687	M2688	E2689	K2690	Q2691	M2694	ASP	SER	GLY	GLY	ASN	F2700	M2701	P2702	Q2703	P2704	M2705	H2706	L2707	L2707	S2708	M2709	L2710	T2711	L2712	P2713	E2714	K2715	L2716				
E2717	Y2718	F2719	I2720	M2721	K2722	Y2723	A2724	E2725	H2726	S2727	H2728	D2729	K2730	M2731	S2732	M2733	D2734	K2735	L2736	A2737	M2738	G2739	M2740	I2741	Y2742	G2743	E2744	I2745	Y2746	S2747	D2748	S2749	S2750	K2751	I2752	Q2753	P2754	L2755	M2756	K2757	P2758	Y2759	K2760	L2761	L2762	S2763	E2764	K2765	E2766	K2767	E2768	I2769	Y2770	R2771	M2772	P2773	K2775	E2776		
S2777	L2778	K2779	T2780	M2781	L2782	A2783	W2784	G2785	W2786	R2787	I2788	E2789	R2790	T2791	R2792	E2793	G2794	D2795	S2796	M2797	A2798	L2799	Y2800	N2801	ARG	THR	ARG	ARG	ILE	ASP	GLN	THR	SER	GLN	VAL	ASP	ILE	ASP	A2816	A2817	H2818	G2819	Y2820	S2821	P2822	R2823	A2824	I2825	D2826	M2827	S2828	N2829	Y2830	T2831	L2832	S2833	R2834	D2835	L2836	
H2837	A2838	M2839	A2840	E2841	M2842	M2843	A2844	E2845	M2846	Y2847	H2848	M2849	L2850	M2851	A2852	K2854	K2855	K2856	L2857	L2858	E2858	L2859	E2860	S2861	K2862	G2863	G2864	G2865	H2866	H2867	P2868	L2869	L2870	V2871	P2872	Y2873	D2874	T2875	L2876	T2877	A2878	K2879	E2880	K2881	K2882	D2883	D2884	L2885	E2886	K2887	A2888	Q2889	D2890	L2891	F2892	K2893	L2895	Q2896		
I2897	S2898	G2899	Y2900	V2901	V2902	S2903	R2904	GLY	PHE	LYS	ASP	LEU	ASP	LEU	ASP	ASP	PRU	ILE	THR	SER	ILE	GLU	LYS	ARG	PHE	ALA	TYR	SER	PHE	GLN	GLM	ARG	THR	ARG	ARG	ILE	ARG	TYR	VAL	ASP	GLU	ALA	ARG	GLY	ASP	GLY	ASP	A2924	I2925	D2926	M2927	S2928	N2929	Y2930	T2931	L2932	S2933	R2934	D2935	L2936
GLN	GLU	ILE	LYS	PHE	ALA	LYS	VAL	VAL	LEU	PRO	GLN	LEU	LEU	ILE	ASP	GLN	TYR	ALA	TYR	SER	PHE	GLN	LYS	L2982	S2983	A2984	A2985	S2986	R2987	P2988	L2989	H2994	L3006	F3007	G3008	V3012	L3013	V3014	R3015	H3016	ARG	ILE	SER	LEU	PHE	GLY	ASN	ASP	ALA	THR	SER	ILE	VAL	ASN	CYS					
LEU	HIS	ILE	L3035	G3036	V3044	G3048	L3049	D3050	S3051	V3052	K3053	K3054	A3055	A3058	F3059	L3060	D3061	N3062	A3063	A3064	E3065	K3069	Q3078	F3079	T3080	H3081	Q3085	P3086	K3087	G3088	V3089	T3090	Q3091	I3092	Y3095	T3096	A3099	P3102	M3103	SER	SER	PHE	GLU	THR	SER	ILE	VAL	ASN	ASN	GLY	GLN	HIS								
GLN	PHE	GLY	ASP	LEU	ILE	LEU	ASP	VAL	VAL	LEU	VAL	PRO	VAL	SER	CYS	TYR	ARG	ILE	LEU	THR	THR	SER	SER	LEU	VAL	ARG	GLN	SER	ALA	LEU	GLY	CYS	LEU	ALA	ALA	ALA	GLY	ALA	PHE	PRO	ILE	ALA	ALA	PHE	LEU	GLU	THR	HIS	L3174											
D3175	K3176	H3177	N3178	V3179	N3184	S3188	L3194	S3195	L3196	P3197	A3198	N3199	V3200	E3201	D3202	V3203	C3204	P3205	N3206	I3207	L3210	L3213	M3214	T3215	I3218	E3219	I3225	R3226	Q3229	M3230	P3231	Y3232	K3233	M3234	E3235	V3236	V3237	L3238	P3239	C3242	S3243	Y3244	M3245	S3246	R3247	H3248	W3249	E3250												
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L3314	K3315	T3316	H3317	F3318	L3319	P3320	L3321	M3322	E3323	K3324	L3325	K3326	K3327	K3328	A3329	A3330	K3331	V3332	S3333	S3334	E3335	E3336	L3337	H3338	L3339	K3340	A3343	K3344	G3345	D3346	M3347	S3348	E3349	A3350	E3351	L3352	L3353	I3354	L3355	D3356	E3357	F3358	T3359	T3360	L3361	A3362	K3363	D3364	L3365	Y3366	A3367	P3370	L3371	L3372	I3373	R3374	F3375			



MET	ALA	ASP	ALA	GLY	GLY	GLY	ASP	E10	Q23	H29	R30	F42	L69	L73	L82	ALA	ASN	THR	VAL	GLU	LYS	SER	GLY	GLU	GLN	VAL	ASP	VAL	GLU	GLY	TRP	LYS	LYS	PHE	MET	MET	LYS	THR	ALA	ALA	G107	A118	I119	L120	L121	R122	H123	S124	Y125	M128																																					
C131	C132	L133	S134	R137	S138	S139	A144	L149	Q150	E156	W159	W160	S166	K167	Q168	R169	S170	E173	R176	S188	E189	R190	GLN	Y191	M198	S199	S200	D204	A205	A206	A215	S221	Y227	L234	H238	G239	H240	E243	C244	L245	P248	G253	E254	E255	Q256	R257	Y262	G265	A266	V267	R272	W275	L280	R290	R296	M309	E310	L315	V324	T327	E336	K337	L338	ASP	VAL	GLY	VAL	R343	K344	E345	G348	M349	G350	T351	D446	S352	E353	D367	T373	M434	R435	Q487	M488	F489	Q490	M494	I495
ARG	MET	GLY	SER	I387	K390	A391	I392	H395	M399	G402	Q409	H410	E411	S412	R414	T415	A416	R417	V418	I419	T422	V423	F424	L425	F426	N427	R431	L436	V440	K441	L442	P443	T444	I445	D446	L447	E468	M484	R485	Q487	M488	F489	Q490	M494	I495																																										
M496	L497	V498	L499	E500	R504	S509	F514	A515	E521	A522	K527	N531	S532	L533	Y534	E535	L536	E537	D534	A539	L540	F541	R542	G543	N544	R545	K546	A549	S552	G553	S554	L555	D556	W557	R561	L565	E566	A567	L572	E573	C577	L488	F489	Q490	S582	P583	E584																																								
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I1308	GLU	CYS	ALA	GLU	VAL	PHE	SER	LYS	SER	VAL	ALA	GLY	GLY	LEU	PRO	GLY	ALA	GLY	PHE	TYR	GLY	PRO	LYS	ASN	ASP	LEU	LEU	ASP	PHE	ASP	VAL	ASP	PHE	R1272	I1273	D1274	G1275	T1276	I1277	S1279	C1282	L1283	K1284	V1285	T1286	Q1287	K1288	S1289	Q1293	N1294	M1295	D1298	I1299	R1303																																	

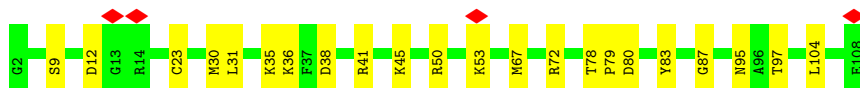
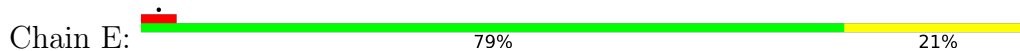




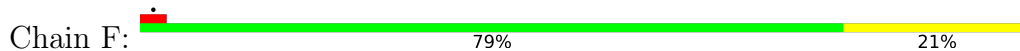
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H2463	K2464	M2467	V2468	R2473	E2478	D2481	L2484	E2488	F2491	L2492	L2495	A2498	A2499	D2502	A2505	L2506	L2527	THR	ARG	CYS	ALA	PRO	PRO	LEU	PHE	ALA	ASP	D2429	D2430	S2436	F2442	T2443	L2444	A2445	K2446	K2449	V2450	V2451	E2452	P2453	D2454	C2460																
SER	LYS	GLY	CYS	SER	LEU	THR	LYS	ALA	GLN	ARG	ASP	SER	ILE	GLU	VAL	CYS	LEU	THR	THR	ILE	C2576	G2577	Q2578	R2579	L2580	P2581	S2582	M2583	M2584	L2587	L2588	R2589	L2591	V2592	F2593	K2594	V2595	P2596	L2597	H2601	THR	GLY	THR	HIS	ALA	SER	SER	LEU	LEU	HIS	THR	VAL	ARG	LEU				
A2632	S2640	R2641	K2642	F2644	W2645	G2646	L2647	L2651	S2652	Q2653	K2654	K2655	Y2656	Q2658	E2659	P2666	Y2679	M2680	E2681	S2682	M2683	Y2684	V2685	S2686	M2687	M2688	E2689	Q2691	M2694	ASP	GLY	GLY	ASN	F2700	M2701	P2702	Q2703	P2704	V2705	D2706	T2707	S2708	M2709	I2710	T2711	P2713	E2714	K2715	L2716									
E2717	Y2718	F2719	L2720	N2721	K2722	Y2723	A2724	E2725	H2726	S2727	L2728	D2729	K2730	W2731	S2732	M2733	D2734	K2735	L2736	A2737	N2738	G2739	W2740	I2741	Y2742	G2743	E2744	I2745	S2746	S2747	D2748	S2749	S2750	K2751	I2752	Q2753	P2754	L2755	M2756	K2757	P2758	Y2759	K2760	L2761	L2762	S2763	E2764	K2765	E2766	K2767	E2768	Y2769	R2771	W2772	P2773	I2774	K2775	E2776
S2777	L2778	K2779	T2780	M2781	L2782	A2783	W2784	G2785	W2786	R2787	L2788	E2789	R2790	T2791	R2792	E2793	G2794	D2795	S2796	M2797	A2798	L2799	Y2800	Y2801	ARG	THR	ARG	ARG	ILE	ASP	GLN	THR	GLN	VAL	ASP	ILE	A2816	A2817	H2818	G2819	S2821	P2822	R2823	A2824	L2825	D2826	S2827	K2828	N2829	V2830	T2831	L2832	S2833	R2834	D2835	L2836		
H2837	A2838	M2839	A2840	E2841	M2842	M2843	A2844	E2845	N2846	Y2847	H2848	N2849	R2850	W2851	A2852	K2853	K2854	K2855	K2856	L2857	E2858	L2859	E2860	S2861	K2862	G2863	G2864	G2865	G2866	H2867	L2868	L2869	L2870	V2871	P2872	Y2873	D2874	T2875	L2876	T2877	A2878	K2879	E2880	K2881	A2882	K2883	D2884	R2885	K2886	K2887	A2888	Q2889	D2890	I2891	F2892	K2893	L2895	Q2896
I2897	S2898	G2899	Y2900	V2901	V2902	S2903	R2904	GLY	PHE	LYS	ASP	LEU	ASP	LEU	LEU	ASP	THR	PRO	SER	ARG	ILE	GLU	LYS	ARG	PHE	L2982	S2983	A2984	A2985	S2986	R2987	P2988	F3079	H3080	H3081	Q3085	P3086	K3087	G3088	V3089	T3090	Q3091	I3092	Y3095	T3096	A3099	F3102	M3103	SER	SER	LEU	GLU	THR	HIS	L3174			
GLN	PHE	GLY	LEU	LYS	PHE	ALA	VAL	VAL	LEU	PRO	LEU	ILE	ASP	GLN	THR	PHE	ASN	LYS	HIS	ARG	LEU	TYR	PHE	L2982	S2983	A2984	A2985	S2986	R2987	P2988	F3079	H3080	H3081	Q3085	P3086	K3087	G3088	V3089	T3090	Q3091	I3092	Y3095	T3096	A3099	F3102	M3103	SER	SER	LEU	GLU	THR	HIS	L3174					
ASN	CYS	HIS	ILE	PHE	ALA	VAL	VAL	LEU	PRO	LEU	ILE	ASP	GLN	THR	PHE	ASN	LYS	HIS	ARG	LEU	TYR	PHE	L2982	S2983	A2984	A2985	S2986	R2987	P2988	F3079	H3080	H3081	Q3085	P3086	K3087	G3088	V3089	T3090	Q3091	I3092	Y3095	T3096	A3099	F3102	M3103	SER	SER	LEU	GLU	THR	HIS	L3174						
GLN	PHE	GLY	LEU	LYS	PHE	ALA	VAL	VAL	LEU	PRO	LEU	ILE	ASP	GLN	THR	PHE	ASN	LYS	HIS	ARG	LEU	TYR	PHE	L2982	S2983	A2984	A2985	S2986	R2987	P2988	F3079	H3080	H3081	Q3085	P3086	K3087	G3088	V3089	T3090	Q3091	I3092	Y3095	T3096	A3099	F3102	M3103	SER	SER	LEU	GLU	THR	HIS	L3174					
D3175	K3176	H3177	N3178	V3179	N3184	S3188	R3191	L3194	S3195	H3271	V3200	E3201	D3202	V3203	C3204	P3205	N3206	I3207	L3210	L3282	I3283	M3214	T3215	I3218	E3219	I3225	R3226	Q3229	M3230	P3231	Y3232	M3233	M3234	E3235	V3236	V3237	L3238	P3239	C3242	S3243	Y3244	M3245	S3246	R3247	W3248	W3249	E3250											
H3251	G3252	F3253	E3254	N3255	H3256	P3257	E3258	R3259	A3260	F3261	K3262	C3263	C3264	S3269	E3270	H3271	N3272	N3273	T3274	L3275	LEU	GLY	ASN	ILE	K3281	I3282	I3283	Y3284	N3285	N3286	G3288	I3289	D3290	E3291	G3292	ALA	TRP	NET	LYS	ARG	LEU	ALA	VAL	F3301	S3302	Q3303	P3304	I3305	I3306	N3307	K3308	V3309	K3310	P3311	Q3312	I3313		



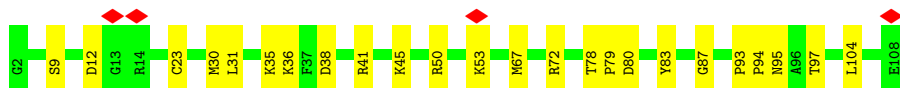
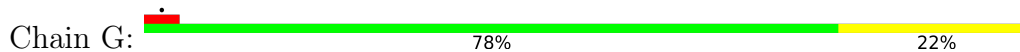
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



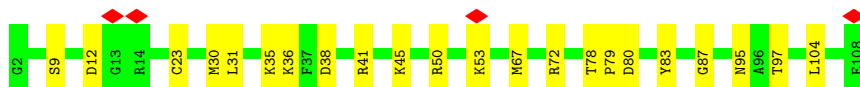
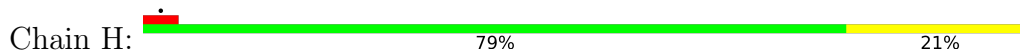
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	406681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.95	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.804	Depositor
Minimum map value	-1.458	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.24	Depositor
Map size (\AA)	496.80002, 496.80002, 496.80002	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.25	0/32026	0.49	7/43315 (0.0%)
1	B	0.26	0/32026	0.49	7/43315 (0.0%)
1	C	0.26	0/32026	0.49	7/43315 (0.0%)
1	D	0.26	0/32026	0.49	7/43315 (0.0%)
2	E	0.27	0/834	0.50	0/1123
2	F	0.27	0/834	0.50	0/1123
2	G	0.27	0/834	0.50	0/1123
2	H	0.27	0/834	0.50	0/1123
All	All	0.26	0/131440	0.49	28/177752 (0.0%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	315	LEU	CA-CB-CG	6.82	130.99	115.30
1	C	315	LEU	CA-CB-CG	6.81	130.95	115.30
1	B	315	LEU	CA-CB-CG	6.79	130.93	115.30
1	A	315	LEU	CA-CB-CG	6.79	130.92	115.30
1	B	1131	ASP	CB-CG-OD1	6.33	124.00	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31374	0	30394	319	0
1	B	31374	0	30394	324	0
1	C	31374	0	30394	328	0
1	D	31374	0	30394	312	0
2	E	818	0	821	12	0
2	F	818	0	821	12	0
2	G	818	0	821	13	0
2	H	818	0	821	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	128772	0	124860	1307	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.

The worst 5 of 1307 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1629:MET:SD	1:A:1629:MET:N	2.61	0.73
1:D:1629:MET:SD	1:D:1629:MET:N	2.61	0.73
1:C:1629:MET:SD	1:C:1629:MET:N	2.61	0.72
1:D:1444:GLY:HA3	1:D:1488:VAL:HA	1.72	0.71
1:A:3843:GLN:HG3	1:A:3921:GLU:HG3	1.73	0.71

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	3952/4966 (80%)	3722 (94%)	224 (6%)	6 (0%)	47 81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	3952/4966 (80%)	3724 (94%)	222 (6%)	6 (0%)	47	81
1	C	3952/4966 (80%)	3725 (94%)	221 (6%)	6 (0%)	47	81
1	D	3952/4966 (80%)	3722 (94%)	224 (6%)	6 (0%)	47	81
2	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	F	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	G	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	H	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
All	All	16228/20292 (80%)	15285 (94%)	919 (6%)	24 (0%)	54	84

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1299	ILE
1	B	1299	ILE
1	C	1299	ILE
1	D	1299	ILE
1	A	1462	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3331/4355 (76%)	3286 (99%)	45 (1%)	67	85
1	B	3331/4355 (76%)	3286 (99%)	45 (1%)	67	85
1	C	3331/4355 (76%)	3286 (99%)	45 (1%)	67	85
1	D	3331/4355 (76%)	3286 (99%)	45 (1%)	67	85
2	E	88/88 (100%)	84 (96%)	4 (4%)	27	61
2	F	88/88 (100%)	84 (96%)	4 (4%)	27	61
2	G	88/88 (100%)	84 (96%)	4 (4%)	27	61
2	H	88/88 (100%)	84 (96%)	4 (4%)	27	61
All	All	13676/17772 (77%)	13480 (99%)	196 (1%)	68	85

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2247	MET
1	D	731	HIS
1	C	2351	LYS
1	C	3635	PHE
1	D	1604	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1685	GLN
1	B	776	GLN
1	B	1685	GLN
1	C	1685	GLN
1	D	1685	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 4 ligands modelled in this entry, 4 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](#)

There are no chain breaks in this entry.

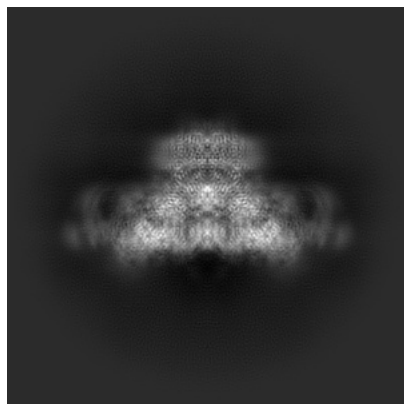
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27711. These allow visual inspection of the internal detail of the map and identification of artifacts.

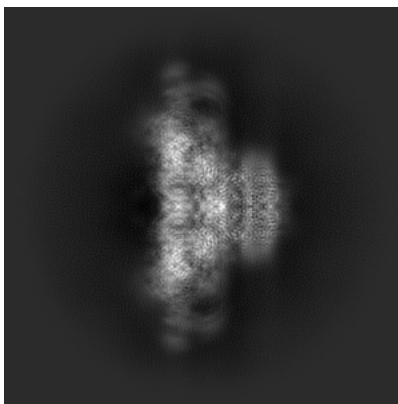
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

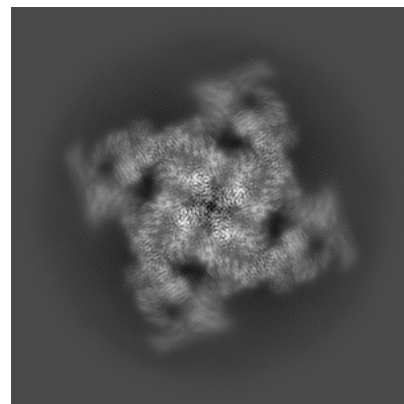
6.1.1 Primary map



X

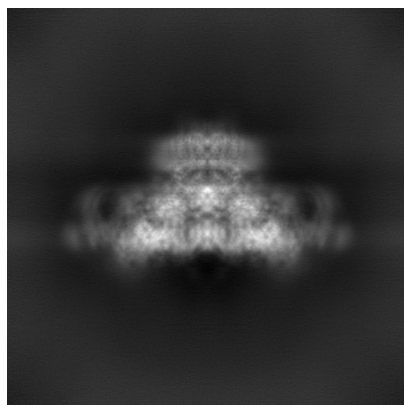


Y

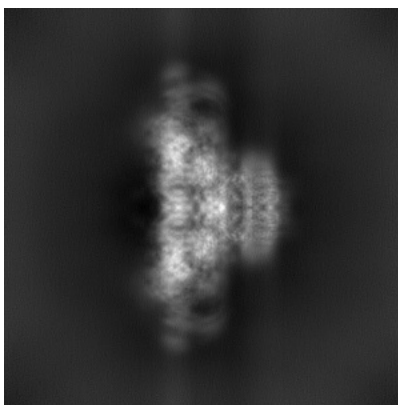


Z

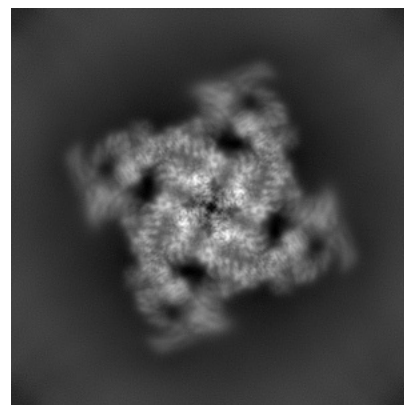
6.1.2 Raw map



X



Y

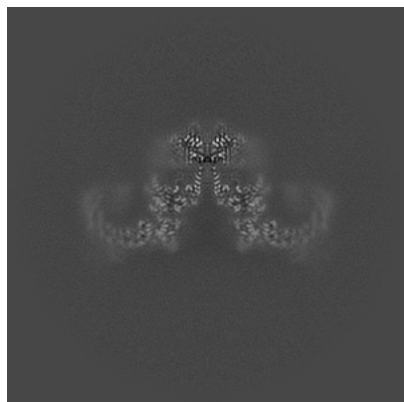


Z

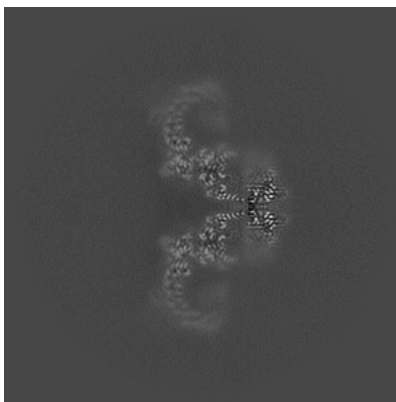
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

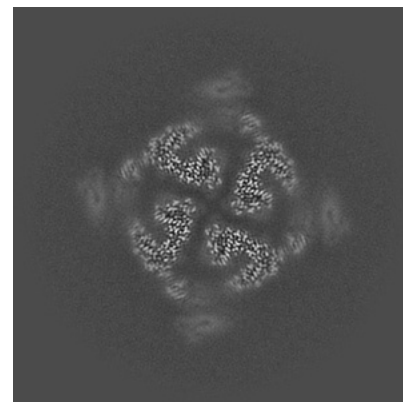
6.2.1 Primary map



X Index: 230

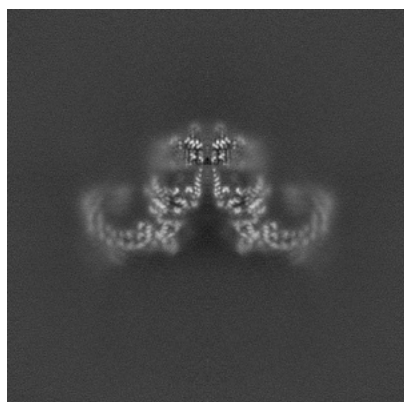


Y Index: 230

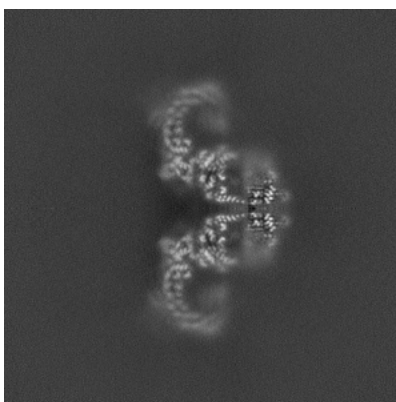


Z Index: 230

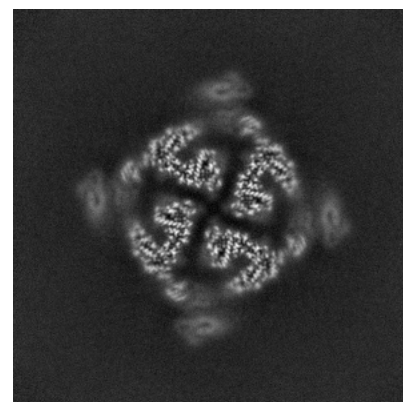
6.2.2 Raw map



X Index: 230



Y Index: 230

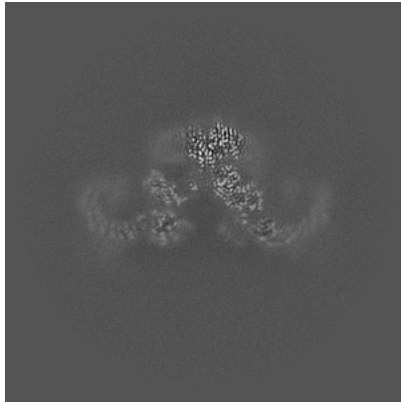


Z Index: 230

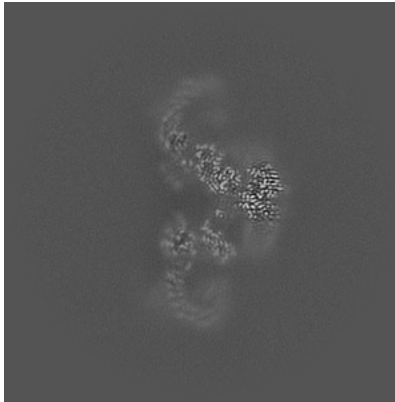
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

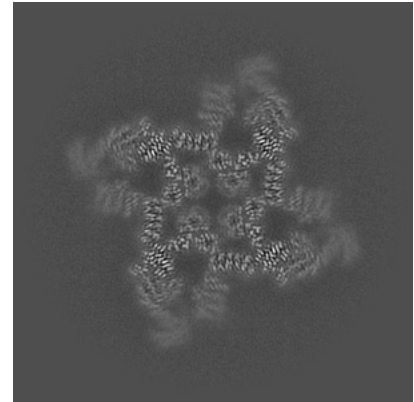
6.3.1 Primary map



X Index: 224

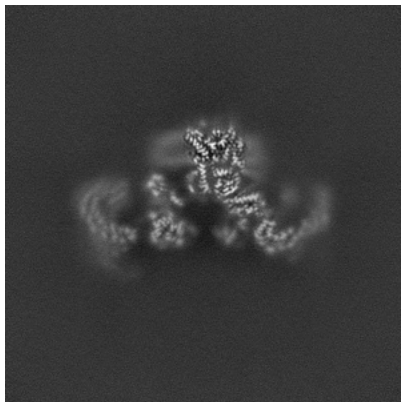


Y Index: 236

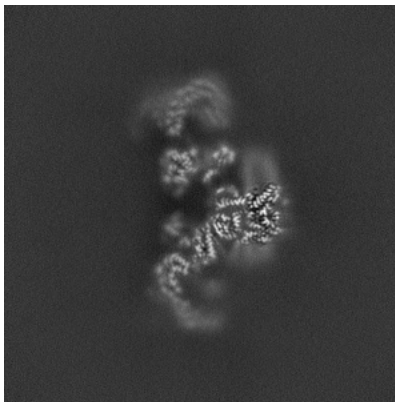


Z Index: 201

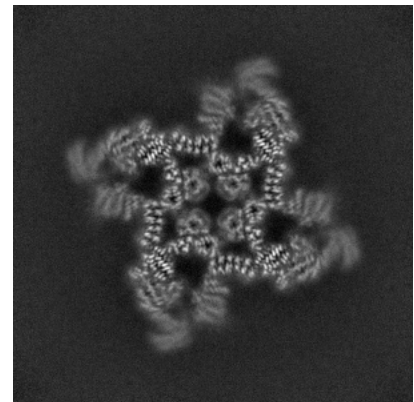
6.3.2 Raw map



X Index: 221



Y Index: 221

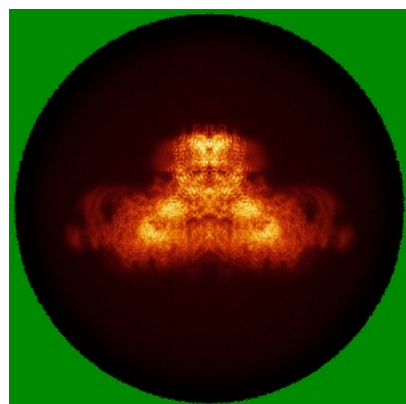


Z Index: 201

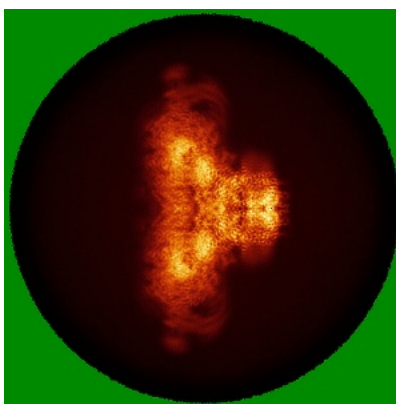
The images above show the largest variance slices of the map in three orthogonal directions.

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

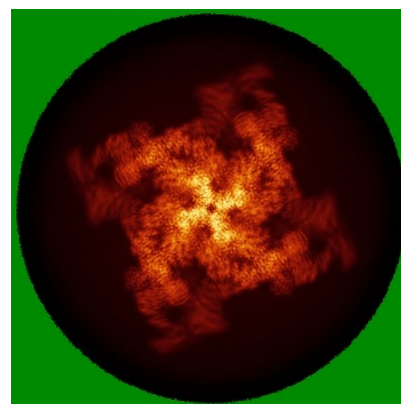
6.4.1 Primary map



X

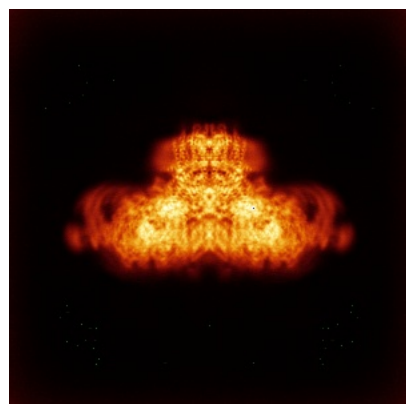


Y

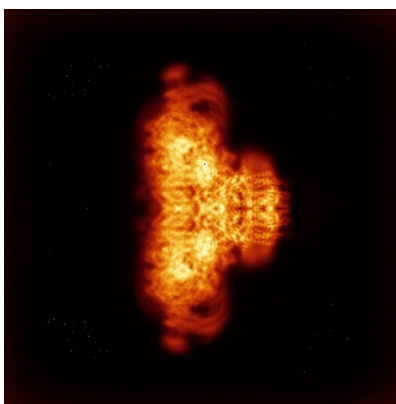


Z

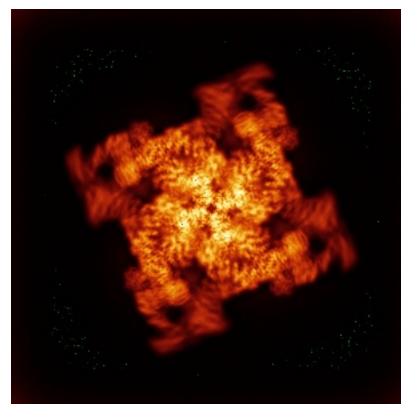
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

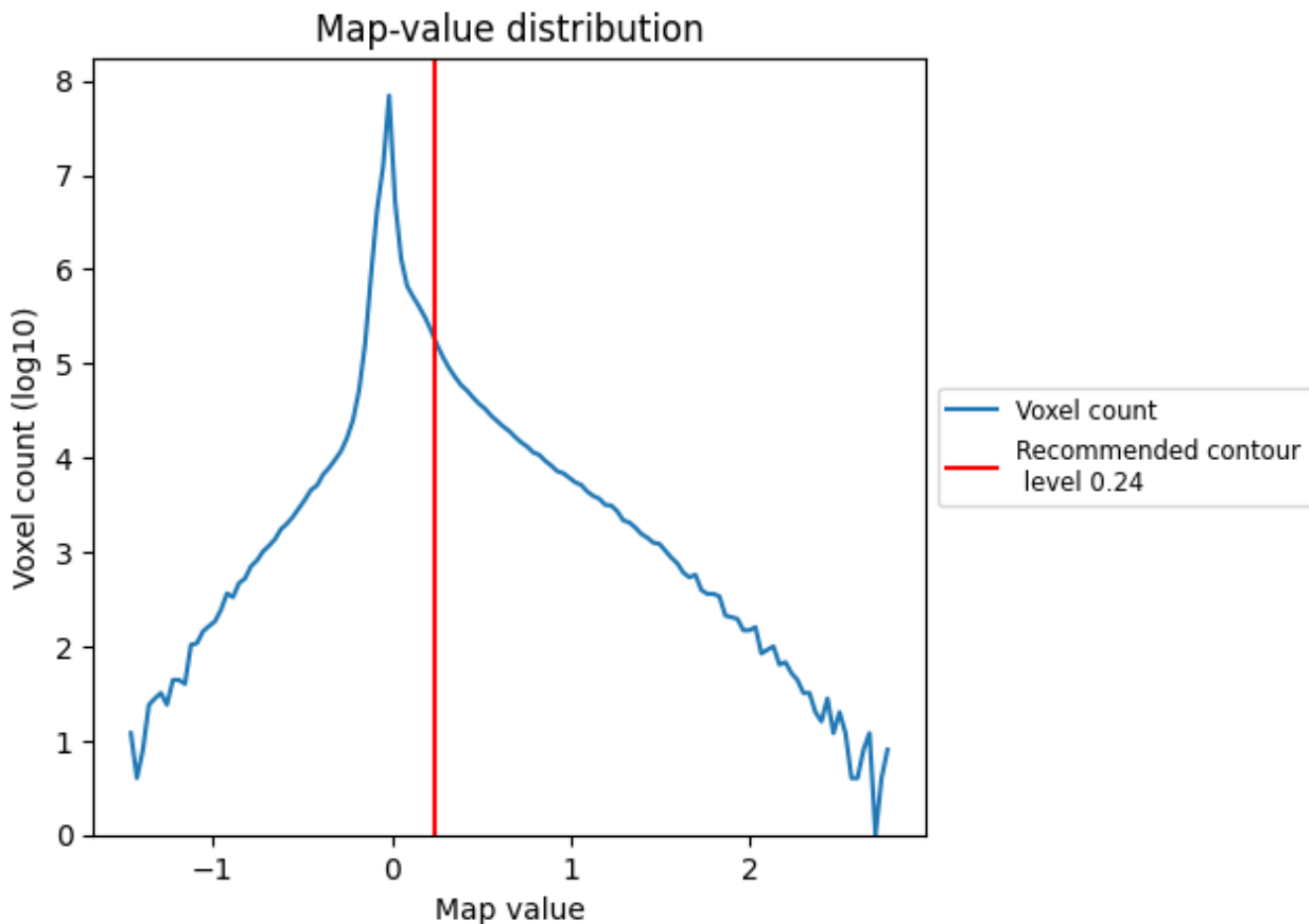
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

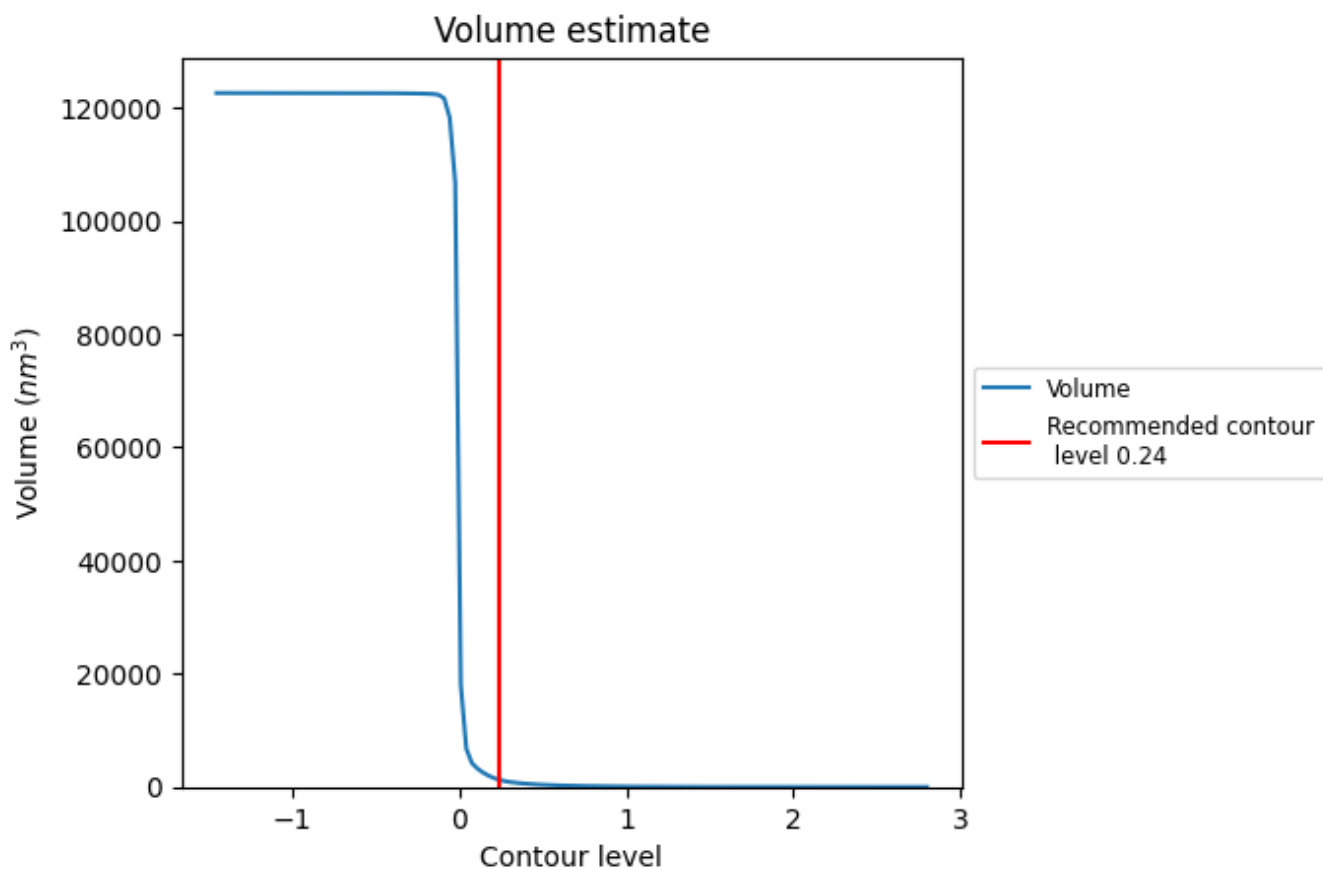
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

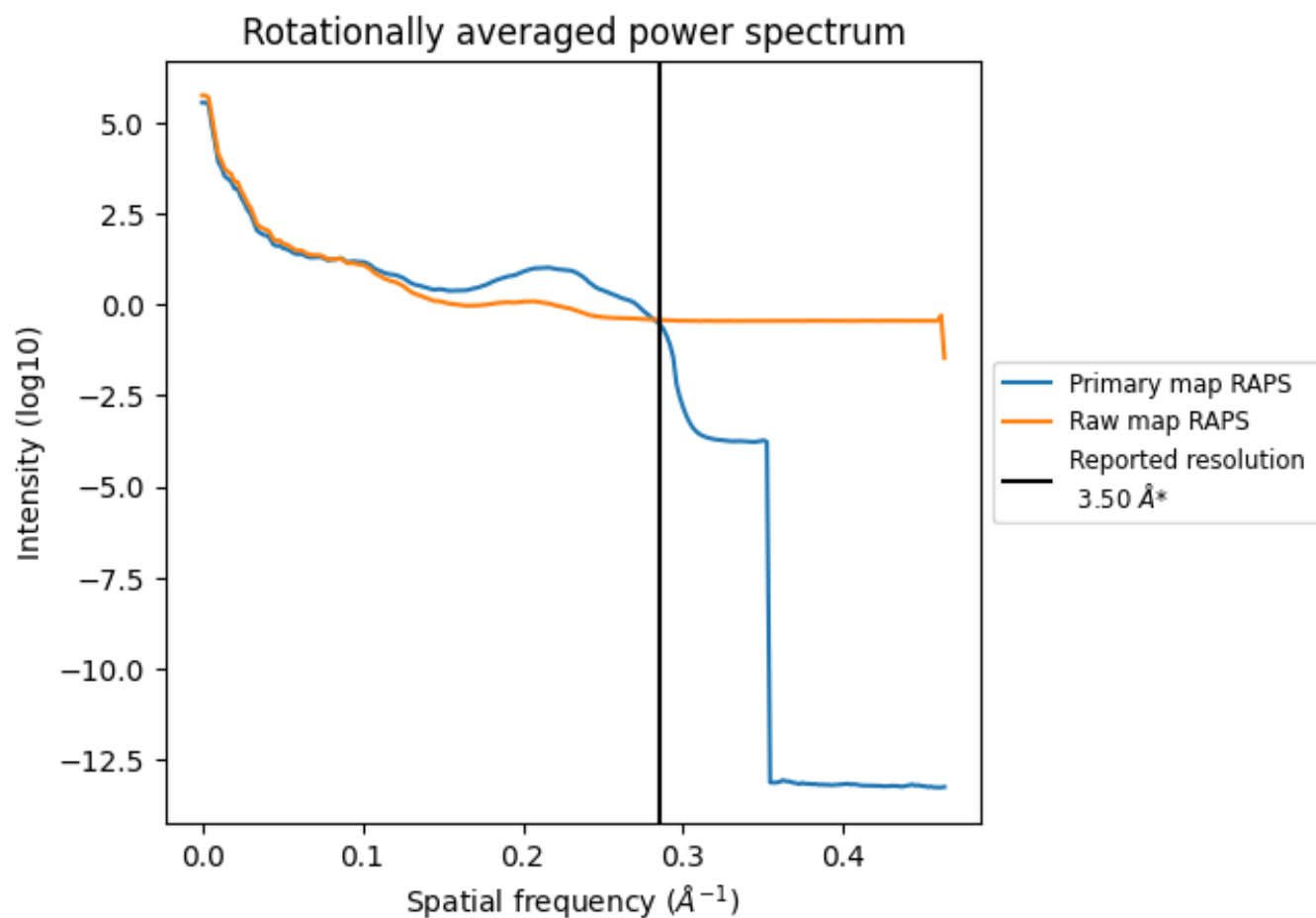
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1250 nm³; this corresponds to an approximate mass of 1129 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

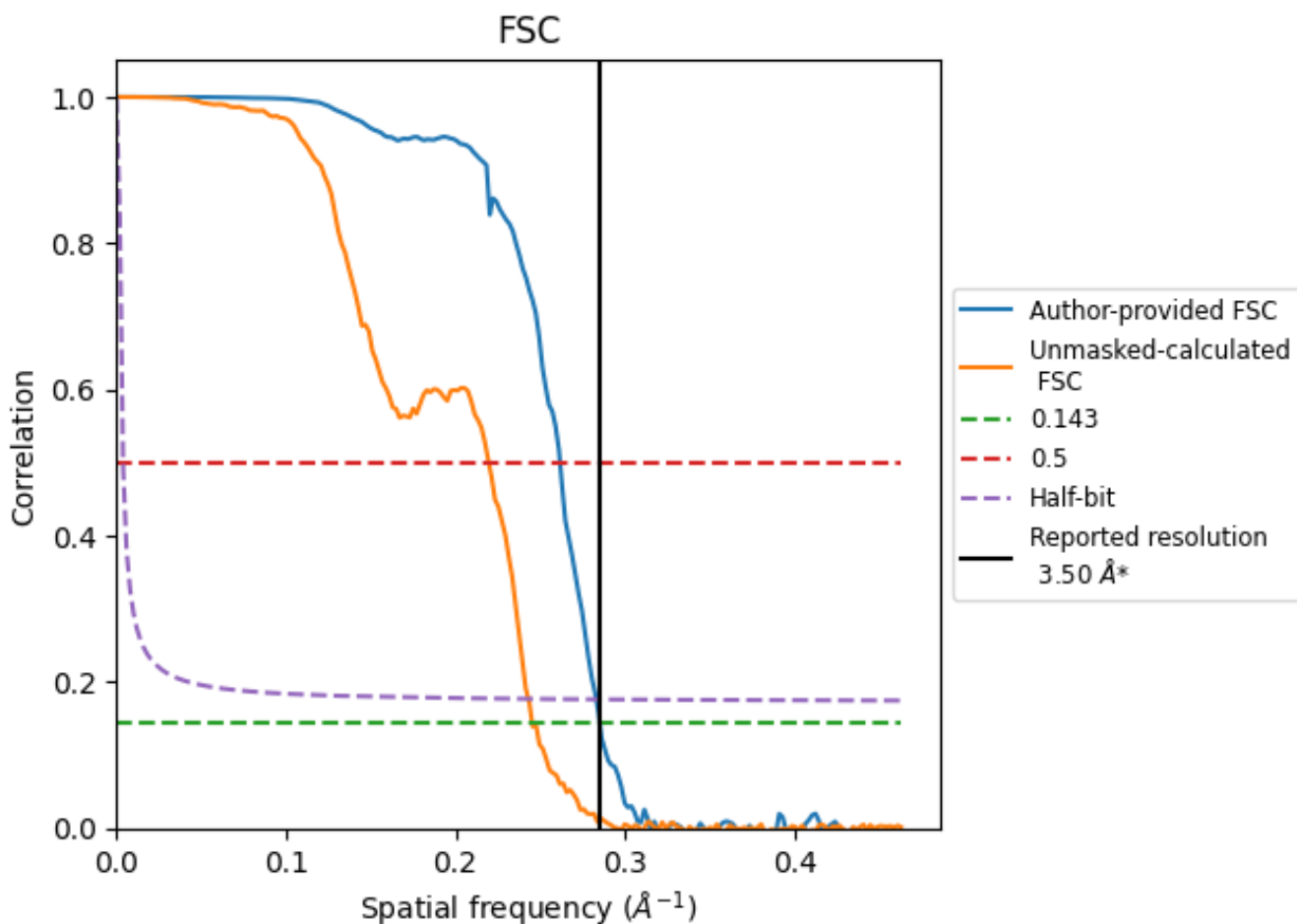


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

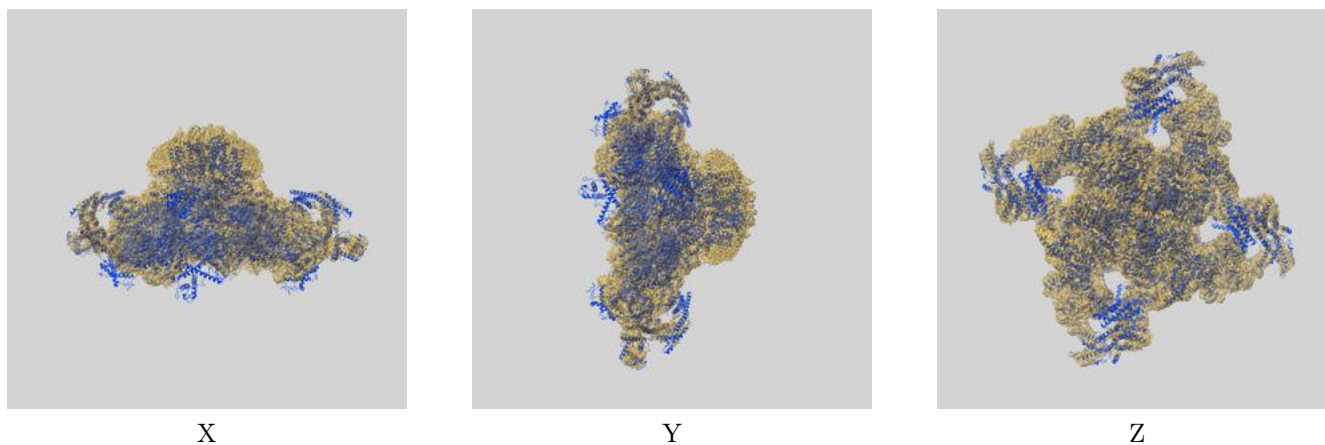
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.82	3.53
Unmasked-calculated*	4.08	4.55	4.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.08 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

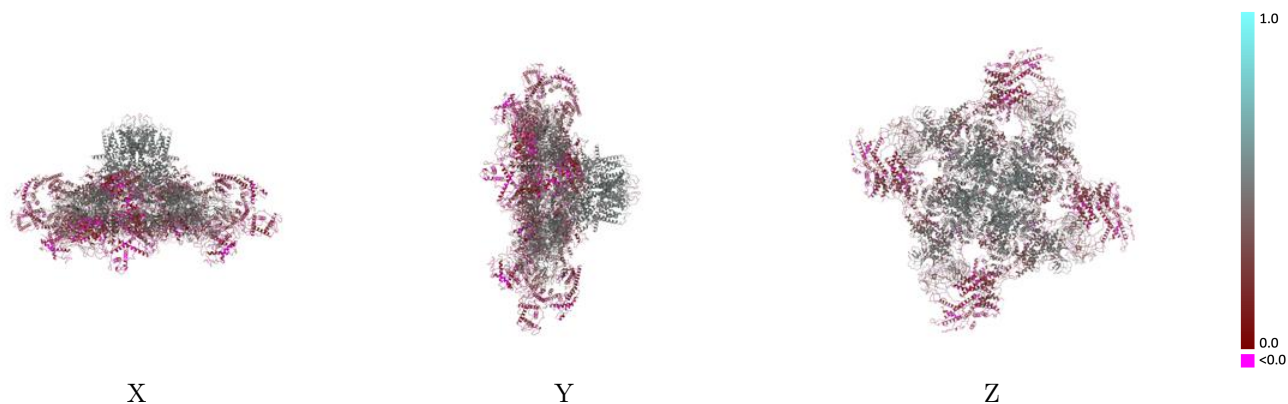
This section contains information regarding the fit between EMDB map EMD-27711 and PDB model 8DTY. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



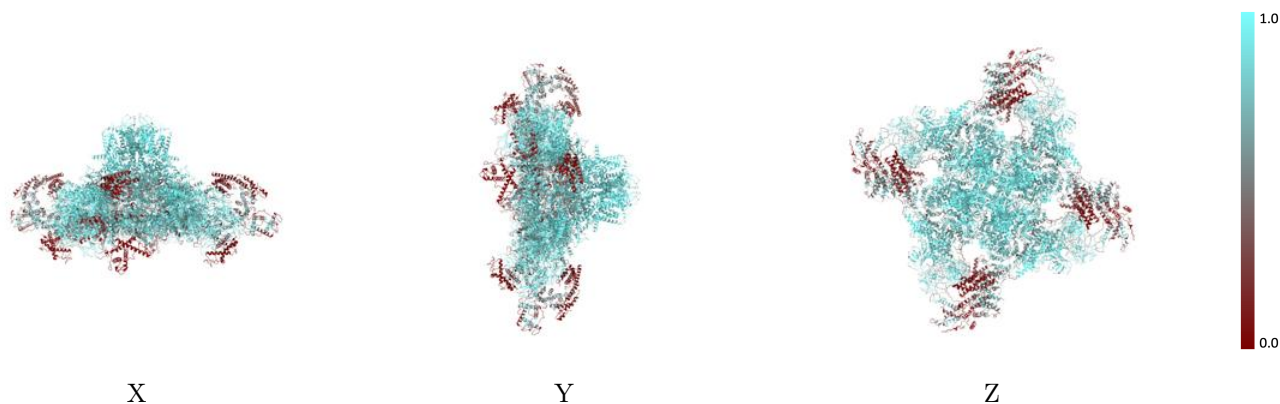
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



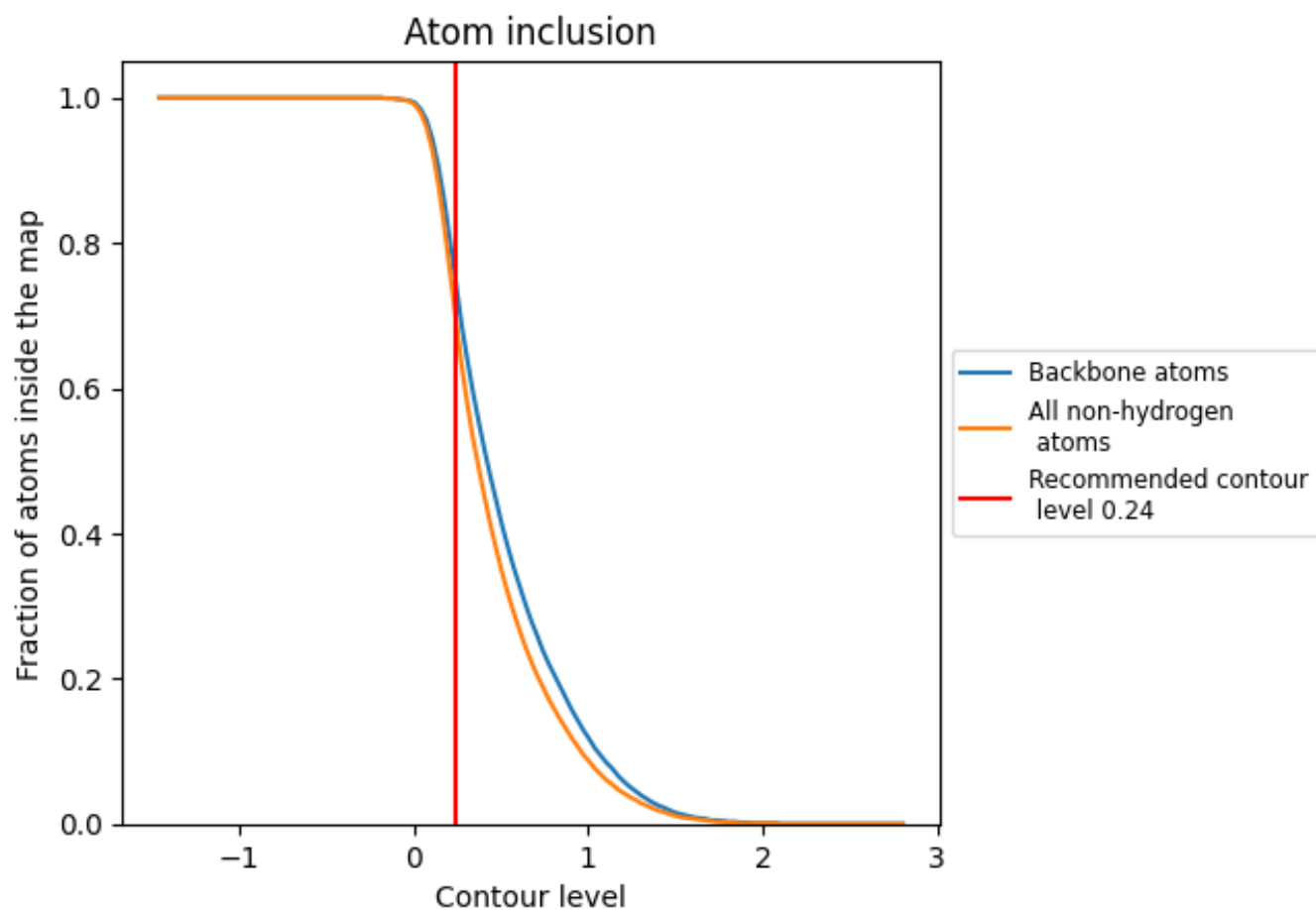
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6970	 0.3090
A	 0.6930	 0.3070
B	 0.6930	 0.3070
C	 0.6930	 0.3070
D	 0.6930	 0.3070
E	 0.8570	 0.3930
F	 0.8590	 0.3950
G	 0.8570	 0.3930
H	 0.8570	 0.3960

