



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 10:20 AM JST

PDB ID : 5GL0
EMDB ID : EMD-9520
Title : Structure of RyR1 in a closed state (C4 conformer)
Authors : Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-07
Resolution : 4.20 Å(reported)

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

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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

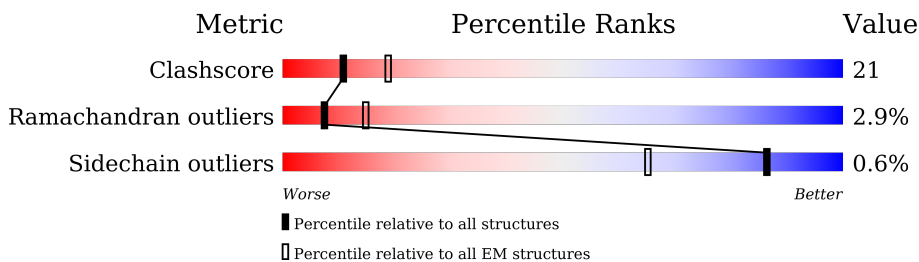
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5037	<div> <div>24%</div> <div>44%</div> <div>26%</div> <div>•</div> <div>27%</div> </div>
1	C	5037	<div> <div>24%</div> <div>44%</div> <div>26%</div> <div>•</div> <div>27%</div> </div>
1	E	5037	<div> <div>24%</div> <div>44%</div> <div>26%</div> <div>•</div> <div>27%</div> </div>
1	G	5037	<div> <div>24%</div> <div>44%</div> <div>27%</div> <div>•</div> <div>27%</div> </div>
2	B	108	<div> <div>36%</div> <div>60%</div> <div>38%</div> <div>••</div> </div>
2	D	108	<div> <div>36%</div> <div>61%</div> <div>37%</div> <div>••</div> </div>
2	F	108	<div> <div>36%</div> <div>63%</div> <div>35%</div> <div>••</div> </div>
2	H	108	<div> <div>31%</div> <div>64%</div> <div>34%</div> <div>••</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 111000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	C	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	E	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	G	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	D	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	F	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	H	107	Total	C	N	O	S	0	0
			832	527	146	155	4		

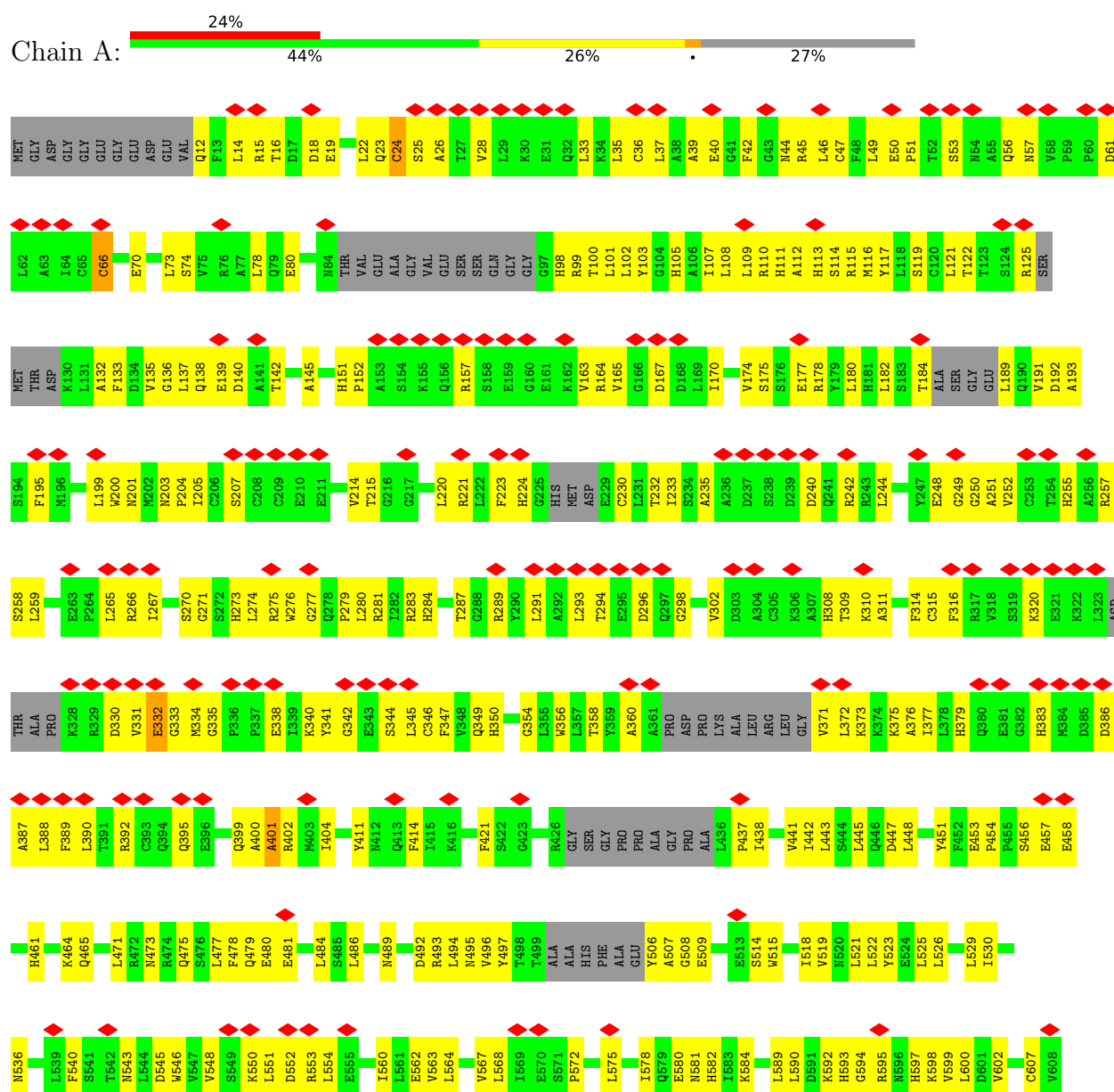
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

• Molecule 1: Ryanodine receptor 1





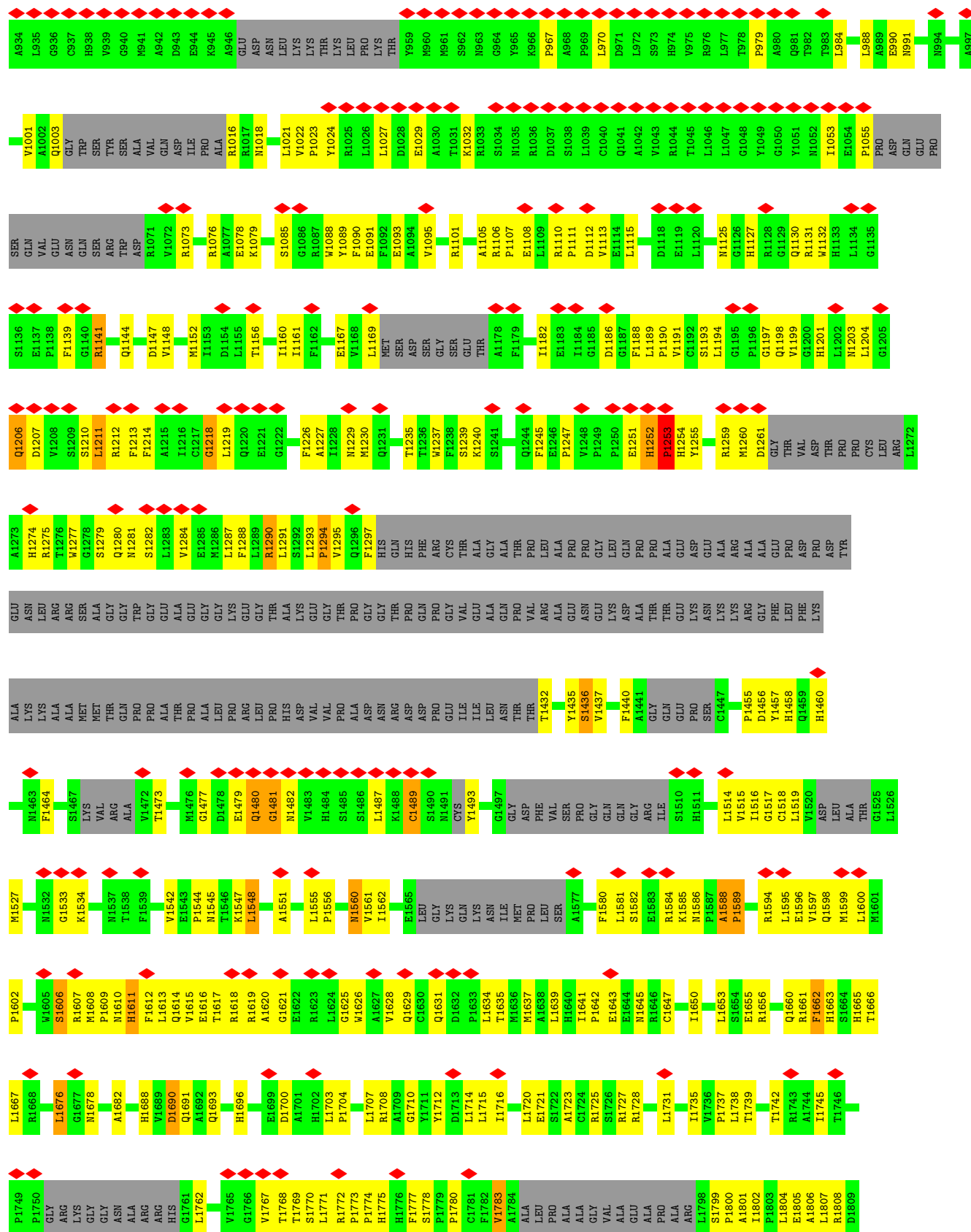


GLN	ALA	GLY	LYS	GLY	E2449	K2450	L2451	R2452	L2453	R2454	K2455	L2456	L2457	R2458	S2459	L2460	VAL	PRO	L2463	D2464	D2465	L2466	V2467	L2470	S2471	L2472	P2473	L2474	L2475	L2476	PRO	THR	LEU	GLY	LYS	ASP	GLY	ALA	LEU	VAL	GLN	PRO	LYS	MET	SER	ALA	SER	F2494	V2495	P2496	D2497	H2498	K2499	A2500	S2501	L2506	D2507		
R2508	V2509	Y2510	GLY	ILE	GLU	N2514	F2517	L2518	L2519	H2520	V2521	L2522	ASP	V2524	A2532	L2536	ASP	THR	ALA	PHE	THR	THR	T2544	E2545	N2546	A2549	L2550	N2551	R2552	Y2553	L2554	C2555	L2556	A2557	V2558	P2560	L2561	I2562	THR	LYS	CYS	ALA	P2567	L2568	F2569	A2570	G2571	T2572	R2575	V2586	TYR								
ARG	LEU	SER	R2591	Q2599	R2600	D2601	M2608	A2609	LEU	CYS	ARG	TYR	ILE	R2615	P2616	S2617	M2618	L2619	Q2620	L2623	R2624	R2625	L2626	V2627	F2628	D2629	V2630	P2631	N2634	GLU	PHE	ALA	K2638	M2639	P2640	L2641	Y2648	Y2654	Y2655	C2656	L2657	P2658	T2659	TRP	ALA	ASN	PHE	GLY	VAL	T2667	S2668	E2669							
F2679	T2682	F2683	S2685	L2686	ALA	HIS	L2751	LYS	Y2691	D2692	Q2693	R2697	P2701	C2702	L2703	C2704	A2705	L2706	K2707	Q2708	A2709	L2710	P2711	P2712	ASP	TYR	VAL	ALA	ALA	SER	THR	SER	SER	LYS	LYS	LYS	THR	ALA	VAL	ASP	ALA	GLU	GLY	N2734	F2735	D2736	P2737	R2738	P2739	V2740	E2741	T2742							
L2743	N2744	V2745	L2746	I2747	P2748	E2749	K2750	L2751	D2752	S2753	F2754	I2755	N2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	I2771	Q2772	N2773	N2774	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	H2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802
E2803	T2804	Y2805	R2806	W2807	P2808	L2809	K2810	S2811	E2812	L2813	K2814	A2815	M2816	L2817	A2818	W2819	E2820	W2821	T2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	GLU	GLU	ARG	THR	GLY	LYS	LYS	THR	ARG	ILE	GLN	THR	ALA	GLN	THR	Y2849	D2850	P2851	R2852	E2853	G2854	N2855	P2857	Q2858	P2859	D2860	K2861	L2862				
S2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	Y2882	H2883	T2884	T2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	K2897	G2898	G2899	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	P2860	K2916	A2917	R2918	D2919	E2921	K2922		
A2923	Q2924	E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	LEU	LYS	ASP	MET	GLU	THR	LEU	ASP	SER	SER	ILE	GLU	LYS	ARG	PHE	PHE	GLY	PHE	LEU	GLN	LEU	GLN	TRP	MET	ASP	ILE	GLN	GLU	PHE	ILE	ALA	ALA	VAL	VAL	SER								
SER	GLY	ARG	VAL	GLU	LYS	SER	PRO	HIS	GLN	GLU	GLU	ILE	LYS	PHE	ASN	ALA	LYS	LYS	ILE	LEU	LEU	PRO	PRO	ILE	ASN	GLN	TYR	PHE	THR	THR	ASN	HIS	CYS	LEU	Y3016	F3017	L3018	S3019	T3020	P3021	A3022	K3023	V3024	L3025	H3030	A3031	S3032	N3033	K3036	E3037	K3038	I3039	THR	SER	LEU	F3043	C3044	K3045	L3046
V3050	R3051	H3052	S3055	D3060	A3061	P3062	ALA	VAL	VAL	ASN	CYS	L3068	H3069	I3070	L3071	A3072	R3073	S3074	D3076	A3077	R3078	T3079	V3080	K3081	K3082	S3083	G3084	P3085	E3086	I3087	V3088	K3089	A3090	GLY	LEU	ARG	SER	F3095	F3096	E3097	S3098	A3099	S3100	E3101	D3102	I3103	E3104	K3105	E3108	N3109	L3110	R3111	L3112	G3113					
K3114	V3115	S3116	GLN	ALA	ARG	THR	GLN	VAL	GLY	VAL	GLY	GLN	ASN	LEU	THR	T3132	T3133	V3134	A3135	P3138	V3139	L3140	T3141	T3142	L3143	F3144	Q3145	H3146	I3147	A3148	Q3149	H3150	Q3151	F3152	GLY	ASP	ASP	VAL	ILE	L3158	D3159	D3160	V3161	Q3162	V3163	S3164	C3165	V3166	R3167	T3168	L3169	T3172	V3173	S3174	L3175				
G3176	T3177	T3178	LYS	ASN	THR	TYR	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	L3194	A3195	R3196	A3198	A3199	MET	PRO	VAL	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	S3213	N3214	A3215	C3216	S3217	VAL	TYR	THR	THR	LYS	SER	PRO	GLU	ARG	ALA	ARG	PRO	ILE	LEU	GLY	LEU	PRO	ASN	SER	VAL	GLU		
GLU	MET	CYS	PRO	ASP	ILE	PRO	VAL	LEU	ASP	ARG	MET	ALA	ASP	ILE	GLY	LEU	ALA	GLU	SER	GLY	ARG	TYR	THR	GLU	MET	PRO	PRO	HIS	VAL	T3273	L3274	P3275	N3276	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	W3284	W3285	E3286	R3287	G3288	P3289	E3290	ALA	PRO	P3294	A3295	L3296	P3297						











A3484	Q3485	S3486	G3487	G3488	S3489	D3490	Q3491	GLU	ARG	T3494	K3495	K3496	K3497	K3498	R3499	G3500	Y3503	S3504	VAL	GLN	THR	SER	ILE	VAL	ALA	T3513	L3514	L3518	P3519	T3520	G3521	L3522	N3523	M3524	C3525	A3526	P3527	THR	ASP	GLN	ASP	LEU	ILE	MET	LEU	ALA	K3537	T3538	R3539	Y3540	A3541	L3542	K3543	D3544	THR	ASP										
G3363	ARG	LEU	ARG	K3367	K3368	A3369	G3370	K3371	V3372	V3373	A3374	E3375	E3376	E3377	Q3378	L3379	R3380	L3381	E3382	A3383	K3384	A3385	E3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395	D3396	E3397	PHE	SER	VAL	LEU	C3402	R3403	D3404	L3405	M3406	M3407	L3408	Y3409	P3410	L3411	L3412	L3413	R3414	Y3415	V3416	D3417	N3418	N3419	R3420	A3421	H3422							
A3300	P3301	P3302	P3303	C3304	T3305	A3306	D3310	H3311	L3312	N3313	SER	LEU	G3317	G3318	N3319	L3320	R3321	I3322	I3323	V3324	N3325	N3326	L3327	G3328	E3331	A3332	T3333	T3334	N3335	K3336	R3337	L3338	A3339	VAL	PHE	ALA	GLN	PRO	ILE	V3346	S3347	R3348	A3349	R3350	P3351	E3352	L3353	L3354	H3355	S3356	H3357	F3358	L3359	P3360	T3361	I3362										
CYS	PRO	ASP	ILE	VAL	VAL	ASP	ARG	MET	LEU	ASP	ASP	ILE	GLY	GLY	ALA	ALA	ARG	THR	THR	GLU	MET	PRO	VAL	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	L3213	N3214	A3215	C3216	S3217	VAL	TYR	THR	THR	LYS	SER	PRO	ARG	GLU	ARG	ALA	ILE	LEU	LEU	PRO	P3294	A3295	L3296	H3297	L3298	V3299	P3297	G3299						
T3178	LYS	ASN	THR	TYR	V3183	E3184	K3185	L3186	R3187	P3188	A3189	L3190	L3194	A3195	R3196	L3197	A3198	A3199	A3200	MET	PRO	VAL	A3204	F3205	L3206	E3207	P3208	Q3209	L3210	N3211	E3212	L3213	N3214	A3215	C3216	S3217	VAL	TYR	THR	THR	LYS	SER	PRO	ARG	GLU	ARG	ALA	ILE	LEU	LEU	PRO	A3294	A3295	P3297	G3299											
S3116	GLN	ALA	ARG	THR	GLN	VAL	LYS	VAL	GLY	VAL	GLN	ASN	CYS	L3068	H3069	L3070	L3071	V3134	A3072	R3073	S3074	ARG	L3075	D3076	A3077	R3078	L3143	F3144	Q3145	H3146	I3147	A3148	Q3149	H3150	Q3151	F3152	GLY	ASP	ASP	VAL	ILE	L3158	D3159	L3160	V3161	Q3162	V3163	E3101	C3165	Y3166	R3167	T3168	L3169	I3172	Y3173	S3174	L3175	G3176	T3177							
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ARG	VAL	GLU	LYS	SER	PRO	HIS	GLU	GLN	ILE	ILE	LYS	PHE	PHE	ALA	LYS	ILE	LEU	LEU	PRO	ILE	LYS	ASP	MET	GLU	LEU	GLY	F3016	F3017	L3018	S3019	PHE	THR	GLY	PHE	GLY	PHE	LEU	GLN	GLN	ARG	LEU	LEU	ARG	TRP	MET	ASP	ILE	GLN	GLN	THR	Y2849	D2850	K2851	P2852	H2853	F2854	G2855	Y2856	N2857	Q2858	P2859	D2860	L2861	L2862	S2863	G2864
E2925	L2926	L2927	K2928	F2929	L2930	Q2931	M2932	G2933	M2934	Y2935	A2936	V2937	T2938	R2939	G2940	LEU	LYS	ASP	MET	GLU	THR	PHE	THR	ASN	ILE	LEU	Y3016	F3017	L3018	S3019	PHE	THR	GLY	PHE	GLY	PHE	LEU	GLN	GLN	ARG	LEU	LEU	ARG	TRP	MET	ASP	ILE	GLN	GLN	THR	Y2849	D2850	K2851	P2852	H2853	F2854	G2855	Y2856	N2857	Q2858	P2859	D2860	L2861	L2862	S2863	G2864
V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	N2881	L2882	H2883	N2884	L2885	W2886	G2887	R2888	K2889	K2890	K2891	Q2892	L2893	E2894	E2895	A2896	K2897	L2898	L2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	Y2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	K2916	A2917	D2918	D2919	R2920	E2921	K2922	A2923	Q2924							
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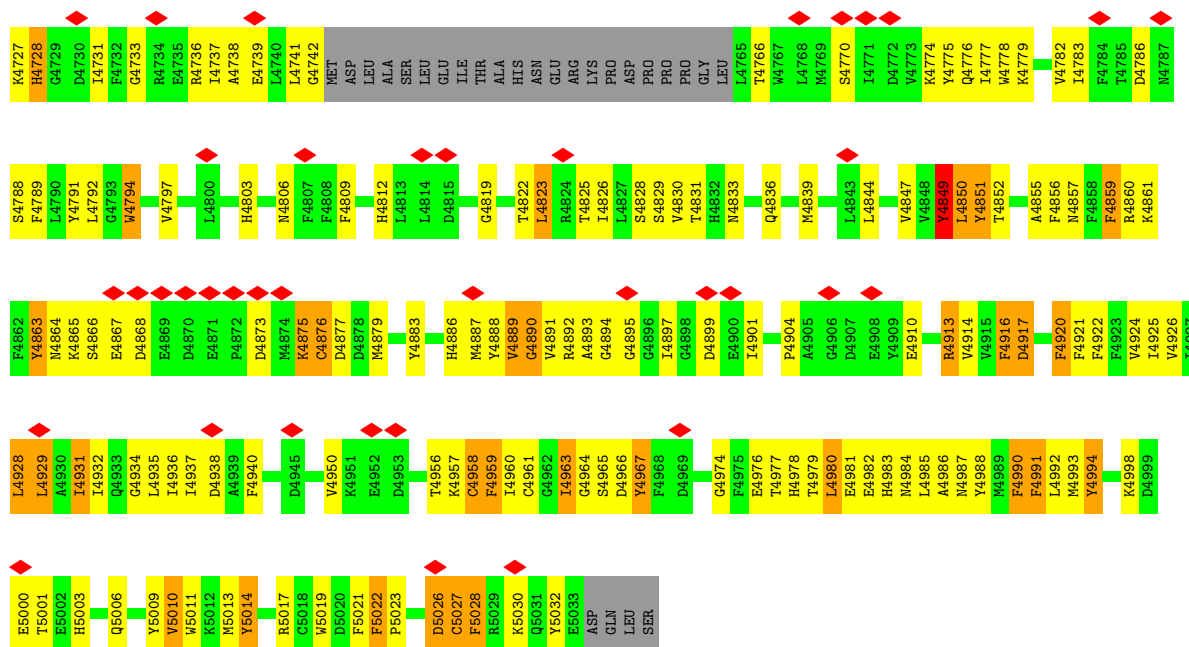




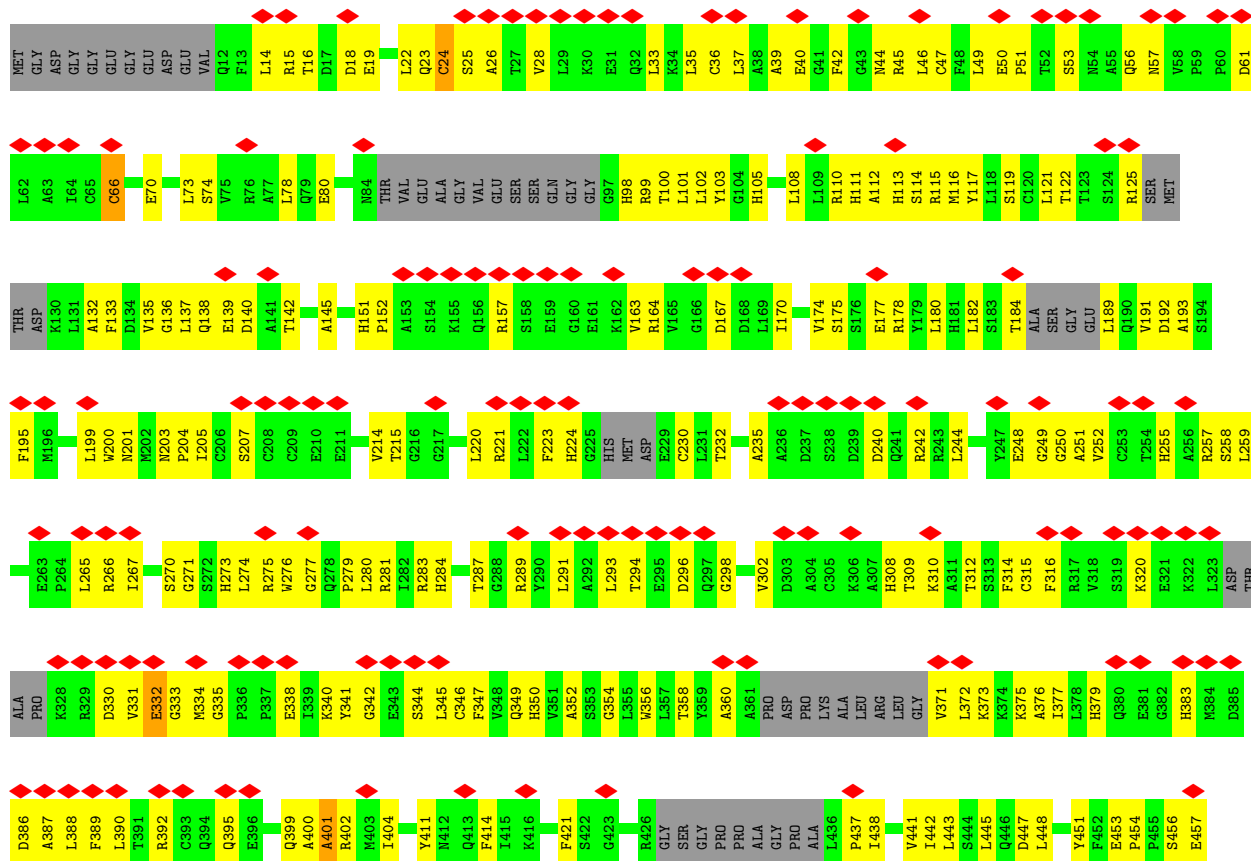
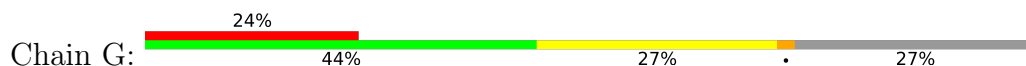
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L2743	N2744	V2745	L2746	I2747	D2748	E2749	K2750	L2751	D2752	S2753	F2754	L2755	I2756	K2757	F2758	A2759	E2760	Y2761	T2762	H2763	E2764	K2765	W2766	A2767	F2768	D2769	K2770	L2771	Q2772	N2773	N2774	S2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	E2784	L2785	K2786	L2787	H2788	P2789	M2790	L2791	T2792	P2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	
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GLN	ALA	GLY	LYS	GLY	E2449	A2450	L2451	R2452	I2453	R2454	A2455	L2456	L2457	R2458	S2459	L2460	VAL	PRO	D2463	D2464	D2465	L2466	V2467	I2470	S2471	L2472	P2473	L2474	Q2475	I2476	PRO	THR	LEU	GLY	LYS	ASP	GLY	ALA	LEU	VAL	GLN	PRO	LYS	MET	ALA	SER	F2494	V2495	P2496	D2497	H2498	K2499	A2500	S2501	L2506	D2507				
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ALA	ASP	GLU	PRO	ASP	CYS	PRO	LEU	PRO	GLU	ASP	ILE	ARG	GLN	ASP	LEU	GLN	Q2045	L2046	E2047	GLY	GLU	GLU	GLU	PRO	GLU	GLU	T2057	S2060	S2061	R2062	L2063	R2064	S2065	L2066	T2069	V2070	R2071	L2072	VAL	LYS	LYS	LYS	GLU	LYS	PRO	GLU	GLU	LEU	PRO	ALA	GLU									







• Molecule 1: Ryanodine receptor 1



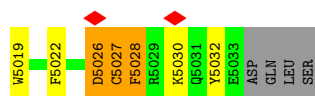




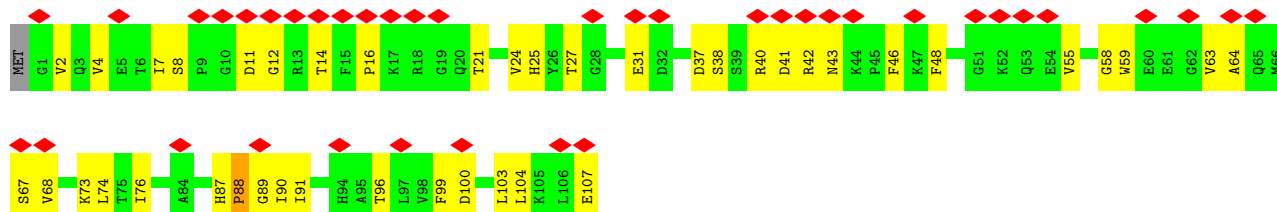
WORLDWIDE
PDB
PROTEIN DATA BANK

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GLU	HIS	PRO	TYR	LYS	SER	LYS	LYS	ALA	VAL	TRP	HIS	LYS	LEU	SER	LYS	ARG	ARG	ALA	VAL	VAL	VAL	ALA	CYS	PHE	ARG	MET	THR	LEU	TYR	ARG	GLY	LEU	PRO	GLY	P3645	T3646	H3647	R3648	N3651	L3654	Y3657	K3658	A3659	A3660	V3661	L3662	L3663	T3664	E3665	D3666	H3667	E3670	T3674	D3675					
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CYS	PRO	ILE	PRO	VAL	LEU	ASP	ARG	LEU	MET	ALA	ASP	ILE	GLY	GLY	ALA	GLU	SER	ALA	ARG	TYR	THR	GLU	MET	PRO	HIS	VAL	ILE	GLU	ILE	L3273	L3274	P3275	M3276	L3277	C3278	S3279	Y3280	L3281	P3282	R3283	W3284	W3285	E3286	R3287	G3288	P3289	E3290	ALA	PRO	P3294	A3295	L3296	P3297	A3298	G3299				
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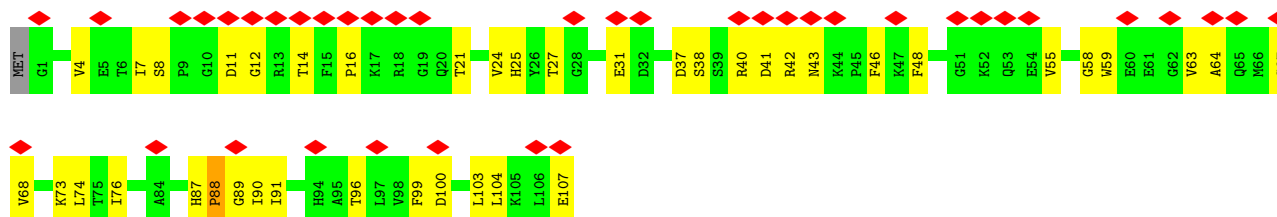
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F4125	P4208	GLY	ASP	ASP	ASP	ASP	K4670	H4728	G4934	
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F4127				GLY	ALA	ALA	R4673	Y4733	I4936	
F4128					GLY	GLY	E4674	Y4795	I4937	
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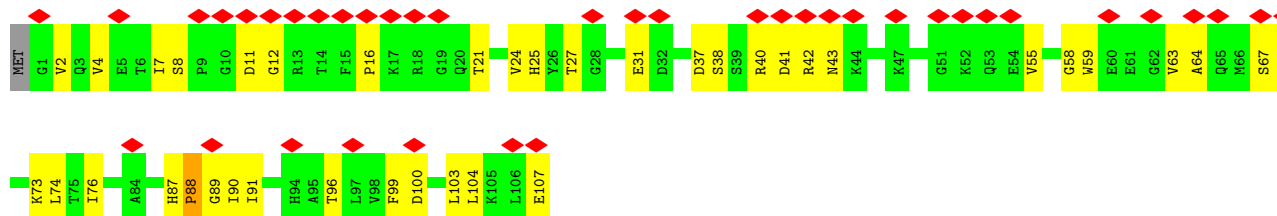
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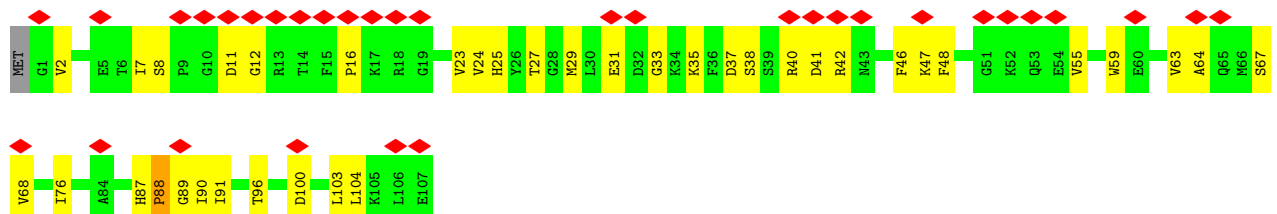
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.324	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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

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	0.93	55/27385 (0.2%)	0.86	90/37104 (0.2%)
1	C	0.93	56/27385 (0.2%)	0.87	92/37104 (0.2%)
1	E	0.93	53/27385 (0.2%)	0.86	91/37104 (0.2%)
1	G	0.93	55/27385 (0.2%)	0.85	90/37104 (0.2%)
2	B	0.58	0/851	0.67	0/1146
2	D	0.58	0/851	0.67	0/1146
2	F	0.58	0/851	0.67	0/1146
2	H	0.60	0/851	0.67	0/1146
All	All	0.92	219/112944 (0.2%)	0.86	363/153000 (0.2%)

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
1	A	0	19
1	C	0	19
1	E	0	19
1	G	0	19
All	All	0	76

The worst 5 of 219 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4988	TYR	CG-CD2	-12.12	1.23	1.39
1	A	5014	TYR	CG-CD1	-11.55	1.24	1.39
1	E	5014	TYR	CG-CD1	-11.43	1.24	1.39
1	C	3922	TYR	CE1-CZ	-11.19	1.24	1.38
1	E	3922	TYR	CE1-CZ	-11.12	1.24	1.38

The worst 5 of 363 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4128	PHE	CB-CG-CD2	-10.00	113.80	120.80
1	E	4128	PHE	CB-CG-CD2	-9.73	113.99	120.80
1	C	4128	PHE	CB-CG-CD2	-9.69	114.02	120.80
1	A	4128	PHE	CB-CG-CD2	-9.62	114.07	120.80
1	E	4064	MET	CG-SD-CE	8.87	114.39	100.20

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1252	HIS	Peptide
1	A	1253	PRO	Peptide
1	A	1464	PHE	Mainchain
1	A	332	GLU	Mainchain,Peptide
1	A	841	GLY	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	26917	0	24461	1094	0
1	C	26917	0	24461	1105	0
1	E	26917	0	24461	1108	0
1	G	26917	0	24461	1100	0
2	B	832	0	831	38	0
2	D	832	0	831	37	0
2	F	832	0	831	36	0
2	H	832	0	831	34	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111000	0	101168	4395	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 21.

The worst 5 of 4395 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:E:4826:ILE:CG2	1:G:4931:ILE:HD11	1.79	1.10
1:A:4879:MET:SD	1:G:4578:LEU:HA	1.92	1.10
1:A:4826:ILE:CG2	1:C:4931:ILE:HD11	1.86	1.05
1:E:4578:LEU:HA	1:G:4879:MET:SD	1.99	1.03
1:C:4826:ILE:CG2	1:E:4931:ILE:HD11	1.91	1.00

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	3496/5037 (69%)	3173 (91%)	220 (6%)	103 (3%)	4	32
1	C	3496/5037 (69%)	3169 (91%)	223 (6%)	104 (3%)	4	32
1	E	3496/5037 (69%)	3169 (91%)	223 (6%)	104 (3%)	4	32
1	G	3496/5037 (69%)	3169 (91%)	226 (6%)	101 (3%)	4	32
2	B	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	15	54
2	D	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	15	54
2	F	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	15	54
2	H	105/108 (97%)	89 (85%)	15 (14%)	1 (1%)	15	54
All	All	14404/20580 (70%)	13045 (91%)	943 (6%)	416 (3%)	7	32

5 of 416 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	689	THR
1	A	720	HIS
1	A	806	PRO

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Mol	Chain	Res	Type
1	A	916	PRO
1	A	1253	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	2500/4276 (58%)	2486 (99%)	14 (1%)	86	92
1	C	2501/4276 (58%)	2487 (99%)	14 (1%)	86	92
1	E	2502/4276 (58%)	2486 (99%)	16 (1%)	86	92
1	G	2501/4276 (58%)	2482 (99%)	19 (1%)	81	89
2	B	89/90 (99%)	89 (100%)	0	100	100
2	D	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10360/17464 (59%)	10297 (99%)	63 (1%)	86	92

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	806	PRO
1	G	1513	ASP
1	E	979	PRO
1	G	1055	PRO
1	G	3926	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	203	ASN
1	G	3699	HIS
1	G	465	GLN

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Mol	Chain	Res	Type
1	G	1631	GLN
1	G	5031	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.

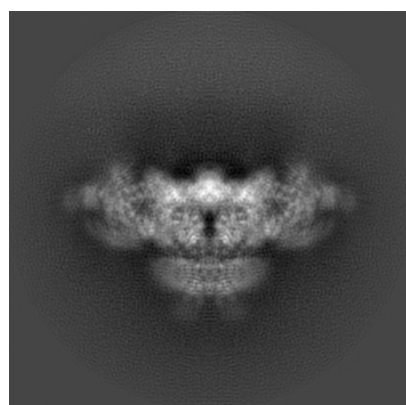
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9520. These allow visual inspection of the internal detail of the map and identification of artifacts.

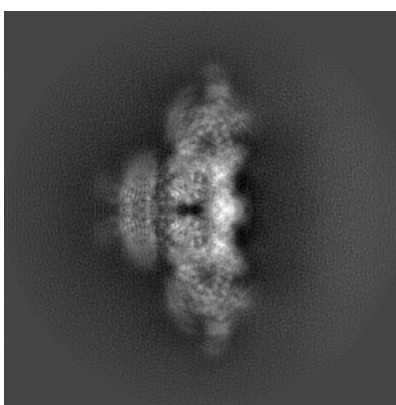
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

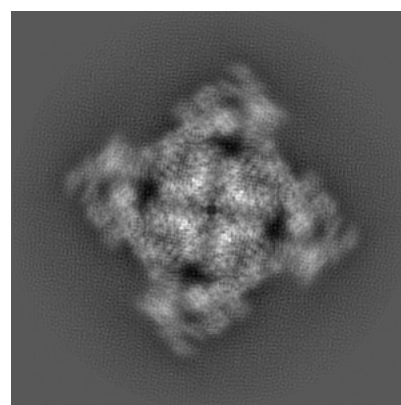
6.1.1 Primary map



X



Y

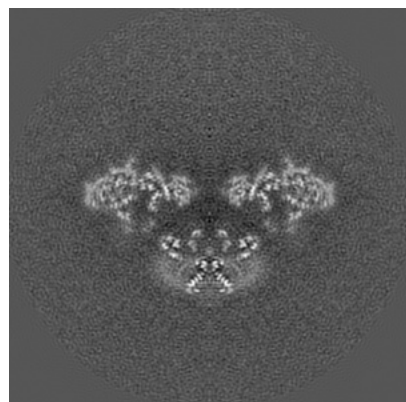


Z

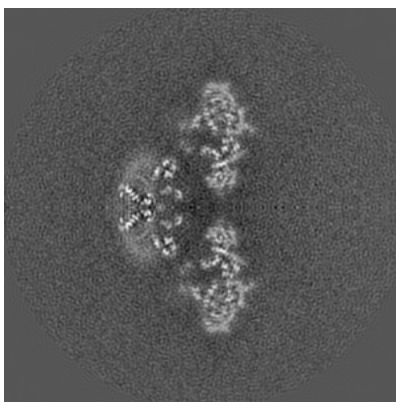
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

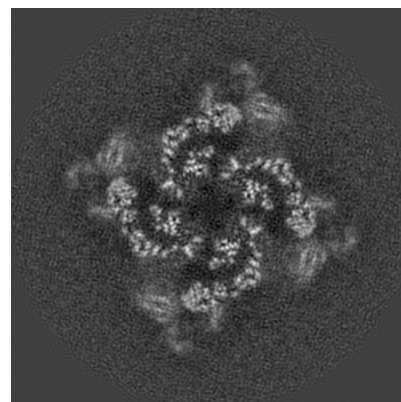
6.2.1 Primary map



X Index: 180



Y Index: 180

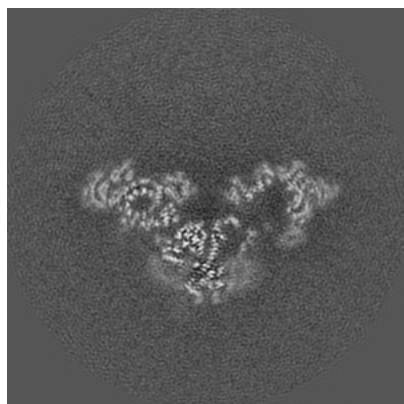


Z Index: 180

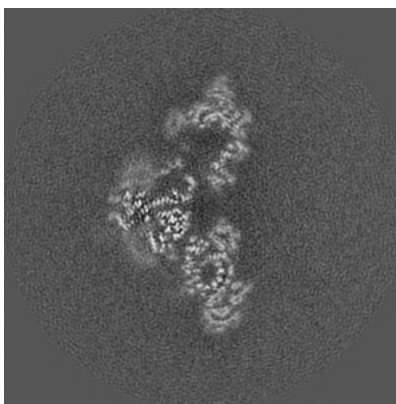
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

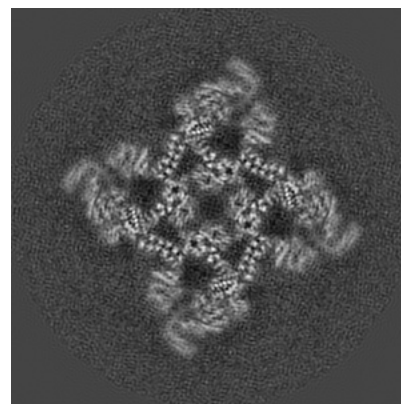
6.3.1 Primary map



X Index: 187



Y Index: 173



Z Index: 191

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 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

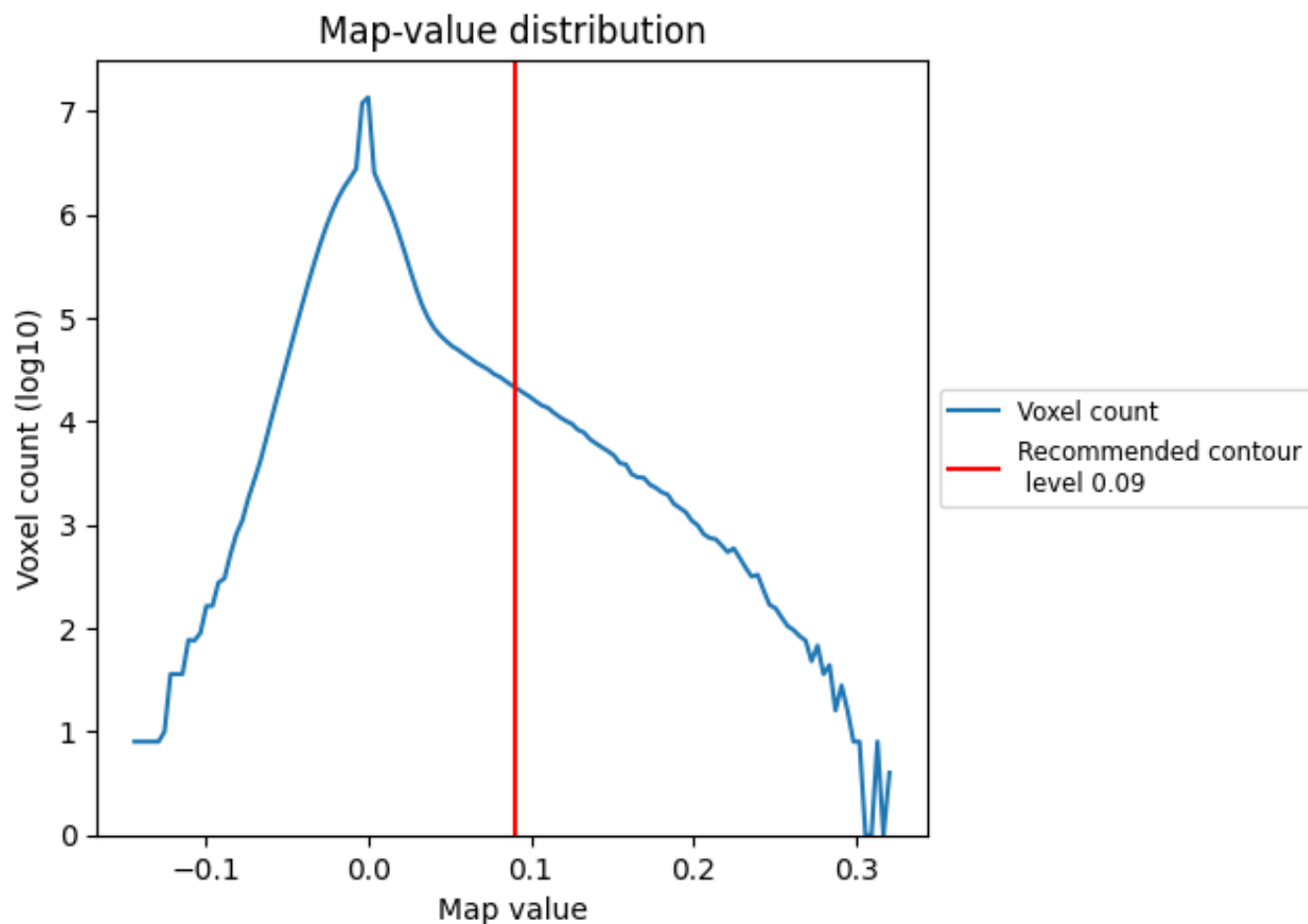
6.5 Mask visualisation

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

7 Map analysis [i](#)

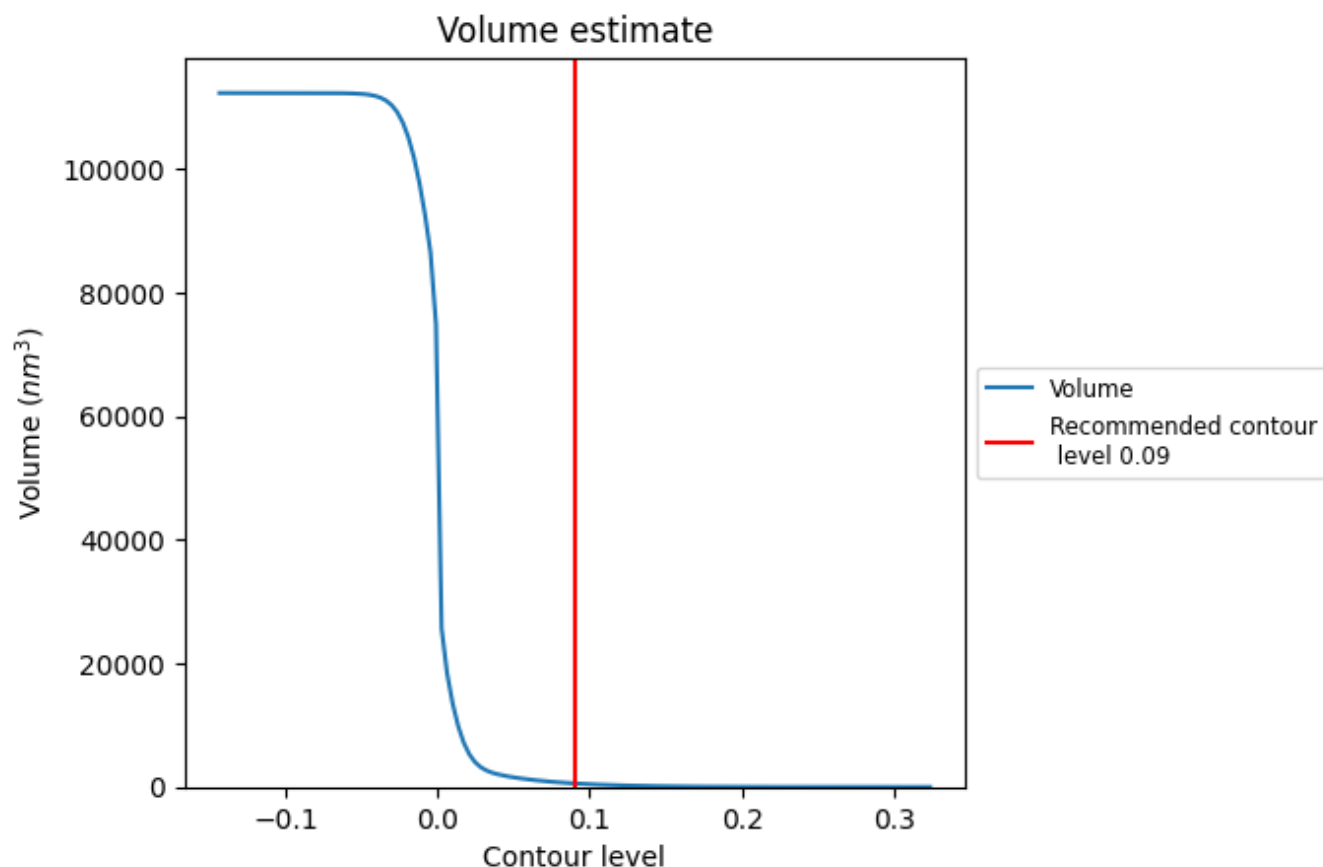
This section contains the results of statistical analysis of the map.

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.

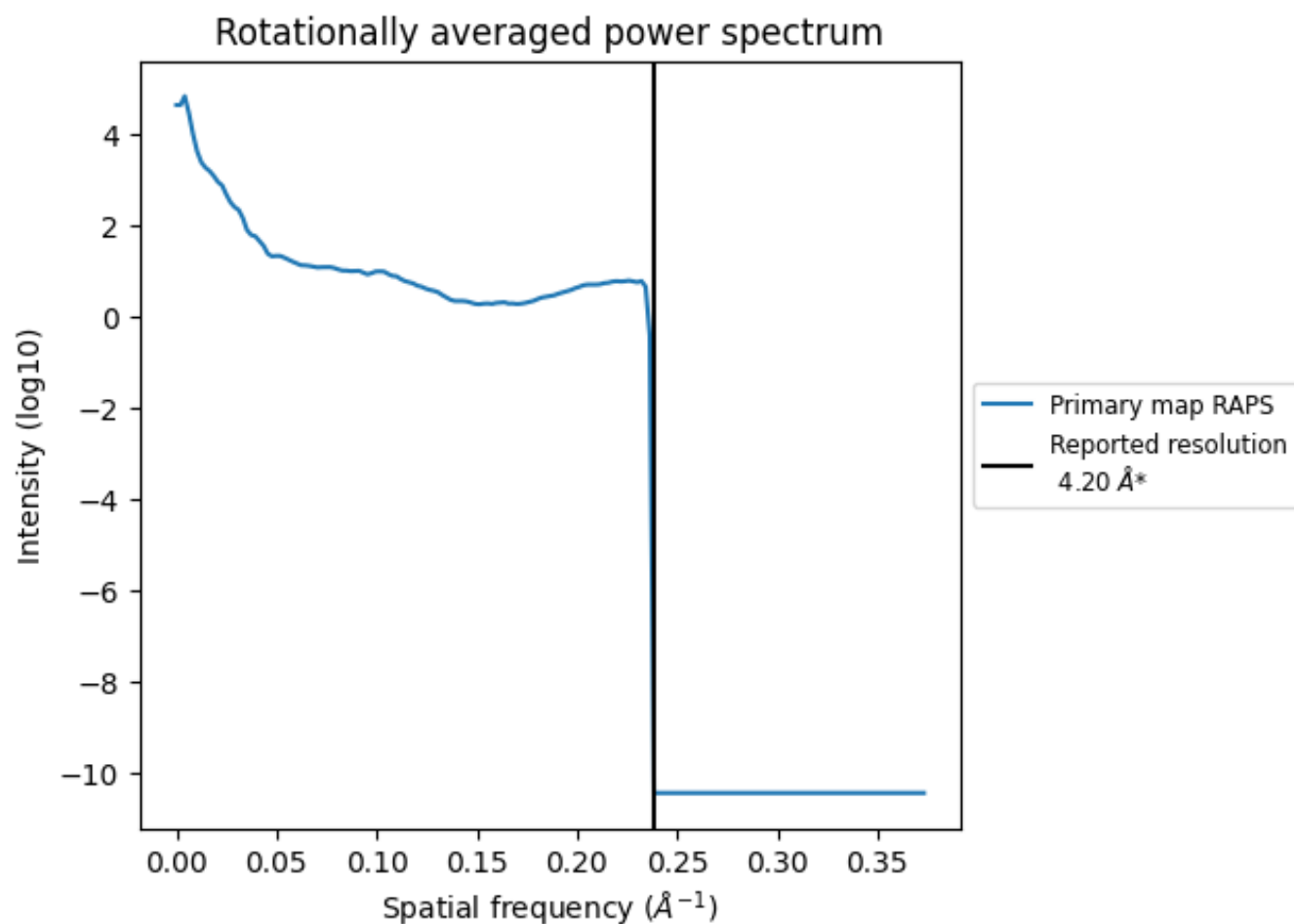
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 572 nm³; this corresponds to an approximate mass of 517 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 0.238 Å⁻¹

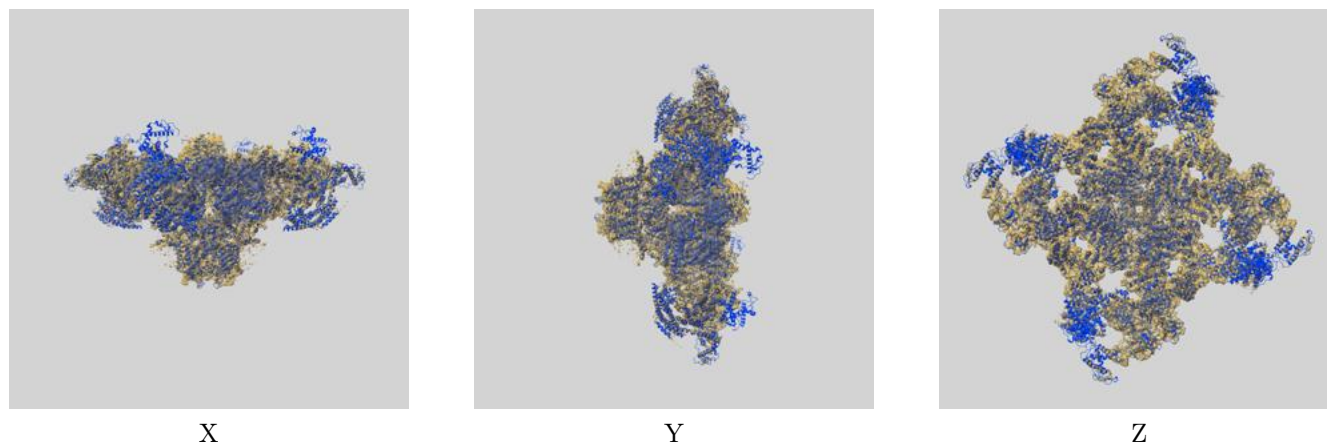
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

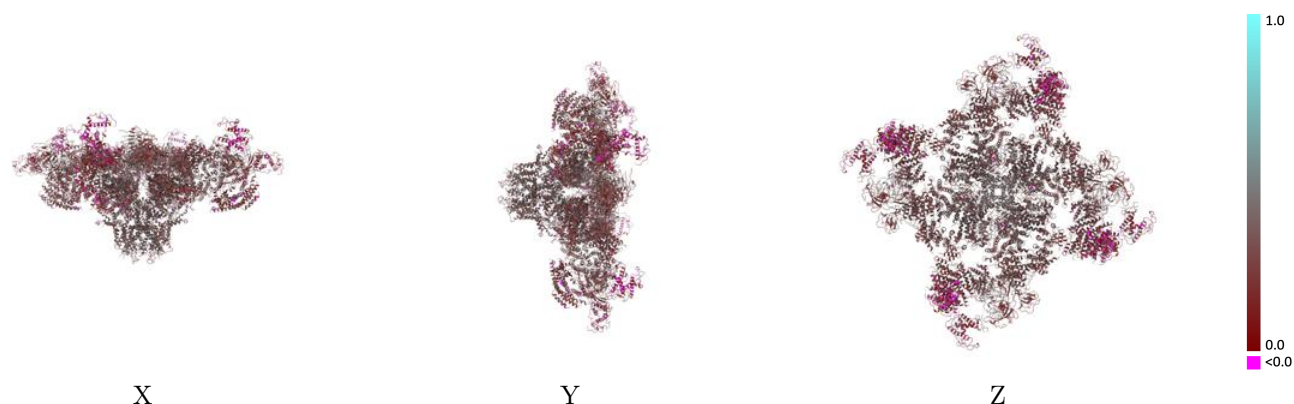
This section contains information regarding the fit between EMDB map EMD-9520 and PDB model 5GL0. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



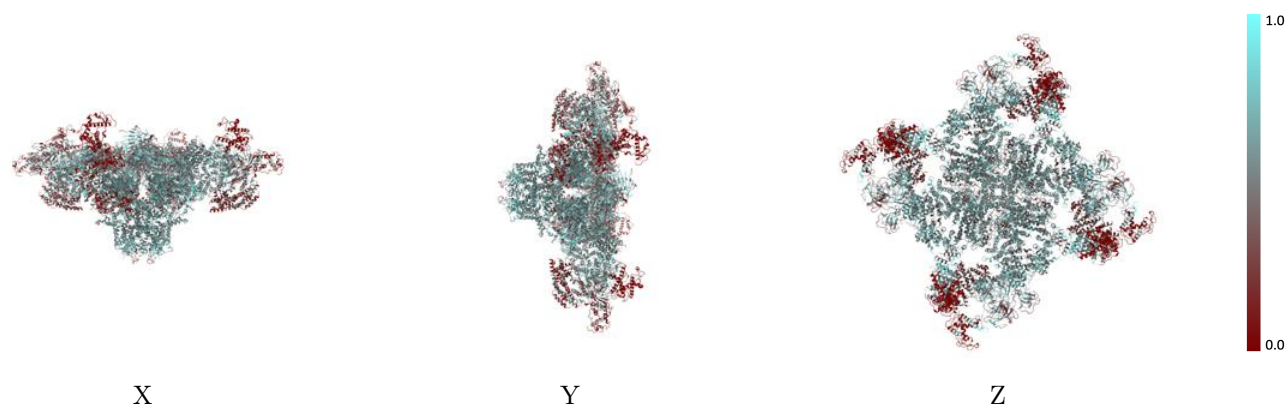
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



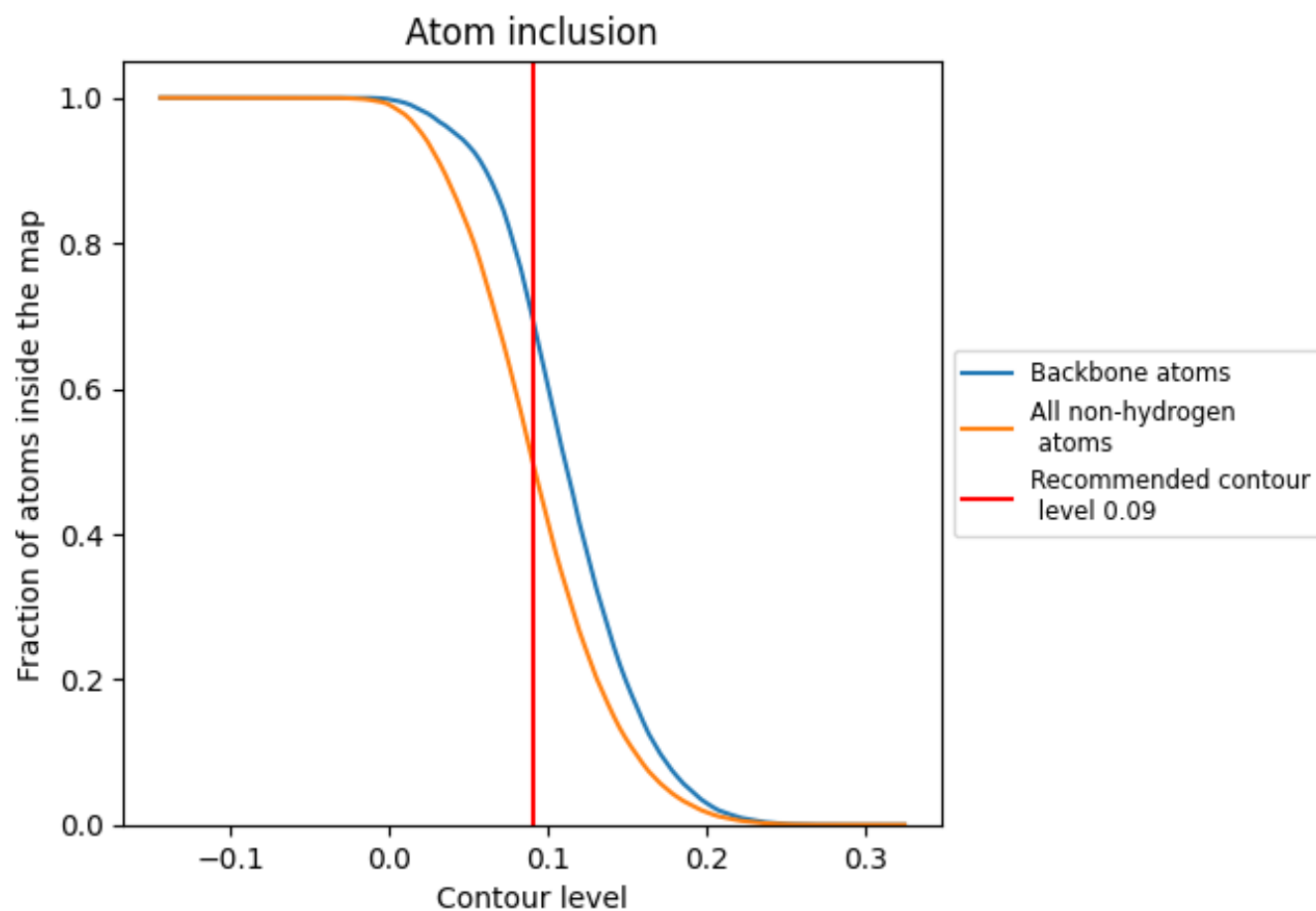
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 50% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.5020	<div><div></div></div> 0.3090
A	<div><div></div></div> 0.5028	<div><div></div></div> 0.3090
B	<div><div></div></div> 0.4669	<div><div></div></div> 0.3060
C	<div><div></div></div> 0.5024	<div><div></div></div> 0.3090
D	<div><div></div></div> 0.4669	<div><div></div></div> 0.3070
E	<div><div></div></div> 0.5027	<div><div></div></div> 0.3090
F	<div><div></div></div> 0.4657	<div><div></div></div> 0.3010
G	<div><div></div></div> 0.5042	<div><div></div></div> 0.3100
H	<div><div></div></div> 0.4706	<div><div></div></div> 0.3070

1.0

0.0

<0.0