



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 05:00 AM EST

PDB ID : 8SEQ
EMDB ID : EMD-40425
Title : Cryo-EM Structure of RyR1 + AMP
Authors : Cholak, S.; Saville, J.W.; Zhu, X.; Berezuk, A.M.; Tuttle, K.S.; Haji-Ghassemi, O.; Van Petegem, F.; Subramaniam, S.
Deposited on : 2023-04-10
Resolution : 3.40 Å(reported)

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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

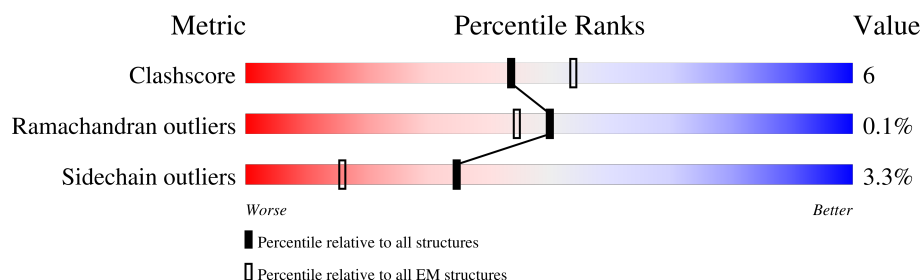
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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>18%</div> <div>70%</div> <div>16%</div> <div>13%</div> </div>
1	B	5037	<div> <div>18%</div> <div>70%</div> <div>16%</div> <div>13%</div> </div>
1	C	5037	<div> <div>18%</div> <div>70%</div> <div>17%</div> <div>13%</div> </div>
1	D	5037	<div> <div>18%</div> <div>70%</div> <div>16%</div> <div>13%</div> </div>
2	E	350	<div> <div>26%</div> <div>69%</div> </div>
2	F	350	<div> <div>26%</div> <div>69%</div> </div>
2	G	350	<div> <div>26%</div> <div>69%</div> </div>
2	H	350	<div> <div>26%</div> <div>69%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 142952 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	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	B	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	C	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		
1	D	4376	Total	C	N	O	S	9	0
			34896	22197	6022	6441	236		

- Molecule 2 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-242	MET	-	expression tag	UNP P08515
E	-241	LYS	-	expression tag	UNP P08515
E	-240	SER	-	expression tag	UNP P08515
E	-239	SER	-	expression tag	UNP P08515
E	-238	HIS	-	expression tag	UNP P08515
E	-237	HIS	-	expression tag	UNP P08515
E	-236	HIS	-	expression tag	UNP P08515
E	-235	HIS	-	expression tag	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-234	HIS	-	expression tag	UNP P08515
E	-233	HIS	-	expression tag	UNP P08515
E	-232	GLY	-	expression tag	UNP P08515
E	-231	SER	-	expression tag	UNP P08515
E	-230	SER	-	expression tag	UNP P08515
E	-11	GLY	-	linker	UNP P08515
E	-10	ILE	-	linker	UNP P08515
E	-9	GLU	-	linker	UNP P08515
E	-8	GLU	-	linker	UNP P08515
E	-7	ASN	-	linker	UNP P08515
E	-6	LEU	-	linker	UNP P08515
E	-5	TYR	-	linker	UNP P08515
E	-4	PHE	-	linker	UNP P08515
E	-3	GLN	-	linker	UNP P08515
E	-2	SER	-	linker	UNP P08515
E	-1	ASN	-	linker	UNP P08515
E	0	ALA	-	linker	UNP P08515
F	-242	MET	-	expression tag	UNP P08515
F	-241	LYS	-	expression tag	UNP P08515
F	-240	SER	-	expression tag	UNP P08515
F	-239	SER	-	expression tag	UNP P08515
F	-238	HIS	-	expression tag	UNP P08515
F	-237	HIS	-	expression tag	UNP P08515
F	-236	HIS	-	expression tag	UNP P08515
F	-235	HIS	-	expression tag	UNP P08515
F	-234	HIS	-	expression tag	UNP P08515
F	-233	HIS	-	expression tag	UNP P08515
F	-232	GLY	-	expression tag	UNP P08515
F	-231	SER	-	expression tag	UNP P08515
F	-230	SER	-	expression tag	UNP P08515
F	-11	GLY	-	linker	UNP P08515
F	-10	ILE	-	linker	UNP P08515
F	-9	GLU	-	linker	UNP P08515
F	-8	GLU	-	linker	UNP P08515
F	-7	ASN	-	linker	UNP P08515
F	-6	LEU	-	linker	UNP P08515
F	-5	TYR	-	linker	UNP P08515
F	-4	PHE	-	linker	UNP P08515
F	-3	GLN	-	linker	UNP P08515
F	-2	SER	-	linker	UNP P08515
F	-1	ASN	-	linker	UNP P08515
F	0	ALA	-	linker	UNP P08515

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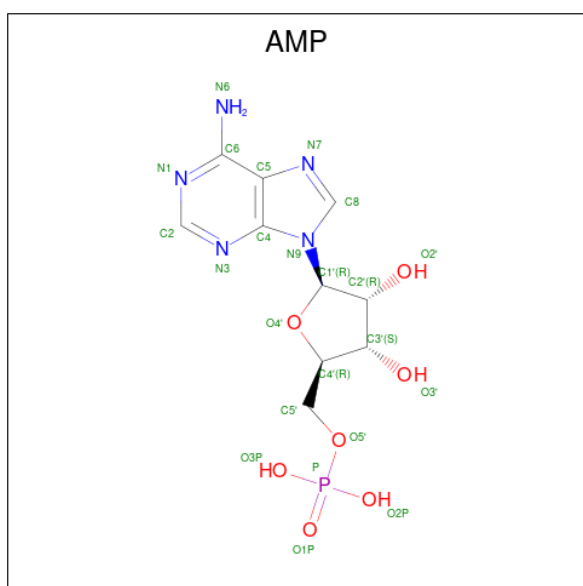
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression tag	UNP P08515
G	-235	HIS	-	expression tag	UNP P08515
G	-234	HIS	-	expression tag	UNP P08515
G	-233	HIS	-	expression tag	UNP P08515
G	-232	GLY	-	expression tag	UNP P08515
G	-231	SER	-	expression tag	UNP P08515
G	-230	SER	-	expression tag	UNP P08515
G	-11	GLY	-	linker	UNP P08515
G	-10	ILE	-	linker	UNP P08515
G	-9	GLU	-	linker	UNP P08515
G	-8	GLU	-	linker	UNP P08515
G	-7	ASN	-	linker	UNP P08515
G	-6	LEU	-	linker	UNP P08515
G	-5	TYR	-	linker	UNP P08515
G	-4	PHE	-	linker	UNP P08515
G	-3	GLN	-	linker	UNP P08515
G	-2	SER	-	linker	UNP P08515
G	-1	ASN	-	linker	UNP P08515
G	0	ALA	-	linker	UNP P08515
H	-242	MET	-	expression tag	UNP P08515
H	-241	LYS	-	expression tag	UNP P08515
H	-240	SER	-	expression tag	UNP P08515
H	-239	SER	-	expression tag	UNP P08515
H	-238	HIS	-	expression tag	UNP P08515
H	-237	HIS	-	expression tag	UNP P08515
H	-236	HIS	-	expression tag	UNP P08515
H	-235	HIS	-	expression tag	UNP P08515
H	-234	HIS	-	expression tag	UNP P08515
H	-233	HIS	-	expression tag	UNP P08515
H	-232	GLY	-	expression tag	UNP P08515
H	-231	SER	-	expression tag	UNP P08515
H	-230	SER	-	expression tag	UNP P08515
H	-11	GLY	-	linker	UNP P08515
H	-10	ILE	-	linker	UNP P08515
H	-9	GLU	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	SER	-	linker	UNP P08515
H	-1	ASN	-	linker	UNP P08515
H	0	ALA	-	linker	UNP P08515

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
3	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

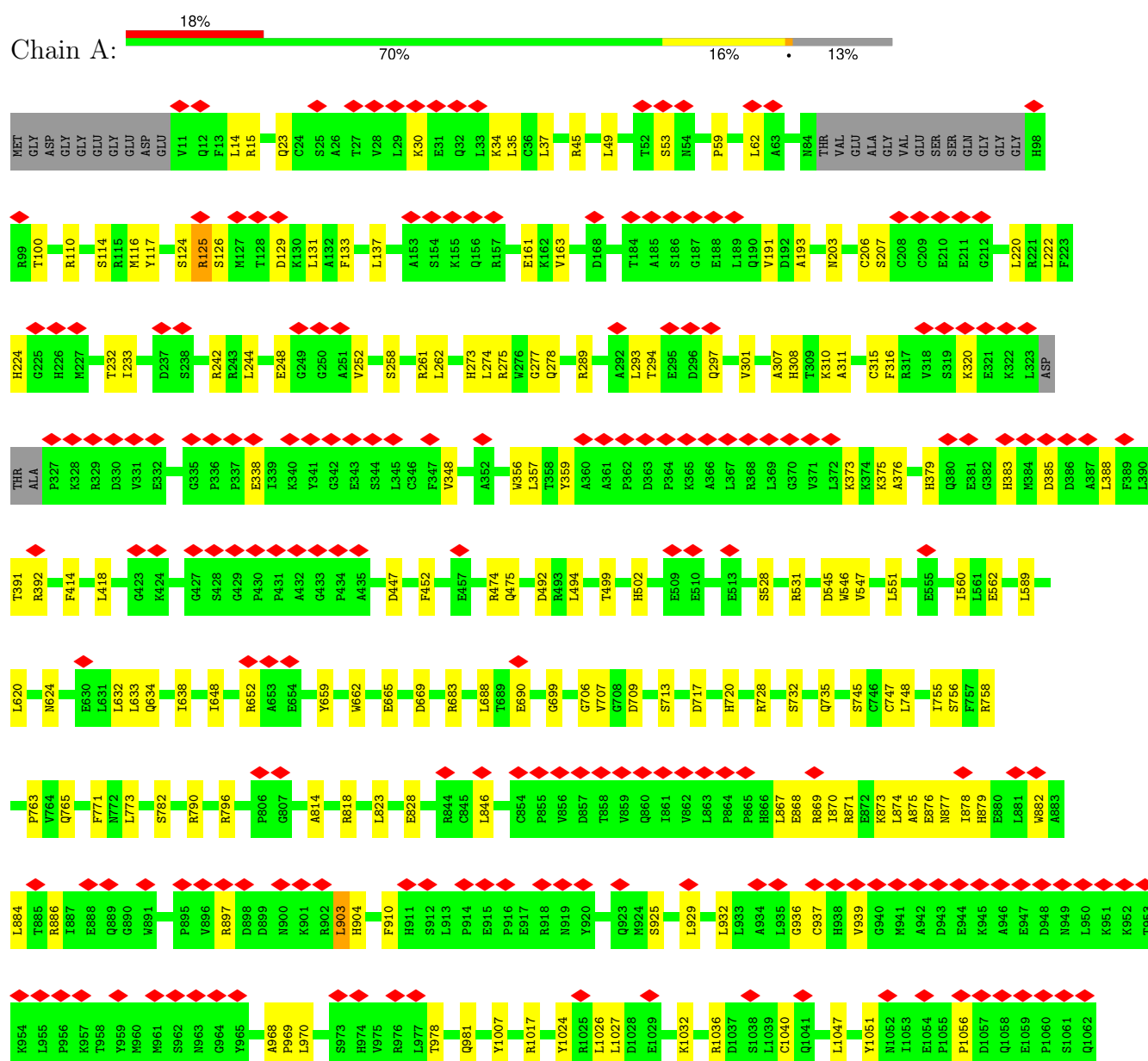
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

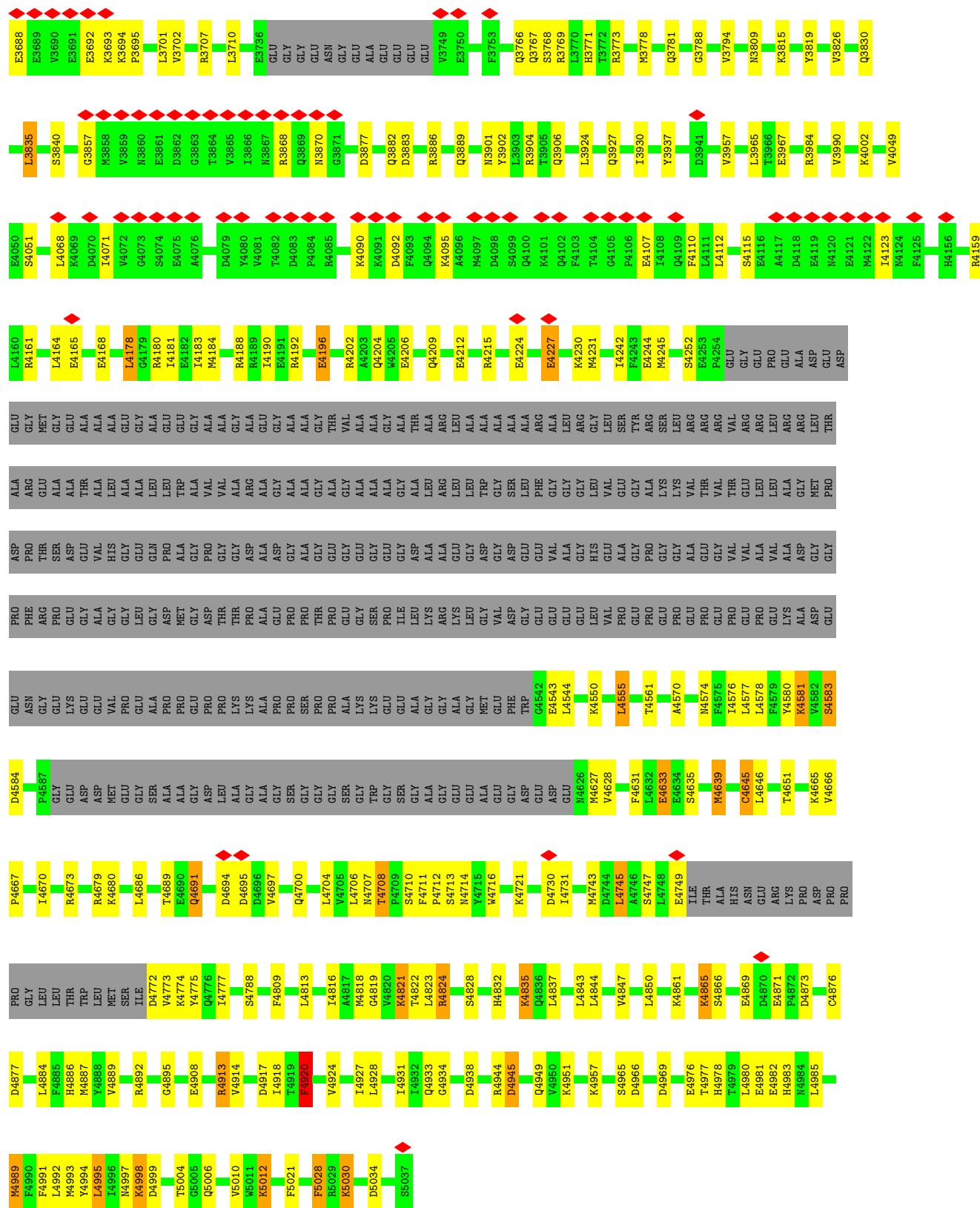
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





V3593	N3523	V3459	G3363	E3290	Y3213	R3111	T3020	L2927	L2867	W2807	I2747	K2662
R3594	M3524	V3460	R3366	A3291	N3214	L3112	P3021	K2928	S2868	P2808	P2748	N2663
R3595	Q3530	Q3461	R3367	P3292	A3215	G3113	A3022	F2929	R2869	T2809	E2749	V2666
S3600	D3531	E3463	R3368	P3293	C3216	V3114	K3023	L2930	E2870	K2810	K2750	T2667
A3601		T3464	V3373	P3294	S3217	V3115	V3024	Q2931	L2871	E2811	L2751	S2668
V3603	M3534	N3465	E3376	L3296	Y3219	GLN	V3024	M2932	Q2872	S2812	D2752	E2669
H3605	L3535	N3466	E3377	P3297	T3220	ALA	L3026	N2933	A2873	L2813	L2753	E2670
L3606	A3536	N3467	Q3378	A3298	T3221	ARG	G3026	Q2934	M2874	K2814	F2754	E2671
L3607	K3537	S3468	L3379	G3299	K3222	THR	S3027	G2936	A2875	L2815	I2755	L2672
Q3608	T3538	F3469	R3380	A3300	S3223	VAL	G3028	A2936	E2876	M2816	T2756	H2673
R3539	R3539	R3470	R3381	P3301	P3224	K3123	G3029	V2937	Q2877	L2817	K2757	L2674
A3540	Y3540	T3471	L3382	P3302	R3225	G3124		T2938	L2878	A2818	F2758	L2678
T3609	A3541	A3472	E3383	P3303	E3226	N3128	E3037	GLY	A2879	W2819	E2759	L2682
E3610	D3473	D3473	E3382	C3304	R3227		M3038	LEU	E2880	E2820	E2760	S2685
H3611	S3474	A3472	K3384	T3305	R3228	V3134	L3042	LYS	M2881	W2821	Y2761	S2686
P3612	K3475	A3474	A3385	T3306	L3229	A3135	L3046	ASP	Y2882	T2822	T2762	A2687
V3613	E3386	S3476	E3386	A3306	L3230	L3136	A3047	MET	H2883	L2823	H2763	K2689
K3614	A3387	A3477	A3387	S3309	G3231	H3146	A3048	D2946	T2885	K2825	E2764	K2690
S3615	E3388	K3477	E3388	L3316	L3232	Q3149	R3051	L2947	V2886	A2826	K2765	K2691
R3616	E3389	K3478	E3389	G3317	P3233	H3150	H3052	T2948	G2887	R2827	A2767	Y2691
K3617	G3390	A3479	E3391	N3318	N3234	Q3151	R3053	E2952	K2888	E2828	F2768	Q2693
A3618	E3391	L3392	L3392	T3319	S3235				K2889	G2829	D2769	E2694
V3619	L3392	L3320	L3320	R3321	V3236	D3154	G3058	G2958	K2890	E2830	K2770	L2695
W3620	L3392	L3320	L3320	R3321	V3236	D3155	T3059	F2959	K2891	GLU	I2771	V2715
H3621	L3392	L3320	L3320	R3321	V3236	D3156	T3059	L2960	Q2772	GLU	Q2772	S2718
K3622	L3392	L3320	L3320	R3321	V3236	D3157	T3059	Q2961	THR	ARG	N2773	L2719
L3623	L3392	L3320	L3320	R3321	V3236	D3158	T3059	Q2962	THR	THR	N2774	S2720
L3624	L3392	L3320	L3320	R3321	V3236	D3159	T3059	L2963	THR	GLU	W2775	S2721
S3625	L3392	L3320	L3320	R3321	V3236	D3160	T3059	W2966	THR	LYS	S2776	S2722
K3626	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	LYS	Y2777	K2722
ASP	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	ARG	E2778	A2723
K3627	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	ILE	E2779	E2724
V3632	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	THR	N2780	K2725
V3633	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLN	V2781	LYS
A3634	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	ALA	D2782	ALA
C3635	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	ALA	E2783	VAL
F3636	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLN	E2784	ASP
K3637	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	THR	L2785	ALA
K3638	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	TVR	K2786	GLU
R3648	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	PRO	T2787	GLY
M3652	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	ARG	W2788	W2734
K3659	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLU	H2788	F2735
T3662	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	P2789	D2736
L3663	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	M2790	F2737
G3681	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	L2791	R2738
E3682	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	R2792	P2739
Q3683	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	P2793	V2740
Q3684	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	E2741	E2741
E3685	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	T2742	T2742
E3686	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	K2795	L2743
E3687	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	F2797	W2744
E3688	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	S2798	V2745
E3689	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	E2799	K2800
E3690	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	D2801	K2802
K3691	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	E2803	E2803
L3692	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	Q2924	Q2924
E3687	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	E2925	E2925
E3687	L3392	L3320	L3320	R3321	V3236	D3160	T3059		THR	GLY	L2926	L2926



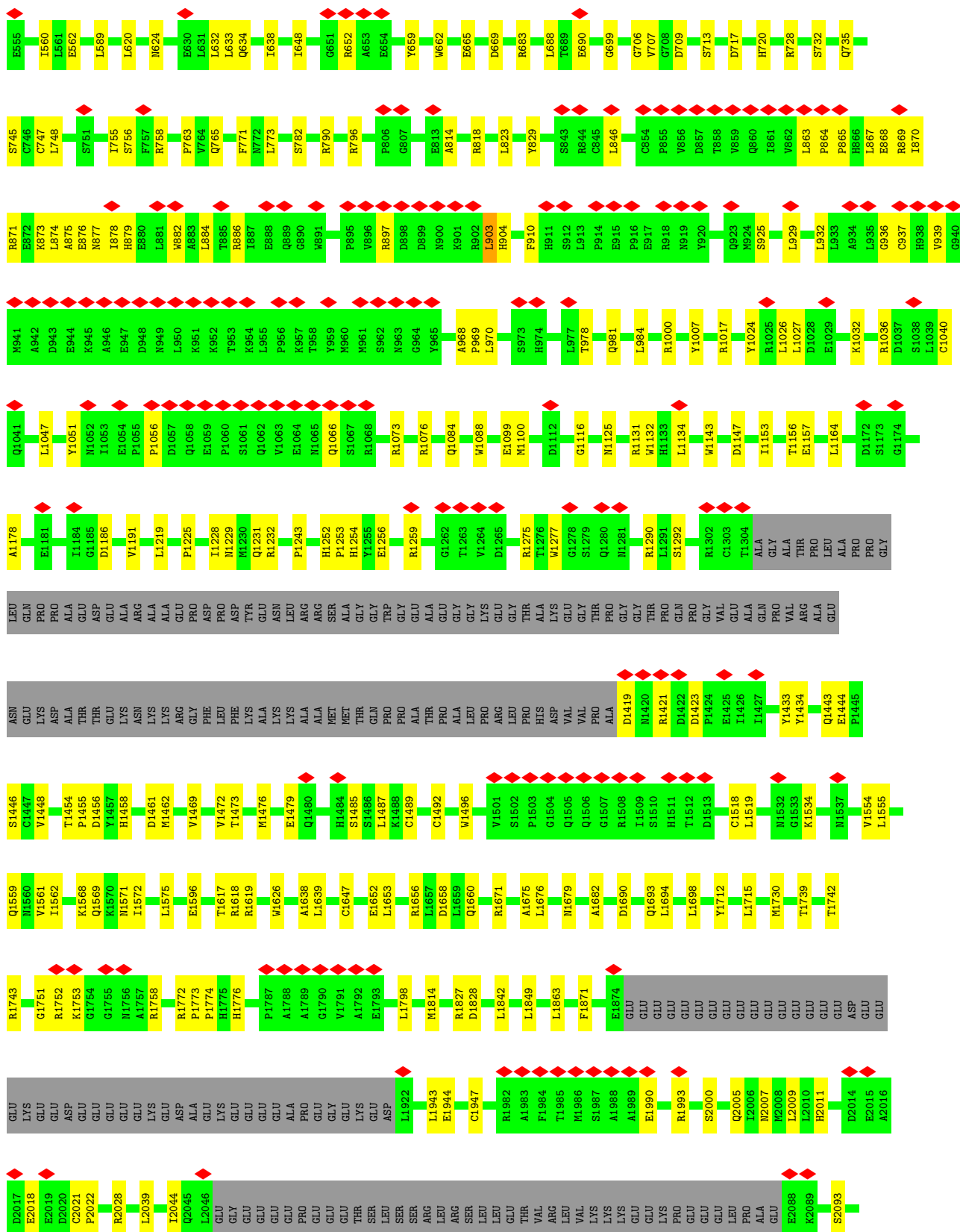
- Molecule 1: Ryanodine receptor 1

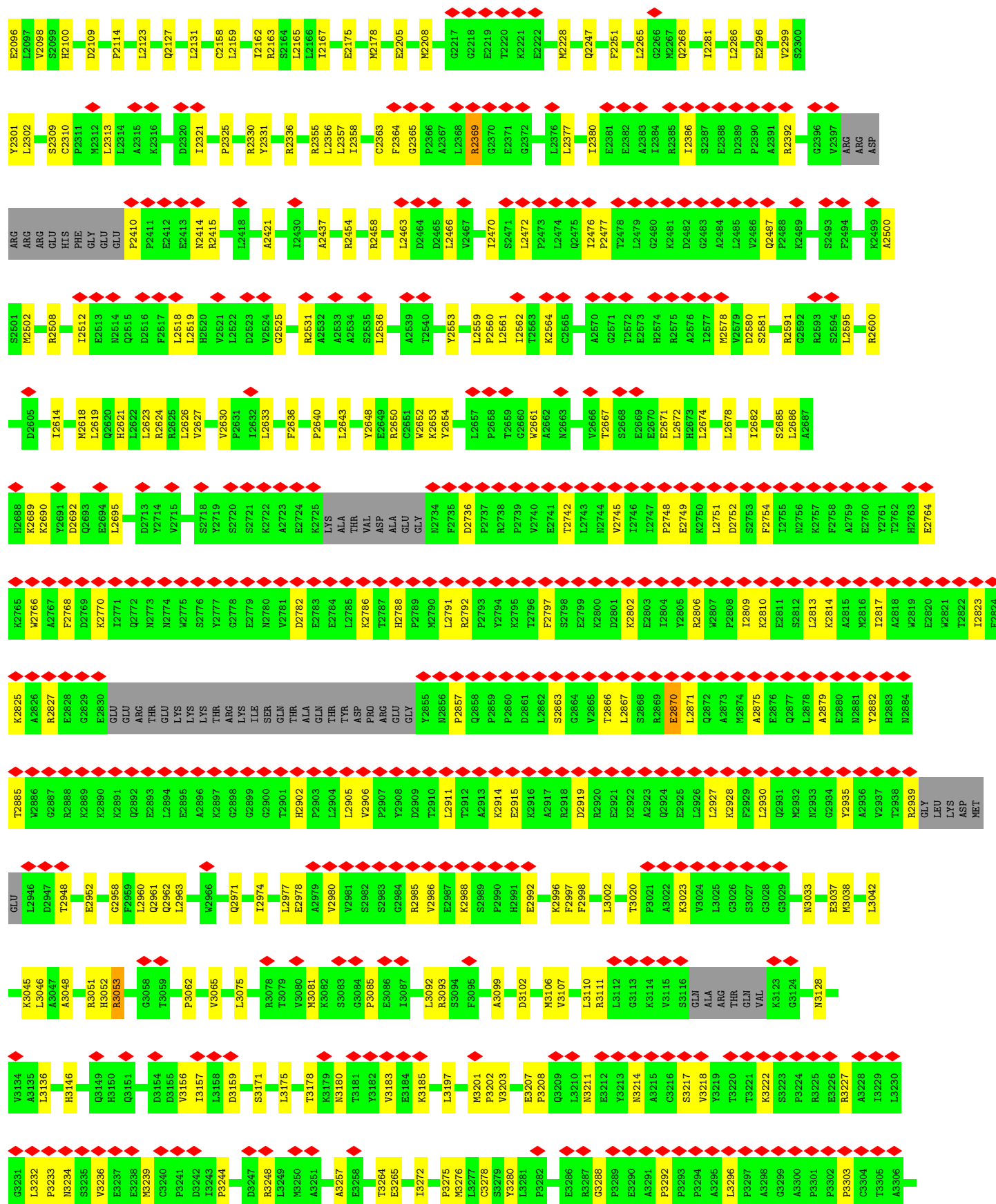




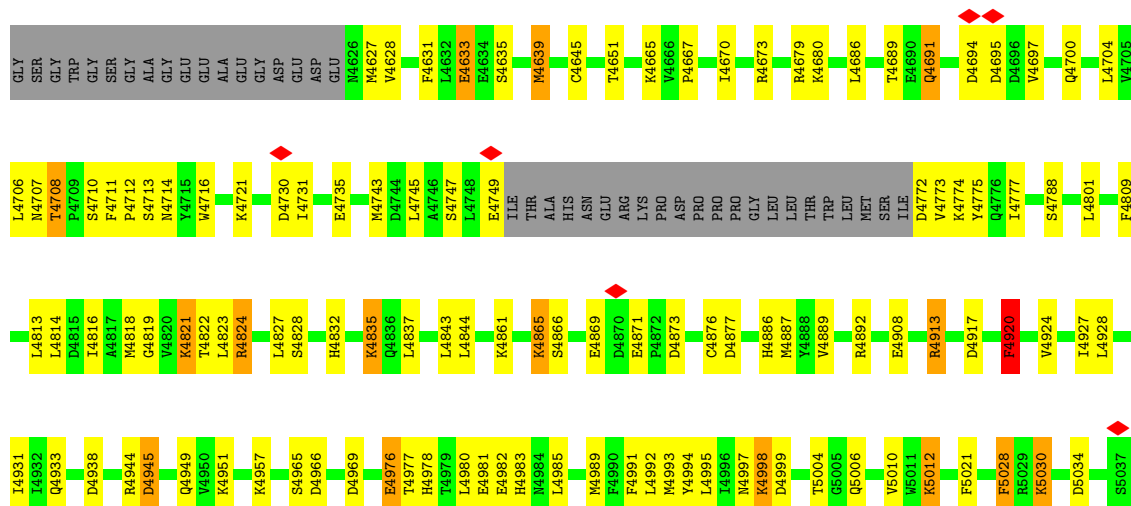


WORLDWIDE
PDB
PROTEIN DATA BANK

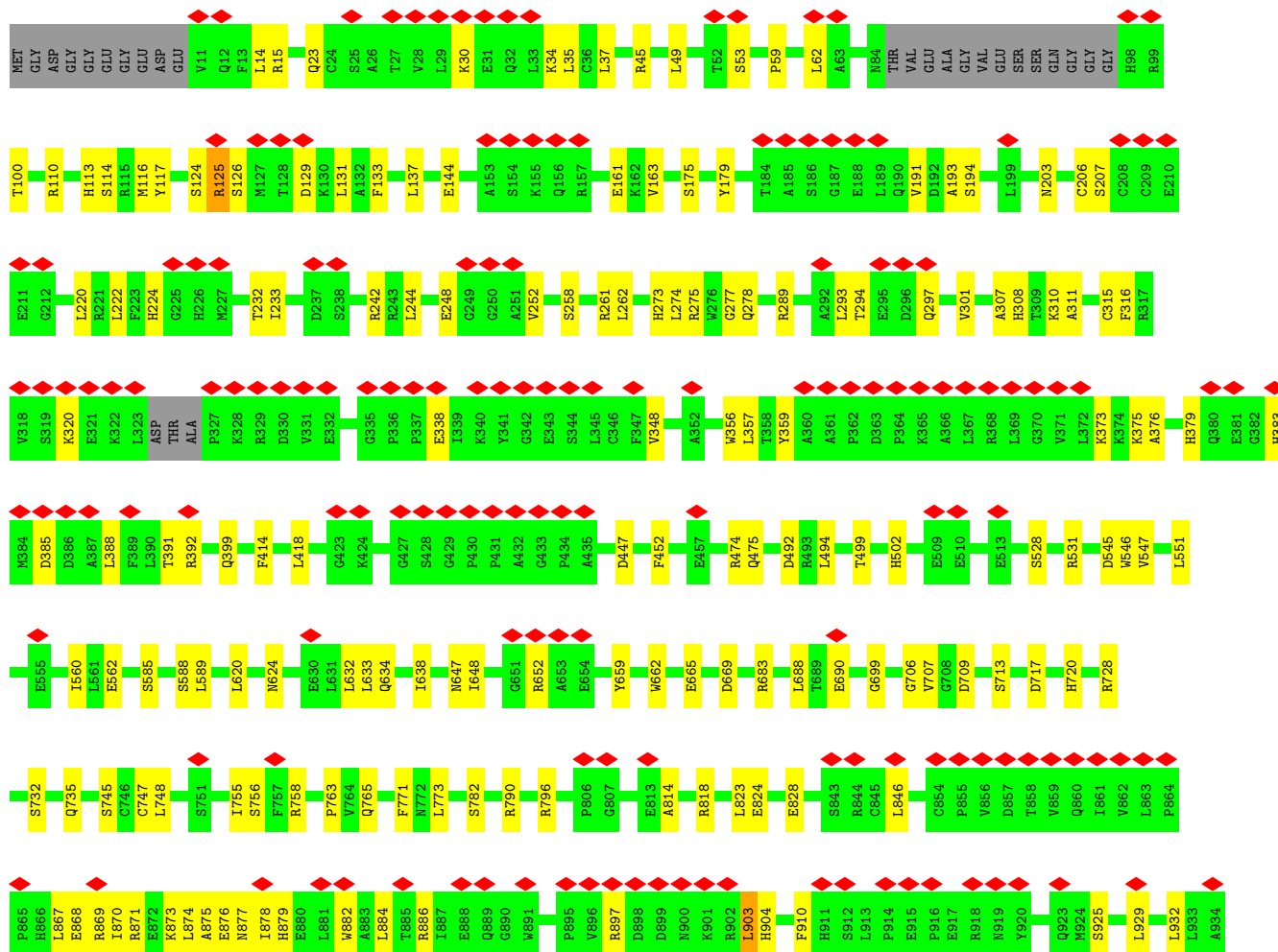








• Molecule 1: Ryanodine receptor 1



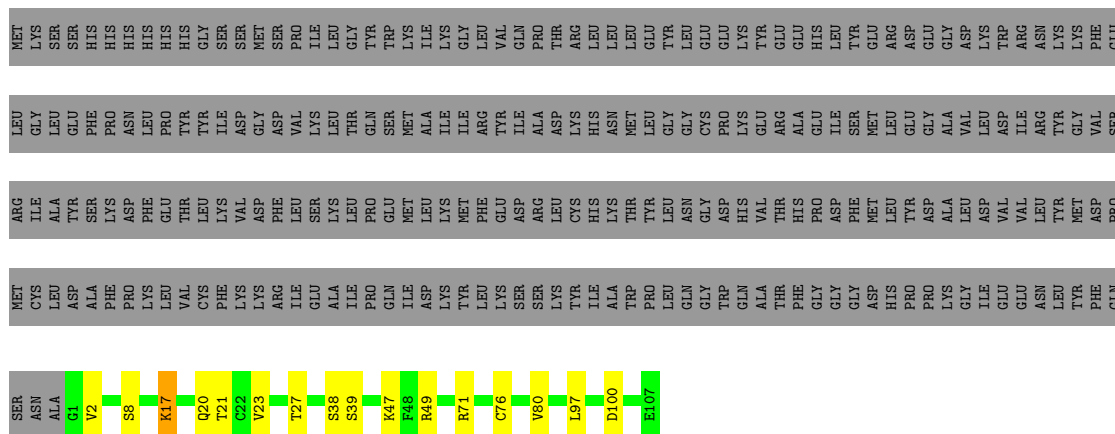


SER	R3403	V3324	M3239	H3150	H3052	G2958	K2881	GLU	L2710	L3623	M2514
ASP	D3404	N3325	C3240	Q3151	R3053	F2959	Q2882	GLU	P2711	R2624	Q2515
GLN	I3413	N3326	P3241	D3154	G3058	L2960	E2883	ARG	P2712	R2625	D2516
ARG	R3414	G3327	D3242	D3155	T3059	Q2961	L2884	THR	L2626	V2627	F2517
THR	D3417	I3328	I3243	V3156	P3062	Q2962	E2885	LYS	V2715	L2518	L2518
LYS	D3418	D3330	P3244	T3157	V3065	L2963	A2886	LYS	V2630	P2631	V2521
LYS	N3419	E3331	D3247	L3158	L3075	V2966	K2887	THR	F2631	L2522	L2522
R3498	R3420	A3332	R3248	D3159	L3076	I2974	G2888	ARG	L2633	D2523	D2523
R3499	A3421	T3333	L3249	S3171	R3078	L2977	G2889	LYS	F2636	V2524	V2524
G3500	H3422	M3334	M3250	S3172	V3080	E2978	G2900	ILE	P2640	G2525	G2525
D3501	W3423	K3335	A3251	L3175	K3081	A2979	T2901	GLN	L2643	R2531	R2531
R3498	L3424	R3337	A3257	T3178	V3082	V2980	P2903	ALA	E2724	A2532	A2532
R3499	E3426	E3258	E3258	K3179	K3082	V2981	L2904	GLN	K2725	A2533	A2533
G3500	V3340	T3264	T3264	N3180	S3083	S2982	L2905	TYR	E2784	A2534	A2534
V3505	A3342	E3265	E3265	T3181	G3084	S2983	V2906	ASP	L2785	S2535	S2535
Q3506	A3342	I3272	I3272	V3182	P3085	Q2984	P2907	PRO	K2786	L2536	L2536
S3508	Q3343	P3275	P3275	V3183	E3086	Q2984	V2908	ARG	W2652	A2539	A2539
L3509	P3344	M3276	M3276	E3184	I3087	R2985	D2909	GLU	K2653	T2540	T2540
L3510	I3345	L3277	L3277	K3185	L3092	V2986	T2910	GLY	Y2654	Y2553	Y2553
V3511	V3346	C3278	C3278	L3197	R3093	E2987	L2911	GLY	C2655	C2553	C2553
A3512	S3347	P3282	P3282	K3201	S3094	K2988	T2912	N2734	L2657	L2559	L2559
T3513	R3348	E3286	E3286	P3202	F3095	S2989	A2913	D2736	P2658	P2560	P2560
L3514	P3351	R3287	R3287	V3203	A3099	P2990	K2914	P2737	T2659	L2561	L2561
K3515	I3359	G3288	G3288	P3208	D3102	H2991	E2915	K2795	W2661	T2562	T2562
P3519	V3459	E3288	E3288	P3208	D3102	E2992	K2916	T2796	A2662	T2563	T2563
N3523	F3459	R3287	R3287	Q3209	M3106	K2996	A2917	F2797	K2564	K2564	K2564
K3524	V3460	G3288	G3288	N3210	V3107	F2997	R2918	E2741	N2663	C2565	C2565
D3530	Q3461	E3289	E3289	E3212	L3110	L3002	D2919	T2742	V2666	V2666	V2666
D3531	E3463	A3291	A3291	E3212	R3111	H3013	E2921	L2743	T2667	T2667	T2667
I3464	I3464	P3292	P3292	V3213	L3112	L3002	K2922	N2744	S2668	S2668	S2668
N3465	N3465	P3293	P3293	N3214	G3113	T3020	K2922	V2745	E2670	E2670	E2670
N3466	N3466	P3294	P3294	A3215	G3113	P3021	A2923	L2746	L2671	L2671	L2671
M3467	M3467	A3295	A3295	C3216	K3114	P3021	Q2924	L2747	H2672	H2672	H2672
S3468	S3468	L3296	L3296	S3217	V3115	A3022	E2925	P2748	L2674	L2674	L2674
F3469	F3469	P3297	P3297	V3218	S3116	K3023	L2926	E2749	L2678	L2678	L2678
L3470	L3470	A3298	A3298	V3219	GLN	V3024	L2927	K2750	L2682	L2682	L2682
T3471	T3471	G3299	G3299	T3220	ALA	L3025	Q2872	L2751	T2682	T2682	T2682
A3472	A3472	A3300	A3300	T3221	ARG	L3025	A2875	D2752	S2685	S2685	S2685
D3473	D3473	P3301	P3301	K3222	THR	G3026	K2810	S2753	L2686	L2686	L2686
S3474	S3474	P3302	P3302	S3223	VAL	S3027	E2811	P2754	A2687	A2687	A2687
K3475	K3475	P3303	P3303	P3224	K3123	G3028	S2812	L2755	H2688	H2688	H2688
S3476	S3476	C3304	C3304	R3225	G3124	G3029	Q2877	L2756	K2689	K2689	K2689
K3477	K3477	T3305	T3305	E3226	G3124	G3029	L2878	K2757	K2690	K2690	K2690
M3478	M3478	A3306	A3306	R3227	N3128	N3033	A2879	P2758	Y2691	Y2691	Y2691
A3479	A3479	S3309	S3309	A3228	V3134	E3037	E2880	A2815	D2692	D2692	D2692
LYS	ALA	G3317	G3317	L3229	A3135	M3038	N2881	A2759	Q2693	Q2693	Q2693
GLY	GLY	L3316	L3316	L3230	L3136	L3042	Y2882	E2760	E2694	E2694	E2694
ASP	ASP	G3317	G3317	G3231	H3146	L3046	H2883	L2761	L2695	L2695	L2695
ALA	ALA	N3318	N3318	L3232	Q3149	A3047	N2884	Y2761	L2614	L2614	L2614
GLN	GLN	I3319	I3319	L3233	Q3149	A3048	A2818	E2768	L2619	L2619	L2619
SER	SER	L3320	L3320	N3234	Q3149	A3048	E2820	K2765	L2620	L2620	L2620
GLY	GLY	R3321	R3321	S3235	Q3149	R3051	W2886	W2766	H2621	H2621	H2621
GLY	GLY	I3322	I3322	V3236	Q3149	R3051	G2887	A2767	L2622	L2622	L2622
L3559	L3559	I3323	I3323	E3237	Q3149	R3051	K2889	D2769			
		E3238	E3238	E3238	E3238	E3238	E2824	K2770			
							K2825				
							A2826				
							R2827				
							G2829				
							E2830				



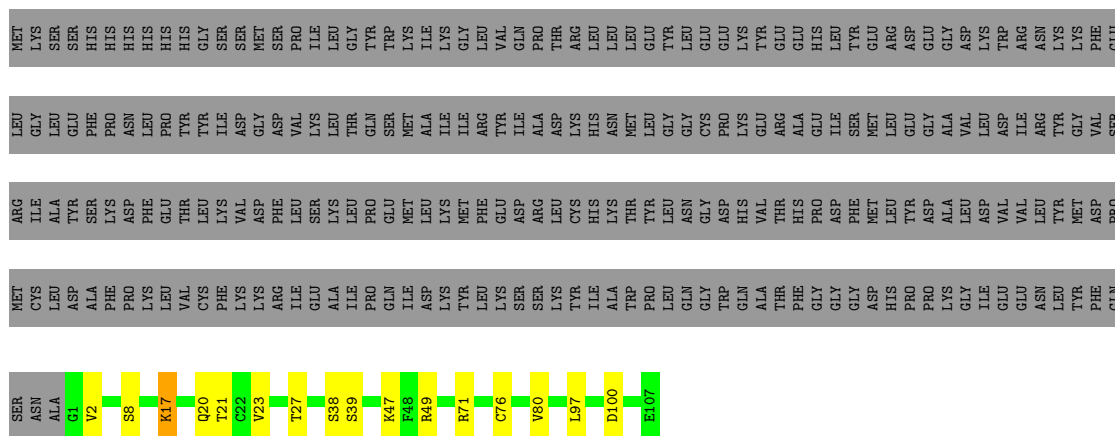
- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 26% 1% 69%



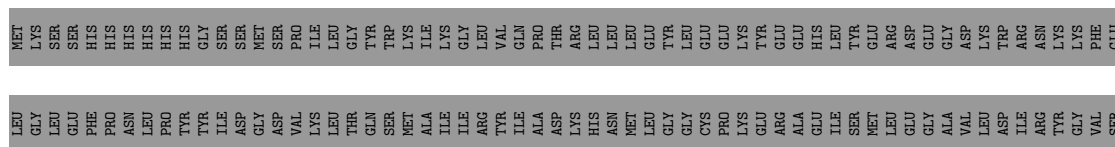
- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 26% 69%



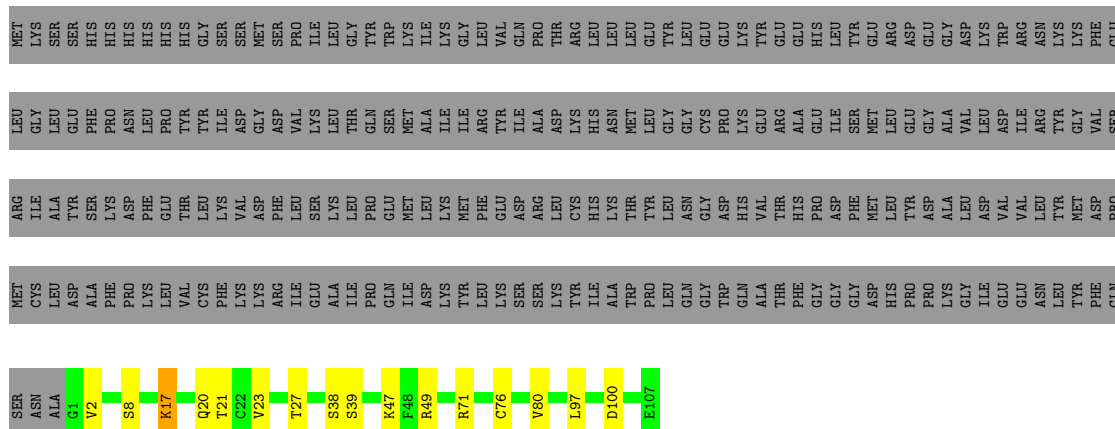
- Molecule 2: Glutathione S-transferase class-mu 26 kDa isozyme,Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 26% . 69%





- Chain H: 26% 1% 69%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133836	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.741	Depositor
Minimum map value	-0.326	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.288, 1.288, 1.288	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, AMP

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	0.34	0/35710	0.66	21/48359 (0.0%)
1	B	0.34	0/35710	0.66	21/48359 (0.0%)
1	C	0.34	0/35710	0.66	20/48359 (0.0%)
1	D	0.34	0/35710	0.66	20/48359 (0.0%)
2	E	0.31	0/834	0.64	0/1123
2	F	0.31	0/834	0.64	0/1123
2	G	0.31	0/834	0.64	0/1123
2	H	0.31	0/834	0.64	0/1123
All	All	0.34	0/146176	0.66	82/197928 (0.0%)

There are no bond length outliers.

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4945	ASP	CB-CG-OD1	10.69	127.92	118.30
1	C	4945	ASP	CB-CG-OD1	10.66	127.90	118.30
1	A	4945	ASP	CB-CG-OD1	10.58	127.82	118.30
1	D	4945	ASP	CB-CG-OD1	10.58	127.82	118.30
1	B	3417	ASP	CB-CG-OD1	8.19	125.67	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	34896	0	34522	451	0
1	B	34896	0	34522	440	0
1	C	34896	0	34522	448	0
1	D	34896	0	34522	451	0
2	E	818	0	824	8	0
2	F	818	0	824	8	0
2	G	818	0	824	8	0
2	H	818	0	824	8	0
3	A	23	0	12	1	0
3	B	23	0	12	1	0
3	C	23	0	12	1	0
3	D	23	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	142952	0	141432	1789	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 6.

The worst 5 of 1789 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:B:4242:ILE:HG12	1:B:4993:MET:HG2	1.71	0.73
1:A:4242:ILE:HG12	1:A:4993:MET:HG2	1.71	0.72
1:D:4242:ILE:HG12	1:D:4993:MET:HG2	1.71	0.72
1:C:4242:ILE:HG12	1:C:4993:MET:HG2	1.71	0.71
1:D:233:ILE:HD12	1:D:242:ARG:HB3	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	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48	78
1	B	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48	78
1	C	4353/5037 (86%)	4200 (96%)	148 (3%)	5 (0%)	48	78
1	D	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	48	78
2	E	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	F	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	G	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
2	H	105/350 (30%)	102 (97%)	3 (3%)	0	100	100
All	All	17832/21548 (83%)	17205 (96%)	607 (3%)	20 (0%)	50	78

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3692	GLU
1	A	4691	GLN
1	B	3692	GLU
1	B	4691	GLN
1	C	3692	GLU

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	3805/4276 (89%)	3675 (97%)	130 (3%)	32	57
1	B	3805/4276 (89%)	3675 (97%)	130 (3%)	32	57
1	C	3805/4276 (89%)	3674 (97%)	131 (3%)	32	57
1	D	3805/4276 (89%)	3674 (97%)	131 (3%)	32	57
2	E	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	F	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	G	88/304 (29%)	87 (99%)	1 (1%)	70	81
2	H	88/304 (29%)	87 (99%)	1 (1%)	70	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15572/18320 (85%)	15046 (97%)	526 (3%)	35 57

5 of 526 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4706	LEU
1	D	4747	SER
1	D	4704	LEU
1	D	5030	LYS
1	B	4667	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	533	ASN
1	C	4728	HIS
1	C	877	ASN
1	C	2962	GLN
1	D	475	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AMP	B	5101	-	21,25,25	0.74	0	23,38,38	1.26	2 (8%)
3	AMP	C	5101	-	21,25,25	0.74	0	23,38,38	1.26	2 (8%)
3	AMP	A	5101	-	21,25,25	0.74	0	23,38,38	1.26	2 (8%)
3	AMP	D	5101	-	21,25,25	0.74	0	23,38,38	1.26	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	B	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	C	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	A	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	D	5101	-	-	2/6/26/26	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5101	AMP	N3-C2-N1	-3.81	123.50	128.67
3	D	5101	AMP	N3-C2-N1	-3.81	123.50	128.67
3	C	5101	AMP	N3-C2-N1	-3.81	123.50	128.67
3	A	5101	AMP	N3-C2-N1	-3.81	123.51	128.67
3	A	5101	AMP	C4-C5-N7	-2.20	107.01	109.34

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

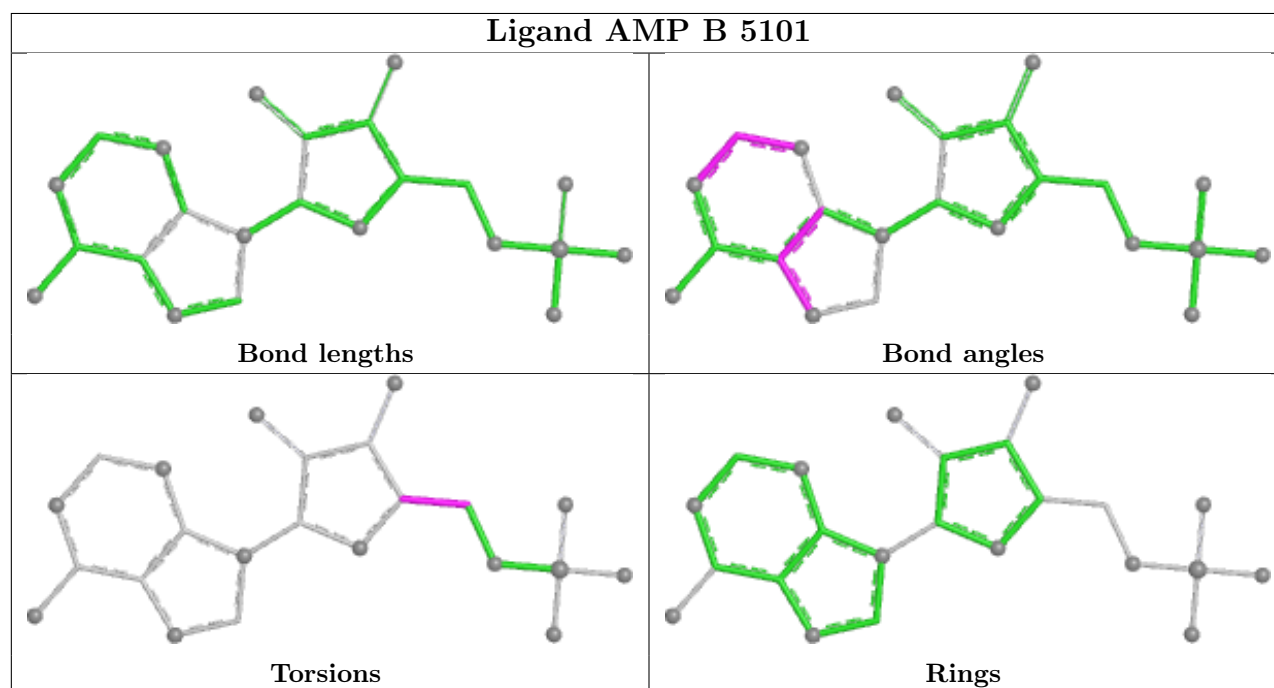
Mol	Chain	Res	Type	Atoms
3	A	5101	AMP	O4'-C4'-C5'-O5'
3	B	5101	AMP	O4'-C4'-C5'-O5'
3	C	5101	AMP	O4'-C4'-C5'-O5'
3	D	5101	AMP	O4'-C4'-C5'-O5'
3	A	5101	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

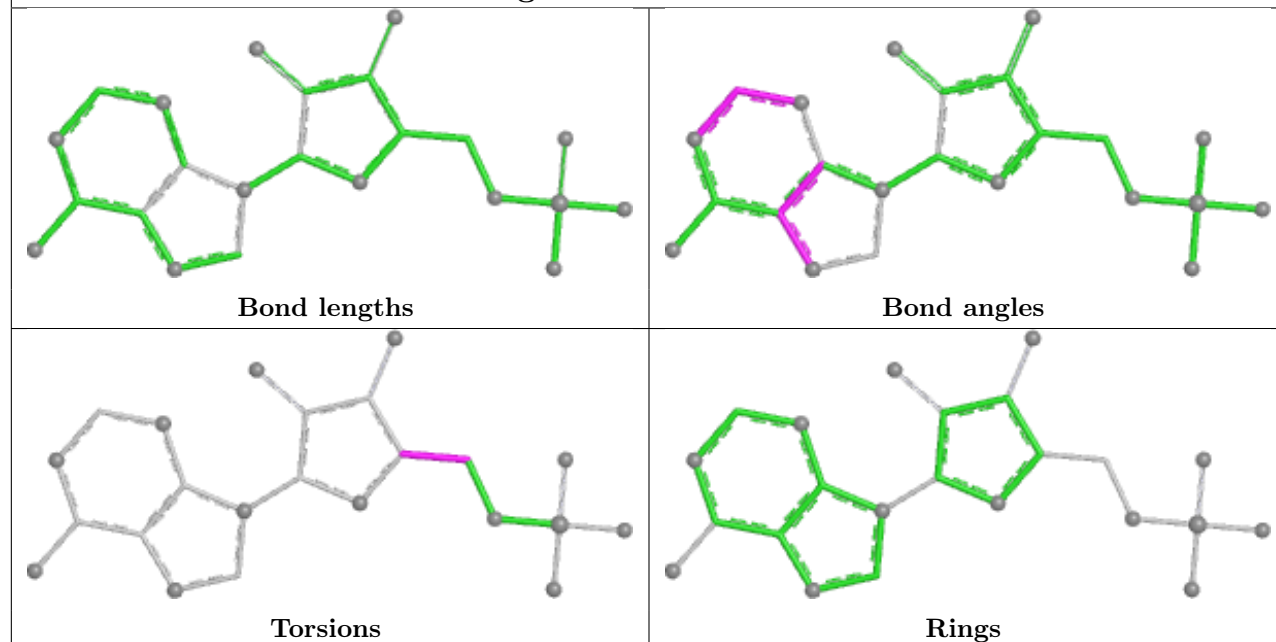
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	AMP	1	0
3	C	5101	AMP	1	0
3	A	5101	AMP	1	0
3	D	5101	AMP	1	0

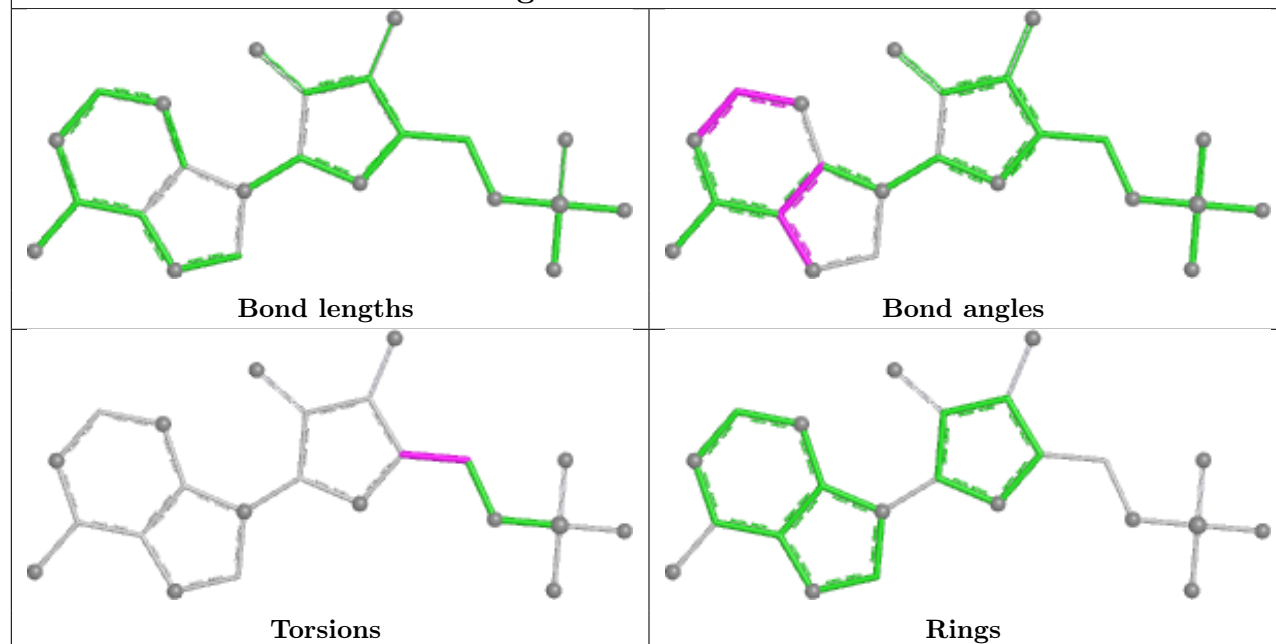
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

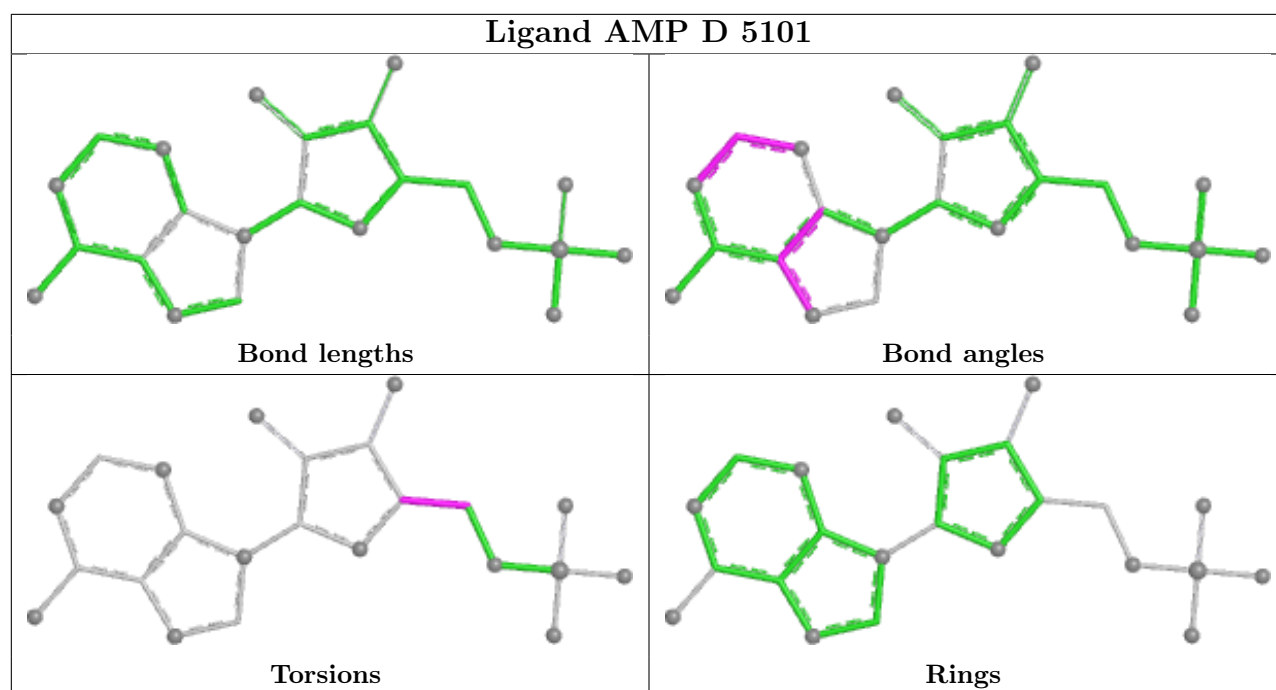


Ligand AMP C 5101



Ligand AMP A 5101





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.

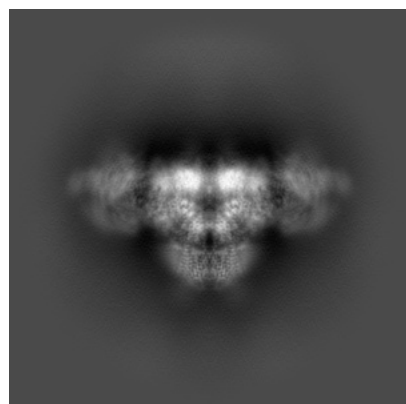
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40425. These allow visual inspection of the internal detail of the map and identification of artifacts.

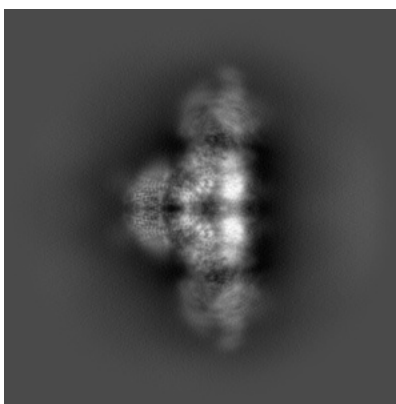
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

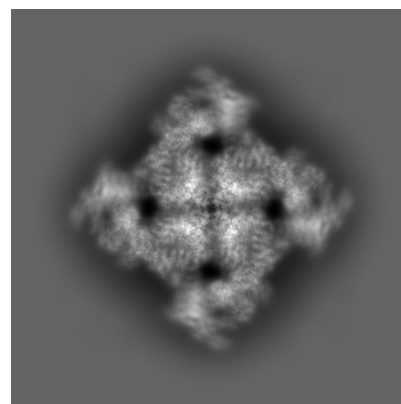
6.1.1 Primary map



X

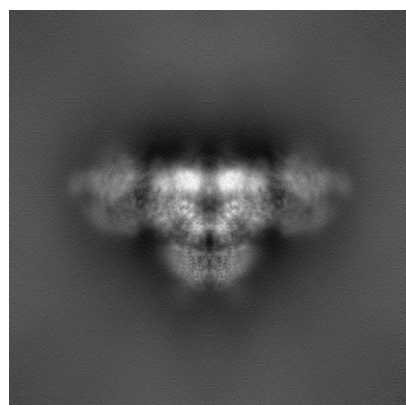


Y

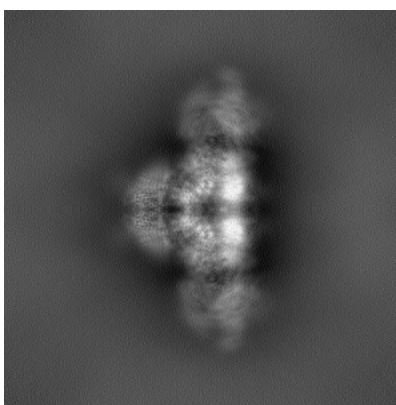


Z

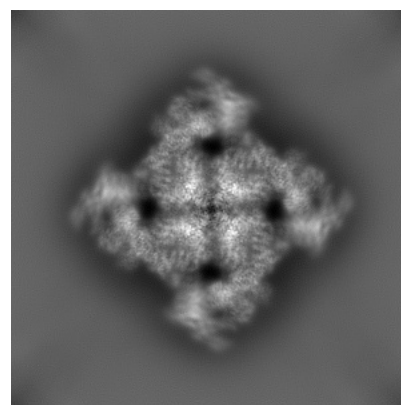
6.1.2 Raw map



X



Y

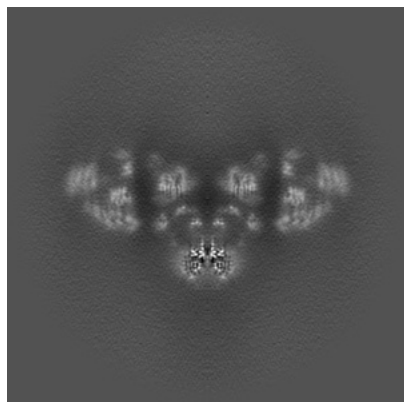


Z

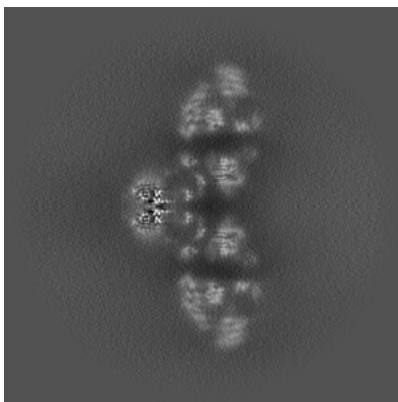
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

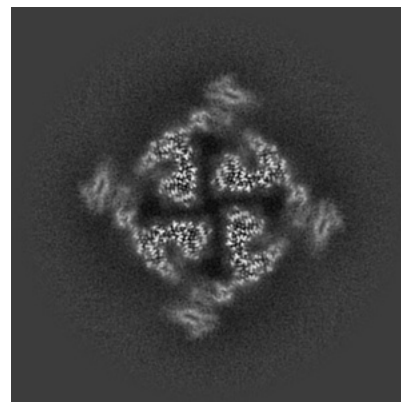
6.2.1 Primary map



X Index: 200

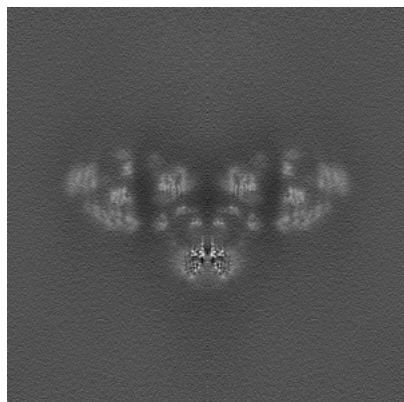


Y Index: 200

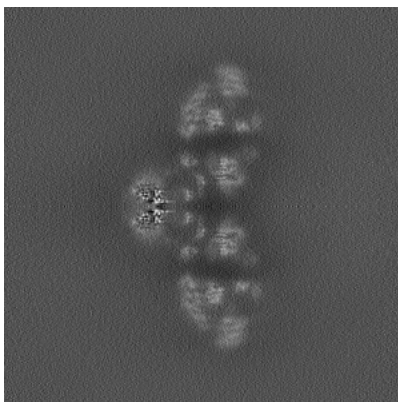


Z Index: 200

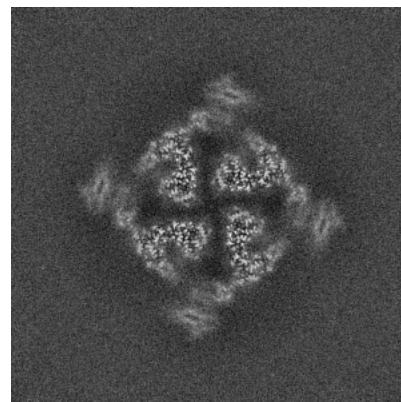
6.2.2 Raw map



X Index: 200



Y Index: 200

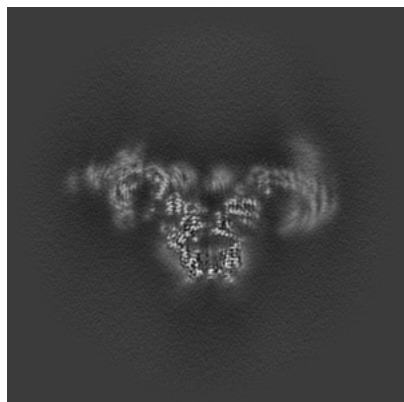


Z Index: 200

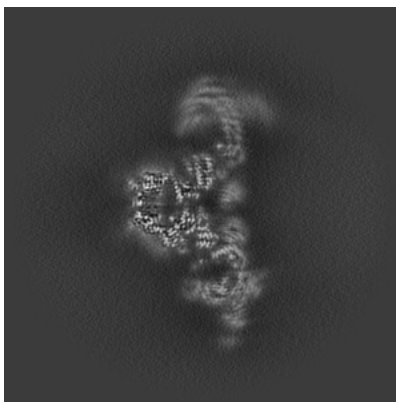
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

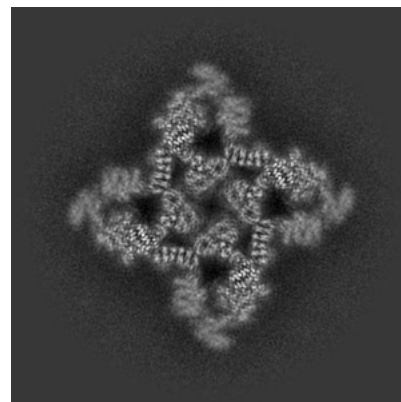
6.3.1 Primary map



X Index: 218

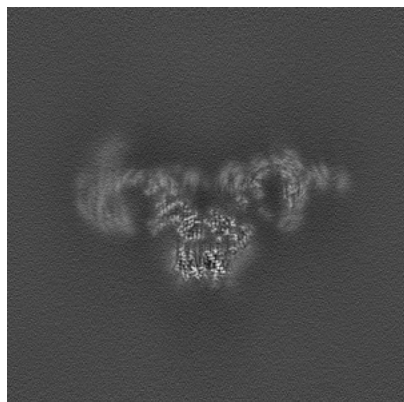


Y Index: 182

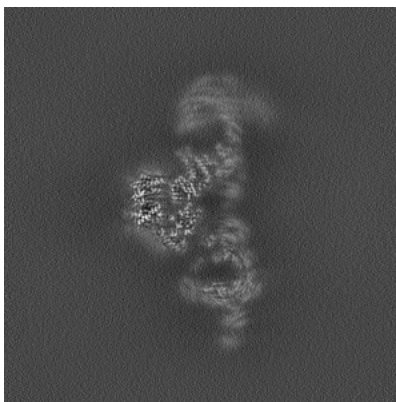


Z Index: 223

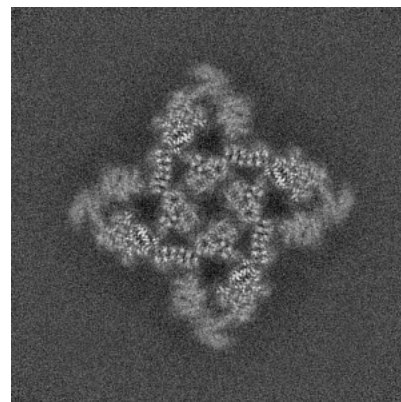
6.3.2 Raw map



X Index: 186



Y Index: 186

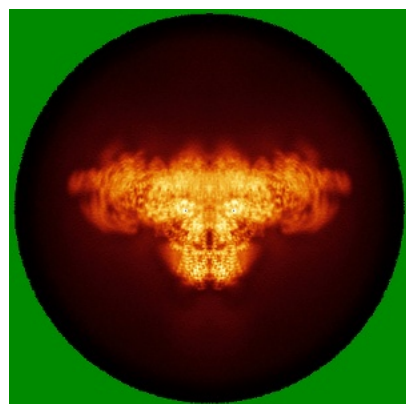


Z Index: 222

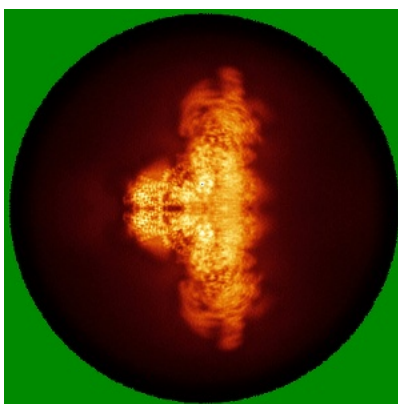
The images above show the largest variance slices of the map in three orthogonal directions.

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

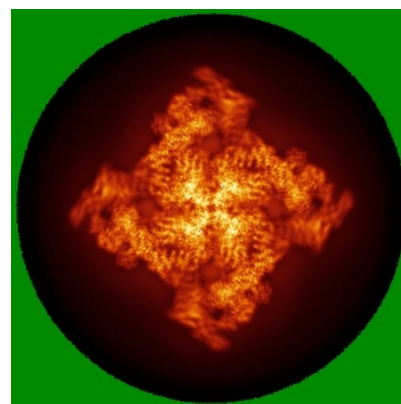
6.4.1 Primary map



X

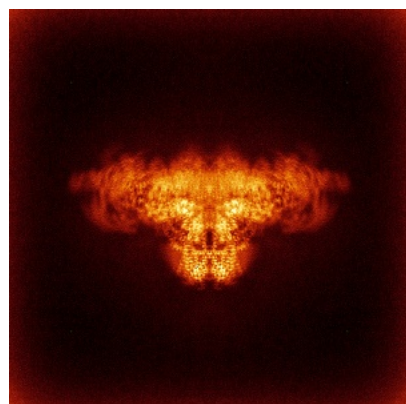


Y

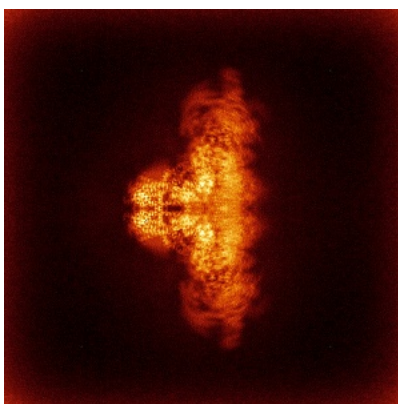


Z

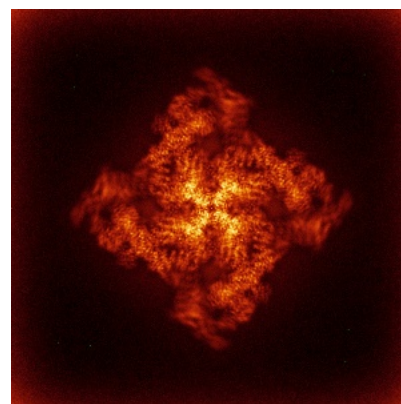
6.4.2 Raw map



X



Y

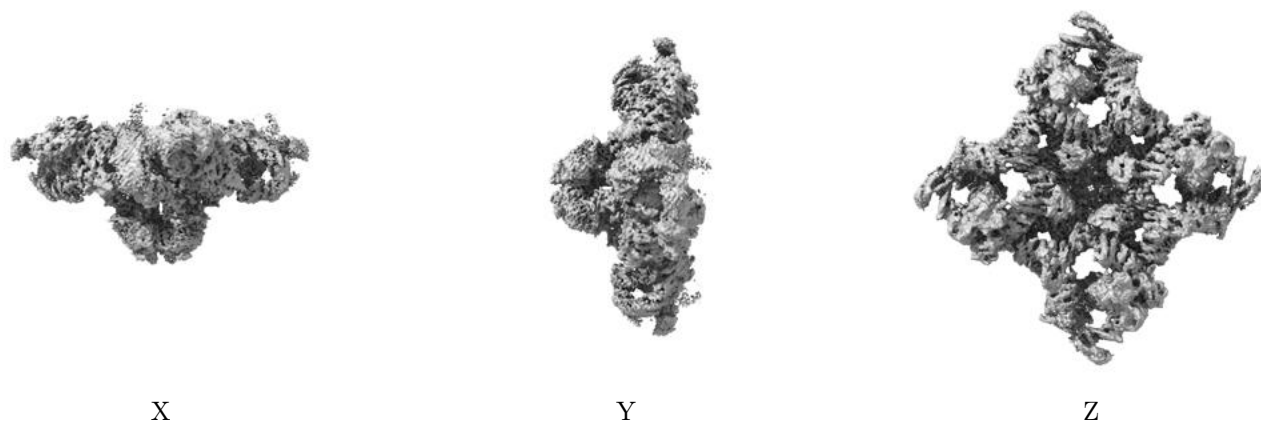


Z

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.

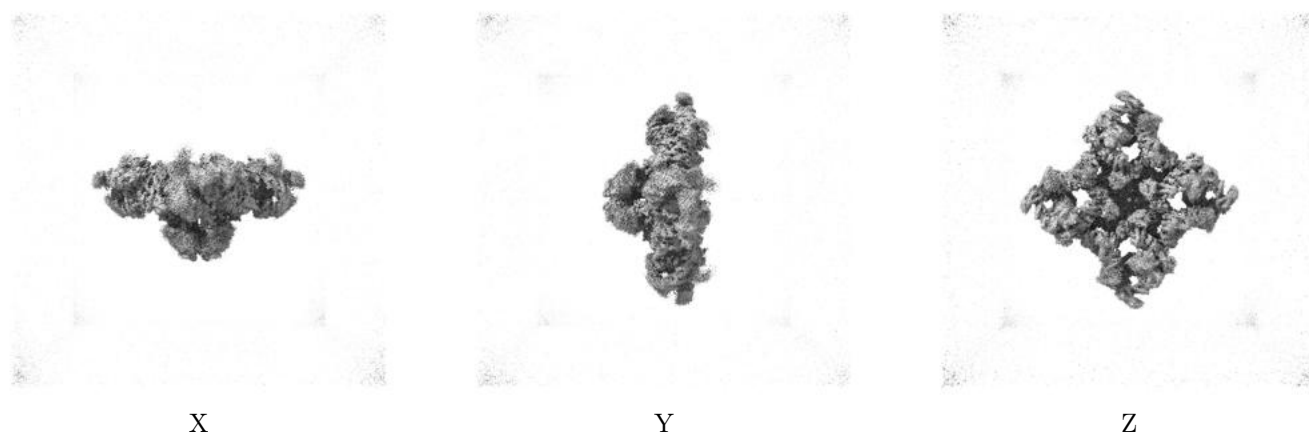
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.132. 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.

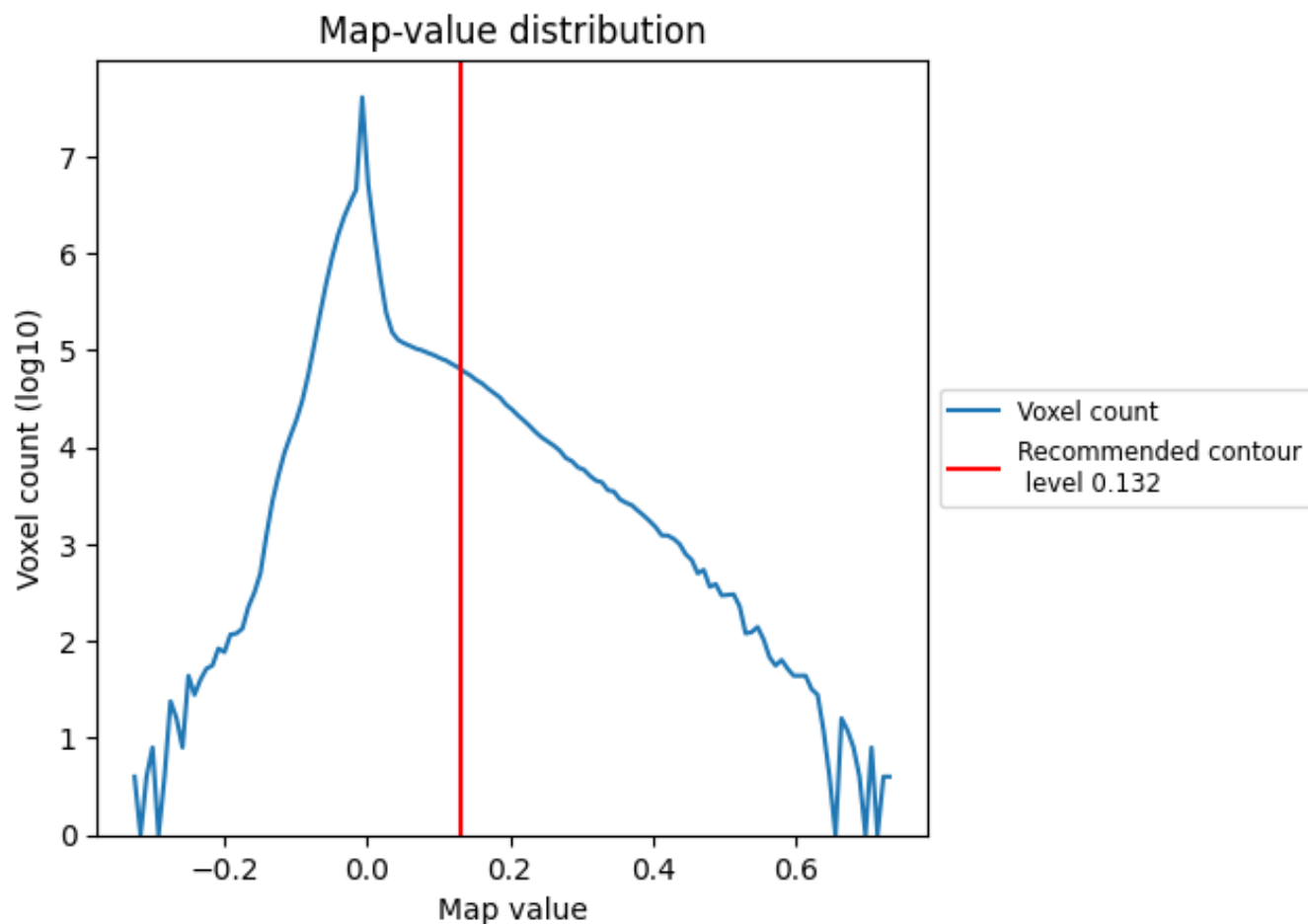
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

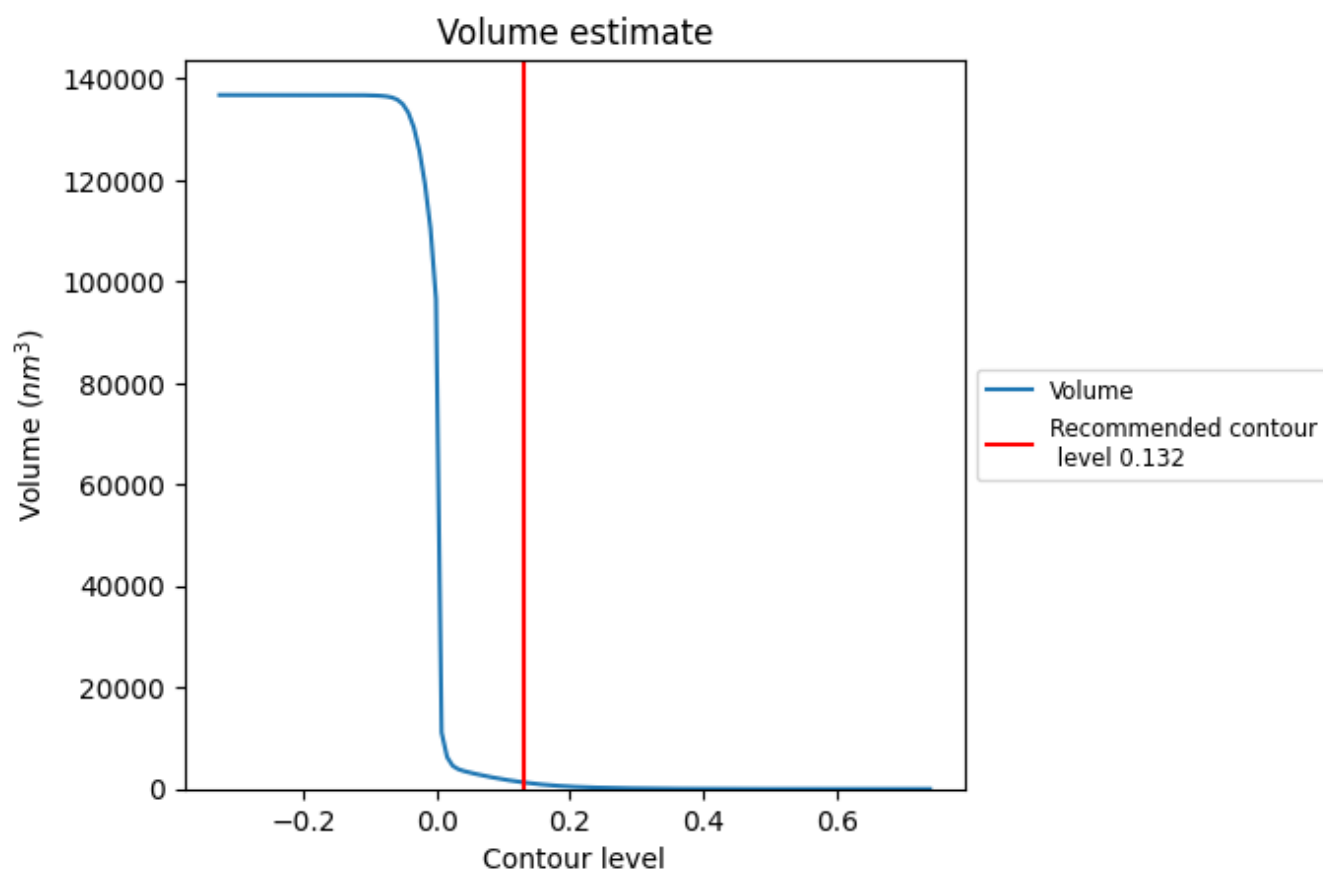
This section contains the results of statistical analysis of the map.

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.

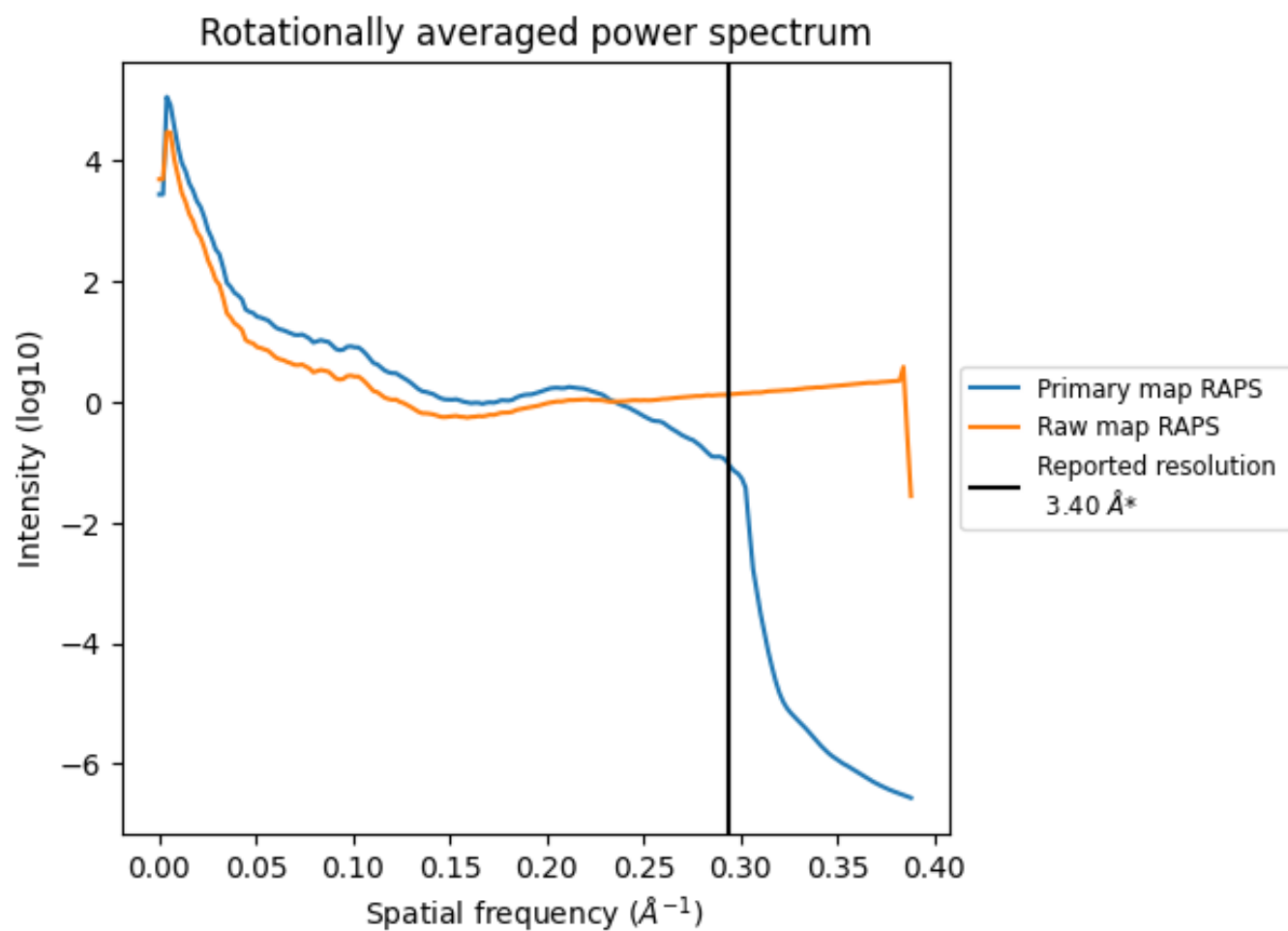
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1261 nm^3 ; this corresponds to an approximate mass of 1139 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 ⓘ

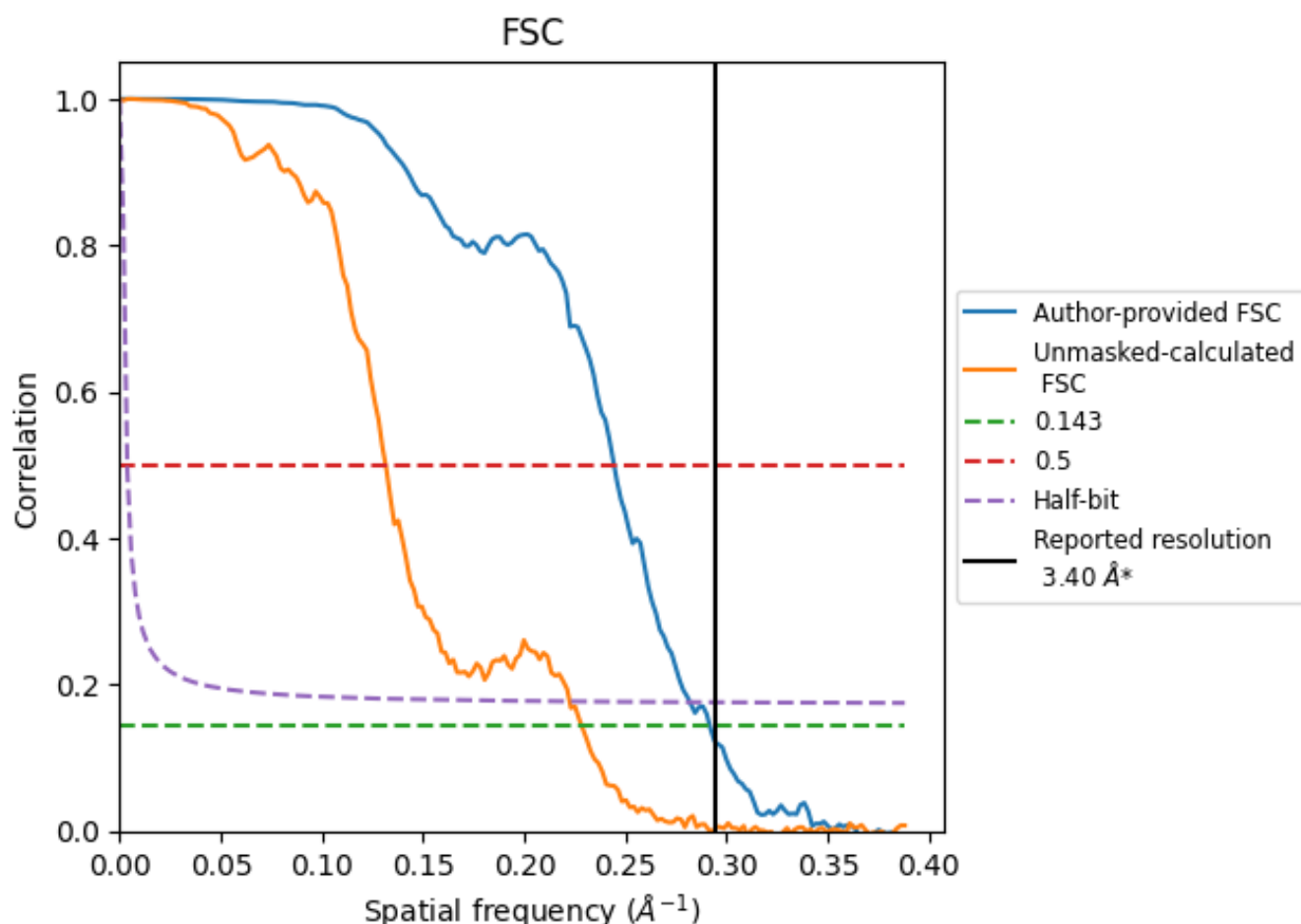


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

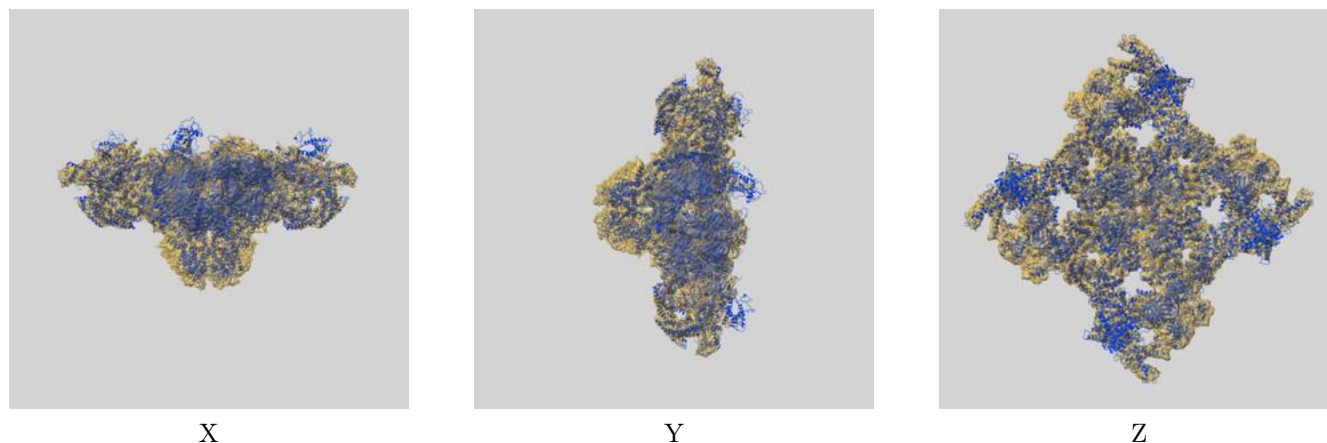
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.09	3.55
Unmasked-calculated*	4.37	7.60	4.49

*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 4.37 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

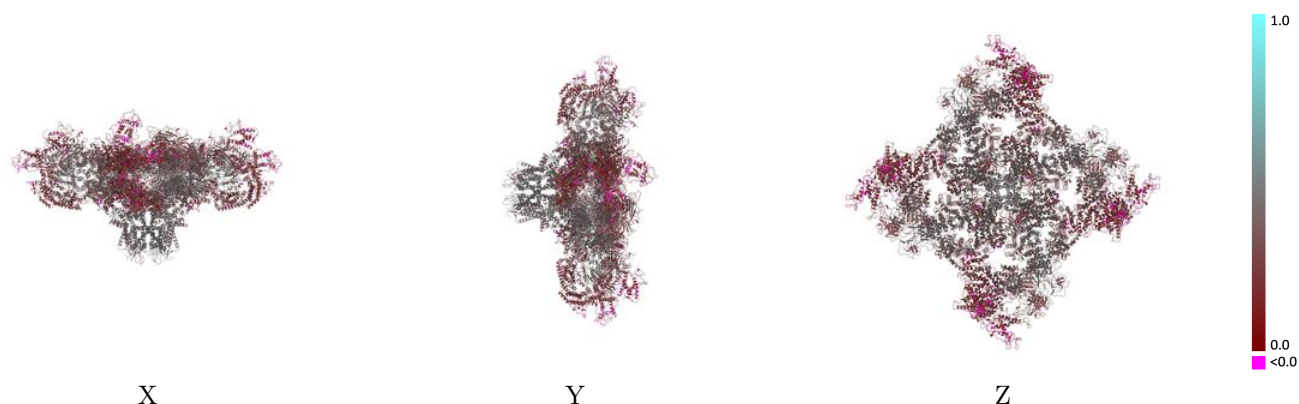
This section contains information regarding the fit between EMDB map EMD-40425 and PDB model 8SEQ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



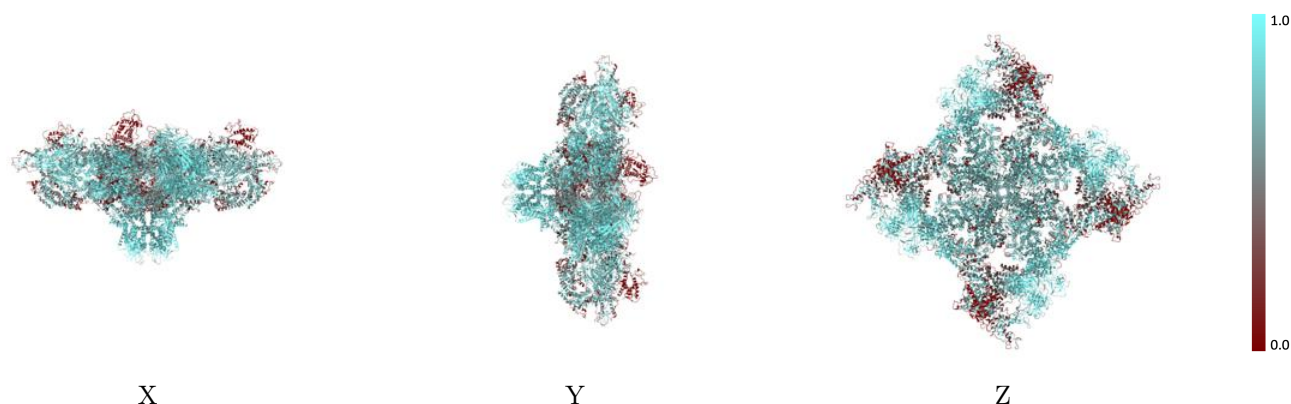
The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



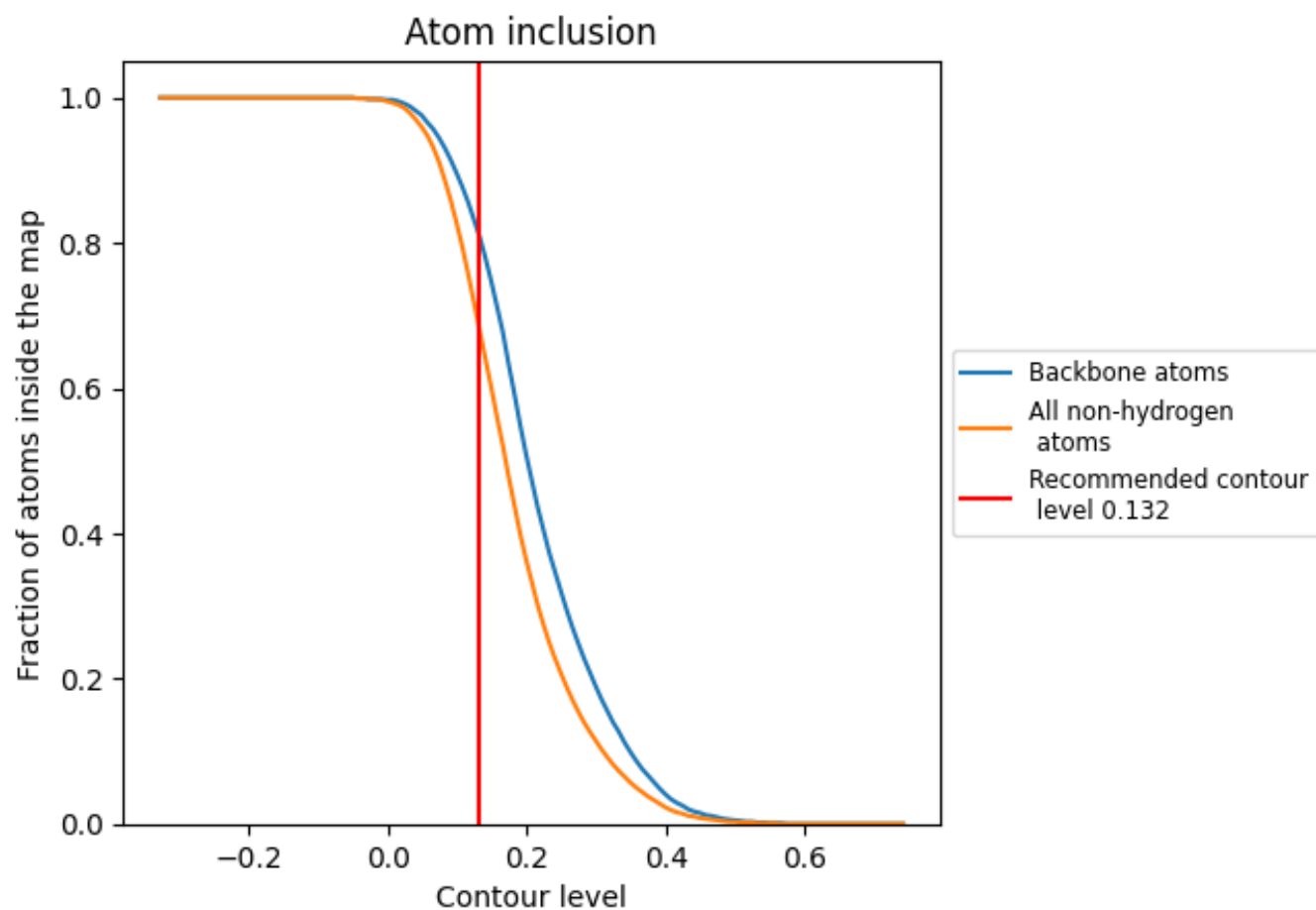
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.132).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6820	<div></div> 0.3220
A	<div></div> 0.6780	<div></div> 0.3210
B	<div></div> 0.6790	<div></div> 0.3200
C	<div></div> 0.6790	<div></div> 0.3200
D	<div></div> 0.6790	<div></div> 0.3200
E	<div></div> 0.8500	<div></div> 0.3890
F	<div></div> 0.8500	<div></div> 0.3880
G	<div></div> 0.8500	<div></div> 0.3900
H	<div></div> 0.8500	<div></div> 0.3920

1.0

0.0

<0.0