



wwPDB EM Validation Summary Report ⓘ

Jul 10, 2023 – 03:00 PM EDT

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.

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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.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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) : 2.34

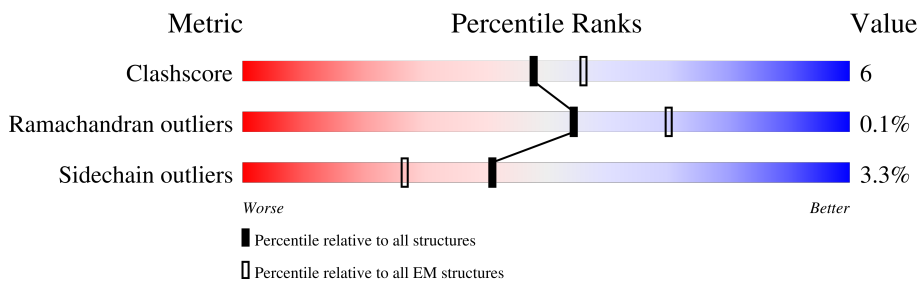
1 Overall quality at a glance

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	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	
1	B	5037	
1	C	5037	
1	D	5037	
2	E	350	
2	F	350	
2	G	350	
2	H	350	

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
			Total	C	N	O	S		
1	A	4376	34896	22197	6022	6441	236	9	0
1	B	4376	34896	22197	6022	6441	236	9	0
1	C	4376	34896	22197	6022	6441	236	9	0
1	D	4376	34896	22197	6022	6441	236	9	0

- 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
			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
2	H	107	818	516	144	154	4	0	0

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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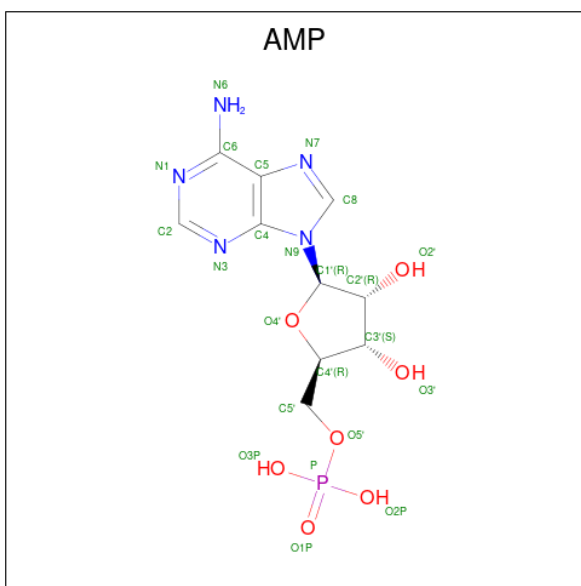
Chain	Residue	Modelled	Actual	Comment	Reference
G	-242	MET	-	expression tag	UNP P08515
G	-241	LYS	-	expression tag	UNP P08515
G	-240	SER	-	expression tag	UNP P08515
G	-239	SER	-	expression tag	UNP P08515
G	-238	HIS	-	expression tag	UNP P08515
G	-237	HIS	-	expression tag	UNP P08515
G	-236	HIS	-	expression 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: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
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).

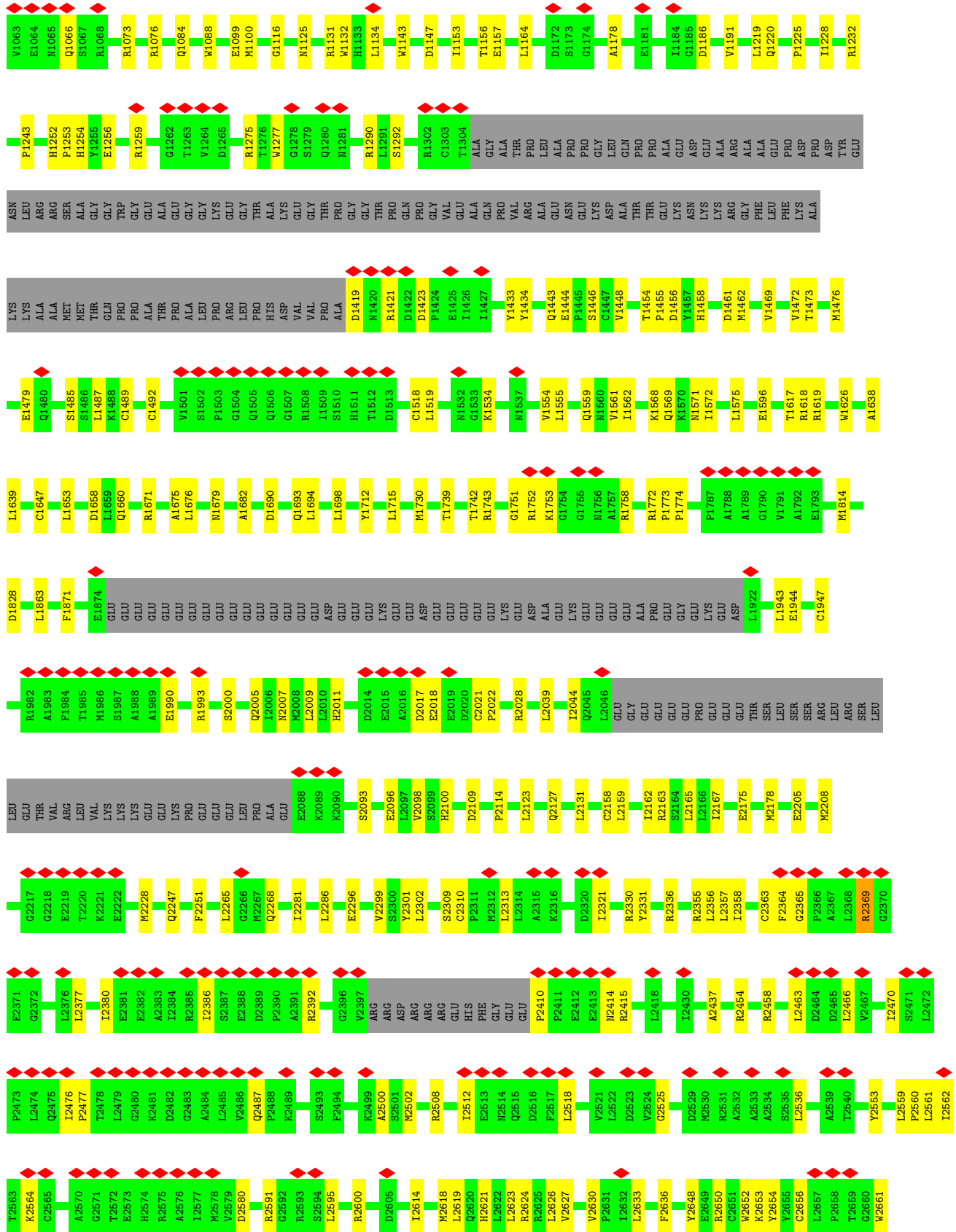
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

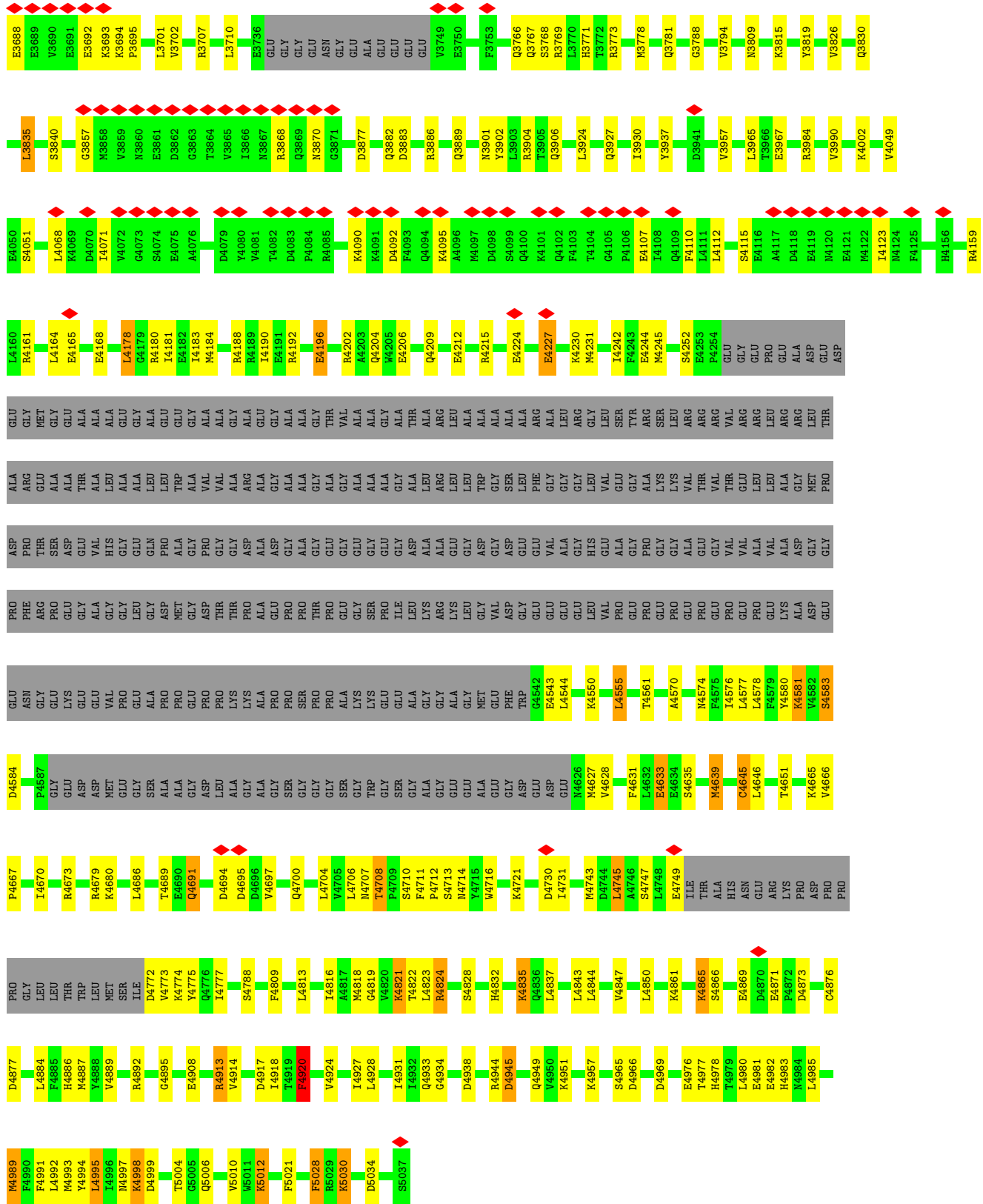
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 1



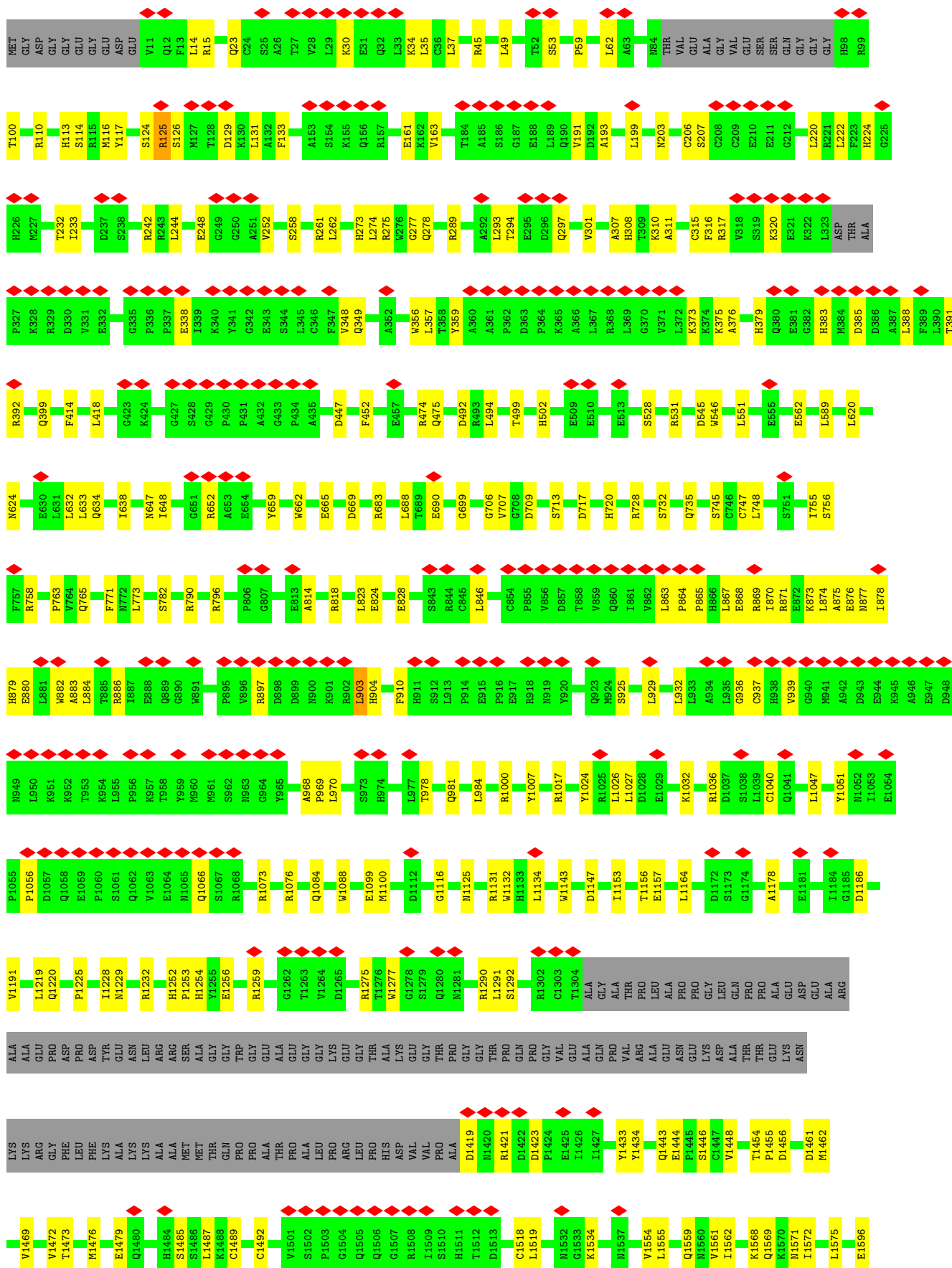


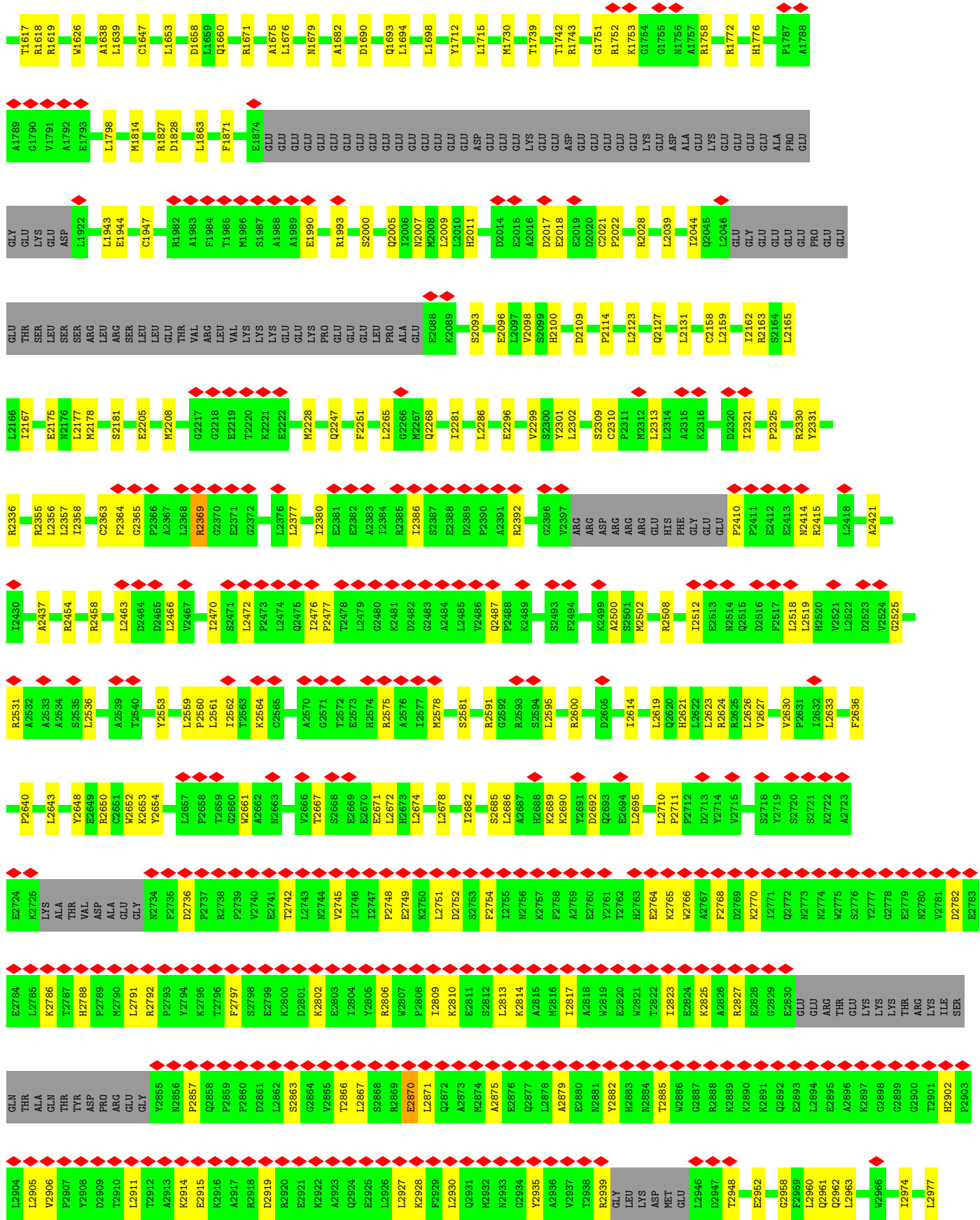
V3593	N3523	V3459	G3363	E5290	Y3213	R3111	T3020	L2927	L2867	W2807	I2747	A2662
R3594	M3524	V3460	R3366	A3291	N3214	L3112	P3021	K2928	S2868	P2808	P2748	I2663
R3595	Q3530	Q3461	R3367	P3292	A3215	G3113	A3021	F2929	R2869	I2809	E2749	V2666
S3600	D3531	N3462	R3368	P3293	C3216	K3114	K3022	L2930	E2870	K2810	K2750	T2667
A3601	D3531	I3464	V3373	P3294	S3217	V3115	V3024	Q2932	L2871	E2811	L2751	S2668
L3603	M3534	N3465	E3376	A3295	V3218	GLN	V3024	M2932	Q2872	S2812	D2752	E2669
H3605	L3535	M3466	E3377	L3296	Y3219	ALA	L3025	N2933	A2873	L2813	D2752	E2670
A3606	A3536	M3467	E3378	P3297	T3220	ARG	G3026	N2934	M2874	K2814	F2754	E2671
L3606	K3537	S3468	Q3378	A3298	T3221	THR	S3027	G2935	A2875	A2815	I2755	L2672
Q3607	T3538	S3469	L3379	G3299	K3222	THR	G3028	A2936	E2876	M2816	N2756	H2673
Q3608	R3539	F3469	R3380	A3300	S3223	VAL	G3029	V2937	A2877	I2817	F2756	L2674
Q3609	R3540	L3470	R3381	P3301	P3224	K3123	G3029	T2938	Q2877	L2818	N2757	L2678
A3541	L3541	T3471	E3382	P3302	R3225	G3124	R3033	R2939	L2878	A2819	F2758	I2682
L3542	A3472	A3472	E3383	P3303	E3226	M3128	E3037	W2879	A2879	W2819	E2760	I2682
K3543	D3473	D3473	R3383	C3304	R3227	V3134	M3038	E2880	E2880	E2820	E2760	S2685
D3544	K3474	S3474	K3384	T3305	L3229	A3135	L3042	M2881	M2881	W2821	Y2761	L2686
E3548	S3476	S3476	A3385	A3306	L3230	L3136	L3046	Y2882	Y2882	T2822	T2762	A2687
E3651	A3477	K3477	E3386	S3309	G3231	H3146	A3047	H2883	H2883	E2824	E2764	H2688
F3552	M3478	M3478	E3387	L3316	L3232	Q3149	A3048	K2889	K2889	K2825	K2765	K2690
L3553	L3479	A3479	E3388	G3317	L3233	H3150	R3051	K2890	K2890	A2826	A2766	Y2691
Q3554	L3479	L3479	E3389	N3318	P3233	H3150	H3052	K2891	K2891	R2827	A2767	Q2693
N3555	E3391	E3391	E3391	I3319	N3234	Q3151	R3053	Q2892	Q2892	E2828	F2768	E2694
N3556	L3392	L3392	L3392	T3320	S3235	Q3151	G3058	K2893	K2893	G2829	D2769	L2695
L3557	V3394	V3394	V3394	R3321	V3236	D3154	T3059	K2894	K2894	E2830	K2770	L2715
H3558	R3395	R3395	R3395	E3238	E3237	D3156	T3059	L2894	L2894	R2827	Q2772	S2718
L3559	S3395	S3395	S3395	M3239	M3239	R3156	P3062	E2895	E2895	E2828	N2773	L2719
Q3560	R3403	V3324	R3403	C3240	C3240	L3158	V3065	K2896	K2896	K2890	N2774	S2720
Q3561	D3404	N3326	D3404	P3241	P3241	D3159	L3075	A2897	A2897	K2890	W2775	S2721
N3562	I3413	L3327	I3413	D3242	D3242	D3160	L3075	V2980	V2980	L2902	Y2777	S2722
V3563	R3414	G3328	R3414	G3328	L3243	D3160	L3075	V2981	V2981	H2902	K2778	K2725
E3564	D3417	D3330	D3417	D3330	P3244	S3171	R3078	V2982	V2982	D2782	ARG	LYS
R3629	N3418	E3331	N3418	E3331	D3247	L3175	T3079	E2978	E2978	E2783	THR	ALA
R3630	M3419	A3332	M3419	A3332	R3248	V3080	V3080	A2979	A2979	E2784	ALA	VAL
A3631	R3420	T3333	R3420	T3333	K3249	K3081	K3081	G2989	G2989	E2784	THR	ASP
V3632	A3421	K3334	A3421	K3334	M3250	K3082	K3082	G2988	G2988	L2785	ALA	ALA
V3633	H3422	K3335	H3422	K3335	A3257	T3181	P3085	R2985	R2985	L2905	GLY	GLY
A3634	W3423	L3338	W3423	L3338	E3258	V3182	E3086	V2986	V2986	P2907	ARG	THR
F3636	L3424	L3338	L3424	L3338	T3264	E3184	I3087	E2987	E2987	H2788	ARG	THR
R3648	P3427	A3339	P3427	A3339	E3265	K3185	L3092	K2988	K2988	P2789	GLY	GLY
M3573	N3430	V3340	N3430	V3340	I3272	L3197	S3094	G2989	G2989	M2790	THR	THR
A3574	F3435	F3343	F3435	F3343	P3275	M3201	F3095	S2989	S2989	M2790	THR	THR
L3575	F3442	F3344	F3442	F3344	M3276	P3202	A3099	P2990	P2990	L2791	THR	THR
R3577	F3444	F3346	F3444	F3346	L3277	V3203	D3102	H2991	H2991	R2792	THR	THR
G3578	H3449	R3347	H3449	R3347	C3278	E3207	E2992	K2988	K2988	Q2858	THR	THR
P3580	N3450	R3348	N3450	R3348	S3279	P3208	K3106	V2986	V2986	Q2859	THR	THR
G3581	K3453	R3351	K3453	R3351	Y3280	Q3209	V3107	E2987	E2987	P2857	THR	THR
R3582	R3453	L3354	R3453	L3354	L3281	L3210	L3110	K2996	K2996	Q2858	THR	THR
G3583	R3453	L3354	R3453	L3354	P3282	N3211	L3110	F2997	F2997	Q2859	THR	THR
E3584	R3453	L3354	R3453	L3354	P3282	E3286	L3110	P2998	P2998	D2861	THR	THR
D3585	R3453	L3354	R3453	L3354	E3286	R3287	L3110	L3002	L3002	L2862	THR	THR
A3586	R3453	L3354	R3453	L3354	R3287	E3212	L3110	H3013	H3013	S2863	THR	THR
D3588	R3453	L3354	R3453	L3354	G3288	P3289	L3110	R2920	R2920	Q2864	THR	THR
P3589	R3453	L3354	R3453	L3354	P3289	P3289	L3110	E2921	E2921	G2865	THR	THR
E3590	R3453	L3354	R3453	L3354	P3289	P3289	L3110	K2922	K2922	E2800	THR	THR
K3591	R3453	L3354	R3453	L3354	P3289	P3289	L3110	A2923	A2923	D2801	THR	THR
I3592	R3453	L3354	R3453	L3354	P3289	P3289	L3110	Q2924	Q2924	E2801	THR	THR
E3687	R3453	L3354	R3453	L3354	P3289	P3289	L3110	E2925	E2925	R2806	THR	THR



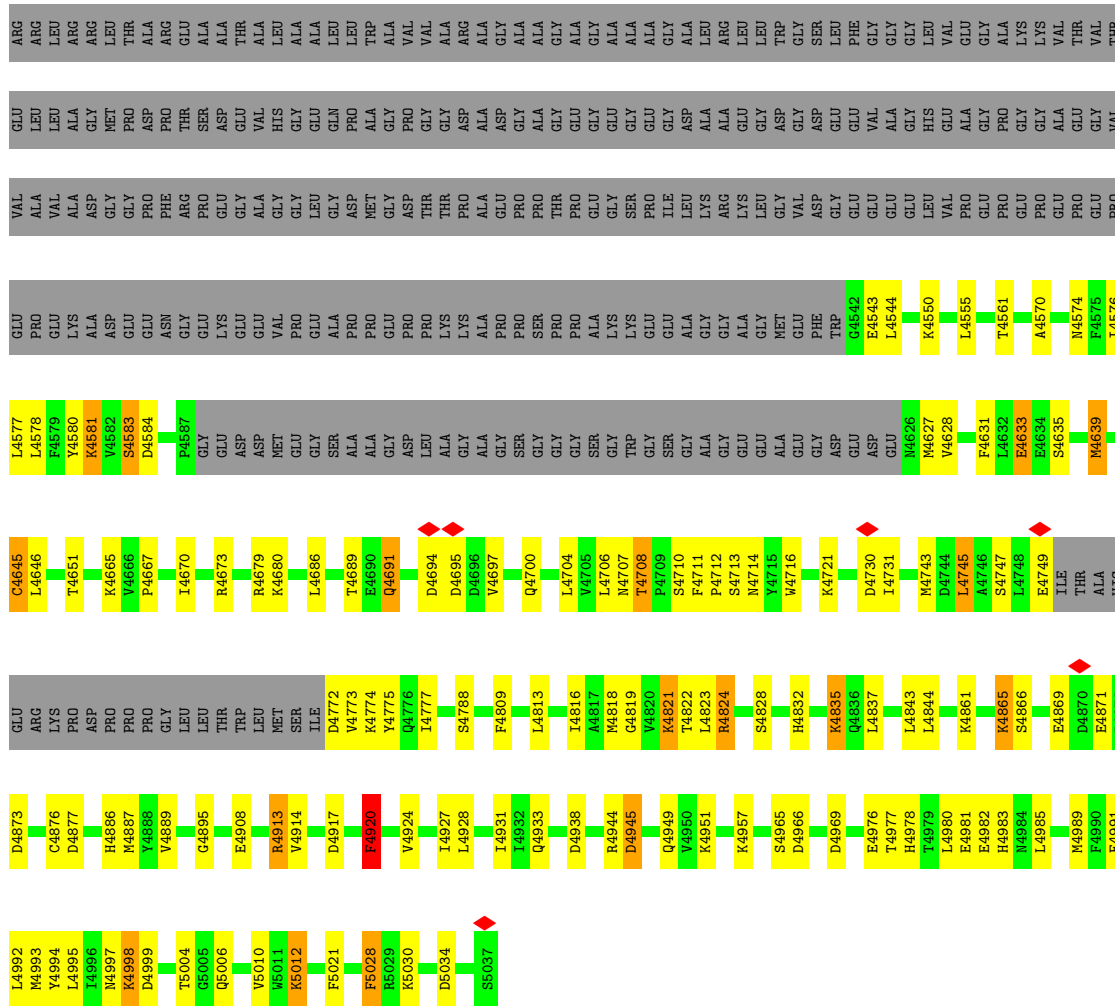
• Molecule 1: Ryanodine receptor 1



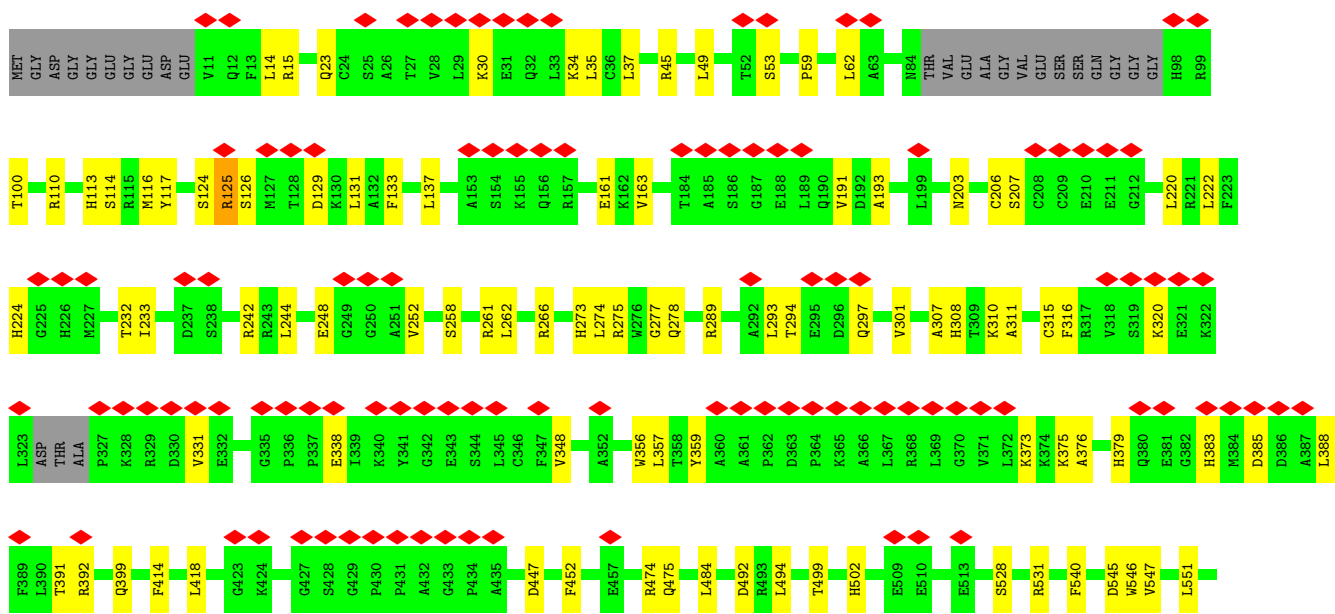


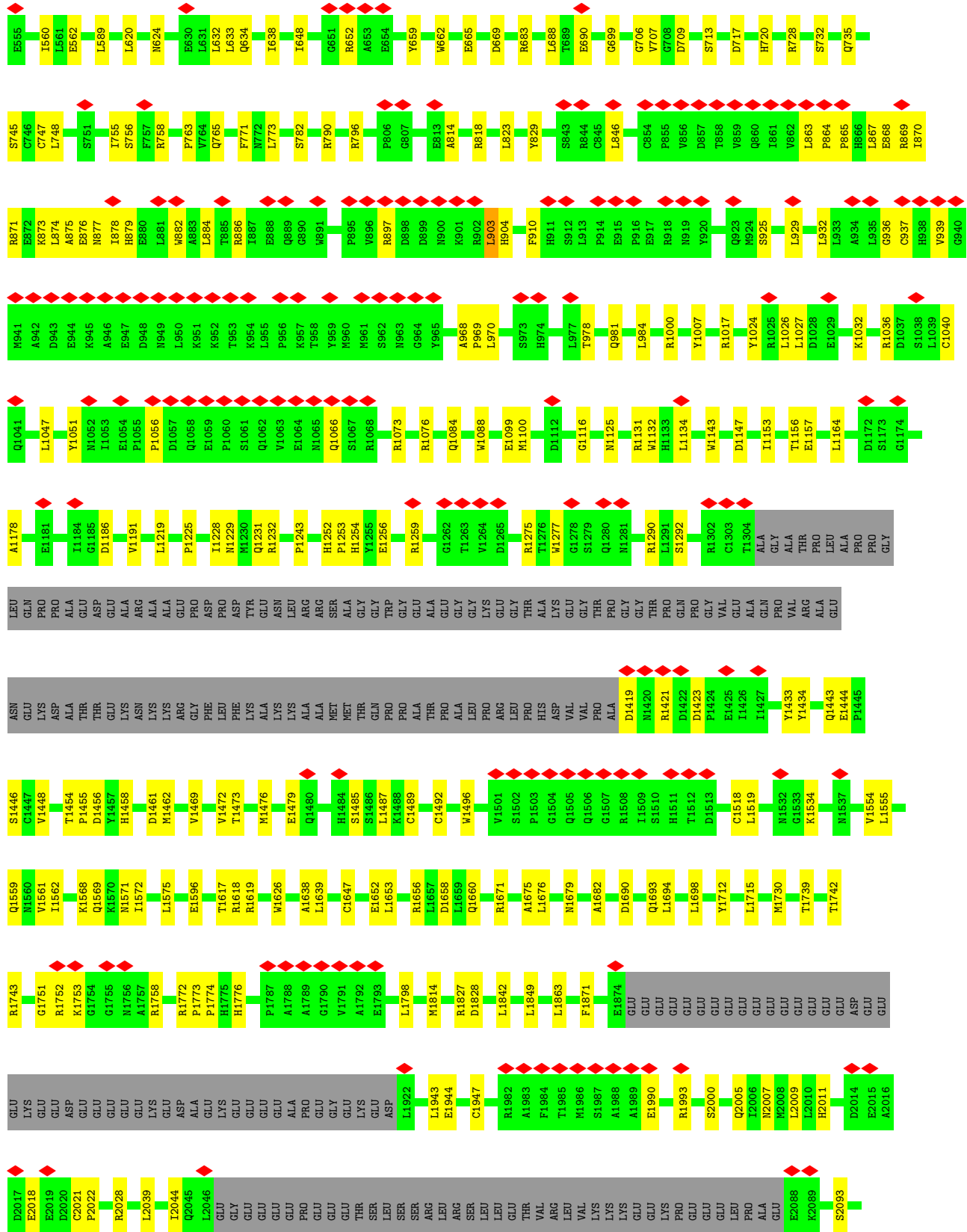


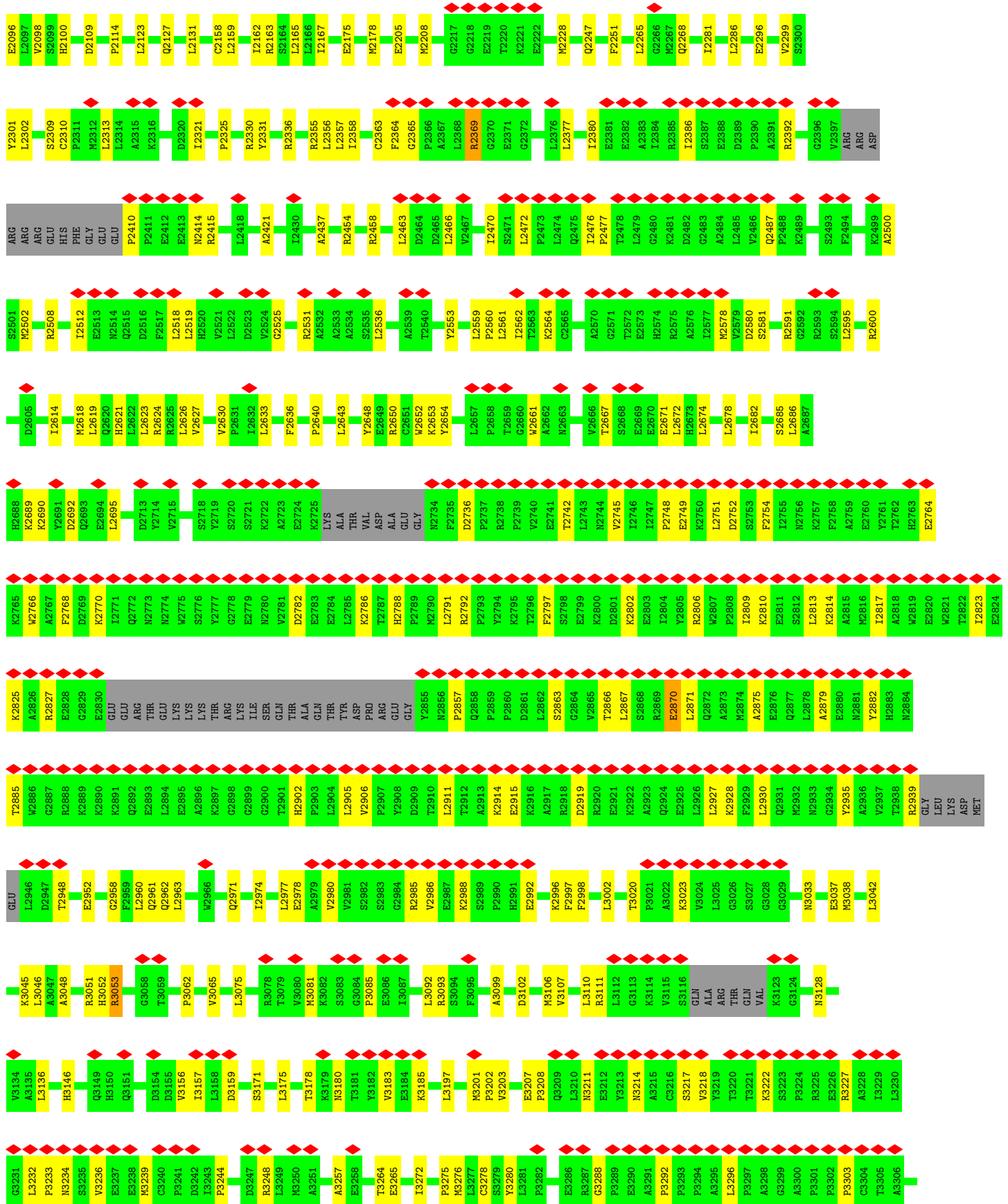
GLU	M4000	V3794	Y3576	Y3503	T3425	L3338	E5258	T3178	M3081	E2978
PRD	F4126	M3809	R3577	S3504	E3426	A3339	E3286	K3179	K3082	A2979
ALA	L4016	K3815	G3578	V3505	F3427	V3340	T3264	N3180	S3083	V2980
ASP	H4156	K3815	L3579	V3506	F3427	F3341	E3265	T3181	G3084	V2981
GLU	R4159	Y3819	P3580	T3507	N3430	A3342	T3272	Y3182	P3085	S2982
ASP	E4050	K3823	G3581	S3508	F3435	Q3343	Y3275	V3183	E3086	S2983
GLY	S4051	K3823	R3582	L3509	F3435	P3344	M3276	E3184	I3087	G2984
MET	L4068	L3835	E3583	I3510	F3442	I3346	L3277	K3185	L3092	R2985
GLY	K4069	L3835	E3584	A3512	H3449	S3347	C3278	L3197	R3093	V2986
GLU	D4070	S3240	D3585	T3513	N3450	S3348	P3282	M3201	S5094	E2987
ALA	L4071	E3688	D3587	L3514	N3450	R3348	P3282	F3095	F3095	V2988
ALA	V4072	E3688	D3588	K3515	R3453	P3351	P3282	A3099	A3099	K2988
ALA	G4073	V3690	D3588	P3519	F3458	P3351	E2286	D3102	D3102	S2989
GLY	S4074	E3691	P3589	M3523	V3459	I3359	G3288	M3106	M3106	S2989
ALA	E4075	E3692	E3590	M3524	V3460	G3363	R3289	V3107	V3107	P2990
GLU	A4076	K3693	K3591	Q3530	Q3461	R3364	E3290	L3210	L3210	H2991
GLY	D4079	L3701	V3593	D3531	N3462	R3366	A3291	L3110	L3110	E2992
ALA	Y4080	L3703	R3594	R3537	E3463	K3367	P3292	R3111	R3111	K2996
ALA	V4081	R3707	R3595	K3534	I3464	R3368	P3293	L3112	L3112	F2997
GLY	T4082	E3710	S3600	L3536	N3465	R3368	P3294	G3113	G3113	F2998
GLU	D4083	L3710	H3605	A3536	N3466	V3373	P3295	L3216	L3216	L3002
GLY	P4084	D3717	L3606	K3537	N3467	E3376	L3296	E3212	E3212	T3020
ALA	R4085	E3736	T3609	T3538	S3468	E3377	P3297	S3217	S3217	A3022
THR	K4090	GLU	E3610	R3539	F3469	E3377	A3298	V3218	V3218	K3023
VAL	K4091	GLY	H3611	Y3540	F3469	G3378	G3299	V3219	V3219	V3024
ALA	D4092	GLY	P3612	L3541	T3470	L3379	A3300	ALA	ALA	L3024
ALA	F4093	GLU	Y3613	K3543	A3472	R3380	A3300	ARG	ARG	G3026
ALA	Q4094	ASN	K3614	D3544	D3473	L3381	P3301	THR	THR	G3026
ALA	K4095	GLY	K3614	E3544	S3474	R3380	P3302	GLN	GLN	S3027
ARG	A4096	ALA	S3615	E3547	S3475	A3383	P3303	K3123	K3123	G3028
LEU	M4097	GLU	K3616	E3548	S3477	K3384	C3304	G3124	G3124	G3029
ALA	D4098	GLU	A3618	E3548	K3477	A3385	T3305	N3128	N3128	M3033
ALA	S4099	GLU	A3618	E3551	R3477	A3386	T3305	V3134	V3134	E3037
ALA	Q4100	GLU	V3619	F3552	N3478	E3386	T3305	A3135	A3135	M3038
ALA	K4101	GLU	H3620	F3553	L3479	A3387	T3305	L3136	L3136	L3042
ALA	Q4102	GLU	H3621	Q3554	LYS	E3388	T3305	H3146	H3146	L3046
ALA	F4103	GLU	K3622	N3555	ALA	E3388	T3305	L3047	L3047	L3046
LEU	T4104	GLU	L3623	N3556	GLY	E3389	T3305	A3048	A3048	A3048
ARG	G4105	GLU	L3624	L3557	ASP	G3390	T3305	Q3149	Q3149	A3048
LEU	G4106	GLU	L3624	L3557	ALA	G3390	T3305	H3150	H3150	A3048
LEU	P4107	GLU	S3625	H3558	ALA	E3391	T3305	Q3151	Q3151	R3051
SER	E4107	GLU	K3626	H3558	SER	L3392	T3305	Q3151	Q3151	R3051
TRP	I4108	GLU	K3627	L3559	GLY	L3323	T3305	D3154	D3154	R3053
ARG	I4109	GLU	Q3627	Q3560	SER	V3324	T3305	D3154	D3154	R3053
ARG	F4110	GLU	Q3627	Q3560	ASP	N3325	T3305	D3154	D3154	R3053
LEU	M4110	GLU	R3628	G3561	GLN	N3326	T3305	V3156	V3156	G3058
ARG	L4111	GLU	R3629	K3562	THR	L3327	T3305	I3157	I3157	T3059
ARG	L4112	GLU	R3630	V3563	ARG	G3328	T3305	C3240	C3240	P3062
ARG	E4115	GLU	A3631	E3564	LYS	I3413	T3305	D3159	D3159	P3062
VAL	S4116	GLU	V3632	G3565	LYS	R3414	T3305	D3160	D3160	V3065
VAL	A4117	GLU	V3633	S3566	LYS	D3417	T3305	S3171	S3171	L3075
VAL	D4118	GLU	A3634	P3567	LYS	N3418	T3305	L3175	L3175	L3075
VAL	E4119	GLU	C3635	R3570	R3498	N3418	T3305	D3247	D3247	R3078
VAL	M4120	GLU	F3636	R3570	R3499	R3419	T3305	R3248	R3248	R3078
VAL	E4121	GLU	M3637	M3573	G3500	R3420	T3305	R3249	R3249	T3079
VAL	M4122	GLU	M3638	L3574	D3501	H3421	T3305	M3250	M3250	V3080
VAL	I4123	GLU	R3648	L3575	R3502	H3422	T3305	A3251	A3251	V3080
VAL		GLU	M3652		R3502	L3424	T3305	A3257	A3257	V3080
VAL		GLU			R3502		T3305			

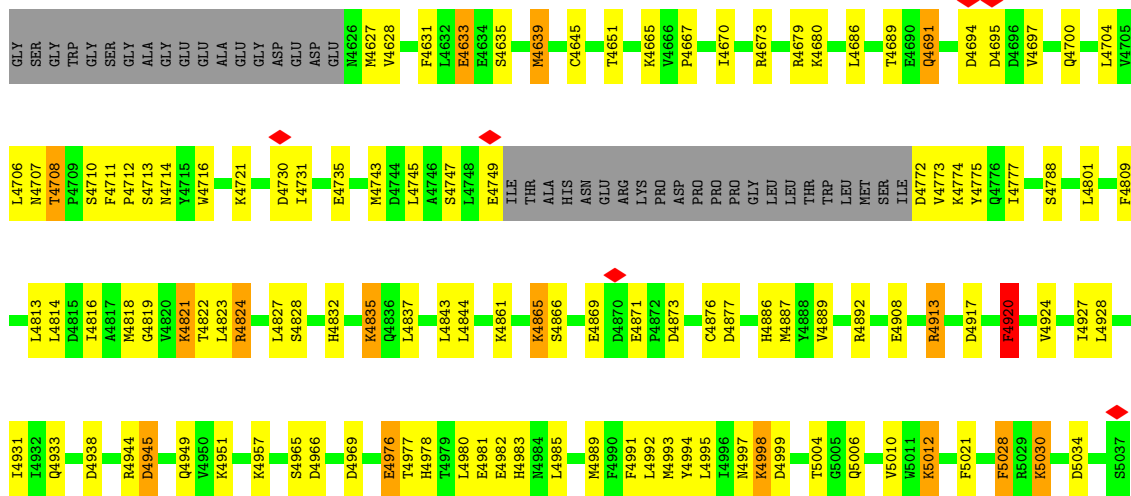


• Molecule 1: Ryanodine receptor 1

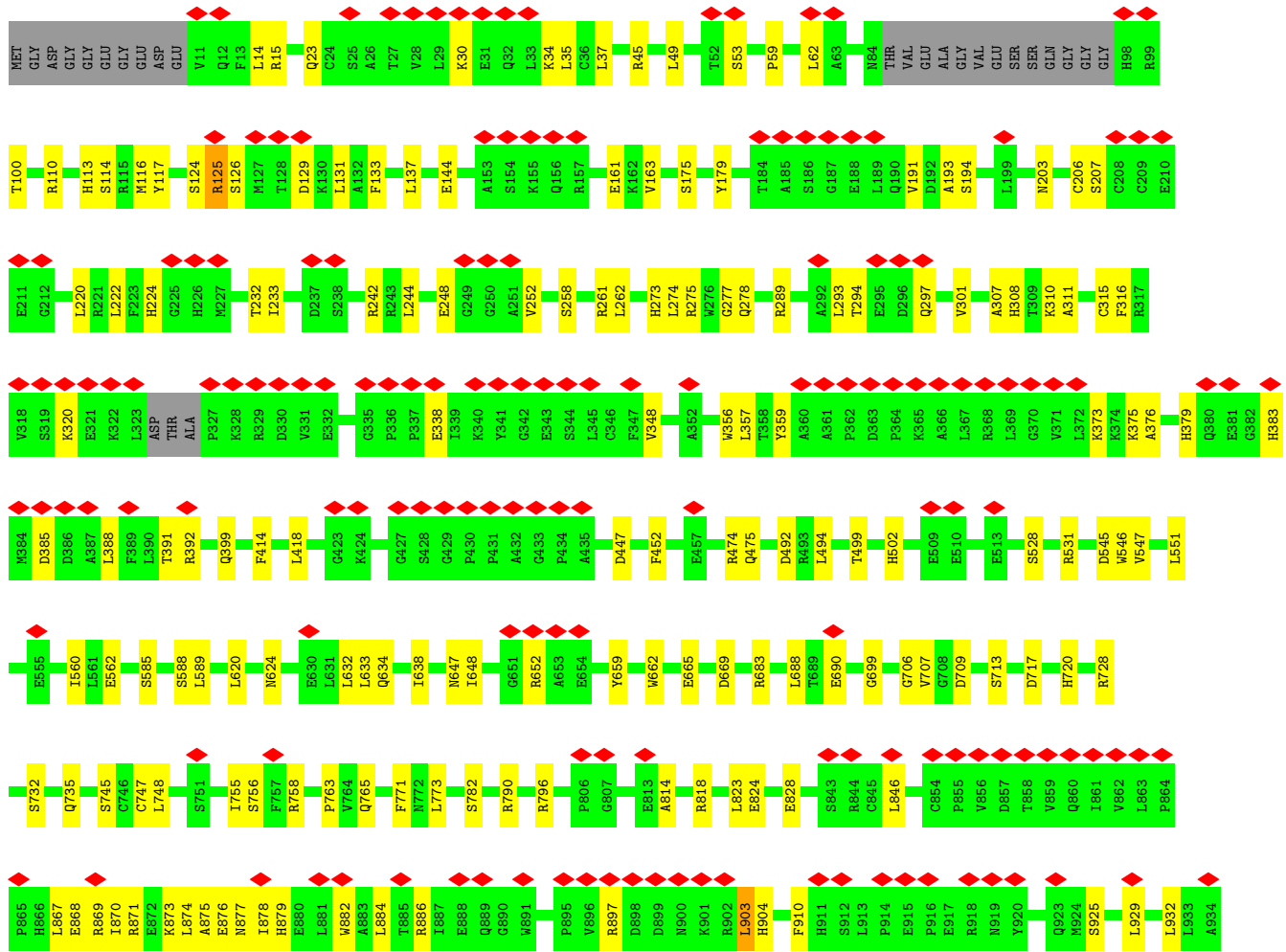


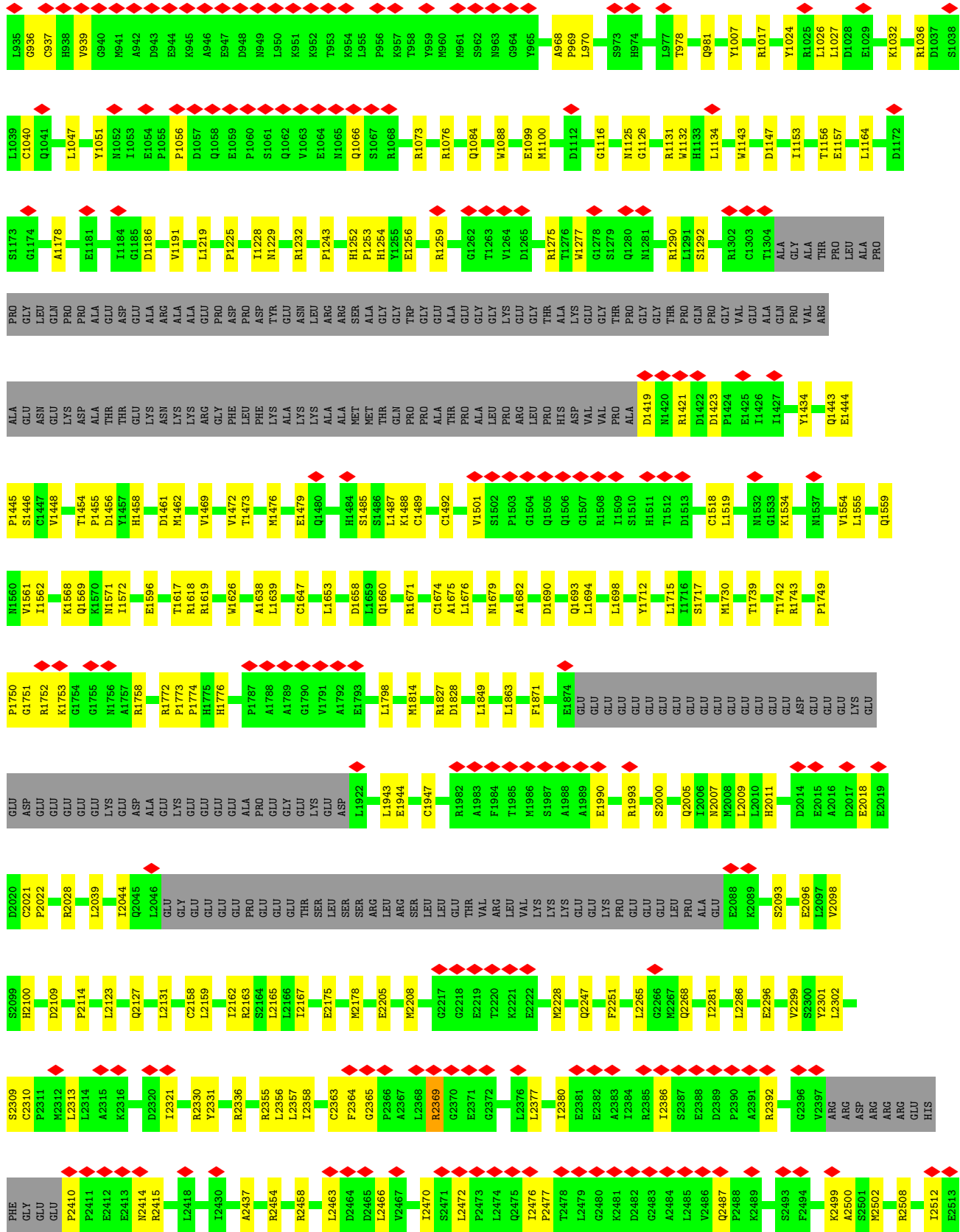




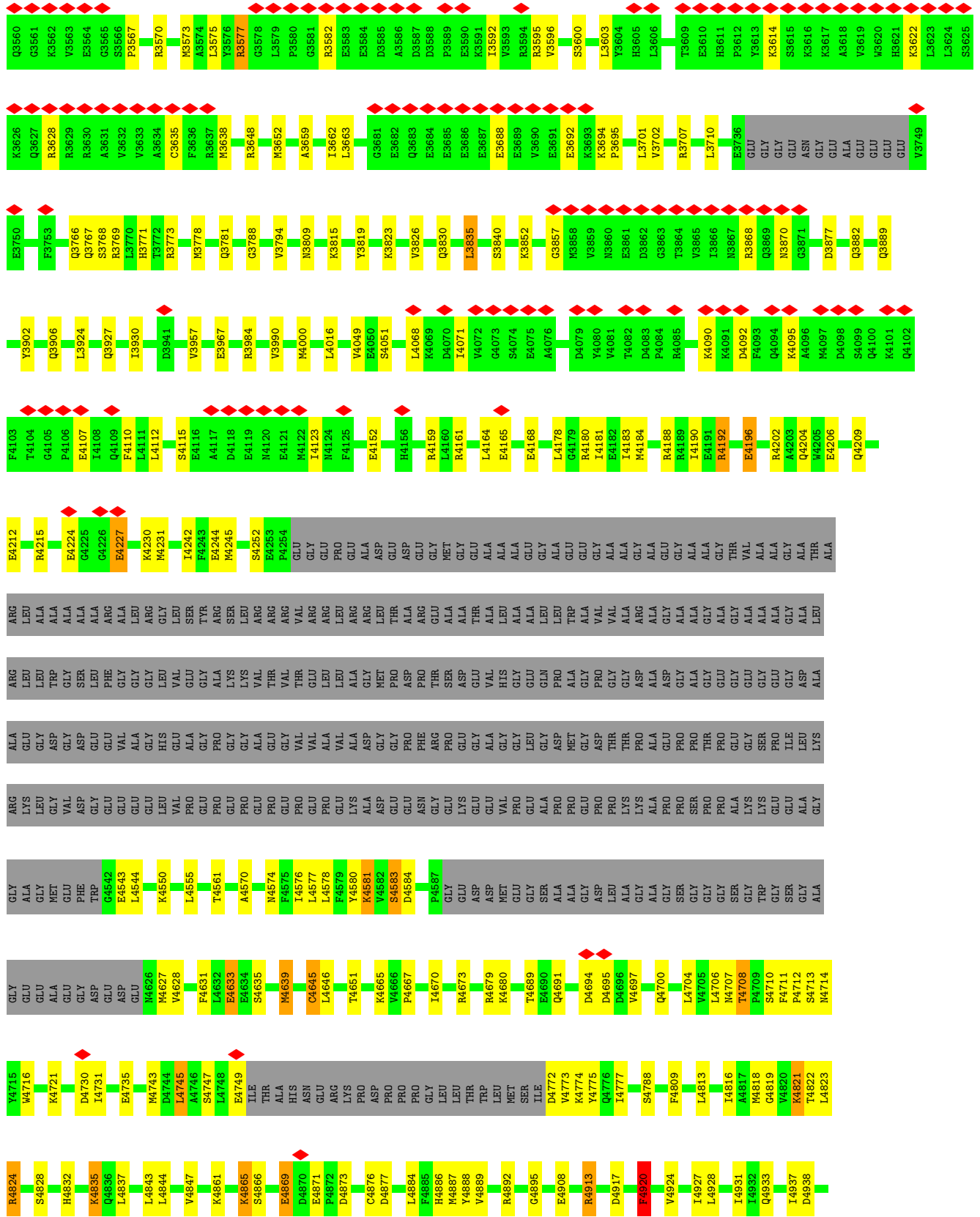


• Molecule 1: Ryanodine receptor 1





SER	R3403	R3404	I3413	R3414	D3417	N3418	R3420	A3421	H3422	W3423	L3424	E3426	P3427	N3430	F3435	F3442	H3449	N3450	R3453	F3458	V3459	V3460	Q3461	M3462	E3463	I3464	N3465	N3466	M3467	S3468	F3469	L3470	T3471	A3472	D3473	K3475	S3476	K3477	M3478	A3479	LYS	ALA	GLY	ASP	ASP	GLN	SER	GLY	SER	GLY	L3559												
	V3324	N3325	L3327	G3328	I3329	D3330	E3331	A3332	W3334	K3336	R3337	L3338	A3339	V3340	F3341	A3342	Q3343	P3344	I3345	V3346	S3347	R3348	P3351	I3359	G3363	R3364	L3365	R3366	K3367	R3368	V3373	E3376	E3377	Q3378	L3379	R3380	E3382	A3383	K3384	A3385	K3386	A3387	E3388	E3389	G3390	E3391	L3392	L3393	V3394	R3395													
	M3239	C3240	P3241	D3242	I3243	P3244	D3247	R3248	L3249	M3250	A3251	A3257	E3258	T3264	E3265	I3272	P3275	M3276	L3277	C3278	P3282	E3286	R3287	G3288	P3289	E3290	A3291	P3292	P3293	P3294	A3295	L3296	P3297	A3298	G3299	A3300	P3301	P3302	P3303	C3304	T3305	A3306	S3309	L3316	M3317	I3319	L3320	L3321	R3322	L3323	R3324	I3325											
	H3150	Q3151	D3154	D3155	V3156	I3157	L3158	D3159	S3171	L3175	T3178	K3179	N3180	T3181	Y3182	V3183	E3184	K3185	L3197	M3201	P3202	V3203	P3208	Q3209	L3210	N3211	E3212	Y3213	N3214	A3215	C3216	S3217	V3218	Y3219	T3220	T3221	K3222	S3223	P3224	R3225	E3226	R3227	A3228	I3229	L3230	G3231	L3232	P3233	N3234	S3235	V3236	E3237											
	H3052	R3053	G3058	T3059	P3062	V3065	L3075	R3078	T3079	M3081	K3082	S3083	G3084	P3085	E3086	R3087	L3092	R3098	S3094	F3095	A3099	D3102	M3106	V3107	L3110	R3111	L3112	G3113	K3114	V3115	S3116	GLN	ALA	ARG	THR	VAL	K3123	G3124	N3128	V3134	A3135	L3136	H3146	Q3149																			
	K2881	Q2882	E2883	L2884	E2885	A2886	K2887	G2888	G2889	G2900	T2901	H2902	P2903	V2904	V2981	S2982	S2983	G2984	R2985	V2986	E2987	K2988	S2989	P2990	H2991	E2992	K2996	F2997	F2998	L3002	H3013	T3020	P3021	E2925	L2926	L2927	K2928	F2929	Q2931	M2932	M2933	G2934	Y2935	M3008	L3042	L3046	A3047	A3048	R3051														
	L2710	P2711	D2712	Q2713	Y2714	V2715	S2718	Y2719	S2720	S2721	K2722	A2723	E2724	K2725	LYS	ALA	TYR	L2785	K2786	VAL	ASP	ASP	ALA	GLU	GLY	M2734	P2735	D2736	P2737	K2738	P2739	V2740	E2741	T2742	L2743	E2744	V2745	L2746	L2747	E2671	H2673	L2674	L2678	T2682	S2685	L2686	A2687	H2688	K2689	L2690	R2600	D2692	E2693	F2694	L2695								
	L2623	Q2514	D2516	F2517	L2518	V2521	L2522	D2523	V2524	G2525	R2531	A2532	A2533	A2534	S2535	L2536	A2539	T2540	Y2553	L2559	P2560	L2561	I2562	T2563	K2564	C2565	A2570	G2571	T2572	E2573	H2574	R2575	A2576	T2577	H2578	S2581	R2591	G2592	R2593	S2594	L2595	R2600	D2605	L2614	L2619	Q2620	H2621	L2622															
	L2771	Q2772	M2773	N2774	S2775	M2776	Y2777	G2778	E2779	M2780	V2781	D2782	E2783	E2784	L2785	K2786	T2787	H2788	P2789	M2790	L2791	R2792	F2793	Y2794	K2795	T2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	L2804	L2805	R2806	M2807	P2808	L2809	K2810	E2811	S2812	L2813	K2814	A2815	E2816	M2816	L2817	A2818	M2819	E2820	M2821	G2822	I2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830		
	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	SER	GLN	THR	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU	GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	S2863	V2865	E2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	N2884	T2885	W2886	L2887	LYS	ASP	MET	GLU	L2946	D2947	T2948	E2952



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

Chain H:  26% • 69%

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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 (\AA)	515.2, 515.2, 515.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: AMP, 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	0.34	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%)	51	82
1	B	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	51	82
1	C	4353/5037 (86%)	4200 (96%)	148 (3%)	5 (0%)	51	82
1	D	4353/5037 (86%)	4199 (96%)	149 (3%)	5 (0%)	51	82
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%)	54	82

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 [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	3805/4276 (89%)	3675 (97%)	130 (3%)	37	65
1	B	3805/4276 (89%)	3675 (97%)	130 (3%)	37	65
1	C	3805/4276 (89%)	3674 (97%)	131 (3%)	37	65
1	D	3805/4276 (89%)	3674 (97%)	131 (3%)	37	65
2	E	88/304 (29%)	87 (99%)	1 (1%)	73	86
2	F	88/304 (29%)	87 (99%)	1 (1%)	73	86
2	G	88/304 (29%)	87 (99%)	1 (1%)	73	86
2	H	88/304 (29%)	87 (99%)	1 (1%)	73	86

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	15572/18320 (85%)	15046 (97%)	526 (3%)	41 65

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 monosaccharides 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	-	22,25,25	0.83	1 (4%)	25,38,38	1.23	2 (8%)
3	AMP	C	5101	-	22,25,25	0.83	1 (4%)	25,38,38	1.23	2 (8%)
3	AMP	D	5101	-	22,25,25	0.83	1 (4%)	25,38,38	1.23	2 (8%)
3	AMP	A	5101	-	22,25,25	0.83	1 (4%)	25,38,38	1.23	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	D	5101	-	-	2/6/26/26	0/3/3/3
3	AMP	A	5101	-	-	2/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5101	AMP	C5-C4	2.18	1.46	1.40
3	D	5101	AMP	C5-C4	2.18	1.46	1.40
3	C	5101	AMP	C5-C4	2.17	1.46	1.40
3	B	5101	AMP	C5-C4	2.17	1.46	1.40

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	-3.31	123.50	128.68
3	D	5101	AMP	N3-C2-N1	-3.31	123.50	128.68
3	C	5101	AMP	N3-C2-N1	-3.31	123.50	128.68
3	A	5101	AMP	N3-C2-N1	-3.31	123.51	128.68
3	A	5101	AMP	C4-C5-N7	-2.29	107.01	109.40

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

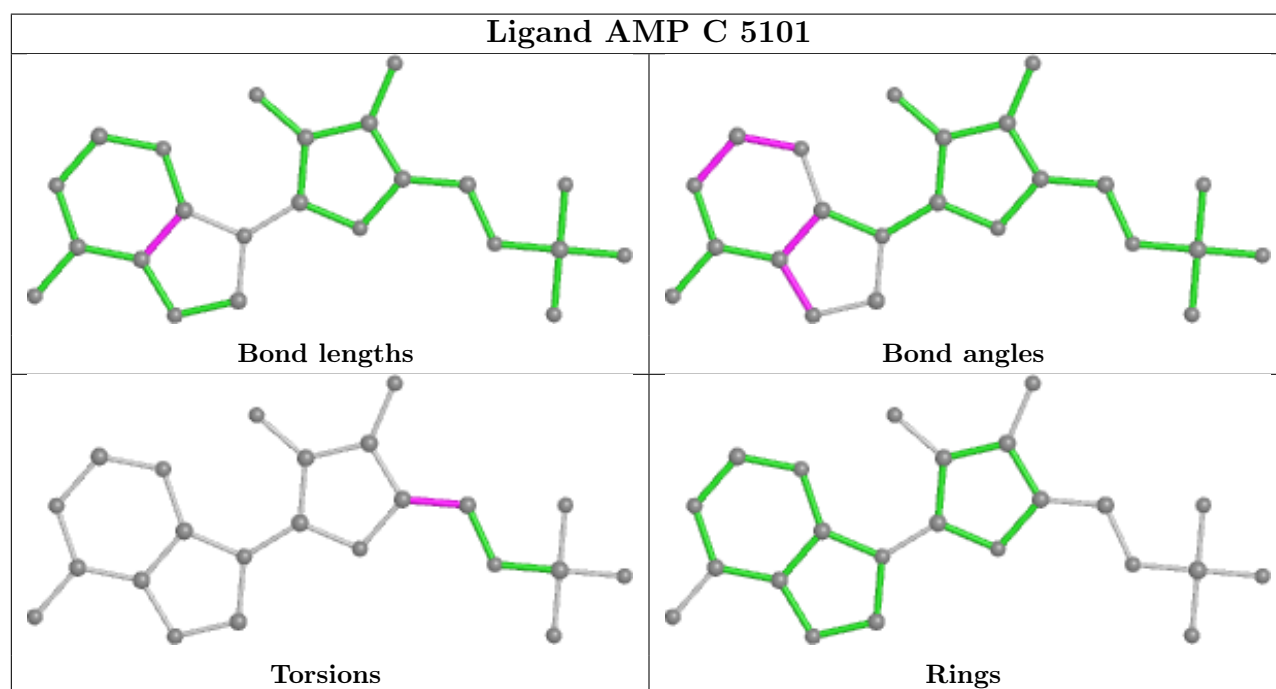
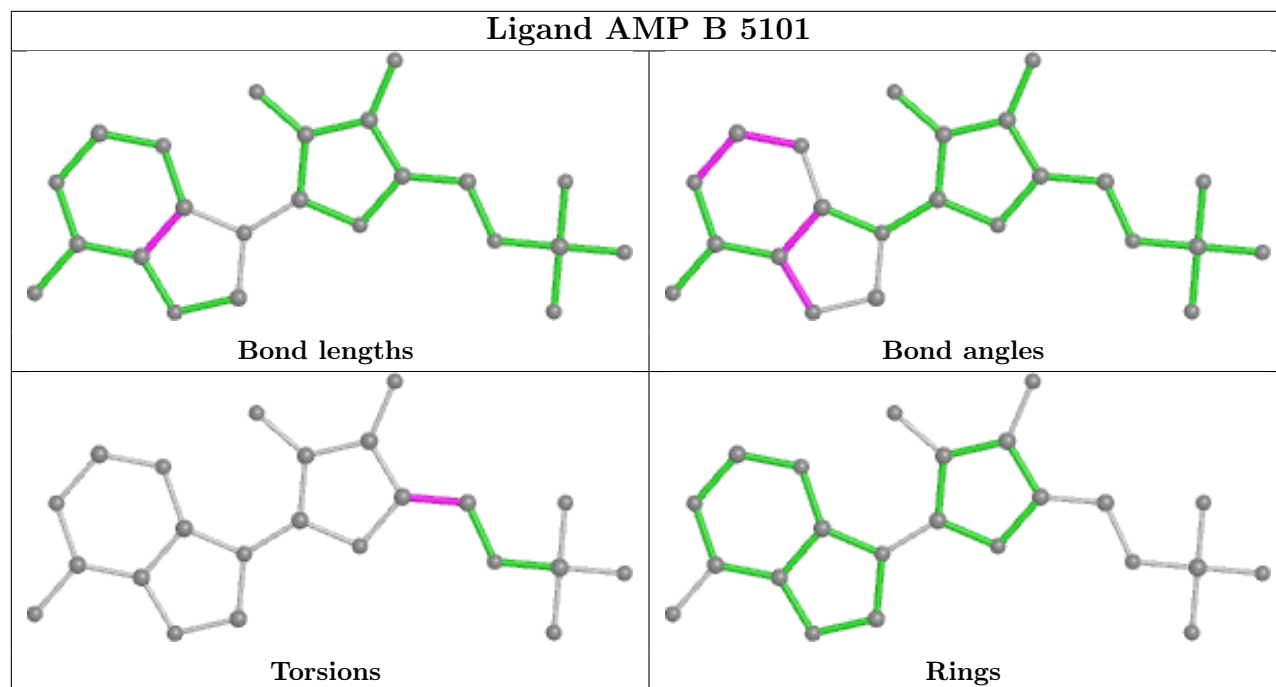
Mol	Chain	Res	Type	Atoms
3	A	5101	AMP	O4'-C4'-C5'-O5'
3	B	5101	AMP	O4'-C4'-C5'-O5'
3	C	5101	AMP	O4'-C4'-C5'-O5'
3	D	5101	AMP	O4'-C4'-C5'-O5'
3	A	5101	AMP	C3'-C4'-C5'-O5'

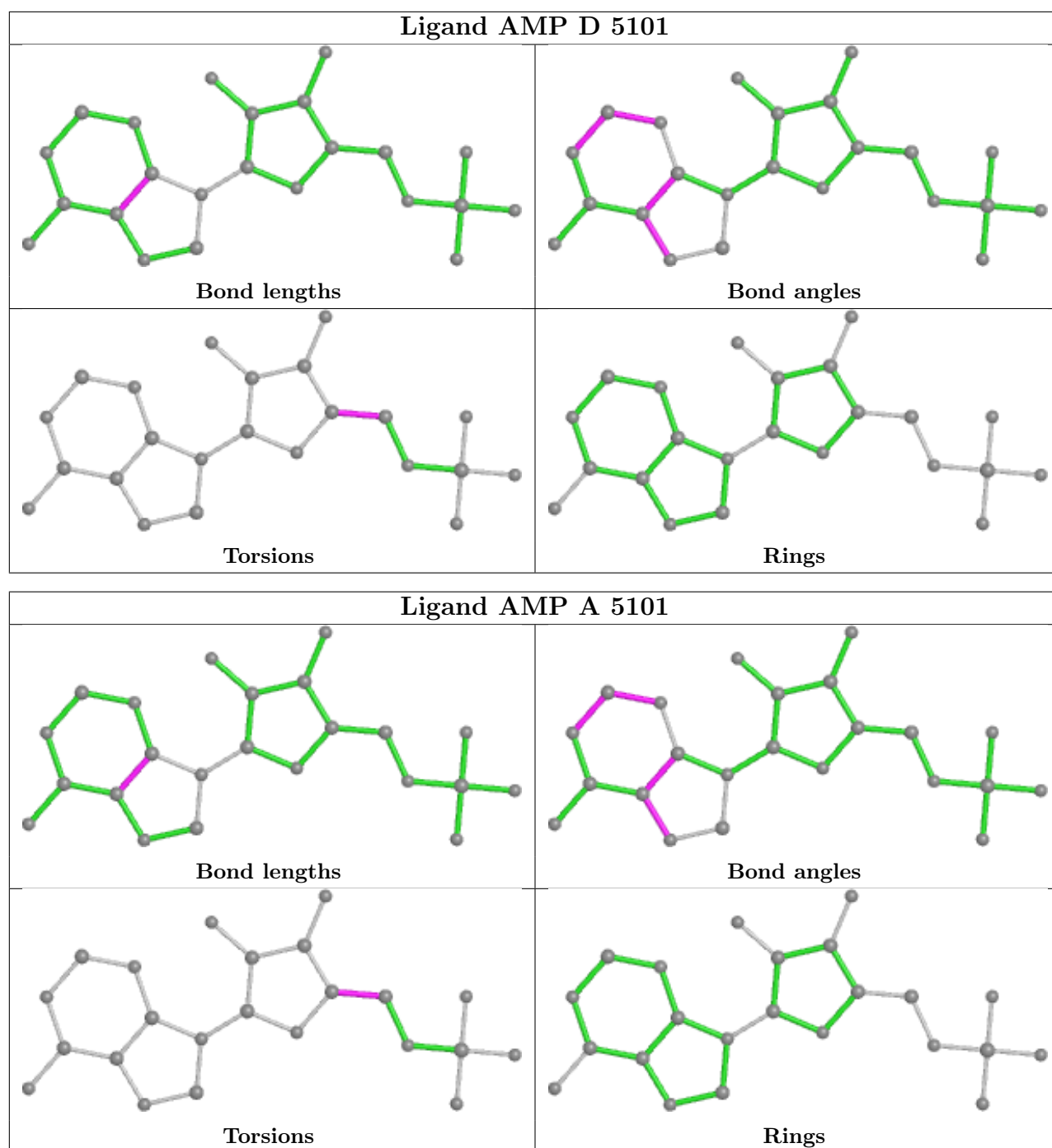
There are no ring outliers.

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	D	5101	AMP	1	0
3	A	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.





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.

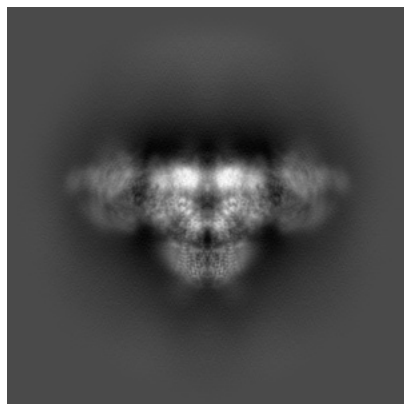
6 Map visualisation [i](#)

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.

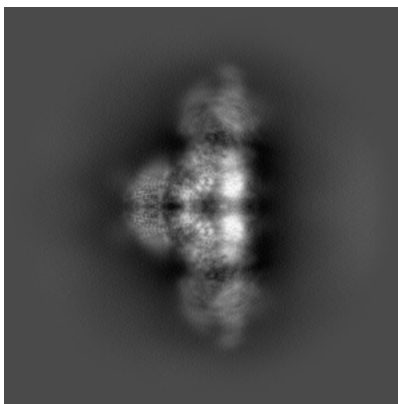
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

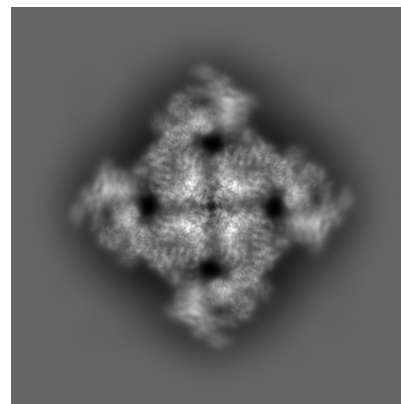
6.1.1 Primary map



X

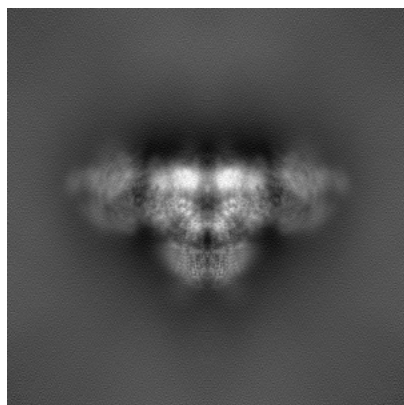


Y

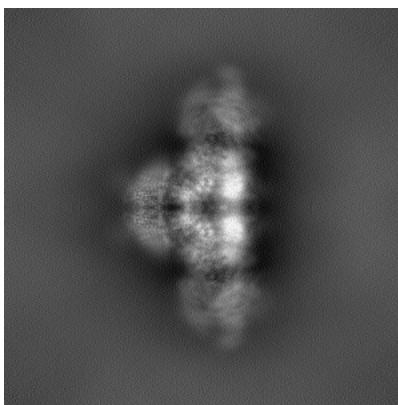


Z

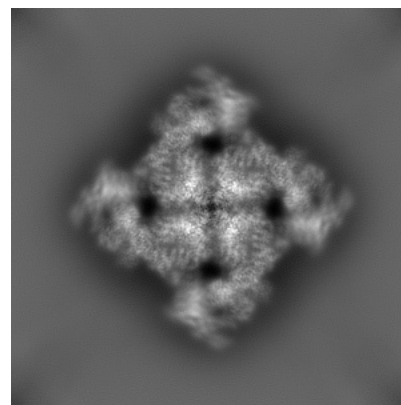
6.1.2 Raw map



X



Y

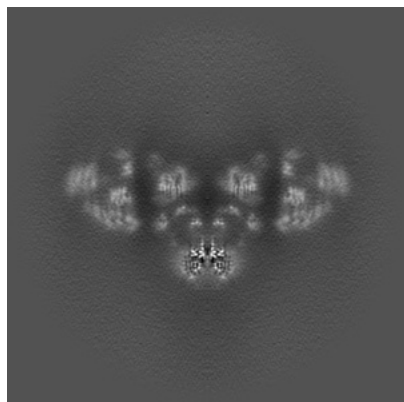


Z

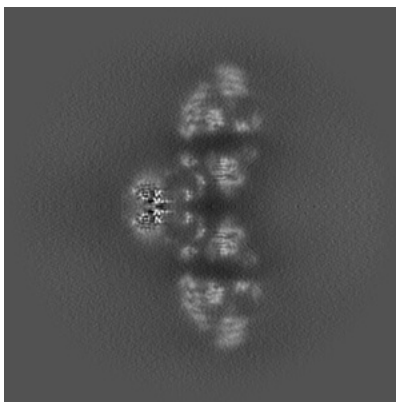
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

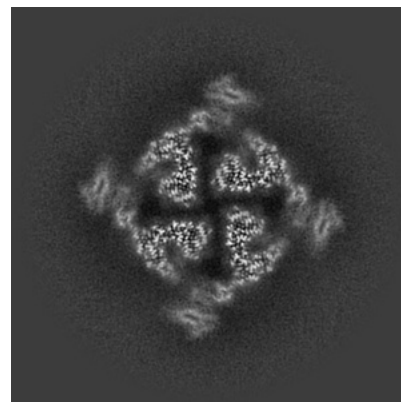
6.2.1 Primary map



X Index: 200

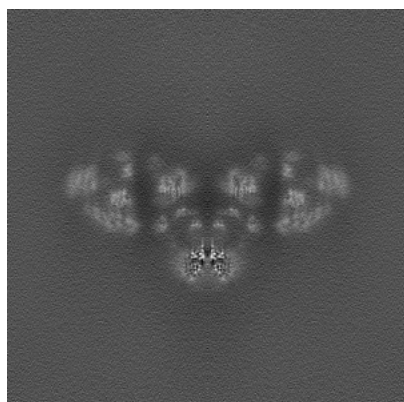


Y Index: 200

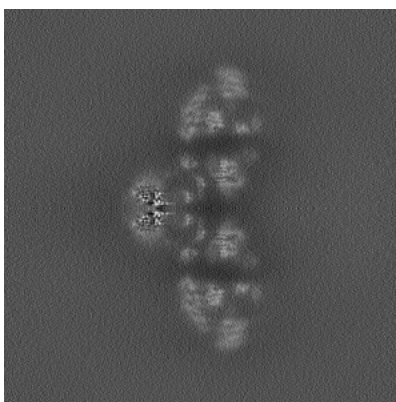


Z Index: 200

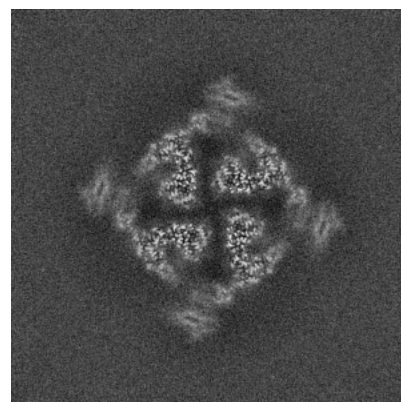
6.2.2 Raw map



X Index: 200



Y Index: 200

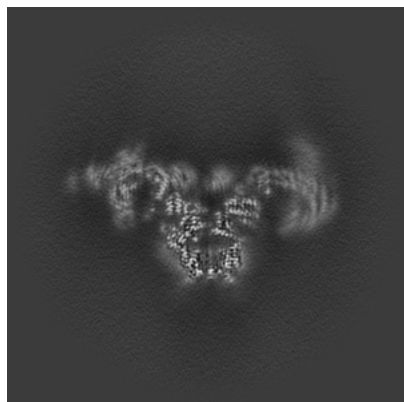


Z Index: 200

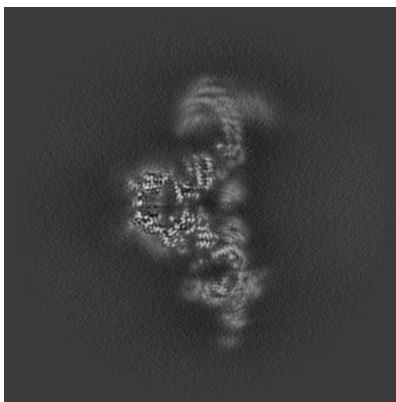
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

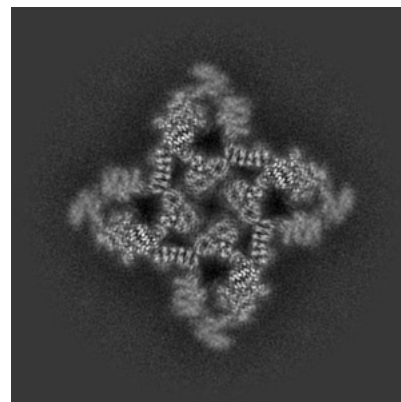
6.3.1 Primary map



X Index: 218

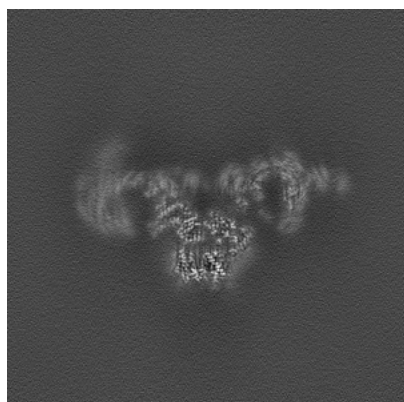


Y Index: 182

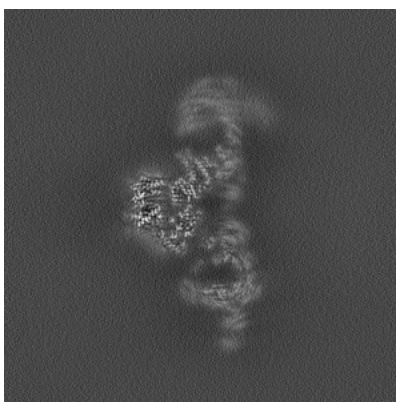


Z Index: 223

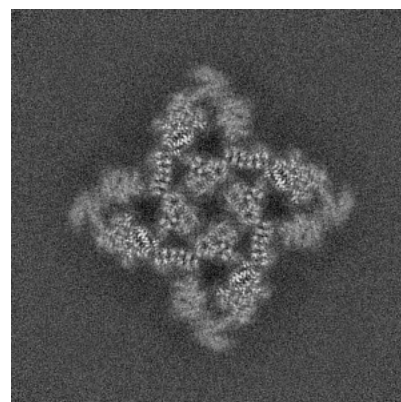
6.3.2 Raw map



X Index: 186



Y Index: 186

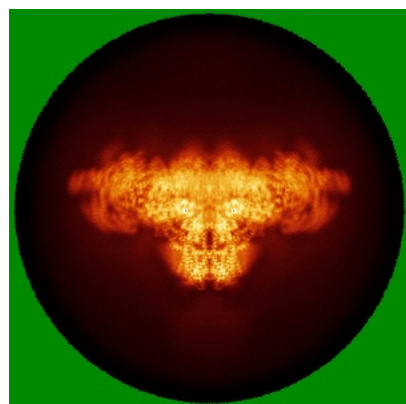


Z Index: 222

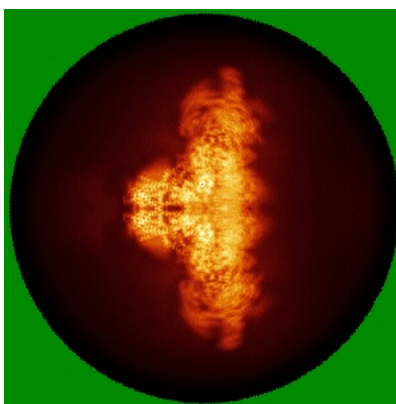
The images above show the largest variance slices of the map in three orthogonal directions.

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

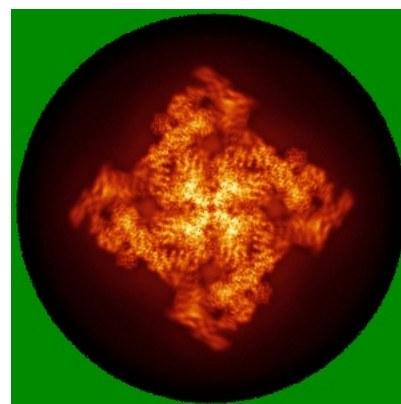
6.4.1 Primary map



X

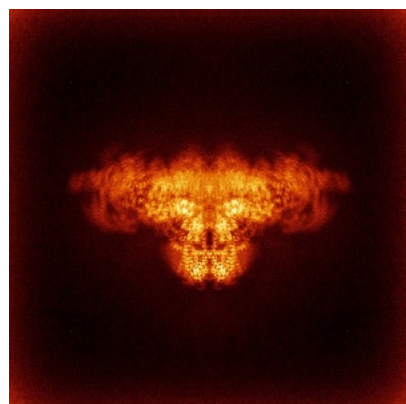


Y

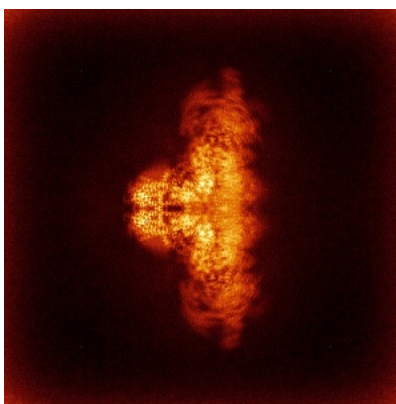


Z

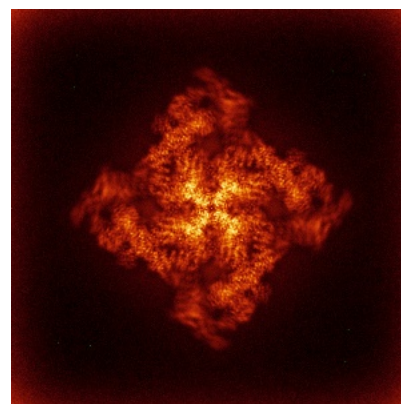
6.4.2 Raw map



X



Y

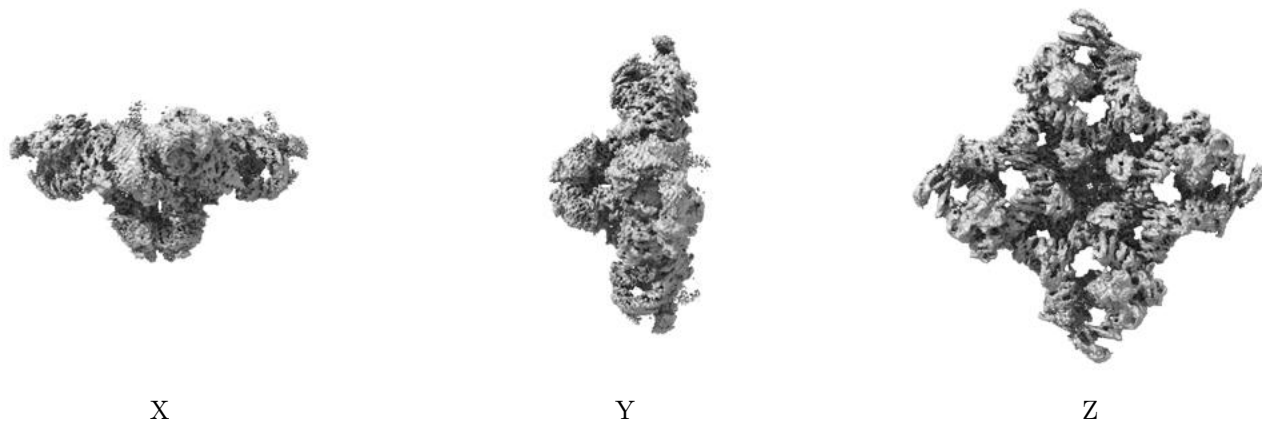


Z

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.

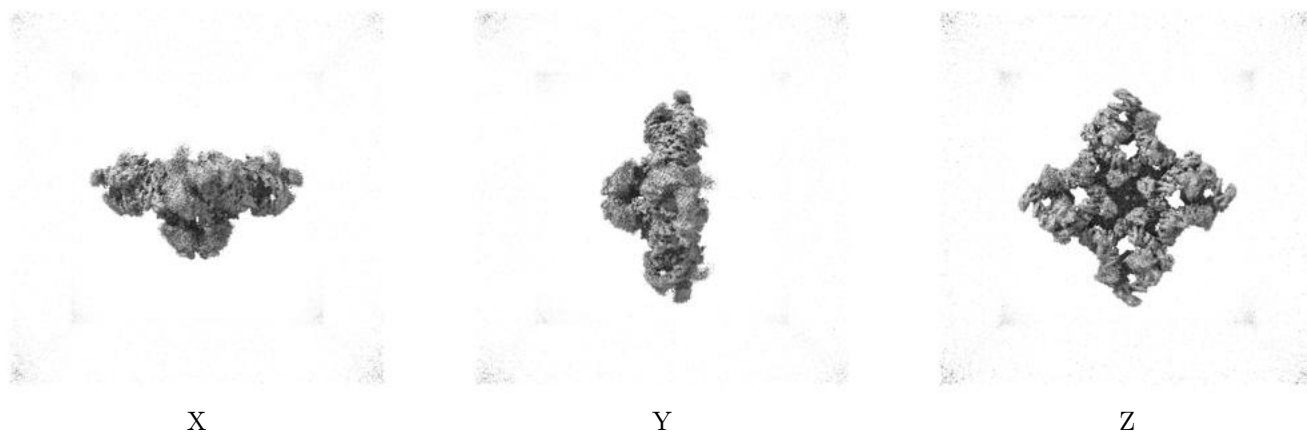
6.5 Orthogonal surface views [i](#)

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.

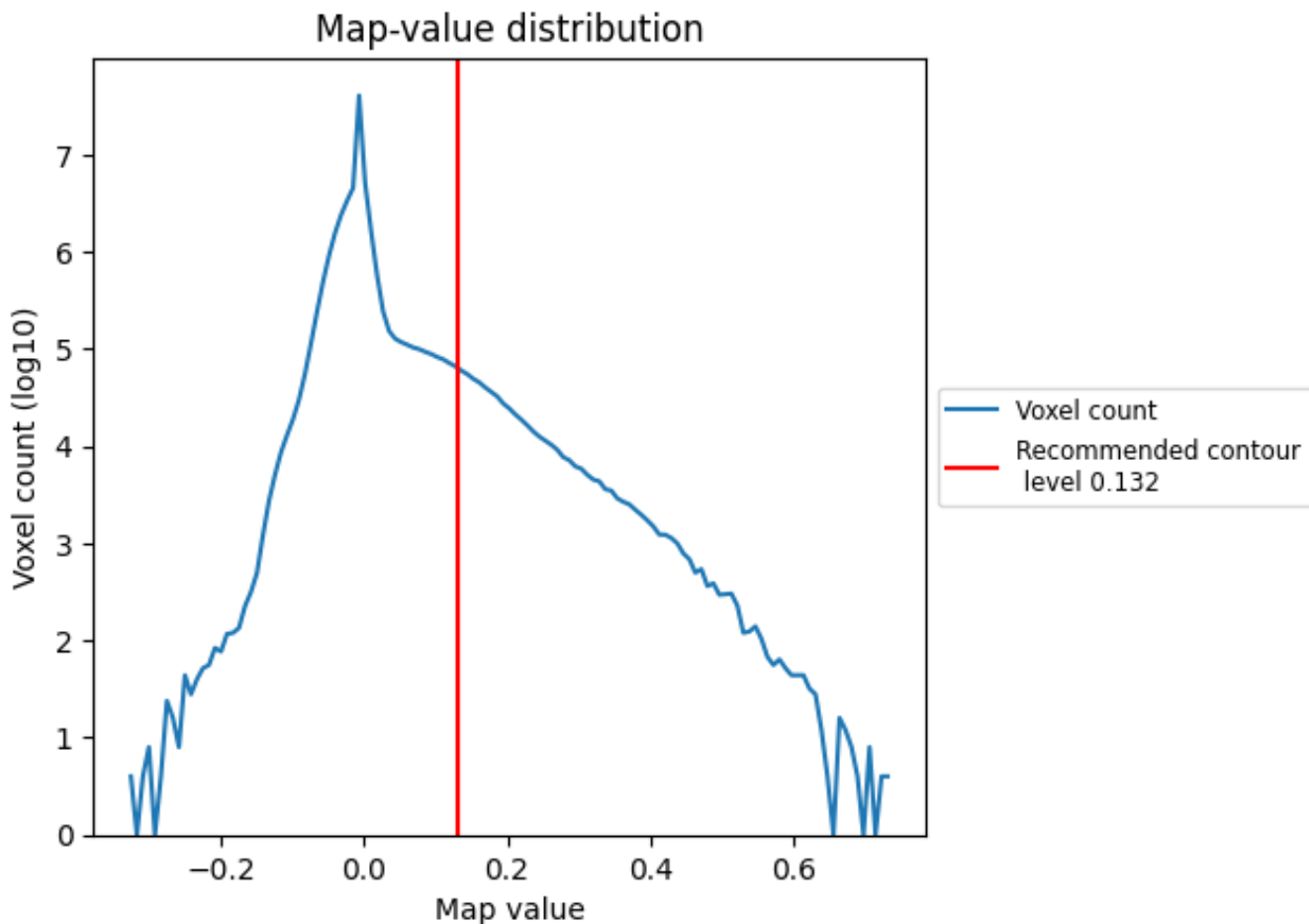
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

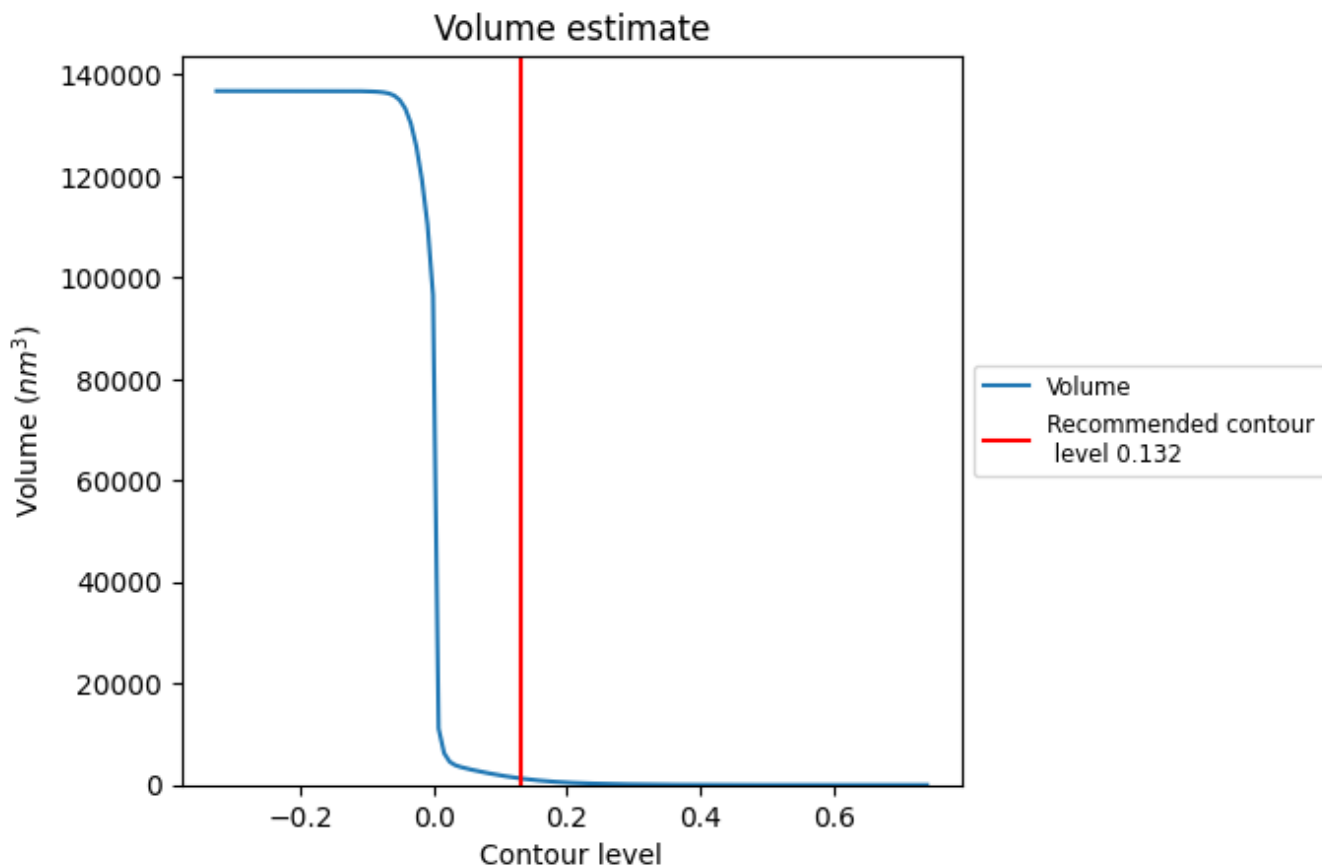
This section contains the results of statistical analysis of the map.

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.

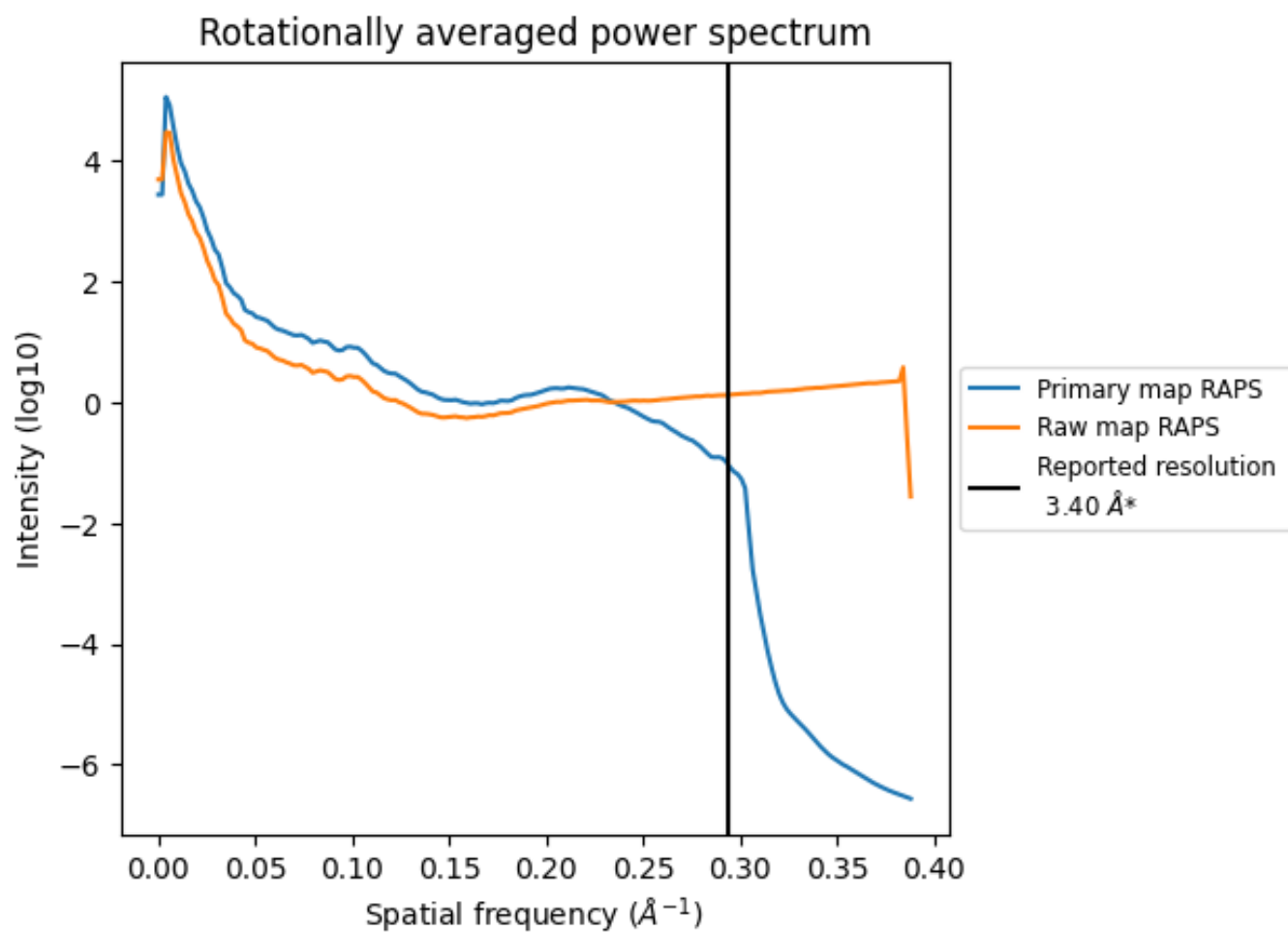
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1261 nm³; 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 i

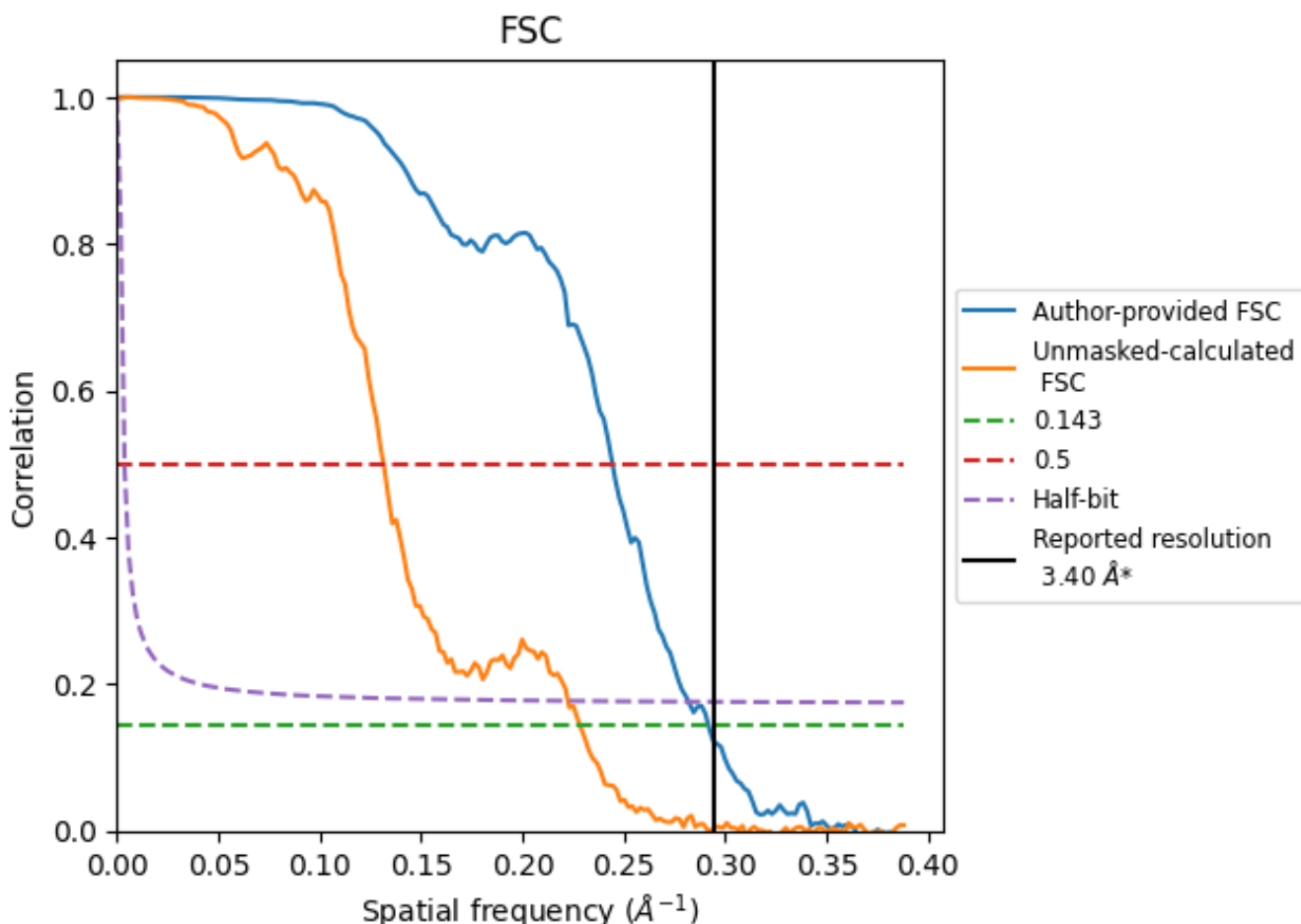


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

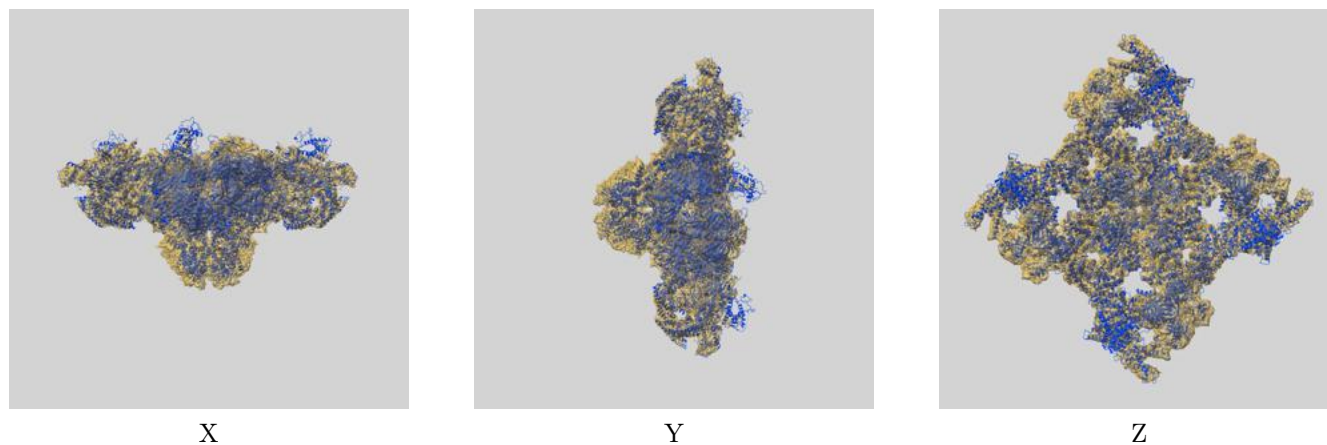
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.09	3.55
Unmasked-calculated*	4.37	7.60	4.49

*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](#)

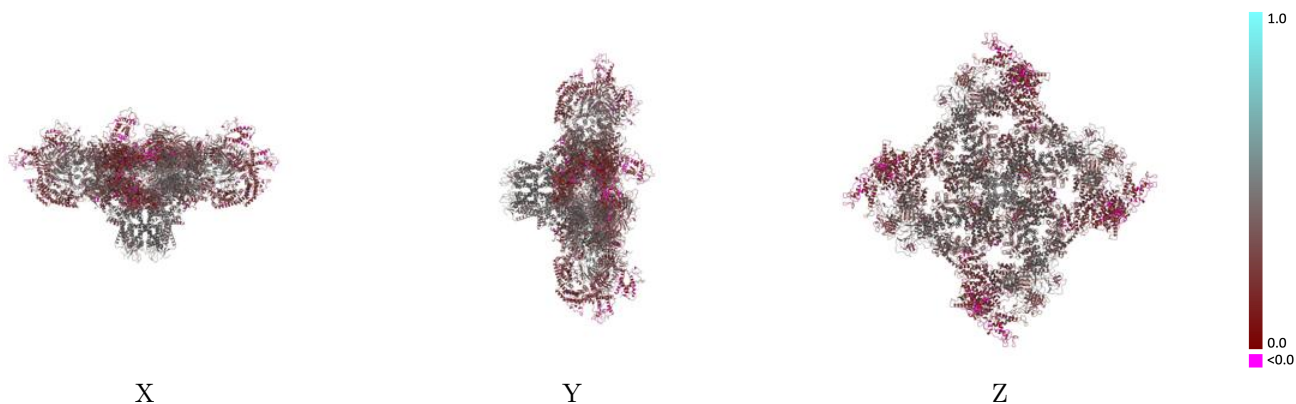
This section contains information regarding the fit between EMDB map EMD-40425 and PDB model 8SEQ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



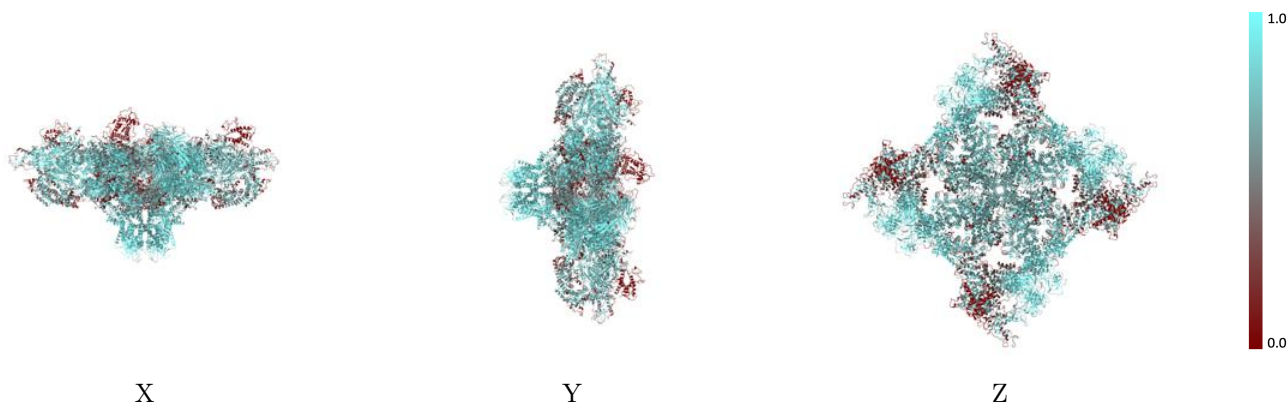
The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



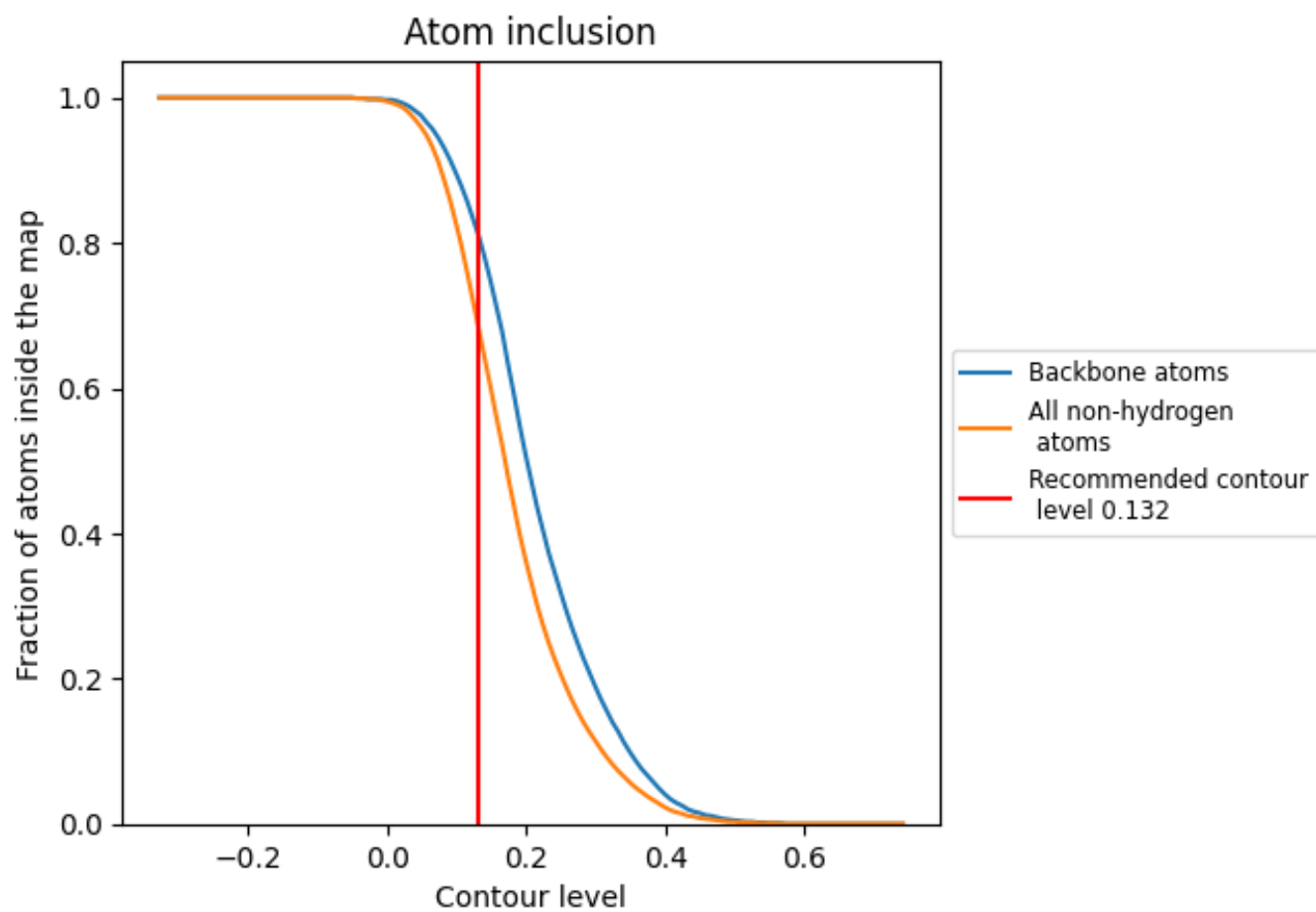
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



















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	 0.6820	 0.3220
A	 0.6780	 0.3210
B	 0.6790	 0.3200
C	 0.6790	 0.3200
D	 0.6790	 0.3200
E	 0.8500	 0.3890
F	 0.8500	 0.3880
G	 0.8500	 0.3900
H	 0.8500	 0.3930

