



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 11:22 PM EST

PDB ID : 6WOV
EMDB ID : EMD-21862
Title : Cryo-EM structure of recombinant mouse Ryanodine Receptor type 2 wild type in complex with FKBP12.6
Authors : Iyer, K.A.; Hu, Y.; Nayak, A.R.; Kurebayashi, N.; Murayama, T.; Samsó, M.
Deposited on : 2020-04-25
Resolution : 5.10 Å (reported)
Based on initial model : 5L1D

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

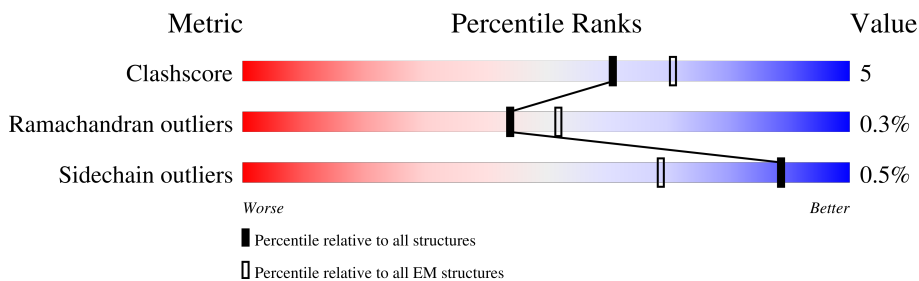
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4966	
1	B	4966	
1	C	4966	
1	D	4966	
2	E	107	
2	F	107	
2	G	107	
2	H	107	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 245656 atoms, of which 120412 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	3921	59769	19350	29277	5253	5698	191	0	0
1	B	3921	59772	19350	29280	5253	5698	191	0	0
1	C	3921	59773	19350	29281	5253	5698	191	0	0
1	D	3921	59770	19350	29278	5253	5698	191	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	107	1642	516	824	144	154	4	0	0
2	F	107	1642	516	824	144	154	4	0	0
2	G	107	1642	516	824	144	154	4	0	0
2	H	107	1642	516	824	144	154	4	0	0

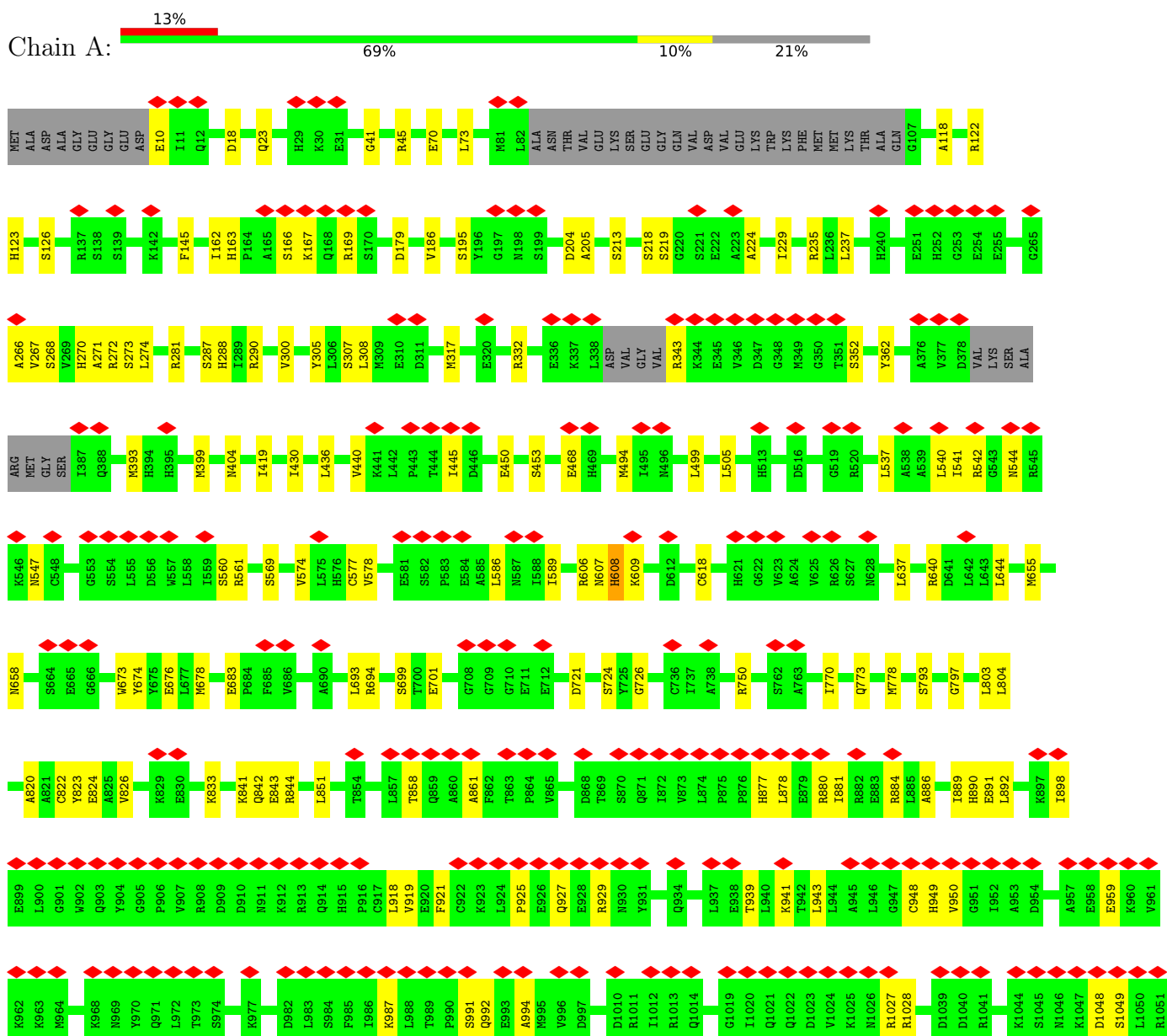
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

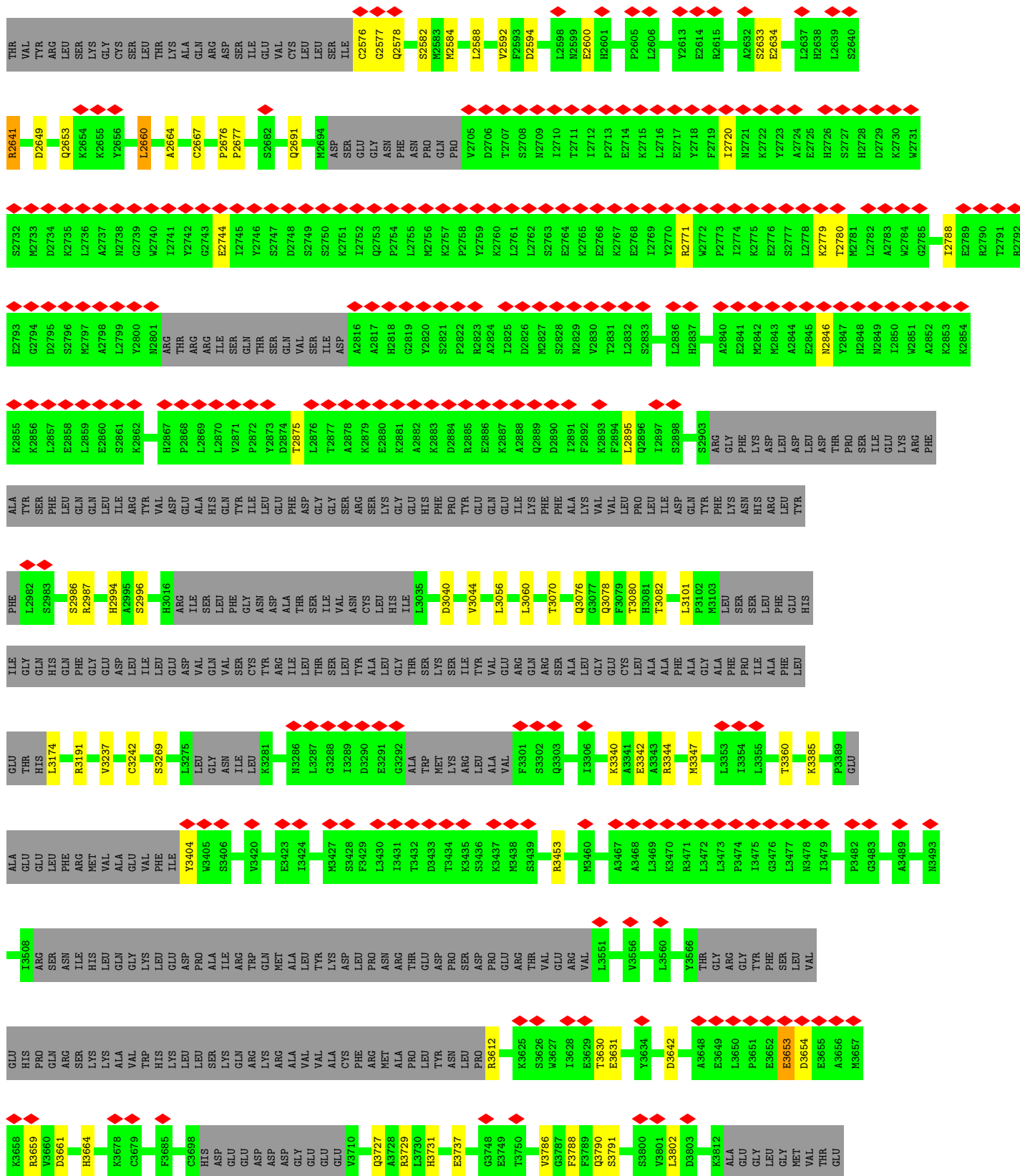
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

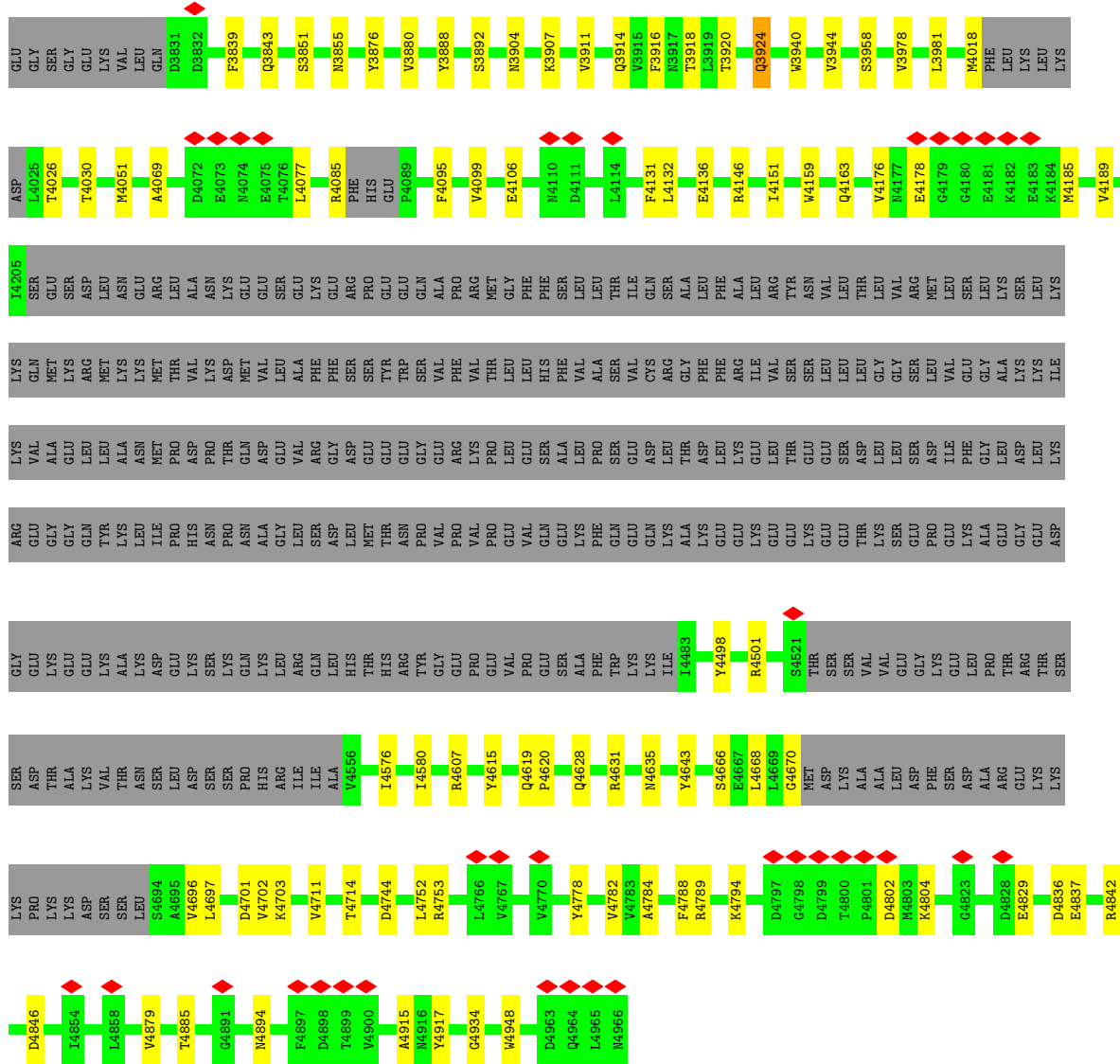
3 Residue-property plots [i](#)

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

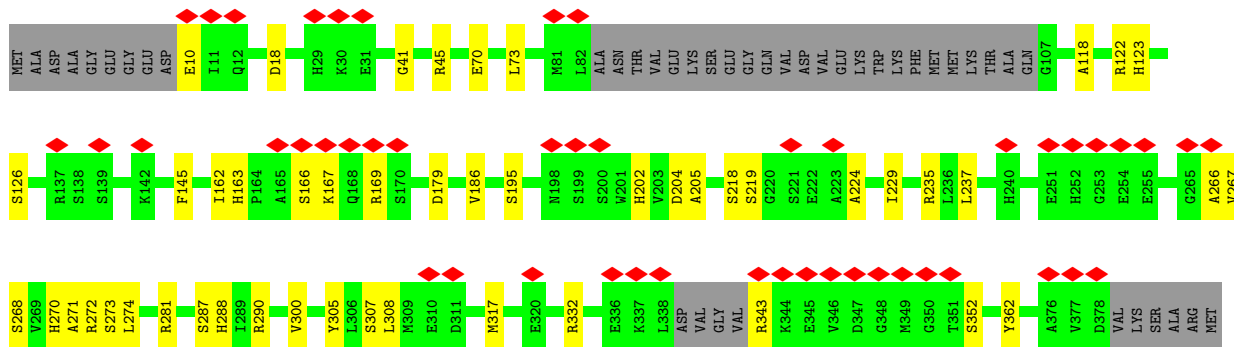
- Molecule 1: Ryanodine receptor 2

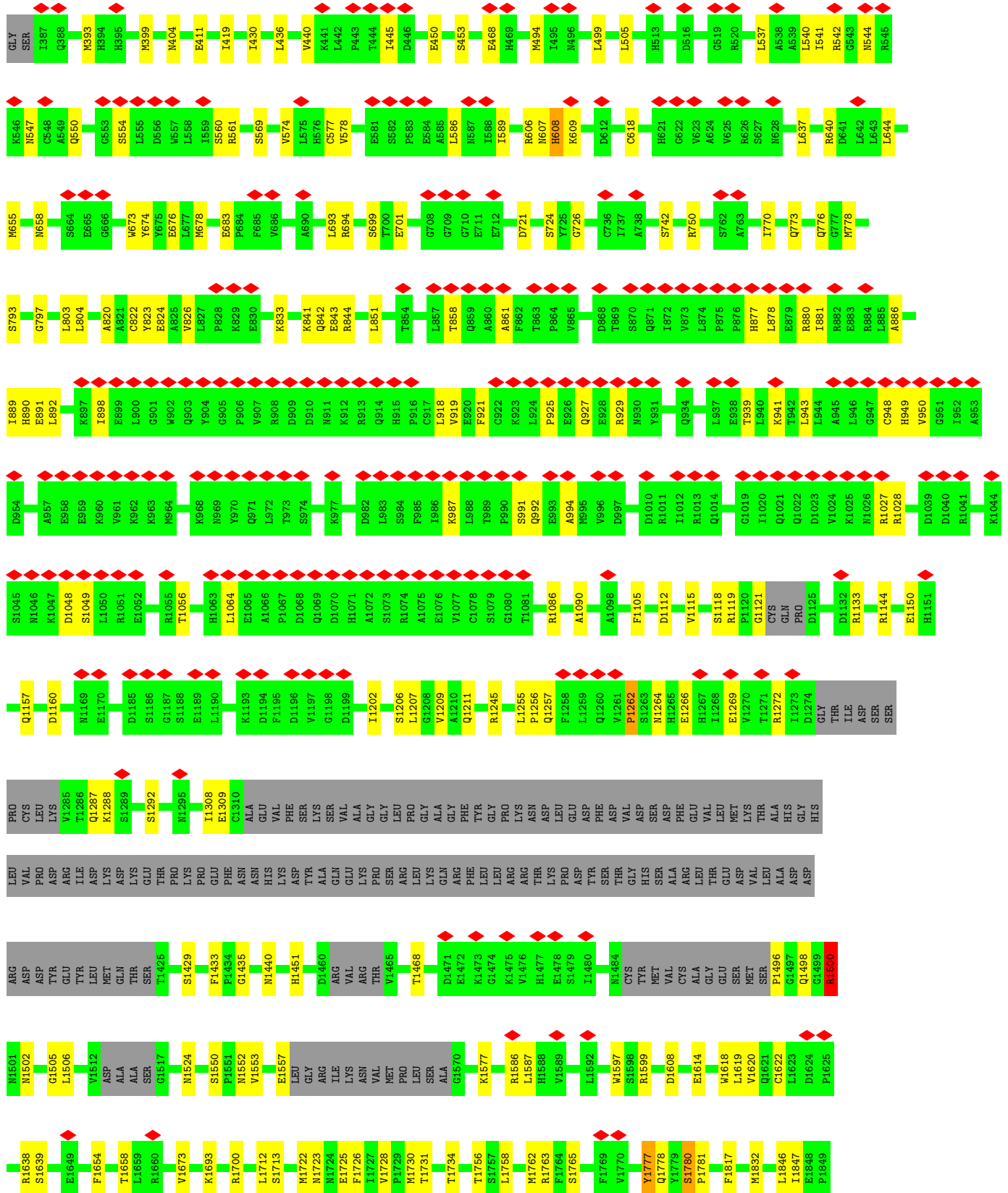


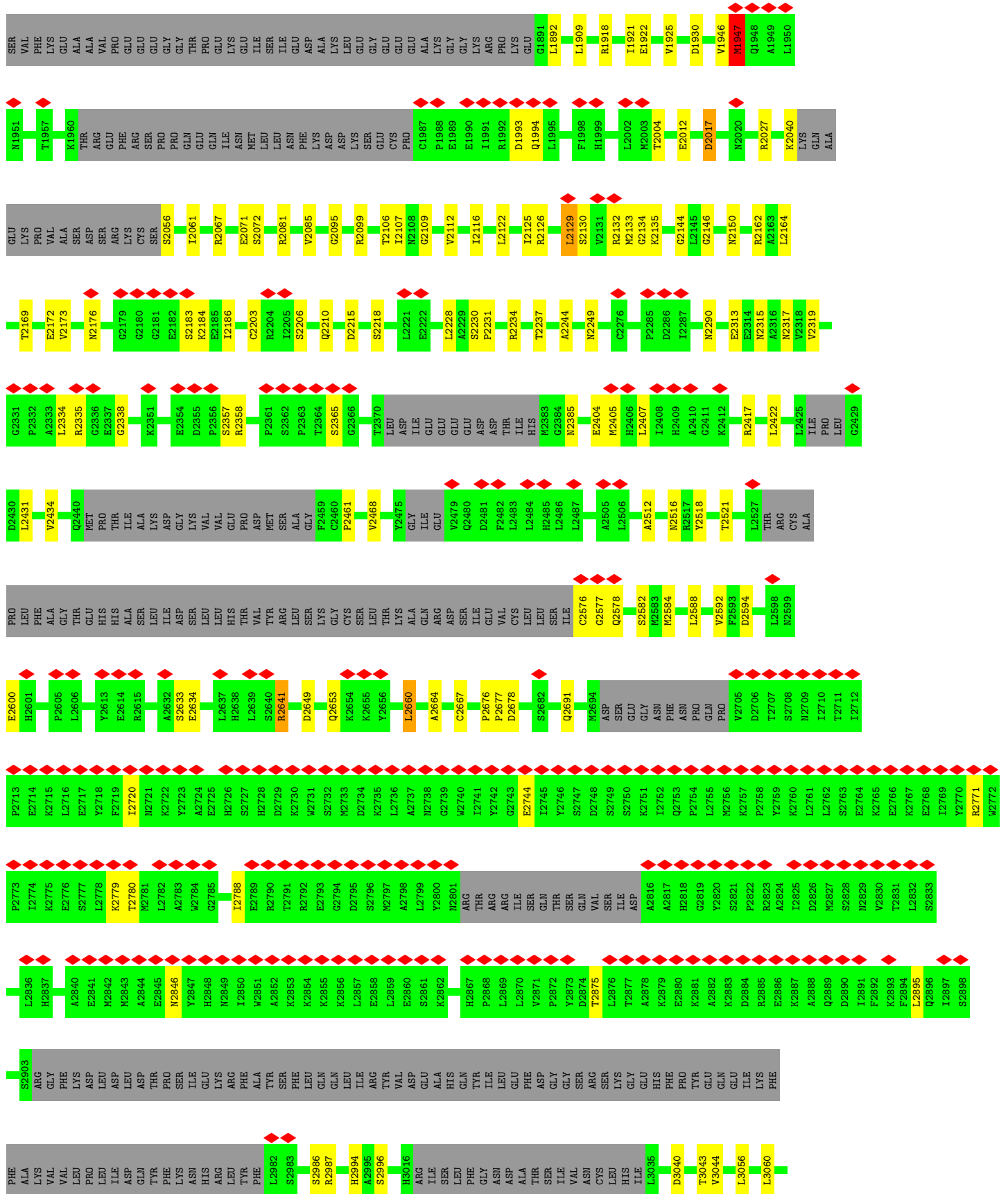


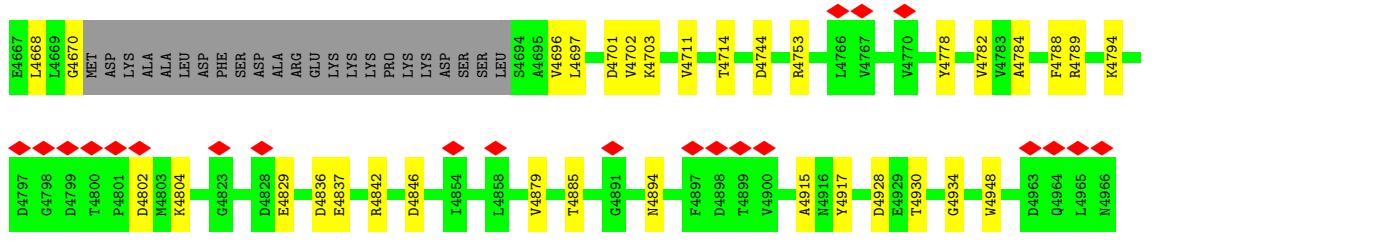


● Molecule 1: Ryanodine receptor 2

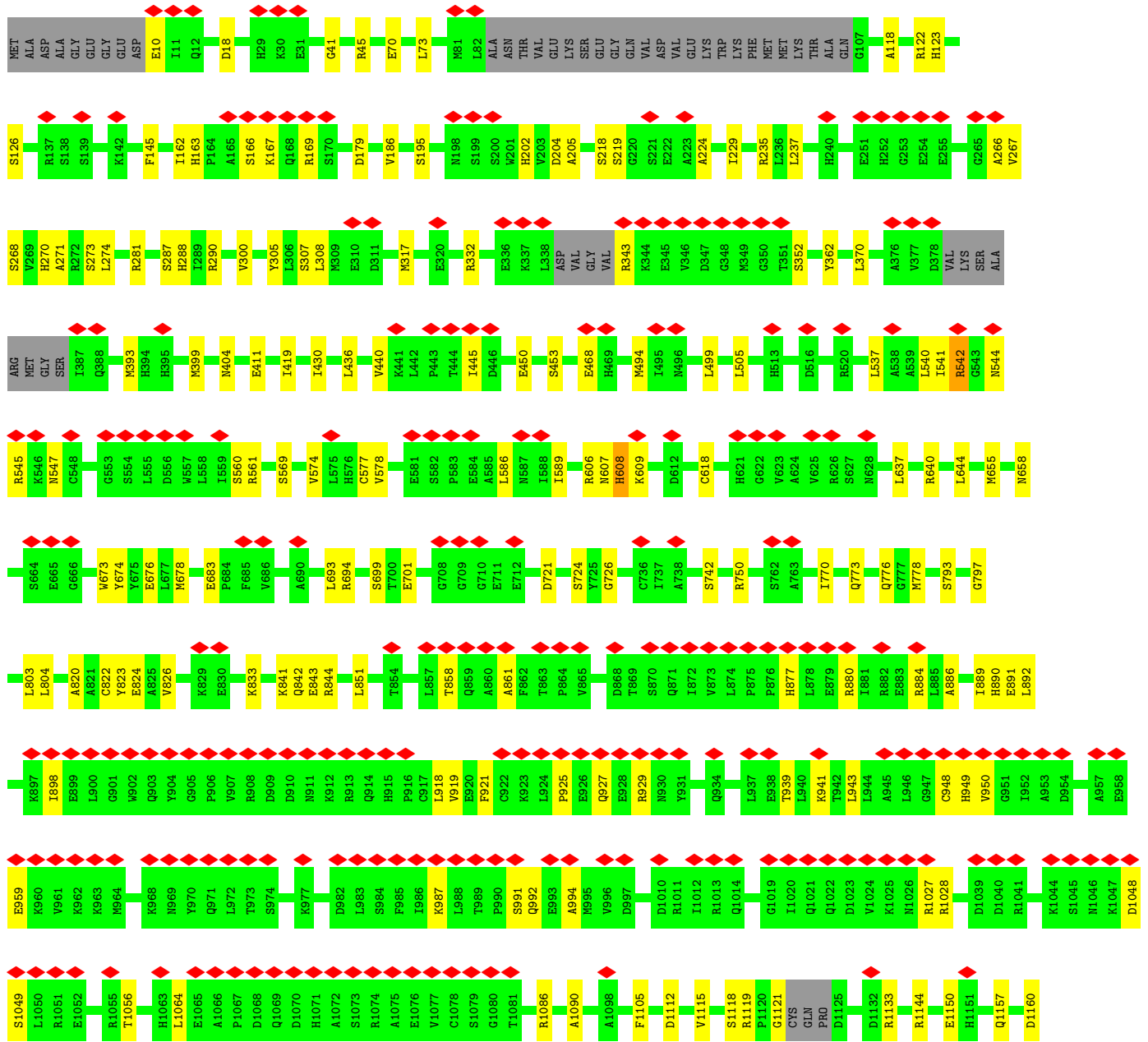




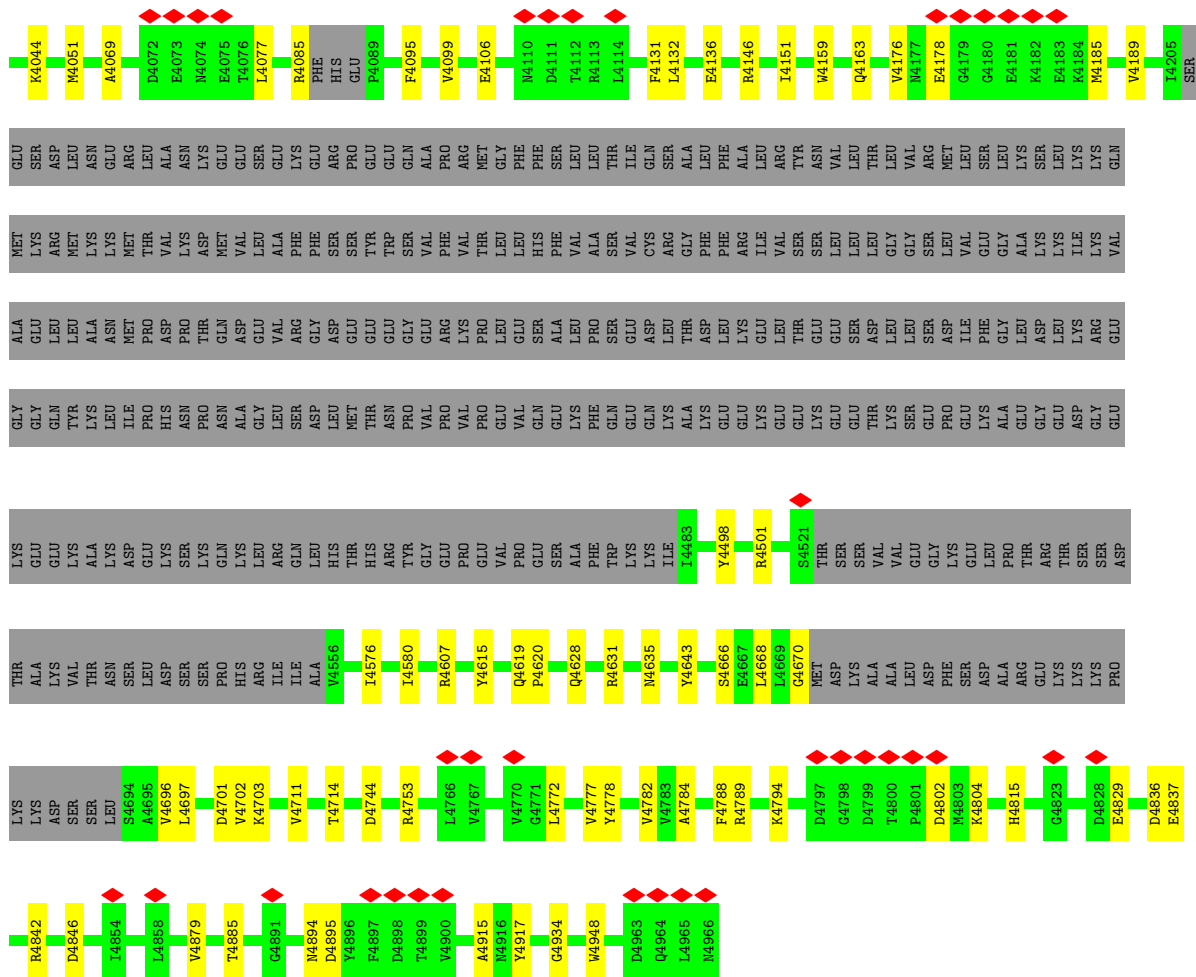




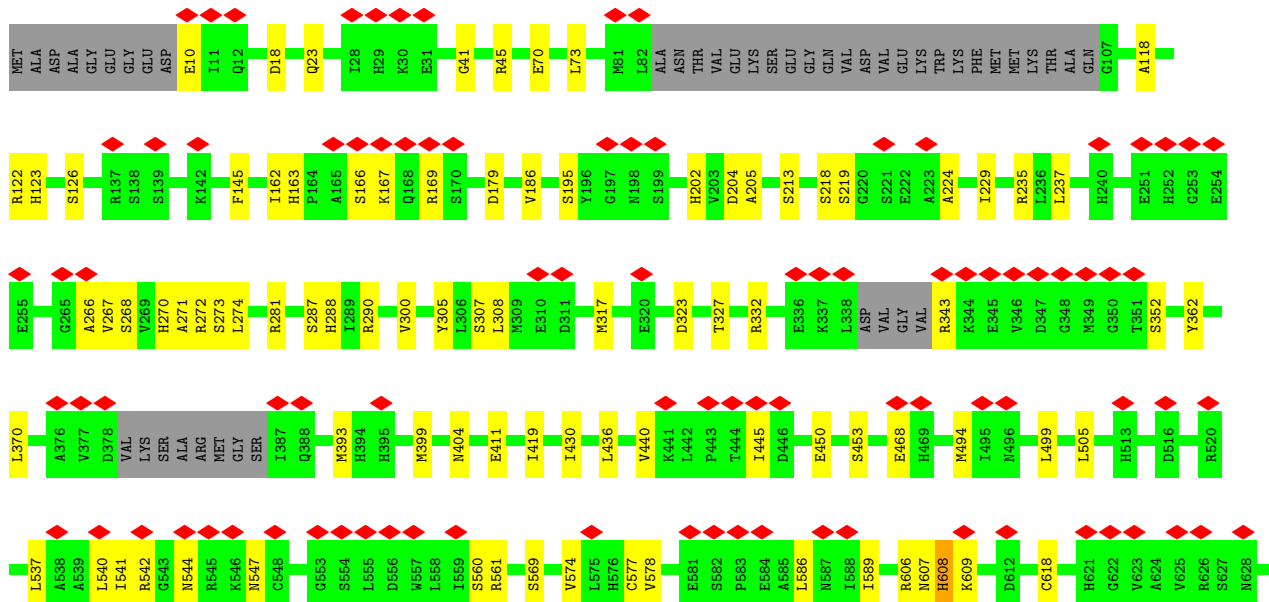
• Molecule 1: Ryanodine receptor 2

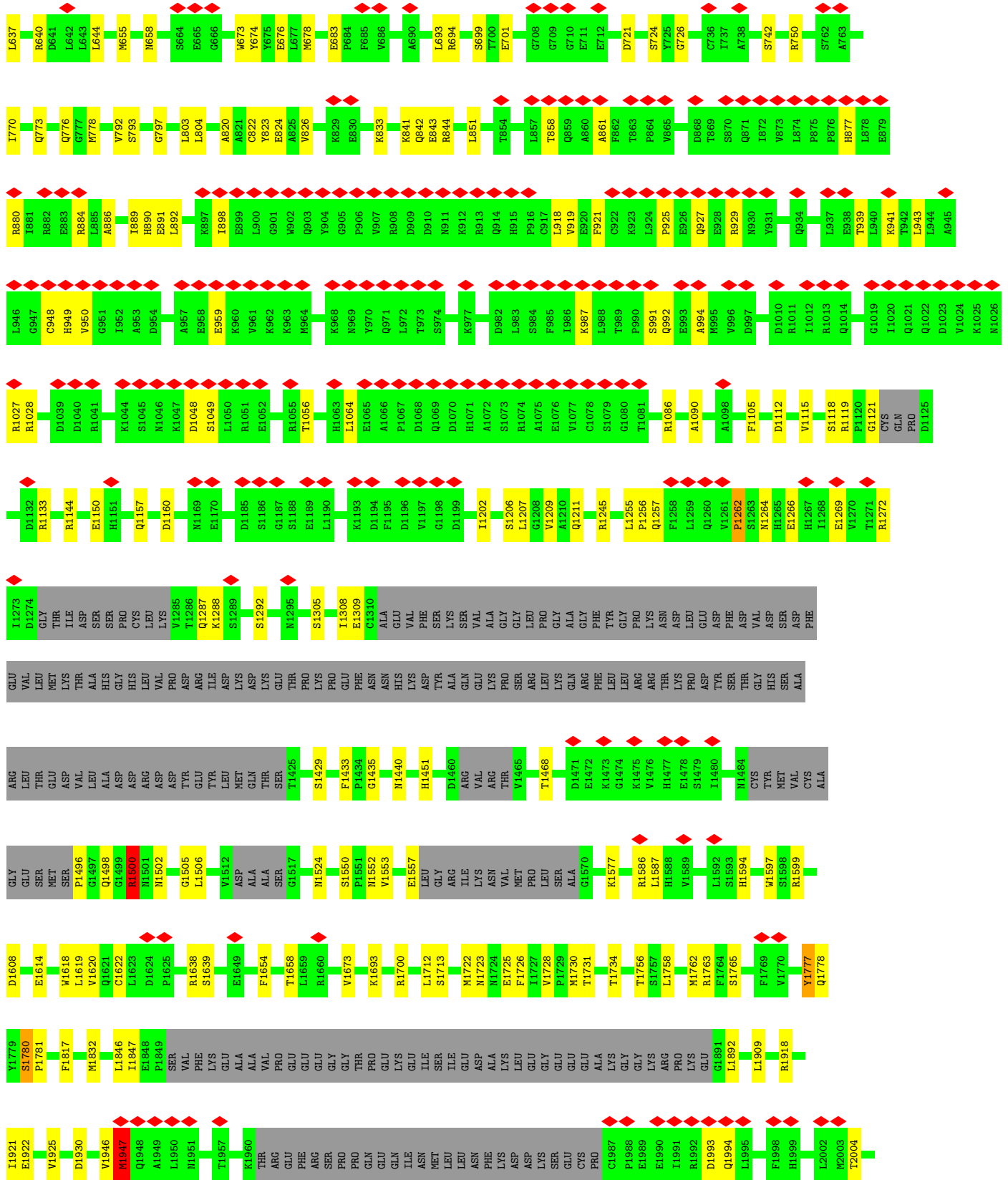


H2638	L2639	S2640	R2641	D2649	Q2653	K2654	Y2656	L2660	A2664	C2667	P2676	P2677	D2678	S2682	Q2691	W0694	ASP	SER	GLU	GLY	ASN	PHE	ASN	PRO	GLN	PRO	V2705	D2706	Y2707	S2708	L2709	I2710	T2711	I2712	P2713	E2714	K2715	L2716	E2717	Y2718	F2719	I2720	N2721	K2722	Y2723	A2724	E2725	H2726	S2727									
H2728	D2729	K2730	W2731	S2732	M2733	D2734	K2735	L2736	A2737	N2738	G2739	W2740	I2741	Y2742	G2743	Y2744	I2745	Y2746	S2747	D2748	S2749	S2750	K2751	I2752	Q2753	P2754	L2755	M2756	P2758	Y2759	K2760	L2761	L2762	S2763	E2764	K2765	E2766	E2768	I2769	R2771	W2772	P2773	I2774	K2775	E2776	S2777	L2778	K2779	Y2780	M2781	L2782	A2783	W2784	G2785	I2788			
E2789	R2790	T2791	R2792	E2793	G2794	D2795	S2796	M2797	A2798	L2799	Y2800	N2801	ARG	THR	ARG	ARG	ILE	SER	GLN	THR	THR	GLN	VAL	A2816	A2817	H2818	G2819	Y2820	S2821	P2822	R2823	A2824	I2825	D2826	M2827	S2828	N2829	V2830	T2831	L2832	S2833	L2836	H2837	A2840	E2841	M2842	M2843	A2844	E2845	N2846	Y2847	H2848	N2849	I2850				
W2851	A2852	K2853	K2854	K2855	K2856	L2857	E2858	L2859	E2860	S2861	K2862	H2867	P2868	L2869	L2870	V2871	P2872	Y2873	D2874	T2875	L2876	T2877	A2878	K2879	E2880	K2881	A2882	K2883	D2884	R2885	E2886	K2887	A2888	Q2889	D2890	I2891	F2892	K2893	L2895	Q2896	I2897	S2898	S2903	GLY	PHE	LYS	ASP	ASP	LEU	ASP	THR	PRO	SER	ILE				
GLU	LYS	ARG	ALA	THR	SER	PHE	GLN	GLY	ILE	ARG	TYR	VAL	GLU	ASN	GLU	ALA	HIS	GLN	TYR	ILE	ASP	PHE	GLY	GLY	SER	ARG	ARG	SER	THR	HIS	GLY	GLU	LEU	PHE	HIS	LYS	VAL	LEU	PRO	TYR	SER	GLY	PHE	LEU	GLN	ASN												
HIS	ARG	LEU	TYR	PHE	L2982	S2983	S2986	R2987	H2994	A2995	S2996	H3016	ARG	ASN	GLU	ASP	ILE	GLY	ASP	VAL	ASP	LEU	VAL	ASP	SER	GLY	GLY	CYS	ASP	ALA	THR	SER	ILE	THR	VAL	VAL	LYS	HIS	ILE	L3085	D3040	T3043	V3044	L3056	L3060	T3070	Q3076	G3077	Q3078	F3079	T3080	H3081	T3082	L3101	P3102	M3103	LEU	SER
SER	PHE	GLU	HIS	ILE	GLY	GLN	HIS	PHE	GLY	ASP	ILE	LEU	GLY	GLU	ASP	VAL	LEU	VAL	VAL	CYS	ARG	ILE	THR	THR	LEU	LYS	ALA	LEU	GLY	THR	SER	THR	LYS	ILE	SER	THR	VAL	TYR	TYR	VAL	VAL	VAL	GLU	VAL	GLY	CYS	ALA	ALA	PHE	ALA	GLY	PHE						
PRO	ILE	ALA	PHE	GLU	THR	HIS	L3174	R3191	S3269	L3275	R3281	N3286	L3287	G3288	I3289	D3290	E3291	G3292	ALA	THR	MET	TRP	ALA	F3301	S3302	Q3303	I3306	K3340	R3344	M3347	L3353	I3354	L3355	T3360	K3385	P3389	GLU	ALA																				
GLU	GLU	PHE	ARG	MET	VAL	ALA	L3404	W3405	S3406	E3423	I3424	M3427	S3428	F3429	L3430	I3431	T3432	D3433	T3434	K3435	S3436	K3437	M3438	S3439	R3453	M3460	A3467	A3468	L3469	K3470	R3471	L3472	L3473	P3474	I3475	G3476	L3477	N3478	L3479	P3482	G3483	A3489	N3493	I3508	ARG													
SER	ASN	ILE	HIS	LEU	GLY	LYS	GLU	GLU	ASP	PRO	ALA	ALA	ILE	ARG	PRO	ASP	ALA	THR	GLU	ASP	PRO	ASN	ARG	THR	GLU	VAL	ARG	ARG	ARG	THR	VAL	GLU	VAL	VAL	VAL	VAL	VAL	VAL	HIS	PRO																		
GLN	ARG	SER	LYS	ALA	VAL	TRP	ALA	TRP	LYS	LEU	SER	LYS	GLN	GLM	ARG	V3710	Q3727	A3728	R3729	L3730	H3731	E3737	G3748	E3749	T3750	V3786	V3915	F3916	N3917	T3918	L3919	T3920	Q3924	W3940	V3944	S3968	V3978	L3981	M4018	PHE	LEU	LYS	LEU	LYS	ASP	L4025	T4026	T4030										
F3685	C3698	HIS	ASP	GLU	GLU	ASP	ASP	GLY	GLU	GLU	V3710	Q3727	A3728	R3729	L3730	H3731	E3737	G3748	E3749	T3750	V3786	V3915	F3916	N3917	T3918	L3919	T3920	Q3924	W3940	V3944	S3968	V3978	L3981	M4018	PHE	LEU	LYS	LEU	LYS	ASP	L4025	T4026	T4030															
F3685	C3698	HIS	ASP	GLU	GLU	ASP	ASP	GLY	GLU	GLU	V3710	Q3727	A3728	R3729	L3730	H3731	E3737	G3748	E3749	T3750	V3786	V3915	F3916	N3917	T3918	L3919	T3920	Q3924	W3940	V3944	S3968	V3978	L3981	M4018	PHE	LEU	LYS	LEU	LYS	ASP	L4025	T4026	T4030															
F3685	C3698	HIS	ASP	GLU	GLU	ASP	ASP	GLY	GLU	GLU	V3710	Q3727	A3728	R3729	L3730	H3731	E3737	G3748	E3749	T3750	V3786	V3915	F3916	N3917	T3918	L3919	T3920	Q3924	W3940	V3944	S3968	V3978	L3981	M4018	PHE	LEU	LYS	LEU	LYS	ASP	L4025	T4026	T4030															

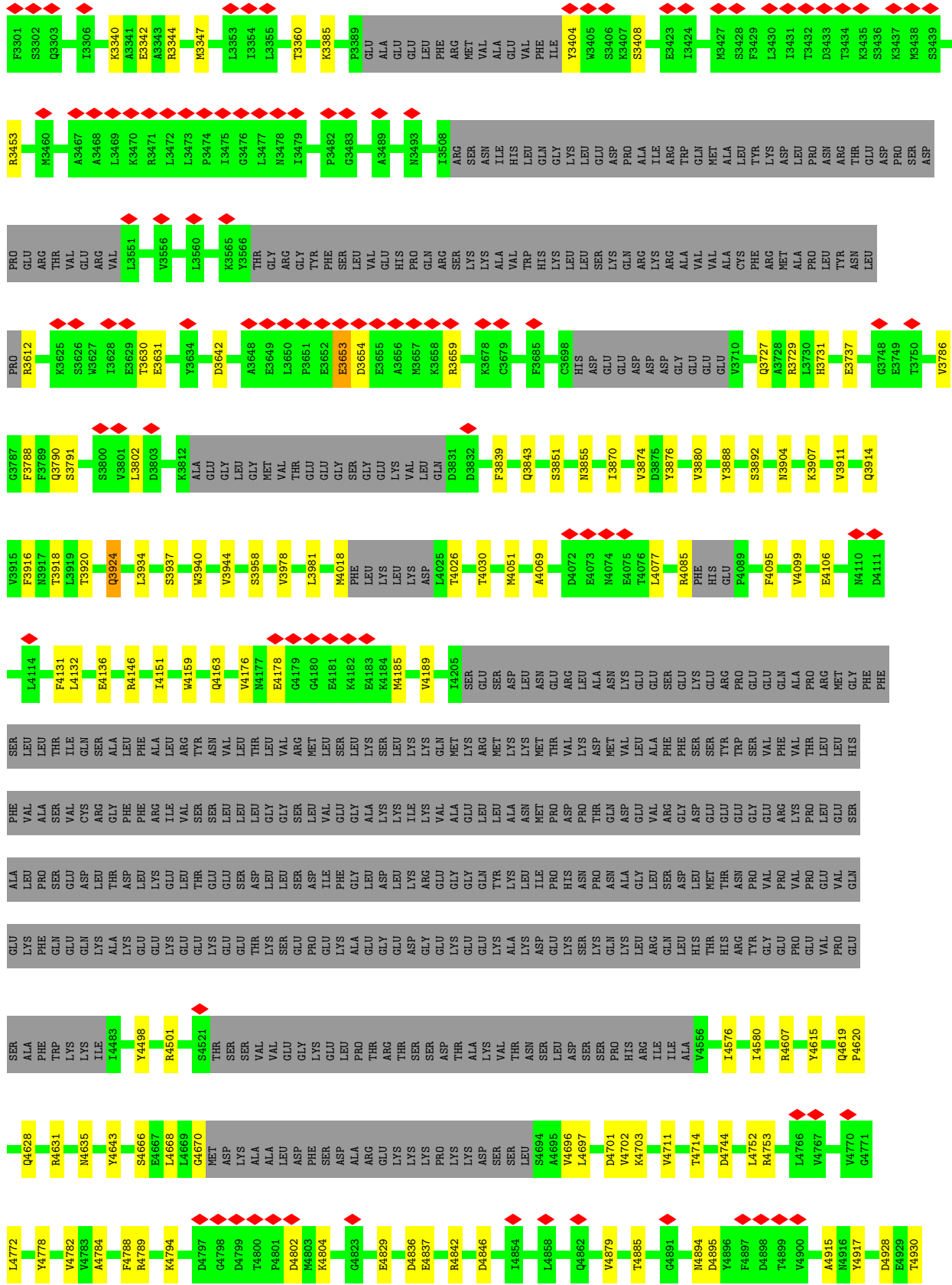


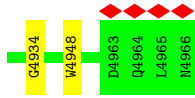
• Molecule 1: Ryanodine receptor 2



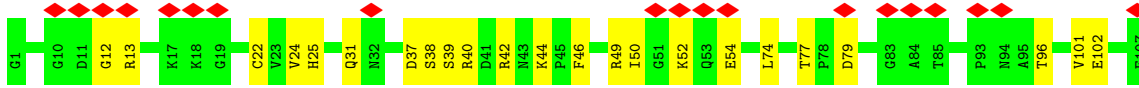
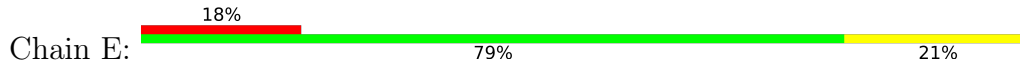


E2012	E2017	E2020	R2027	R2040	GLN	LYS	ALA	GLU	LYS	PRO	VAL	ALA	SER	ASP	ARG	LYS	CYS	SER	S2056	I2061	R2067	E2071	S2072	H2088	G2095	R2099	T2106	I2107	H2108	G2109	V2112	I2116	L2122	I2125	R2126	L2129	S2130	V2131	R2132	H2133	G2134	K2135																		
G2144	L2145	G2146	N2150	R2162	A2163	L2164	T2169	E2172	V2173	N2176	G2179	G2180	G2181	E2182	S2183	K2184	E2186	C2203	R2204	I2205	S2206	Q2210	L2221	E2222	L2228	A2229	S2230	P2231	R2234	T2237	A2244	N2249	L2268	C2276	H2285	P2285	D2286	I2287	N2290																					
Y2297	E2313	E2314	N2315	A2316	N2317	V2318	V2319	G2331	P2332	A2333	L2334	R2335	G2336	E2337	G2338	K2351	E2354	D2355	P2356	S2357	R2358	P2361	S2362	P2363	T2364	S2365	G2366	T2370	LEU	ASP	ILE	GLU	GLU	GLU	ASP	THR	ILE	HIS	M2383	G2384	N2385	E2404	M2405	H2406	L2407	I2408	H2409	A2410	G2411	K2412										
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R2517	Y2518	T2521	L2527	THR	ARG	CYS	ALA	PRO	LEU	PHE	GLY	THR	HIS	THR	ALA	SER	LYS	ILE	ASP	SER	LEU	LEU	HIS	THR	VAL	TYR	ARG	LEU	LEU	SER	LYS	GLY	CYS	SER	THR	THR	LEU	LEU	LEU	SER	ILE	C2576	G2577	Q2578	M2582	N2583														
H2584	L2588	V2592	F2593	D2594	E2600	H2601	P2605	L2606	V2613	E2614	H2615	A2632	E2633	E2634	L2637	H2638	L2639	S2640	R2641	D2649	Q2653	K2654	K2655	Y2656	L2660	A2664	C2667	P2676	F2677	D2678	S2682	Q2691	H2694	ASP	SER	GLU	GLY	PHE	ASN	PRO	GLN	PRO																		
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I2891	F2892	K2893	L2894	Q2896	I2897	S2898	S2903	ARG	PHE	LYS	ASP	LEU	ASP	LEU	ASP	THR	LYS	PRO	SER	ASN	ILE	GLU	LYS	ARG	ALA	TYR	SER	PHE	LEU	GLN	GLN	GLN	TYR	VAL	ASP	ALA	ALA	ASP	GLY	GLY	GLY	ARG	VAL	VAL	LYS	VAL	ILE	GLY	GLY	HIS	PHE									
PRO	TYR	GLU	GLN	GLU	ILE	LYS	PHE	ALA	LYS	VAL	VAL	LEU	PRO	LEU	ILE	ASP	GLN	TYR	PHE	THR	ASN	ARG	LEU	PHE	L2982	S2983	S2986	R2987	H2994	A2995	S2996	H3016	ARG	ILE	ASP	SER	VAL	GLN	VAL	GLY	ASN	CYS	TYR	ALA	THR	SER	ILE	THR	VAL	ASN	CYS	LEU	ALA	LEU	ILE	GLY	THR	SER		
T3043	V3044	L3056	L3060	T3070	Q3076	G3077	Q3078	F3079	H3080	H3081	T3082	L3101	F3102	M3103	LEU	SER	SER	PRO	ILE	ALA	PHE	GLU	HIS	ILE	GLY	GLN	HIS	GLN	PHE	GLY	GLY	ASP	LEU	ILE	LEU	VAL	VAL	VAL	SER	CYS	TYR	ARG	ILE	ILE	THR	THR	THR	THR	ALA	ALA	ALA	ALA	ALA	VAL						
LYS	SER	ILE	TYR	VAL	GLU	ARG	GLN	ARG	SER	ALA	LYS	ALA	LEU	GLY	CYS	ALA	ALA	PHE	ALA	GLY	PHE	LEU	THR	HIS	THR	HIS	GLN	HIS	GLN	PHE	GLY	ASP	LEU	ILE	LEU	VAL	VAL	VAL	SER	CYS	TYR	ARG	ILE	ILE	THR	THR	THR	THR	ALA	ALA	ALA	ALA	VAL							

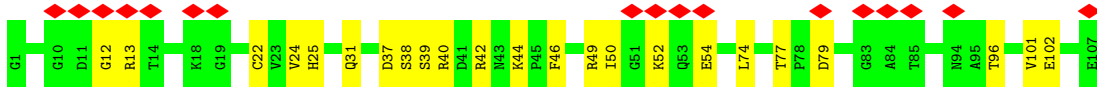
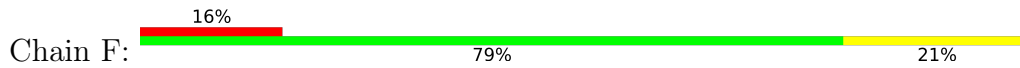




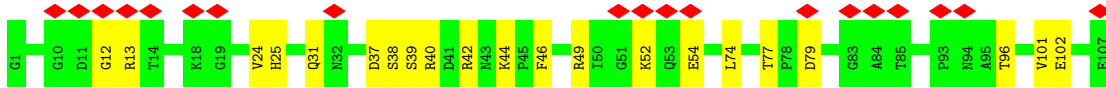
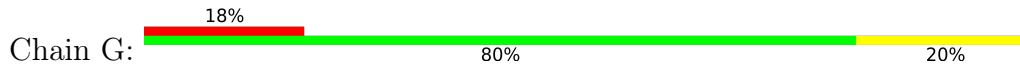
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



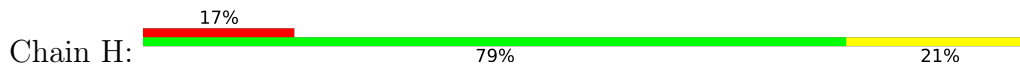
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	103845	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	24.070	Depositor
Minimum map value	-7.125	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (\AA)	484.70398, 484.70398, 484.70398	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.377, 1.377, 1.377	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/31108	0.68	15/42056 (0.0%)
1	B	0.35	0/31108	0.68	14/42056 (0.0%)
1	C	0.35	0/31108	0.68	13/42056 (0.0%)
1	D	0.35	0/31108	0.68	14/42056 (0.0%)
2	E	0.35	0/834	0.67	0/1123
2	F	0.35	0/834	0.67	0/1123
2	G	0.35	0/834	0.67	0/1123
2	H	0.35	0/834	0.67	0/1123
All	All	0.35	0/127768	0.68	56/172716 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
1	B	0	15
1	C	0	15
1	D	0	15
All	All	0	60

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2660	LEU	CA-CB-CG	9.27	136.63	115.30
1	D	2660	LEU	CA-CB-CG	9.27	136.63	115.30
1	A	2660	LEU	CA-CB-CG	9.27	136.62	115.30
1	B	2660	LEU	CA-CB-CG	9.25	136.57	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1500	ARG	N-CA-C	7.46	131.14	111.00

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1266	GLU	Peptide
1	A	1500	ARG	Peptide
1	A	544	ASN	Peptide
1	A	608	HIS	Peptide
1	A	618	CYS	Peptide

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	30492	29277	29270	263	0
1	B	30492	29280	29270	272	0
1	C	30492	29281	29270	269	0
1	D	30492	29278	29270	276	0
2	E	818	824	824	14	0
2	F	818	824	824	14	0
2	G	818	824	824	13	0
2	H	818	824	824	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	125244	120412	120376	1129	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1129 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:644:LEU:HD11	1:B:1658:THR:HG21	1.70	0.74
1:C:644:LEU:HD11	1:C:1658:THR:HG21	1.69	0.73
1:A:644:LEU:HD11	1:A:1658:THR:HG21	1.69	0.73
1:C:2106:THR:OG1	1:C:3612:ARG:O	2.06	0.73
1:B:288:HIS:O	1:B:290:ARG:NH1	2.22	0.72

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	3849/4966 (78%)	3357 (87%)	482 (12%)	10 (0%)	41	76
1	B	3849/4966 (78%)	3358 (87%)	481 (12%)	10 (0%)	41	76
1	C	3849/4966 (78%)	3358 (87%)	481 (12%)	10 (0%)	41	76
1	D	3849/4966 (78%)	3359 (87%)	480 (12%)	10 (0%)	41	76
2	E	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	F	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	G	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	H	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
All	All	15816/20292 (78%)	13816 (87%)	1960 (12%)	40 (0%)	44	76

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1500	ARG
1	B	1500	ARG
1	C	1500	ARG
1	D	1500	ARG
1	A	607	ASN

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	3178/4355 (73%)	3164 (100%)	14 (0%)	91	94
1	B	3178/4355 (73%)	3164 (100%)	14 (0%)	91	94
1	C	3178/4355 (73%)	3164 (100%)	14 (0%)	91	94
1	D	3178/4355 (73%)	3164 (100%)	14 (0%)	91	94
2	E	88/88 (100%)	87 (99%)	1 (1%)	73	85
2	F	88/88 (100%)	87 (99%)	1 (1%)	73	85
2	G	88/88 (100%)	87 (99%)	1 (1%)	73	85
2	H	88/88 (100%)	87 (99%)	1 (1%)	73	85
All	All	13064/17772 (74%)	13004 (100%)	60 (0%)	89	93

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	343	ARG
1	D	3654	ASP
1	C	2203	CYS
1	D	3653	GLU
2	H	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2210	GLN
1	D	2317	ASN
1	D	4878	GLN
1	B	2176	ASN
1	B	2150	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

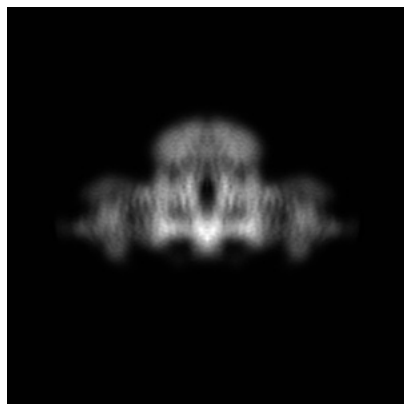
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21862. These allow visual inspection of the internal detail of the map and identification of artifacts.

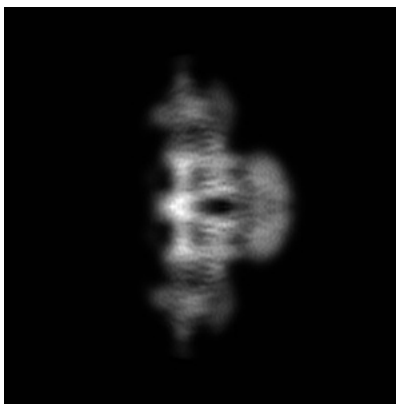
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

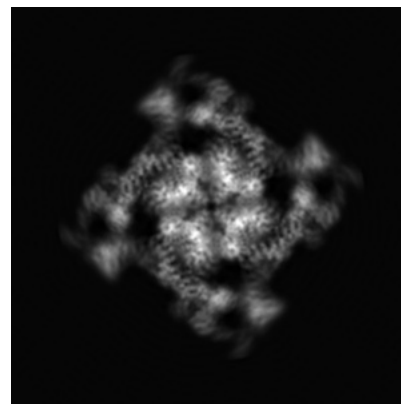
6.1.1 Primary map



X

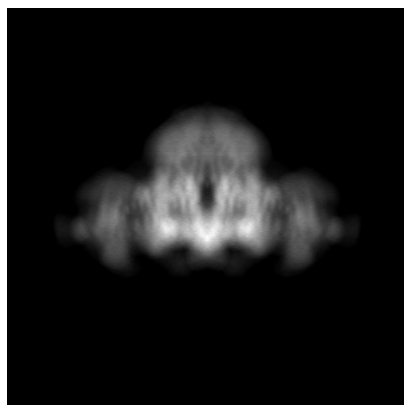


Y

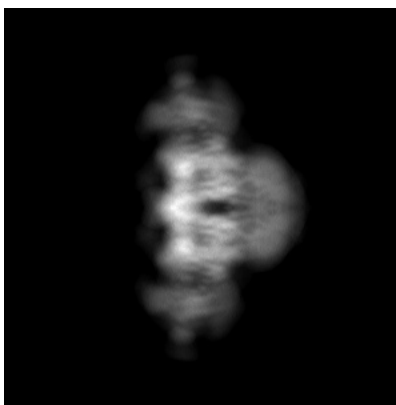


Z

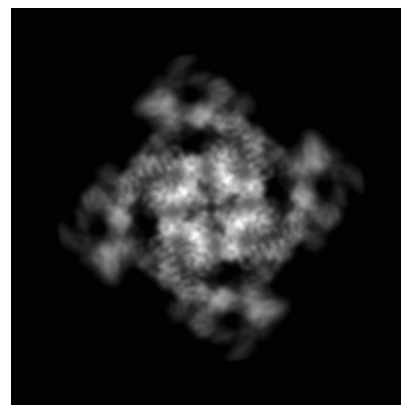
6.1.2 Raw map



X



Y

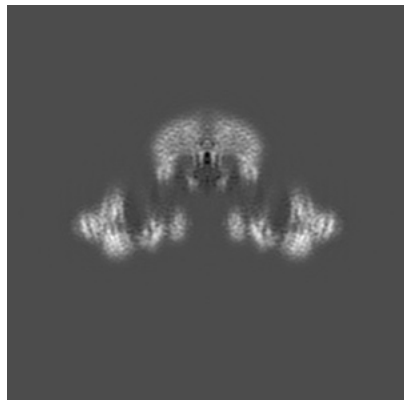


Z

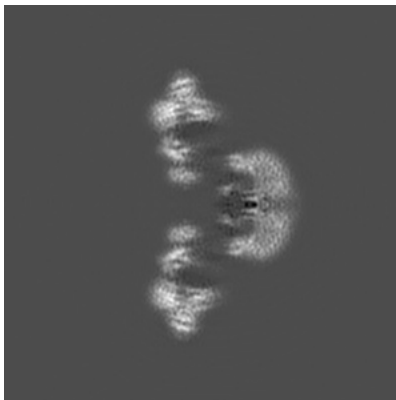
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

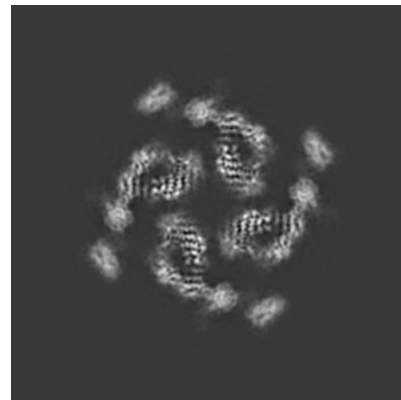
6.2.1 Primary map



X Index: 176

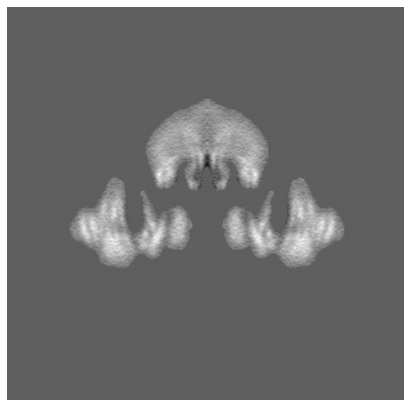


Y Index: 176

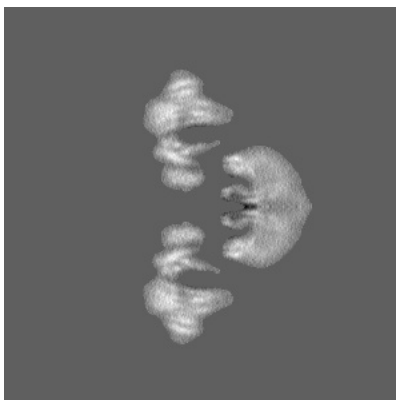


Z Index: 176

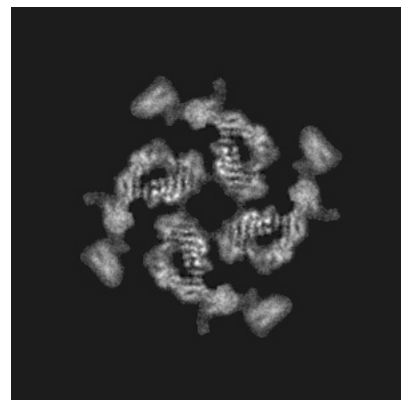
6.2.2 Raw map



X Index: 352



Y Index: 352

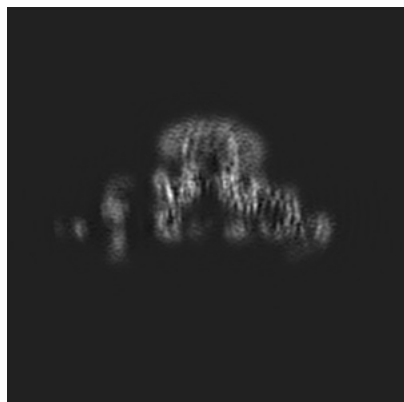


Z Index: 352

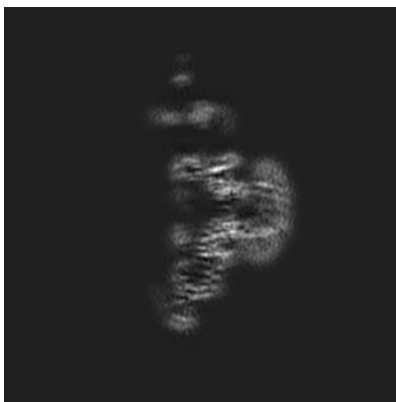
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

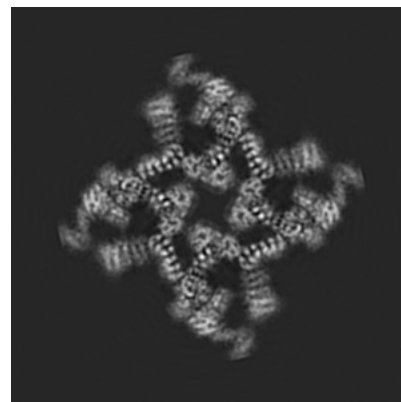
6.3.1 Primary map



X Index: 191



Y Index: 191



Z Index: 159

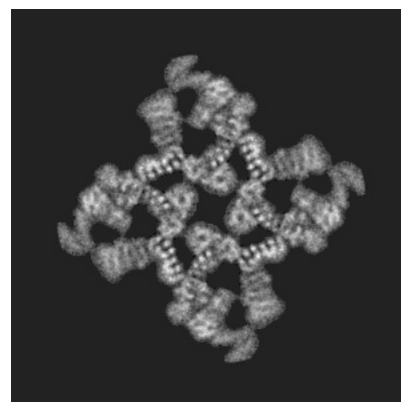
6.3.2 Raw map



X Index: 330



Y Index: 330

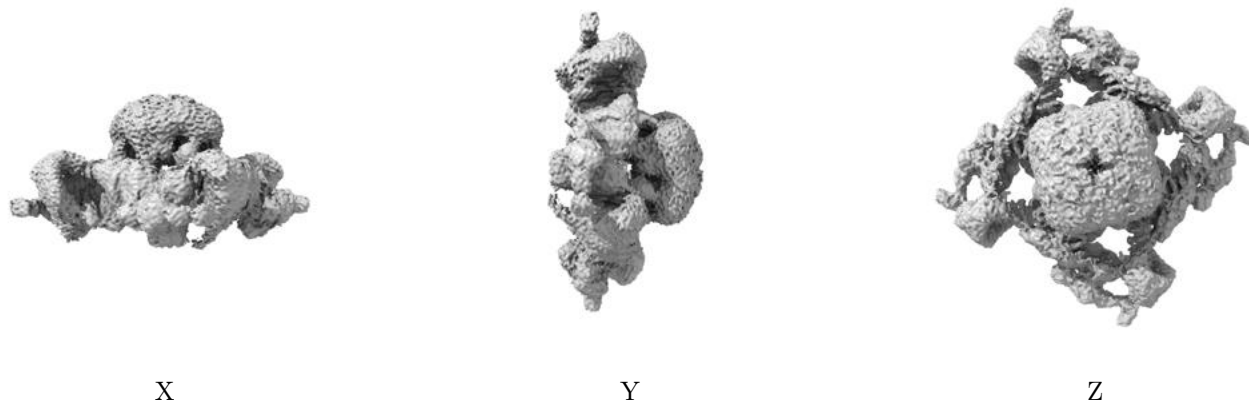


Z Index: 318

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

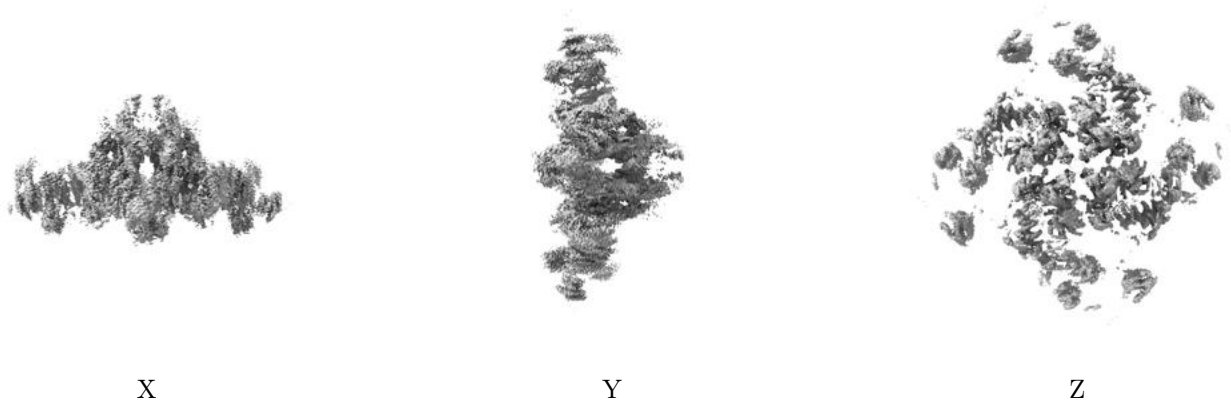
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

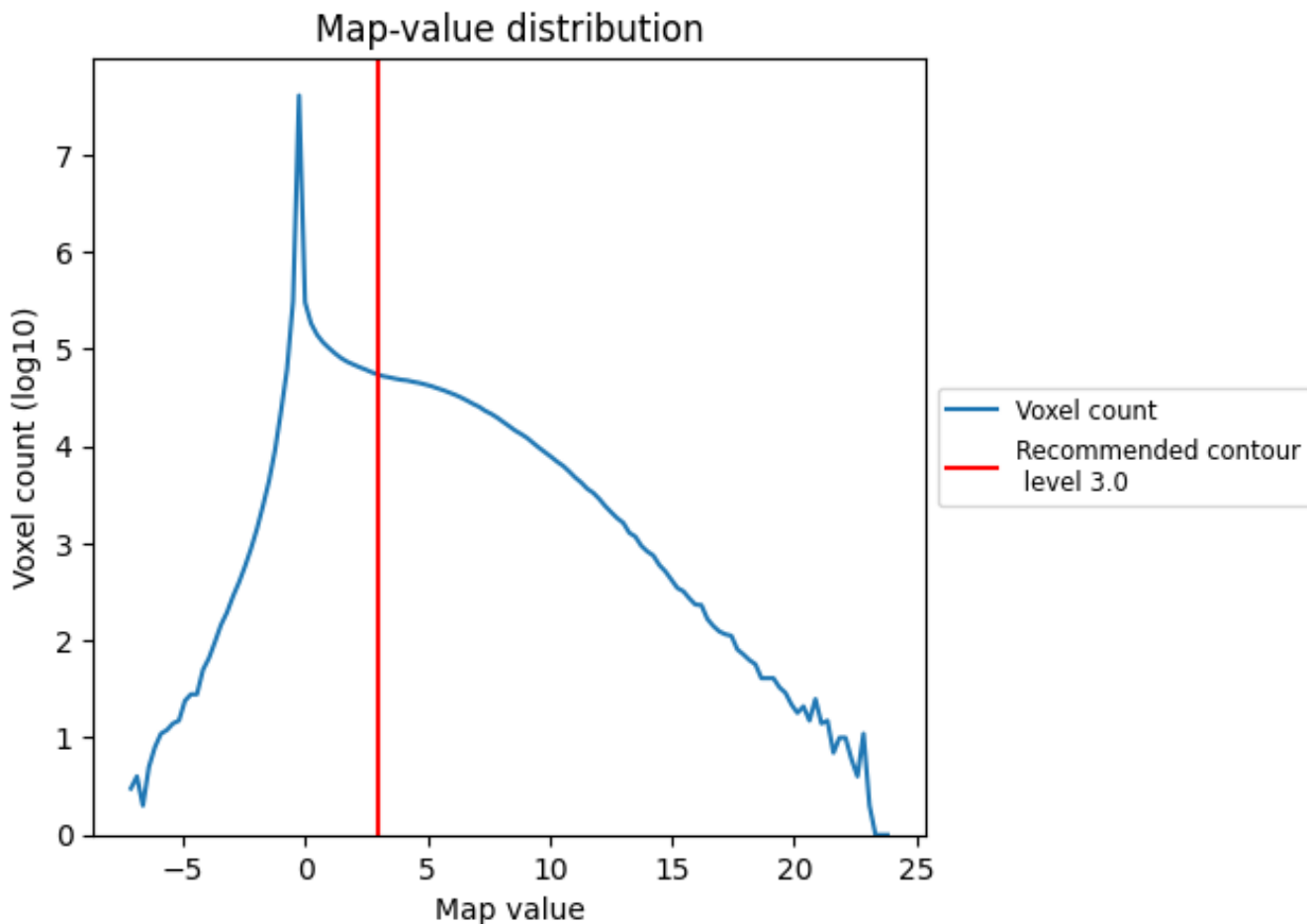
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

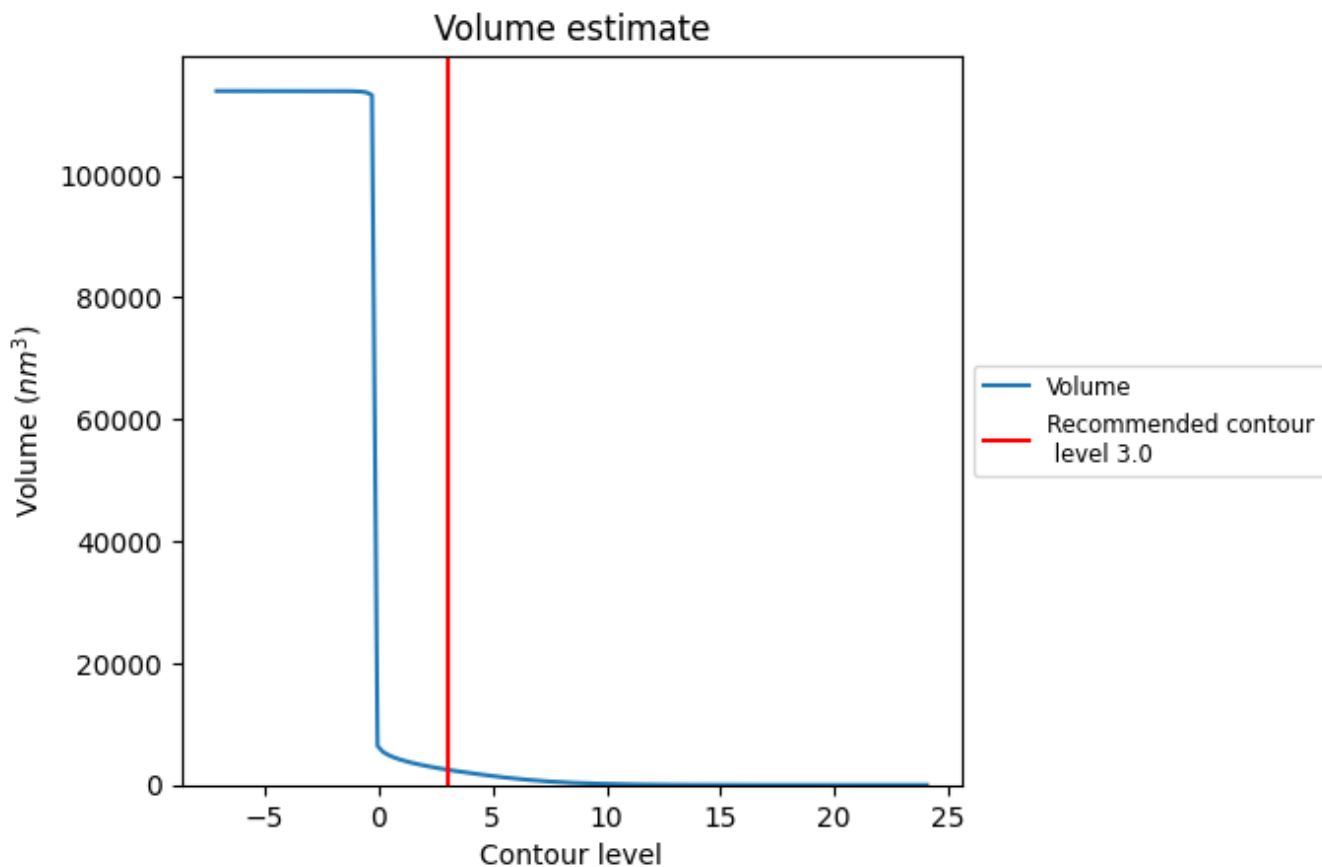
This section contains the results of statistical analysis of the map.

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.

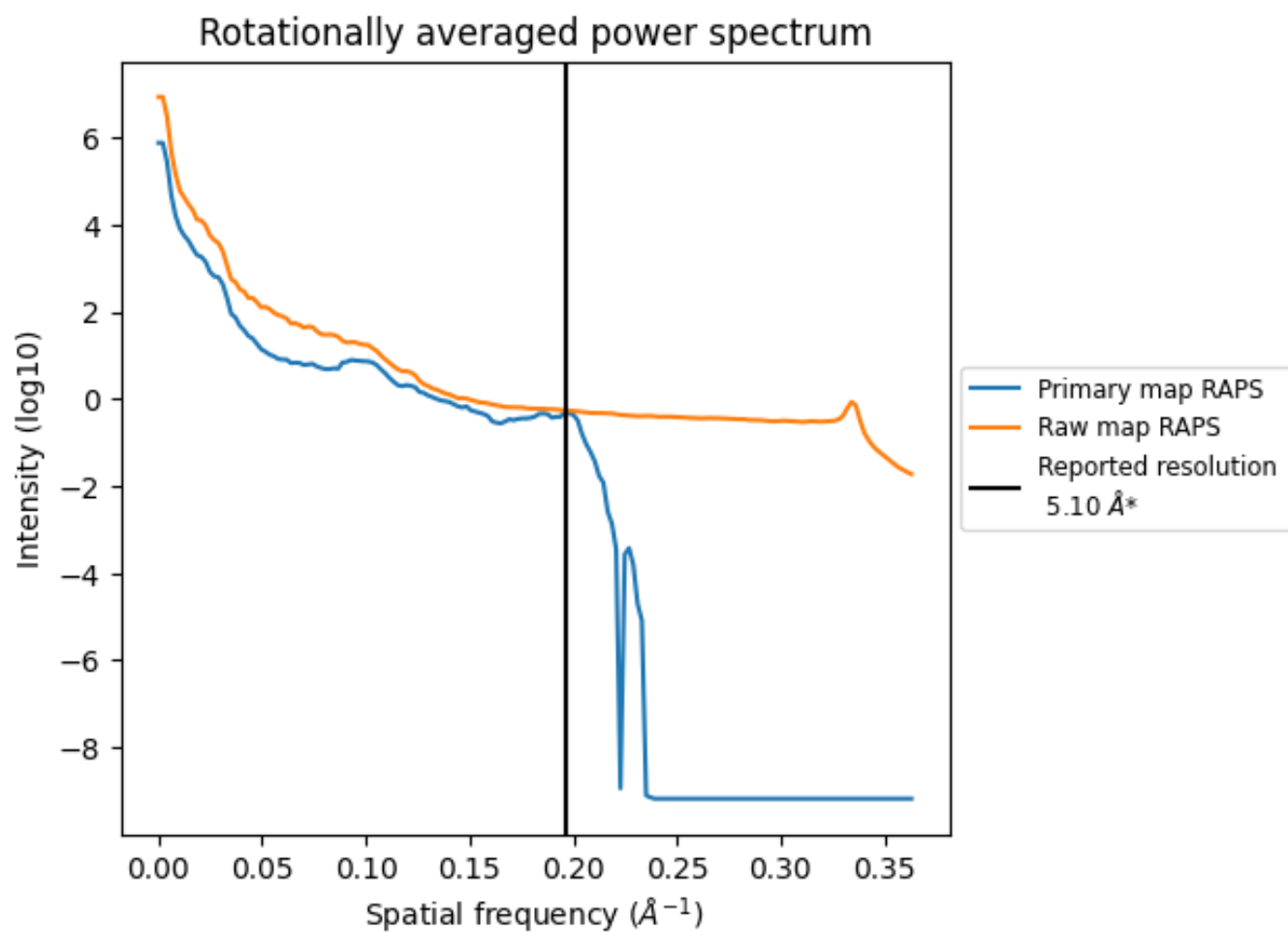
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2507 nm^3 ; this corresponds to an approximate mass of 2265 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](#)

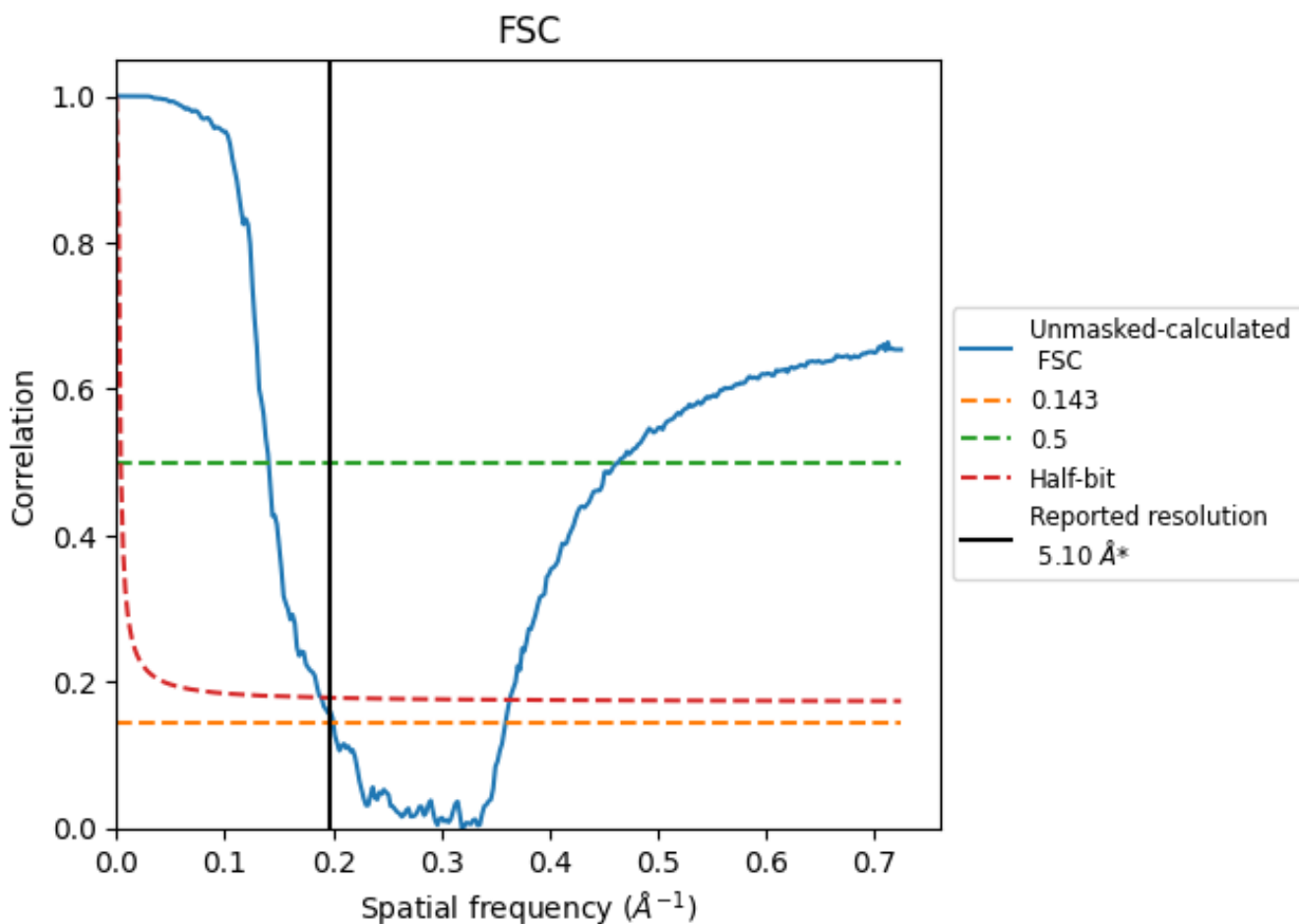


*Reported resolution corresponds to spatial frequency of 0.196 Å⁻¹

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 0.196 Å⁻¹

8.2 Resolution estimates [i](#)

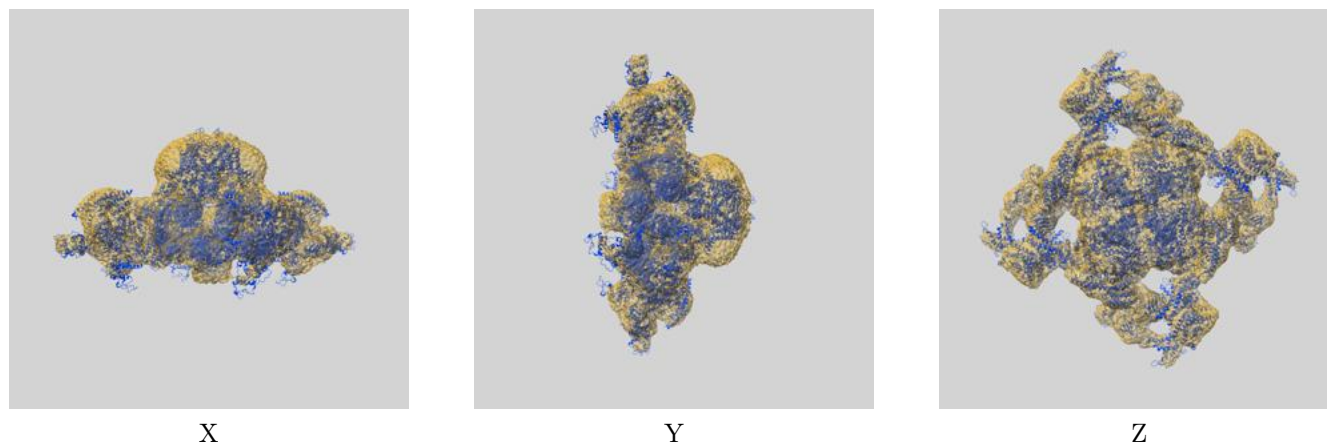
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.99	7.12	5.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

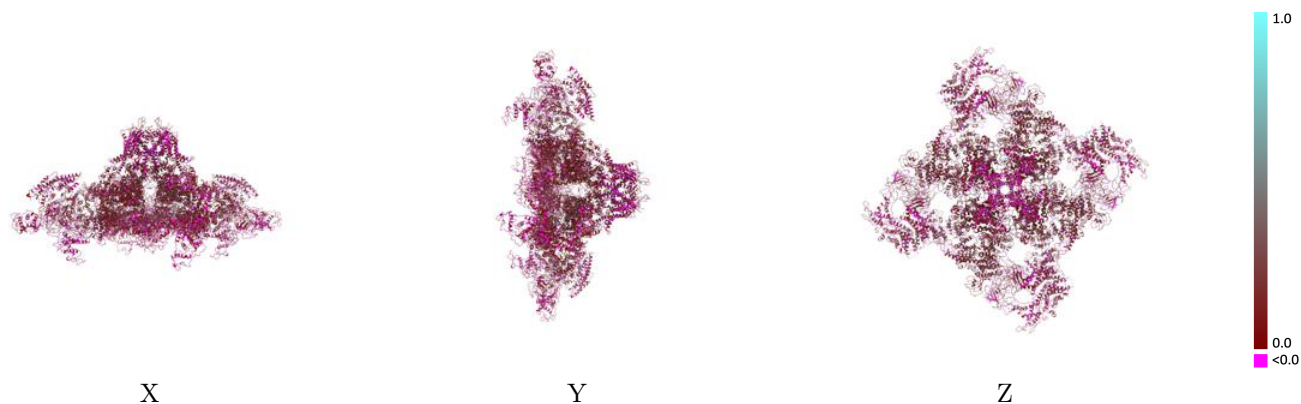
This section contains information regarding the fit between EMDB map EMD-21862 and PDB model 6WOV. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



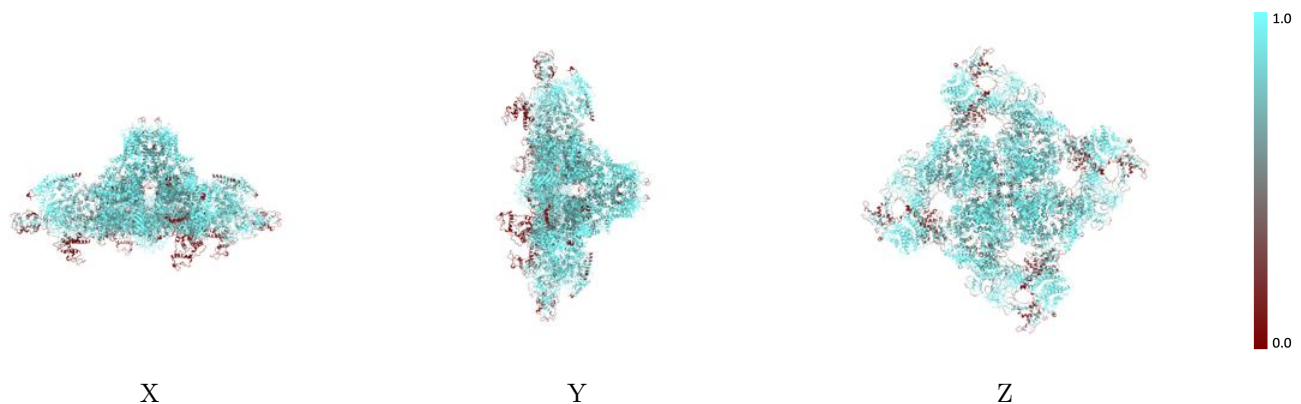
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



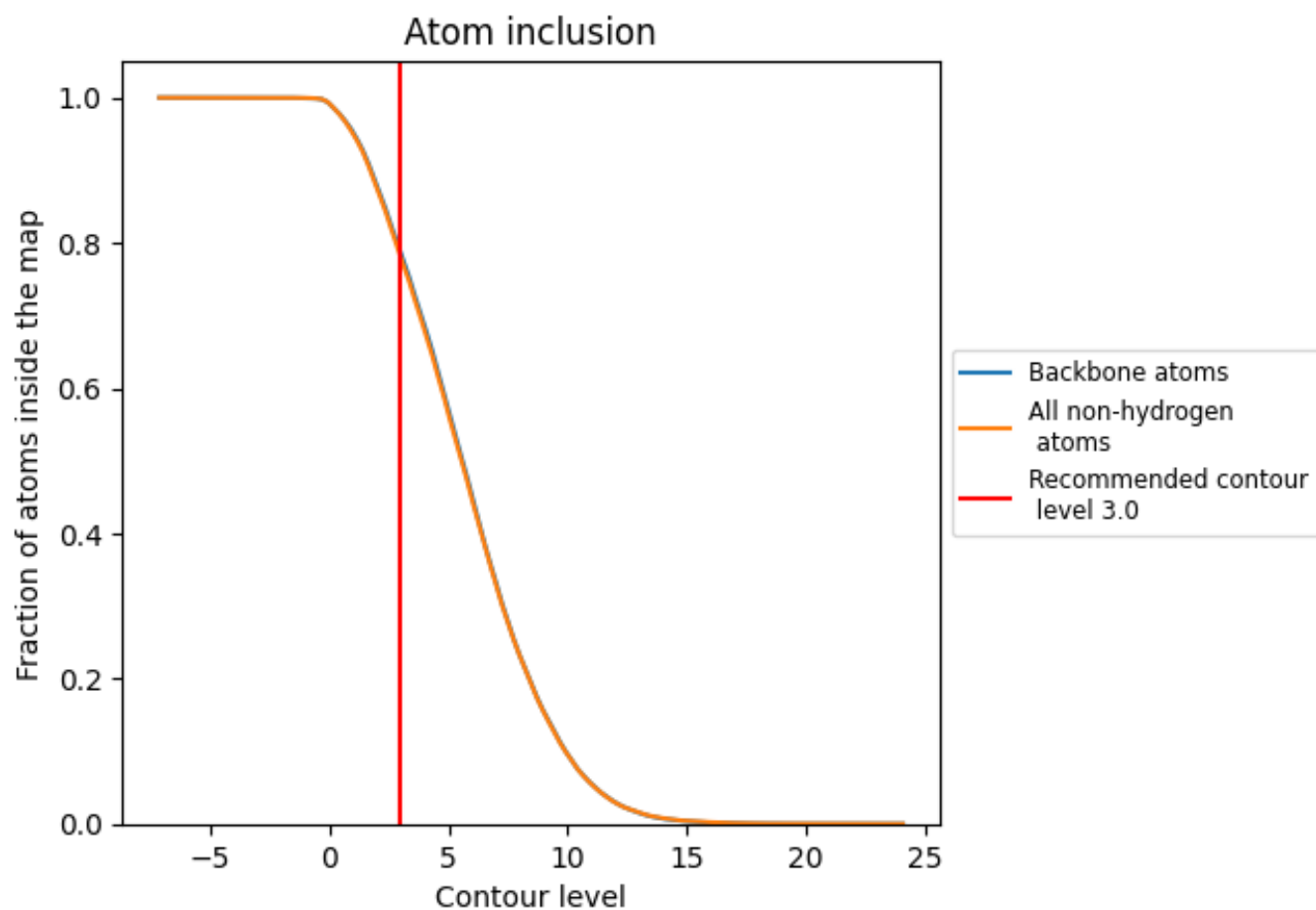
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.0).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7802	 0.1330
A	 0.7819	 0.1330
B	 0.7813	 0.1330
C	 0.7820	 0.1330
D	 0.7822	 0.1330
E	 0.7667	 0.1520
F	 0.7717	 0.1540
G	 0.7643	 0.1470
H	 0.7643	 0.1430

