



wwPDB EM Validation Summary Report ⓘ

Oct 31, 2024 – 03:20 PM EDT

PDB ID : 6X33
EMDB ID : EMD-22016
Title : Wt pig RyR1 in complex with apoCaM, EGTA condition (class 3, open)
Authors : Woll, K.W.; Haji-Ghassemi, O.; Van Petegem, F.
Deposited on : 2020-05-21
Resolution : 4.20 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
MolProbity : 4.02b-467
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

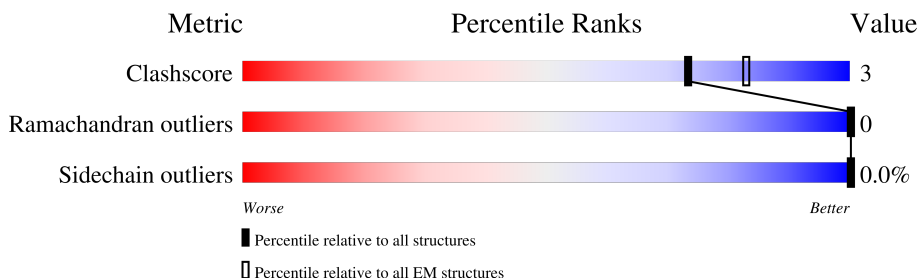
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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





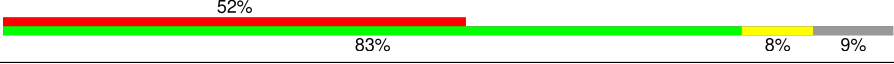
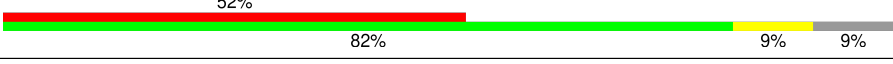
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	107	
1	D	107	
1	G	107	
1	J	107	
2	B	3816	
2	E	3816	
2	H	3816	
2	K	3816	

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Mol	Chain	Length	Quality of chain
3	C	148	
3	F	148	
3	I	148	
3	L	148	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 112372 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	106	Total	C	N	O	S	0	0
			727	460	124	139	4		
1	D	106	Total	C	N	O	S	0	0
			727	460	124	139	4		
1	G	106	Total	C	N	O	S	0	0
			727	460	124	139	4		
1	J	106	Total	C	N	O	S	0	0
			727	460	124	139	4		

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	E	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	H	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		
2	K	3816	Total	C	N	O	S	6	0
			26597	17002	4711	4735	149		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	F	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	I	135	Total	C	N	O	S	0	0
			768	477	138	151	2		
3	L	135	Total	C	N	O	S	0	0
			768	477	138	151	2		

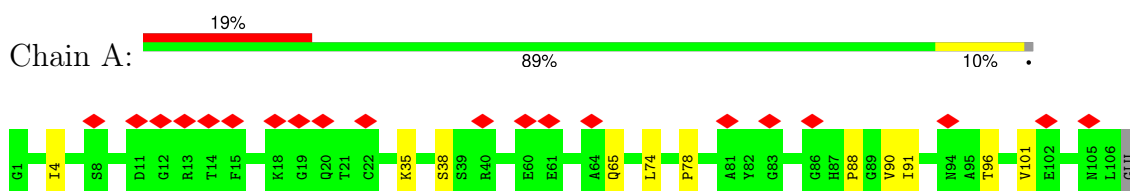
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Zn 1	0
4	E	1	Total 1	Zn 1	0
4	H	1	Total 1	Zn 1	0
4	K	1	Total 1	Zn 1	0

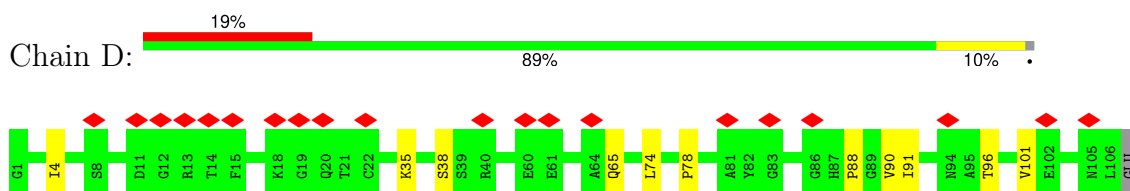
3 Residue-property plots

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.

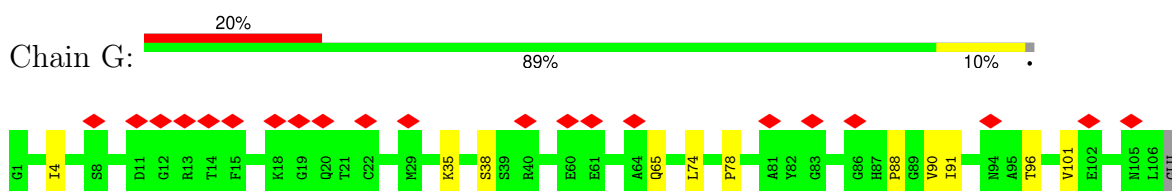
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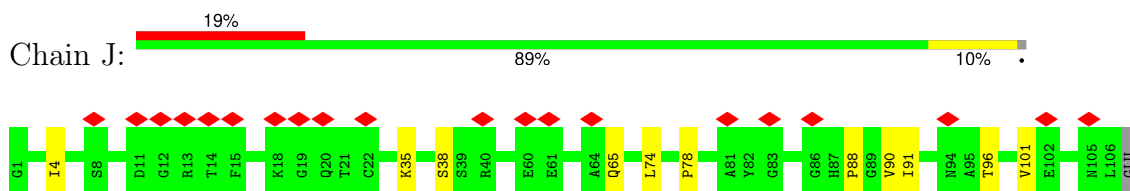
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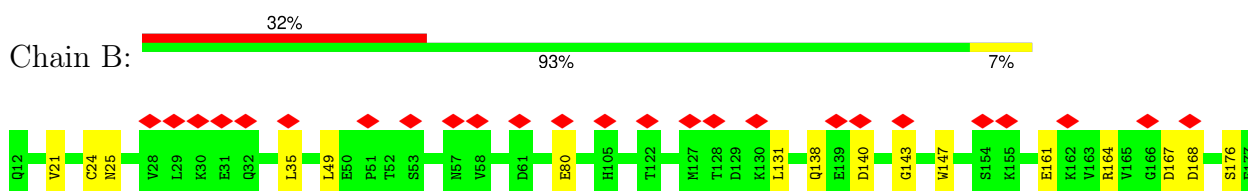
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

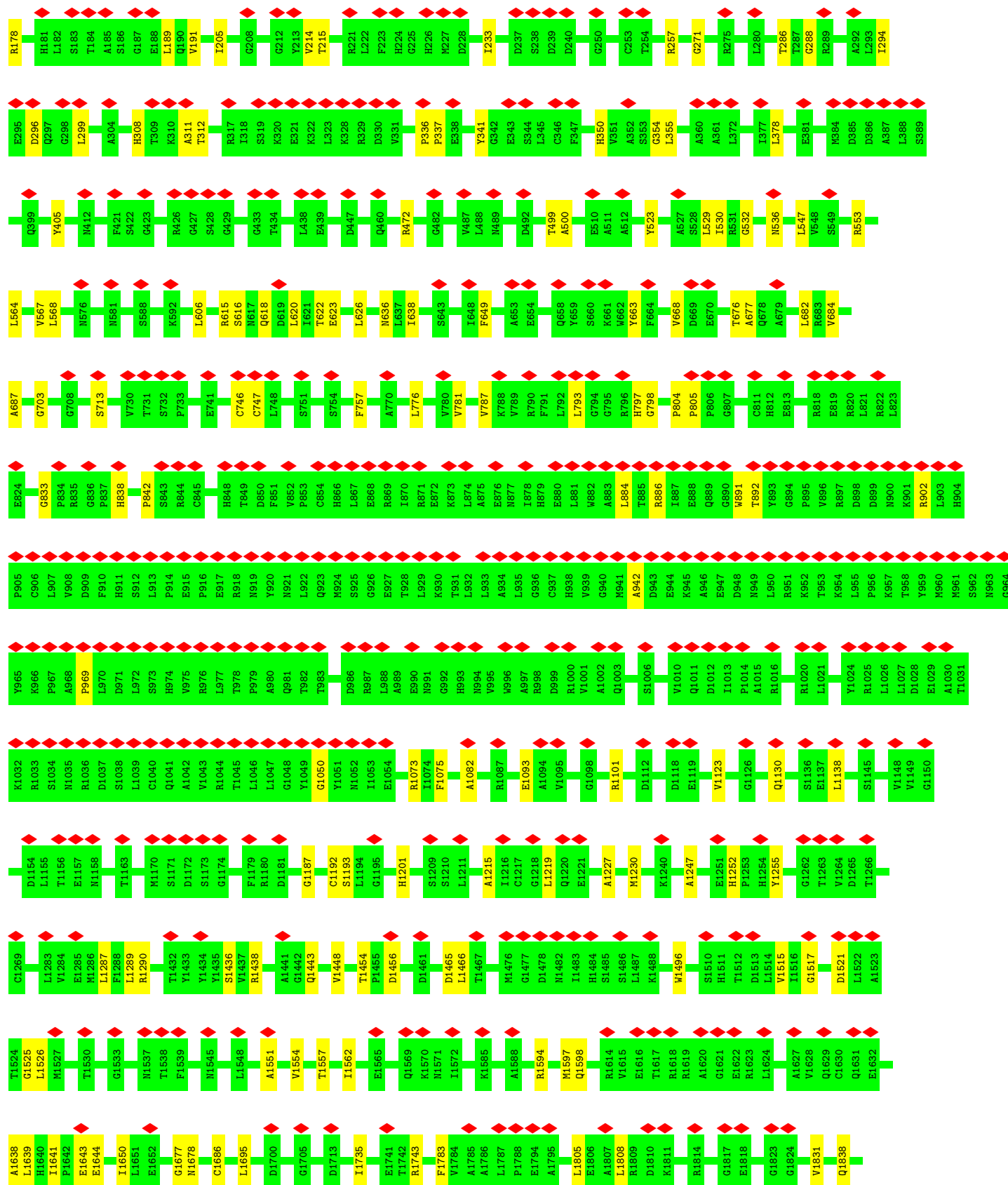


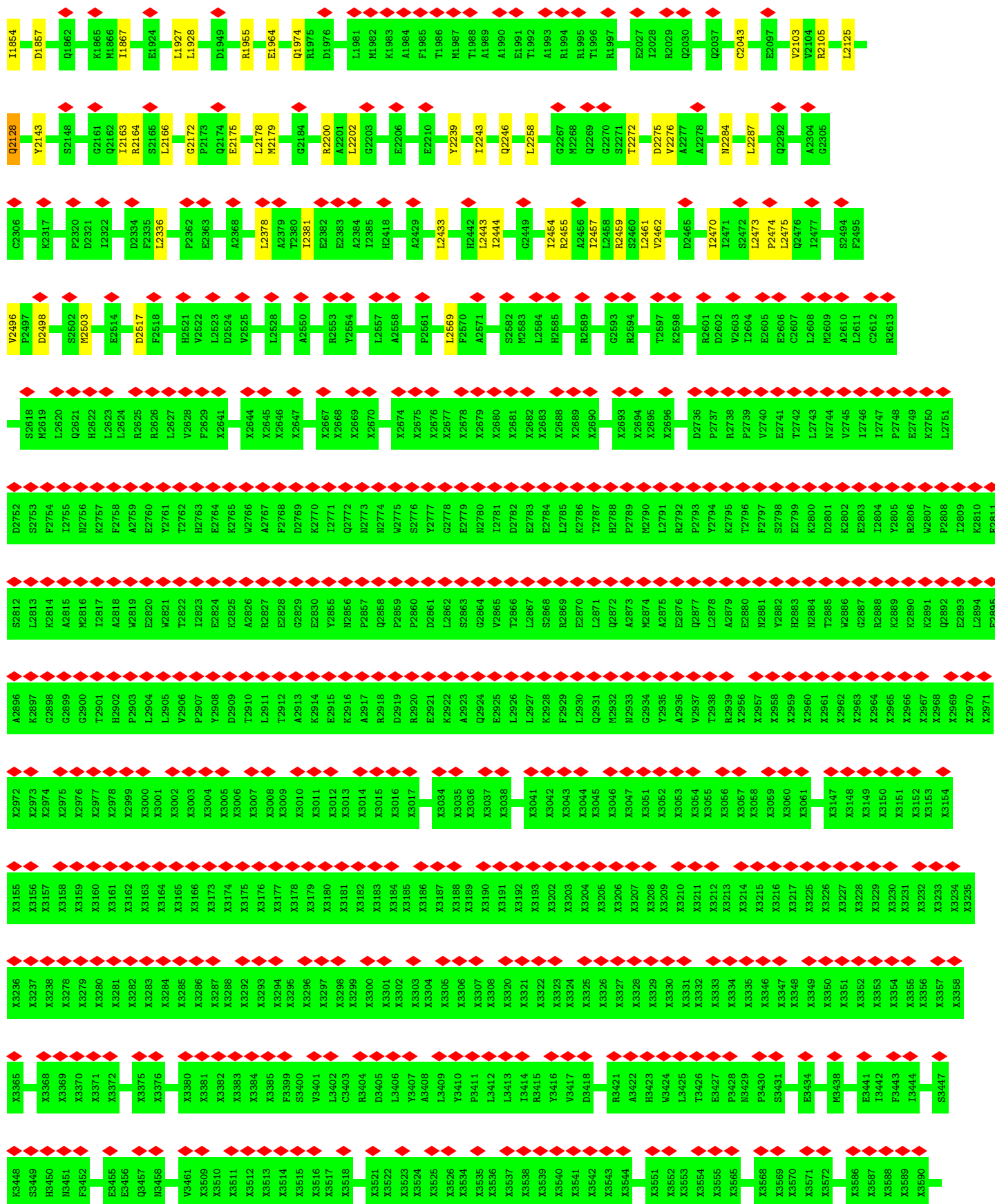
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

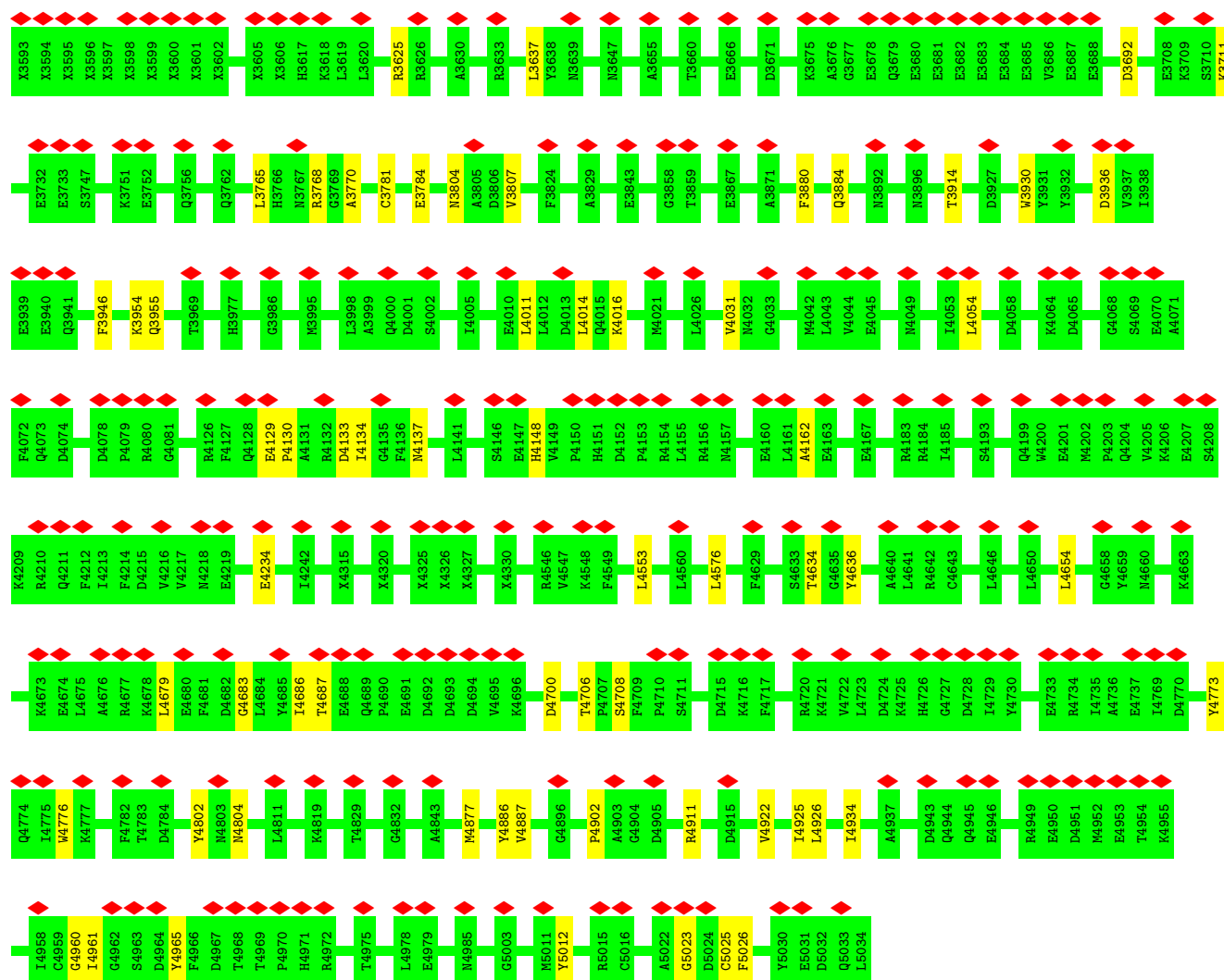


- Molecule 2: Ryanodine Receptor

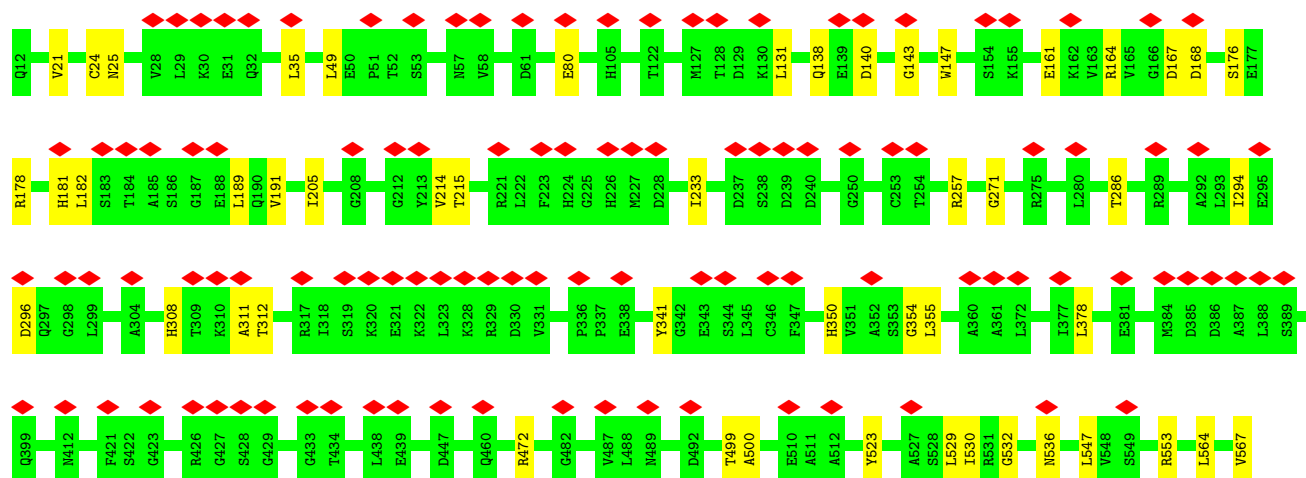
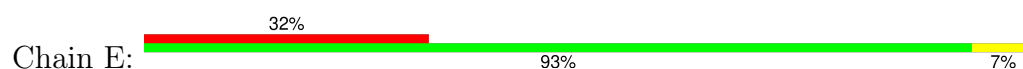


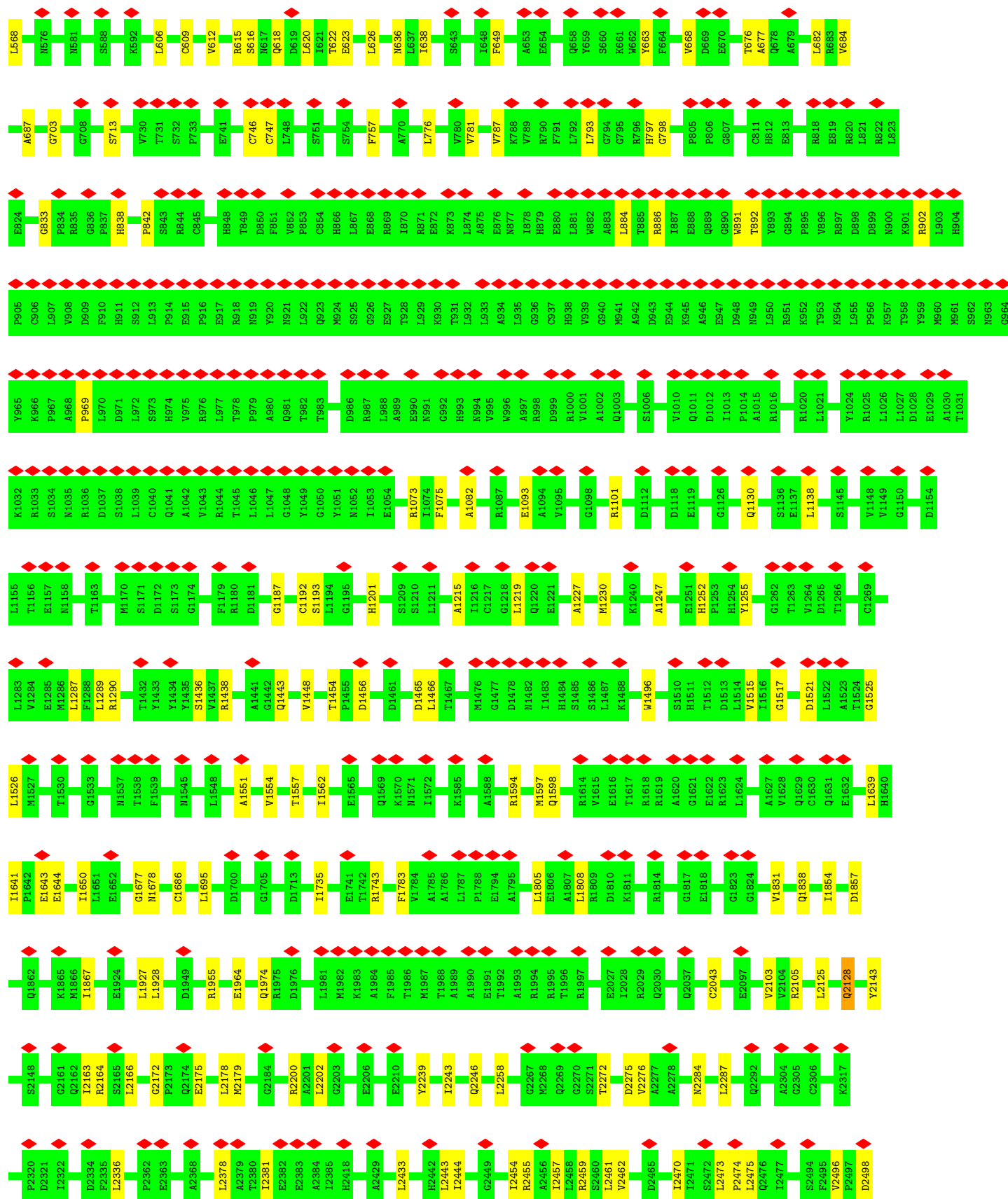




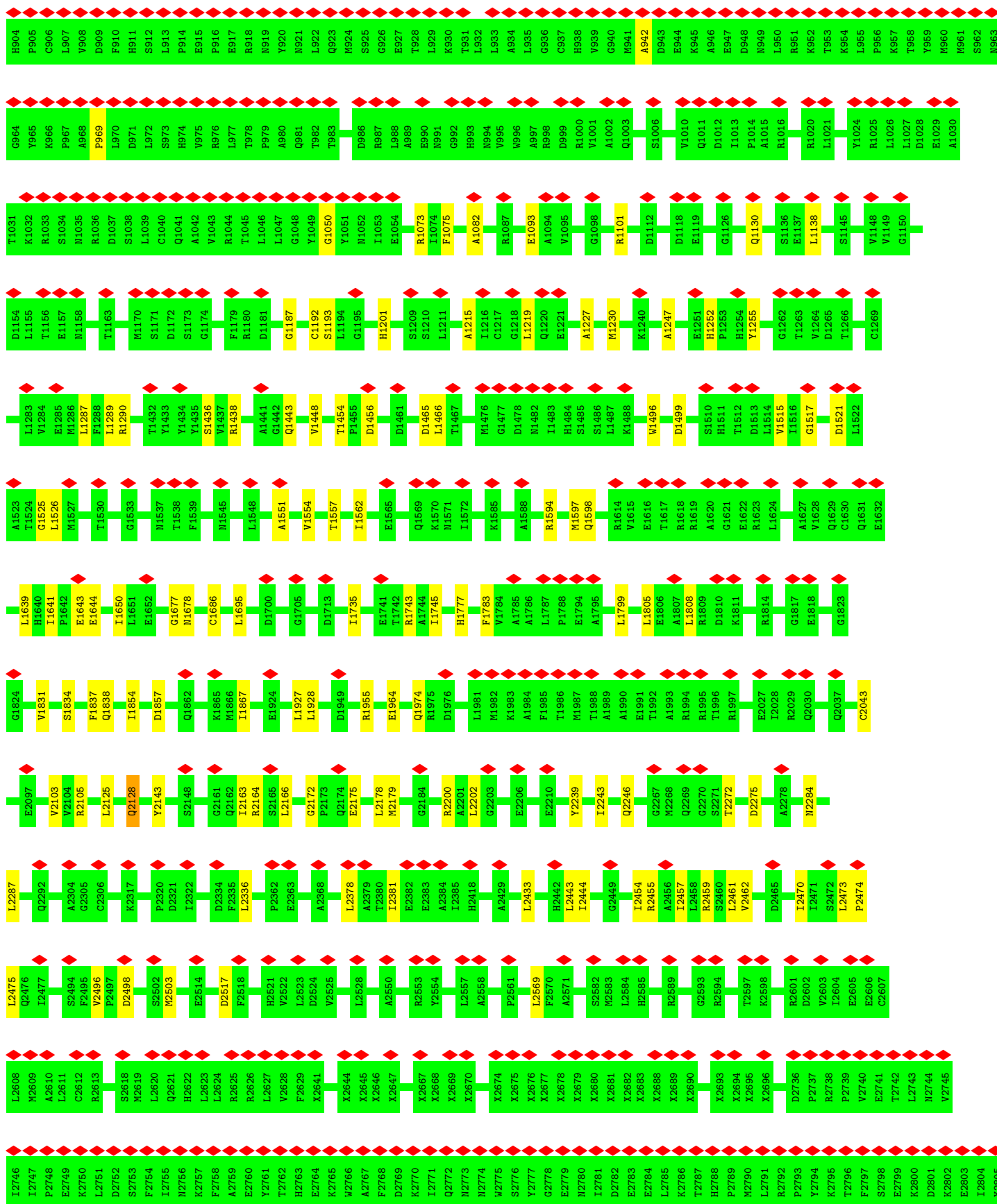


● Molecule 2: Ryanodine Receptor

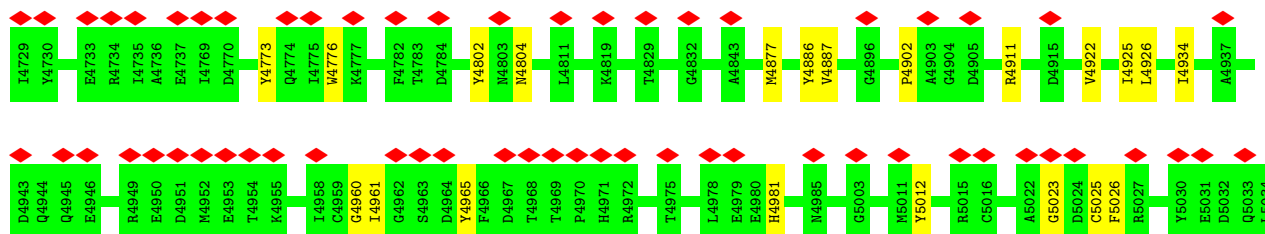




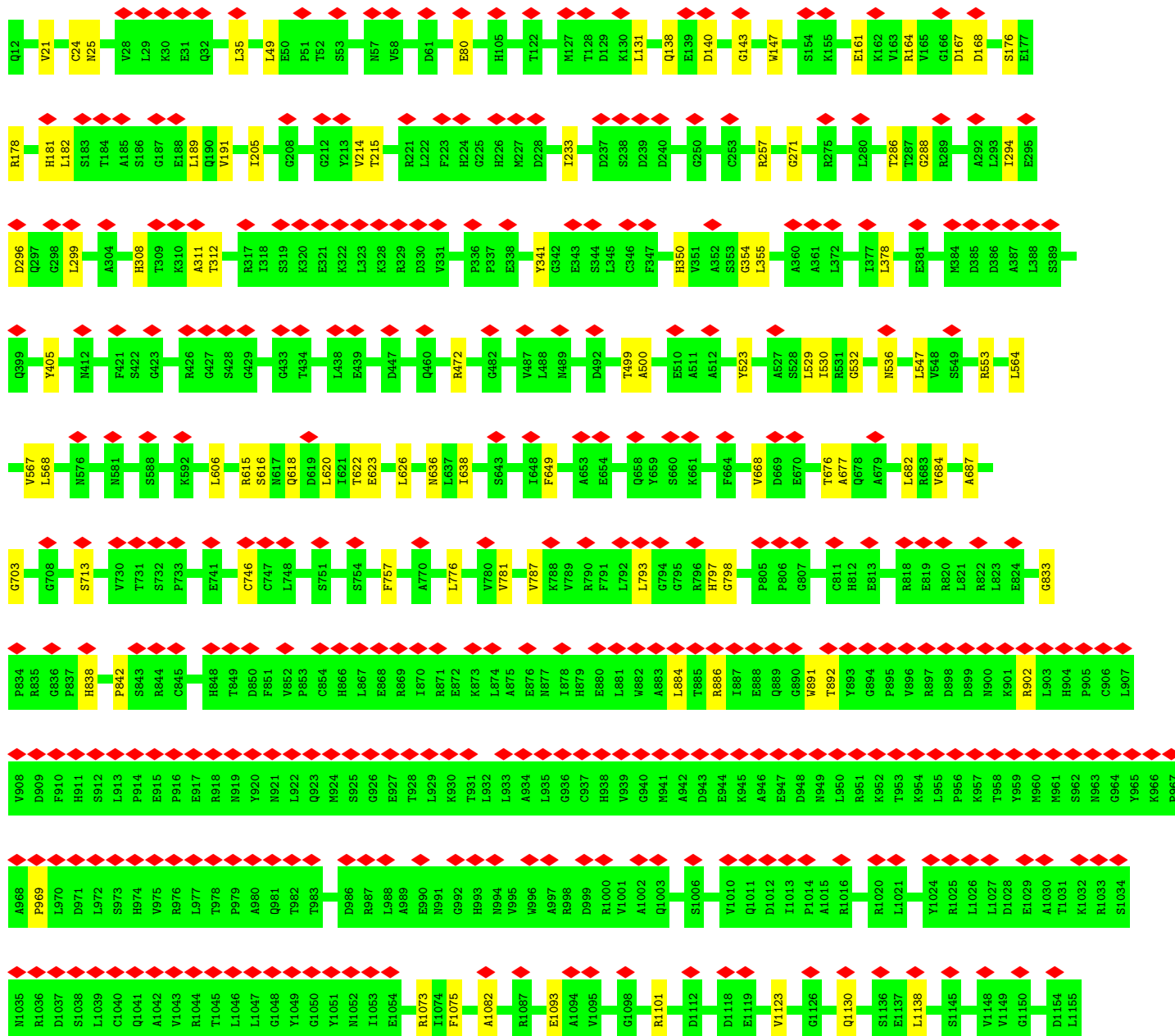
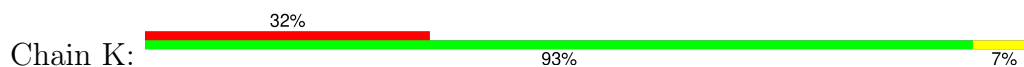
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A2815	M2816	L2817	A2818	L2819	E2820	M2821	L2822	L2823	E2824	K2825	A2826	R2827	E2828	G2829	E2830	Y2855	N2856	P2857	Q2858	P2859	D2861	L2862	S2863	Q2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	M2881	Y2882	H2883	N2884	T2885	V2886	G2887	R2888	K2889	L2890	Q2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	
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X3149	X3150	X3151	X3152	X3153	X3154	X3155	X3156	X3157	X3158	X3159	X3160	X3161	X3162	X3163	X3164	X3165	X3166	X3167	X3173	X3174	X3175	X3176	X3177	X3178	X3179	X3180	X3181	X3182	X3183	X3184	X3185	X3186	X3187	X3188	X3189	X3190	X3191	X3192	X3193	X3202	X3203	X3204	X3205	X3206	X3207	X3208	X3209	X3210	X3211	X3212	X3213	X3214	X3215	X3216	X3217	X3225	X3226	X3227	X3228	X3229
X3230	X3231	X3232	X3233	X3234	X3235	X3236	X3237	X3238	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3292	X3293	X3294	X3295	X3296	X3297	X3298	X3299	X3300	X3301	X3302	X3303	X3304	X3305	X3306	X3307	X3308	X3320	X3321	X3322	X3323	X3324	X3325	X3326	X3327	X3328	X3329	X3330	X3331	X3332	X3333	X3334	X3335	X3346	X3347	X3348	X3349	X3350	X3351	X3352	
X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3365	X3368	X3369	X3370	X3371	X3372	X3375	X3376	X3380	X3381	X3382	X3383	X3384	X3385	F3399	S3400	V3401	L3402	C3403	R3404	D3405	L3406	Y3407	A3408	L3409	Y3410	P3411	L3412	L3413	I3414	R3415	Y3416	V3417	D3418	R3421	A3422	H3423	W3424	L3425	T3426	E3427	P3428	N3429	F3430	S3431	E3434	Y3438							
E3441	I3442	F3443	I3444	S3447	K3448	S3449	H3450	N3451	F3452	E3455	E3456	Q3457	N3458	V3461	X3509	X3510	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3521	X3522	X3523	X3524	X3525	X3526	X3534	X3535	X3536	X3537	X3538	X3539	X3540	X3541	X3542	X3543	X3544	X3551	X3552	X3553	X3554	X3555	X3556	X3568	X3569	X3570	X3571	X3572								
X3586	X3587	X3588	X3589	X3590	X3593	X3594	X3595	X3596	X3597	X3598	X3599	X3600	X3601	X3602	X3605	X3606	H3617	K3618	L3619	L3620	S3621	K3622	Q3623	R3624	R3625	R3626	A3630	R3633	L3637	Y3638	X3639	N3647	A3655	T3660	E3666	D3671	K3675	A3676	G3677	E3678	Q3679	E3680	E3681	E3682	E3683	E3684	E3685	V3686												
E3687	E3688	D3692	E3708	K3709	S3710	K3711	E3732	E3733	S3747	K3751	E3752	Q3756	Q3762	L3765	H3766	R3767	R3768	G3769	A3770	C3781	E3784	N3804	A3805	S3806	V3807	A3829	C3834	E3843	G3858	T3859	E3867	A3871	F3880	Q3884	G3677	E3678	N3892	N3896	T3914		L4053	L4054																		
Y3917	D3927	Y3930	Y3931	Y3932	V3937	I3938	E3939	E3940	Q3941	F3946	K3954	Q3955	T3969	H3977	G3986	M3995	L3998	A3999	Q4000	D4001	S4002	I4005	E4010	L4011	L4012	D4013	L4014	Q4015	K4016	M4021	L4026	Y4031	M4032	G4033	M4042	L4043	V4044	E4045	M4049	L4053	L4054																			
D4058	K4064	D4065	G4068	S4069	E4070	A4071	F4072	Q4073	D4074	D4078	P4079	R4080	G4081	R4126	F4127	Q4128	E4129	P4130	A4131	D4132	L4133	I4134	G4135	F4136	N4137	L4141	S4146	E4147	H4148	P4150	H4151	D4152	P4153	R4154	L4155	R4156	N4157	E4160	L4161	A4162	E4163	E4167	E4177	R4183	R4184	L4185														
S4193	Q4199	V4200	E4201	M4202	Q4203	Q4204	V4205	K4206	E4207	S4208	K4209	R4210	Q4211	F4212	L4213	F4214	D4215	V4216	V4217	M4218	E4219	E4234	I4242	X4315	X4320	X4325	X4326	X4327	X4330	R4546	V4547	K4548	F4549	L4553	L4560	L4576	F4629	S4633	T4634	Y4635	Y4636	A4640	L4641	R4642	Q4643															
L4646	L4650	L4654	G4658	Y4659	Y4660	K4663	K4673	E4674	L4675	A4676	R4677	K4678	L4679	F4680	F4681	D4682	C4683	L4684	Y4685	L4686	T4687	E4688	Q4689	F4690	E4691	D4692	D4693	D4694	V4695	K4696	D4700	T4706	P4707	S4708	P4709	P4710	S4711	D4715	K4716	F4717	R4720	K4721	V4722	L4723	D4724	K4725	H4726	G4727	D4728											

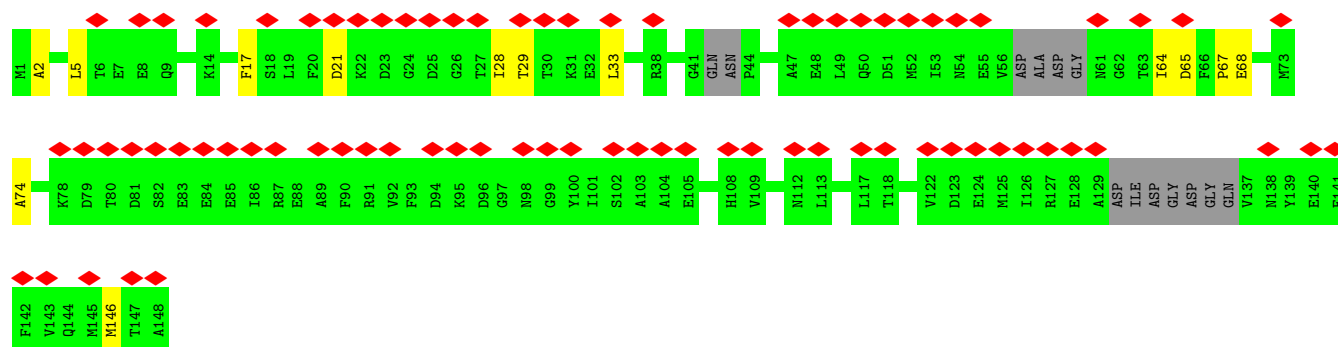


• Molecule 2: Ryanodine Receptor

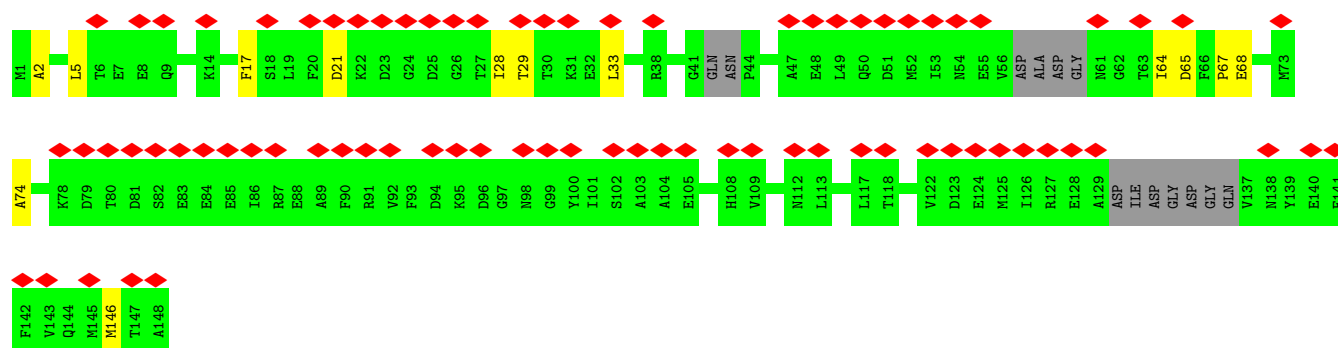


X2971	E2895	E2811	L2751	R2613	F2495	G2305	Q2128	L1639	M1527	V1284	T1156
X2972	A2896	S2812	D2752	S2618	V2496	C2306	Y2143	H1640	T1530	E1285	E1157
X2973	K2897	L2813	S2753	M2619	P2497	K2317	S2148	I1641	G1533	M1286	M1158
X2975	G2898	K2814	F2754	L2620	D2498	P2320	S2148	P1642	E1643	F1288	T1163
X2976	G2899	A2815	L2755	H2621	S2502	D2321	Q2161	E1644	M1537	L1289	G1174
X2977	G2900	M2816	M2756	Q2621	M2503	I2322	Q2162	I1650	T1538	T1432	M1170
X2978	G2899	L2817	K2757	H2622	E2514	D2334	Q2163	L1651	F1539	Y1433	S1171
X2979	H2902	A2818	F2758	L2623	E2514	D2334	R2164	E1652	M1545	Y1434	D1172
X3000	P2903	W2819	A2759	L2624	D2517	F2335	S2165	G1677	L1548	Y1435	S1173
X3001	L2904	E2820	E2760	R2625	F2518	L2336	L2166	M1678	R1438	S1436	G1174
X3002	L2905	W2821	Y2761	L2626	V2518	F2335	L2166	E1924	L1548	S1436	G1174
X3003	V2906	T2822	T2762	L2627	H2521	P2362	G2172	L1927	A1551	A1441	F1179
X3004	P2907	L2823	H2763	V2628	V2522	E2363	P2173	L1928	V1554	Q1442	R1180
X3005	Y2908	E2824	E2764	F2629	D2524	A2368	Q2174	E1949	T1557	Q1443	D1181
X3006	D2909	K2825	K2765	X2641	V2525	A2368	E2175	R1955	I1562	Q1443	G1187
X3007	T2910	A2826	W2766	X2644	L2528	L2378	L2178	G1705	T1562	V1448	C1192
X3008	L2911	R2827	A2767	X2645	L2528	A2379	M2179	E1964	E1569	V1448	S1193
X3009	T2912	E2828	F2768	X2646	L2528	T2380	Q2179	E1964	E1569	T1454	L1194
X3010	A2913	G2829	D2769	X2647	A2550	I2381	G2184	Q1974	E1569	T1454	G1195
X3011	K2914	E2830	K2770	X2667	A2550	E2382	G2184	R1975	E1569	D1456	H1201
X3012	E2915	Y2855	I2771	X2667	R2553	E2382	R2200	D1976	K1570	D1461	S1209
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X3014	A2917	P2857	Q2772	X2669	Y2554	A2384	L2202	M1982	I1572	D1466	L1211
X3015	R2918	Q2858	N2773	X2670	L2557	I2385	G2203	K1983	E1572	L1466	L1211
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X3038	E2925	V2865	L2781	X2680	S2582	I2444	Q2246	A1990	M1597	I1483	Q1220
	L2926	T2866	D2782	X2681	M2583	G2449	L2258	E1991	Q1598	H1484	E1221
X3041	L2927	L2867	E2783	X2682	L2584	G2449	L2258	T1992	M1599	S1485	A1227
X3042	K2928	S2868	E2784	X2683	H2585	I2454	G2267	A1993	L1600	S1486	M1230
X3043	F2929	R2869	L2785	X2688	R2589	R2455	W2268	R1994	R1614	L1487	K1240
X3044	L2930	E2870	K2786	X2689	R2589	A2456	W2268	R1995	V1615	K1488	
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X3051	Q2934	M2874	T2789	X2694	R2594	S2460	T2272	D1810	R1619	H1511	H1252
X3052	Y2935	A2875	L2791	X2695	T2597	L2461	D2275	K1811	A1620	T1512	P1253
X3053	A2936	E2876	R2792	X2696	K2598	V2462	V2276	R1814	G1621	D1513	H1254
X3054	P2937	Q2877	K2793	X2696	K2598	D2465	A2277	G1817	E1622	L1514	Y1255
X3055	T2938	L2878	P2793	X2736	R2601	I2470	A2278	G1817	R1623	I1516	
X3056	R2939	L2878	T2794	D2736	D2602	I2470	A2278	E1818	L1624	G1517	G1262
X3057	X2956	A2879	K2795	P2737	V2602	I2471	N2284	C2043	A1627	T1263	T1263
X3058	X2957	E2880	T2796	R2738	D2603	S2472	L2287	E2097	V1628	V1264	V1264
X3059	X2958	N2881	F2797	P2739	L2604	L2473	Q2292	G1824	Q1529	D1522	D1265
X3060	X2959	Y2882	S2798	V2740	E2605	P2474	Q2292	V1831	Q1630	L1524	T1266
X3061	X2960	E2741	E2799	E2741	E2606	L2475	Q2292	Q1831	T1524	T1524	
	X2961	H2883	T2742	T2742	C2607	Q2476	A2304	R2105	E1632	L1526	
	X2960	N2884	L2743	L2608	L2608	I2477					
	X2961	L2743	L2743	L2608	L2608	I2477					
	X2961	D2801	N2744	M2609	M2609	S2494					
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X3148	X2962	W2886	V2745	A2610	A2610	S2494					
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X3152	X2966	K2890	I2747	L2611	L2611	S2494					
X3153	X2967	L2891	P2748	E2749	E2749	S2494					
	X2968	K2891	K2750								
	X2969	P2808									
	X2970	K2810									

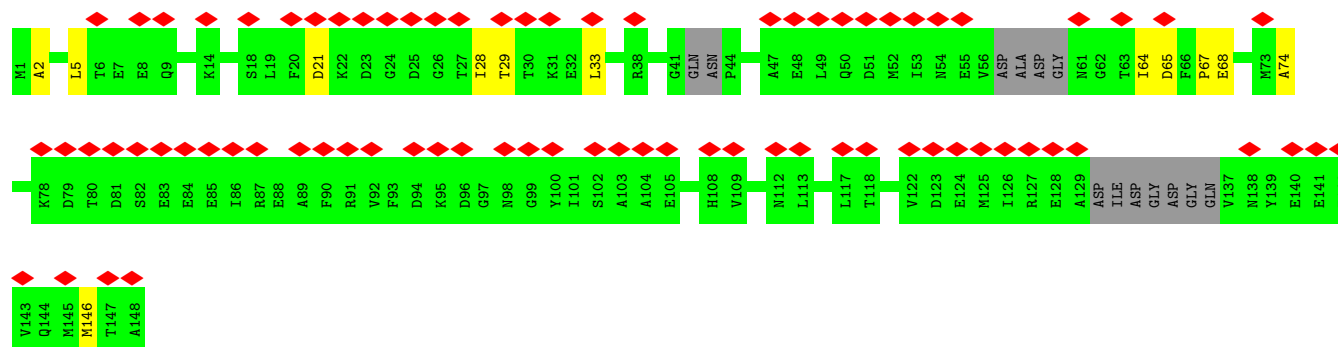
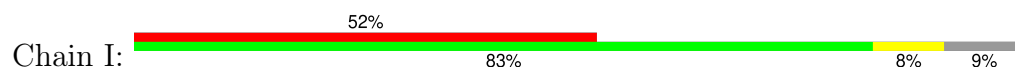




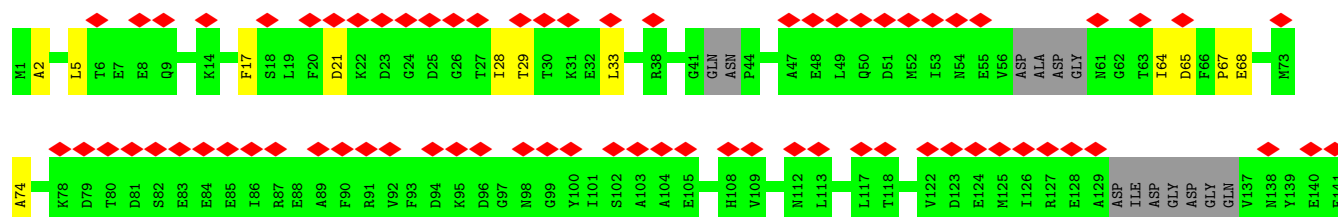
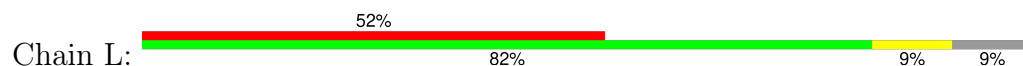
• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



• Molecule 3: Calmodulin-1



F142	V143	Q144	M145	M146	T147	A148
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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	25122	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.136	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	523.2, 523.2, 523.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.09, 1.09, 1.09	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/743	0.42	0/1014
1	D	0.25	0/743	0.42	0/1014
1	G	0.25	0/743	0.42	0/1014
1	J	0.25	0/743	0.42	0/1014
2	B	0.23	0/25353	0.38	0/34606
2	E	0.23	0/25353	0.38	0/34606
2	H	0.23	0/25353	0.38	0/34606
2	K	0.23	0/25353	0.38	0/34606
3	C	0.24	0/772	0.36	0/1059
3	F	0.24	0/772	0.36	0/1059
3	I	0.24	0/772	0.36	0/1059
3	L	0.24	0/772	0.36	0/1059
All	All	0.23	0/107472	0.38	0/146716

There are no bond length outliers.

There are no bond angle outliers.

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	727	0	651	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	727	0	651	8	0
1	G	727	0	651	8	0
1	J	727	0	651	8	0
2	B	26597	0	22867	156	0
2	E	26597	0	22867	153	0
2	H	26597	0	22867	157	0
2	K	26597	0	22867	157	0
3	C	768	0	486	9	0
3	F	768	0	486	9	0
3	I	768	0	486	8	0
3	L	768	0	486	9	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
All	All	112372	0	96016	654	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 3.

The worst 5 of 654 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)
2:E:886:ARG:HB2	2:E:891:TRP:HB2	1.73	0.71
2:B:886:ARG:HB2	2:B:891:TRP:HB2	1.73	0.71
2:H:886:ARG:HB2	2:H:891:TRP:HB2	1.73	0.71
2:K:886:ARG:HB2	2:K:891:TRP:HB2	1.73	0.71
2:E:4706:THR:HG21	2:E:4773:TYR:HB2	1.74	0.70

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	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	D	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	G	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
1	J	104/107 (97%)	98 (94%)	6 (6%)	0	100	100
2	B	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	E	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	H	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
2	K	3396/3816 (89%)	3335 (98%)	61 (2%)	0	100	100
3	C	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	F	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	I	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
3	L	127/148 (86%)	124 (98%)	3 (2%)	0	100	100
All	All	14508/16284 (89%)	14228 (98%)	280 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	66/88 (75%)	66 (100%)	0	100	100
1	D	66/88 (75%)	66 (100%)	0	100	100
1	G	66/88 (75%)	66 (100%)	0	100	100
1	J	66/88 (75%)	66 (100%)	0	100	100
2	B	2222/3025 (74%)	2221 (100%)	1 (0%)	100	100
2	E	2222/3025 (74%)	2221 (100%)	1 (0%)	100	100
2	H	2222/3025 (74%)	2221 (100%)	1 (0%)	100	100
2	K	2222/3025 (74%)	2221 (100%)	1 (0%)	100	100
3	C	29/126 (23%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	29/126 (23%)	29 (100%)	0	100	100
3	I	29/126 (23%)	29 (100%)	0	100	100
3	L	29/126 (23%)	29 (100%)	0	100	100
All	All	9268/12956 (72%)	9264 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2128	GLN
2	E	2128	GLN
2	H	2128	GLN
2	K	2128	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	3955	GLN
2	K	2128	GLN
2	H	838	HIS
2	K	838	HIS
2	E	4981	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	56
2	E	56
2	H	56
2	K	56

The worst 5 of 224 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4331:UNK	C	4543:GLU	N	51.24
1	E	4331:UNK	C	4543:GLU	N	51.24
1	H	4331:UNK	C	4543:GLU	N	51.24
1	K	4331:UNK	C	4543:GLU	N	51.24
1	B	1054:GLU	C	1071:ARG	N	36.98

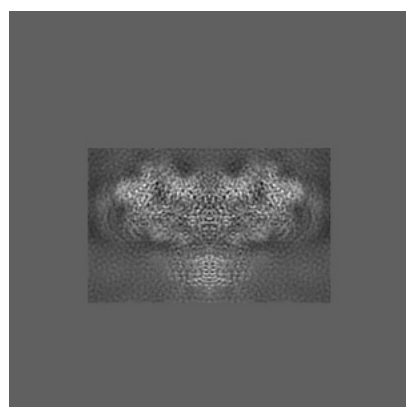
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22016. These allow visual inspection of the internal detail of the map and identification of artifacts.

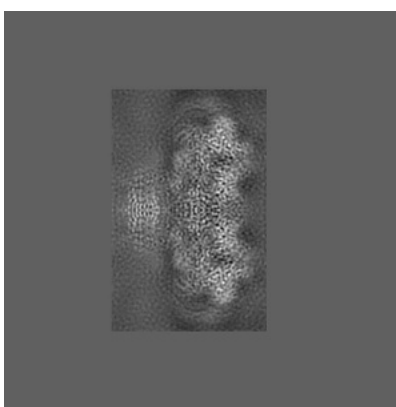
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

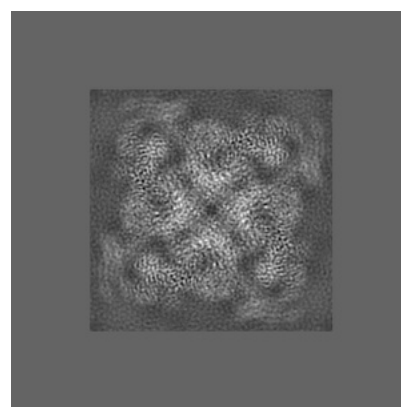
6.1.1 Primary map



X



Y



Z

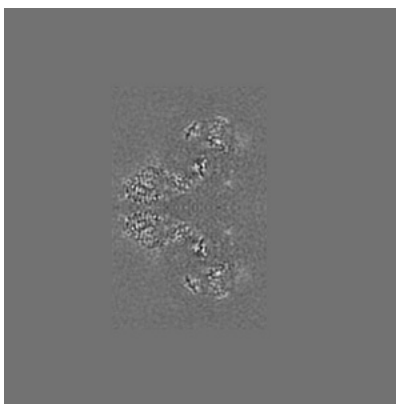
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

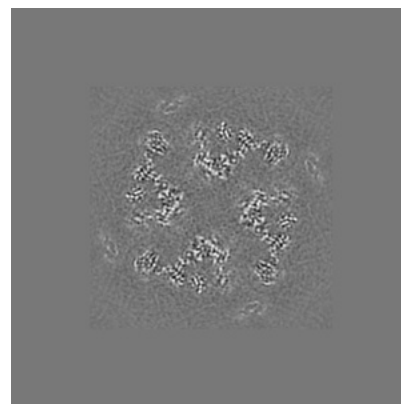
6.2.1 Primary map



X Index: 240



Y Index: 240

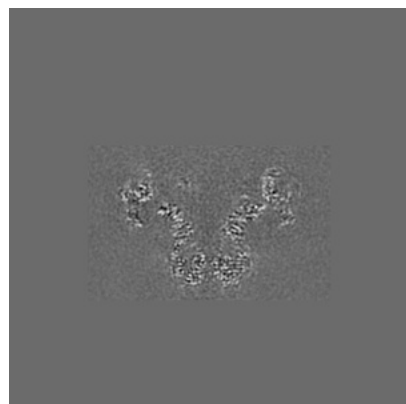


Z Index: 240

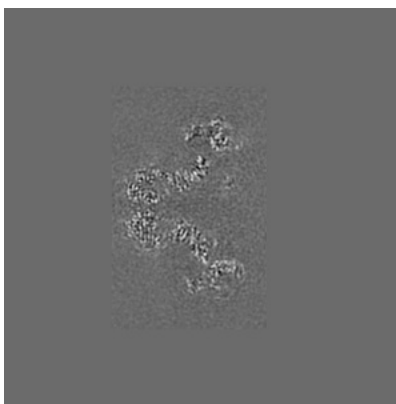
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

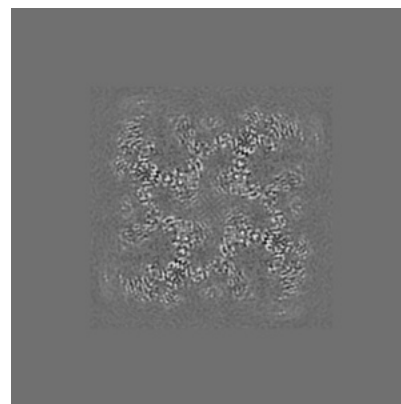
6.3.1 Primary map



X Index: 236



Y Index: 236

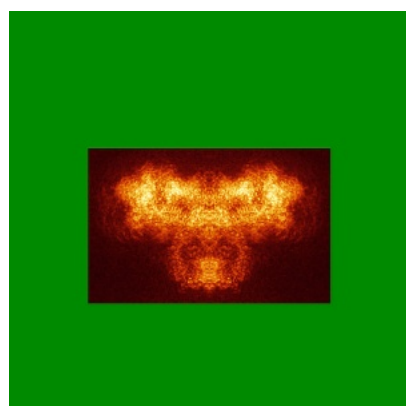


Z Index: 265

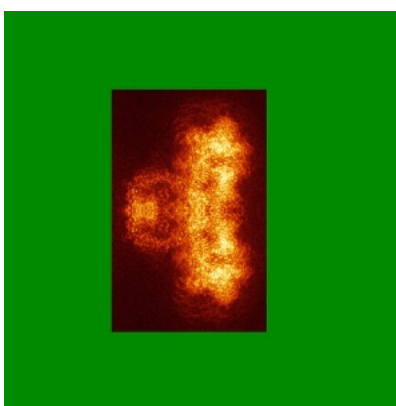
The images above show the largest variance slices of the map in three orthogonal directions.

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

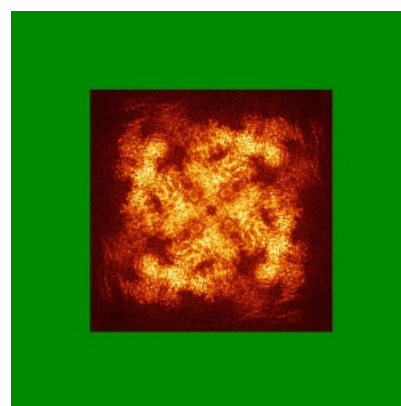
6.4.1 Primary map



X



Y

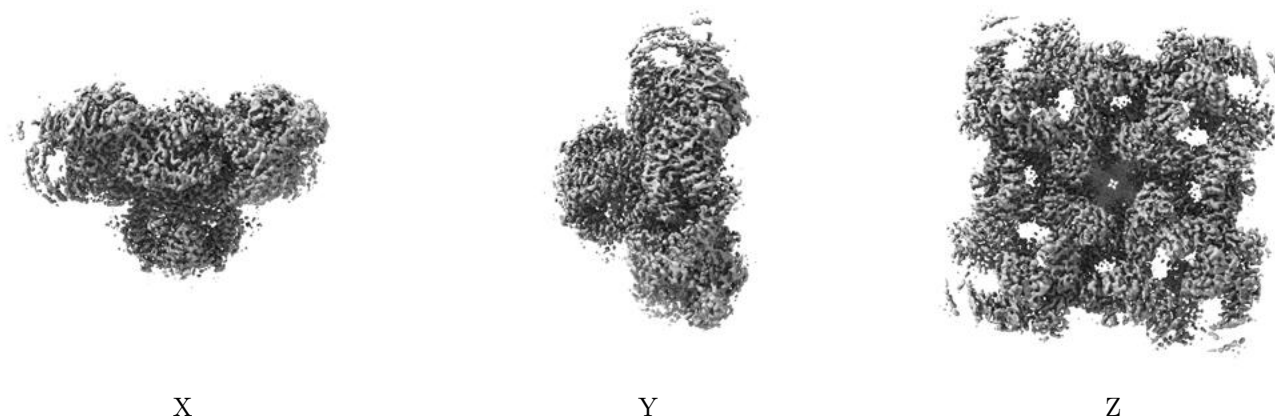


Z

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

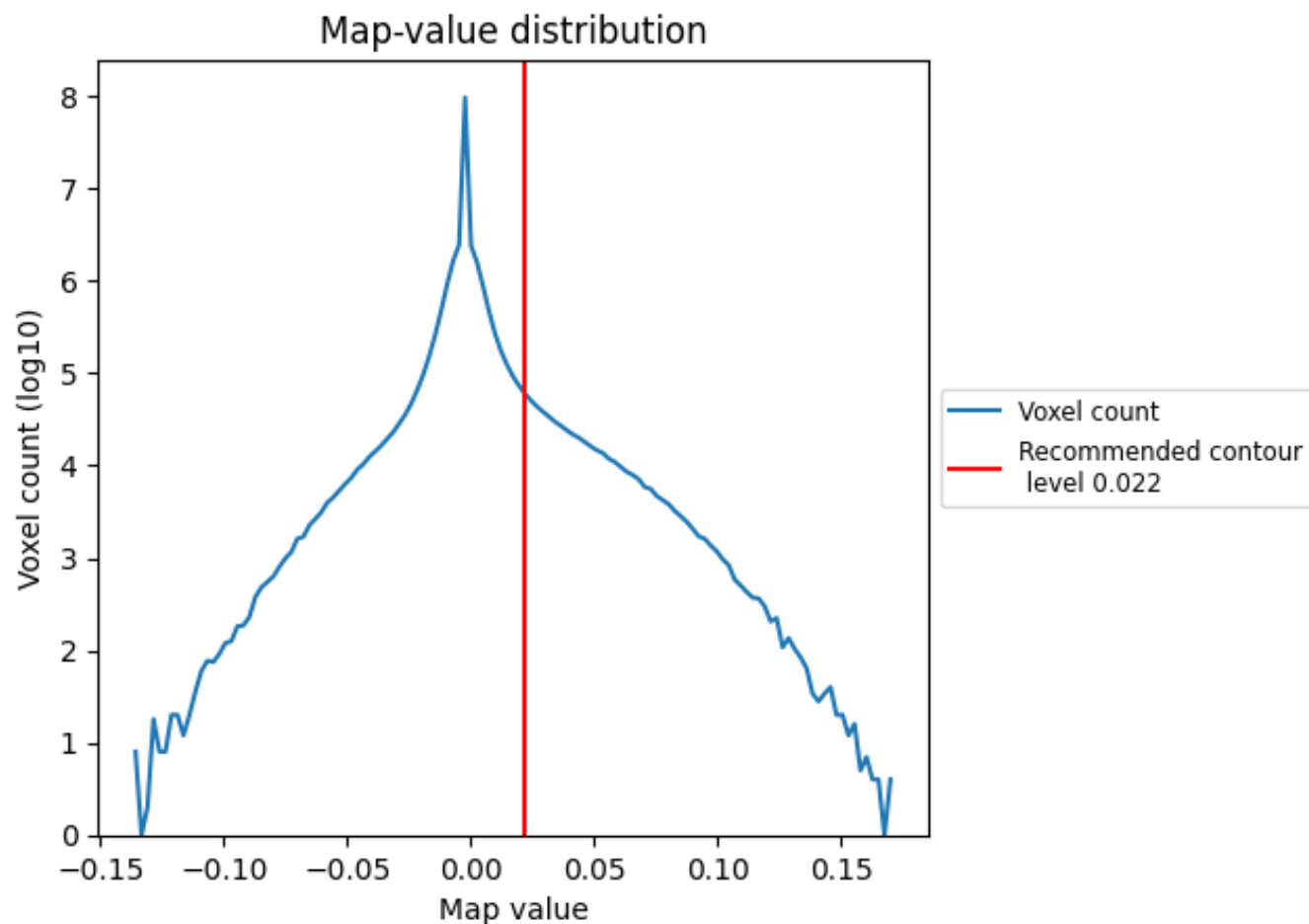
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

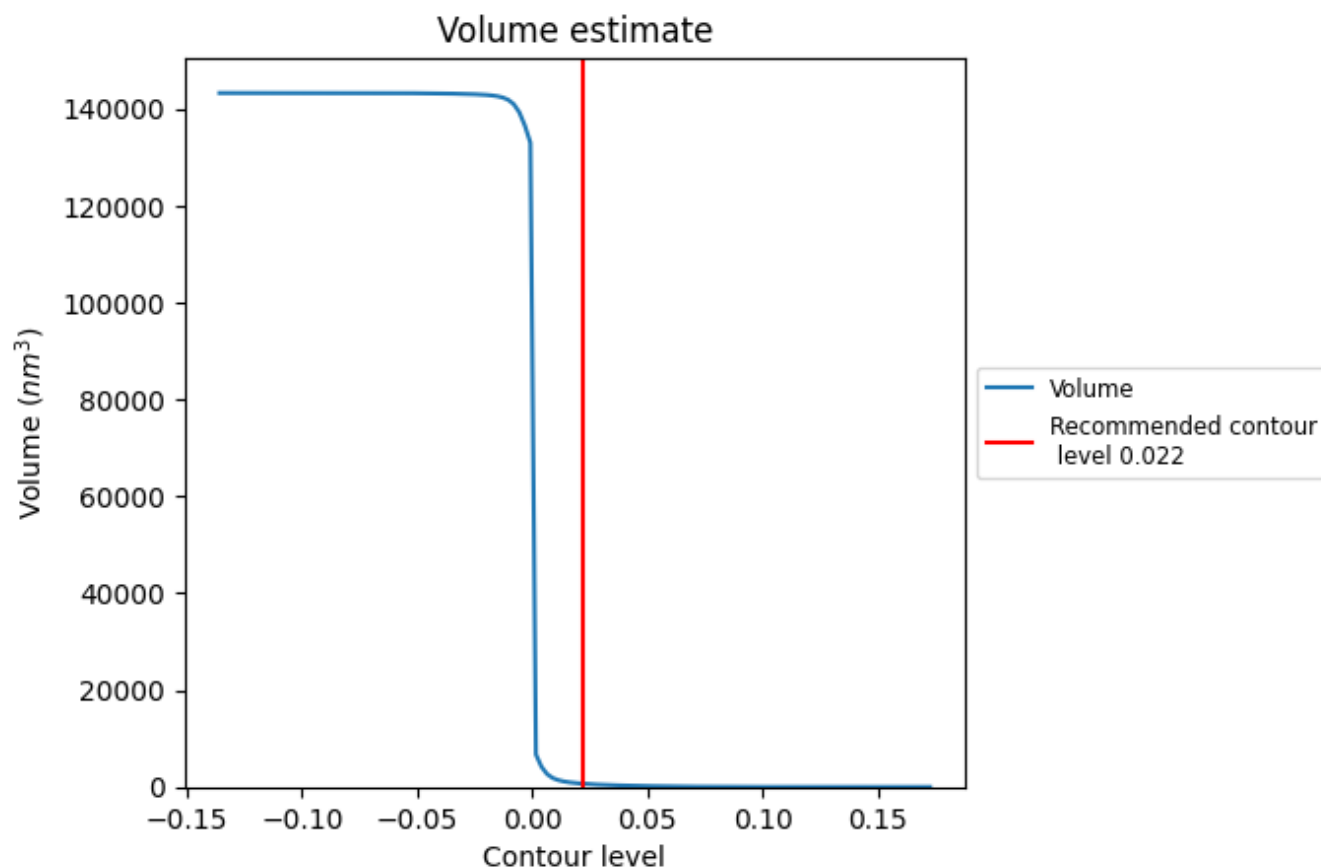
This section contains the results of statistical analysis of the map.

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.

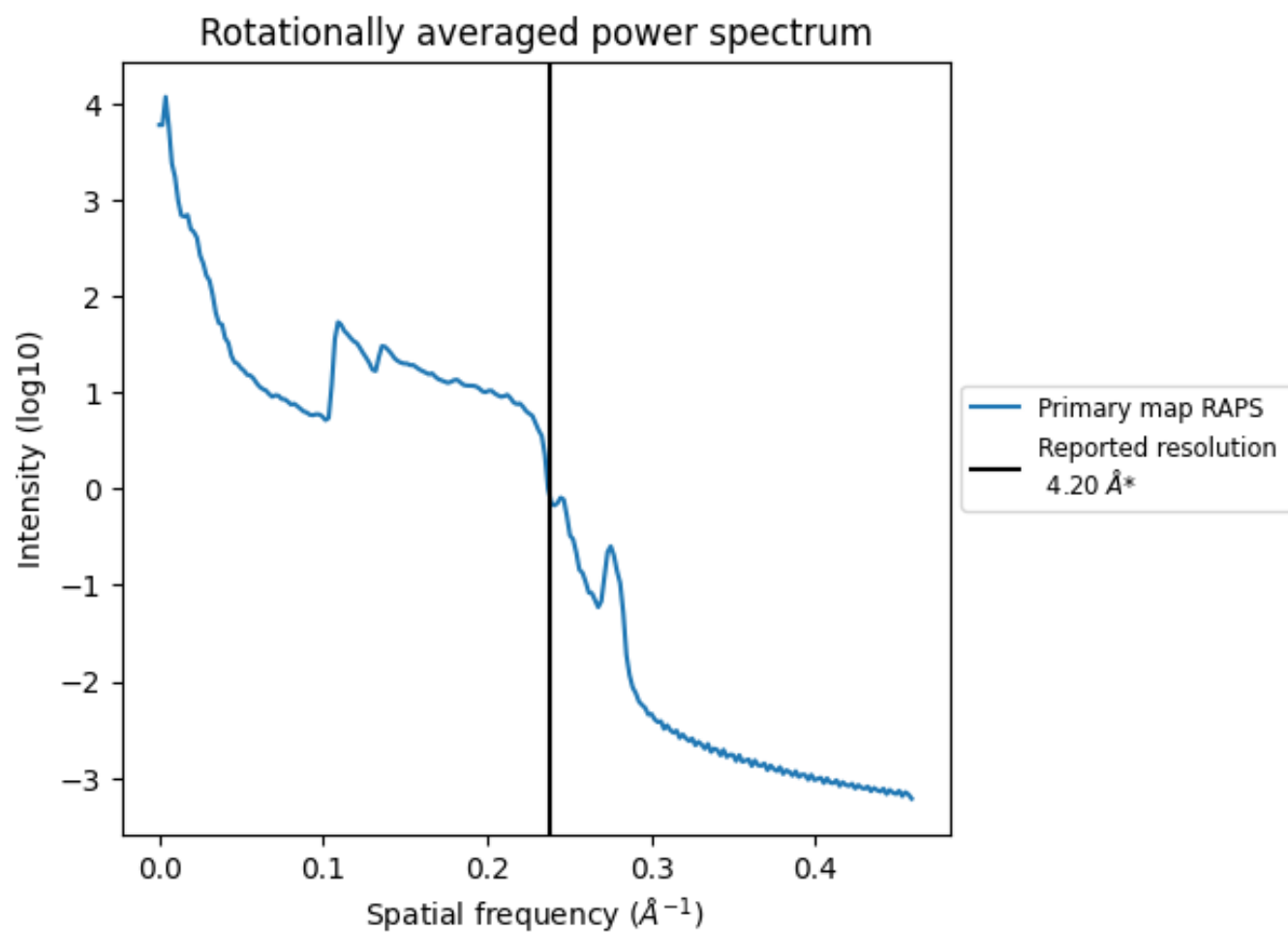
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 672 nm³; this corresponds to an approximate mass of 607 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 \AA^{-1}

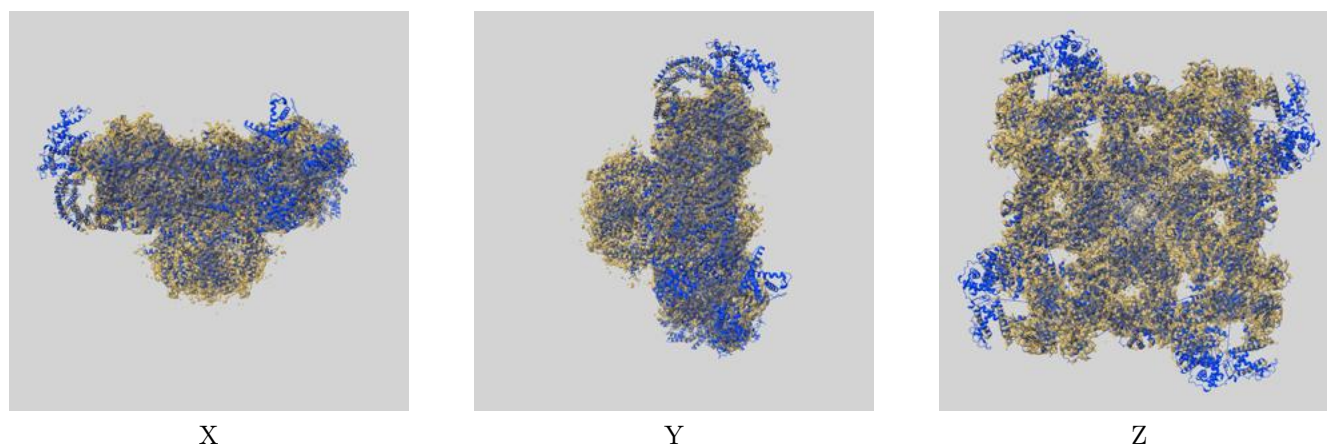
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

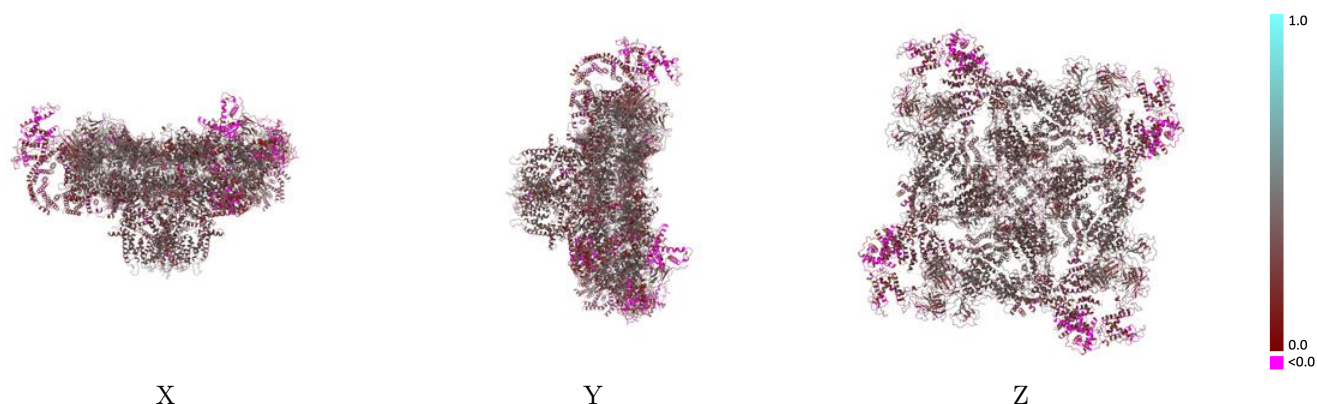
This section contains information regarding the fit between EMDB map EMD-22016 and PDB model 6X33. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



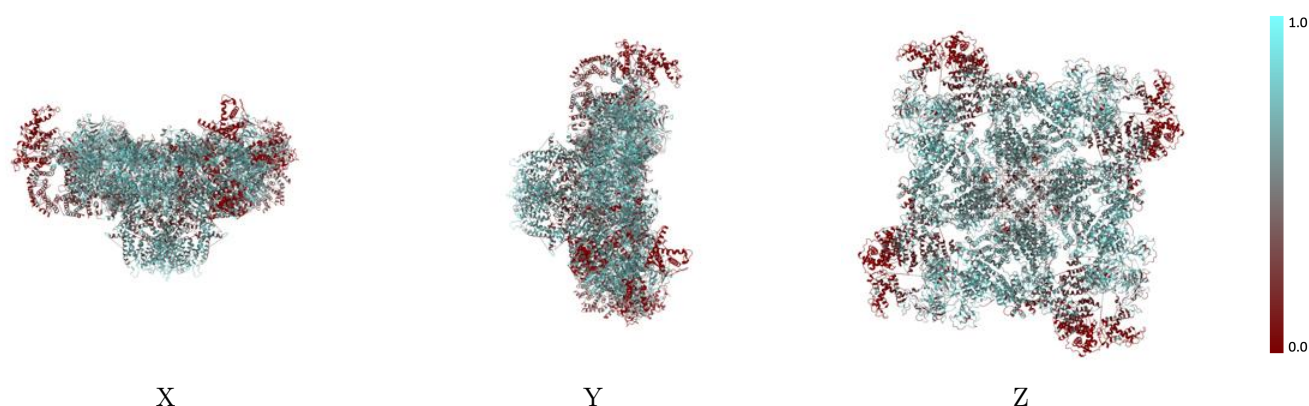
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



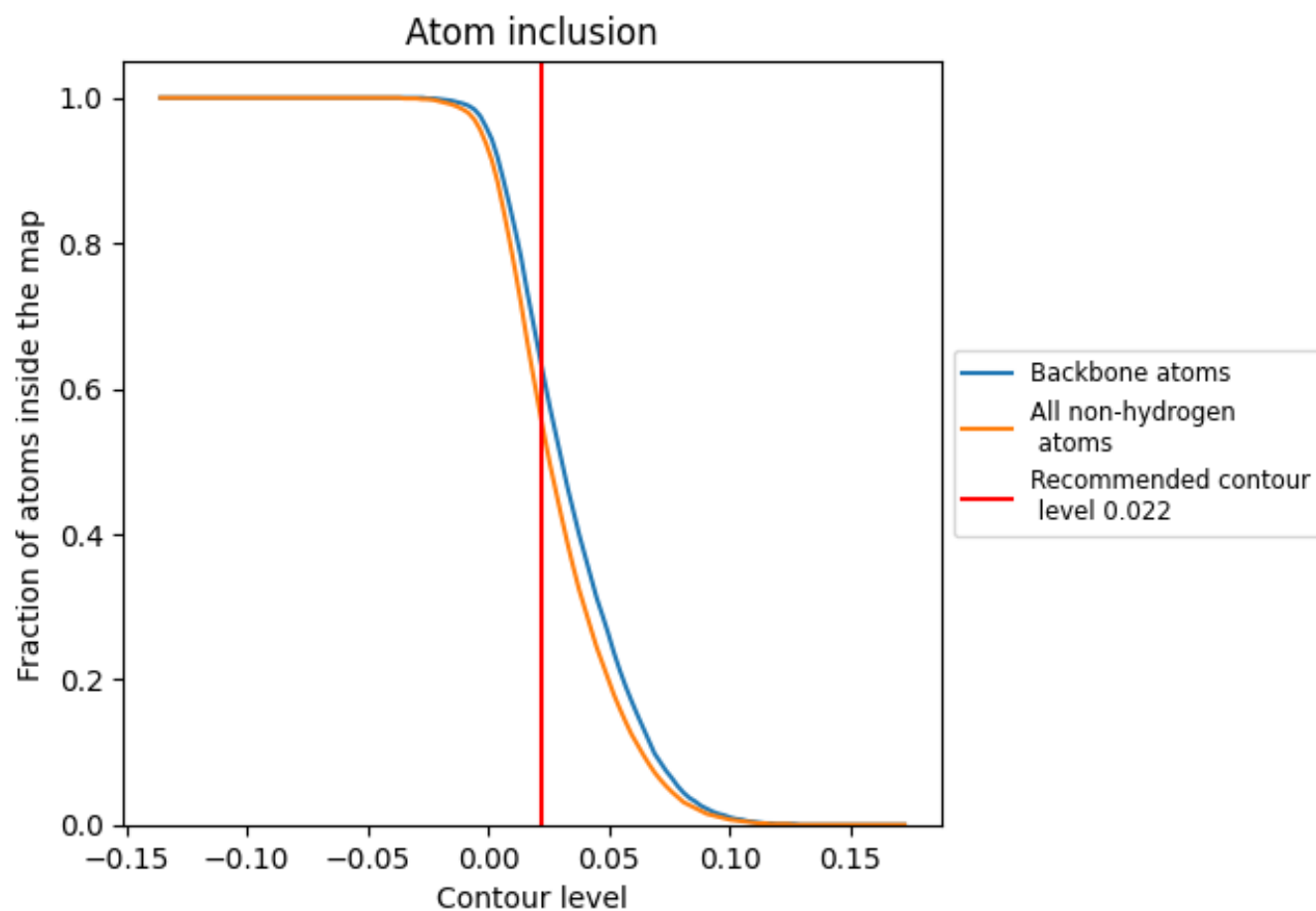
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 56% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5580	<div></div> 0.3230
A	<div></div> 0.6020	<div></div> 0.3810
B	<div></div> 0.5610	<div></div> 0.3230
C	<div></div> 0.4110	<div></div> 0.2760
D	<div></div> 0.6020	<div></div> 0.3780
E	<div></div> 0.5610	<div></div> 0.3230
F	<div></div> 0.4110	<div></div> 0.2740
G	<div></div> 0.6010	<div></div> 0.3780
H	<div></div> 0.5610	<div></div> 0.3230
I	<div></div> 0.4110	<div></div> 0.2720
J	<div></div> 0.6020	<div></div> 0.3790
K	<div></div> 0.5620	<div></div> 0.3220
L	<div></div> 0.4110	<div></div> 0.2750

1.0

0.0

<0.0