



## wwPDB EM Validation Summary Report ⓘ

Oct 12, 2024 – 03:03 PM EDT

PDB ID : 5TAX  
EMDB ID : EMD-8388  
Title : Structure of rabbit RyR1 (ryanodine dataset, class 1)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-10  
Resolution : 6.60 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](mailto: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>.

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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

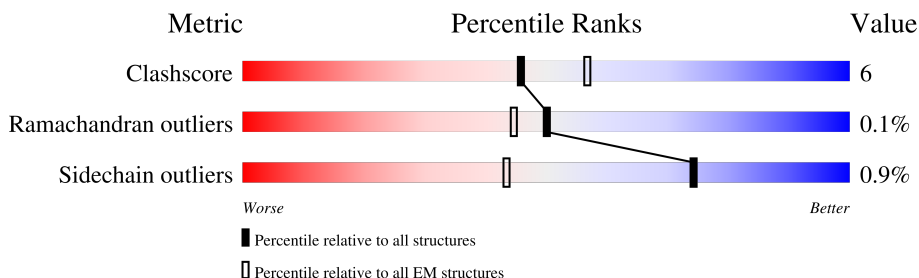
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.60 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  $\geq 3$ , 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	108	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 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	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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

Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

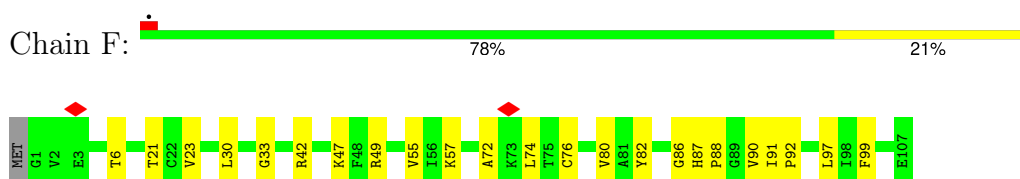
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

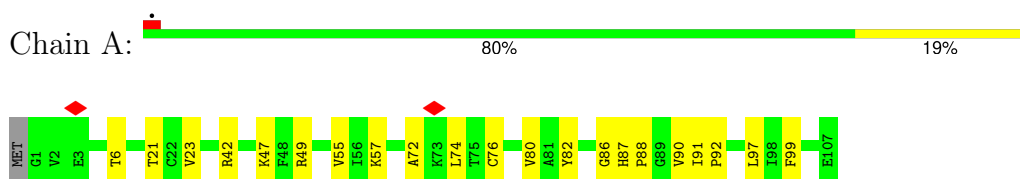
### 3 Residue-property plots

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.

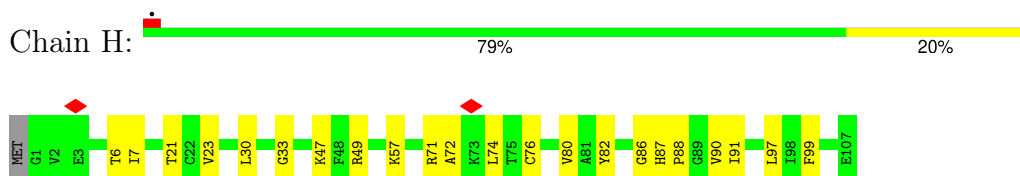
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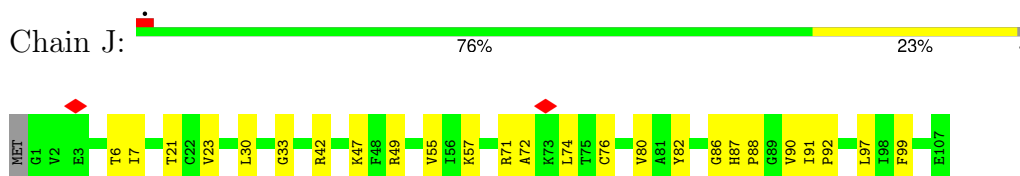
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



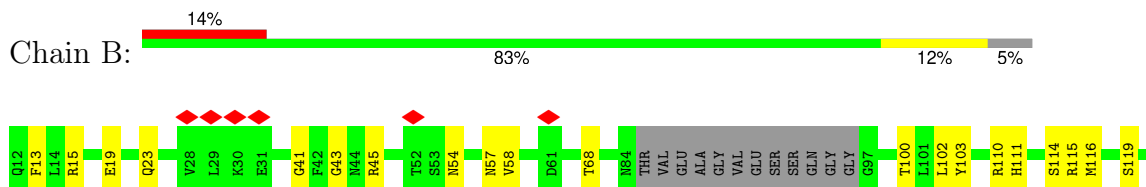
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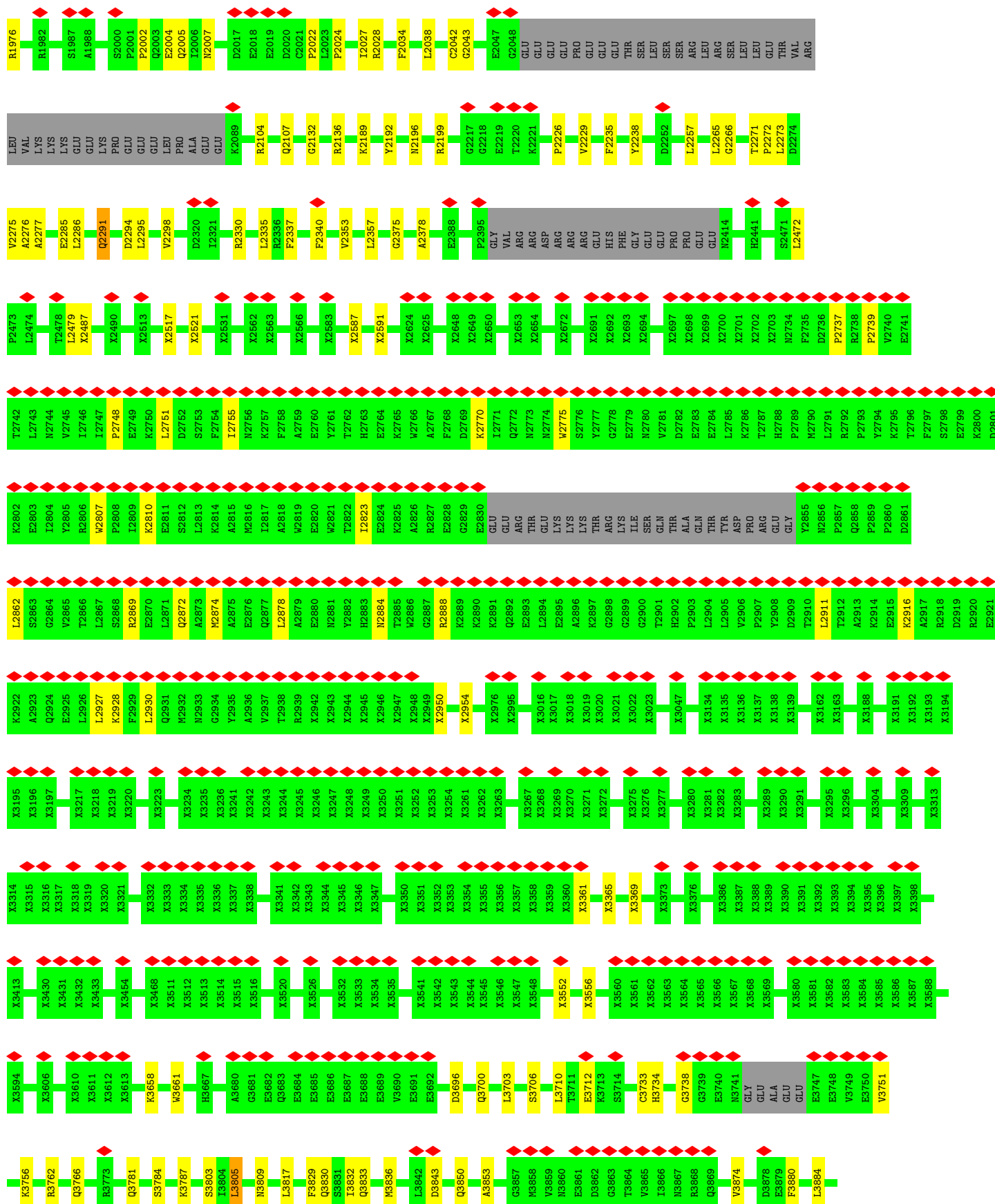
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



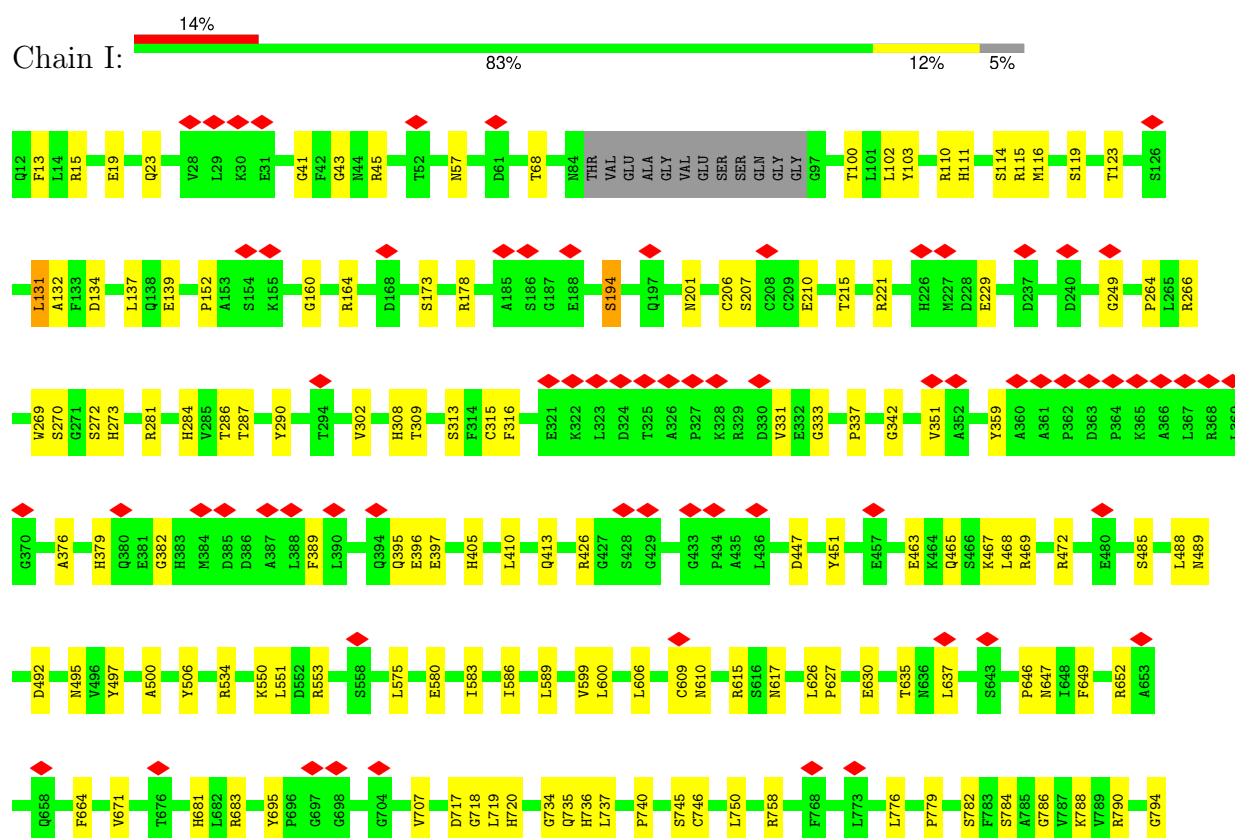
- Molecule 2: Ryanodine receptor 1



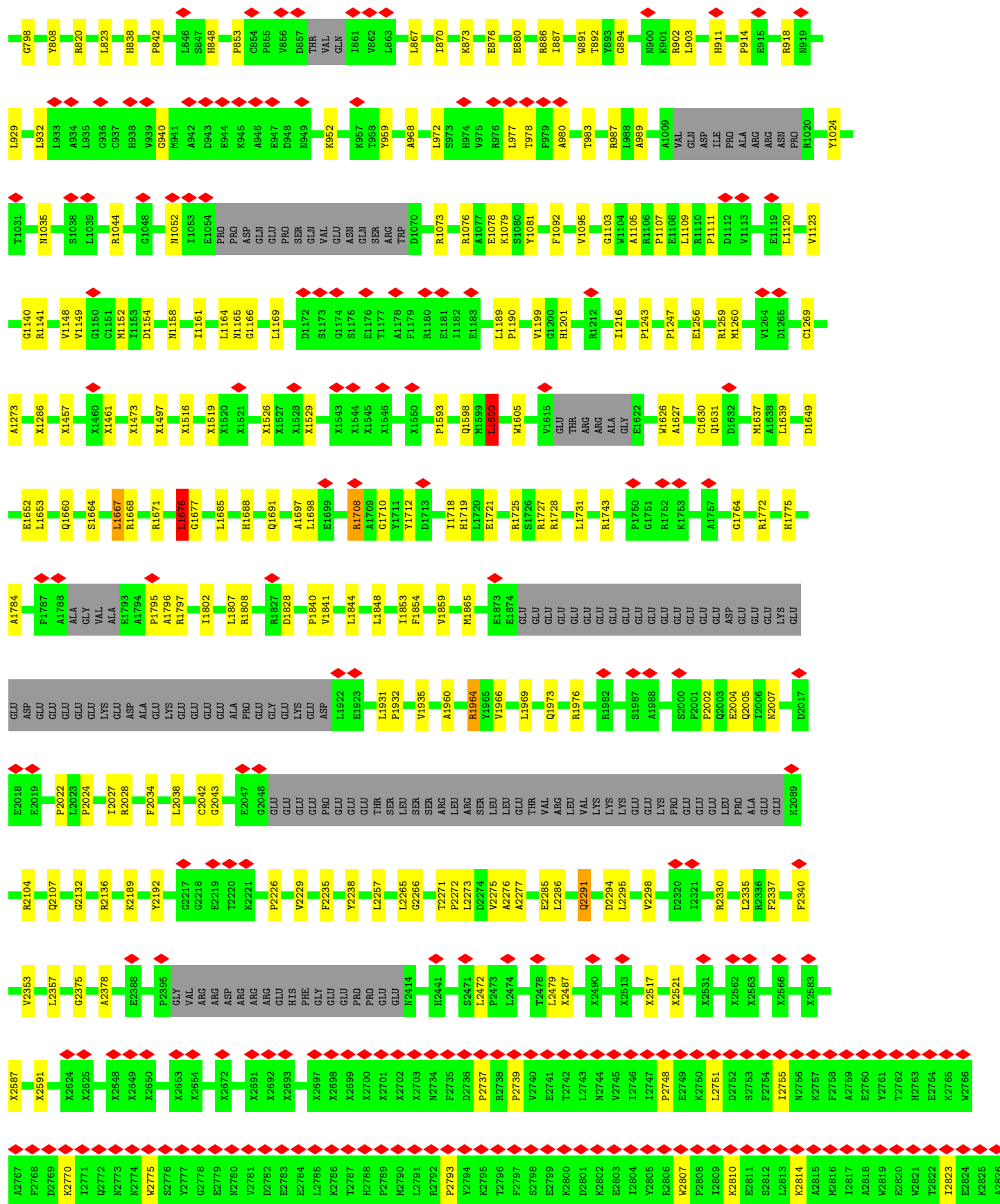




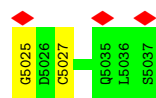
- Molecule 2: Ryanodine receptor 1



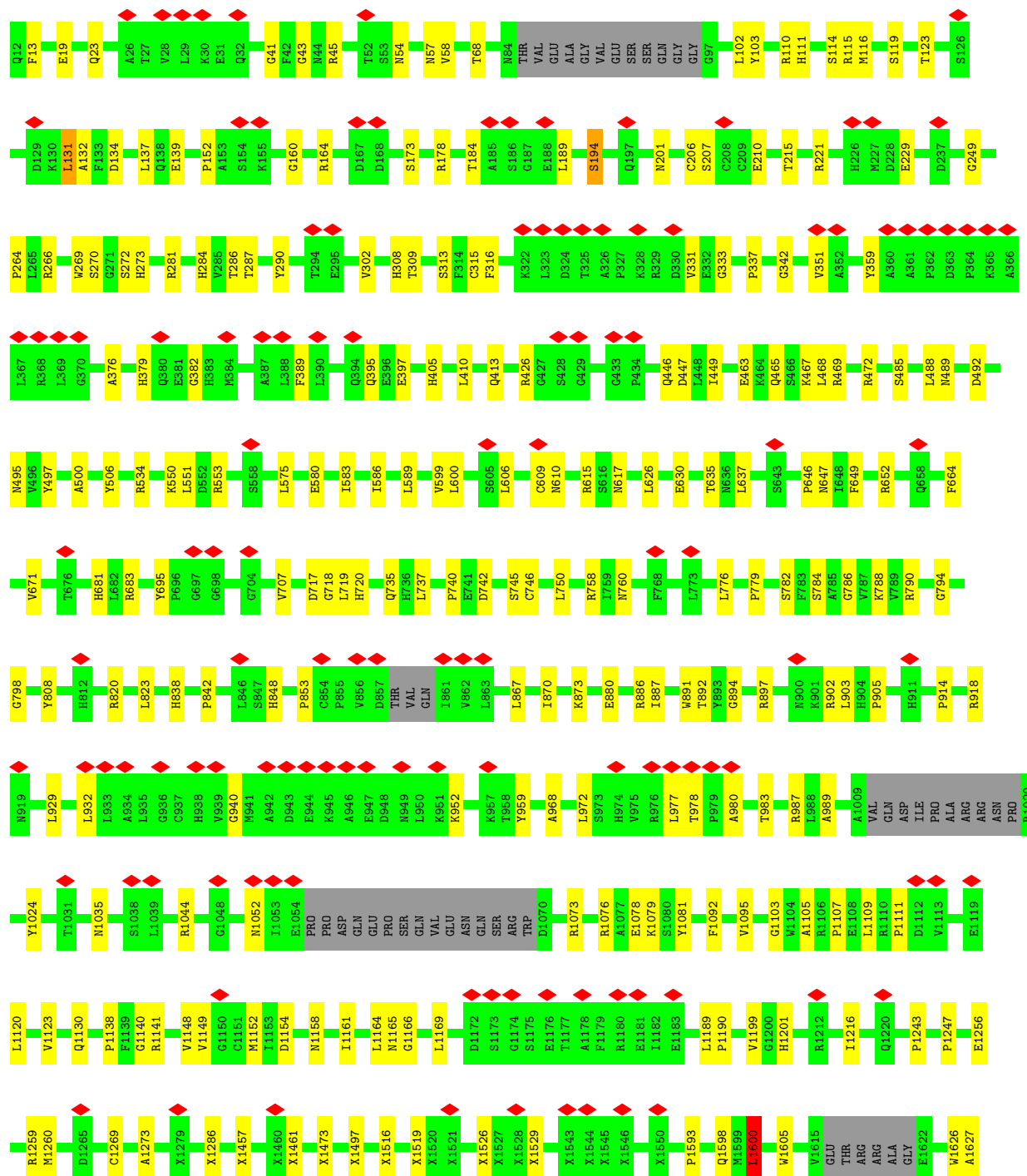
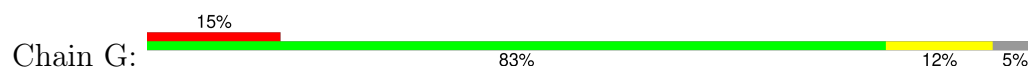


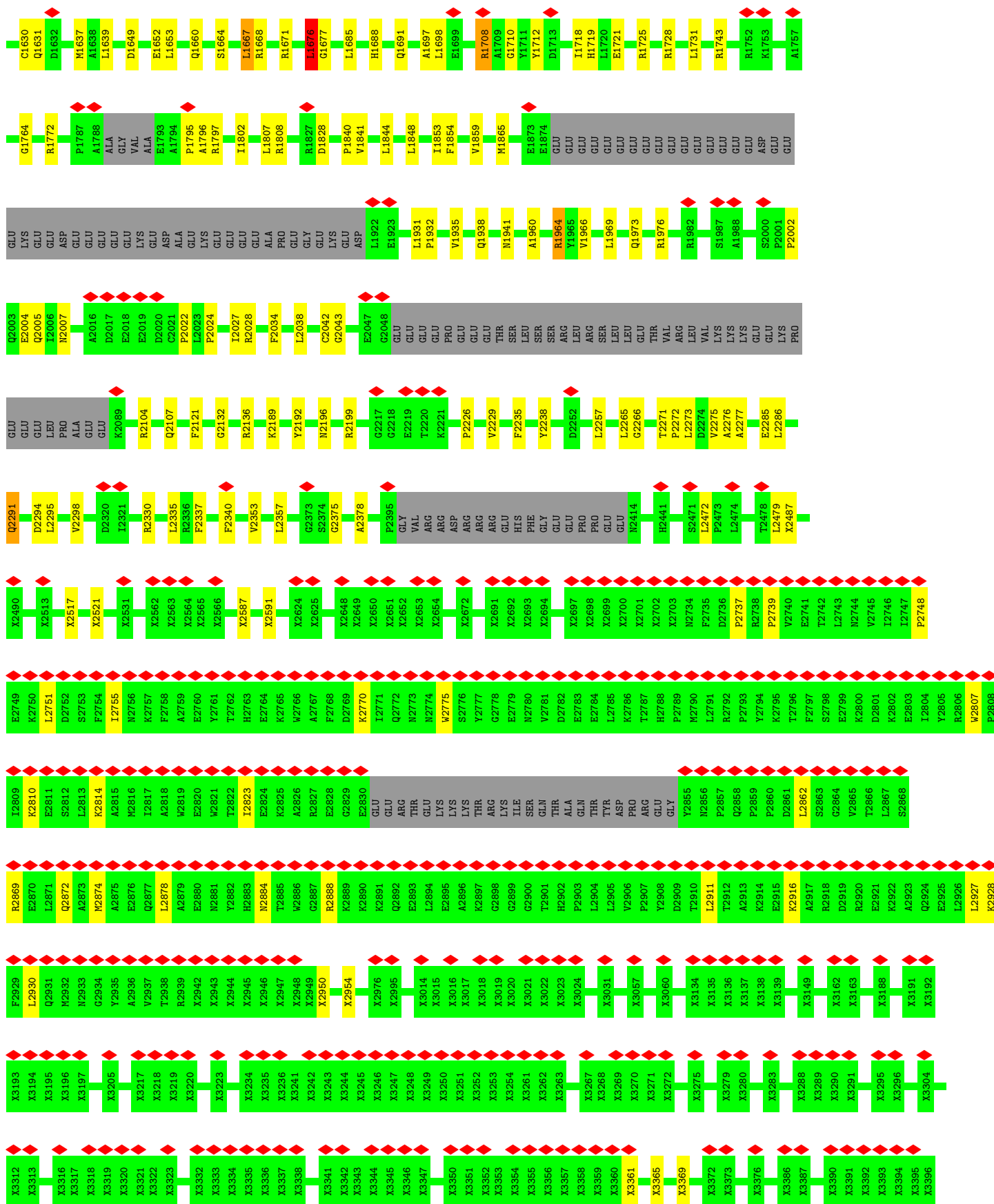


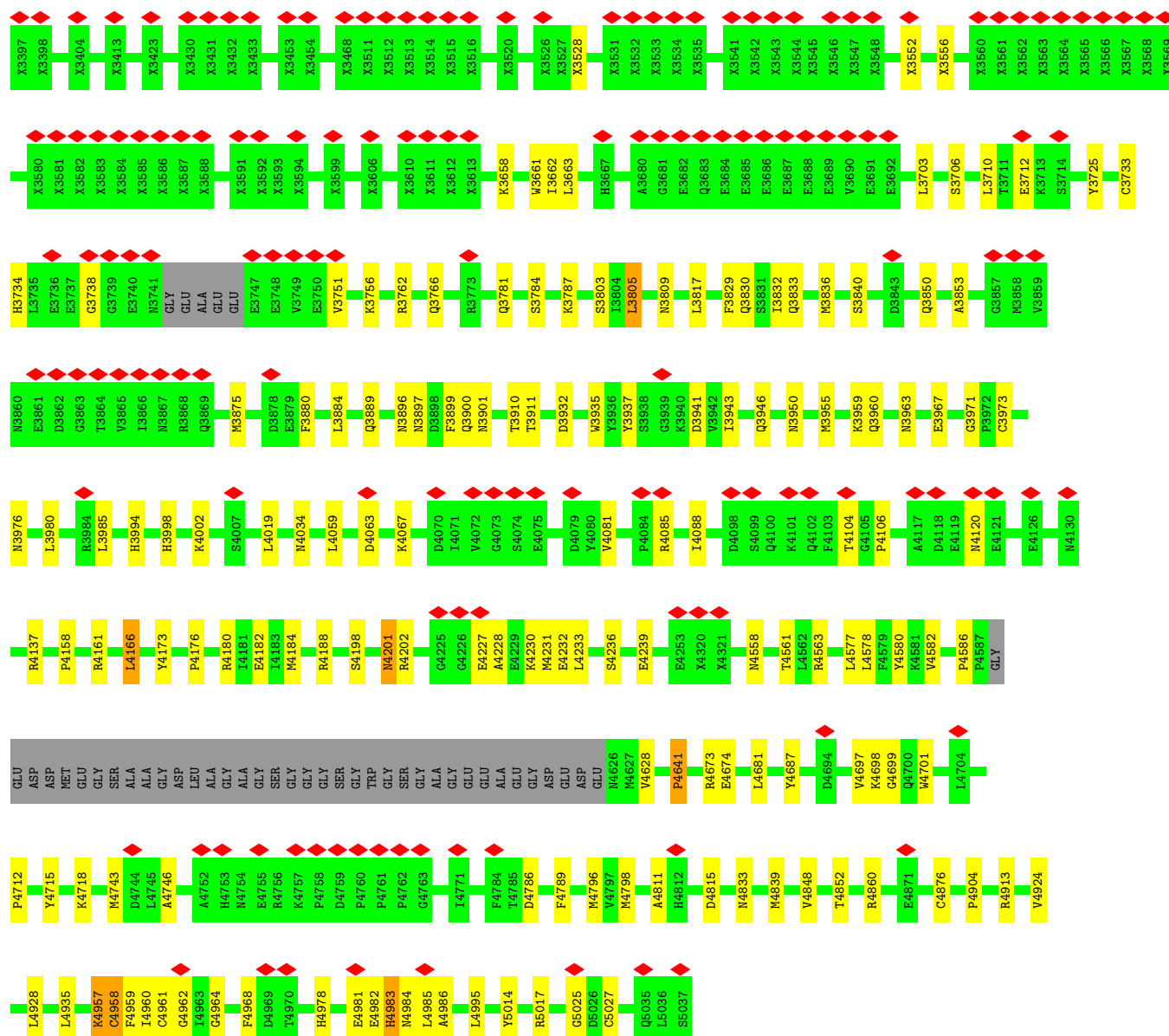
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N4833	K4698	Y4580	P4106	N3963	E3692	X3544	X3356	X2954	G2829
N4839	F4110	Y4581	F4109	E3967	D3696	X3545	X3357	K2890	E2830
V4848	W4701	P4586	A4117	G3971	Q3700	X3546	X3358	X2976	GLU
T4852	R4702	P4587	D4118	F3972	L3703	X3547	X3359	X2995	ARG
R4860	L4704	GLU	E4119	C3973	S3706	X3548	X3360	X3016	THR
C4876	P4712	ASP	M4120	N3976	L3710	X3552	X3361	X3017	GLU
C4882	Y4715	ASP	E4121	L3980	T3711	X3556	X3362	X3018	LYS
Y4718	Y4718	MET	A4126	R3984	E3712	X3560	X3363	X3019	LYS
D4730	D4730	SER	M4130	L3985	K3714	X3561	X3364	X3020	THR
M4743	M4743	ALA	R4137	H3994	C3733	X3562	X3365	X3021	ARG
D4744	D4744	ALA	P4158	H3998	H3734	X3563	X3366	X3022	ILE
L4745	L4745	ASP	R4161	K4002	G3738	X3564	X3367	X3047	GLN
A4746	A4746	LEU	M4162	K4007	G3739	X3565	X3368	X3134	THR
A4752	A4752	GLY	F4163	S4007	E3740	X3566	X3369	X3135	TVR
H4753	H4753	ALA	L4166	L4019	N3741	X3567	X3370	X3136	ASP
H4754	H4754	ALA	L4173	D4022	GLY	X3568	X3371	X3137	PRO
E4755	E4755	SER	Y4173	N4034	GLU	X3569	X3372	X3138	ARG
R4756	R4756	GLY	R4180	N4038	ALA	X3580	X3373	X3139	GLY
K4757	K4757	GLY	F4181	L4059	GLU	X3581	X3374	X3162	N2855
P4758	P4758	GLY	E4182	L4063	GLU	X3582	X3375	X3163	N2856
D4759	D4759	TRP	I4183	D4063	E3747	X3583	X3376	X3188	P2857
P4760	P4760	SER	M4184	K4067	E3748	X3584	X3377	X3191	Q2858
P4761	P4761	GLY	R4188	K4067	V3749	X3585	X3378	X3192	P2859
P4762	P4762	ALA	S4198	D4070	E3750	X3586	X3379	X3193	P2860
G4763	G4763	GLY	N4201	I4071	V3751	X3587	X3380	X3194	D2861
I4771	I4771	GLU	G4225	V4072	K3756	X3588	X3381	X3195	L2862
W4778	W4778	GLU	G4226	V4073	R3762	X3594	X3382	X3196	S2863
F4779	F4779	ASP	E4227	G4074	Q3766	X3601	X3383	X3197	Q2864
F4780	F4780	GLU	E4228	E4075	Q3767	X3608	X3384	X3211	V2865
G4781	G4781	ASP	A4229	D4079	R3773	X3609	X3385	X3217	T2866
I4782	I4782	GLU	E4230	Y4080	Q3781	X3610	X3386	X3218	S2867
I4783	I4783	GLU	M4231	V4081	S3784	X3611	X3387	X3219	R2868
T4785	T4785	GLU	E4232	F4084	K3787	X3612	X3388	X3220	R2869
D4786	D4786	GLU	L4233	R4085	S3803	X3613	X3389	X3234	E2870
P4789	P4789	ASP	S4236	T4088	L3804	X3614	X3390	X3235	L2871
F4796	F4796	GLU	E4253	M4097	L3805	X3615	X3391	X3236	Q2872
W4797	W4797	GLU	X4320	D4098	N3809	X3616	X3392	X3241	A2873
M4798	M4798	ASP	M4558	S4099	L3817	X3617	X3393	X3242	N2874
M4799	M4799	GLU	T4561	K4100	Q3829	X3618	X3394	X3243	A2875
A4811	A4811	GLU	L4562	Q4102	Q3830	X3619	X3395	X3244	E2876
H4812	H4812	GLU				X3620	X3396	X3245	Q2877
D4815	D4815	GLU				X3621	X3397	X3246	L2878
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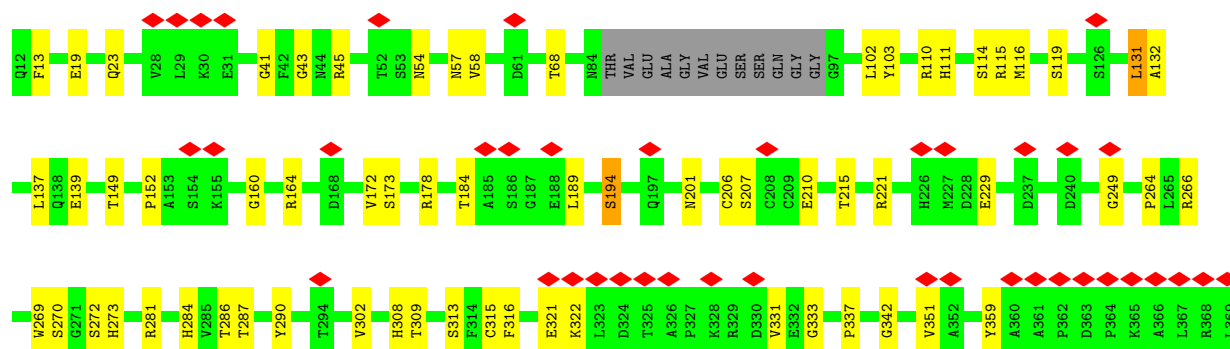
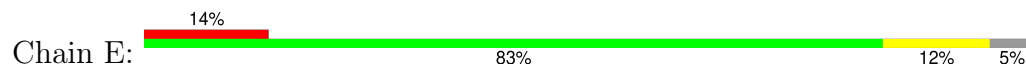
• Molecule 2: Ryanodine receptor 1





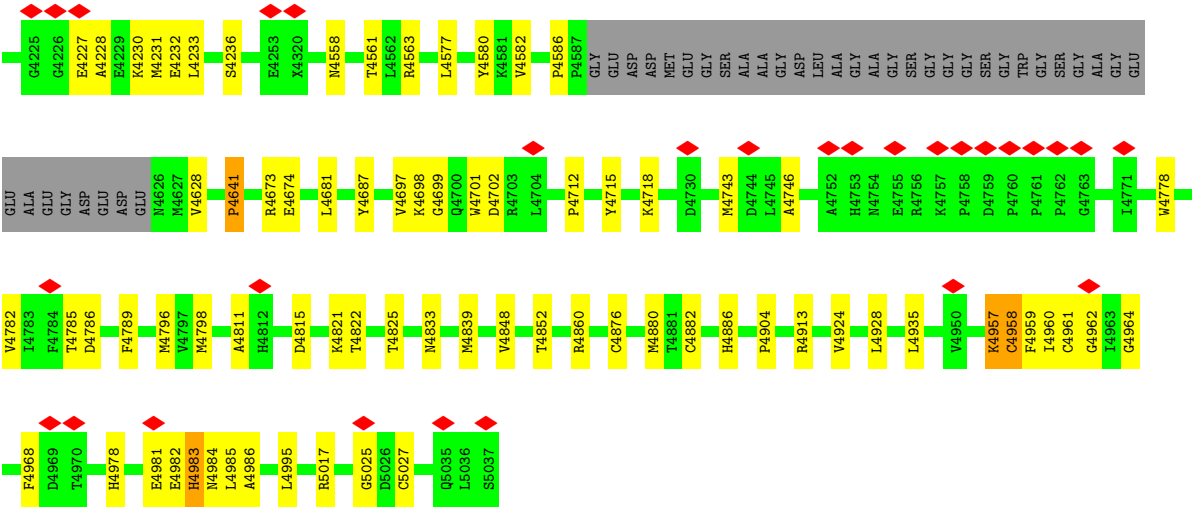


• Molecule 2: Ryanodine receptor 1





V4072	Q3900	X3612	X3337	X3241	A2936	E2876	M2816	N2756	X2521	D2320
G4073	N3901	X3613	X3338	X3242	V2937	Q2877	L2817	K2757	X2531	L2321
S4074	T3910	K3658	X3339	X3243	T2938	L2878	A2818	F2758		R2330
E4075	T3911	W3661	X3340	X3245	R2939	A2879	N2819	A2759	X2562	L2335
	D3932	S3784	X3341	X3246	X2942	E2880	E2820	E2760	X2563	R2336
	W3935	K3787	X3342	X3247	X2943	N2881	N2821	Y2761	X2566	F2337
W3936	Y3937	S3803	X3343	X3248	X2944	Y2882	T2822	T2762		R2337
Y3937	T3804	S3804	X3344	X3249	X2945	H2883	L2823	H2763		F2340
S3938	L3805	L3805	X3345	X3250	X2946	N2884	E2824	E2764		
G3939	L3806	L3806	X3346	X3251	X2947	T2885	K2825	K2765		
K3940	N3809	Q3682	X3347	X3252	X2948	V2886	A2826	W2766		
D3941	L3817	Q3683	X3350	X3253	X2949	G2887	R2827	A2767		
		E3684	X3351	X3254	X2950	R2888	E2828			
		E3685	X3352	X3255	X2954	K2889	Q2829	F2768		
		E3686	X3353	X3256	X2954	K2890	E2830	D2769		
		E3687	X3354	X3257	X2954	K2891	G2830	K2770		
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		E3689	X3356	X3259	X2954	E2893	GLU	Q2772		
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		E3691	X3358	X3261	X2954	E2895	GLU	N2774		
		E3692	X3359	X3262	X2954	E2896	LYS	W2775		
		D3696	X3360	X3263	X2954	K2897	LYS	S2776		
		Q3700	X3361	X3264	X2954	Q2898	THR	Y2777		
		L3703	X3362	X3265	X2954	G2899	ARG	G2778		
		S3706	X3363	X3266	X2954	G2900	LYS	E2779		
		L3710	X3364	X3267	X2954	T2901	LYS	N2780		
		T3711	X3365	X3268	X2954	H2902	THR	W2781		
		E3712	X3366	X3269	X2954	P2903	ALA	D2782		
		K3713	X3367	X3270	X2954	L2904	GLN	E2783		
		S3714	X3368	X3271	X2954	L2905	THR	L2784		
		C3733	X3369	X3272	X2954	V2906	TVR	E2785		
		H3734	X3370	X3273	X2954	P2907	ASP	K2786		
		G3738	X3371	X3274	X2954	Y2908	PRO	X2787		
		C3739	X3372	X3275	X2954	D2909	ARG	X2701		
		E3740	X3373	X3276	X2954	T2910	GLU	X2702		
		H3741	X3374	X3277	X2954	L2911	GLY	P2789		
		GLY	X3375	X3278	X2954	X2912	Y2855	M2790		
		ALA	X3376	X3279	X2954	X2913	N2856	K2793		
		GLU	X3377	X3280	X2954	A2914	P2857	L2791		
		GLU	X3378	X3281	X2954	X2915	Q2858	F2735		
		E3747	X3379	X3282	X2954	E2916	P2859	D2736		
		V3749	X3380	X3283	X2954	K2917	P2860	P2737		
		E3750	X3381	X3284	X2954	X2918	D2861	L2474		
		V3751	X3382	X3285	X2954	A2919	L2862	P2739		
		K3756	X3383	X3286	X2954	R2918	S2863	V2740		
		R3762	X3384	X3287	X2954	D2919	G2864	E2741		
		Q3766	X3385	X3288	X2954	R2920	V2865	T2742		
			X3386	X3289	X2954	E2921	T2866	L2743		
			X3387	X3290	X2954	A2922	L2867	K2801		
			X3388	X3291	X2954	A2923	S2868	K2802		
			X3389	X3292	X2954	Q2924	R2869	E2803		
			X3390	X3293	X2954	E2925	E2870	L2804		
			X3391	X3294	X2954	L2926	L2871	Y2805		
			X3392	X3295	X2954	L2927	Q2872	K2806		
			X3393	X3296	X2954	X2928	A2873	W2807		
			X3394	X3297	X2954	F2929	W2874	P2808		
			X3395	X3298	X2954	L2930	A2875	D2762		
			X3396	X3299	X2954	Q2931	K2810	S2763		
			X3397	X3300	X2954	M2932	E2811	F2754		
			X3398	X3301	X2954	N2933	S2812	I2755		
			X3399	X3302	X2954	G2934	K2814			
			X3400	X3303	X2954	Y2935	A2815			
			X3401	X3304	X2954					
			X3402	X3305	X2954					
			X3403	X3306	X2954					
			X3404	X3307	X2954					
			X3405	X3308	X2954					
			X3406	X3309	X2954					
			X3407	X3310	X2954					
			X3408	X3311	X2954					
			X3409	X3312	X2954					
			X3410	X3313	X2954					
			X3411	X3314	X2954					
			X3412	X3315	X2954					
			X3413	X3316	X2954					
			X3414	X3317	X2954					
			X3415	X3318	X2954					
			X3416	X3319	X2954					
			X3417	X3320	X2954					
			X3418	X3321	X2954					
			X3419	X3322	X2954					
			X3420	X3323	X2954					
			X3421	X3324	X2954					
			X3422	X3325	X2954					
			X3423	X3326	X2954					
			X3424	X3327	X2954					
			X3425	X3328	X2954					
			X3426	X3329	X2954					
			X3427	X3330	X2954					
			X3428	X3331	X2954					
			X3429	X3332	X2954					
			X3430	X3333	X2954					
			X3431	X3334	X2954					
			X3432	X3335	X2954					
			X3433	X3336	X2954					
			X3434	X3337	X2954					
			X3435	X3338	X2954					
			X3436	X3339	X2954					
			X3437	X3340	X2954					
			X3438	X3341	X2954					
			X3439	X3342	X2954					
			X3440	X3343	X2954					
			X3441	X3344	X2954					
			X3442	X3345	X2954					
			X3443	X3346	X2954					
			X3444	X3347	X2954					
			X3445	X3348	X2954					
			X3446	X3349	X2954					
			X3447	X3350	X2954					
			X3448	X3351	X2954					
			X3449	X3352	X2954					
			X3450	X3353	X2954					
			X3451	X3354	X2954					
			X3452	X3355	X2954					
			X3453	X3356	X2954					
			X3454	X3357	X2954					
			X3455	X3358	X2954					
			X3456	X3359	X2954					
			X3457	X3360	X2954					
			X3458	X3361	X2954					
			X3459	X3362	X2954					
			X3460	X3363	X2954					
			X3461	X3364	X2954					
			X3462	X3365	X2954					
			X3463	X3366	X2954					
			X3464	X3367	X2954					
			X3465	X3368	X2954					
			X3466	X3369	X2954					
			X3467	X3370	X2954					
			X3468	X3371	X2954					
			X3469	X3372	X2954					
			X3470	X3373	X2954					
			X3471	X3374	X2954					
			X3472	X3375	X2954					
			X3473	X3376	X2954					
			X3474	X3377	X2954					
			X3475	X3378	X2954					
			X3476	X3379	X2954					
			X3477	X3380	X2954					
			X3478	X3381	X2954					
			X3479	X3382	X2954					
			X3480	X3383	X2954					
			X3481	X3384	X2954					
			X3482	X3385	X2954					
			X3483	X3386	X2954					
			X3484	X3387	X2954					
			X3485	X3388	X2954					
			X3486	X3389	X2954					
			X3487	X3390	X2954					
			X3488	X3391	X2954					
			X3489	X3392	X2954					
			X3490	X3393	X2954					
			X3491	X3394	X2954					
			X3492	X3395	X2954					
			X3493	X3396	X2954					
			X3494	X3397	X2954					
			X3495	X3398	X2954					
			X3496	X3399	X2954					
			X3497	X3400	X2954					
			X3498	X3401	X2954					
			X3499	X3402	X2954					
			X3500	X3403	X2954					
			X3501	X3404	X2954					
			X3502	X3405	X2954					
			X3503	X3406	X2954					
			X3504	X3407	X2954					
			X3505	X3408	X2954					
			X3506	X3409	X2954					
			X3507	X3410	X2954					
			X3508	X3411	X2954					
			X3509	X3412	X2954					
			X3510	X3413	X2954					
			X3511	X3414	X2954					
			X3512	X3415	X2954					





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.100	Depositor
Minimum map value	-0.044	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.29	0/834	0.53	0/1123
1	F	0.29	0/834	0.53	0/1123
1	H	0.29	0/834	0.53	0/1123
1	J	0.29	0/834	0.53	0/1123
2	B	0.29	0/25428	0.54	7/34534 (0.0%)
2	E	0.29	0/25428	0.54	7/34534 (0.0%)
2	G	0.29	0/25428	0.54	7/34534 (0.0%)
2	I	0.29	0/25428	0.54	7/34534 (0.0%)
All	All	0.29	0/105048	0.54	28/142628 (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
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	8.10	133.93	115.30
2	I	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	B	131	LEU	CA-CB-CG	8.08	133.88	115.30
2	G	131	LEU	CA-CB-CG	8.07	133.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4985	LEU	CA-CB-CG	7.05	131.51	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	194	SER	Peptide
2	B	808	TYR	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	14	0
1	H	818	0	824	12	0
1	J	818	0	824	15	0
2	B	29499	0	24741	329	0
2	E	29499	0	24742	325	0
2	G	29499	0	24741	322	0
2	I	29499	0	24742	324	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102262	1338	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 1338 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:I:4182:GLU:OE2	2:I:4983:HIS:NE2	1.64	1.31
2:E:4182:GLU:OE2	2:E:4983:HIS:NE2	1.64	1.29
2:G:4182:GLU:OE2	2:G:4983:HIS:NE2	1.64	1.29
2:B:4182:GLU:OE2	2:B:4983:HIS:NE2	1.64	1.27
2:G:4982:GLU:OE1	2:G:5027:CYS:SG	1.98	1.22

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	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	H	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	J	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4416 (73%)	2899 (90%)	332 (10%)	4 (0%)	48	83
2	E	3235/4416 (73%)	2900 (90%)	331 (10%)	4 (0%)	48	83
2	G	3235/4416 (73%)	2900 (90%)	331 (10%)	4 (0%)	48	83
2	I	3235/4416 (73%)	2900 (90%)	331 (10%)	4 (0%)	48	83
All	All	13360/18096 (74%)	11967 (90%)	1377 (10%)	16 (0%)	50	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	E	1708	ARG

*Continued on next page...*

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Mol	Chain	Res	Type
2	B	4641	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2471 (99%)	22 (1%)	75	83
2	E	2493/3022 (82%)	2471 (99%)	22 (1%)	75	83
2	G	2493/3022 (82%)	2471 (99%)	22 (1%)	75	83
2	I	2493/3022 (82%)	2471 (99%)	22 (1%)	75	83
All	All	10324/12444 (83%)	10236 (99%)	88 (1%)	74	83

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	4120	ASN
2	E	1600	LEU
2	G	4201	ASN
2	G	4995	LEU
2	E	3805	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	1719	HIS
2	E	2127	GLN
2	E	4054	ASN
2	I	1598	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
2	I	479	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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	14
2	I	14

*Continued on next page...*

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Mol	Chain	Number of breaks
2	G	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.58
1	I	4345:UNK	C	4540:PHE	N	74.58
1	G	4345:UNK	C	4540:PHE	N	74.58
1	E	4345:UNK	C	4540:PHE	N	74.58
1	B	3613:UNK	C	3639:THR	N	46.52

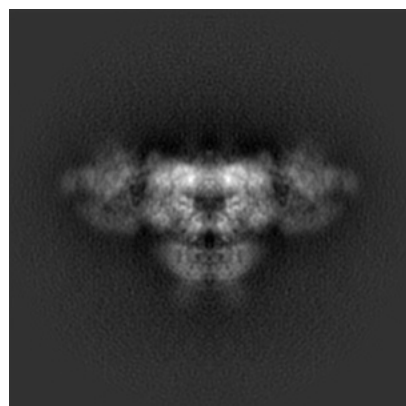
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8388. These allow visual inspection of the internal detail of the map and identification of artifacts.

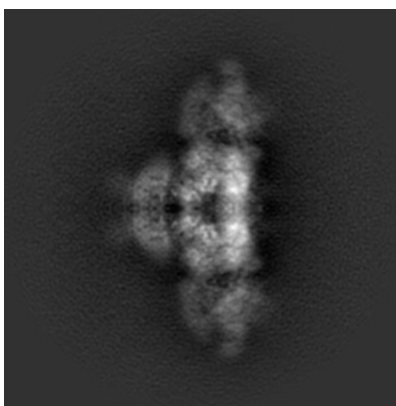
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

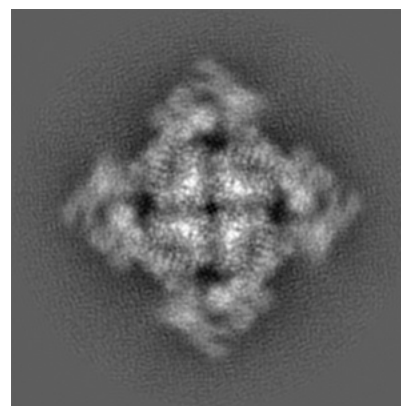
#### 6.1.1 Primary map



X

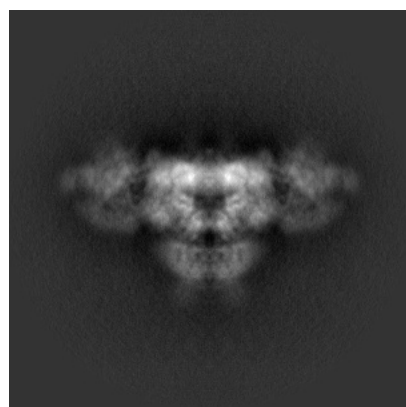


Y

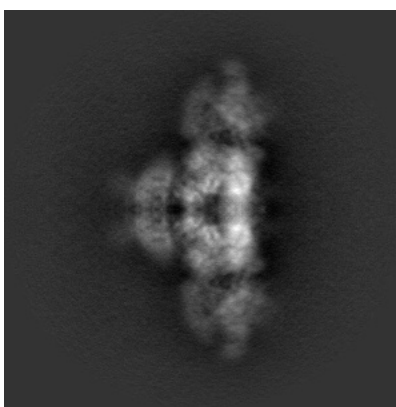


Z

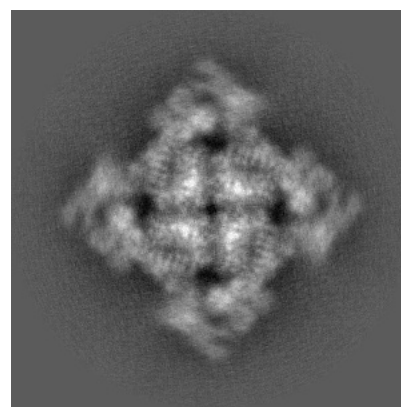
#### 6.1.2 Raw map



X



Y



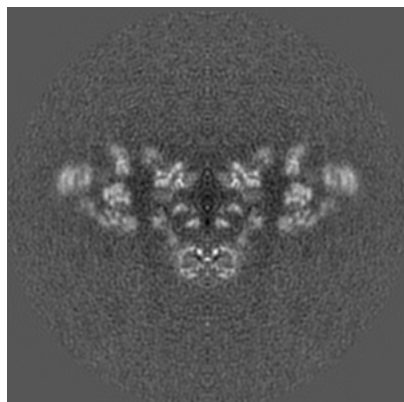
Z

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

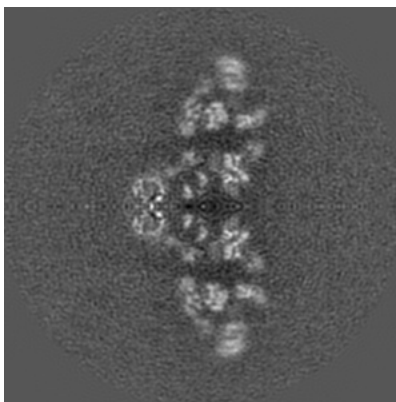


## 6.2 Central slices [i](#)

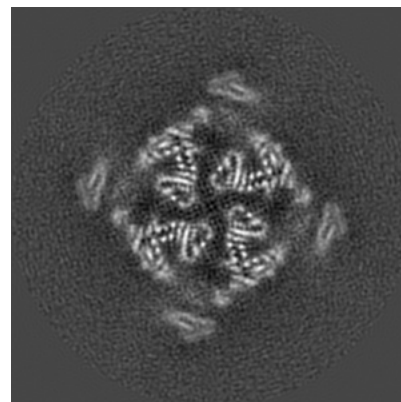
### 6.2.1 Primary map



X Index: 200

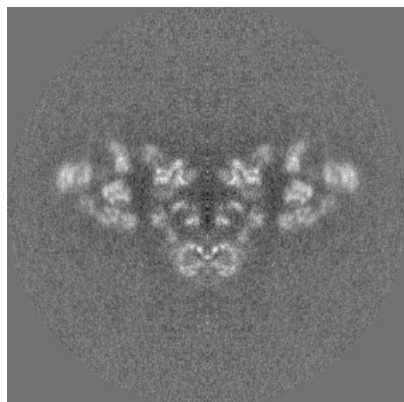


Y Index: 200

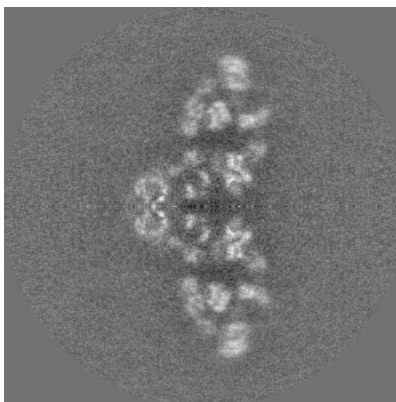


Z Index: 200

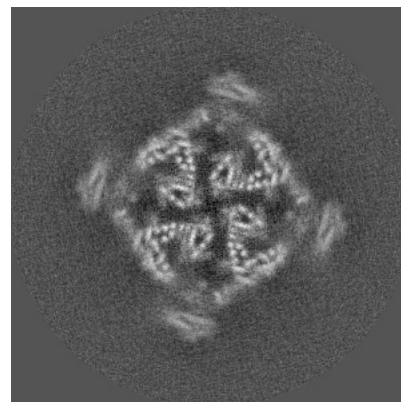
### 6.2.2 Raw map



X Index: 200



Y Index: 200

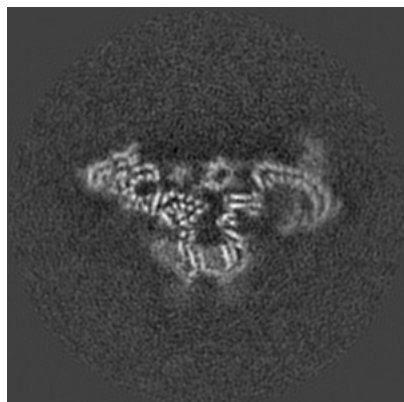


Z Index: 200

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

## 6.3 Largest variance slices [i](#)

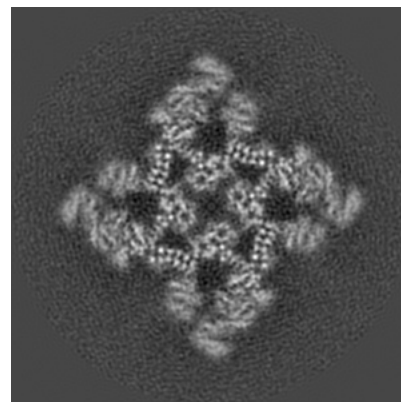
### 6.3.1 Primary map



X Index: 225

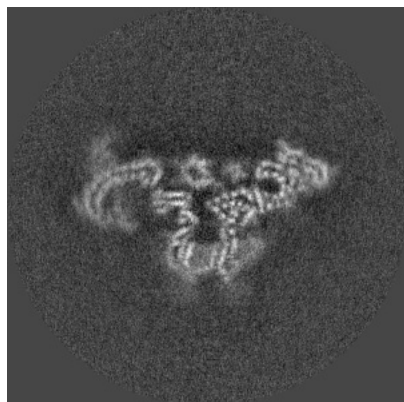


Y Index: 225

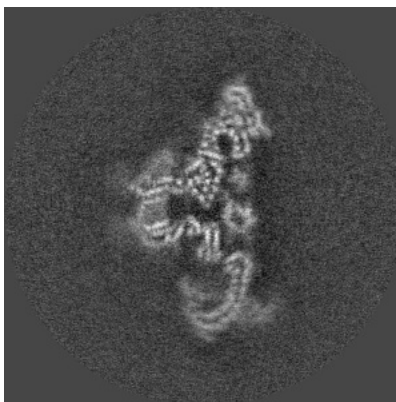


Z Index: 226

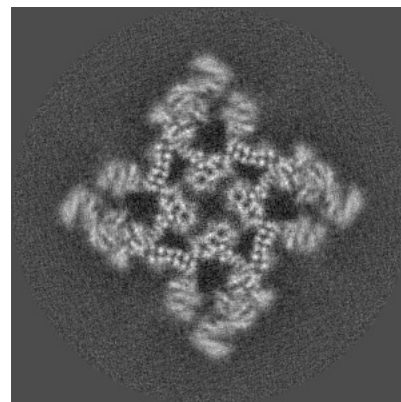
### 6.3.2 Raw map



X Index: 175



Y Index: 225

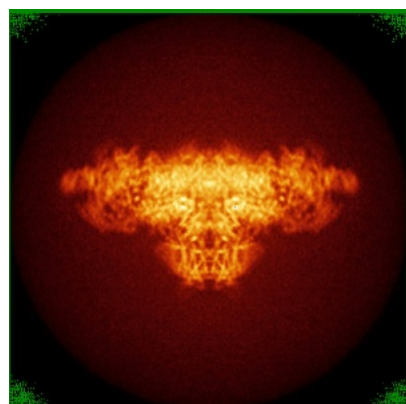


Z Index: 229

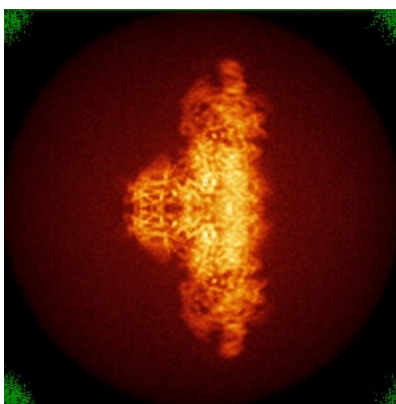
The images above show the largest variance slices of the map in three orthogonal directions.

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

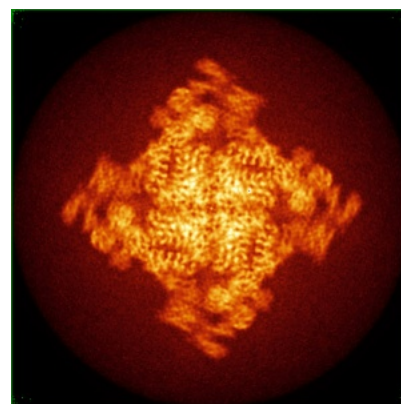
### 6.4.1 Primary map



X

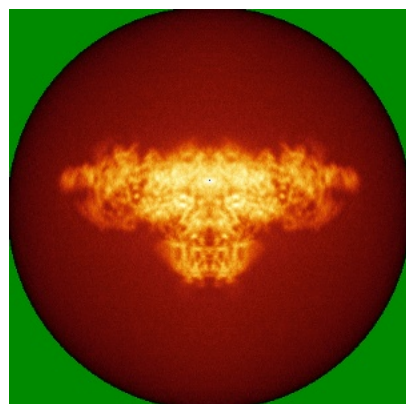


Y

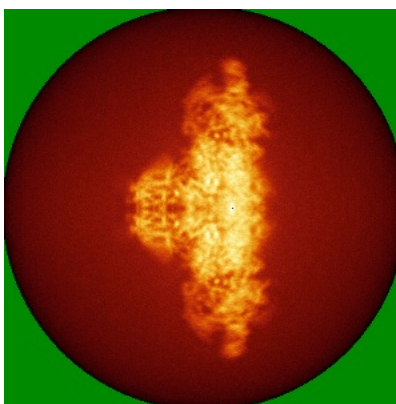


Z

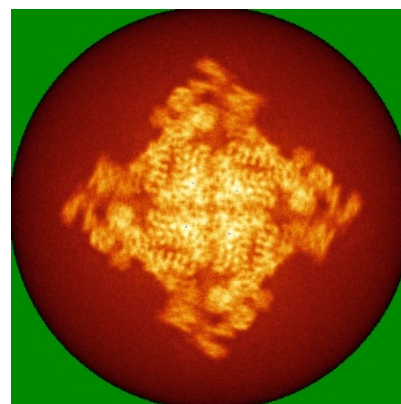
### 6.4.2 Raw map



X



Y

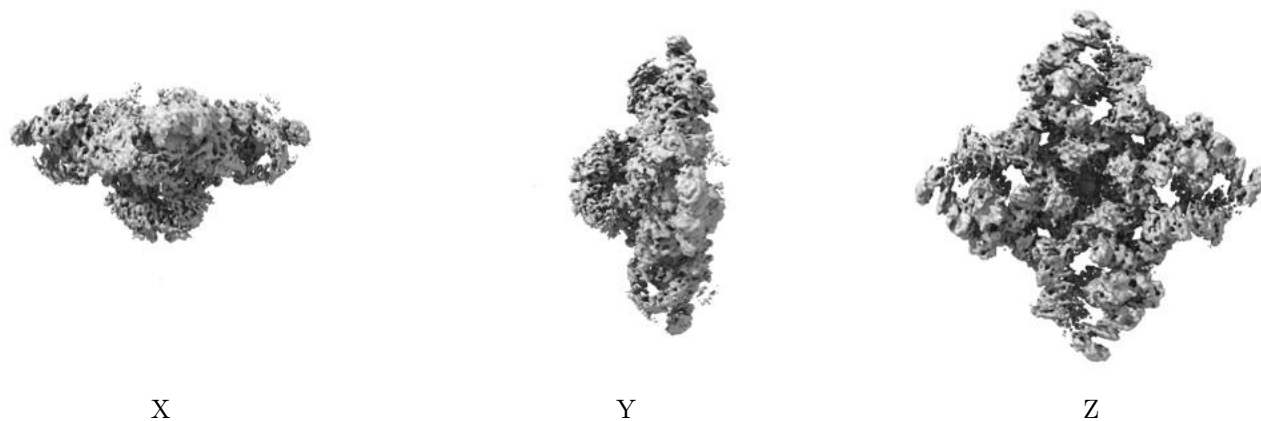


Z

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.

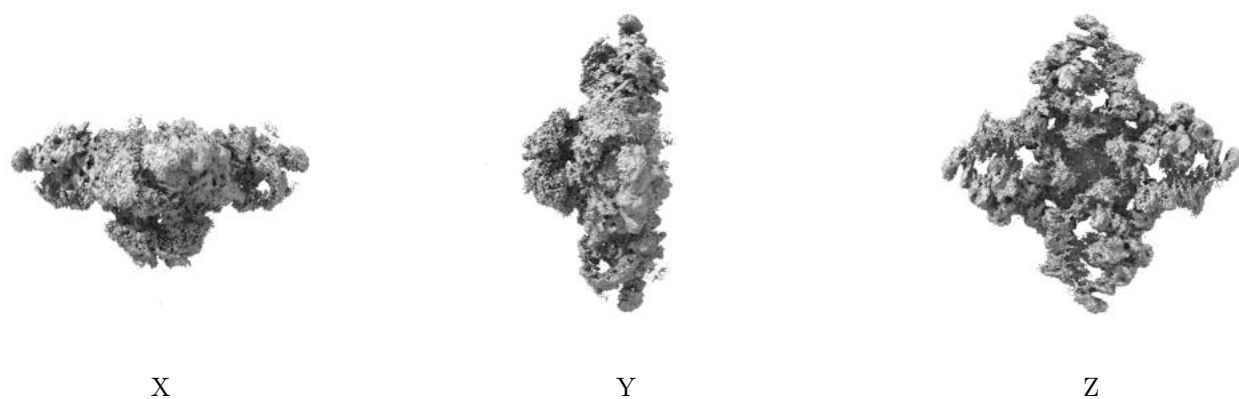
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

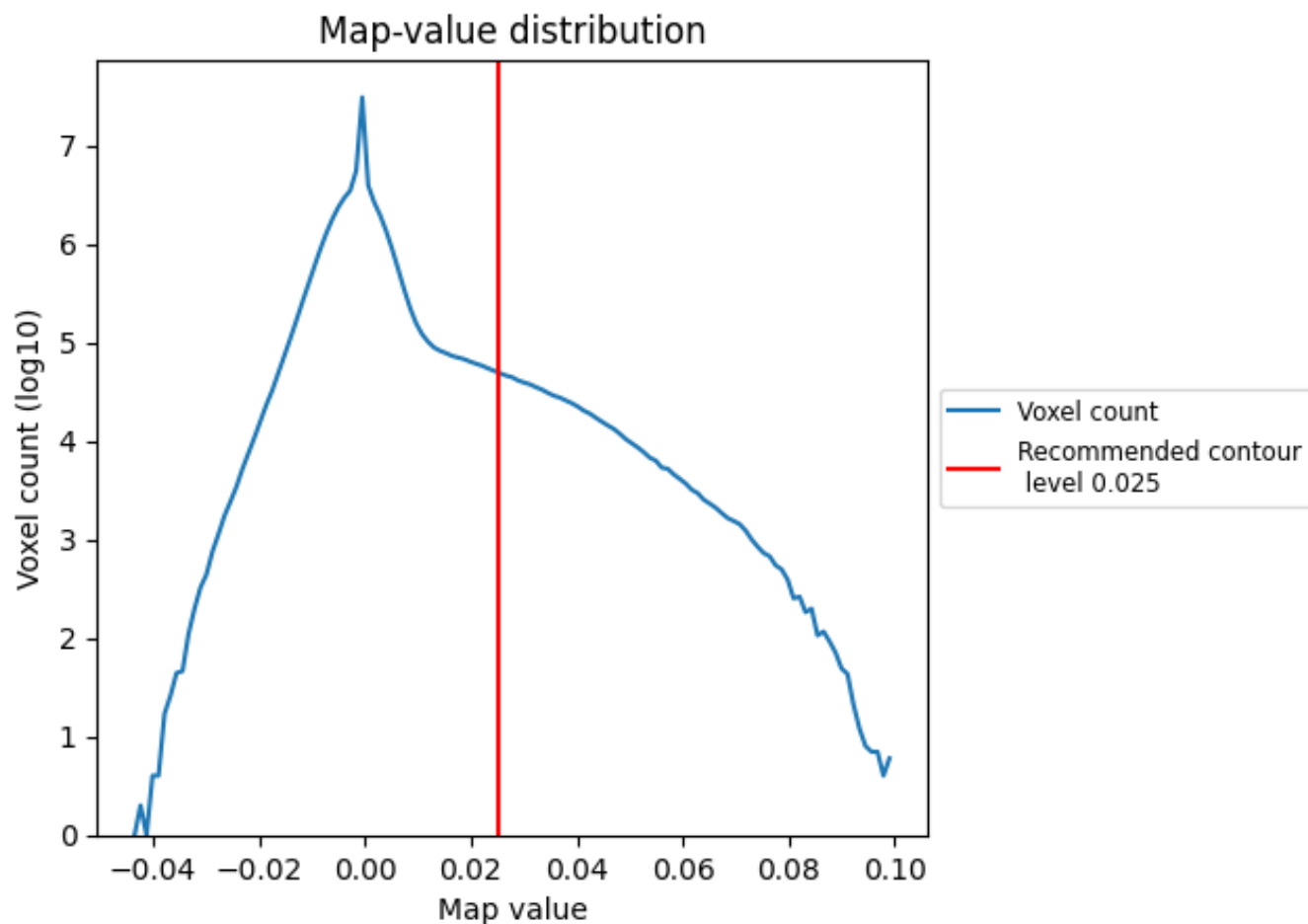
## 6.6 Mask visualisation [i](#)

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.

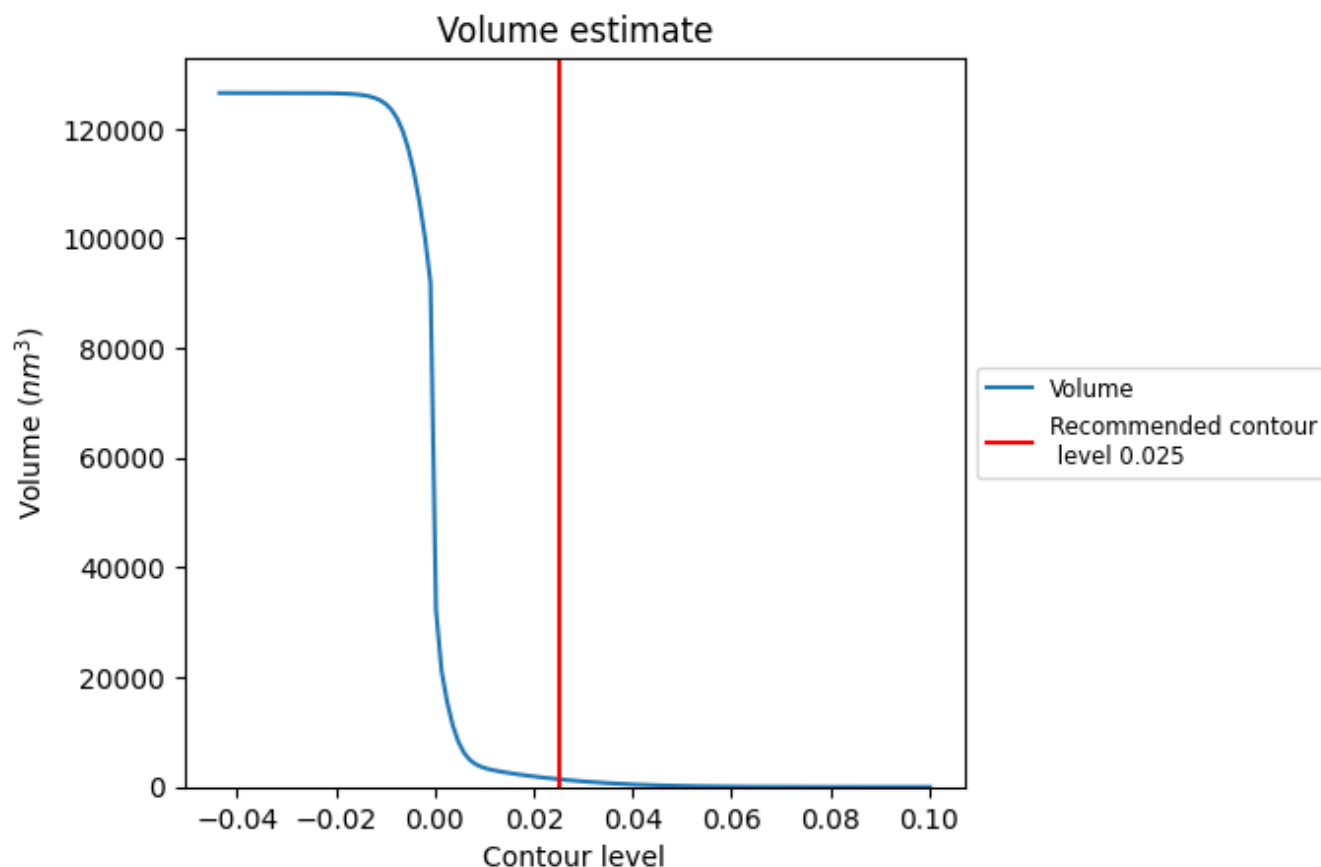
### 7.1 Map-value distribution [i](#)



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.



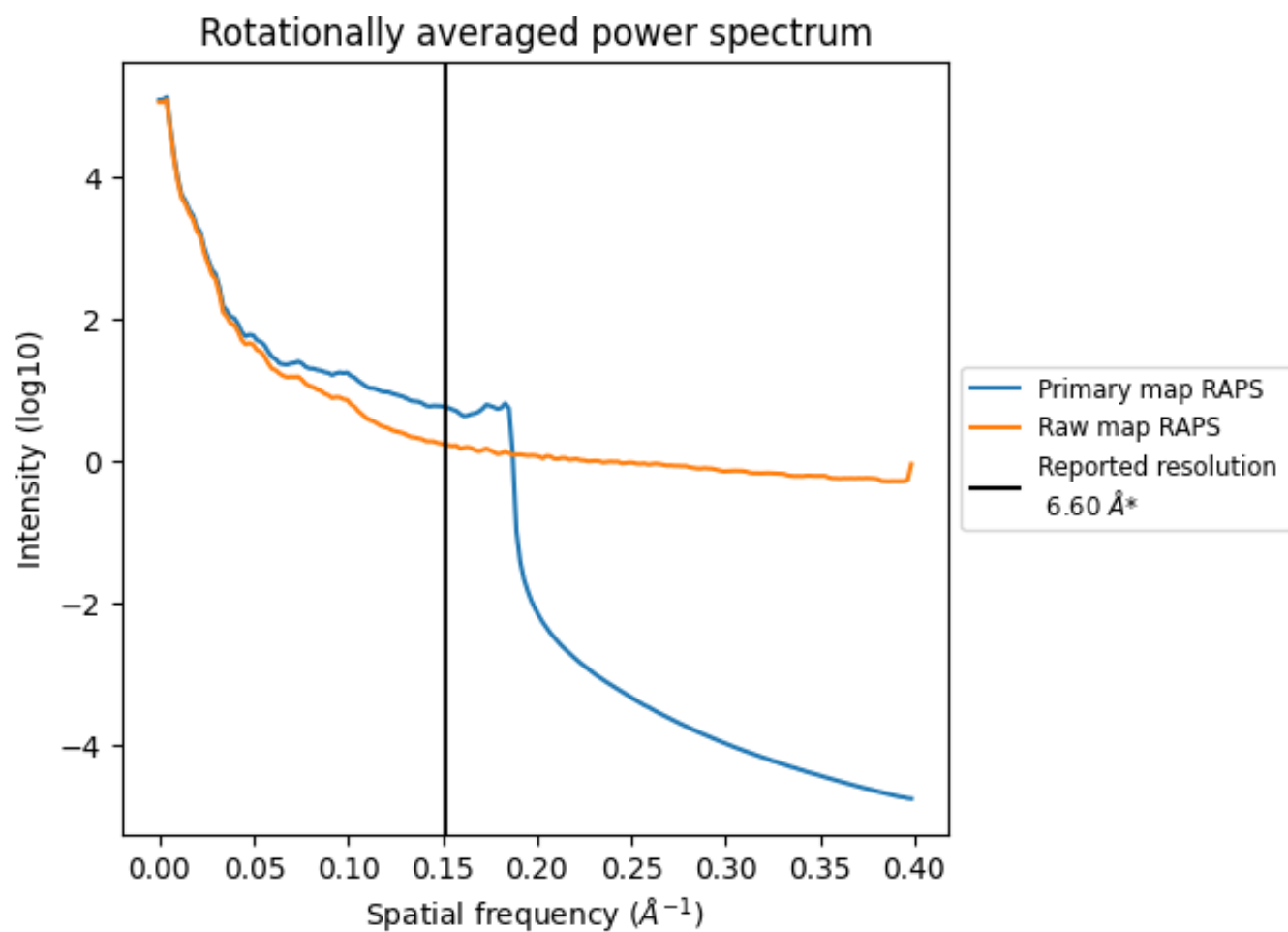
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1411 nm<sup>3</sup>; this corresponds to an approximate mass of 1274 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 ⓘ

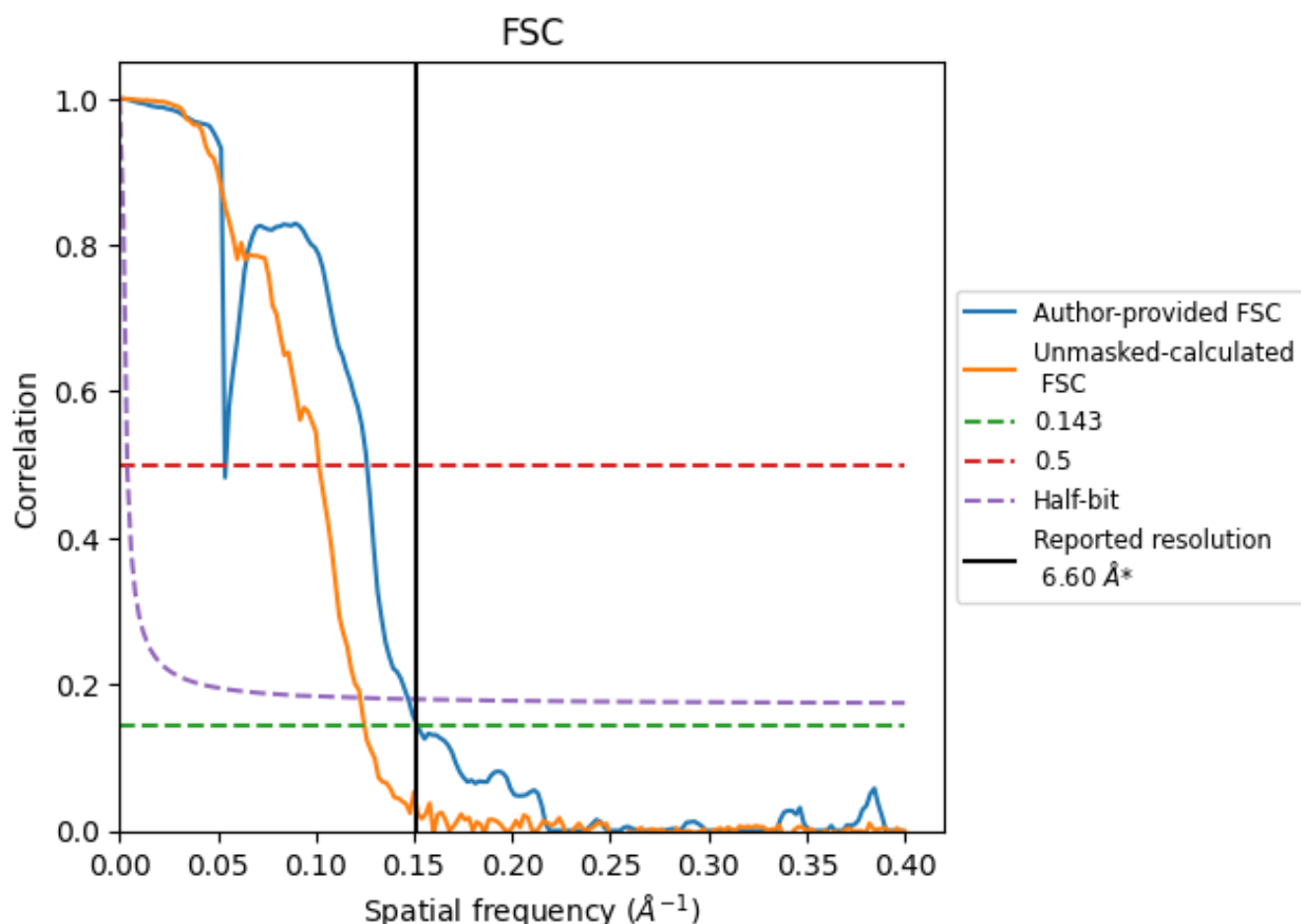


\*Reported resolution corresponds to spatial frequency of 0.152  $\text{\AA}^{-1}$

## 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  $0.152 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

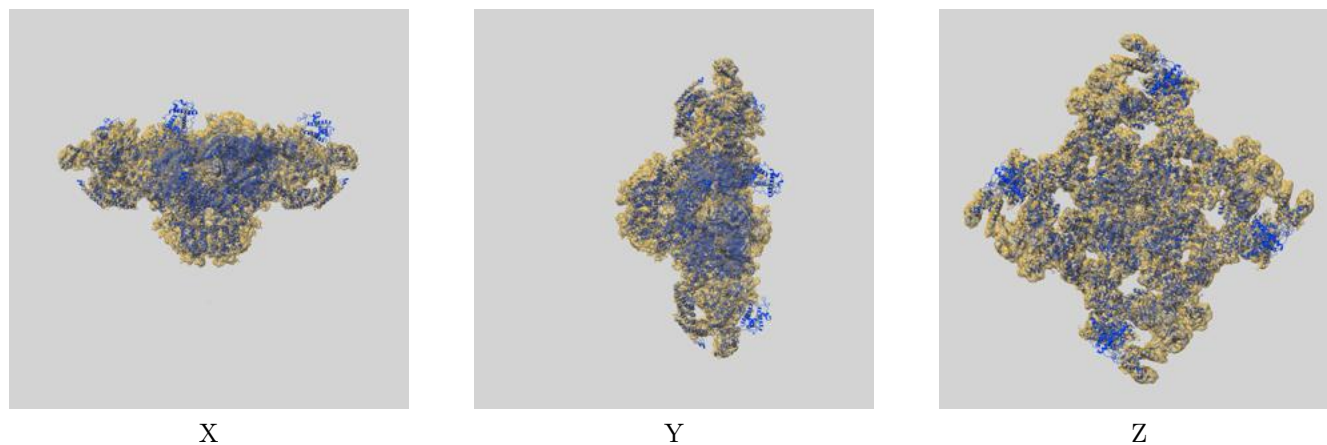
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.58	18.62	6.80
Unmasked-calculated*	8.01	9.83	8.16

\*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 8.01 differs from the reported value 6.6 by more than 10 %

## 9 Map-model fit [i](#)

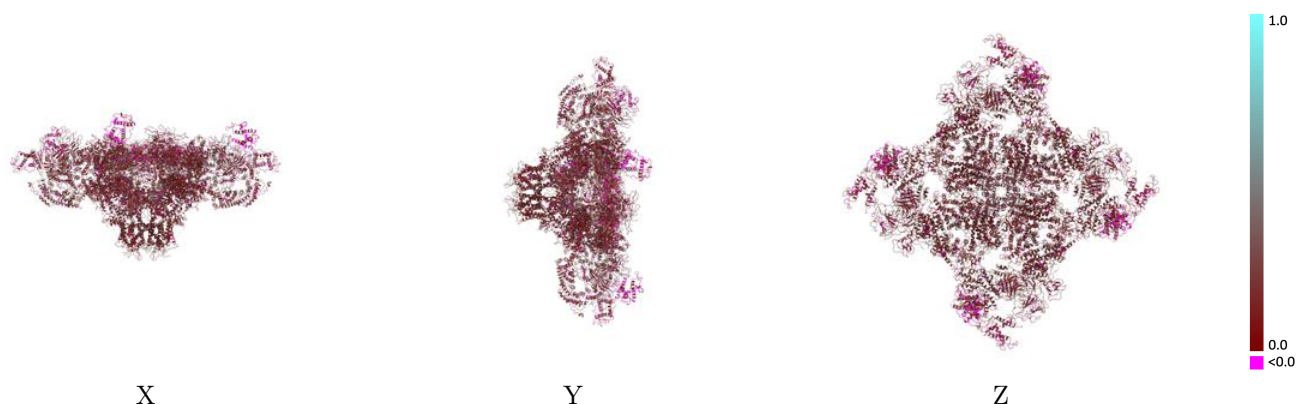
This section contains information regarding the fit between EMDB map EMD-8388 and PDB model 5TAX. Per-residue inclusion information can be found in section 3 on page 5.

### 9.1 Map-model overlay [i](#)



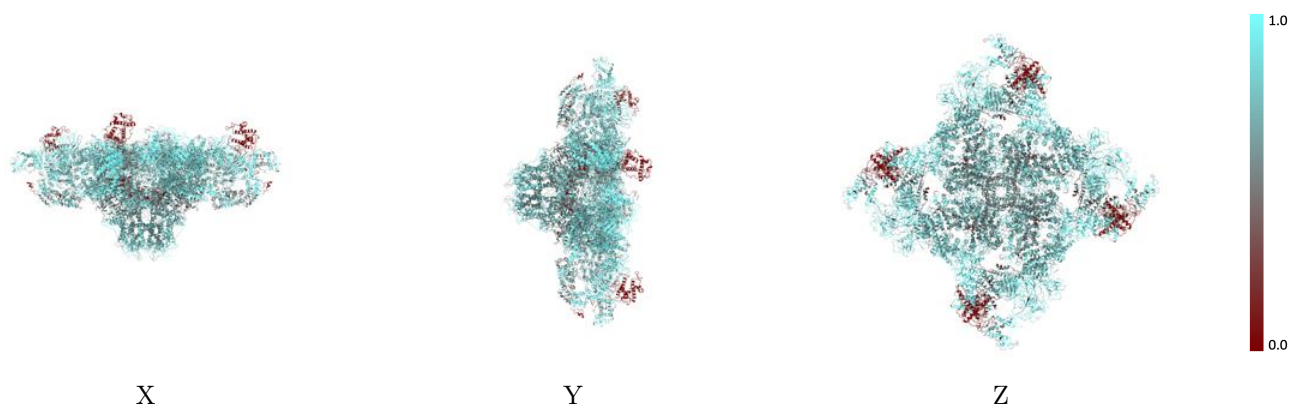
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



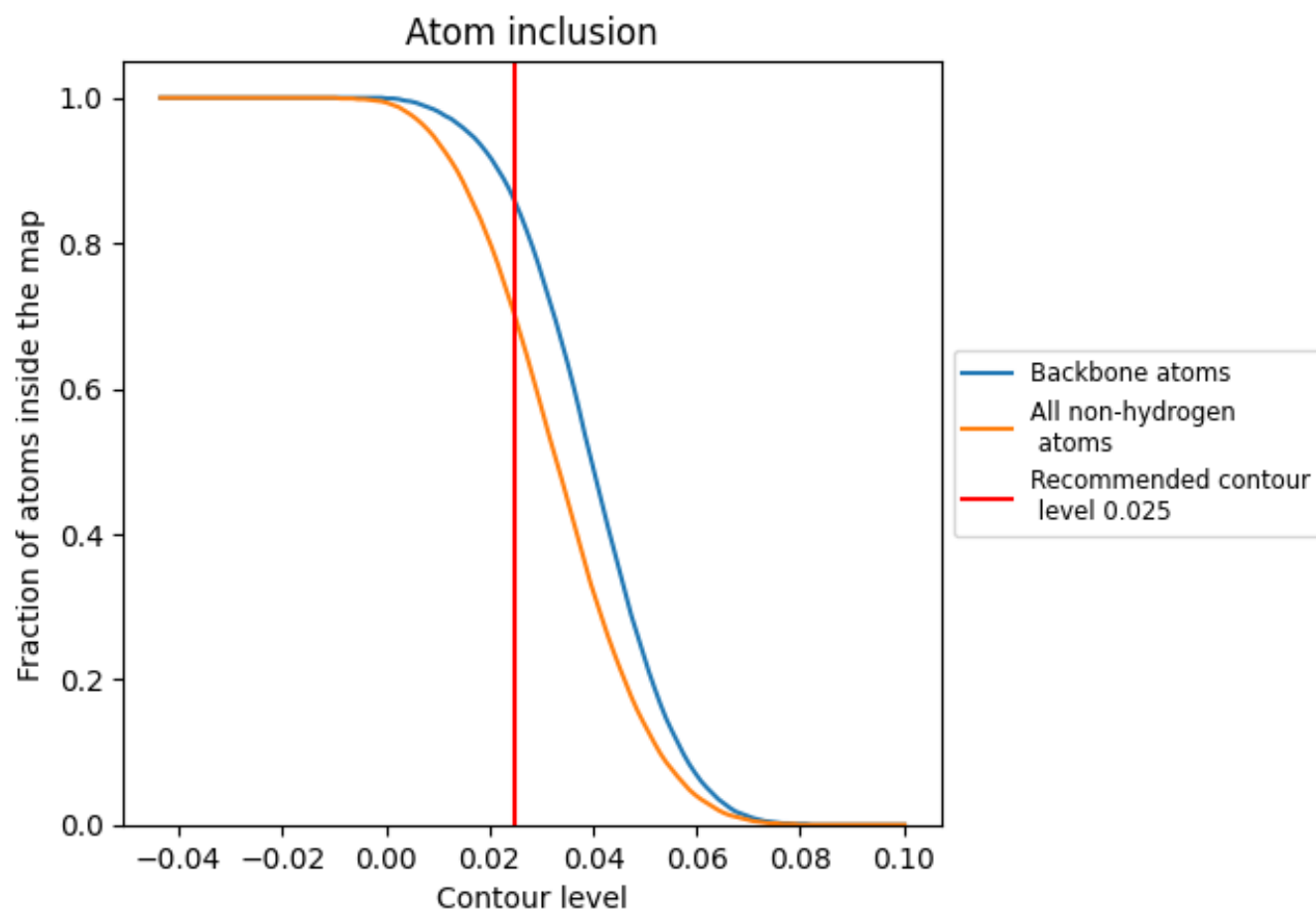
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6980	<div></div> 0.1910
A	<div></div> 0.8060	<div></div> 0.1870
B	<div></div> 0.6950	<div></div> 0.1910
E	<div></div> 0.6960	<div></div> 0.1910
F	<div></div> 0.8060	<div></div> 0.1910
G	<div></div> 0.6930	<div></div> 0.1910
H	<div></div> 0.8080	<div></div> 0.1900
I	<div></div> 0.6960	<div></div> 0.1910
J	<div></div> 0.8080	<div></div> 0.1870

1.0

0.0

<0.0