



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:38 PM UTC

PDB ID : 7JMH / pdb_00007jmh
EMDB ID : EMD-22394
Title : Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots
- Frame 35 - State 4 (S4)
Authors : Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on : 2020-07-31
Resolution : 4.50 Å(reported)
Based on initial model : 5TB4

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:

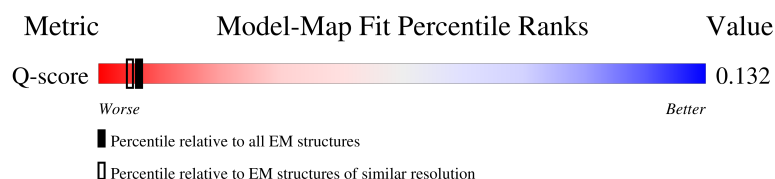
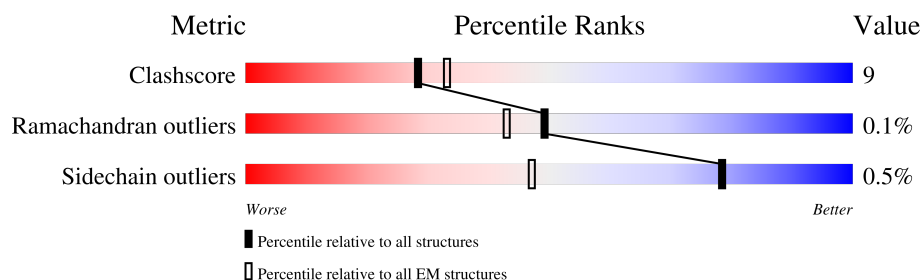
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.50 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.



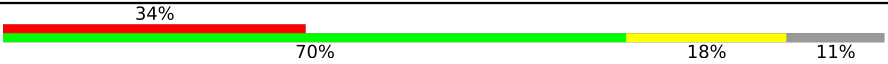
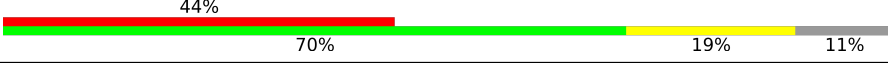
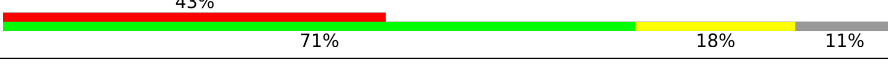
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	30% 68% 31% .
1	F	107	44% 67% 33%
1	H	107	46% 69% 31%
1	J	107	43% 66% 34%

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Mol	Chain	Length	Quality of chain
2	B	4687	
2	E	4687	
2	G	4687	
2	I	4687	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	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 type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest")

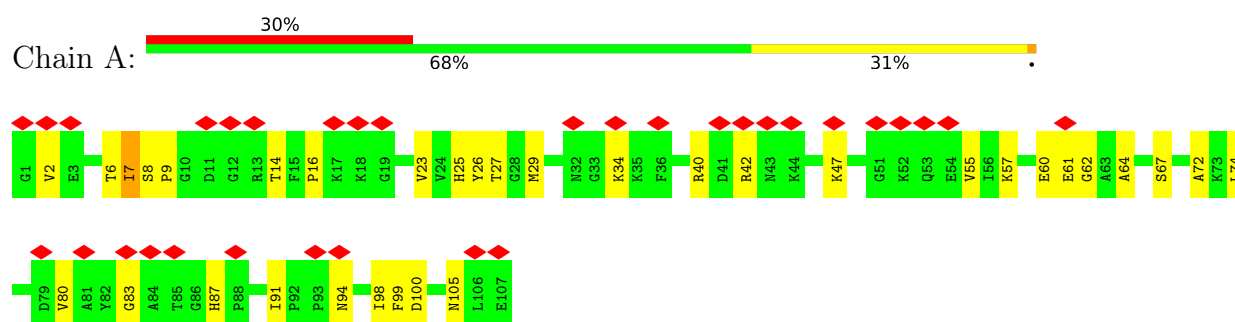
by depositor).

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

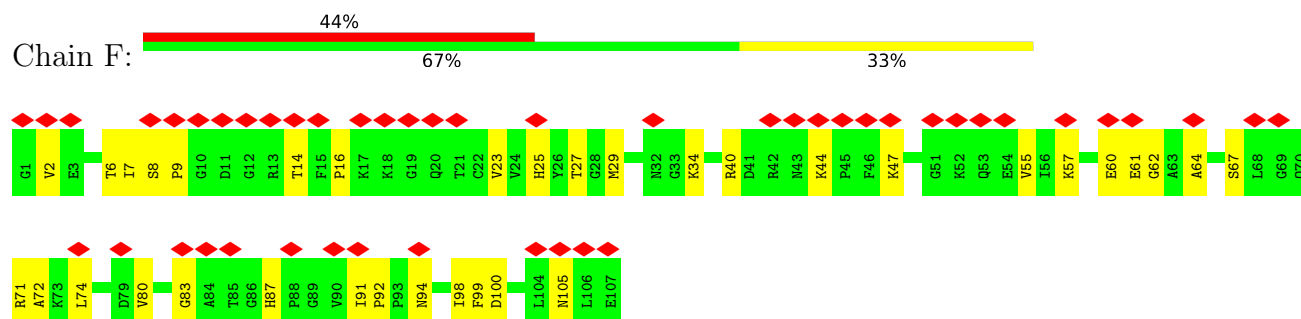
3 Residue-property plots [i](#)

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

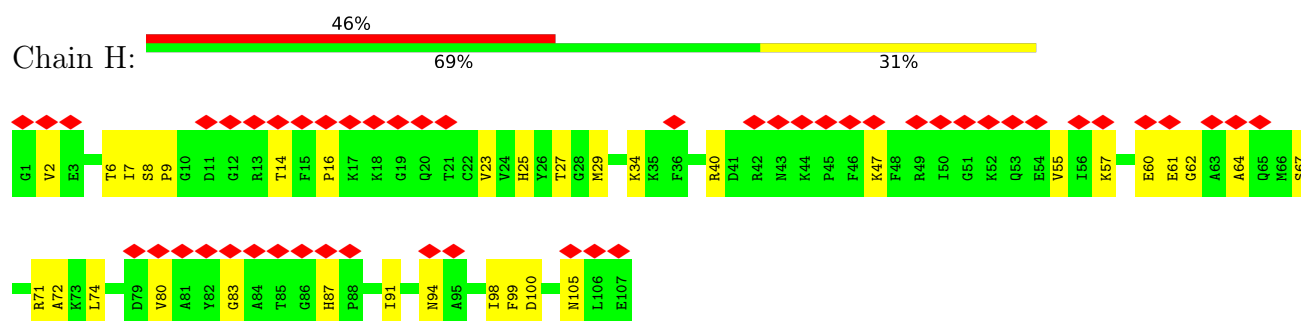
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



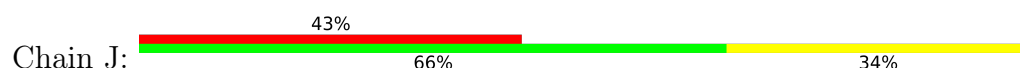
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

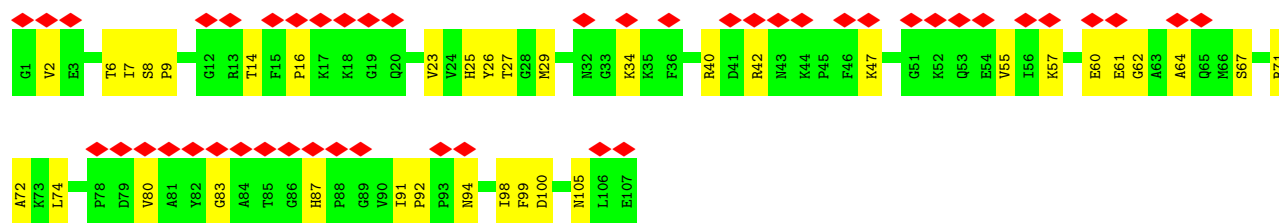


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

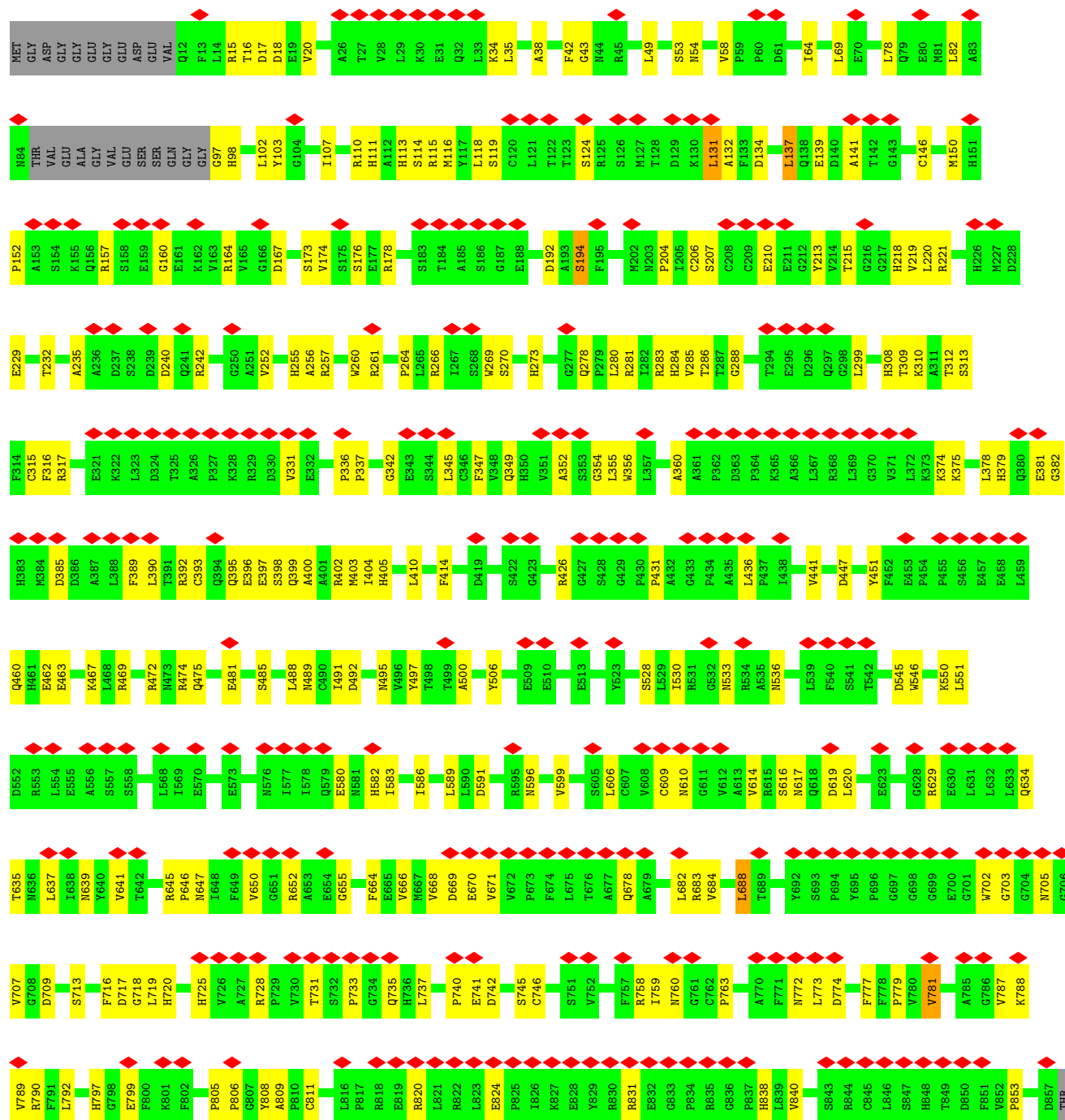


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

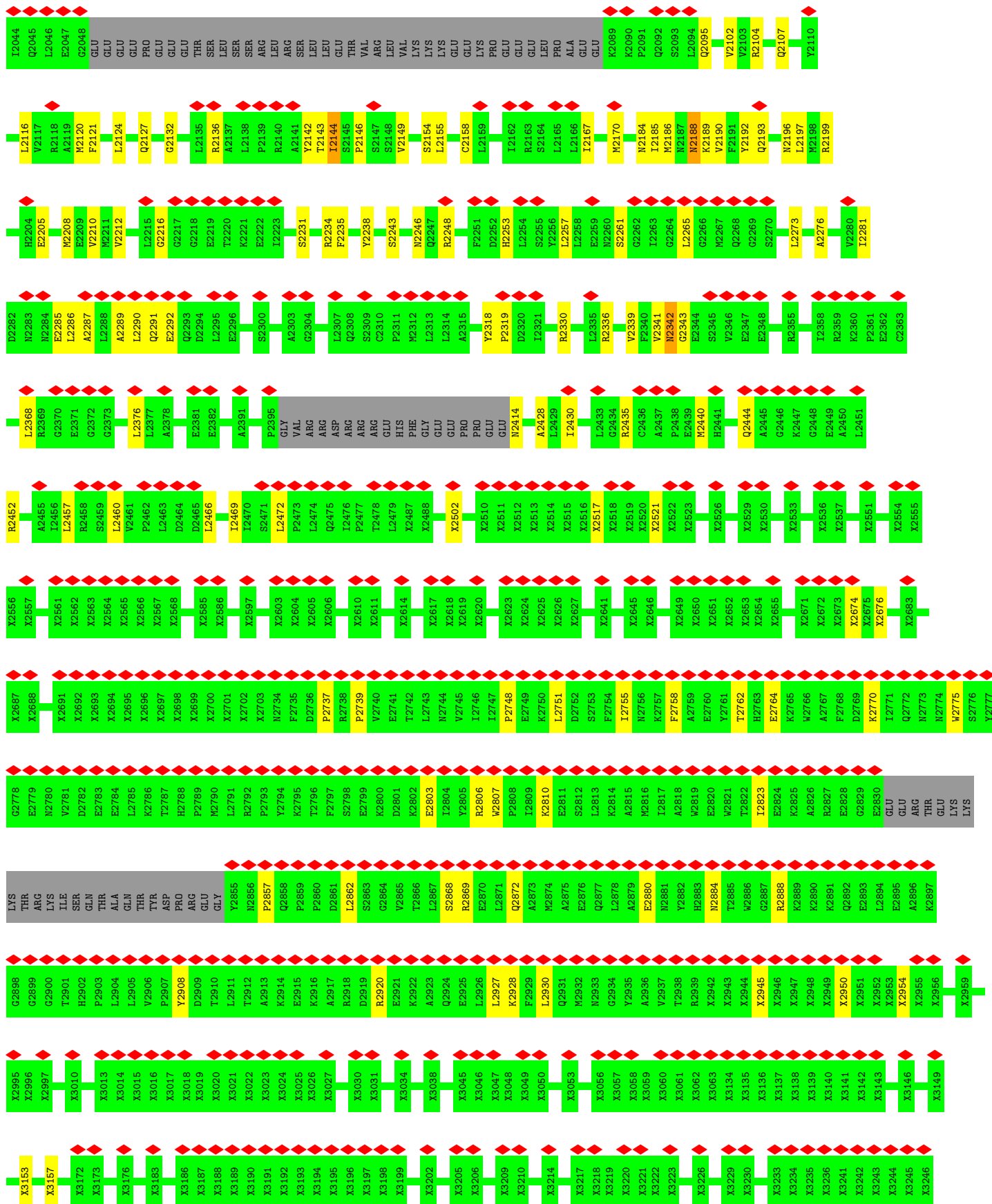




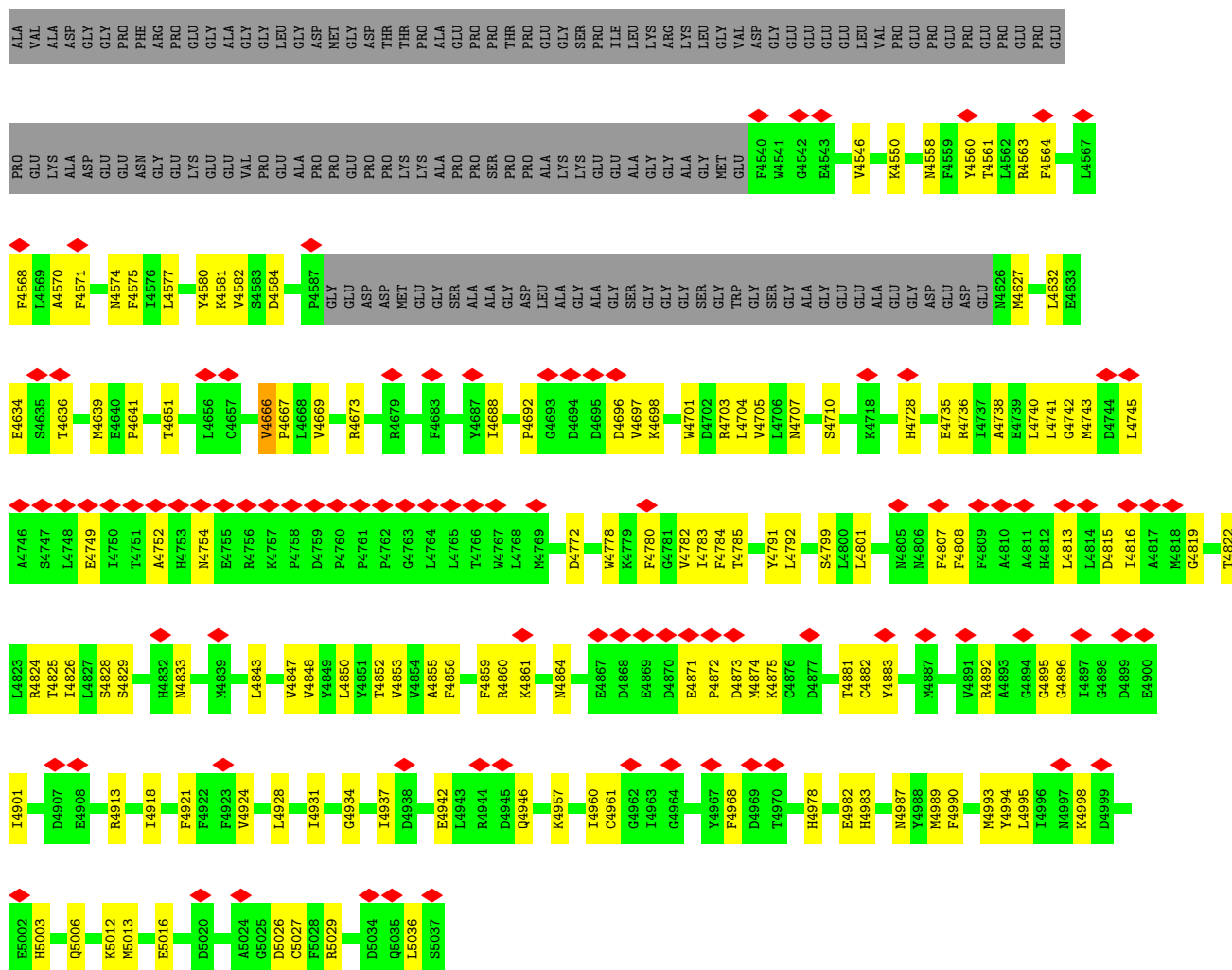
• Molecule 2: ryanodine receptor type 1



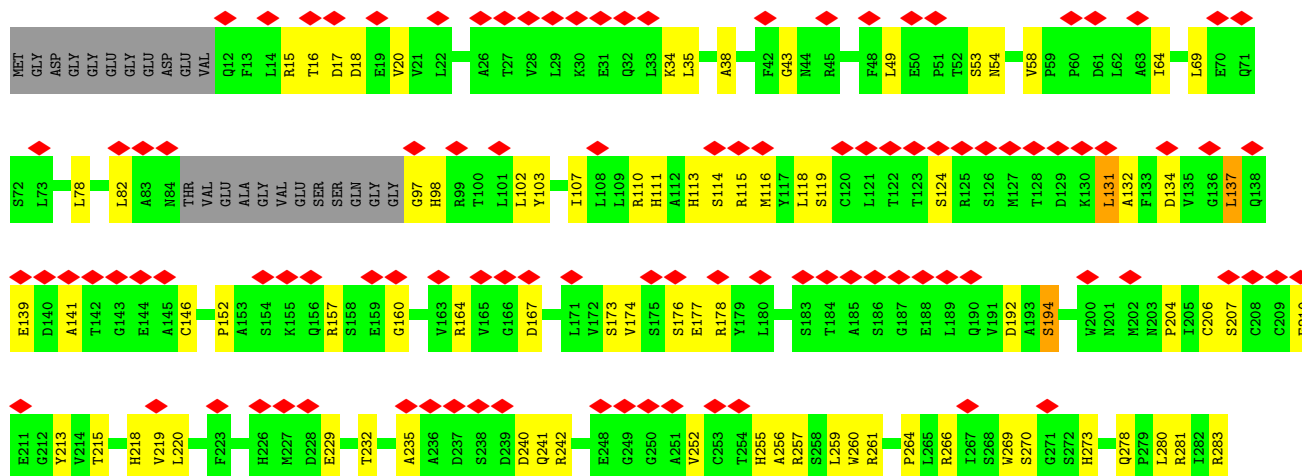
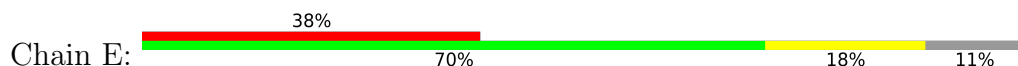


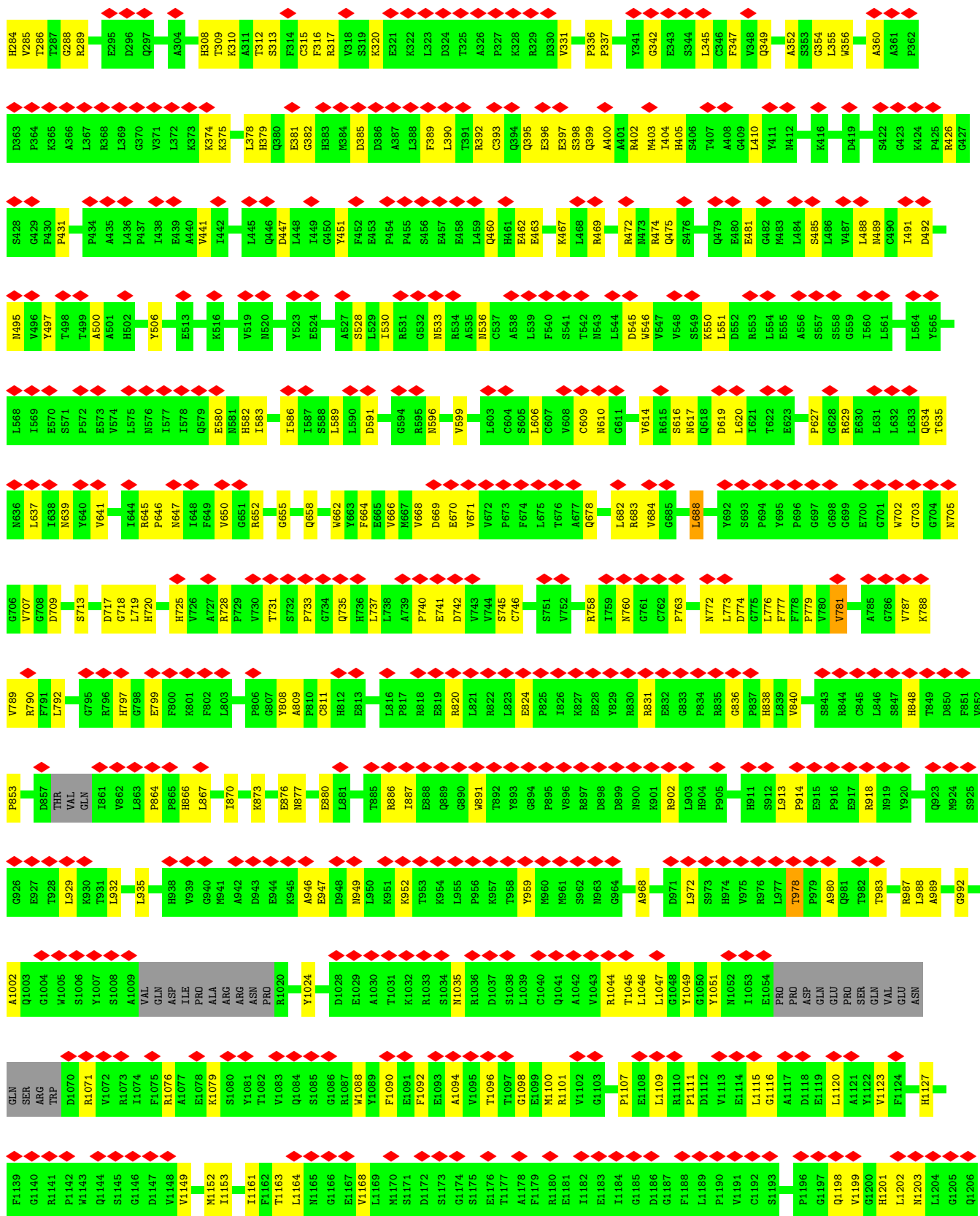


LEU	ARG	PRO	P4155	E4075	V3990	F3899	L3817	E3737	N3651	X3552	X3420	X3330	X3247
LEU	LEU	GLU	H4156	Q4076	G3991	L3903	K3821	G3738	M3652	X3557	X3421	X3337	X3248
ALA	ARG	ALA	F3992	D4078	F3992	L3904	E3826	G3739	F3653	X3556	X3422	X3338	X3249
GLY	ARG	ASP	L4160	D4079	H3994	T3905	F3829	E3740	L3654	X3558	X3423	X3341	X3250
THR	THR	ASP	L4161	T4082	V3996	Q3906	Q3830	N3741	E3655	X3559	X3424	X3342	X3251
ALA	ALA	GLY	F3997	D4083	M4000	T3907	Q3831	GLU	A3659	X3560	X3425	X3343	X3252
GLY	GLY	MET	A4167	P4084	M4001	T3910	Q3832	ALA	I3662	X3561	X3426	X3344	X3253
THR	GLU	GLY	E4168	P4085	M4002	T3911	I3832	GLU	L3663	X3562	X3427	X3345	X3254
ALA	ALA	GLU	L4169	R4086	K4002	T3912	Q3833	GLU	T3664	X3563	X3428	X3346	X3255
VAL	ALA	ALA	L4170	L4088	L4003	T3915	S3840		D3665	X3564	X3429	X3347	X3256
HIS	LEU	ALA	L4171	L4089	A4004				H3667	X3565	X3430	X3348	X3263
GLY	ALA	GLY	E4172	K4091	L4012	D3921	D3843	E3747	S3668	X3566	X3431	X3349	X3264
GLY	ALA	GLY	L4175	Q4094	L4013	L3924	N3844	E3748	M3673	X3567	X3432	X3350	X3265
GLN	LEU	ALA	P4176	K4095	L4016	Q3927	L3845	V3749	I3674	X3568	X3433	X3351	X3266
PRO	LEU	GLY	L4177	A4096	L4019	S3931	N3846	V3750	D3675	X3569	X3434	X3352	
ALA	TRP	GLY	L4178	M4097	Q4020	D3932	F3847	F3752	D3676	X3570	X3435	X3353	X3269
ALA	ALA	ALA	M4184	D4098	K4021	F3933	E3848	E3753	X3679	X3571	X3436	X3354	X3270
ASP	ARG	ALA	R4188	S4099	V4024	F3934	N3851	E3754	K3679	X3572	X3437	X3355	X3271
ALA	ALA	GLY	E4189	Q4100	V4027	Y3934	K3852	E3755	A3680	X3573	X3444	X3356	X3272
GLY	GLY	GLY	I4190	K4101	L4027	W3936	A3853	E3756	G3681	X3574	X3452	X3357	X3273
ALA	ALA	ALA	E4191	Q4102	L4028	Y3937	E3854	Q3760	E3682	X3575	X3462	X3358	X3274
GLY	GLY	GLY	L4178	F4103	L4031	S3938	L3856	Q3761	Q3683	X3576	X3465	X3359	X3275
GLY	GLY	THR	F4195	F4104	E4032	Q3939	G3857	Q3766	E3684	X3577	X3466	X3360	X3276
VAL	GLY	VAL	E4199	Q4105	M4034	K3940	M3858	Q3767	E3685	X3578	X3467	X3361	X3277
ALA	ALA	ALA	T4200	P4106	N4037	D3941	V3859	Q3768	E3686	X3579	X3468	X3362	X3278
ALA	ALA	GLY	R4202	E4107	M4037	N3950	N3860	L3770	E3687	X3580	X3469	X3363	X3279
ASP	ALA	ALA	W4205	E4108	L4040	K3953	E3861	H3771	E3688	X3581	X3470	X3364	X3280
ALA	LEU	ALA	E4206	Q4109	A4041	A3954	D3862	T3772	E3689	X3582	X3471	X3365	X3281
ALA	ARG	LEU	M4207	S4113	A4044	M3955	G3863	T3773	V3690	X3583	X3472	X3366	X3282
GLY	LEU	ALA	P4208	C4114	M4044	S3956	T3864	G3774	E3691	X3584	X3473	X3367	X3283
ASP	TRP	ALA	K4211	A4117	M4047	V3957	V3865	A3775	E3692	X3585	X3474	X3368	X3284
ASP	SER	ALA	R4215	D4118	M4047	Q3960	V3866	A3776	K3693	X3586	X3475	X3369	X3285
GLY	LEU	ALA	I4218	E4119	E4050	N3963	N3867	L3780	E3712	X3587	X3476	X3370	X3286
VAL	PHE	ARG	E4223	M4120	S4051	T3966	R3868	Q3781	K3713	X3588	X3477	X3371	X3287
ALA	GLY	ALA	E4224	E4121	E4056	G3971	Q3869	S3784	G3714	X3589	X3478	X3372	X3288
HIS	GLY	ARG	E4225	I4123	M4057	P3972	N3870	A3785	K3715	X3590	X3479	X3373	X3297
GLU	VAL	LEU	G4226	M4124	I4058	C3973	G3871	C3786	L3716	X3591	X3480	X3383	X3301
ALA	GLY	SER	E4227	F4125	L4059	C3974	E3872	K3787	D3717	X3602	X3481	X3384	X3304
PRO	ALA	ARG	A4228	E4126	F4062	T3974	K3873	Q3788	E3718	X3605	X3482	X3385	X3307
GLY	LYS	SER	T4241	M4130	D4063	Q3977	V3874	Q3789	D3719	X3606	X3483	X3386	X3308
GLY	LYS	LEU	M4245	M4131	M4064	H3982	M3875	T3790	Y3720	X3607	X3484	X3387	X3309
ALA	THR	ARG	E4253	R4137	M4067	R3984	D3878	L3798	M3723	X3608	X3485	X3388	X3311
GLY	VAL	ARG	PRO	D4138	K4067	F3880	E3879	A3724	Y3725	X3609	X3486	X3389	X3312
GLY	THR	VAL	GLY	I4139	D4070	Q3881	T3880	L3804	A3726	X3610	X3487	X3390	X3313
VAL	GLU	VAL	E4253	E4142	D4074	Q3882	Q3883	N3806	D3727	X3611	X3488	X3391	X3314
			GLY	M4142	G4073	L3884	L3885	G3807	I3728	X3612	X3489	X3392	X3315
			GLY	L4147	S4074	F3886	F3887	G3808	K3731	X3613	X3490	X3393	X3316
				S4151		Q3889	Q3890	N3809	S3732	Y3642	X3491	X3394	X3317
				E4152				N3809	H3734	N3643	X3492	X3395	X3318
				V4154		N3897	D3898	K3815	L3735	L3644	X3493	X3396	X3319
								K3816	E3736	P3645	X3494	X3397	X3320
										R3648	X3495	X3398	X3321
										C3650	X3496	X3399	X3322
											X3415	X3400	X3323
											X3419	X3401	X3324

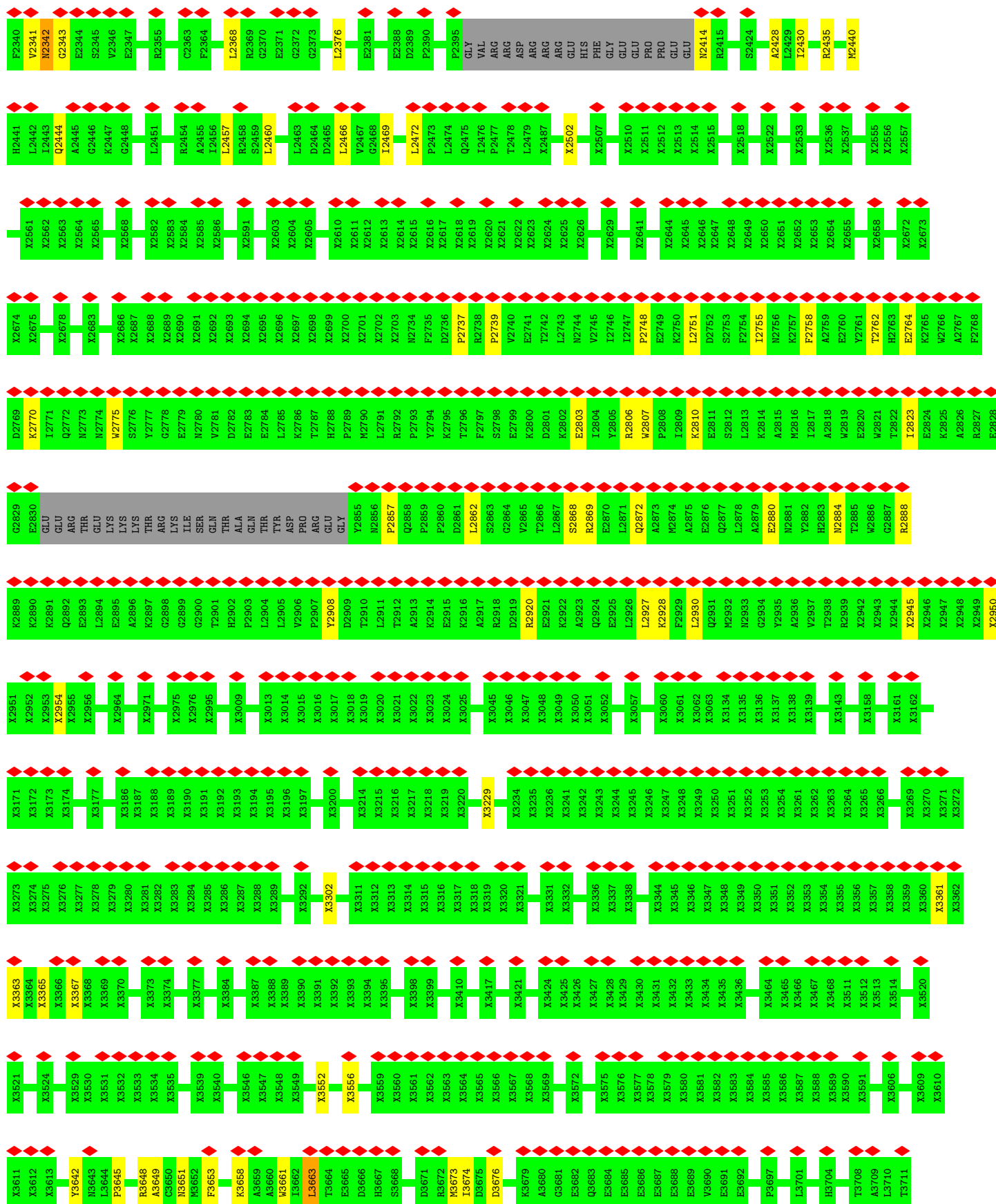


• Molecule 2: ryanodine receptor type 1

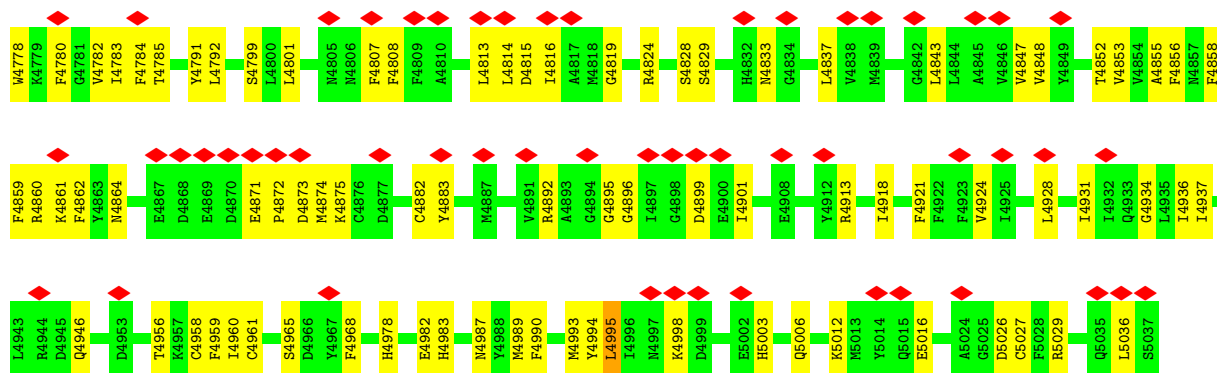




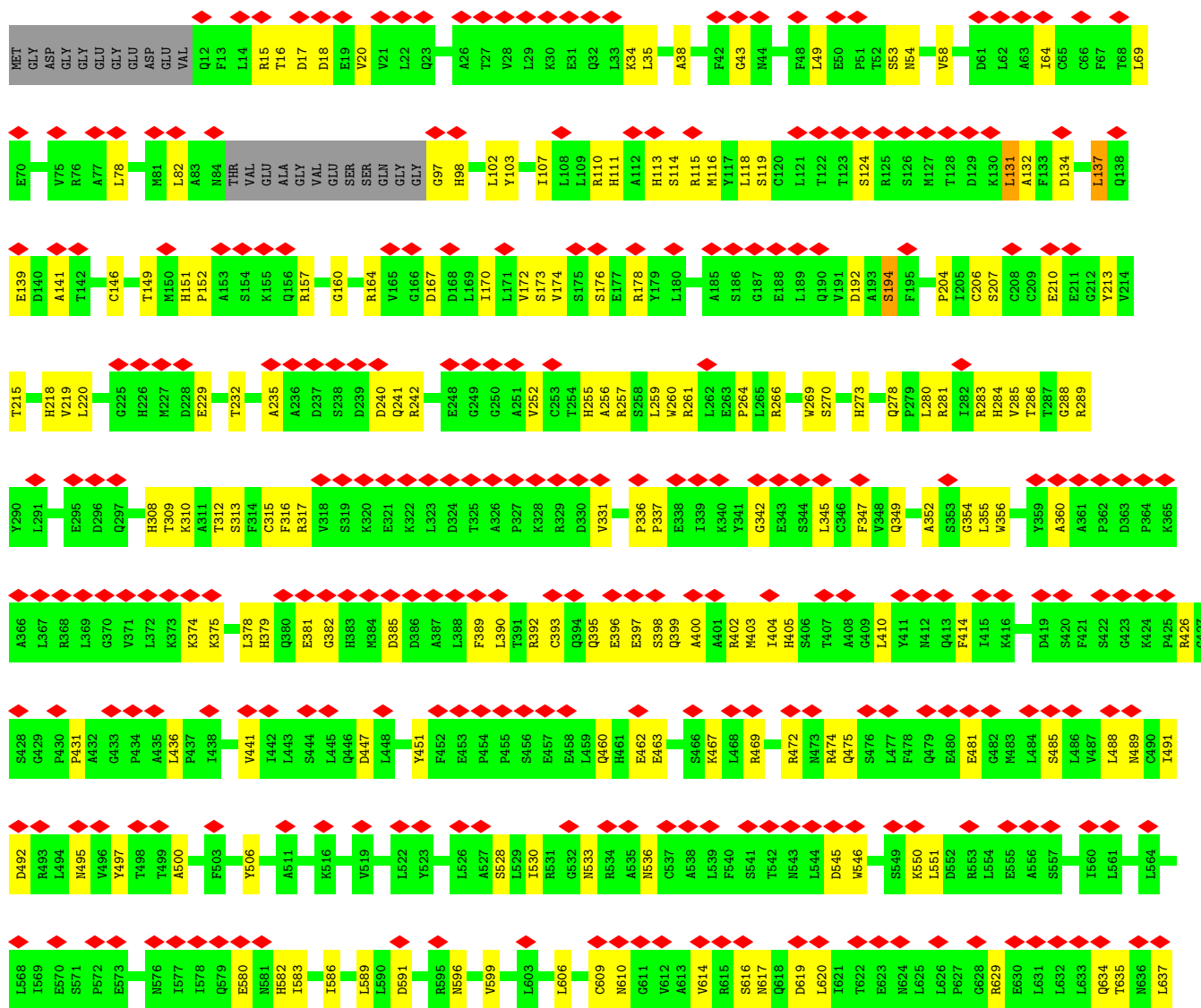
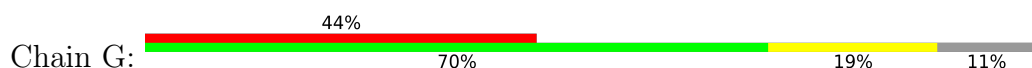


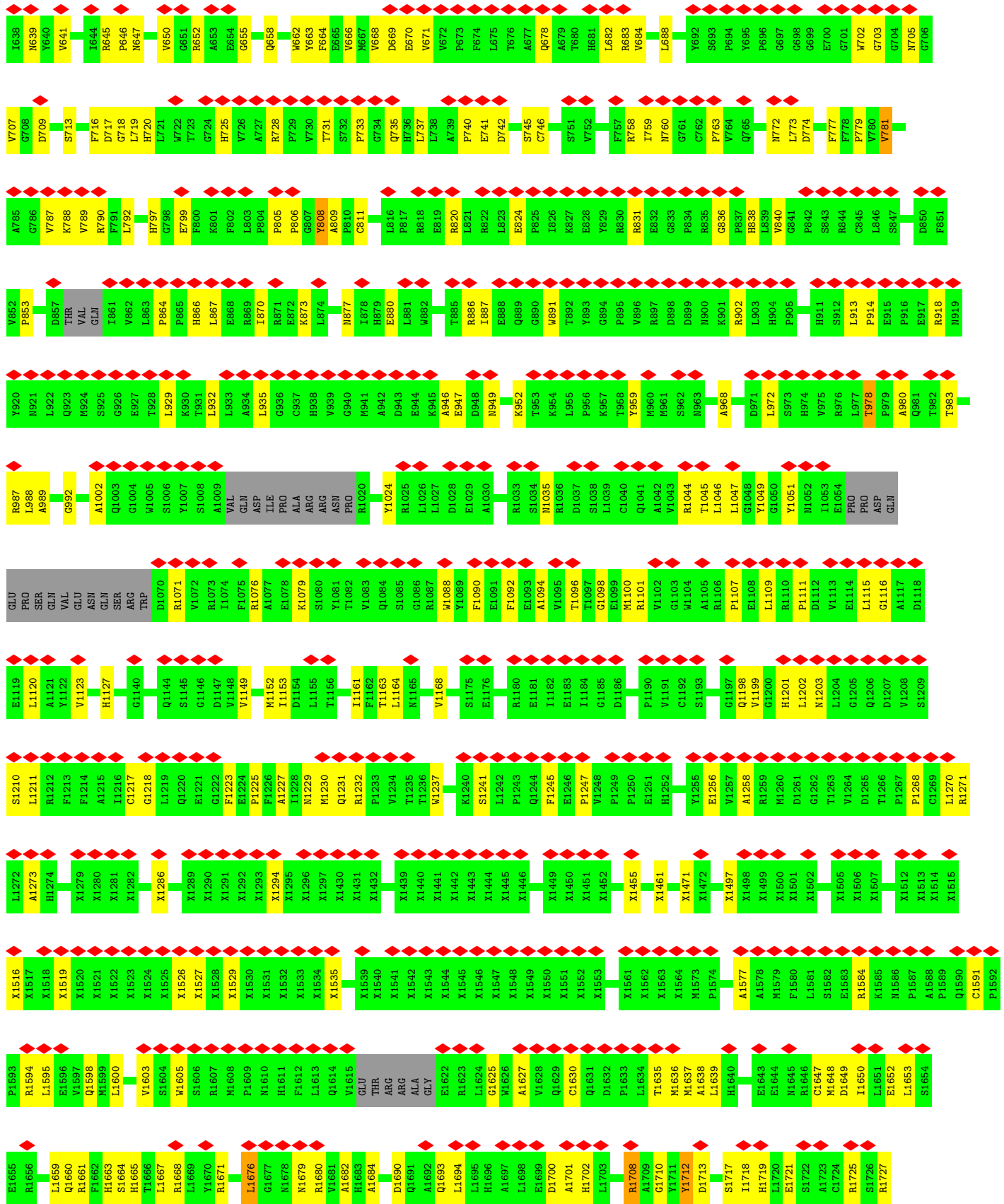






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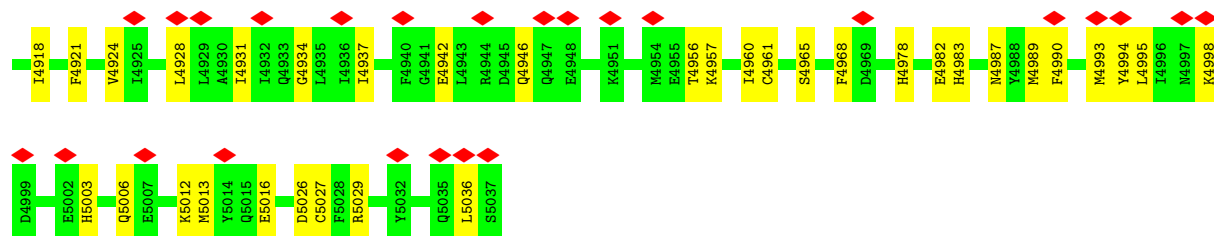




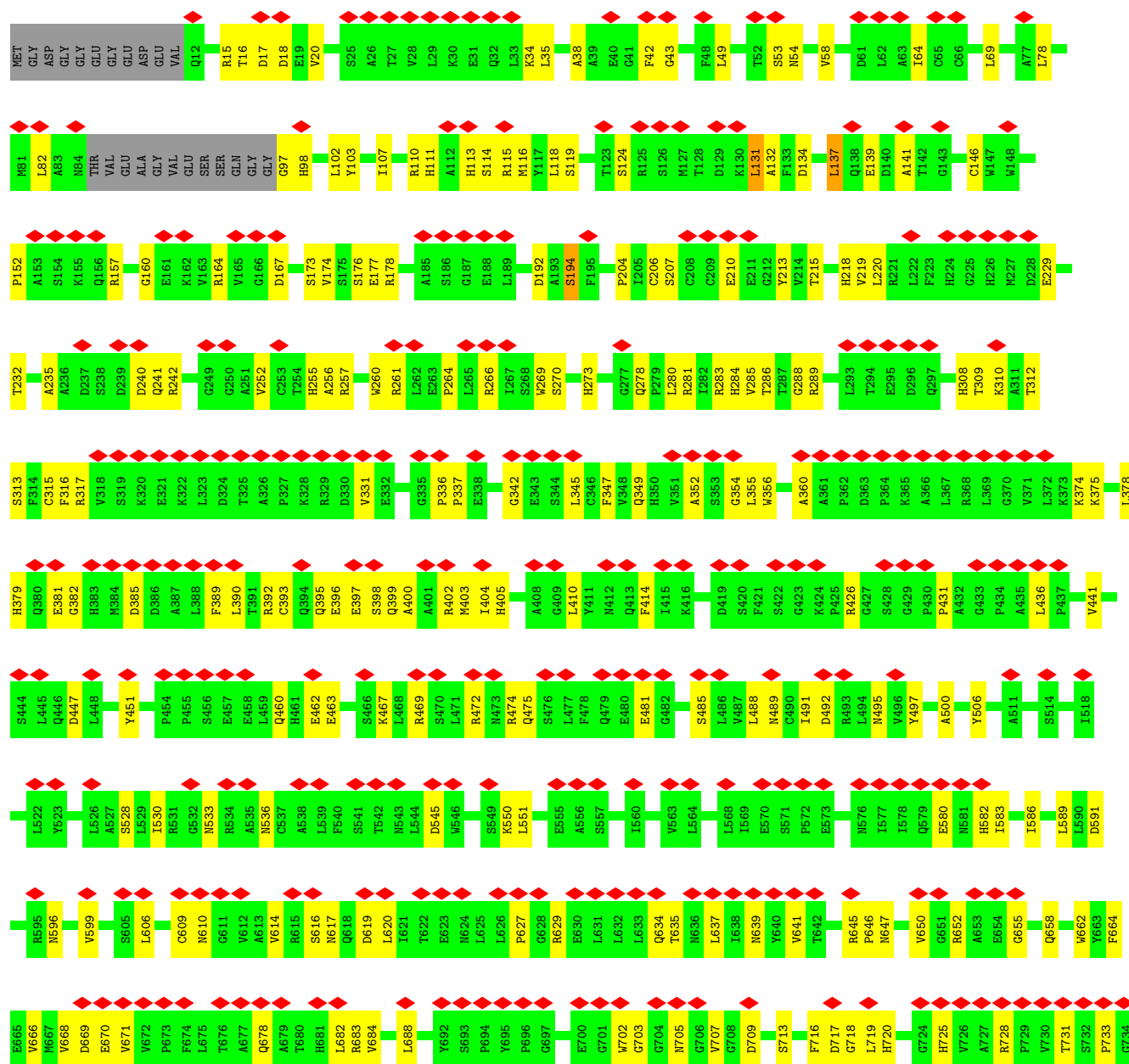
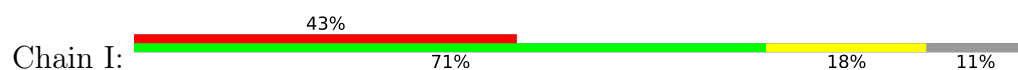


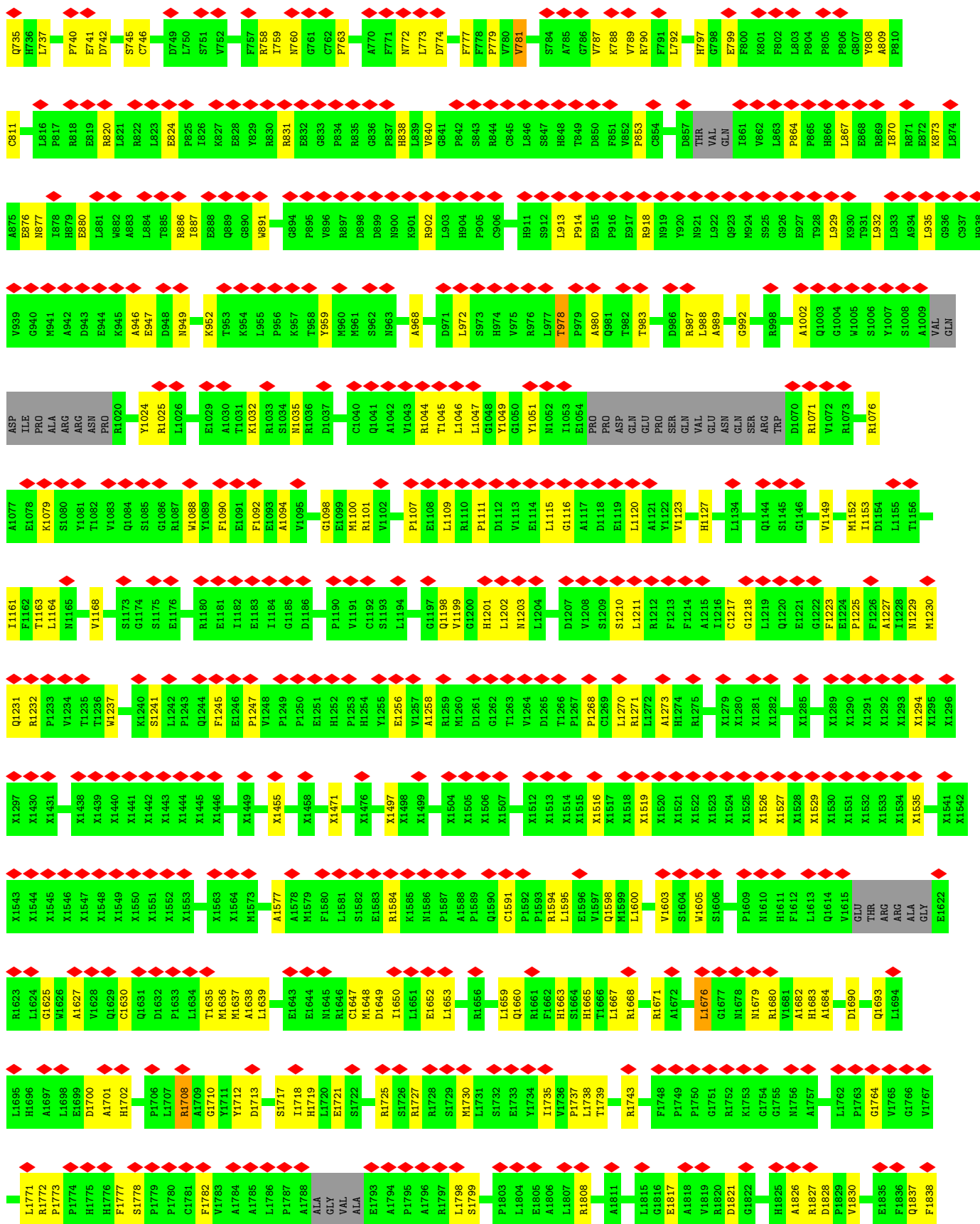
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• Molecule 2: ryanodine receptor type 1







K3948	F3951	A3954	M3955	S3956	V3957	A3958	K3959	F3960	V3961	F3962	S3963	S3964	L3965	T3966	I3969	D3970	C3971	F3972	C3973	T3974	Q3977	Q3978	A3981	H3982	S3983	R3984	D3987	V3990	G3991	F3992	L3993	H3994	V3995	F3996	A3997	H3998	K3999	M4000	M4001	K4002	L4003	A4004	Q4005	L4010	E4011	L4012	L4013	S3998	G3999	E4015	L4016	L4017							
N3870	G3871	E3872	K3873	V3874	N3875	D3878	G3807	F3880	T3881	Q3882	L3883	L3884	F3885	L3888	Q3889	E3893	N3897	D3898	F3899	L3903	R3904	T3905	Q3906	T3907	T3910	T3911	T3912	I3913	N3914	I3915	I3916	I3917	V3920	D3921	L3924	R3925	L3926	Q3927	E3928	S3931	D3932	M4000	V3936	V3937	S3938	G3939	K3940	D3941											
K3799	L3802	S3803	L3804	L3805	N3806	K3807	G3808	N3809	K3815	M3816	L3817	L3820	K3821	K3824	E3825	F3829	Q3830	S3831	L3832	Q3833	M3836	Q3837	S3840	L3841	L3842	D3843	L3844	N3845	A3846	F3847	E3848	R3849	Q3850	N3851	K3852	A3853	E3854	G3855	L3856	G3857	M3858	V3859	K3860	E3861	D3862	L3863	T3864	V3865	L3866	R3867	Q3869								
L3735	E3736	E3737	G3738	G3739	E3740	M3741	GLY	GLU	ALA	GLU	E3747	E3748	V3749	E3750	V3751	S3752	F3753	E3754	E3755	K3756	E3759	K3760	Q3761	R3762	L3763	L3764	V3765	Q3766	Q3767	S3768	R3769	L3770	H3771	G3772	R3773	G3774	A3775	A3776	L3780	Q3781	K3782	S3784	A3785	C3786	K3787	G3788	E3789	T3790	G3791	A3792	K3793	V3794	S3795	L3798					
T3664	E3665	D3666	H3667	S3668	F3669	E3670	M3673	GLU	L3674	D3675	D3676	A3680	G3681	E3682	Q3683	E3684	E3685	E3686	E3687	E3688	E3689	V3690	E3691	E3692	K3693	L3698	V3702	S3706	R3707	T3708	A3709	L3710	L3711	E3712	K3713	S3714	K3715	L3716	D3717	E3718	D3719	V3720	M3723	A3724	V3725	A3726	D3727	I3728	M3729	A3730	K3731	S3732	C3733	H3734					
X3559	X3560	X3561	X3562	X3563	X3564	X3565	X3566	X3567	X3568	X3569	X3570	X3571	X3572	X3573	X3574	X3575	X3576	X3577	X3578	X3579	X3580	X3581	X3582	X3583	X3584	X3585	X3586	X3587	X3588	X3589	X3590	X3591	X3602	X3605	X3606	X3607	X3608	X3609	X3610	X3611	X3612	X3613	N3643	R3648	A3649	C3650	N3651	M3652	E3655	K3658	A3659	L3663							
X3424	X3425	X3426	X3427	X3428	X3429	X3430	X3431	X3432	X3433	X3434	X3435	X3436	X3437	X3444	X3462	X3463	X3464	X3465	X3466	X3467	X3468	X3511	X3512	X3513	X3514	X3515	X3516	X3517	X3518	X3519	X3520	X3521	X3522	X3523	X3524	X3527	X3528	X3532	X3533	X3534	X3535	X3536	X3539	X3540	X3543	X3547	X3552	X3556	X3557	X3558									
X3342	X3343	X3344	X3345	X3346	X3347	X3348	X3349	X3350	X3351	X3352	X3353	X3354	X3355	X3356	X3357	X3358	X3359	X3360	X3361	X3362	X3363	X3364	X3365	X3366	X3369	X3370	X3371	X3372	X3373	X3377	X3380	X3383	X3384	X3385	X3386	X3387	X3388	X3389	X3390	X3391	X3392	X3393	X3394	X3411	X3415	X3416	X3417	X3418	X3419	X3420	X3421	X3422	X3423						
X3252	X3253	X3254	X3261	X3262	X3263	X3264	X3265	X3266	X3269	X3270	X3271	X3272	X3273	X3274	X3275	X3276	X3277	X3278	X3279	X3280	X3281	X3282	X3283	X3284	X3285	X3286	X3287	X3288	X3297	X3302	X3307	X3308	X3309	X3310	X3311	X3312	X3313	X3314	X3315	X3316	X3317	X3318	X3319	X3320	X3321	X3322	X3323	X3324	X3330	X3337	X3338	X3341							
X3143	X3146	X3172	X3173	X3183	X3186	X3187	X3188	X3189	X3190	X3191	X3193	X3194	X3195	X3196	X3197	X3198	X3199	X3200	X3201	X3202	X3206	X3209	X3210	X3214	X3217	X3218	X3219	X3220	X3221	X3226	X3229	X3230	X3233	X3234	X3235	X3236	X3241	X3242	X3243	X3244	X3245	X3246	X3247	X3248	X3249	X3250	X3251												
X2954	X2965	X2968	X2975	X2976	X2995	X2996	X2997	X2998	X3004	X3010	X3013	X3014	X3015	X3016	X3017	X3018	X3019	X3020	X3021	X3022	X3023	X3024	X3025	X3028	X3041	X3045	X3046	X3047	X3048	X3049	X3050	X3053	X3056	X3057	X3060	X3061	X3062	X3063	X3134	X3135	X3136	X3137	X3138	X3139	X3140	X3141	X3142												
Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	G2900	T2901	H2902	P2903	L2904	L2905	V2906	P2907	P2908	D2909	T2910	L2911	T2912	A2913	K2914	E2915	X2916	A2917	R2918	D2919	R2920	E2921	K2922	A2923	Q2924	E2925	L2926	L2927	X2928	F2929	L2930	Q2931	M2932	N2933	G2934	Y2935	A2936	V2937	T2938	R2939	X2942	X2943	X2944	X2945	X2946	X2947	X2948	X2949	X2950	X2951	X2952	X2953



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	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	0.486	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.16	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	0.24	0/834	0.63	3/1123 (0.3%)
1	F	0.23	0/834	0.63	1/1123 (0.1%)
1	H	0.24	0/834	0.63	1/1123 (0.1%)
1	J	0.24	0/834	0.63	1/1123 (0.1%)
2	B	0.28	0/25428	0.64	6/34534 (0.0%)
2	E	0.29	0/25428	0.64	6/34534 (0.0%)
2	G	0.29	0/25428	0.64	6/34534 (0.0%)
2	I	0.28	0/25428	0.64	4/34534 (0.0%)
All	All	0.28	0/105048	0.64	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	23
2	E	0	23
2	G	0	23
2	I	0	23
All	All	0	92

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	G	4872	PRO	N-CA-C	-7.30	103.38	113.53
2	E	4872	PRO	N-CA-C	-7.21	103.50	113.53
2	I	4872	PRO	N-CA-C	-7.21	103.51	113.53
2	B	4872	PRO	N-CA-C	-7.18	103.55	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	8	SER	N-CA-C	5.61	120.54	113.25

There are no chirality outliers.

5 of 92 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	194	SER	Peptide
2	B	240	ASP	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	18	0
1	F	818	0	824	20	0
1	H	818	0	824	18	0
1	J	818	0	824	20	0
2	B	29369	0	24713	512	0
2	E	29369	0	24712	524	0
2	G	29369	0	24716	522	0
2	I	29369	0	24713	508	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	120756	0	102150	2114	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 9.

The worst 5 of 2114 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:G:4859:PHE:HA	2:G:4862:PHE:CD2	1.88	1.08
2:G:4859:PHE:HA	2:G:4862:PHE:HD2	1.28	0.97
2:E:4859:PHE:HA	2:E:4862:PHE:CD2	2.05	0.92
2:E:4859:PHE:HA	2:E:4862:PHE:HD2	1.43	0.83
2:G:4859:PHE:CA	2:G:4862:PHE:HD2	1.99	0.73

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	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	F	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	H	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	J	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4687 (69%)	2848 (88%)	382 (12%)	5 (0%)	43	77
2	E	3235/4687 (69%)	2849 (88%)	381 (12%)	5 (0%)	43	77
2	G	3235/4687 (69%)	2848 (88%)	382 (12%)	5 (0%)	43	77
2	I	3235/4687 (69%)	2850 (88%)	380 (12%)	5 (0%)	43	77
All	All	13360/19176 (70%)	11775 (88%)	1565 (12%)	20 (0%)	49	83

5 of 20 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
2	B	1932	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	88/88 (100%)	88 (100%)	0	100	100
1	F	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	J	88/88 (100%)	88 (100%)	0	100	100
2	B	2493/3209 (78%)	2481 (100%)	12 (0%)	81	81
2	E	2493/3209 (78%)	2481 (100%)	12 (0%)	81	81
2	G	2493/3209 (78%)	2481 (100%)	12 (0%)	81	81
2	I	2493/3209 (78%)	2481 (100%)	12 (0%)	81	81
All	All	10324/13188 (78%)	10276 (100%)	48 (0%)	78	81

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	2144	ILE
2	G	4995	LEU
2	G	2339	VAL
2	G	4154	VAL
2	I	688	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 219 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	224	HIS
2	G	3809	ASN
2	I	3882	GLN
2	G	405	HIS

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Continued from previous page...

Mol	Chain	Res	Type
2	G	1691	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	12
2	I	12

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
2	E	12
2	G	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	44.41
1	I	3613:UNK	C	3639:THR	N	44.36
1	E	3613:UNK	C	3639:THR	N	44.35
1	G	3613:UNK	C	3639:THR	N	44.35
1	B	3163:UNK	C	3170:UNK	N	16.42

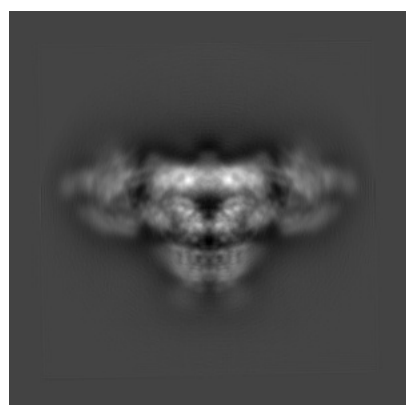
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22394. These allow visual inspection of the internal detail of the map and identification of artifacts.

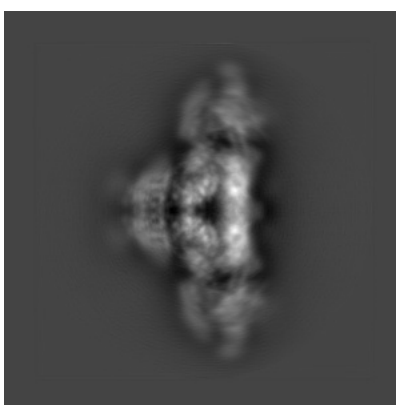
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

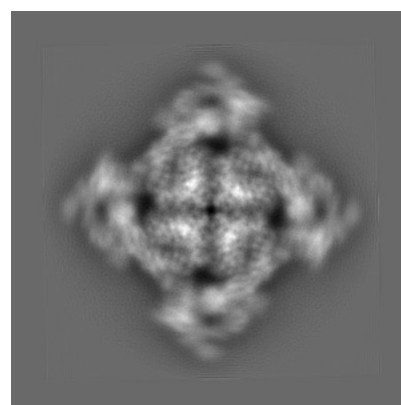
6.1.1 Primary map



X



Y

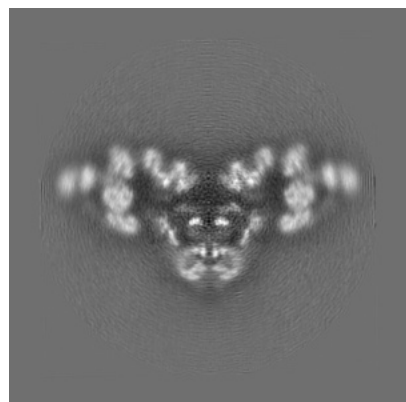


Z

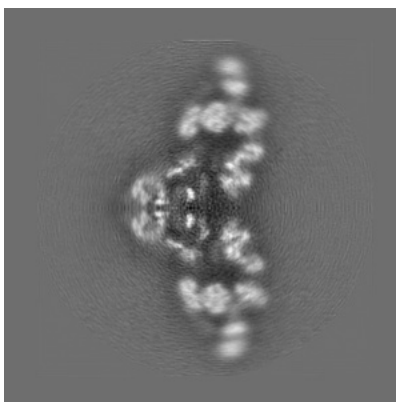
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

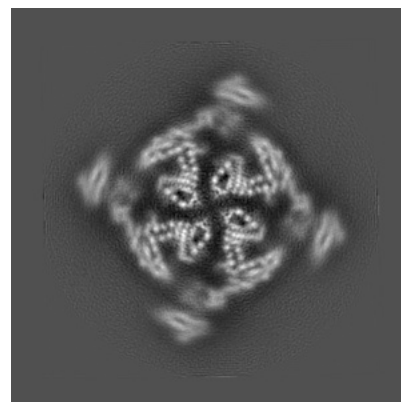
6.2.1 Primary map



X Index: 200



Y Index: 200

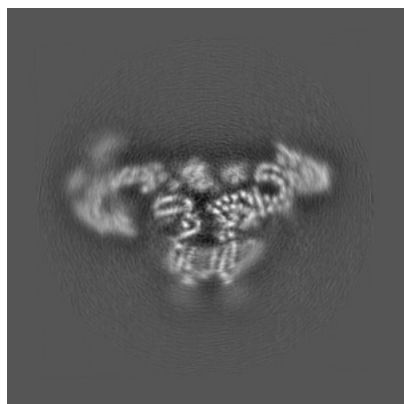


Z Index: 200

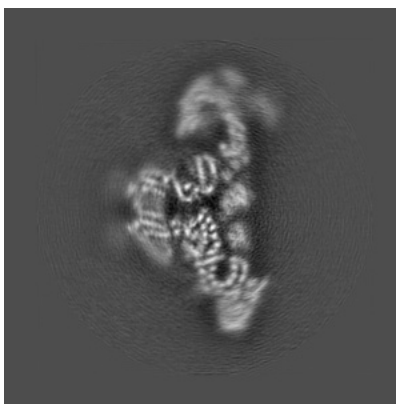
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

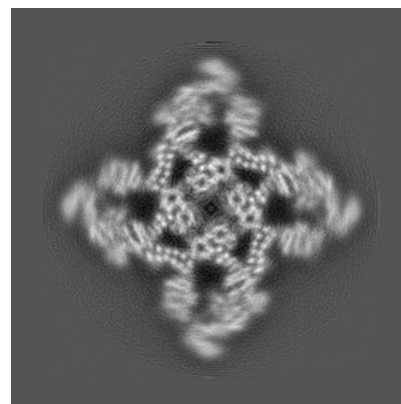
6.3.1 Primary map



X Index: 177



Y Index: 177



Z Index: 227

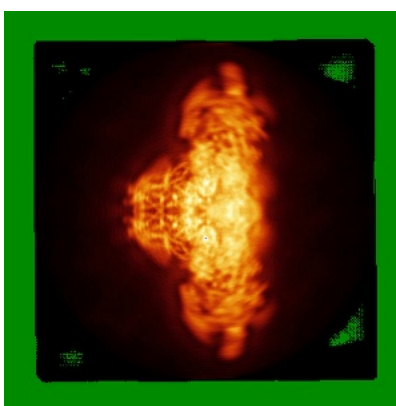
The images above show the largest variance slices of the map in three orthogonal directions.

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

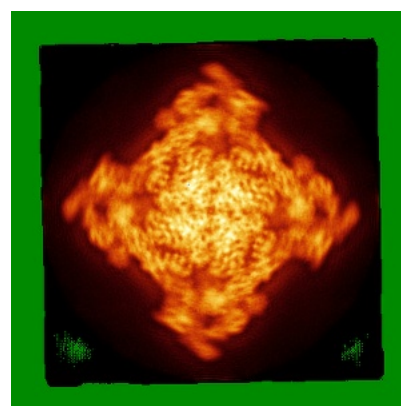
6.4.1 Primary map



X



Y

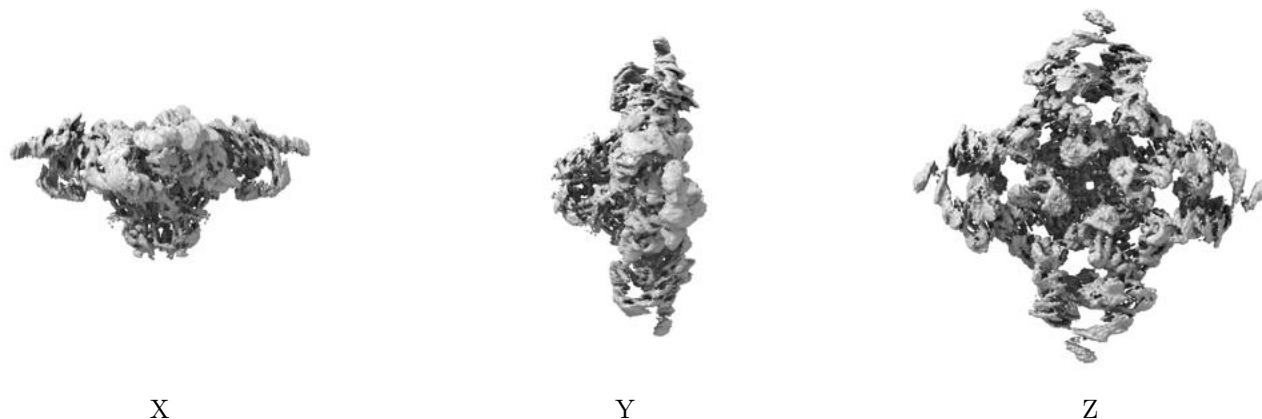


Z

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

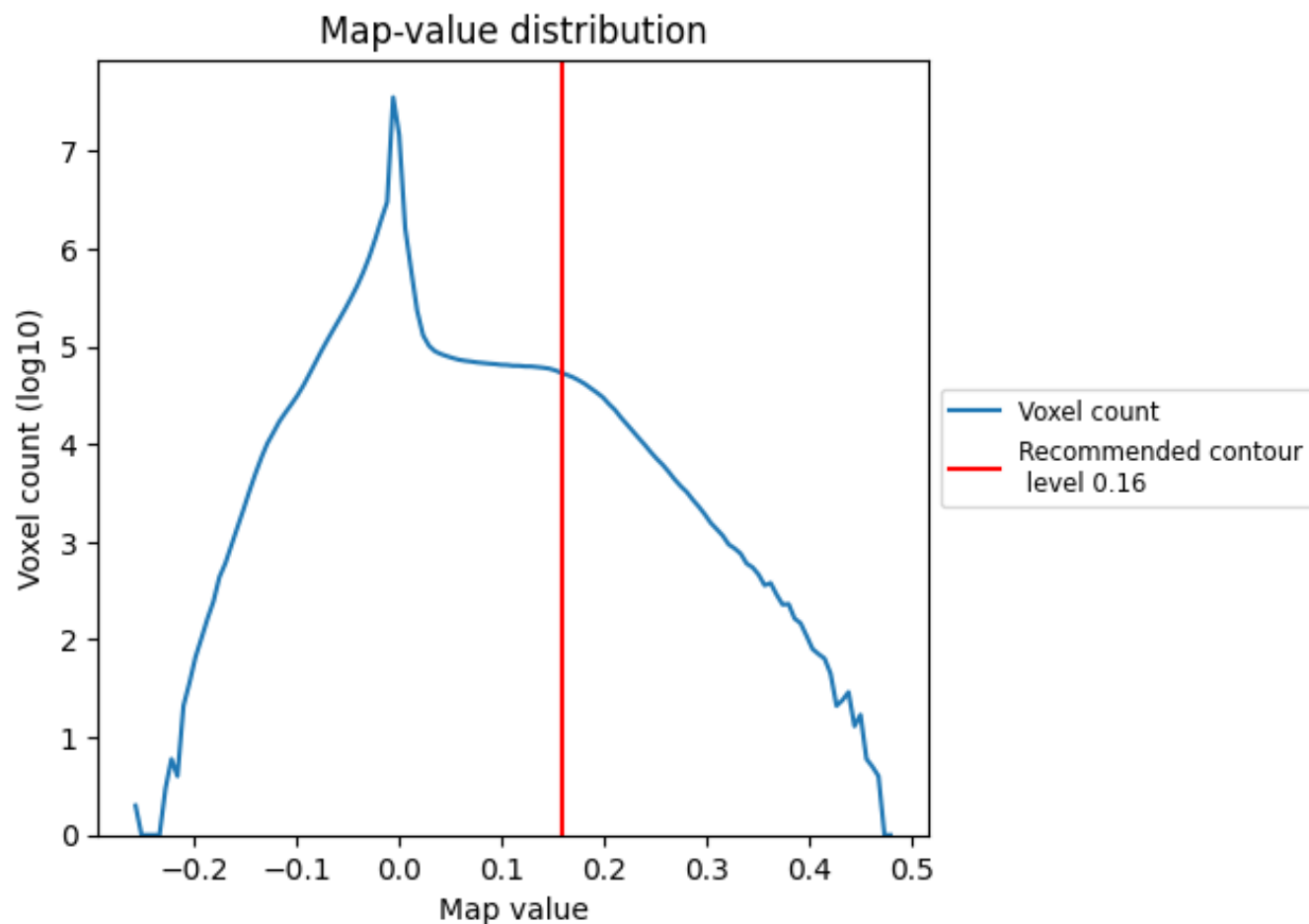
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

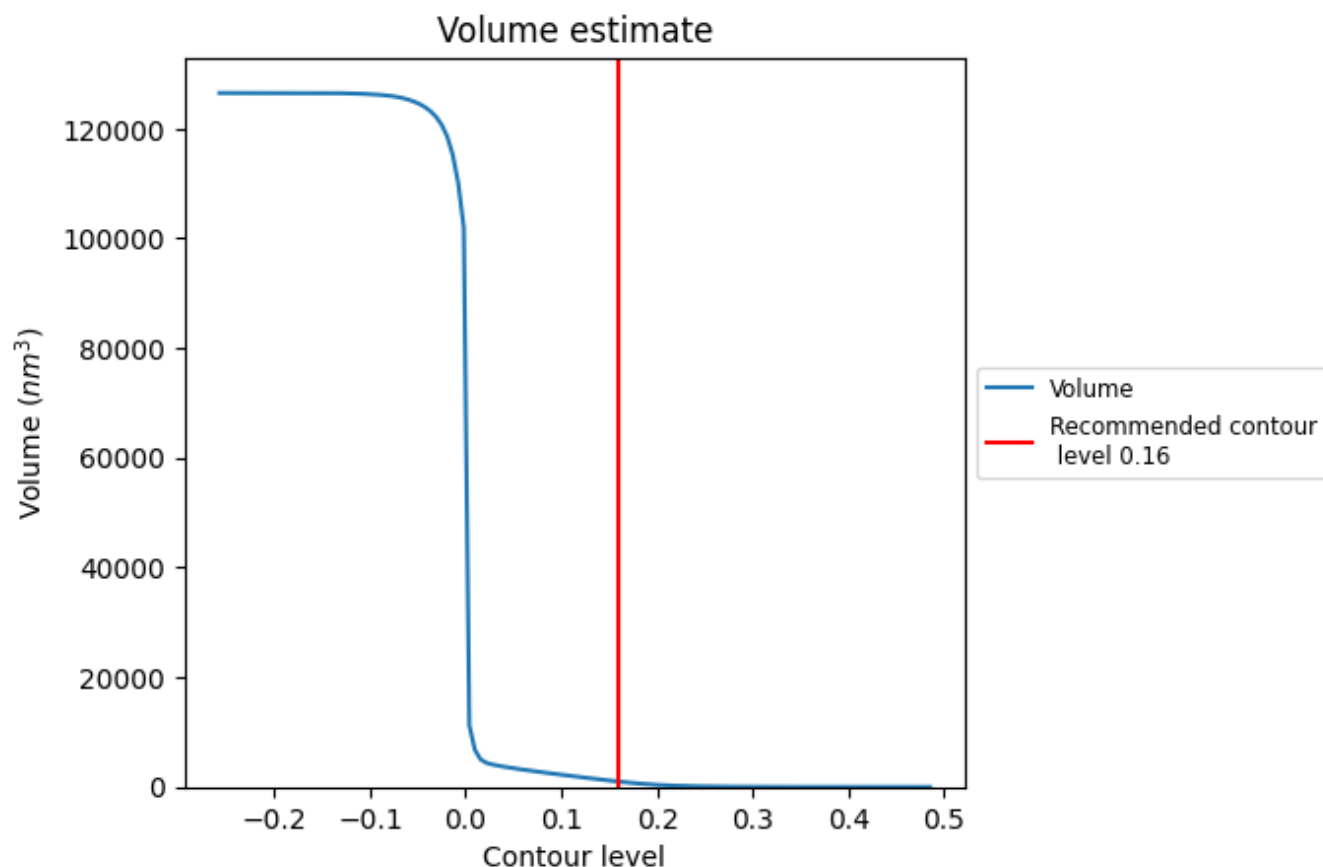
This section contains the results of statistical analysis of the map.

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.

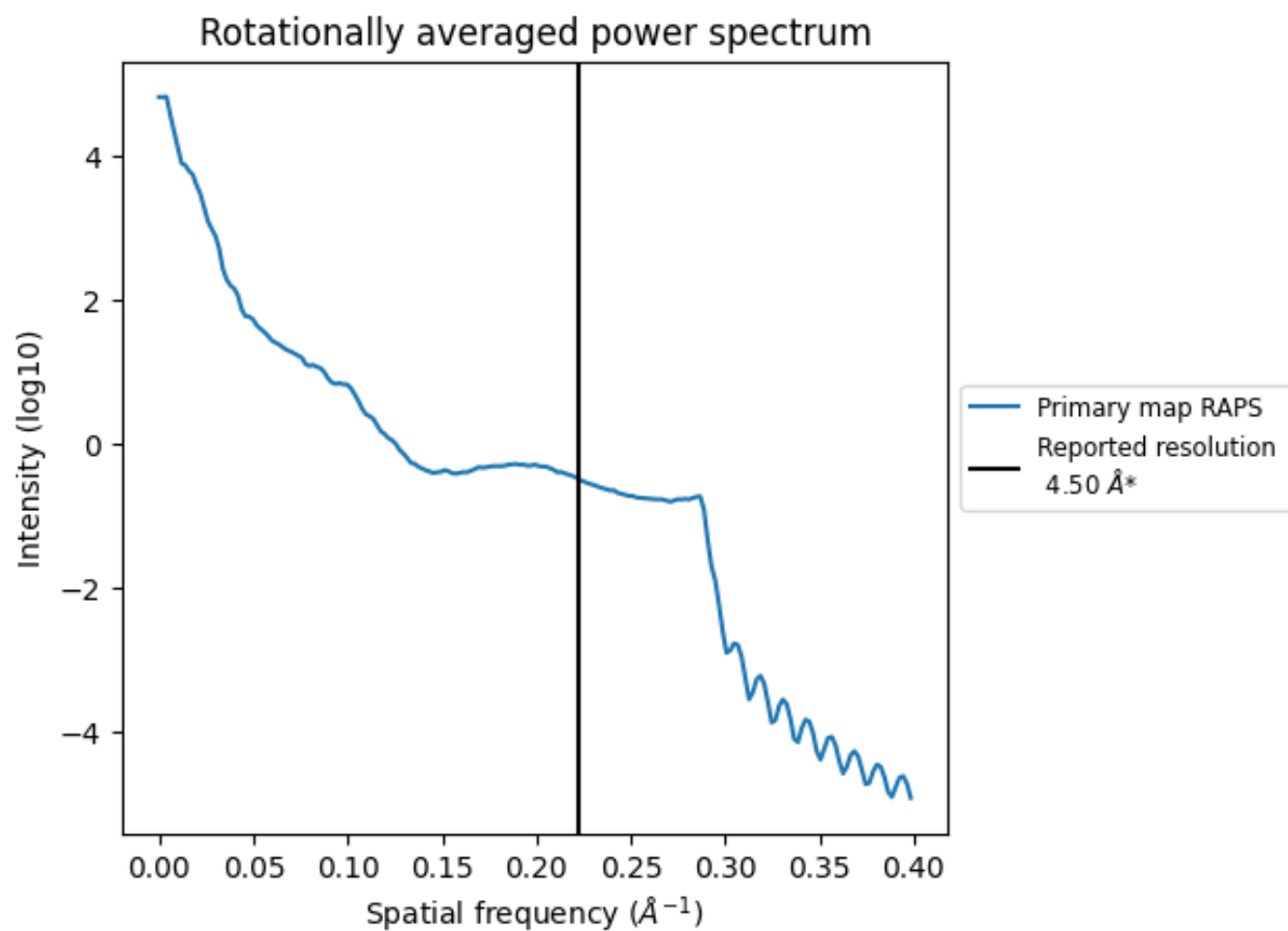
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 979 nm^3 ; this corresponds to an approximate mass of 884 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 0.222 Å⁻¹

8 Fourier-Shell correlation

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

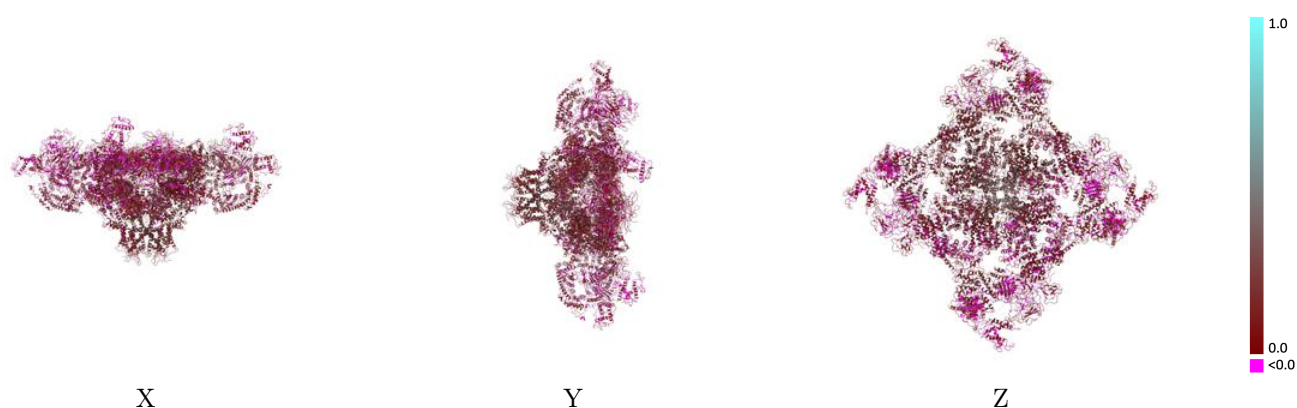
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22394 and PDB model 7JMH. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

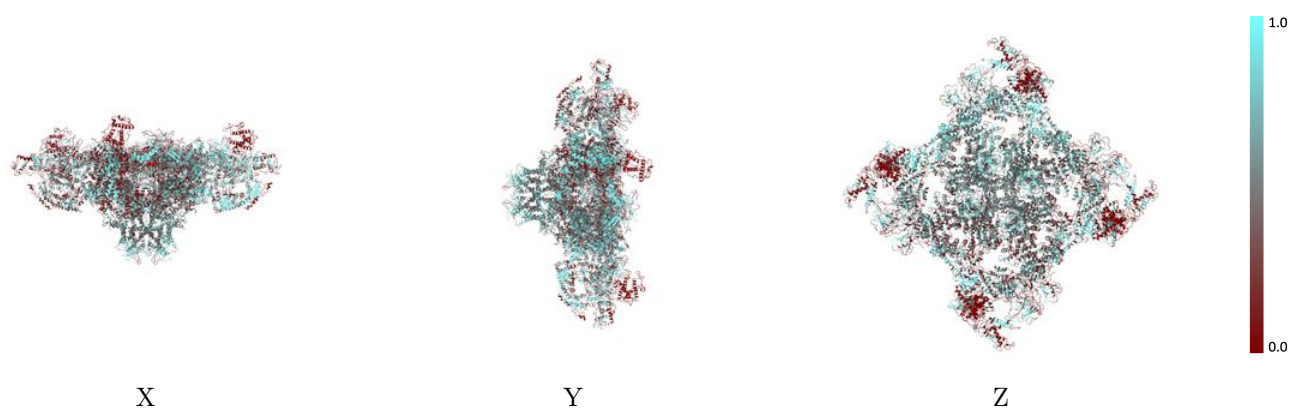
This section was not generated.

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



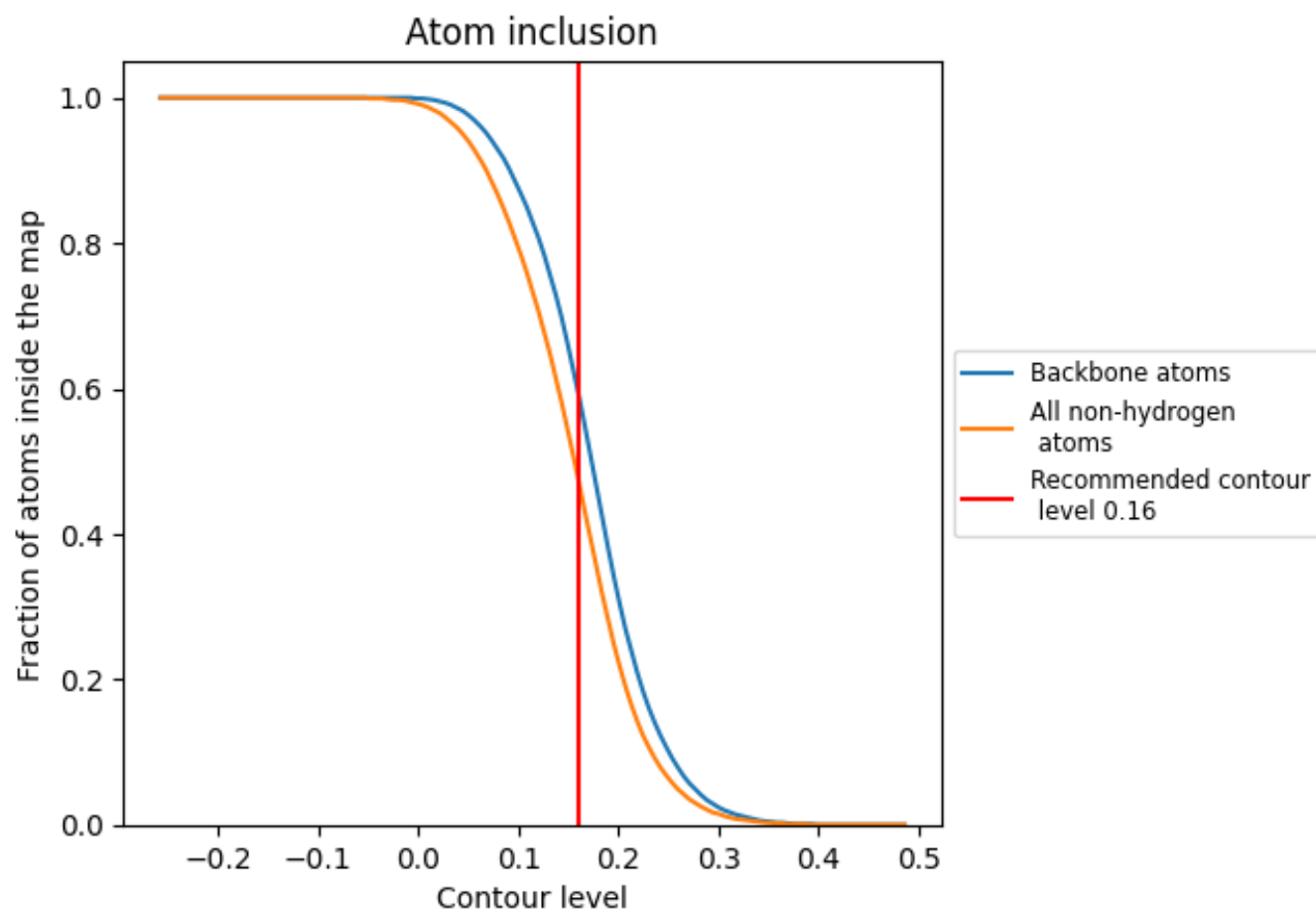
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 48% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4750	0.1320
A	0.5620	0.1390
B	0.5150	0.1680
E	0.4810	0.1330
F	0.4890	0.1070
G	0.4450	0.1070
H	0.4530	0.1190
I	0.4560	0.1230
J	0.4690	0.1180

