



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:55 AM UTC

PDB ID : 5TAW / pdb_00005taw
EMDB ID : EMD-8387
Title : Structure of rabbit RyR1 (ryanodine dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.40 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:

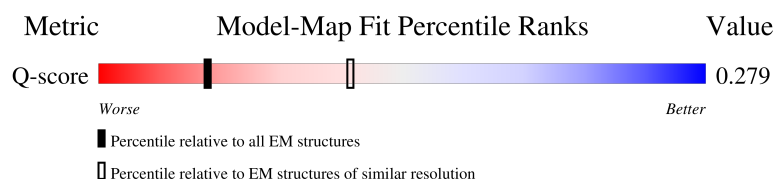
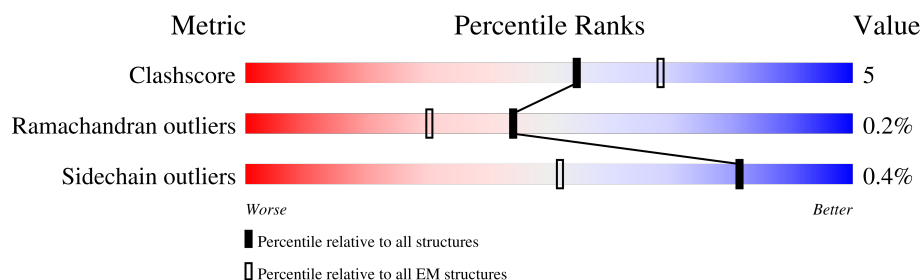
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.40 Å.

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



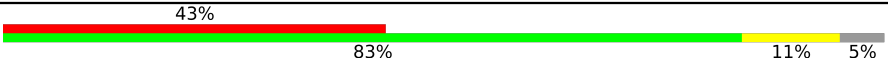
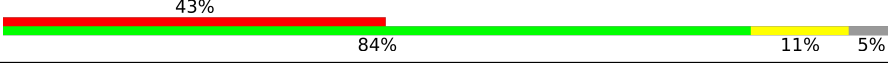
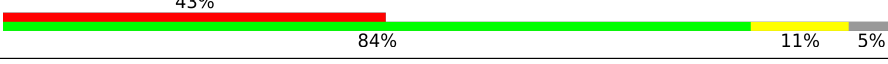
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	108	30% 83% 16% .
1	F	108	31% 81% 18% .
1	H	108	31% 81% 18% .
1	J	108	29% 81% 18% .

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Mol	Chain	Length	Quality of chain
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	G	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	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	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	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

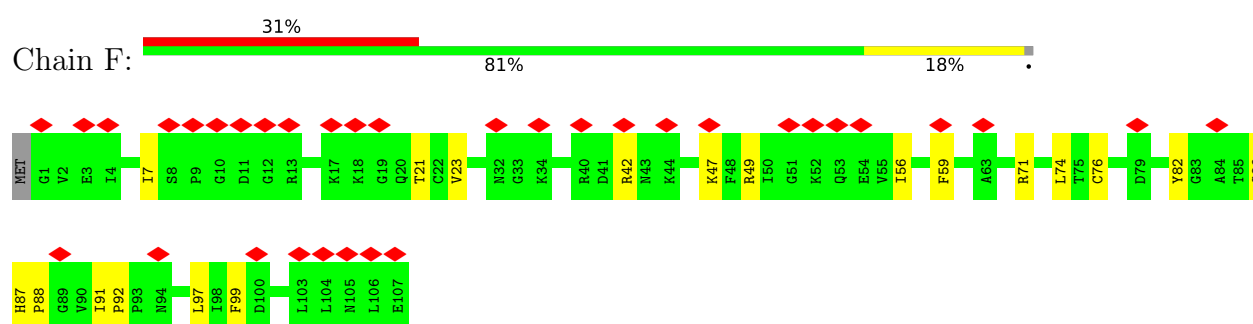
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

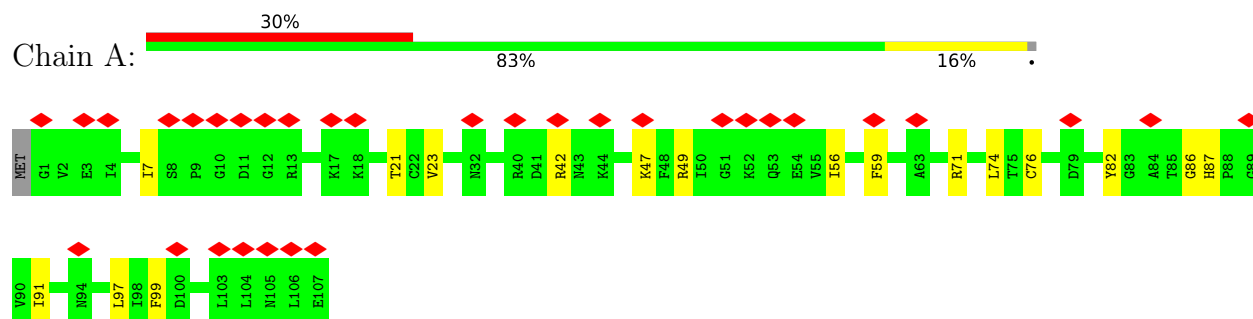
3 Residue-property plots [i](#)

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.

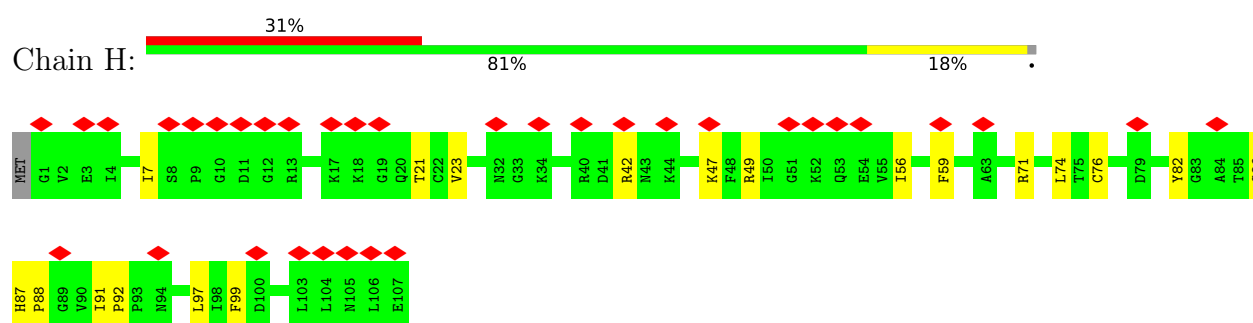
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



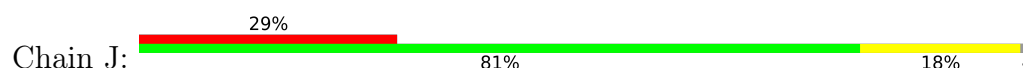
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

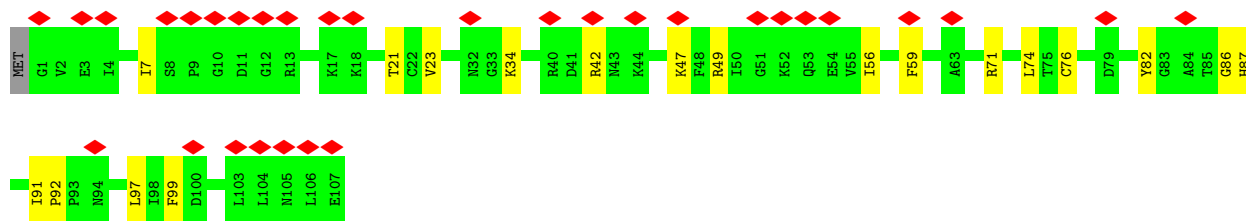


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

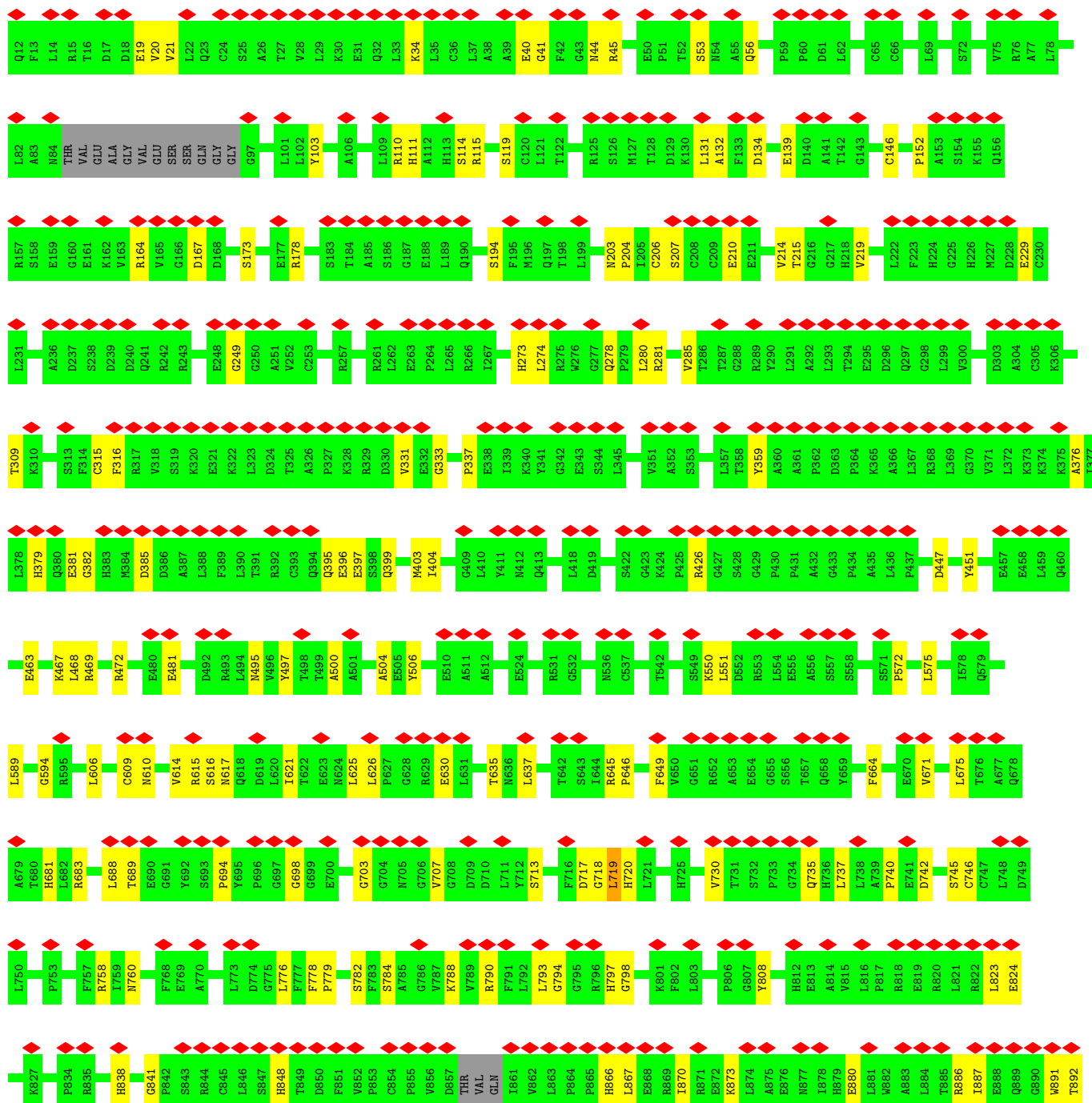
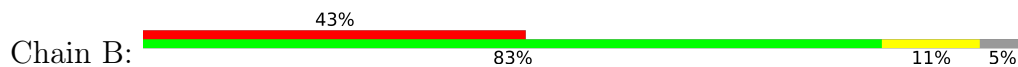


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

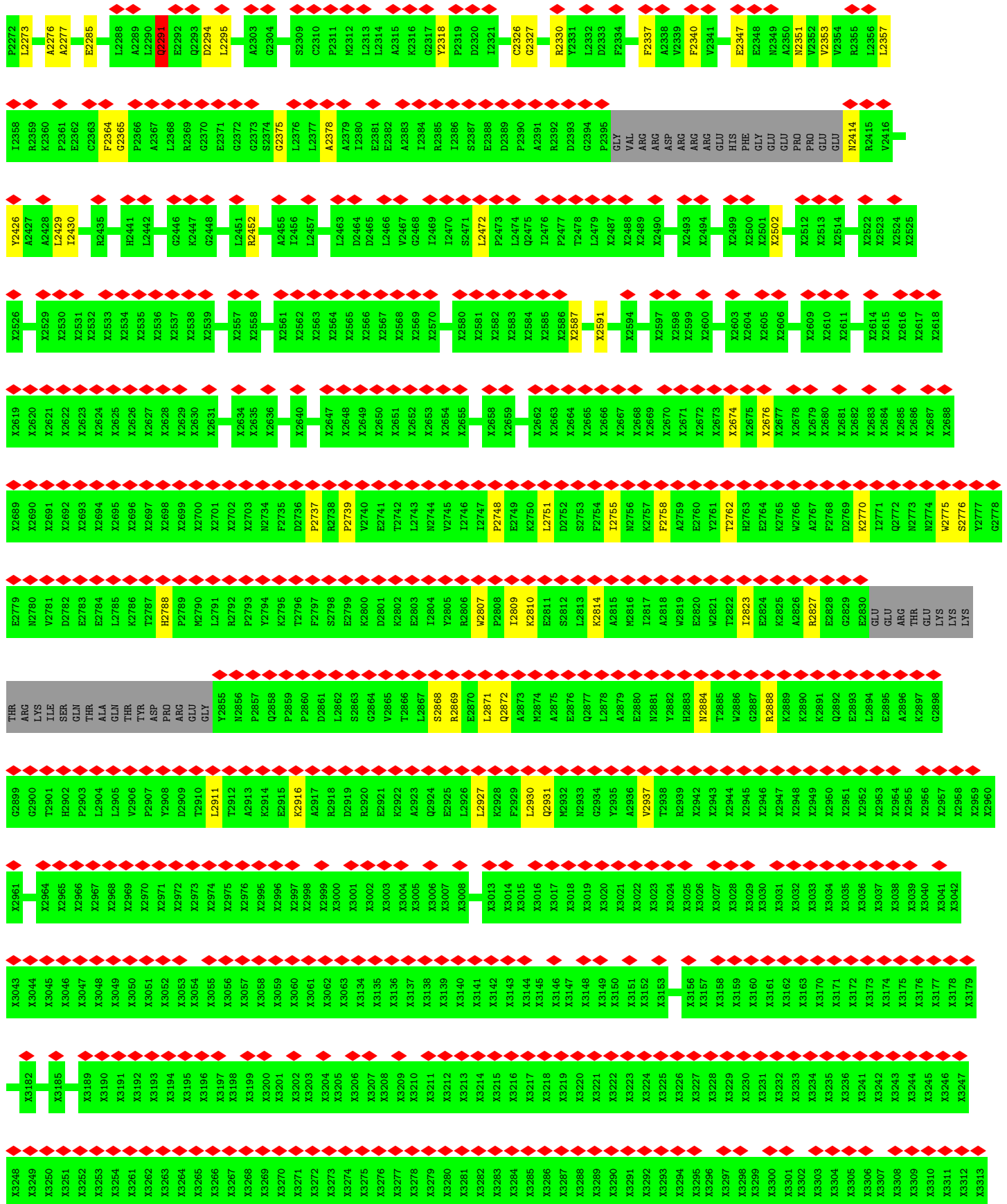




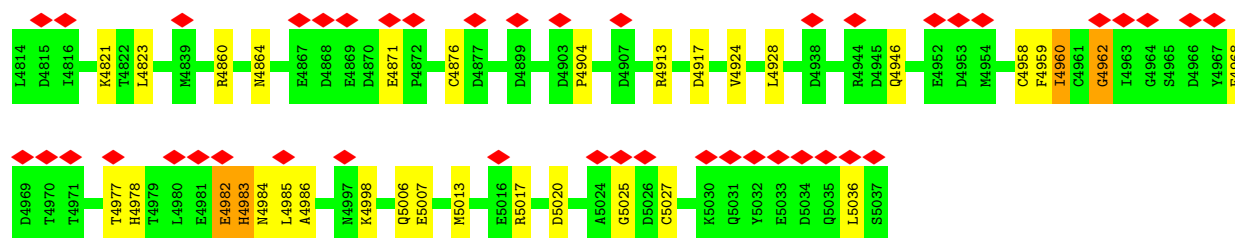
• Molecule 2: Ryanodine receptor 1



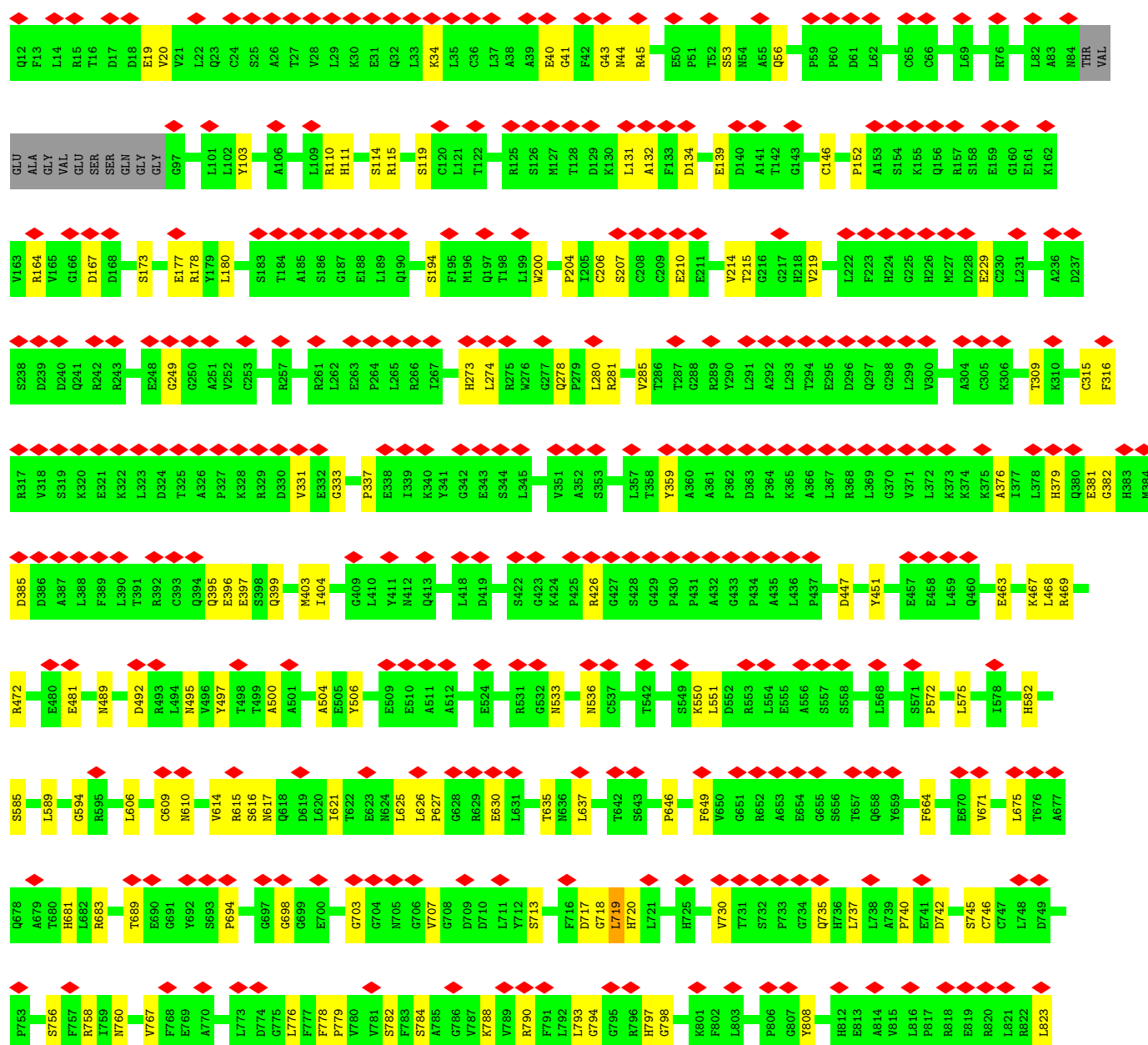
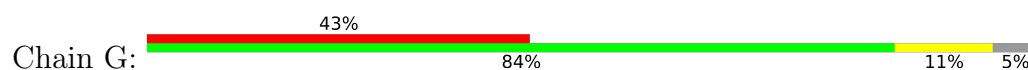




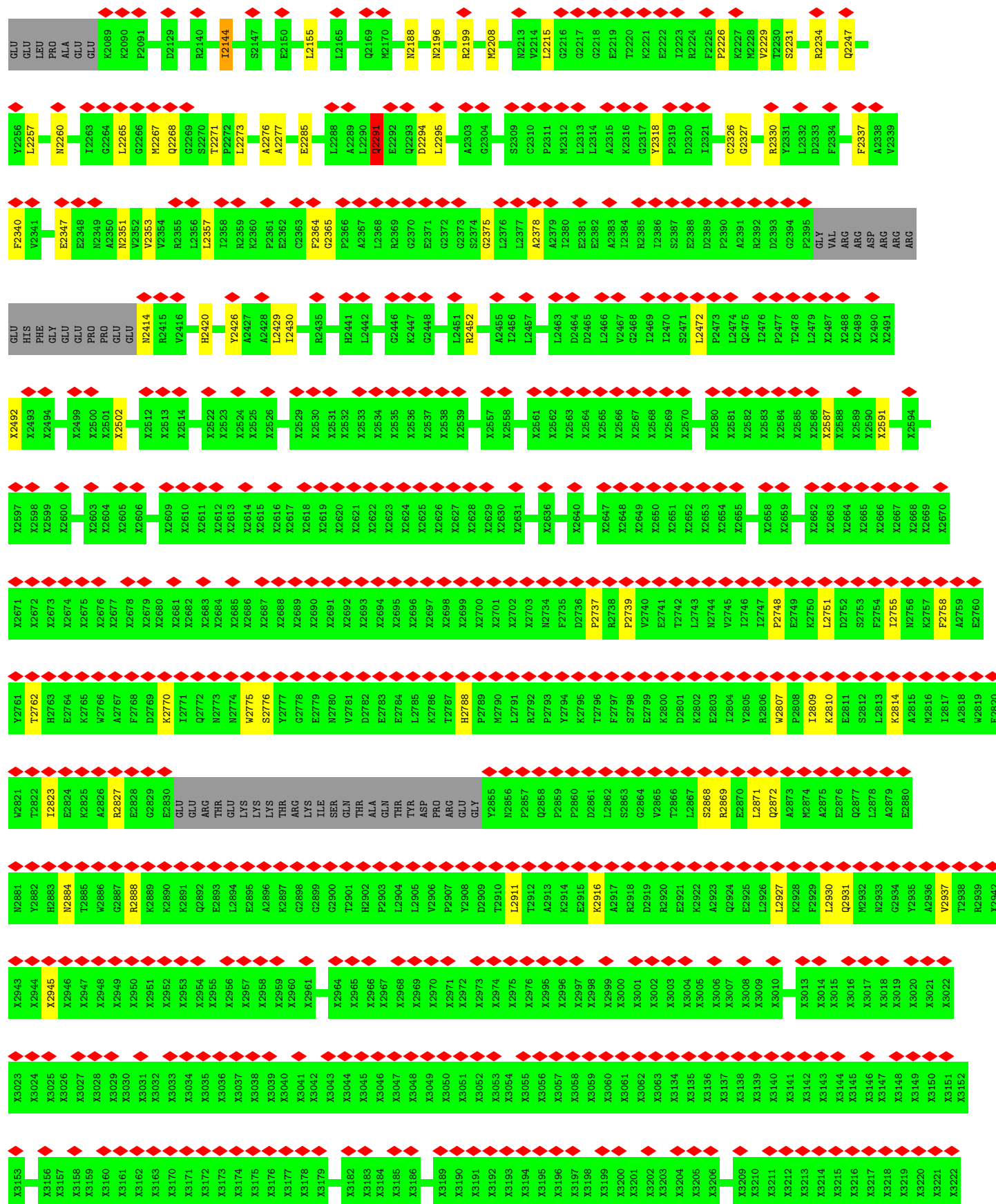




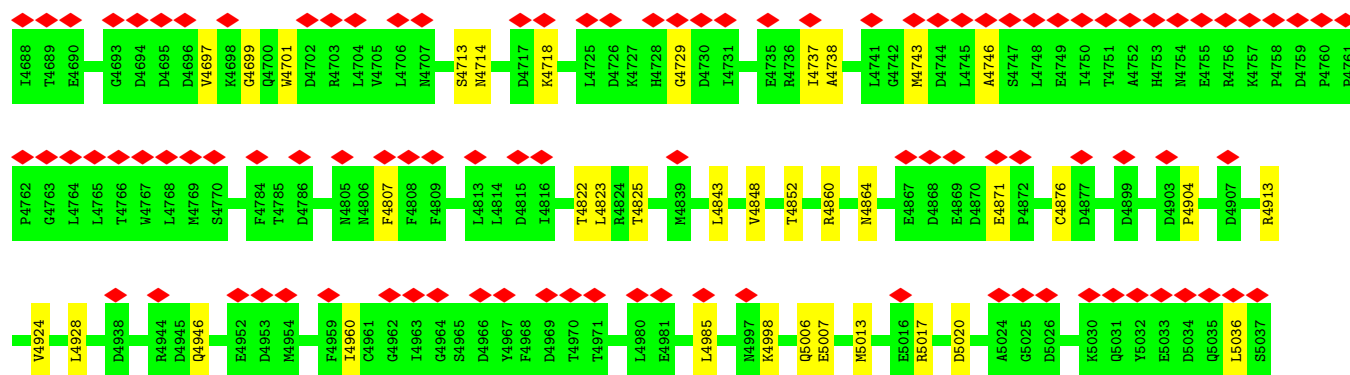
• Molecule 2: Ryanodine receptor 1



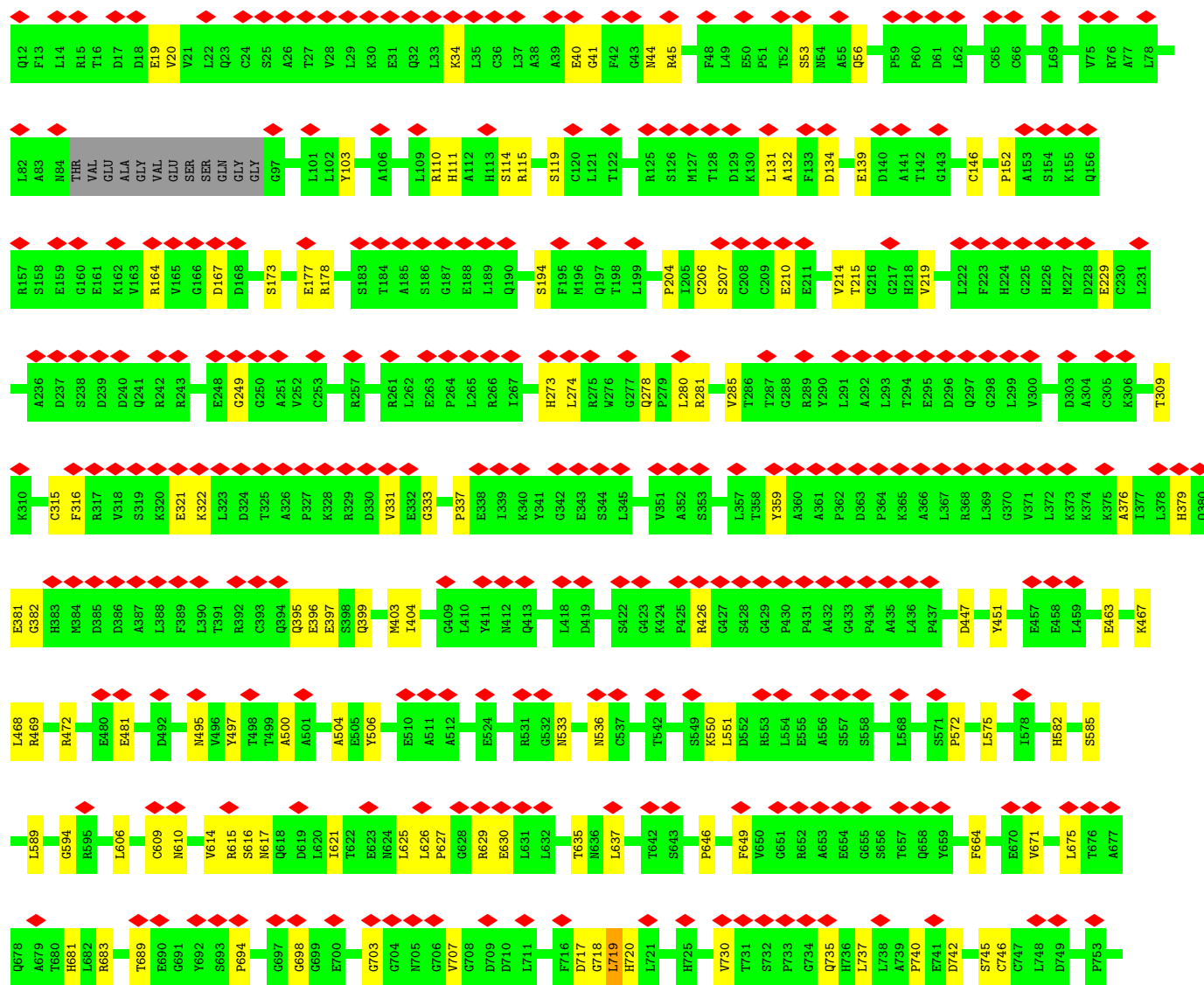
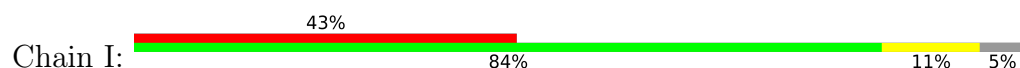




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ALA	E4199	P4106	D4022	T3910	I3763	E3691	X3587	X3526	X3415	X3354	X3362	X3301	X3229	X3227	X3226	X3225	X3224
GLY	E4206	E4107		T3911	S3784	E3692	X3588	X3527	X3416	X3355	X3363	X3302	X3232	X3233	X3234	X3235	X3236
ASP				T3912	I3804	K3693	X3589	X3528	X3417	X3356	X3364	X3303	X3233	X3234	X3235	X3236	X3237
LEU				I3913	L3805	K3694	X3590	X3529	X3418	X3357	X3365	X3304	X3238	X3239	X3240	X3241	X3242
ALA				N3914			X3591	X3530	X3419	X3358	X3366	X3305	X3239	X3240	X3241	X3242	X3243
ALA				I3915	N3809	K3694	X3592	X3531	X3420	X3359	X3367	X3306	X3240	X3241	X3242	X3243	X3244
GLY						R3707	X3592	X3532	X3421	X3360	X3368	X3307	X3241	X3242	X3243	X3244	X3245
GLY				R3925	L3817	E3712	X3595	X3533	X3422	X3361	X3369	X3308	X3242	X3243	X3244	X3245	X3246
GLY				D3932	K3821	K3713	X3596	X3534	X3423	X3362	X3367	X3309	X3243	X3244	X3245	X3246	X3247
GLY				Y3937	D3822	S3714	X3597	X3535	X3424	X3363	X3368	X3310	X3244	X3245	X3246	X3247	X3248
GLY				G3939	E3825	L3716	X3598	X3536	X3425	X3364	X3369	X3311	X3245	X3246	X3247	X3248	X3249
TRP				K3940	V3826	L3717	X3599	X3537	X3426	X3365	X3367	X3312	X3246	X3247	X3248	X3249	X3250
GLY				D3941	G3827	L3718	X3600	X3538	X3427	X3366	X3368	X3313	X3247	X3248	X3249	X3250	X3251
GLY				V3942	F3828	E3718	X3601	X3539	X3428	X3367	X3369	X3314	X3248	X3249	X3250	X3251	X3252
GLY				I3943	F3829	Y3722	X3602	X3540	X3429	X3368	X3367	X3315	X3249	X3250	X3251	X3252	X3253
GLY				E3944	Q3830	N3723	X3606	X3541	X3430	X3369	X3368	X3316	X3250	X3251	X3252	X3253	X3254
GLY				E3945	Q3833	N3723	X3607	X3542	X3431	X3370	X3369	X3317	X3251	X3252	X3253	X3254	X3255
ALA				Q3946	Q3836	I3728	X3608	X3543	X3432	X3371	X3370	X3318	X3252	X3253	X3254	X3255	X3256
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GLY				N3963	Q3850	E3737	X3612	X3547	X3436	X3375	X3374	X3322	X3256	X3257	X3258	X3259	X3260
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GLY				C3973	E3855	GLY	X3615	X3550	X3439	X3378	X3377	X3325	X3259	X3260	X3261	X3262	X3263
GLY				N3976	L3856	ALA	X3616	X3551	X3440	X3379	X3378	X3326	X3260	X3261	X3262	X3263	X3264
GLY				Q3977	G3857	GLY	X3617	X3552	X3441	X3380	X3379	X3327	X3261	X3262	X3263	X3264	X3265
GLY				Q3978	N3859	GLY	X3618	X3553	X3442	X3381	X3380	X3328	X3262	X3263	X3264	X3265	X3266
GLY				Q3979	V3860	ALA	X3619	X3554	X3443	X3382	X3381	X3329	X3263	X3264	X3265	X3266	X3267
GLY				L3980	E3861	E3748	X3620	X3555	X3444	X3383	X3382	X3330	X3264	X3265	X3266	X3267	X3268
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GLY				M4000	Q3871	Q3766	X3631	X3566	X3455	X3394	X3391	X3341	X3275	X3276	X3277	X3278	X3279
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GLY				D4006	D3878	R3773	X3635	X3570	X3459	X3398	X3395	X3345	X3279	X3280	X3281	X3282	X3283
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GLY				L4017	N3880	Q3775	X3637	X3572	X3461	X3400	X3397	X3347	X3281	X3282	X3283	X3284	X3285
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GLY				L4018	N3898	Q3775	X3655	X3590	X3479	X3418	X3415	X3365	X3299	X3300	X3301	X3302	X3303
GLY				L4018	N3899	Q3775	X3656	X3591	X3480	X3419	X3416	X3366	X3300	X3301	X3302	X3303	X3304
GLY				L4018	N3900	Q3775	X3657	X3592	X3481	X3420	X3417	X3367	X3301	X3302	X3303	X3304	X3305
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GLY				L4018	N3902	Q3775	X3659	X3594	X3483	X3422	X3419	X3369	X3303	X3304	X3305	X3306	X3307
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GLY				L4018	N3905	Q3775	X3662	X3597	X3486	X3425	X3422	X3372	X3306	X3307	X3308	X3309	X3310
GLY				L4018	N3906	Q3775	X3663	X3598	X3487	X3426	X3423	X3373	X3307	X3308	X3309	X3310	X3311
GLY				L4018	N3907	Q3775	X3664	X3599	X3488	X3427	X3424	X3374	X3308	X3309	X3310	X3311	X3312
GLY				L4018	N3908	Q3775	X3665	X3600	X3489	X3428	X3425	X3375	X3309	X3310	X3311	X3312	X3313
GLY				L4018	N3909	Q3775	X3666	X3601	X3490	X3429	X3426	X3376	X3310	X3311	X3312	X3313	X3314
GLY				L4018	N3910	Q3775	X3667	X3602	X3491	X3430	X3427	X3377	X3311	X3312	X3313	X3314	X3315
GLY				L4018	N3911	Q3775	X3668	X3603	X3492	X3431	X3428	X3378	X3312	X3313	X3314	X3315	X3316
GLY				L4018	N3912	Q3775	X3669	X3604	X3493	X3432	X3429	X3379	X3313	X3314	X3315	X3316	X3317
GLY				L4018	N3913	Q3775	X3670	X3605	X3494	X3433	X3430	X3380	X3314	X3315	X3316	X3317	X3318
GLY				L4018	N3914	Q3775	X3671	X3606	X3495	X3434	X3431	X3381	X3315	X3316	X3		



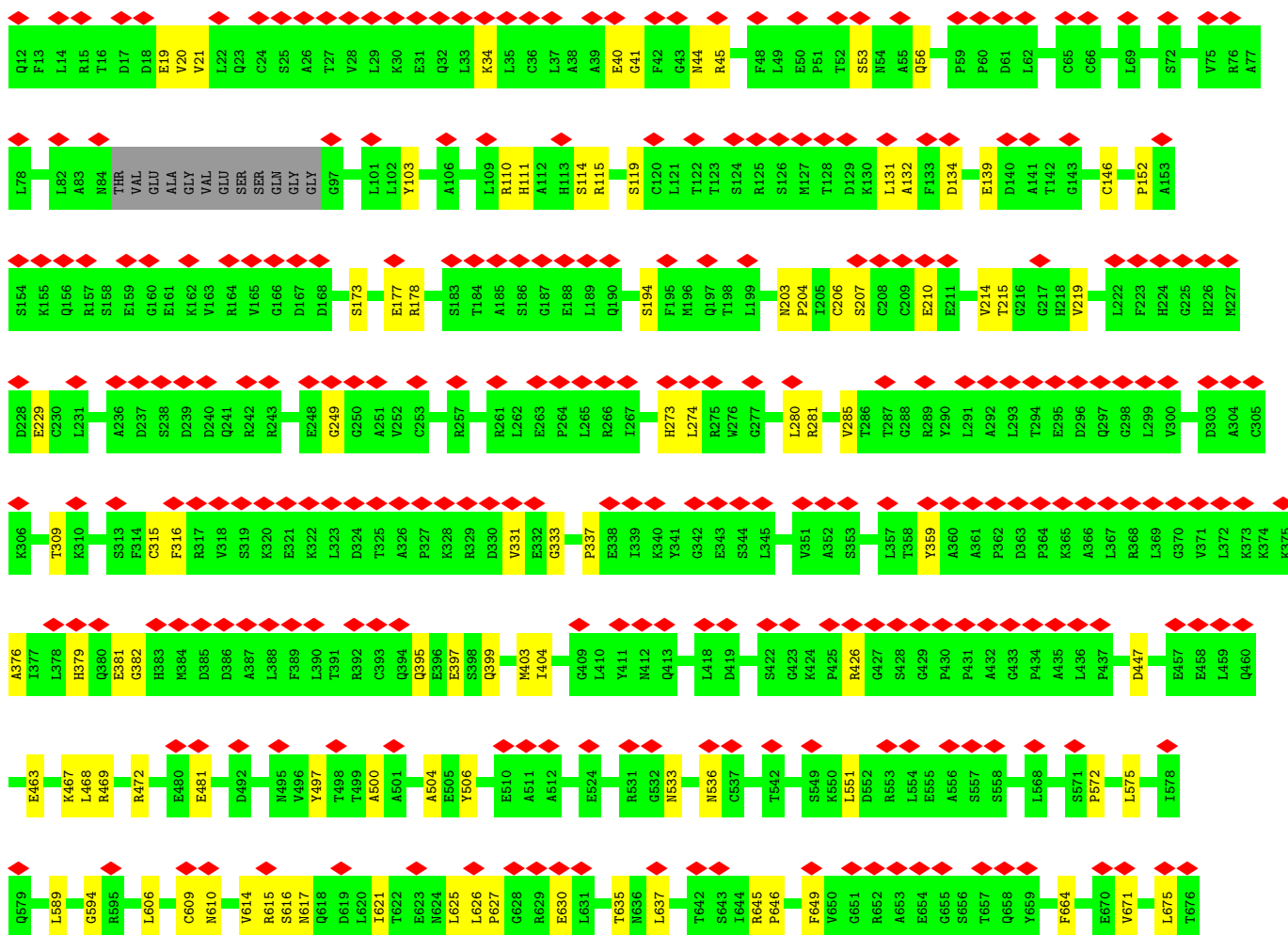
• Molecule 2: Ryanodine receptor 1

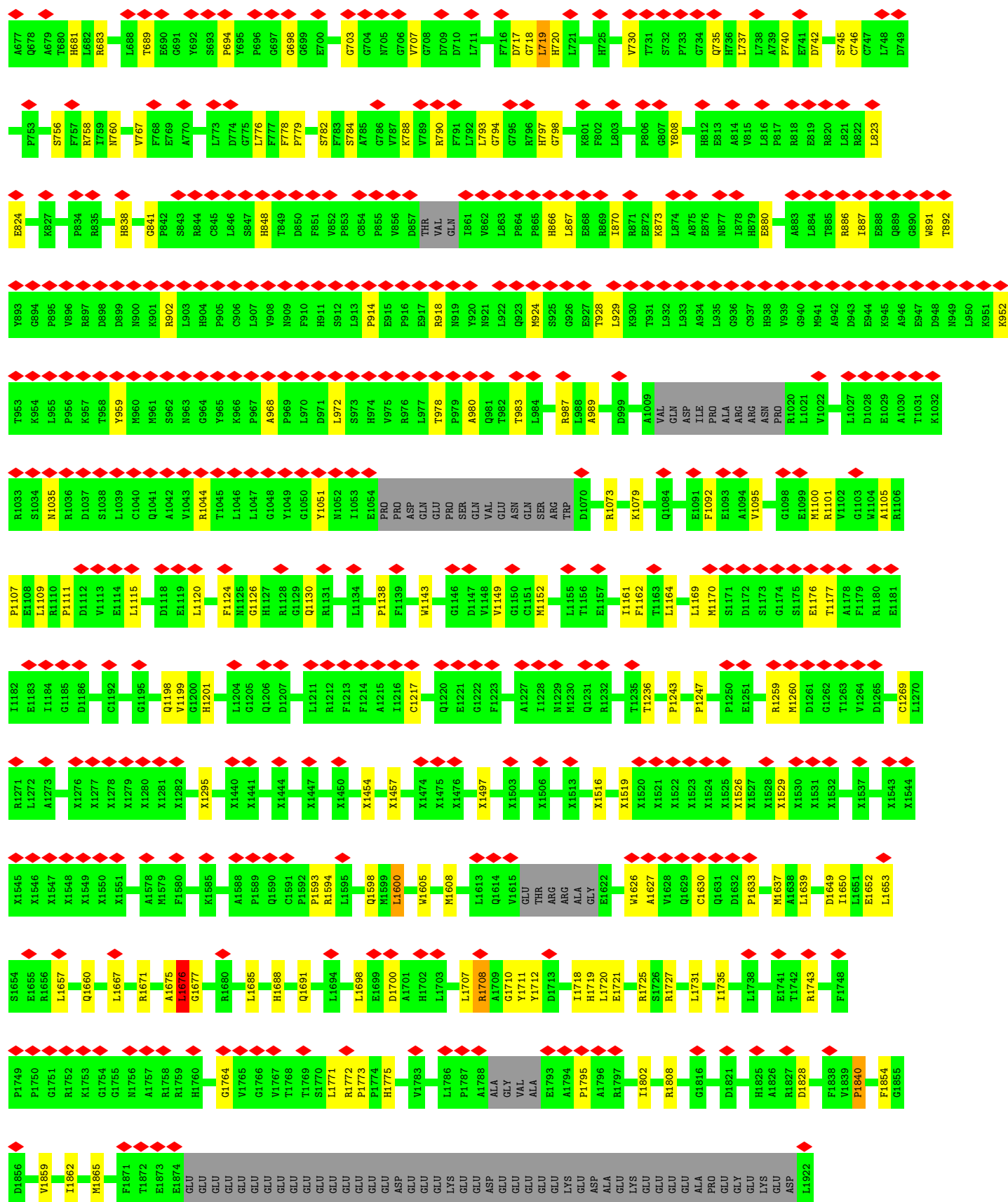


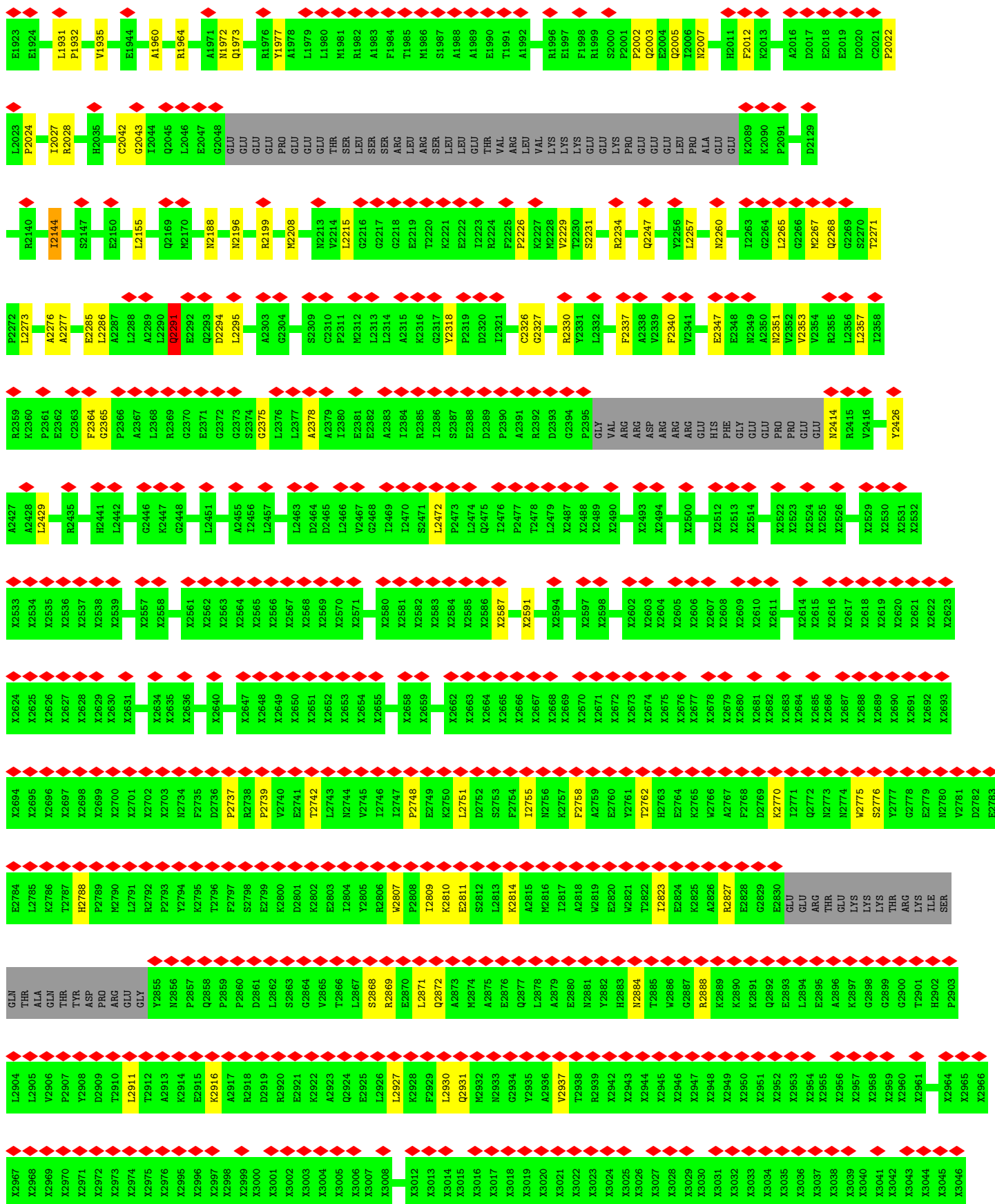




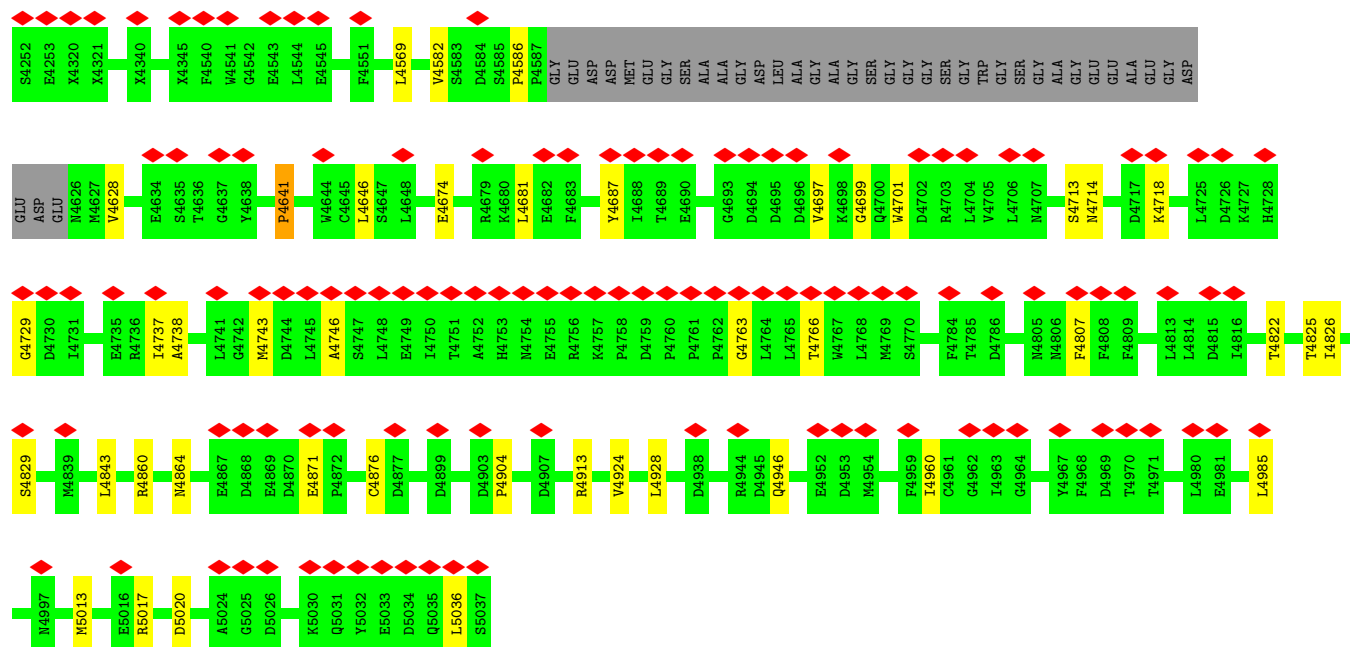








E4134	L4066	D3943	G3738	N3643	X3649	X3379	X3380	X3319	X3253	X3185	X3047
R4137	D4070	Q3350	G3739	L3644	X3650	X3381	X3382	X3320	X3254	X3186	X3048
I4138	I4071	A3853	E3740	M3652	X3651	X3382	X3383	X3321	X3261	X3189	X3049
N4142	G4073	E3854	GLU	M3652	X3652	X3383	X3384	X3322	X3262	X3190	X3050
E4152	S4074	G3855	ALA	S3656	X3653	X3384	X3385	X3323	X3263	X3191	X3051
E4152	E4075	L3856	GLU	Y3657	X3654	X3385	X3386	X3324	X3264	X3192	X3052
P4155	A4076	G3857	E3747	K3658	X3655	X3387	X3387	X3325	X3265	X3193	X3053
H4156	F4077	M3858	E3748	A3659	X3657	X3388	X3388	X3326	X3266	X3194	X3054
H4157	Q4078	V3859	V3749	X3660	X3658	X3389	X3389	X3327	X3267	X3195	X3055
P4158	D4079	N3860	E3750	I3662	X3659	X3390	X3390	X3328	X3268	X3196	X3056
R4159	D4080	E3861	V3751	L3663	X3660	X3391	X3391	X3329	X3269	X3197	X3057
L4160	V4081	D3862	S3752	T3664	X3661	X3392	X3392	X3330	X3270	X3200	X3058
L4161	T4082	G3863	F3753	D3665	X3662	X3393	X3393	X3331	X3271	X3201	X3059
R4161	D4083	T3864	E3753	D3666	X3663	X3394	X3394	X3332	X3272	X3202	X3060
L4164	P4084	V3865	K3756	H3667	X3664	X3395	X3395	X3333	X3273	X3203	X3061
E4165	R4085	I3866	H3667	F3668	X3665	X3396	X3396	X3334	X3274	X3204	X3062
I4170	G4086	N3867	F3669	F3669	X3666	X3397	X3397	X3335	X3275	X3205	X3063
F4174	L4087	R3868	I3674	D3675	X3667	X3398	X3398	X3336	X3276	X3207	X3134
R4180	I4088	Q3869	D3676	D3676	X3668	X3399	X3399	X3337	X3277	X3208	X3135
M4184	K4091	N3870	A3680	A3680	X3669	X3400	X3400	X3338	X3278	X3209	X3136
G4185	D4092	G3871	G3681	G3681	X3670	X3401	X3401	X3339	X3279	X3210	X3137
A4186	F4093	E3872	E3682	E3682	X3671	X3402	X3402	X3340	X3280	X3211	X3138
S4187	Q4094	K3873	E3683	E3683	X3672	X3403	X3403	X3341	X3281	X3212	X3139
R4188	A4095	V3874	Q3683	Q3683	X3673	X3404	X3404	X3342	X3282	X3213	X3140
R4189	M4096	D3875	E3684	E3684	X3674	X3405	X3405	X3343	X3283	X3214	X3141
Y4194	D4097	Q3876	E3685	E3685	X3675	X3406	X3406	X3344	X3284	X3215	X3142
E4199	D4098	Q3882	E3686	E3686	X3676	X3407	X3407	X3345	X3285	X3216	X3143
E4206	S4099	R3886	E3687	E3687	X3677	X3408	X3408	X3346	X3286	X3217	X3144
F4219	Q4100	N3887	E3688	E3688	X3678	X3409	X3409	X3347	X3287	X3218	X3145
N4223	K4101	D3889	E3689	E3689	X3679	X3410	X3410	X3348	X3288	X3219	X3146
E4224	F4102	L3890	E3690	E3690	X3680	X3411	X3411	X3349	X3289	X3220	X3147
Q4225	Q4103	L3891	E3691	E3691	X3681	X3412	X3412	X3350	X3290	X3221	X3148
Q4226	T4104	N3899	E3692	E3692	X3682	X3413	X3413	X3351	X3291	X3222	X3149
E4227	G4105	G3903	E3693	E3693	X3683	X3414	X3414	X3352	X3292	X3223	X3150
A4228	P4106	M3909	E3694	E3694	X3684	X3415	X3415	X3353	X3293	X3224	X3151
E4229	E4107	T3910	E3695	E3695	X3685	X3416	X3416	X3354	X3294	X3225	X3152
M4231	I4108	T3911	E3696	E3696	X3686	X3417	X3417	X3355	X3295	X3226	X3153
E4232	Q4109	T3912	E3697	E3697	X3687	X3418	X3418	X3356	X3296	X3227	X3154
L4233	F4110	I3913	E3698	E3698	X3688	X3419	X3419	X3357	X3297	X3228	X3155
S4236	A4117	I3915	E3699	E3699	X3689	X3420	X3420	X3358	X3298	X3229	X3156
E4239	D4118	R3925	E3700	E3700	X3690	X3421	X3421	X3359	X3299	X3230	X3157
E4250	E4119	D3932	E3701	E3701	X3691	X3422	X3422	X3360	X3300	X3231	X3158
I4251	E4120	T3937	E3702	E3702	X3692	X3423	X3423	X3361	X3301	X3232	X3159
E4251	M4121	G3938	E3703	E3703	X3693	X3424	X3424	X3362	X3302	X3233	X3160
E4251	I4122	N3939	E3704	E3704	X3694	X3425	X3425	X3363	X3303	X3234	X3161
E4251	M4123	G3940	E3705	E3705	X3695	X3426	X3426	X3364	X3304	X3235	X3162
E4251	I4124	K3941	E3706	E3706	X3696	X3427	X3427	X3365	X3305	X3236	X3163
E4251	F4125	D4062	E3707	E3707	X3697	X3428	X3428	X3366	X3306	X3237	X3170
E4251	E4126	D4063	E3708	E3708	X3698	X3429	X3429	X3367	X3307	X3241	X3171
E4251	E4127	M4064	E3709	E3709	X3699	X3430	X3430	X3368	X3308	X3242	X3172
E4251	F4128	F4065	E3710	E3710	X3700	X3431	X3431	X3369	X3309	X3243	X3173
E4251	I4129	E3944	E3711	E3711	X3701	X3432	X3432	X3370	X3310	X3244	X3174
E4251	N4130	E3945	E3712	E3712	X3702	X3433	X3433	X3371	X3311	X3245	X3175
E4251	R4131	Q3946	E3713	E3713	X3703	X3434	X3434	X3372	X3312	X3246	X3176
E4251	F4132	Q3946	E3714	E3714	X3704	X3435	X3435	X3373	X3313	X3247	X3177
E4251	Q4133	Q3946	E3715	E3715	X3705	X3436	X3436	X3374	X3314	X3248	X3178
E4251	E4133	Q3946	E3716	E3716	X3706	X3437	X3437	X3375	X3315	X3249	X3179
E4251	E4133	Q3946	E3717	E3717	X3707	X3438	X3438	X3376	X3316	X3250	X3180
E4251	E4133	Q3946	E3718	E3718	X3708	X3439	X3439	X3377	X3317	X3251	X3181
E4251	E4133	Q3946	E3719	E3719	X3709	X3440	X3440	X3378	X3318	X3252	X3182



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	0.110	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	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	0.20	0/834	0.47	0/1123
1	F	0.20	0/834	0.47	0/1123
1	H	0.20	0/834	0.47	0/1123
1	J	0.20	0/834	0.47	0/1123
2	B	0.21	0/25428	0.51	2/34534 (0.0%)
2	E	0.21	0/25428	0.51	2/34534 (0.0%)
2	G	0.21	0/25428	0.51	2/34534 (0.0%)
2	I	0.21	0/25428	0.51	2/34534 (0.0%)
All	All	0.21	0/105048	0.51	8/142628 (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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2291	GLN	CA-C-N	5.61	132.25	121.54
2	I	2291	GLN	C-N-CA	5.61	132.25	121.54
2	B	2291	GLN	CA-C-N	5.60	132.23	121.54
2	B	2291	GLN	C-N-CA	5.60	132.23	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2291	GLN	CA-C-N	5.59	132.22	121.54

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1720	LEU	Peptide
2	B	694	PRO	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	10	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24749	295	0
2	E	29499	0	24749	266	0
2	G	29499	0	24750	276	0
2	I	29499	0	24749	272	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	102293	1137	0

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

The worst 5 of 1137 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:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.28	1.20
2:B:4230:LYS:HD2	2:B:4959:PHE:HE2	0.99	1.10
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.92	1.04
2:B:4983:HIS:CE1	2:B:5027:CYS:SG	2.57	0.98
2:B:4230:LYS:CD	2:B:4959:PHE:HE2	1.87	0.87

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2894 (90%)	333 (10%)	8 (0%)	43	77
2	E	3235/4416 (73%)	2898 (90%)	332 (10%)	5 (0%)	43	77
2	G	3235/4416 (73%)	2896 (90%)	334 (10%)	5 (0%)	43	77
2	I	3235/4416 (73%)	2898 (90%)	332 (10%)	5 (0%)	43	77
All	All	13360/18096 (74%)	11962 (90%)	1375 (10%)	23 (0%)	44	77

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4962	GLY
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG

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Mol	Chain	Res	Type
2	E	1708	ARG

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%)	2479 (99%)	14 (1%)	78	80
2	E	2493/3022 (82%)	2484 (100%)	9 (0%)	84	82
2	G	2493/3022 (82%)	2484 (100%)	9 (0%)	84	82
2	I	2493/3022 (82%)	2485 (100%)	8 (0%)	86	84
All	All	10324/12444 (83%)	10284 (100%)	40 (0%)	81	82

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	2144	ILE
2	E	1676	LEU
2	I	3663	LEU
2	E	719	LEU
2	E	3663	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 242 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	4120	ASN
2	E	3704	HIS
2	I	1611	HIS
2	E	2772	GLN

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Mol	Chain	Res	Type
2	E	4806	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	G	14
2	B	14

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Mol	Chain	Number of breaks
2	I	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	G	4345:UNK	C	4540:PHE	N	73.65
1	B	4345:UNK	C	4540:PHE	N	73.61
1	I	4345:UNK	C	4540:PHE	N	73.61
1	E	4345:UNK	C	4540:PHE	N	73.59
1	G	3613:UNK	C	3639:THR	N	45.21

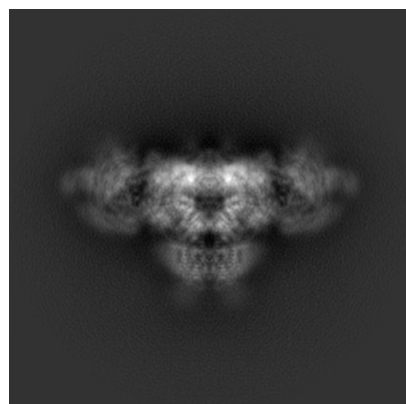
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8387. These allow visual inspection of the internal detail of the map and identification of artifacts.

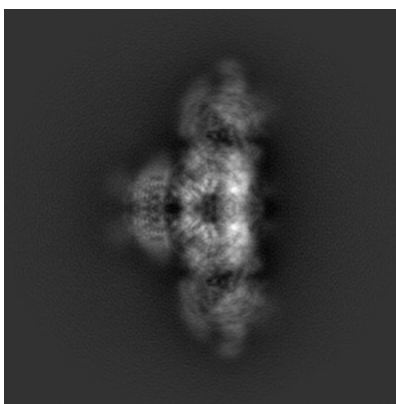
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

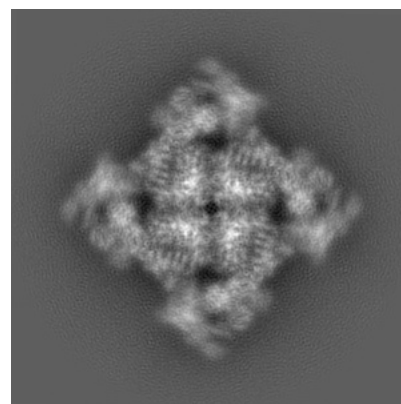
6.1.1 Primary map



X

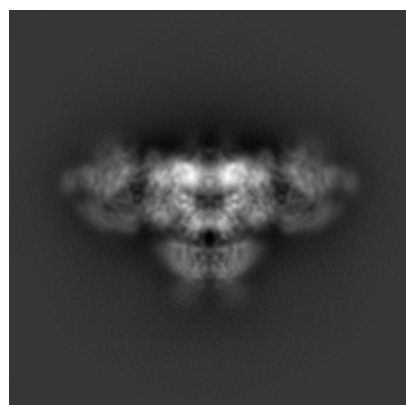


Y

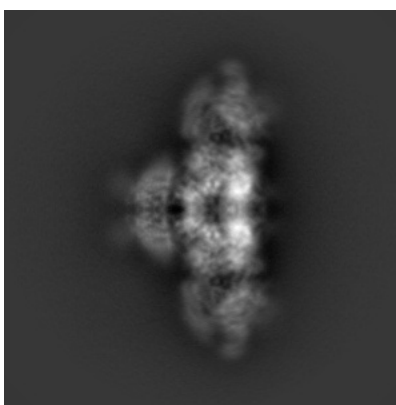


Z

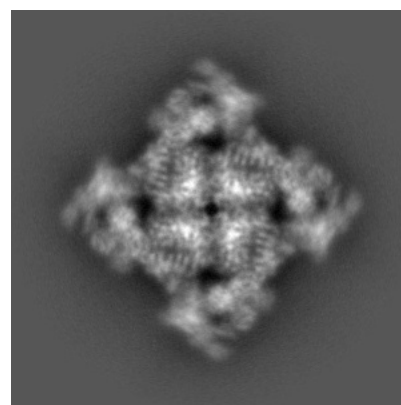
6.1.2 Raw map



X



Y

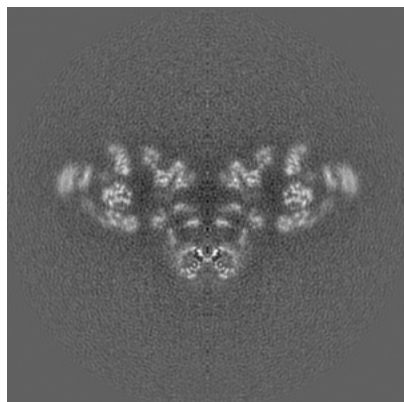


Z

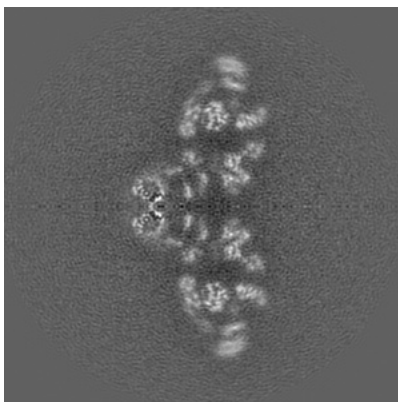
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

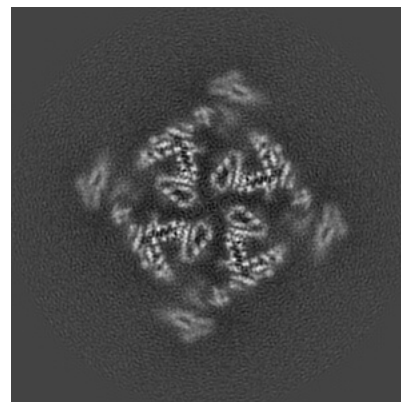
6.2.1 Primary map



X Index: 200

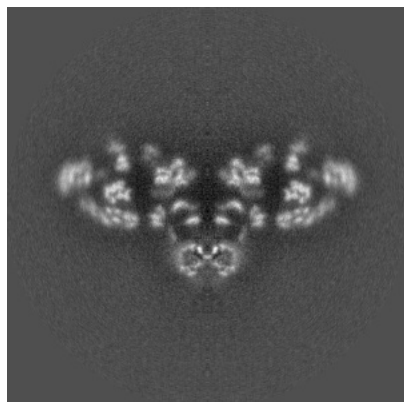


Y Index: 200

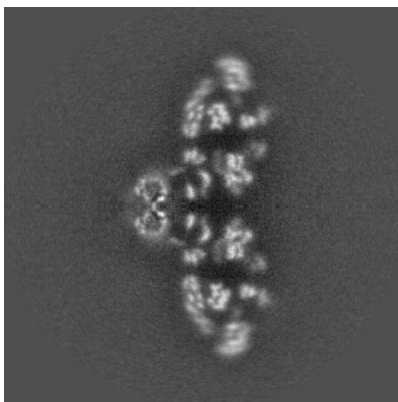


Z Index: 200

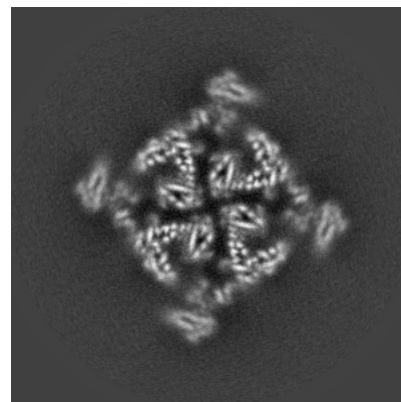
6.2.2 Raw map



X Index: 200



Y Index: 200

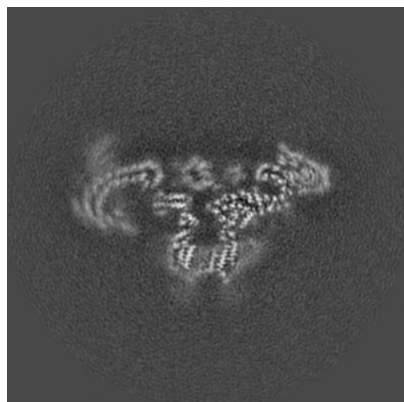


Z Index: 200

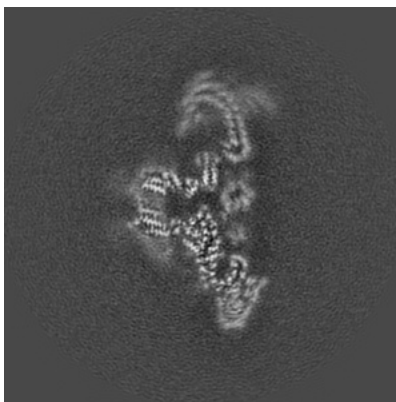
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

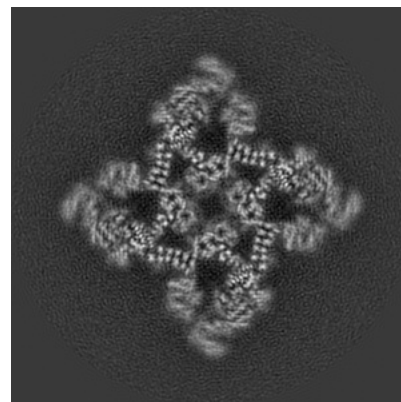
6.3.1 Primary map



X Index: 175

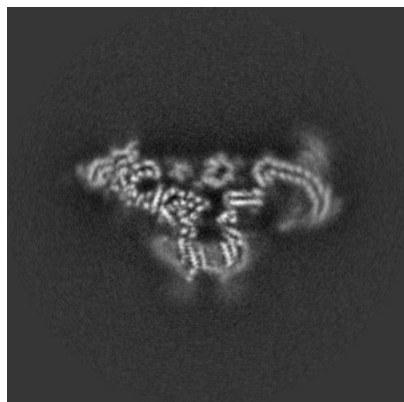


Y Index: 175

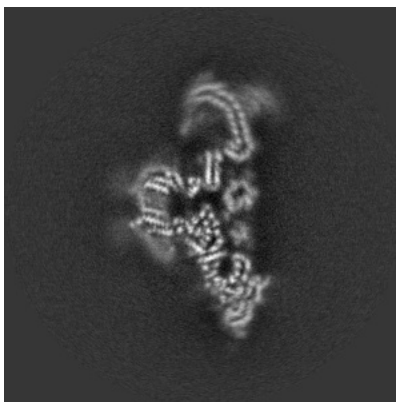


Z Index: 227

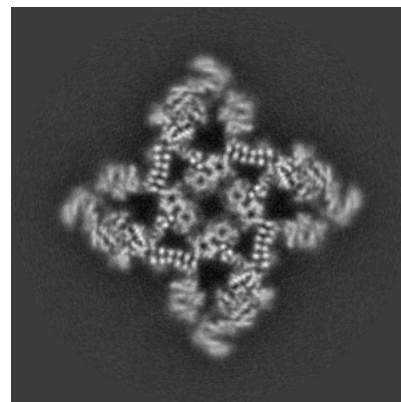
6.3.2 Raw map



X Index: 225



Y Index: 175

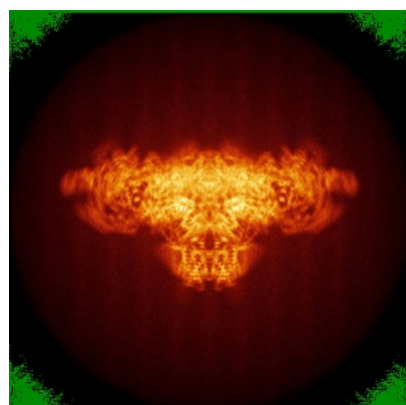


Z Index: 229

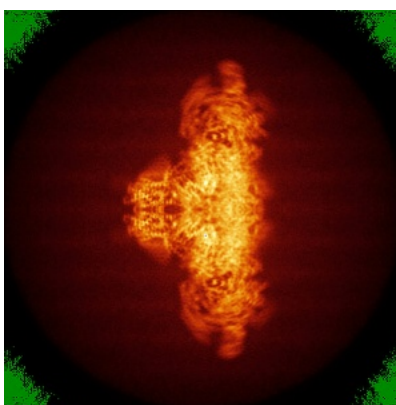
The images above show the largest variance slices of the map in three orthogonal directions.

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

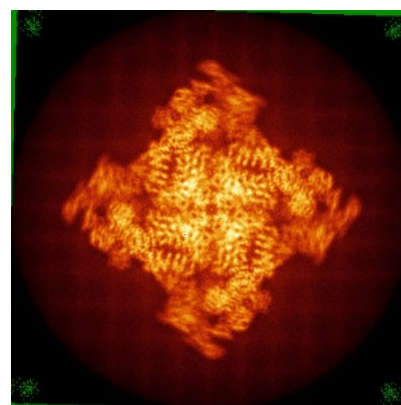
6.4.1 Primary map



X



Y

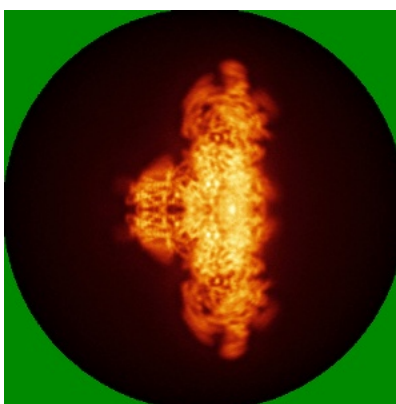


Z

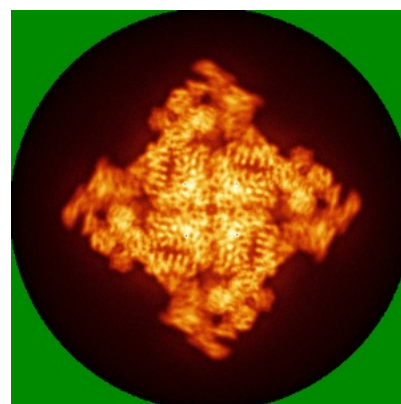
6.4.2 Raw map



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](#)

This section was not generated.

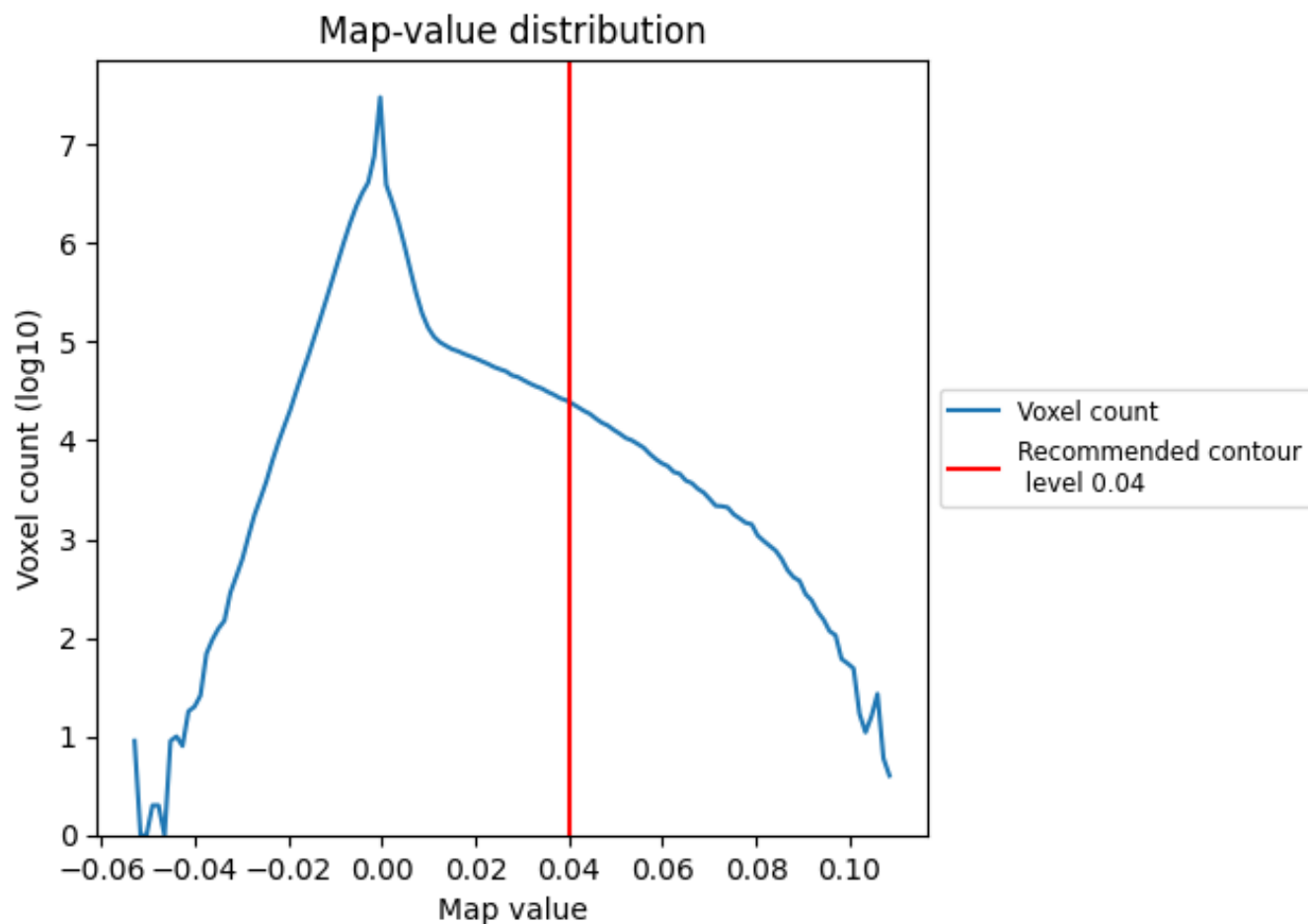
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

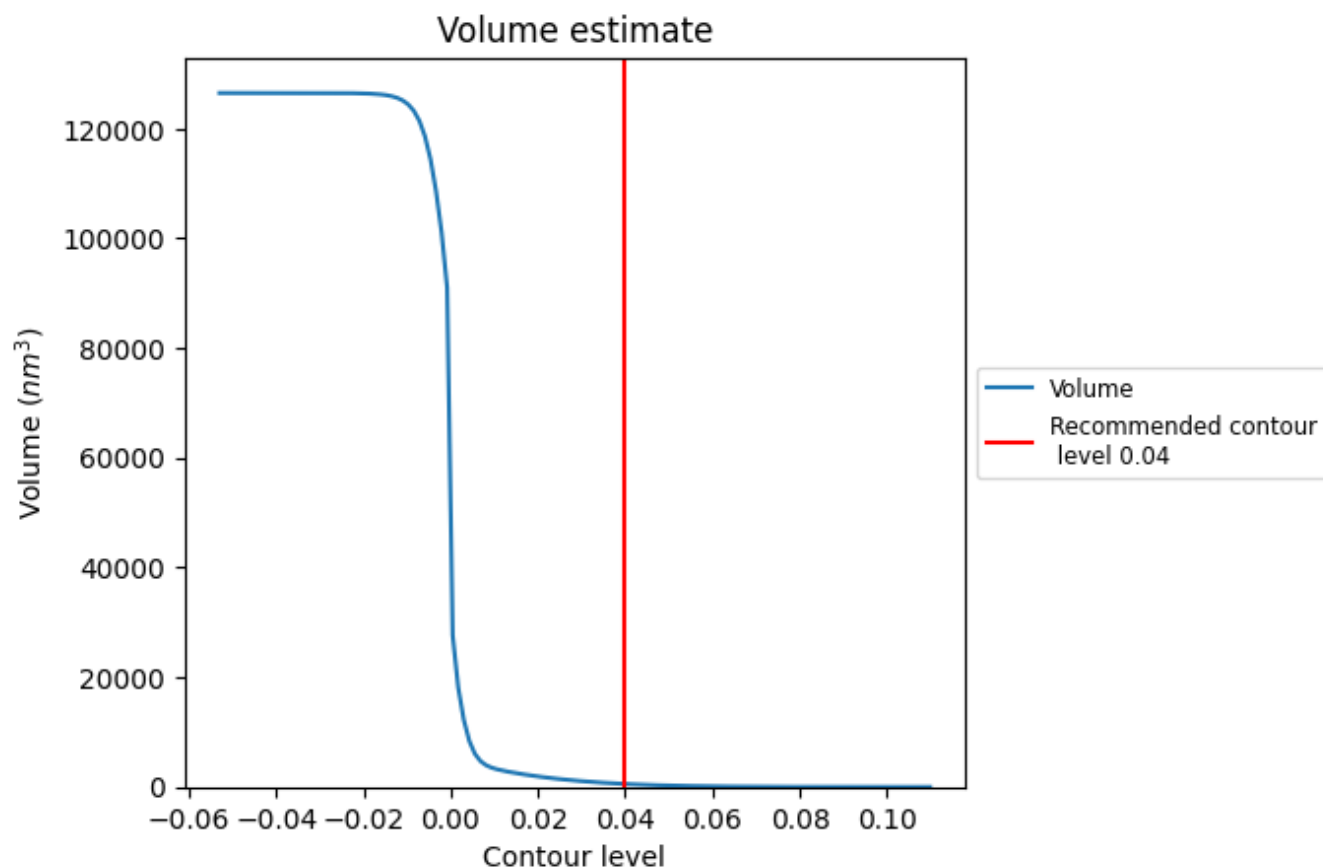
This section contains the results of statistical analysis of the map.

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.

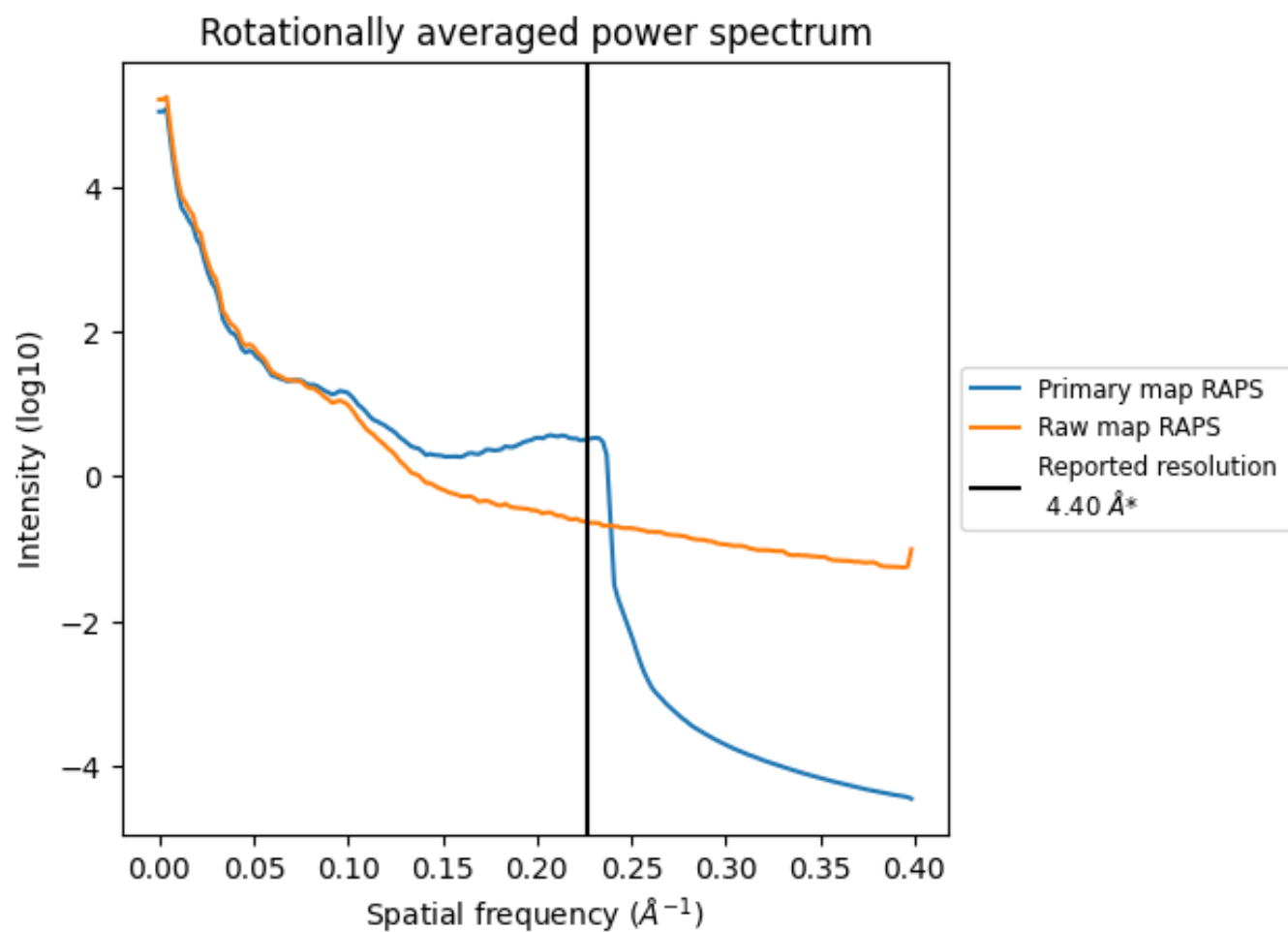
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547 nm³; this corresponds to an approximate mass of 494 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 ⓘ

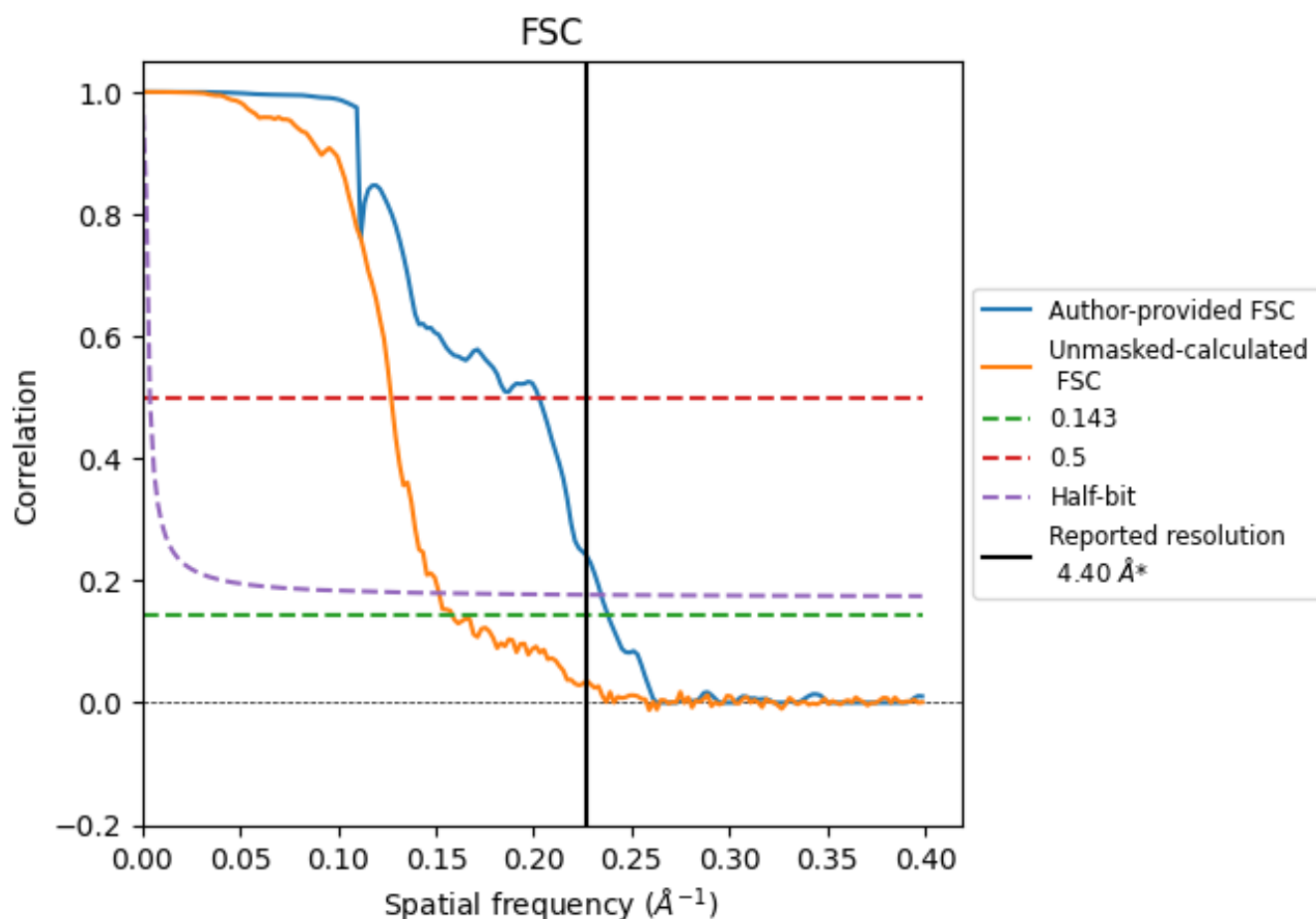


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.20	4.94	4.27
Unmasked-calculated*	6.31	7.87	6.60

*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 6.31 differs from the reported value 4.4 by more than 10 %

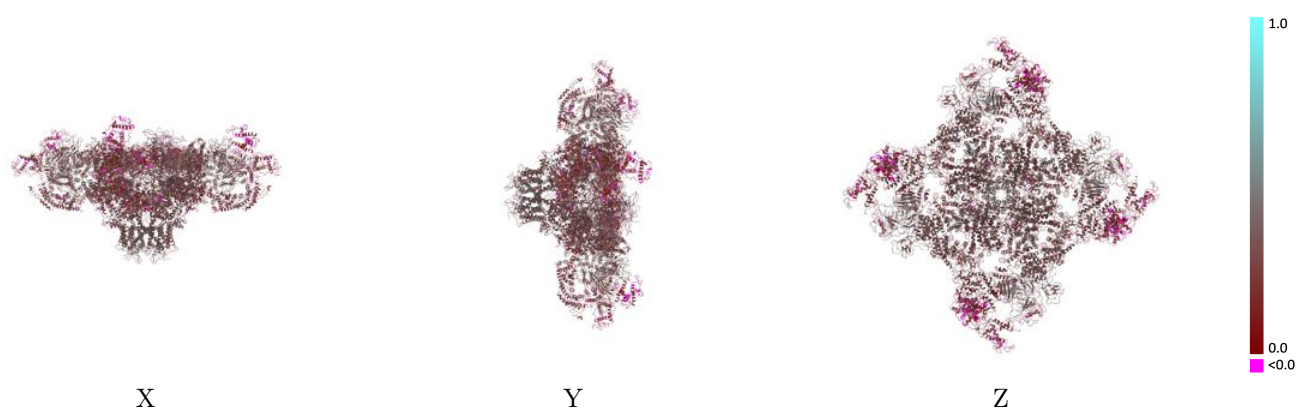
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8387 and PDB model 5TAW. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)

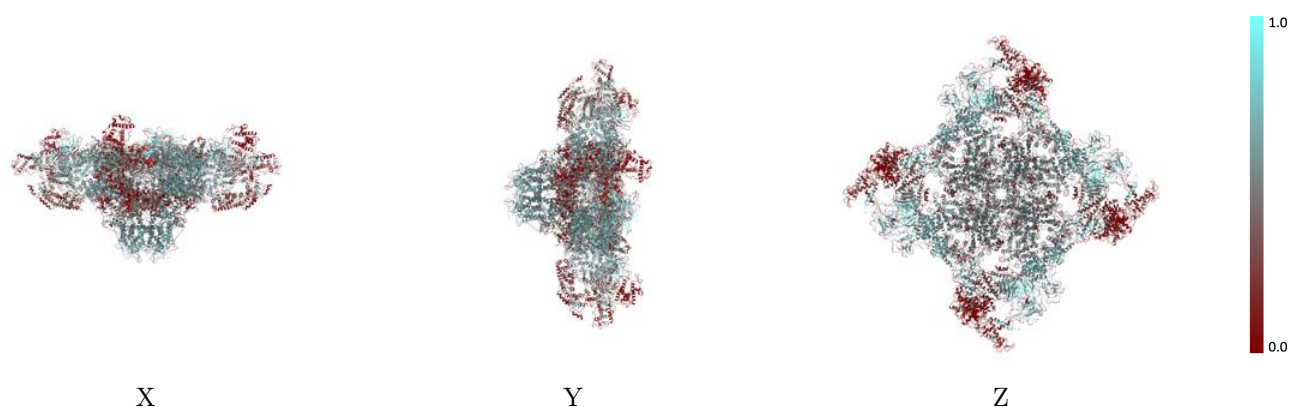
This section was not generated.

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



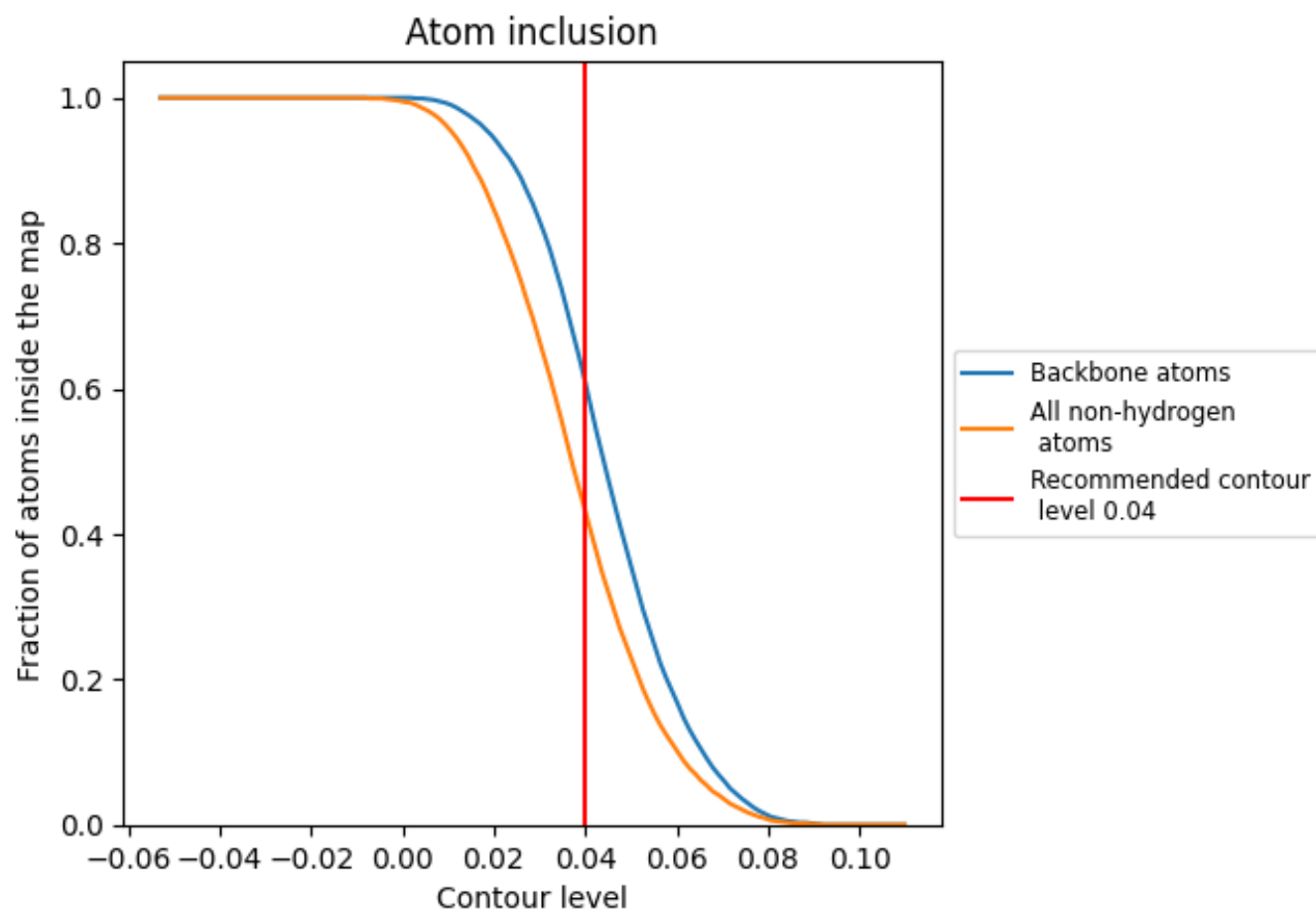
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 43% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4320	0.2790
A	0.4970	0.3250
B	0.4300	0.2780
E	0.4300	0.2780
F	0.4940	0.3290
G	0.4310	0.2780
H	0.4950	0.3280
I	0.4300	0.2780
J	0.4990	0.3270

