wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 05:59 AM EDT

PDB ID	:	5TAV
EMDB ID	:	EMD-8386
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.80 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:

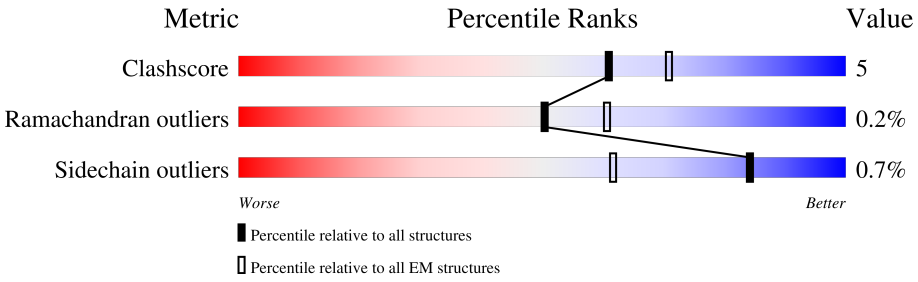
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	32% 92% 7% ·
1	F	108	31% 91% 8% ·
1	H	108	31% 92% 7% ·
1	J	108	31% 93% 6% ·
2	B	4416	39% 84% 10% 5%
2	E	4416	39% 84% 10% 5%
2	G	4416	39% 85% 10% 5%
2	I	4416	39% 84% 10% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

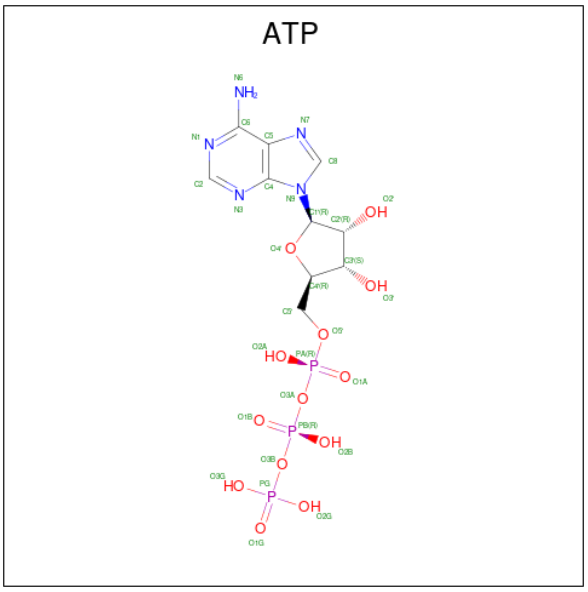
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

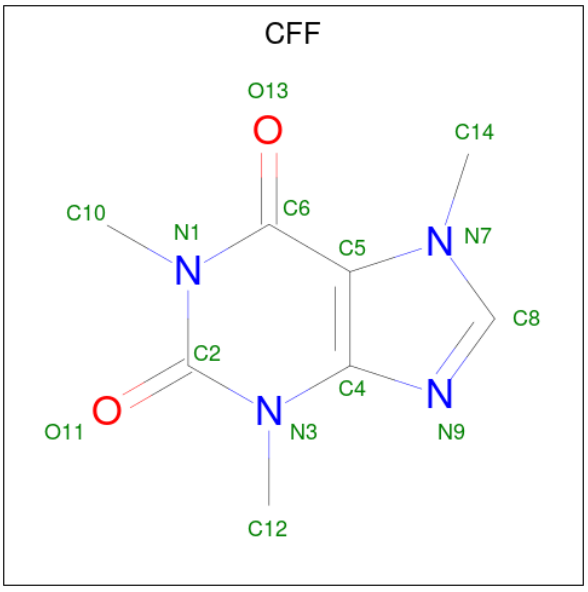
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

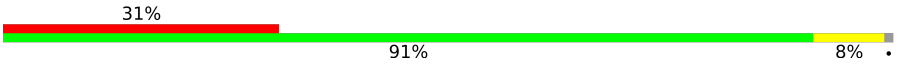
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	

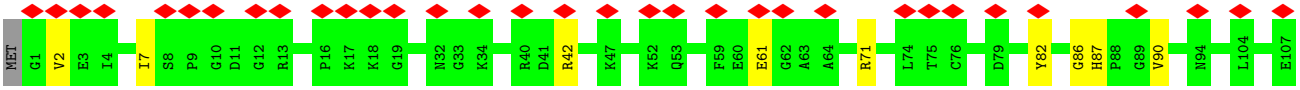
3 Residue-property plots (i)

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

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

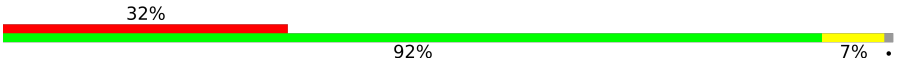
Chain F:

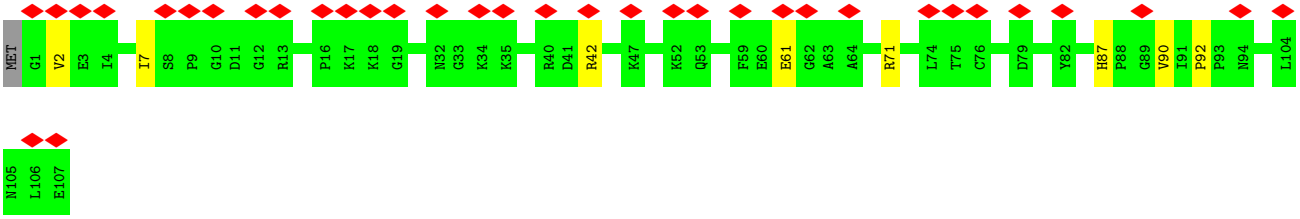




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

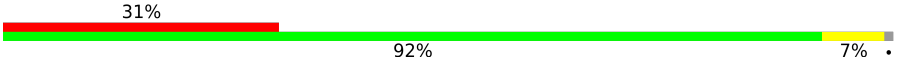
Chain A:

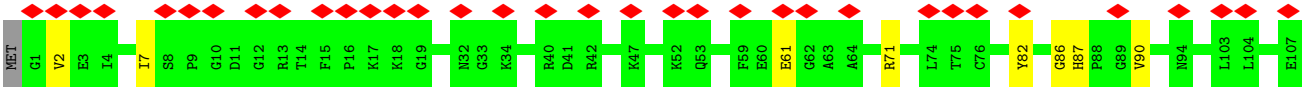




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

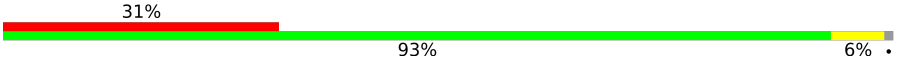
Chain H:

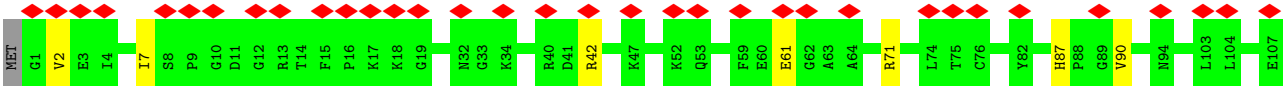




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

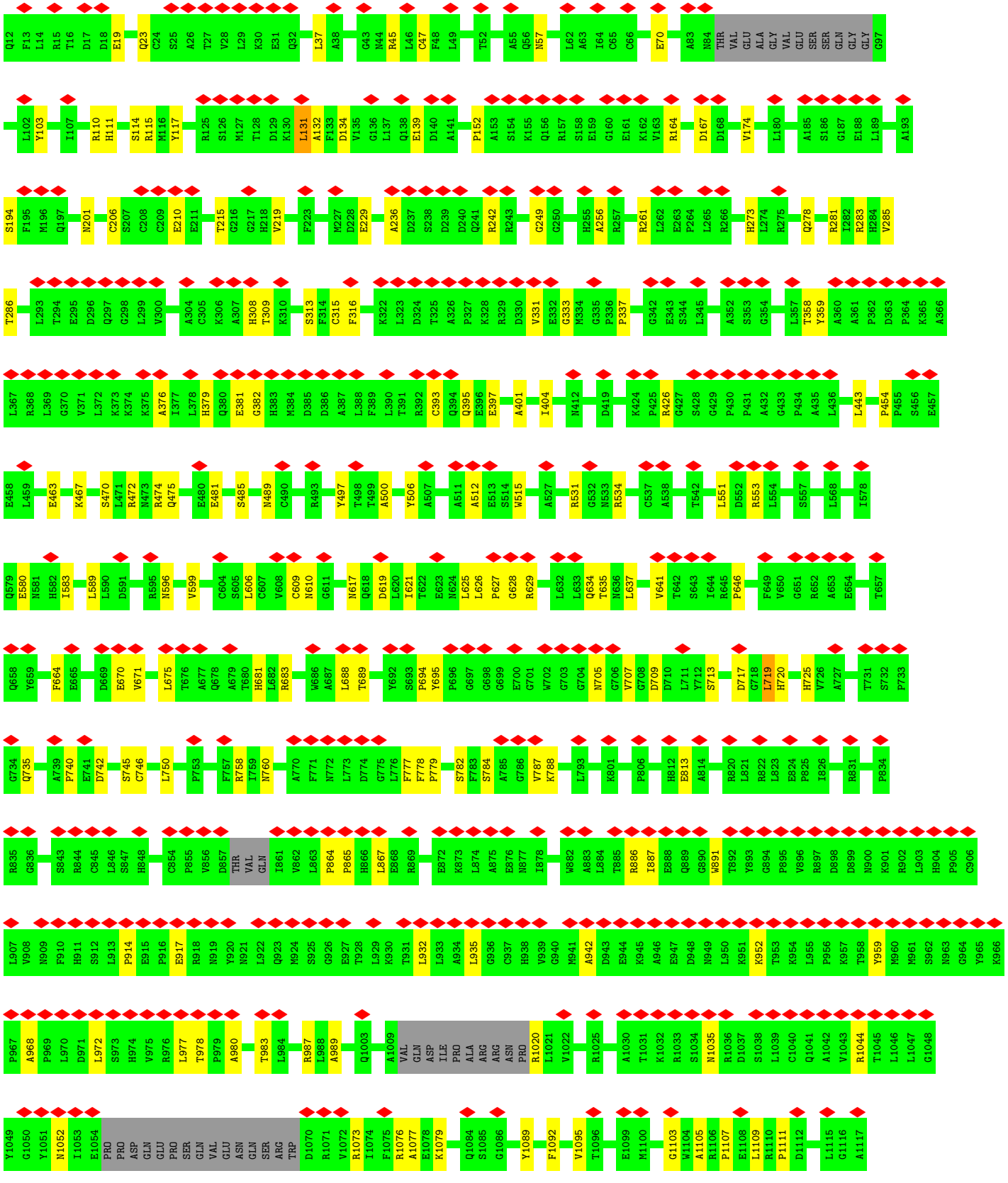
Chain J:





• Molecule 2: Ryanodine receptor 1

Chain B: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L102 Y103 I107 R110 H111 S114 R115 M116 Y117 R125 S126 M127 T128 D129 K130 L131 A132 F133 D134 V135 G136 L137 Q138 E139 D140 A141 P152 A153 S154 K155 Q156 R157 S158 E159 G160 E161 K162 V163 R164 D167 D168 V174 L180 A185 S186 G187 E188 L189 A193
S194 F195 M196 Q197 N201 C206 S207 C208 C209 E210 E211 T215 G216 G217 H218 V219 F223 M227 D228 E229 A236 D237 S238 D239 D240 Q241 R242 R243 G249 G250 H255 A256 R257 R261 L262 E263 P264 L265 R266 H273 L274 R275 Q278 R281 I282 R283 H284 V285
T286 L293 T294 E295 D296 Q297 G298 L299 V300 A304 C305 K306 A307 H308 T309 K310 S313 F314 C315 F316 K322 L323 D324 T325 A326 P327 K328 R329 D330 V331 E332 G333 M334 G335 P336 P337 G342 E343 S344 L345 A352 S353 G354 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366
L367 R368 L369 G370 V371 L372 K373 K374 K375 A376 I377 L378 H379 Q380 E381 G382 H383 M384 D385 D386 A387 L388 F389 L390 T391 R392 C393 Q394 Q395 E396 E397 A401 I404 N412 D419 K424 P425 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 L436 L443 P454 P455 S456 E457
E458 L459 E463 K467 S470 L471 R472 N473 R474 Q475 E480 E481 S485 N489 C490 R493 Y497 T498 T499 A500 Y506 A507 A511 A512 E513 S514 W515 A527 R531 G532 N533 R534 C537 A538 T542 L551 D552 R553 L554 S557 L568 I578
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Q658 Y659 F664 E665 D669 E670 V671 L675 T676 A677 Q678 A679 T680 H681 L682 R683 W686 A687 L688 T689 Y692 S693 P694 Y695 P696 G697 G698 G699 E700 G701 W702 G703 G704 N705 G706 V707 G708 D709 D710 L711 Y712 S713 D717 G718 L719 H720 H725 V726 A727 T731 S732 P733
G734 Q735 A739 P740 E741 D742 S745 C746 L750 P753 F757 R758 I759 N760 A770 F771 N772 L773 D774 G775 L776 F777 F778 P779 S782 F783 S784 A785 G786 V787 K788 L793 K801 P806 H812 E813 A814 R820 L821 R822 L823 E824 P825 I826 R831 P834
R835 G836 S843 R844 C845 L846 S847 H848 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 E872 K873 L874 A875 E876 N877 I878 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906
L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966
P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 T983 L984 R987 L988 A989 Q1003 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 R1025 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048
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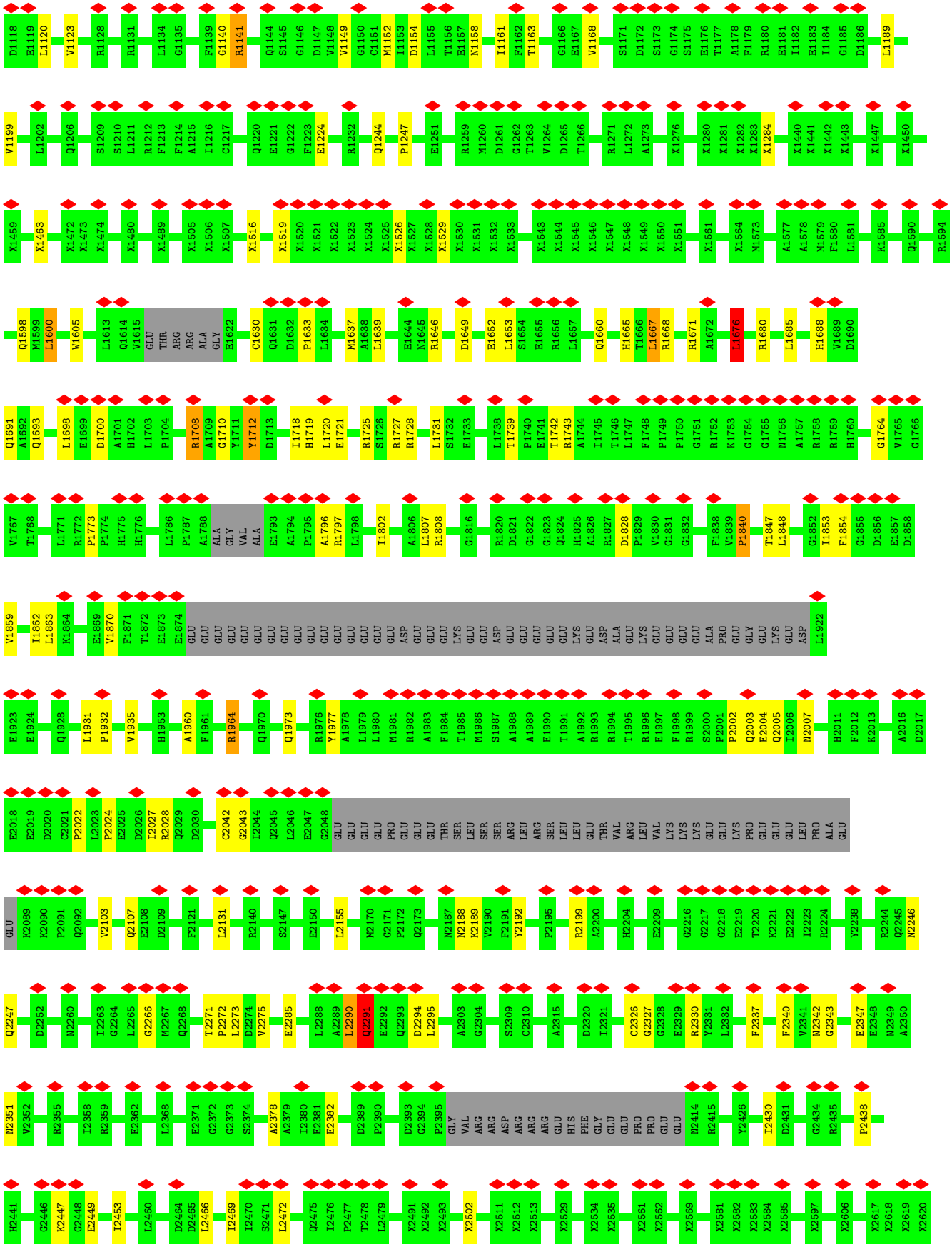

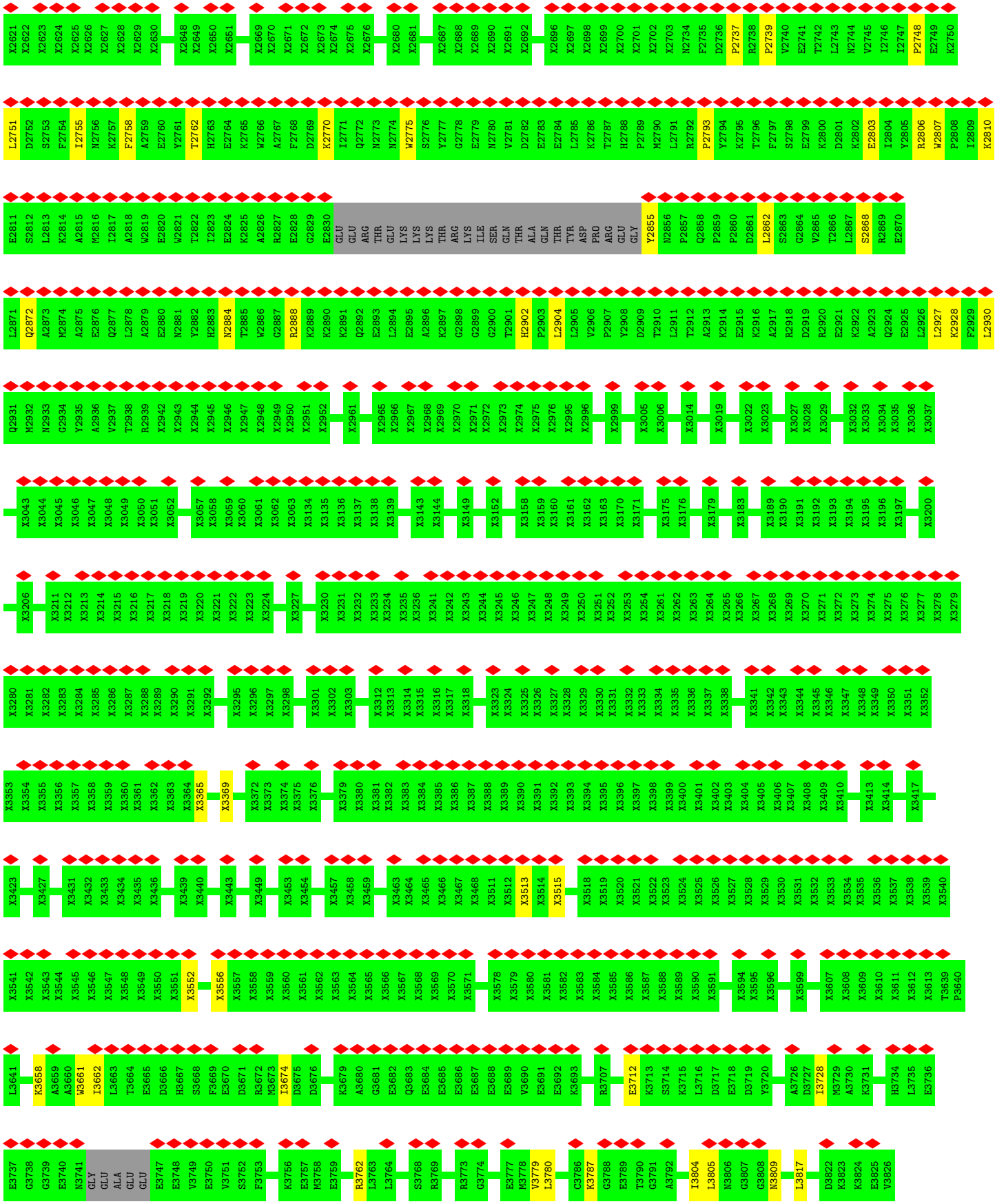
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E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870
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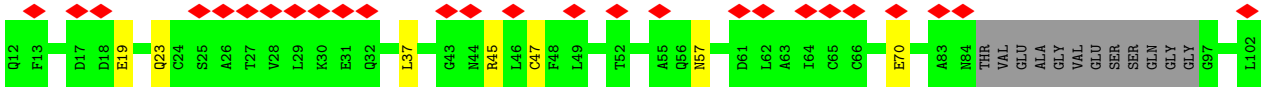
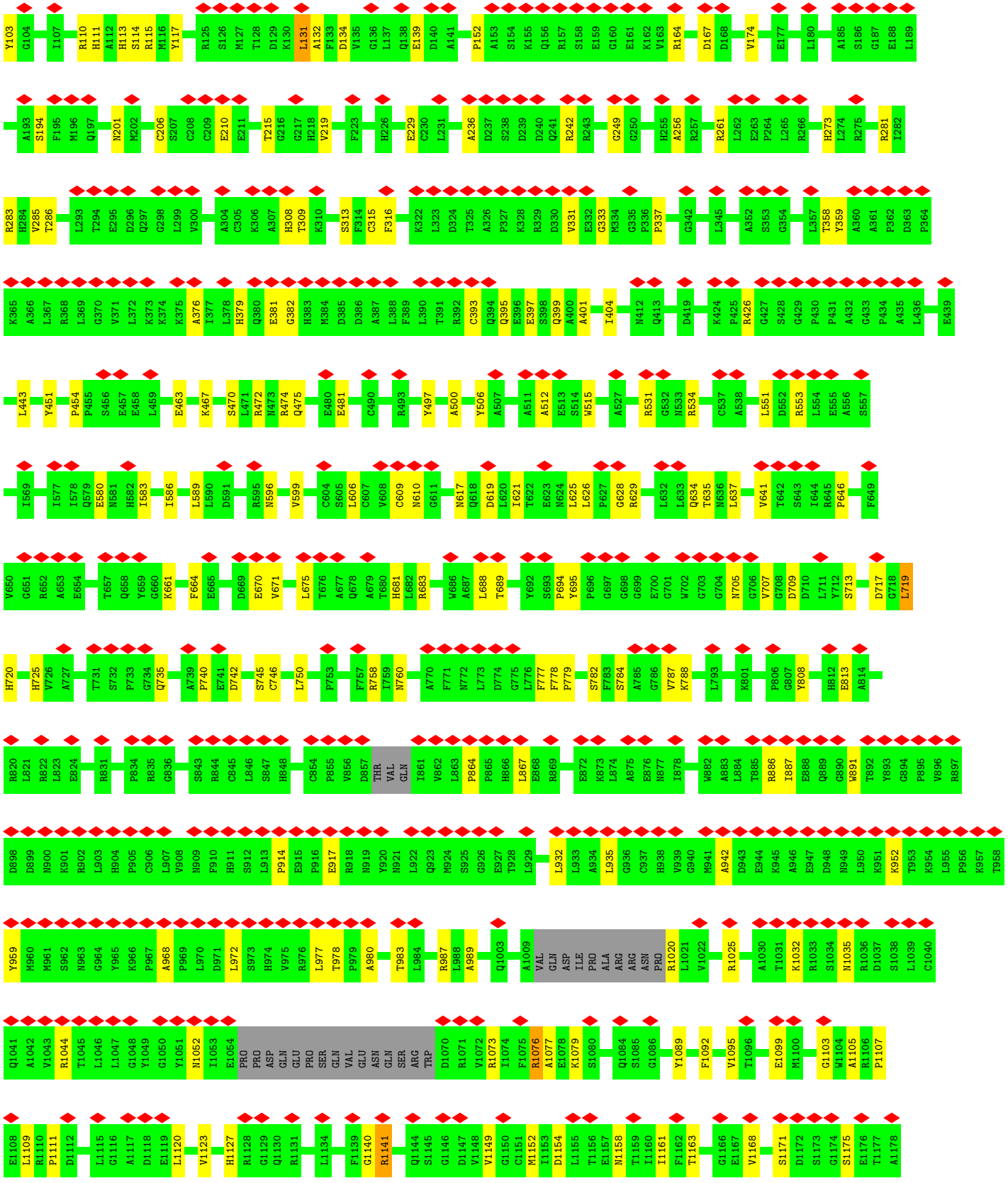
E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 K3756 E3757 M3758 E3759 R3762 L3763 L3764 S3768 R3769 R3773 G3774 E3777 M3778 V3779 L3780 C3786 K3787 G3788 E3789 T3790 G3791 A3792 I3804 L3805 N3806 G3807 G3808 N3809 L3817 D3822 K3823 K3824 E3825 V3826

• Molecule 2: Ryanodine receptor 1

Chain E:

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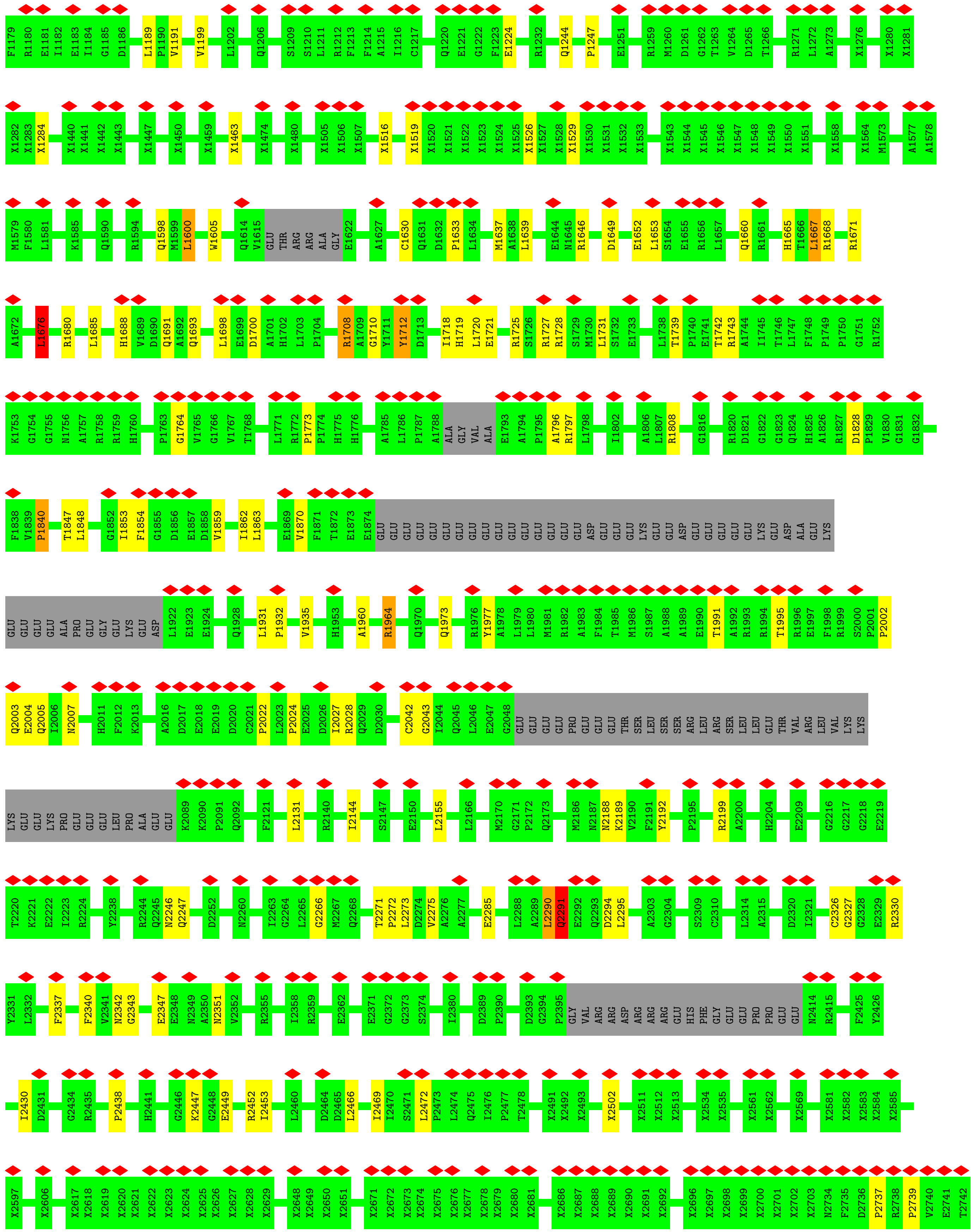
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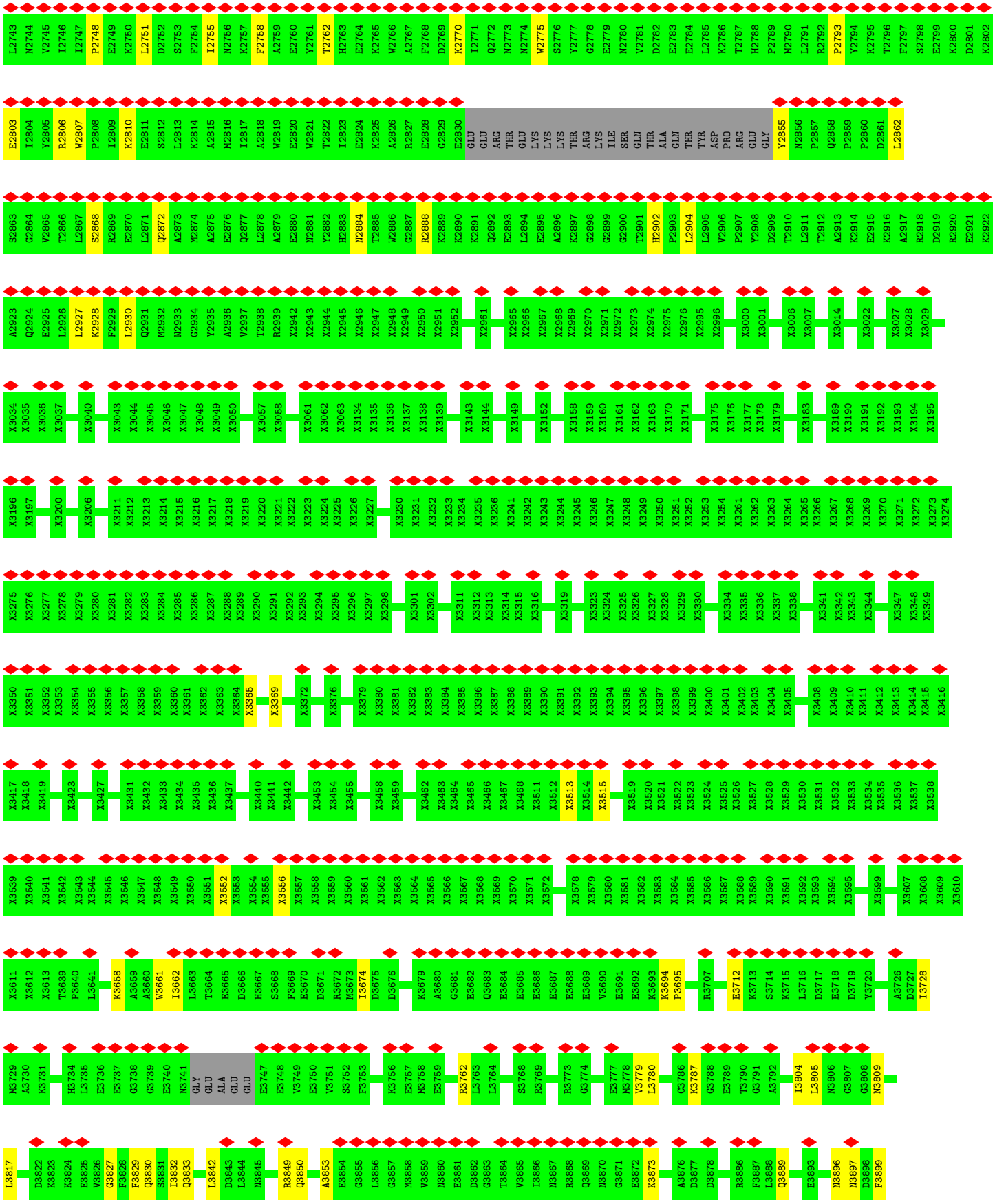
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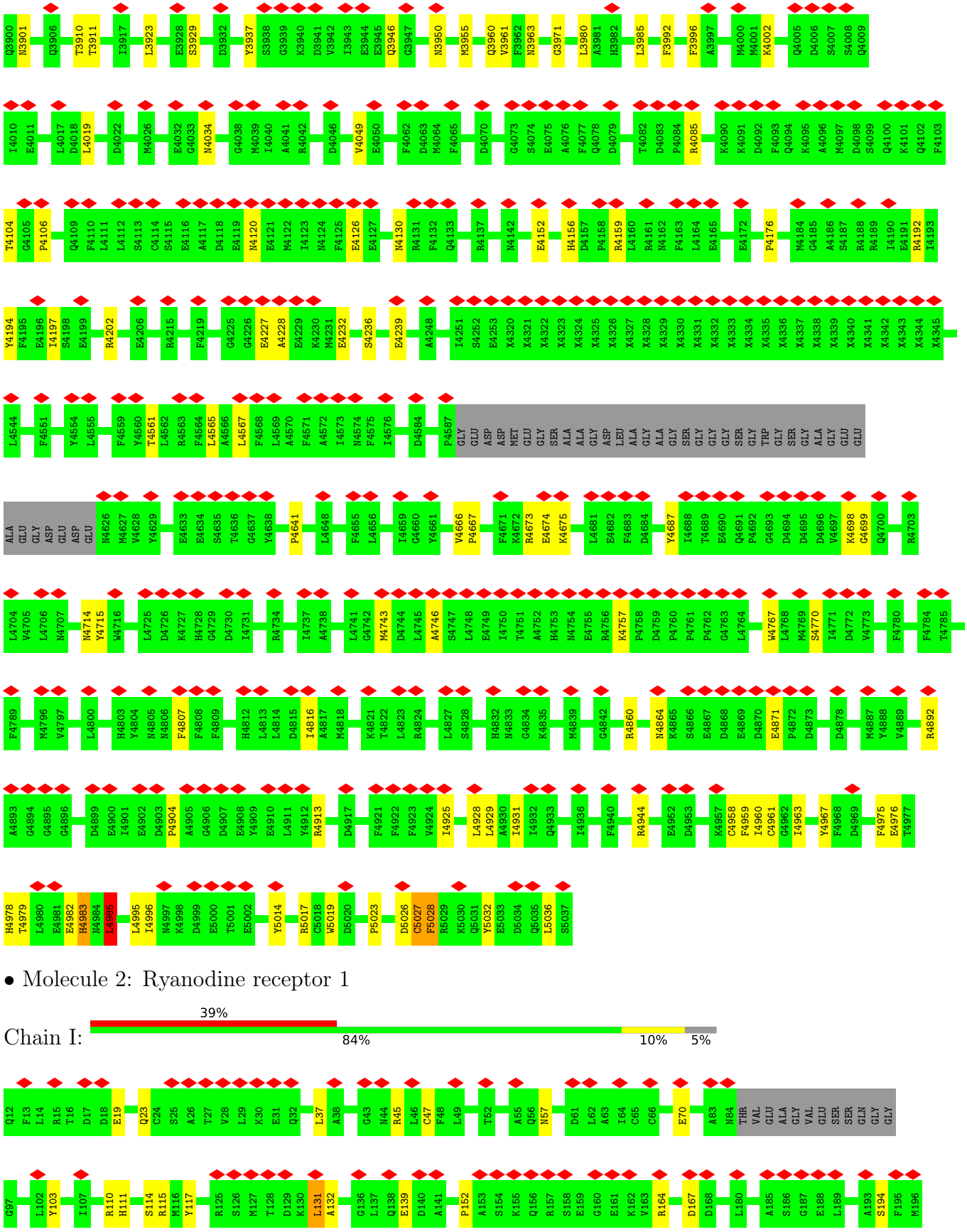
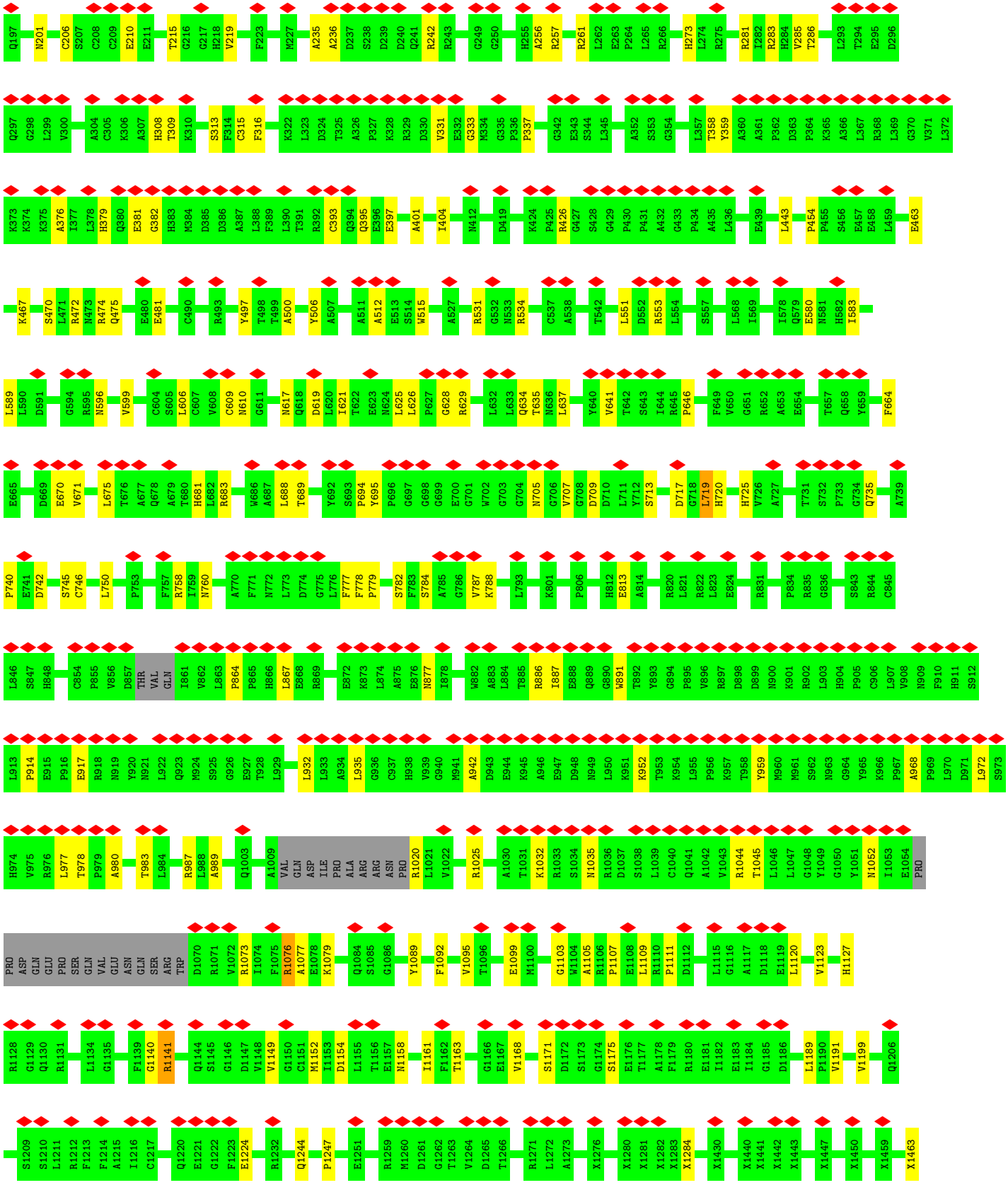


• Molecule 2: Ryanodine receptor 1

Chain I: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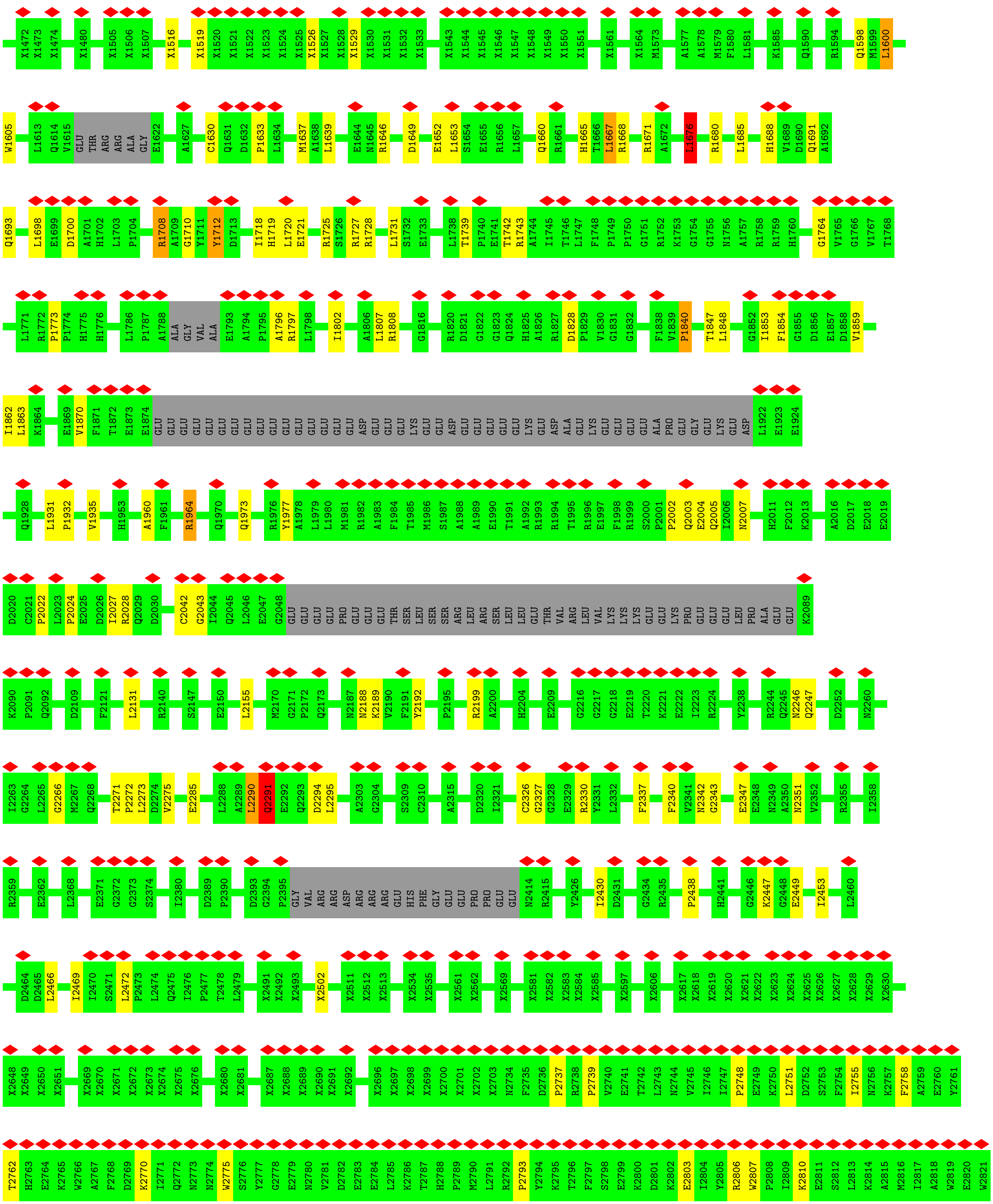
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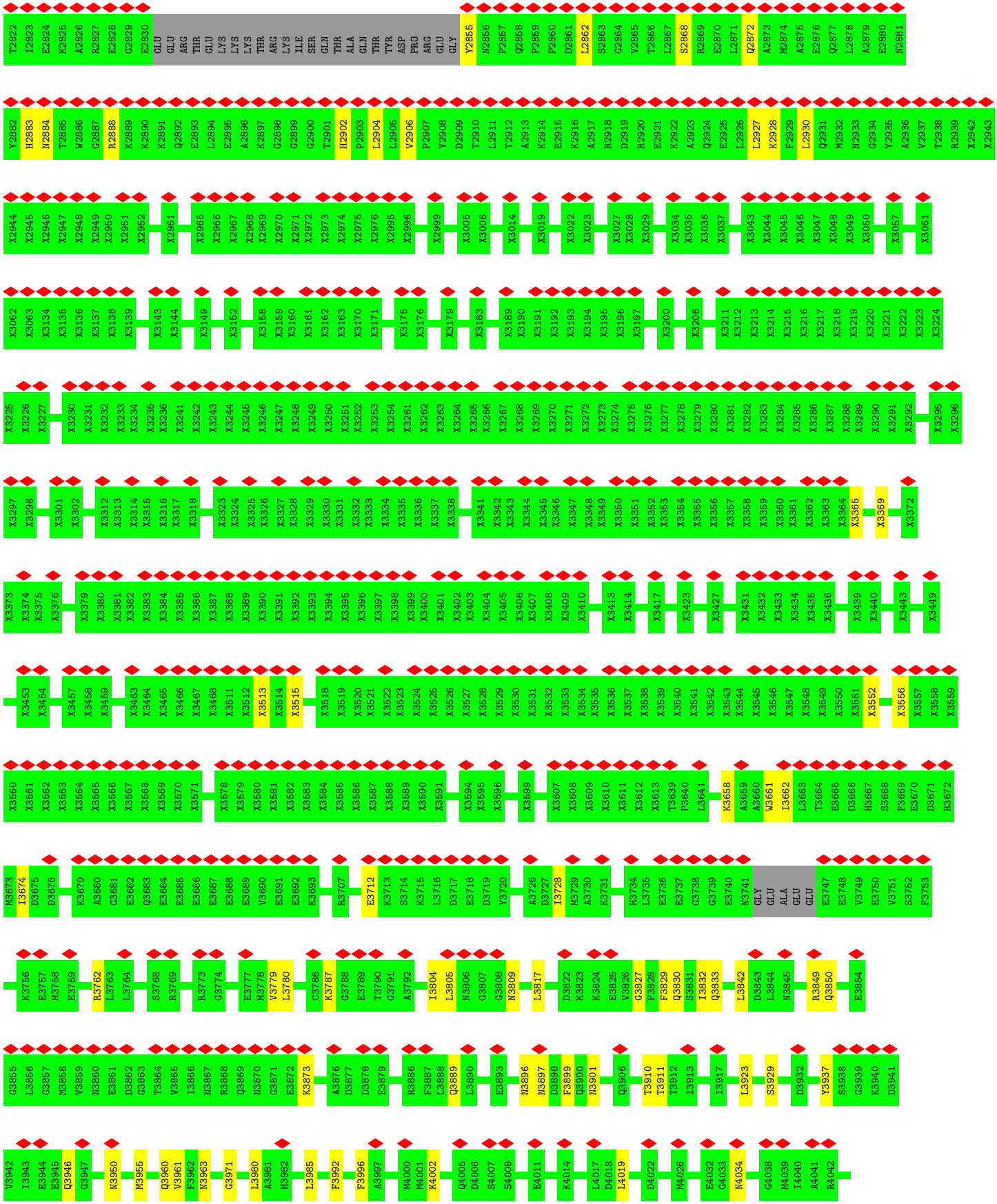
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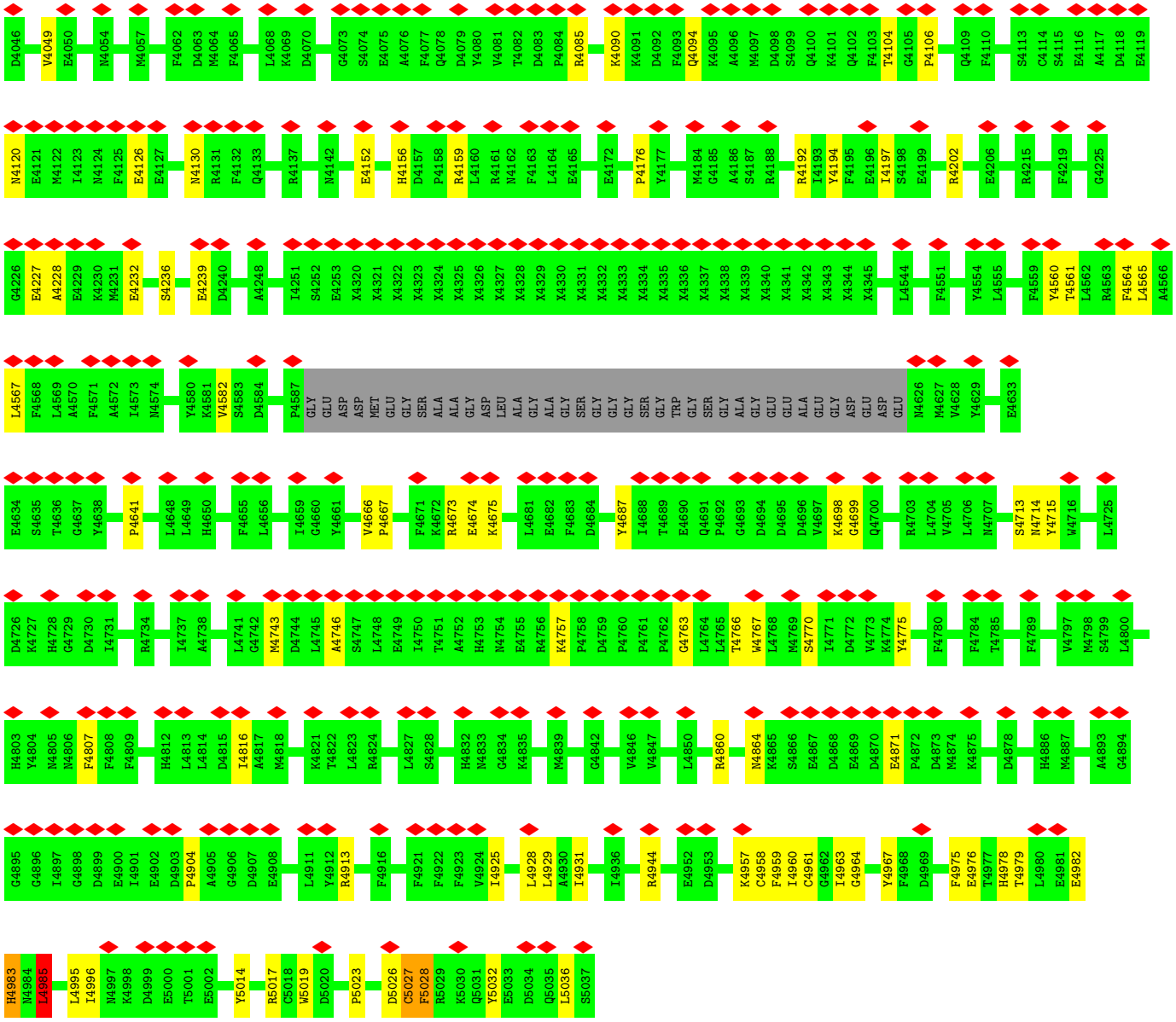

• Molecule 2: Ryanodine receptor 1

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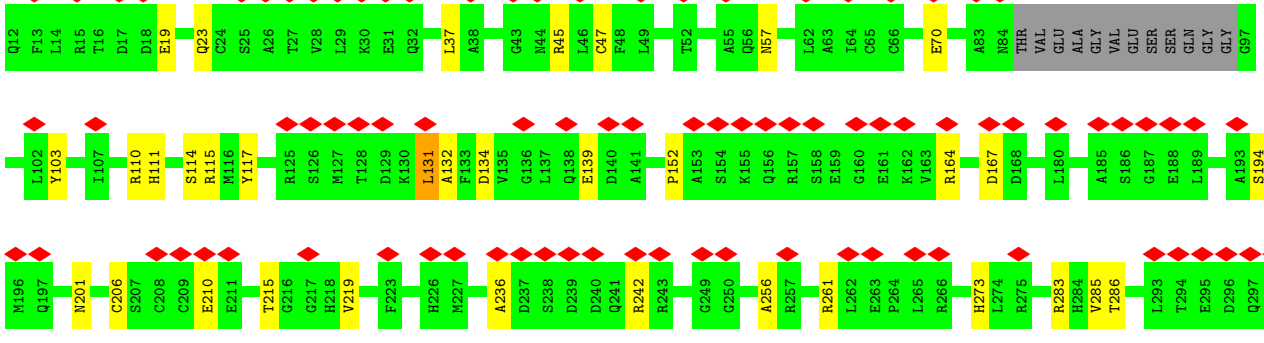

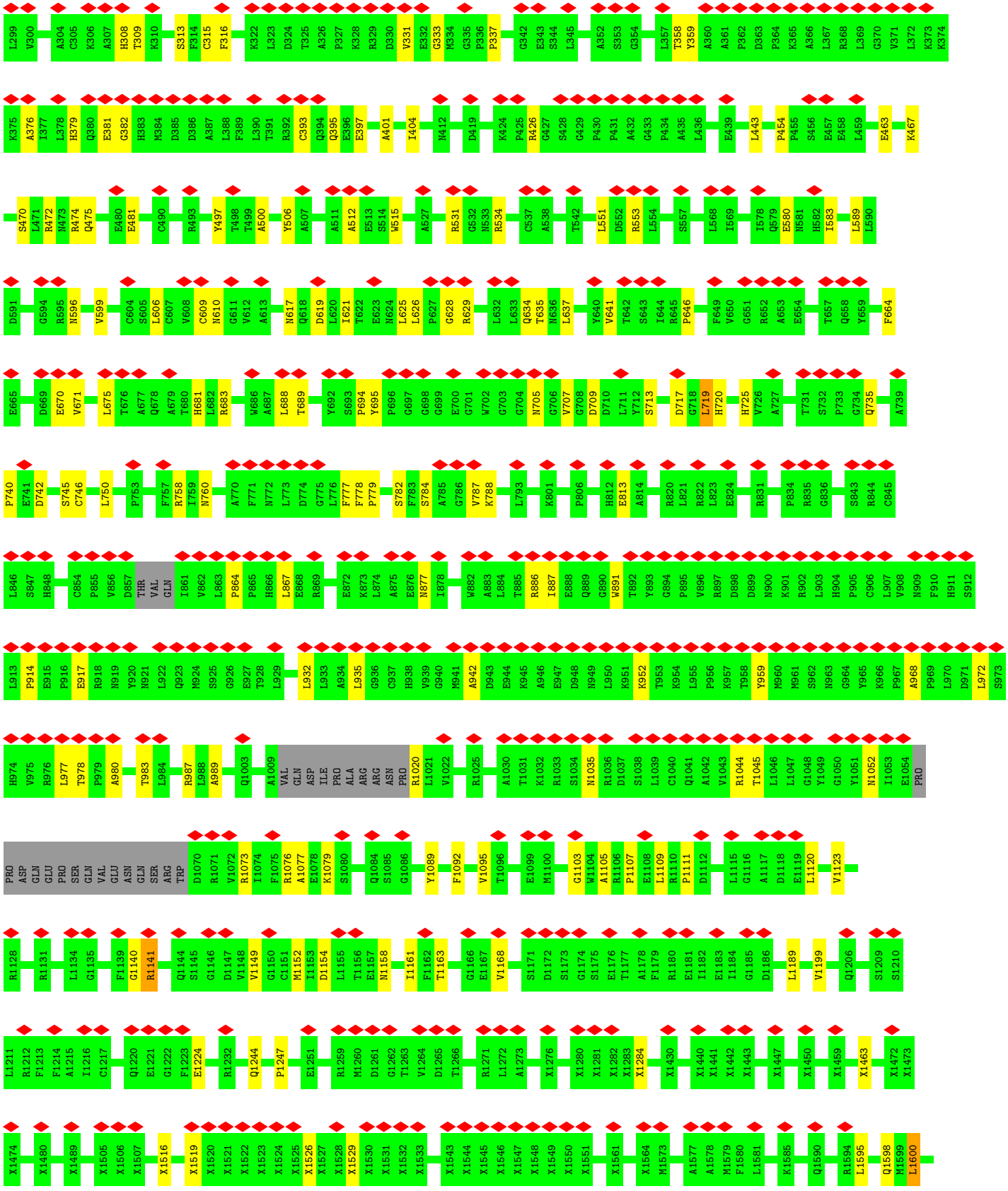
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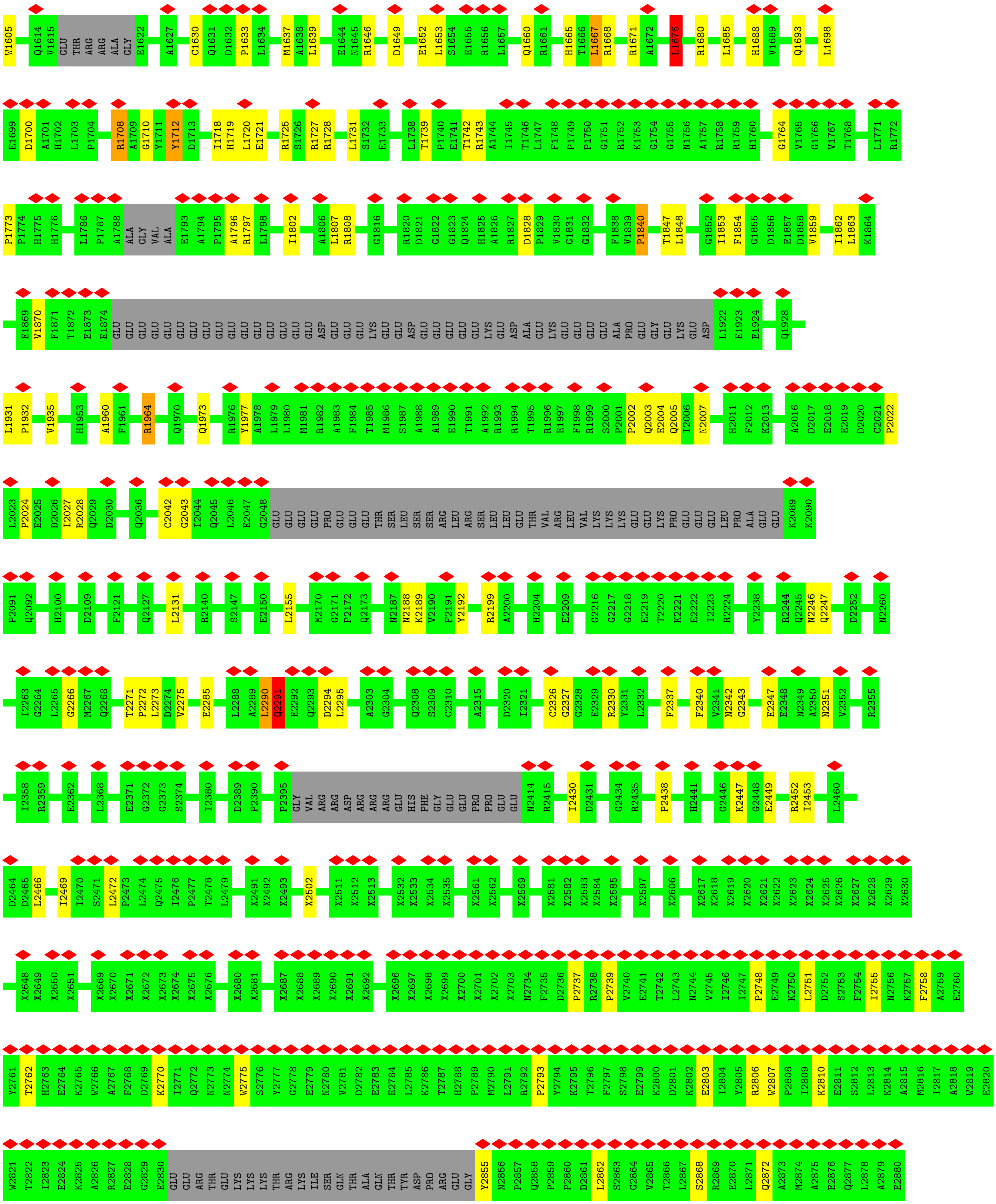
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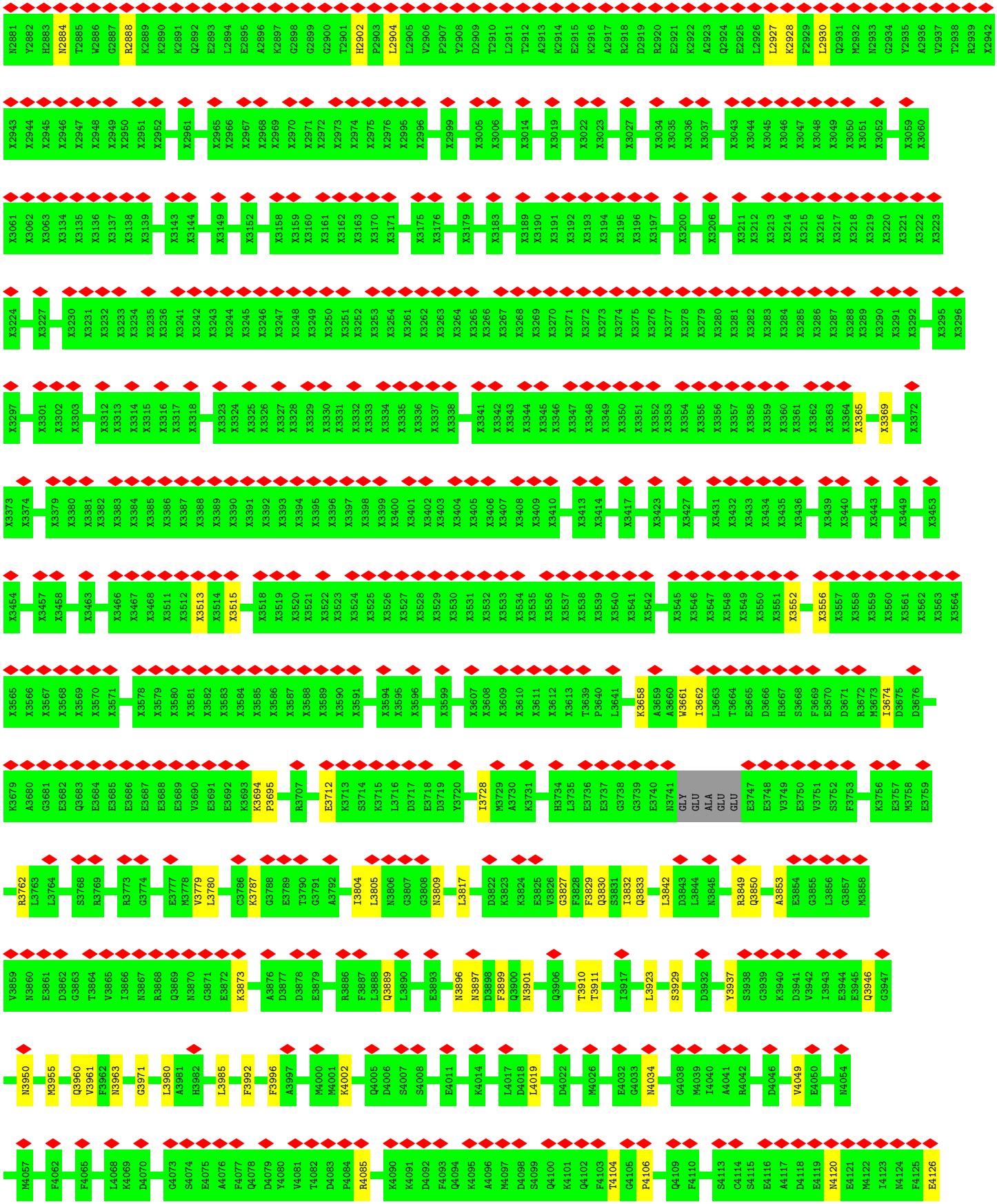
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X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2961 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2995 X2996 X2999 X3005 X3006 X3014 X3019 X3022 X3023 X3027 X3034 X3035 X3036 X3037 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3051 X3052 X3059 X3060
X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3139 X3143 X3144 X3149 X3152 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3175 X3176 X3179 X3183 X3189 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3206 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223
X3224 X3227 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3295 X3296
X3297 X3301 X3302 X3303 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3323 X3324 X3325 X3326 X3327 X3328 X3329 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3341 X3342 X3343 X3344 X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3369 X3372
X3373 X3374 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3413 X3414 X3417 X3423 X3427 X3431 X3432 X3433 X3434 X3435 X3436 X3439 X3440 X3443 X3449 X3453
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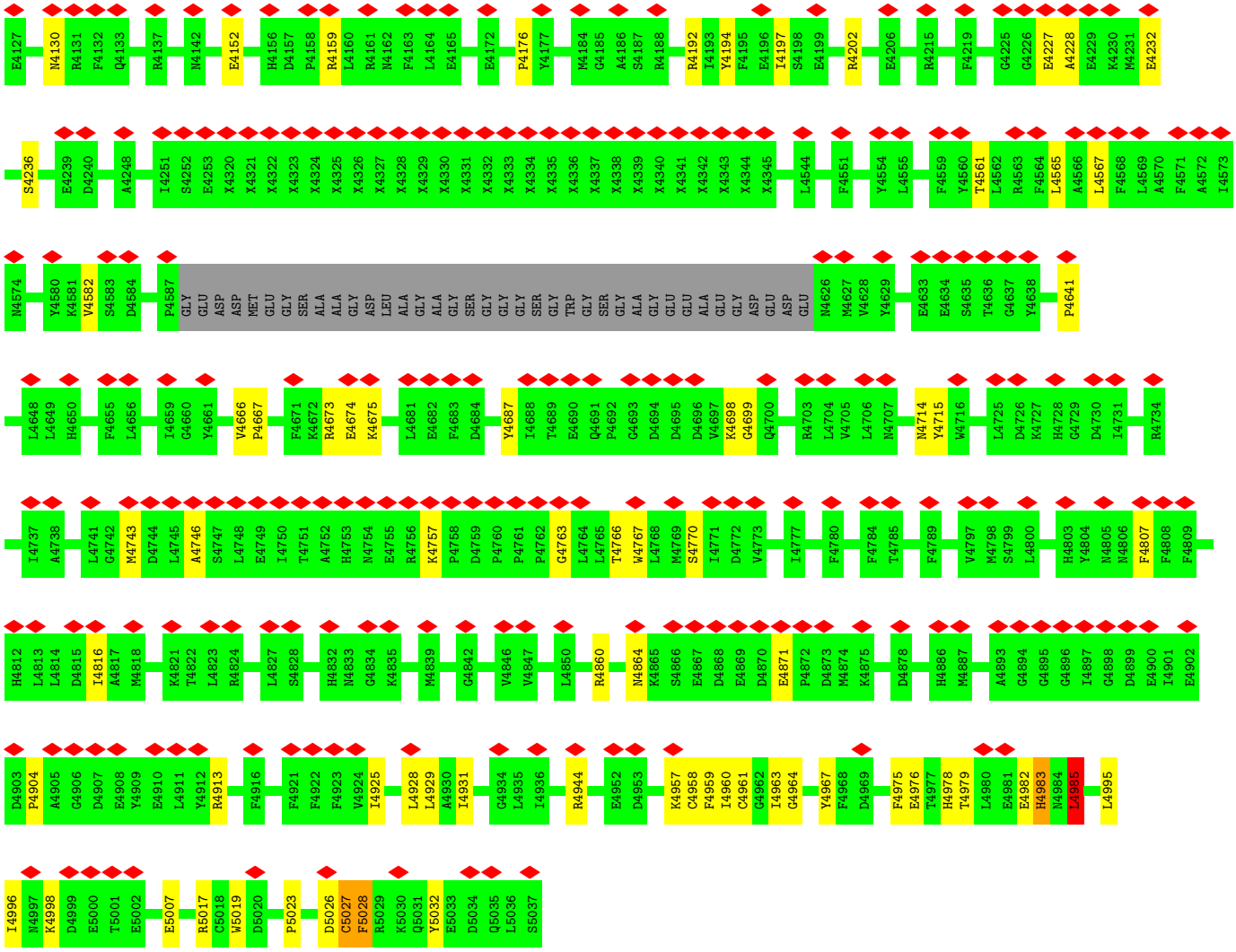
K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695 R3707 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 I3728 M3729 A3730 K3731 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 K3756 E3757 M3758 E3759
R3762 L3763 L3764 S3768 R3769 R3773 G3774 E3777 M3778 V3779 L3780 C3786 K3787 G3788 E3789 T3790 G3791 A3792 I3804 L3805 N3806 G3807 G3808 N3809 L3817 D3822 K3823 K3824 E3825 V3826 G3827 F3828 F3829 Q3830 S3831 I3832 Q3833 L3842 D3843 L3844 N3845 R3849 Q3850 A3853 E3854 G3855 L3856 G3857 M3858
V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 A3876 D3877 D3878 E3879 R3886 F3887 L3888 Q3889 L3890 E3893 N3896 N3897 D3898 F3899 Q3900 N3901 Q3906 T3910 T3911 I3917 L3923 S3929 D3932 Y3937 S3938 G3939 K3940 D3941 V3942 I3943 E3944 E3945 Q3946 G3947
N3950 M3955 Q3960 V3961 F3962 N3963 G3971 L3980 A3981 H3982 L3985 F3992 F3996 A3997 M4000 M4001 K4002 Q4005 D4006 S4007 S4008 E4011 K4014 L4017 D4018 L4019 D4022 M4026 E4032 G4033 N4034 G4038 M4039 I4040 A4041 R4042 D4046 V4049 E4050 N4054
M4057 F4062 F4065 L4068 K4069 D4070 G4073 S4074 E4075 A4076 F4077 Q4078 D4079 Y4080 V4081 T4082 D4083 P4084 R4085 K4090 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 Q4109 F4110 S4113 C4114 S4115 E4116 A4117 D4118 E4119 N4120 E4121 M4122 I4123 N4124 F4125 E4126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S4236 E4239 D4240 A4248 I4251 S4252 E4253 X4320 X4321 X4322 X4323 X4324 X4325 X4326 X4327 X4328 X4329 X4330 X4331 X4332 X4333 X4334 X4335 X4336 X4337 X4338 X4339 X4340 X4341 X4342 X4343 X4344 X4345 L4544 F4551 Y4554 L4555 F4559 Y4560 T4561 L4562 R4563 F4564 L4565 A4566 L4567 F4568 L4569 A4570 F4571 A4572 I4573
N4574 Y4580 K4581 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU N4626 M4627 V4628 Y4629 E4633 E4634 S4635 T4636 G4637 Y4638 P4641
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I4737 A4738 L4741 G4742 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 S4770 I4771 D4772 V4773 I4777 F4780 F4784 T4785 F4789 V4797 M4798 S4799 L4800 H4803 Y4804 N4805 N4806 F4807 F4808 F4809
H4812 L4813 L4814 D4815 I4816 A4817 M4818 K4821 T4822 L4823 R4824 L4827 S4828 H4832 N4833 G4834 K4835 M4839 G4842 V4846 V4847 L4850 R4860 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 D4878 H4886 M4887 A4893 G4894 G4895 G4896 I4897 G4898 D4899 E4900 I4901 E4902
D4903 P4904 A4905 G4906 D4907 E4908 Y4909 E4910 L4911 Y4912 R4913 F4916 F4921 F4922 F4923 V4924 I4925 L4928 L4929 A4930 I4931 G4934 L4935 I4936 R4944 E4952 D4953 K4957 C4958 F4959 I4960 C4961 G4962 I4963 G4964 Y4967 F4968 D4969 F4975 E4976 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 L4995
I4996 M4997 K4998 D4999 E5000 T5001 E5002 E5007 R5017 C5018 W5019 D5020 P5023 D5026 C5027 F5028 R5029 K5030 Q5031 Y5032 E5033 D5034 Q5035 L5036 S5037

4 Experimental information (i)

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 ($e^-/Å^2$)	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	0.105	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	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: ZN, ATP, CFF

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	0.52	0/1123
1	F	0.29	0/834	0.52	0/1123
1	H	0.29	0/834	0.52	0/1123
1	J	0.29	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	10/34534 (0.0%)
2	E	0.29	0/25428	0.54	10/34534 (0.0%)
2	G	0.29	0/25428	0.54	10/34534 (0.0%)
2	I	0.29	0/25428	0.54	10/34534 (0.0%)
All	All	0.29	0/105048	0.54	40/142628 (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	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.42	134.66	115.30
2	B	131	LEU	CA-CB-CG	8.41	134.65	115.30
2	E	131	LEU	CA-CB-CG	8.41	134.63	115.30
2	I	131	LEU	CA-CB-CG	8.39	134.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1600	LEU	CA-CB-CG	6.97	131.33	115.30

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	694	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	5	0
1	F	818	0	824	5	0
1	H	818	0	824	4	0
1	J	818	0	824	4	0
2	B	29499	0	24746	252	0
2	E	29499	0	24746	258	0
2	G	29499	0	24746	248	0
2	I	29499	0	24746	255	0
3	B	31	0	12	0	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102368	1020	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 1020 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:5028:PHE:HE1	2:G:5032:TYR:CD2	1.87	0.93
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.87	0.93
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.87	0.92
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.87	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.58	0.92

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%)	2916 (90%)	311 (10%)	8 (0%)	47	81
2	E	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	47	81
2	G	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	47	81
2	I	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	47	81
All	All	13360/18096 (74%)	12037 (90%)	1291 (10%)	32 (0%)	50	81

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE

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Mol	Chain	Res	Type
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	84	90

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1676	LEU
2	G	3787	LYS
2	G	4983	HIS
2	E	1964	ARG
2	E	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	4034	ASN

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Mol	Chain	Res	Type
2	G	3896	ASN
2	I	1206	GLN
2	G	3889	GLN
2	G	4983	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	B	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.57	5 (16%)
3	ATP	G	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.57	5 (16%)
4	CFF	E	5102	-	8,15,15	2.46	3 (37%)	8,23,23	1.26	1 (12%)
3	ATP	E	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.58	5 (16%)
4	CFF	G	5102	-	8,15,15	2.45	3 (37%)	8,23,23	1.27	1 (12%)
3	ATP	I	5101	-	26,33,33	0.87	1 (3%)	31,52,52	1.57	5 (16%)
4	CFF	I	5102	-	8,15,15	2.46	3 (37%)	8,23,23	1.26	1 (12%)
4	CFF	B	5102	-	8,15,15	2.45	3 (37%)	8,23,23	1.26	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-4.52	1.33	1.39
4	B	5102	CFF	C5-C4	-4.48	1.33	1.39
4	G	5102	CFF	C5-C4	-4.48	1.33	1.39
4	I	5102	CFF	C5-C4	-4.48	1.33	1.39
4	I	5102	CFF	C6-N1	-4.11	1.32	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	5101	ATP	PB-O3B-PG	-3.89	119.47	132.83
3	I	5101	ATP	PB-O3B-PG	-3.89	119.49	132.83
3	B	5101	ATP	PB-O3B-PG	-3.88	119.51	132.83
3	G	5101	ATP	PB-O3B-PG	-3.88	119.51	132.83
3	E	5101	ATP	N3-C2-N1	-3.53	123.17	128.68

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	PB-O3A-PA-O5'
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	PB-O3A-PA-O5'
3	E	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O3A

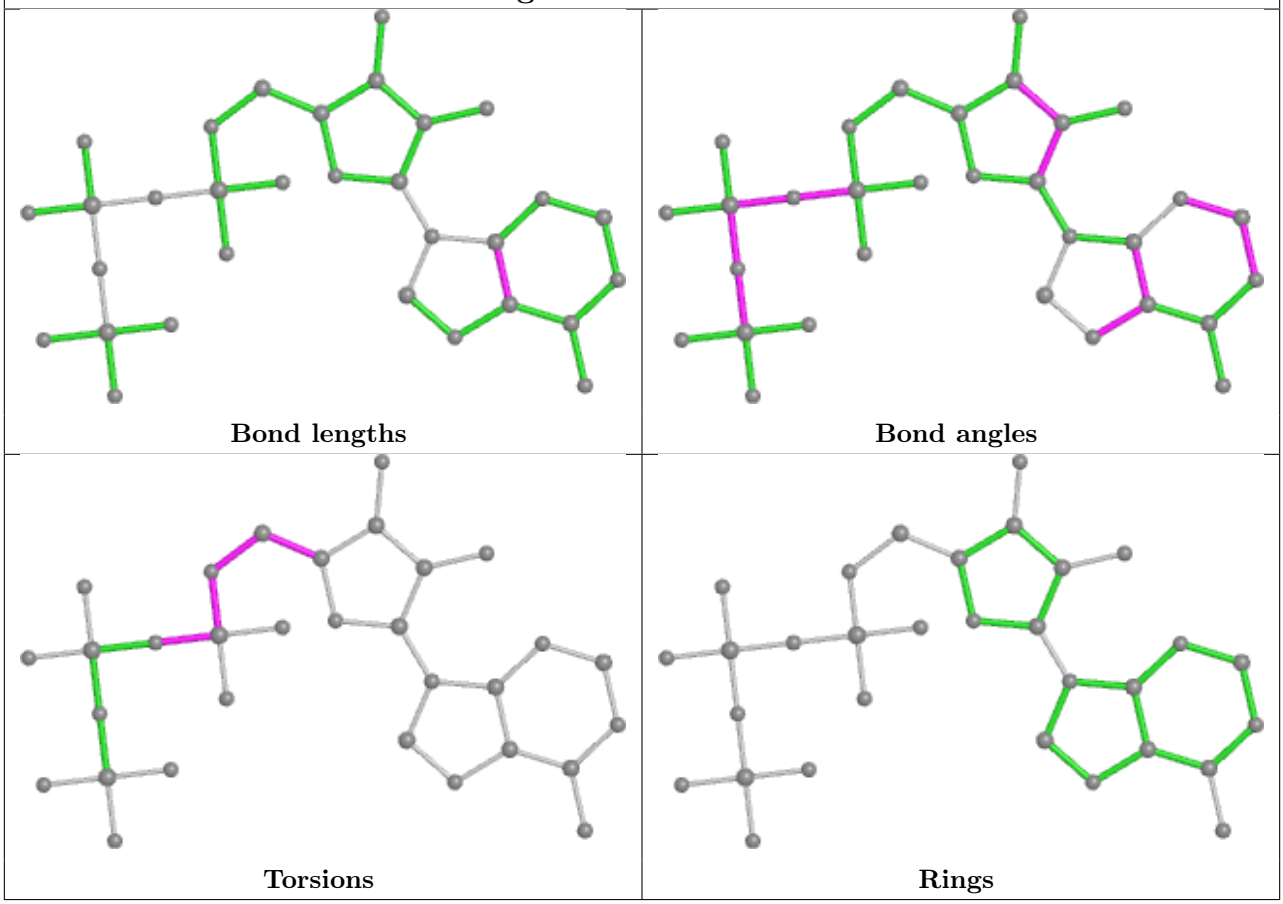
There are no ring outliers.

4 monomers are involved in 4 short contacts:

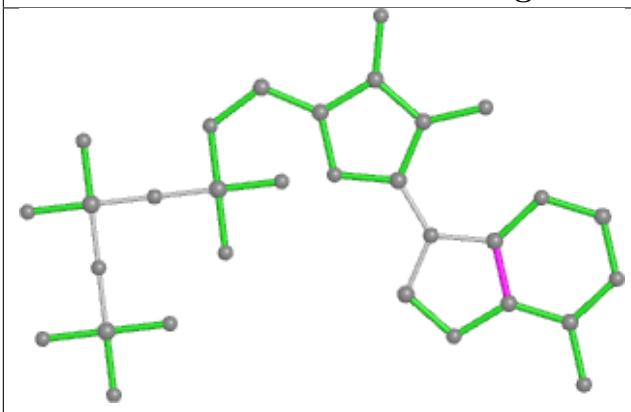
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	5102	CFF	1	0
4	G	5102	CFF	1	0
4	I	5102	CFF	1	0
4	B	5102	CFF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

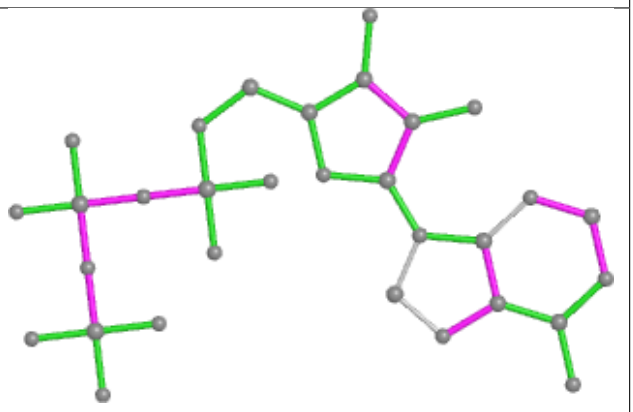
Ligand ATP B 5101



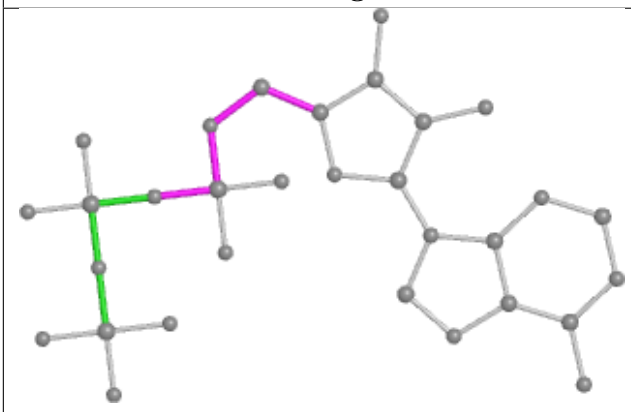
Ligand ATP G 5101



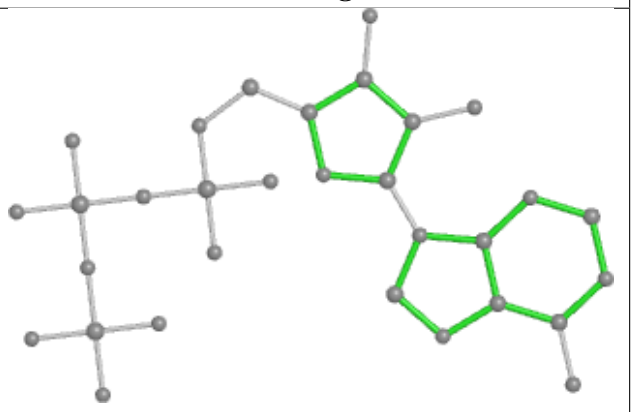
Bond lengths



Bond angles

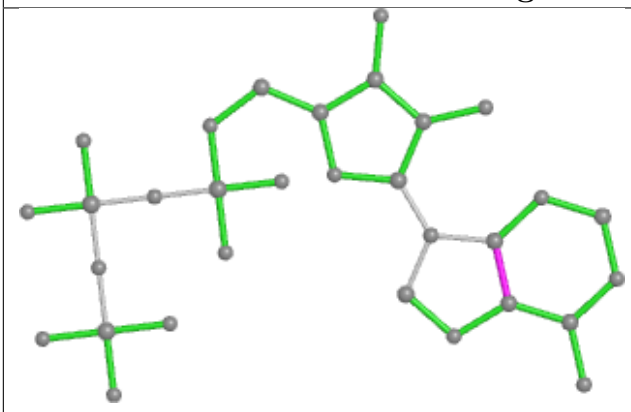


Torsions

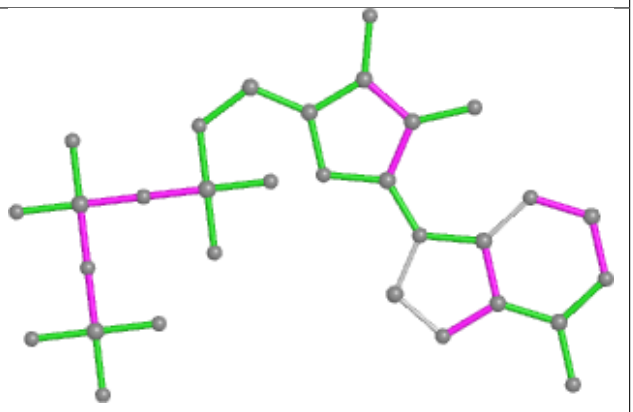


Rings

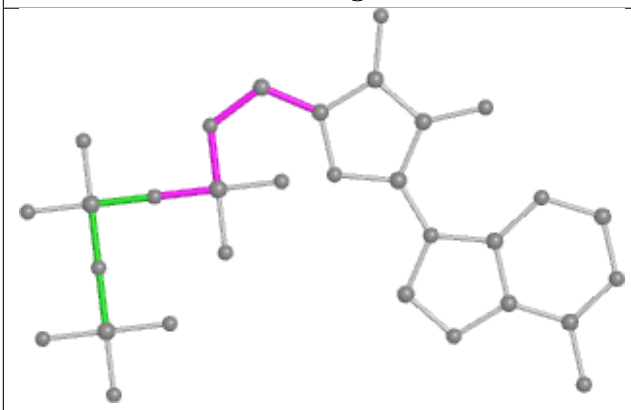
Ligand ATP E 5101



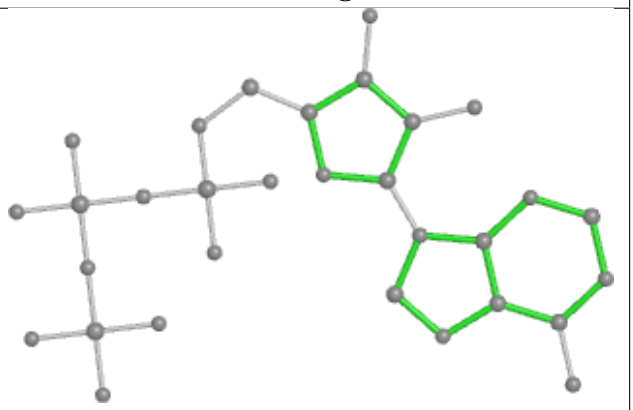
Bond lengths



Bond angles

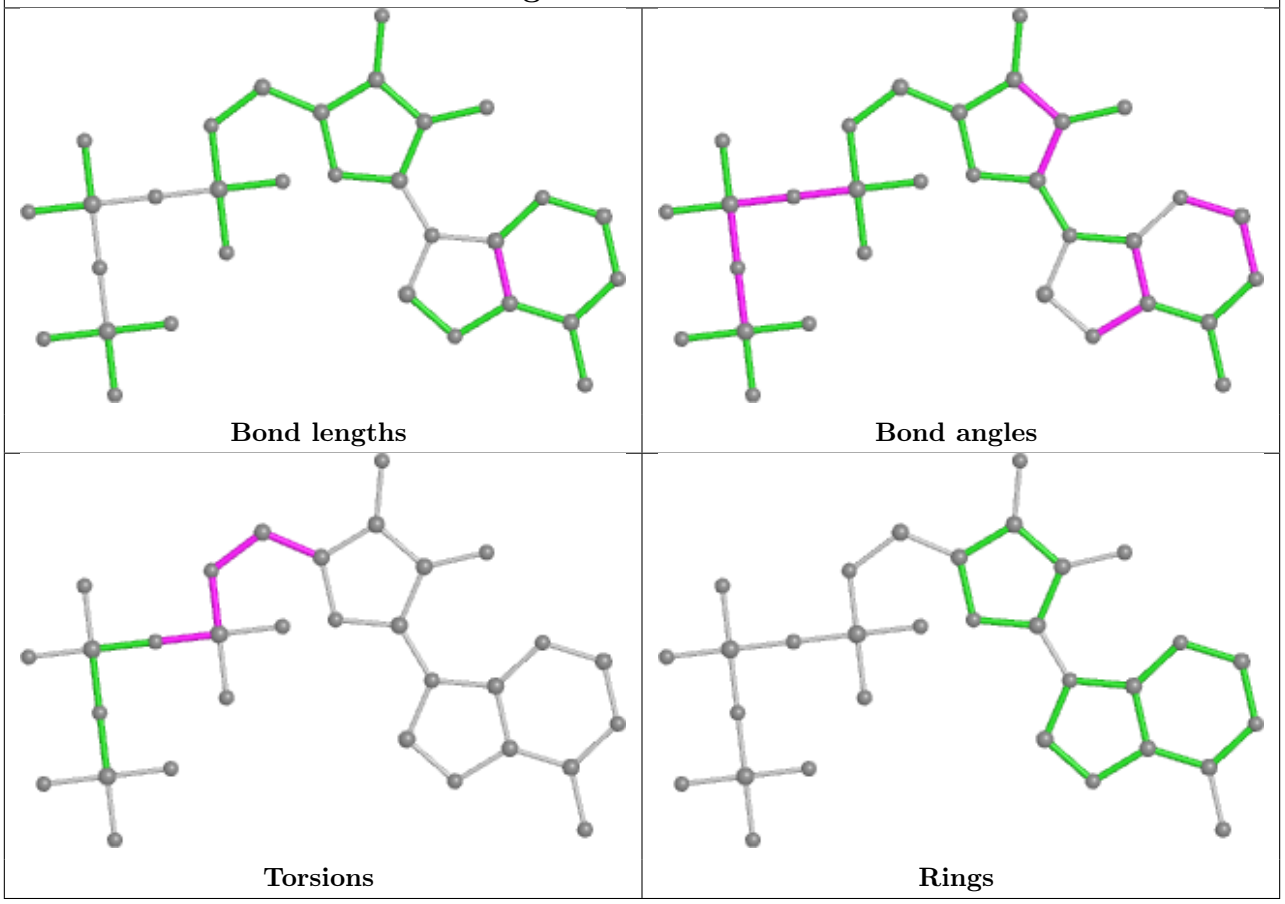


Torsions



Rings

Ligand ATP I 5101



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	E	14
2	I	14
2	G	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	72.89
1	E	4345:UNK	C	4540:PHE	N	72.89

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.89
1	G	4345:UNK	C	4540:PHE	N	72.89
1	B	3613:UNK	C	3639:THR	N	44.63

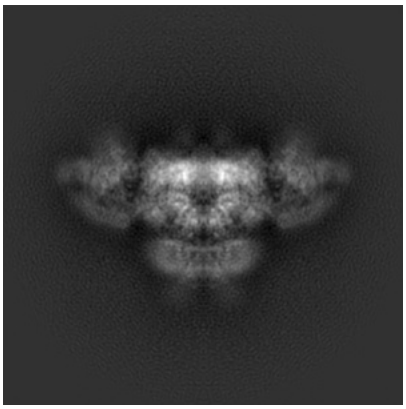
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8386. These allow visual inspection of the internal detail of the map and identification of artifacts.

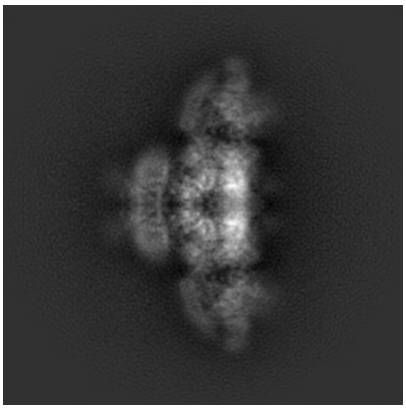
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

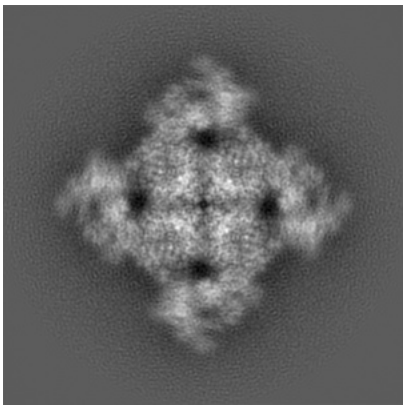
6.1.1 Primary map



X

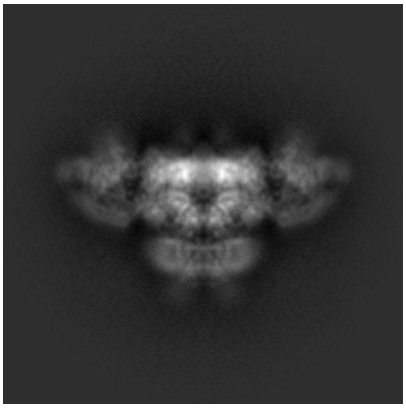


Y

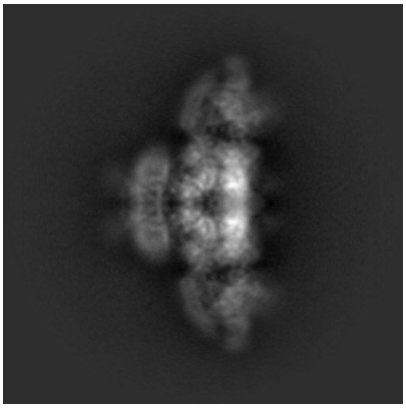


Z

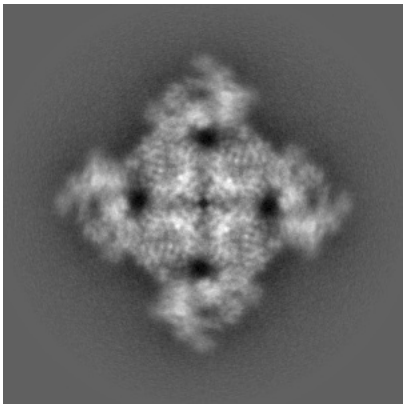
6.1.2 Raw map



X



Y

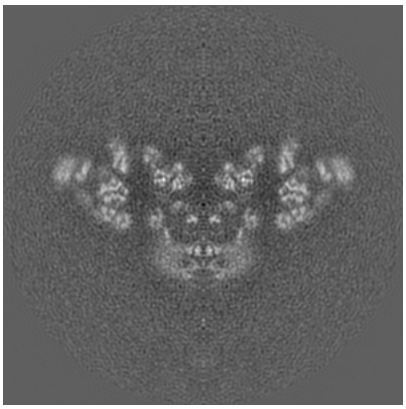


Z

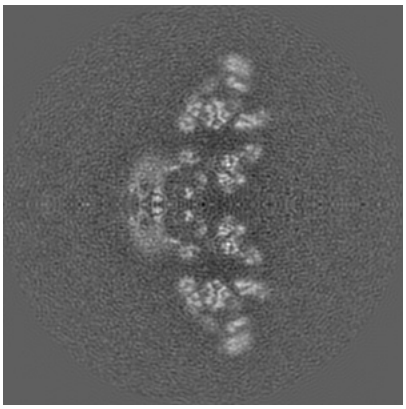
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

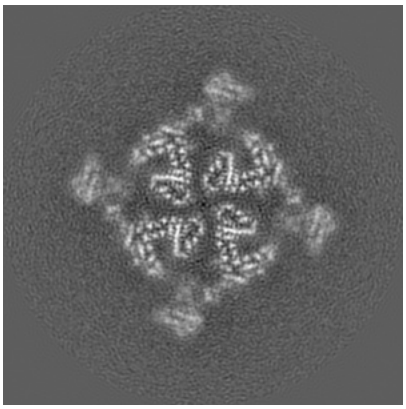
6.2.1 Primary map



X Index: 200

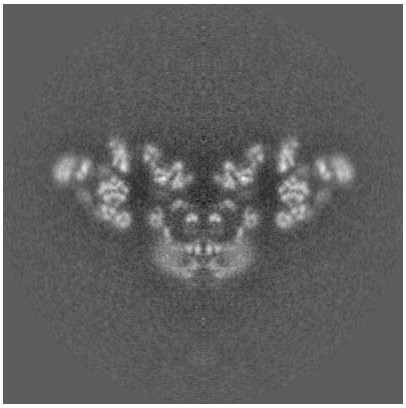


Y Index: 200

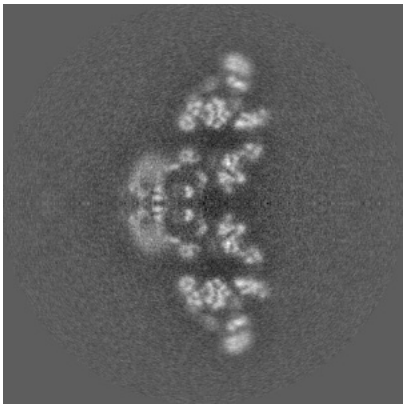


Z Index: 200

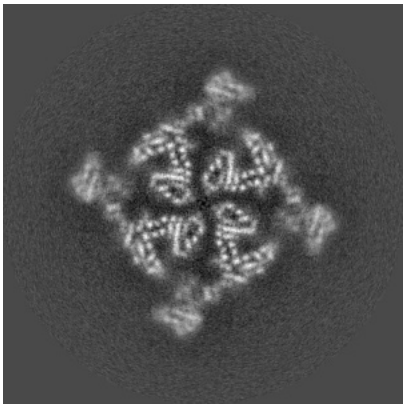
6.2.2 Raw map



X Index: 200



Y Index: 200

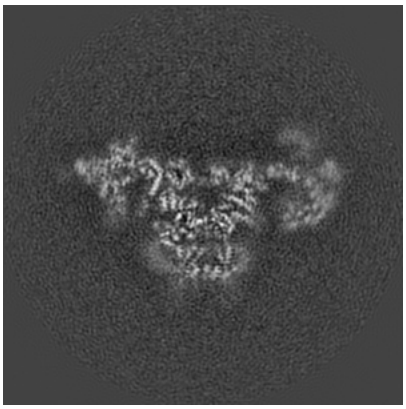


Z Index: 200

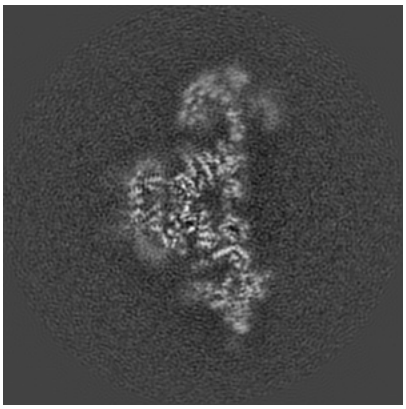
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

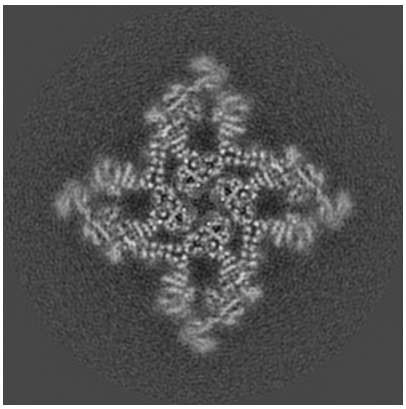
6.3.1 Primary map



X Index: 216

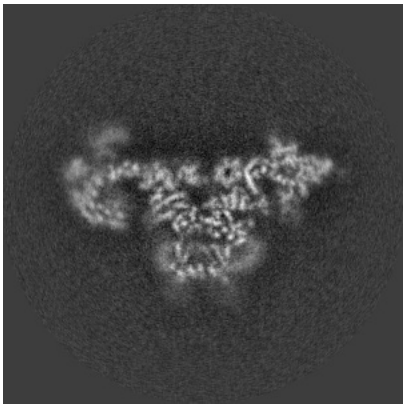


Y Index: 184

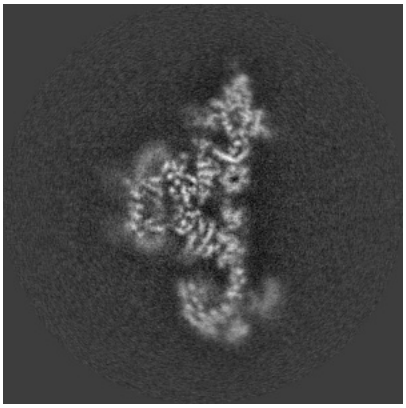


Z Index: 228

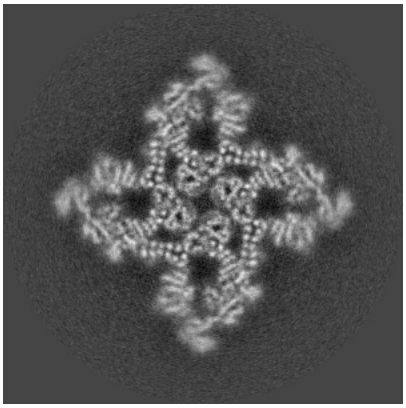
6.3.2 Raw map



X Index: 183



Y Index: 217

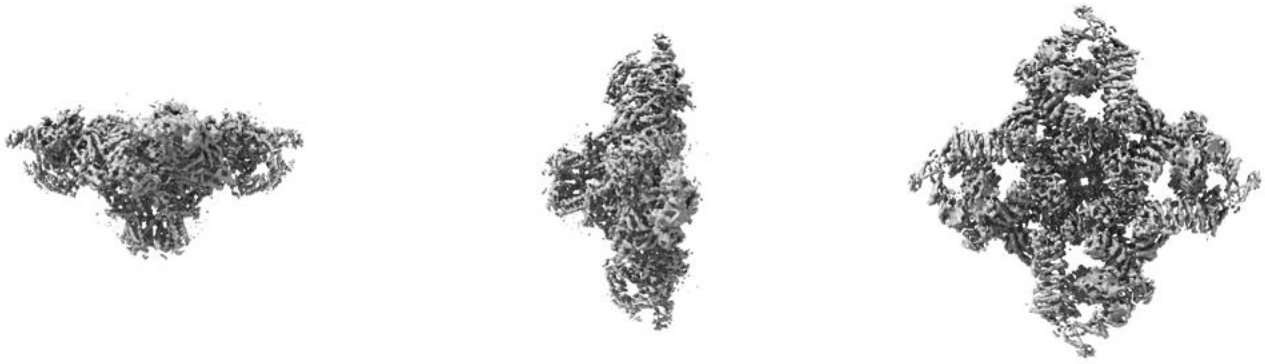


Z Index: 228

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

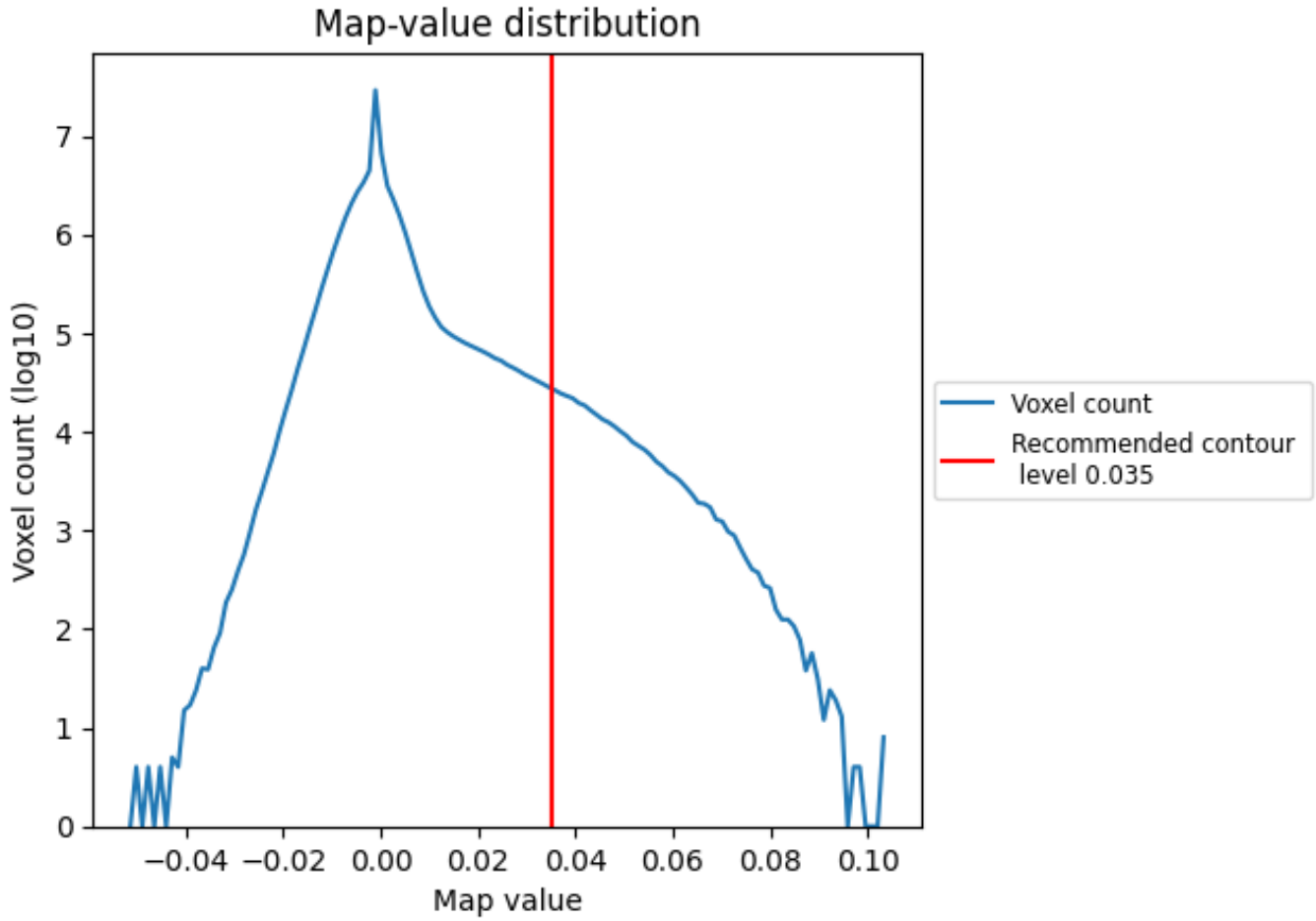
6.5 Mask visualisation (i)

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

7 Map analysis

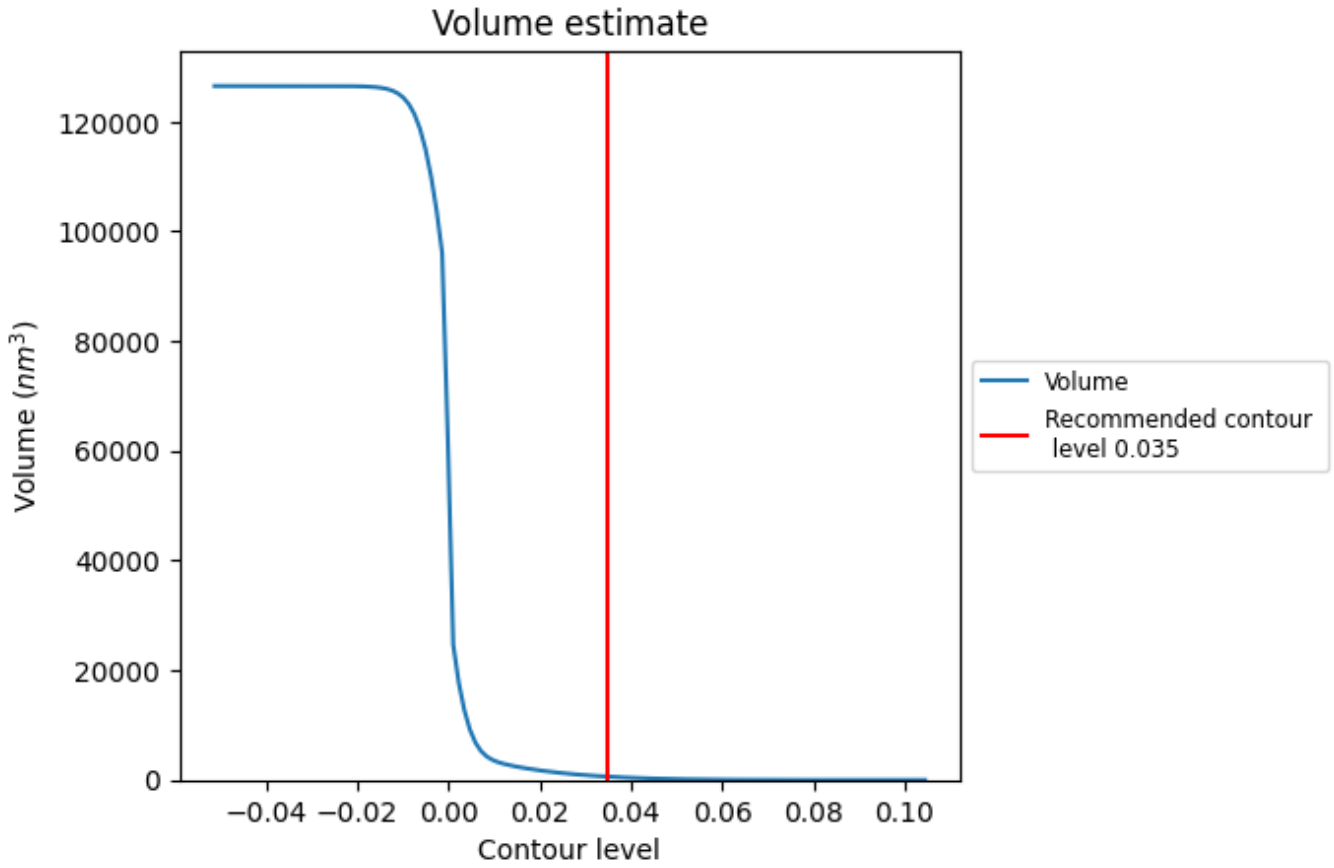
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

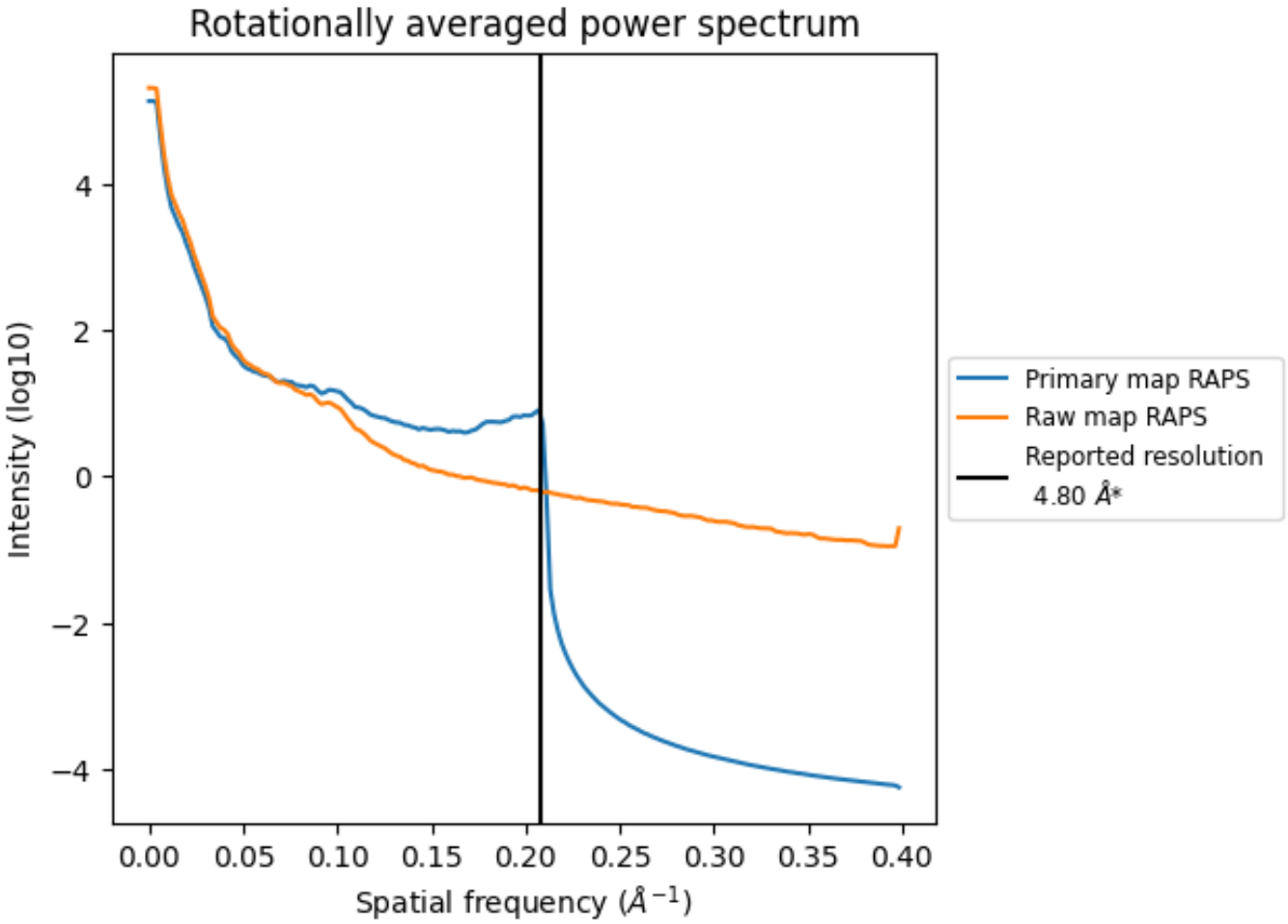
7.2 Volume estimate (i)



The volume at the recommended contour level is 605 nm^3; this corresponds to an approximate mass of 547 kDa.

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

7.3 Rotationally averaged power spectrum (i)

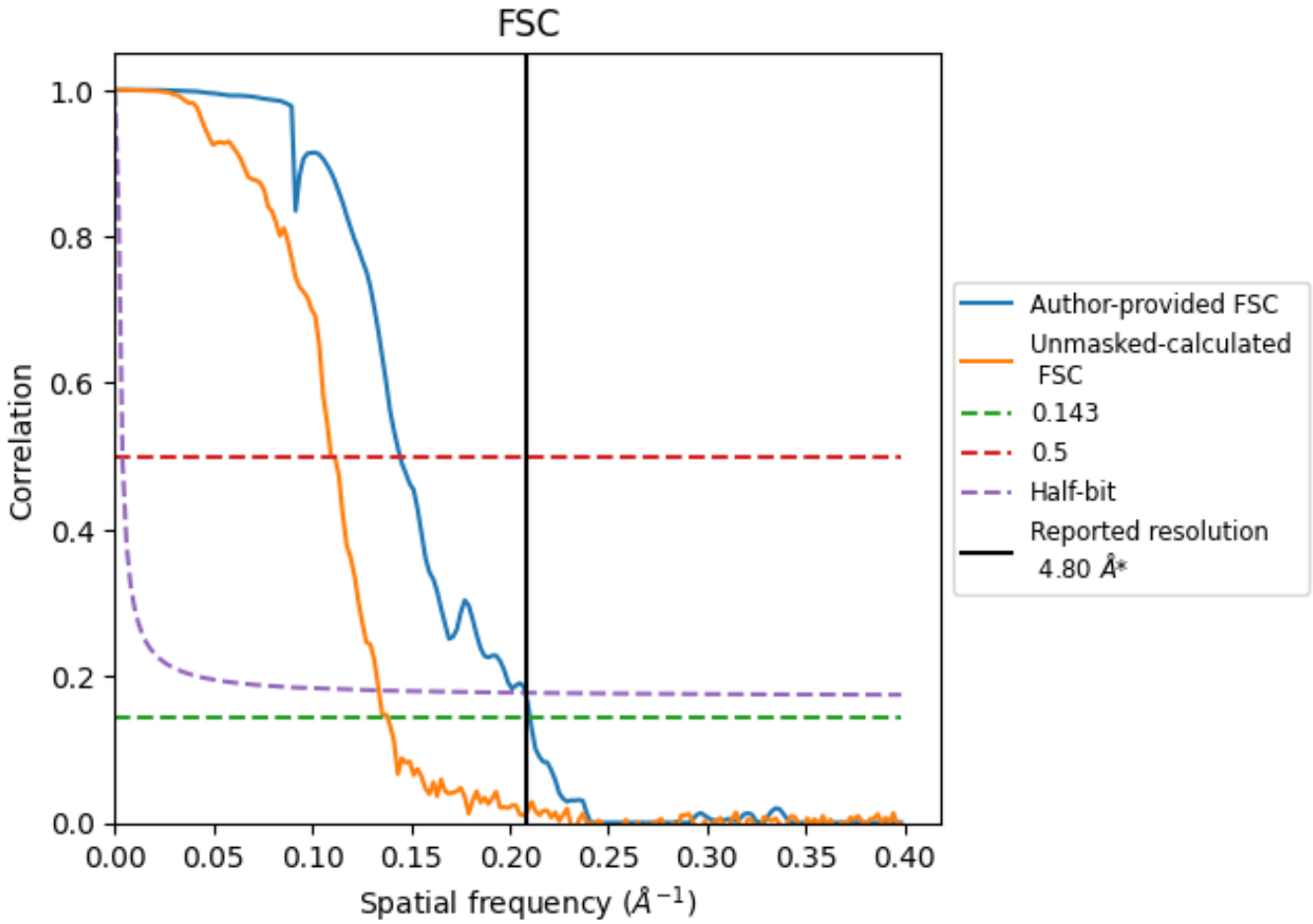


*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

8.2 Resolution estimates (i)

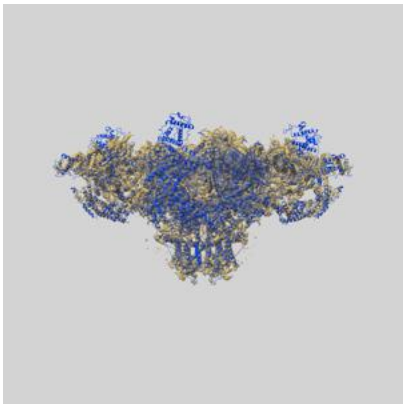
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.76	6.92	4.81
Unmasked-calculated*	7.24	9.13	7.48

*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 7.24 differs from the reported value 4.8 by more than 10 %

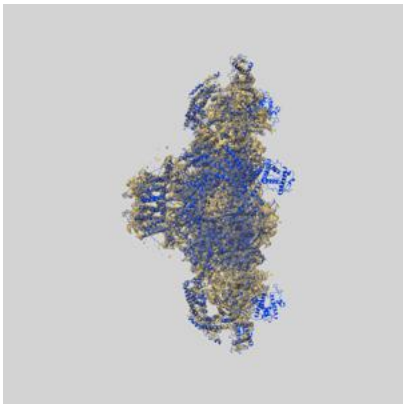
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8386 and PDB model 5TAV. Per-residue inclusion information can be found in section 3 on page 6.

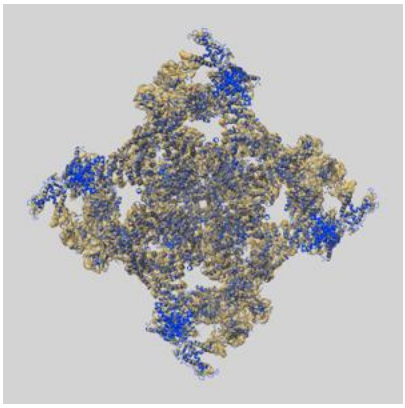
9.1 Map-model overlay



X



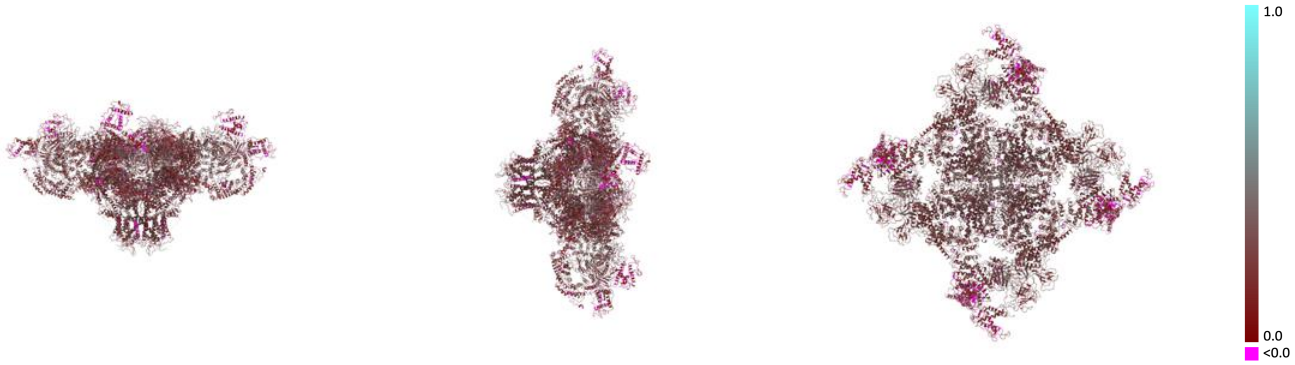
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

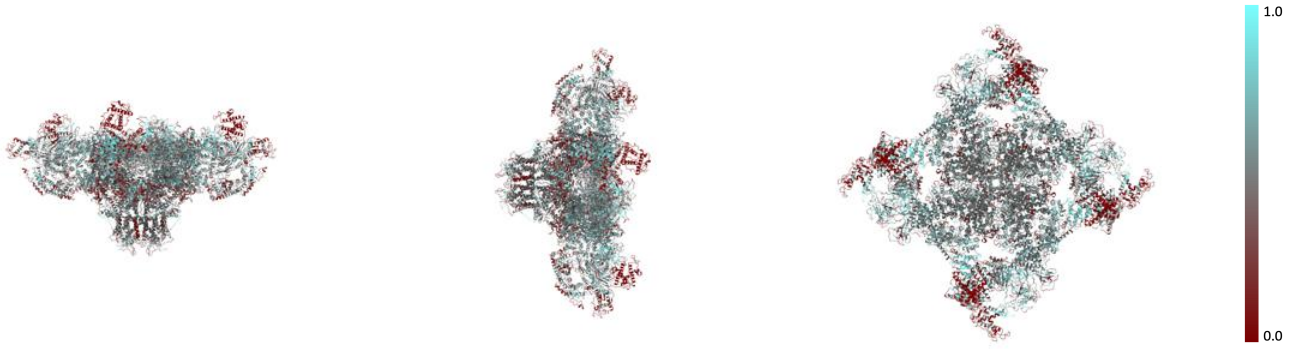
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

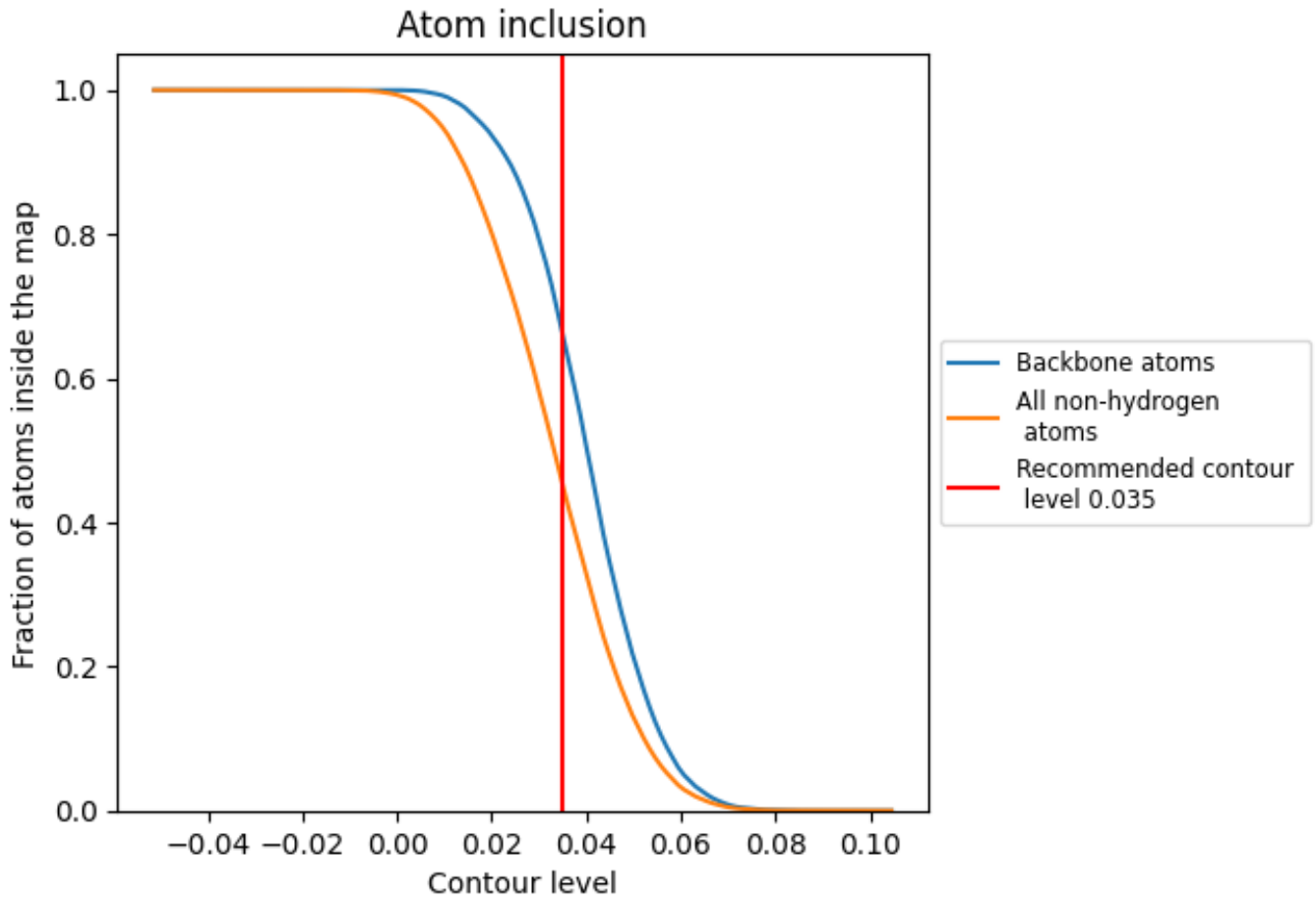
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 45% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4527	0.2520
A	0.4628	0.2710
B	0.4525	0.2520
E	0.4524	0.2520
F	0.4653	0.2720
G	0.4521	0.2510
H	0.4615	0.2720
I	0.4525	0.2520
J	0.4615	0.2720