wwPDB EM Map/Model Validation Report (i)

Sep 14, 2016 – 12:13 PM EDT

PDB ID	:	5GL0
EMDB ID:	:	EMD-9520
Title	:	Structure of RyR1 in a closed state (C4 conformer)
Authors	:	Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on	:	2016-07-07
Resolution	:	4.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

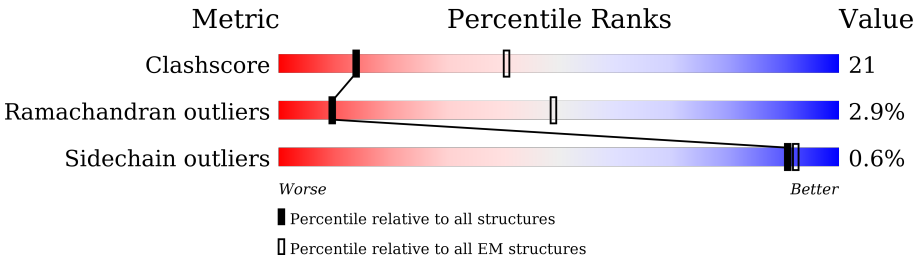
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	5037	44% 26% • 27%
1	C	5037	44% 26% • 27%
1	E	5037	44% 26% • 27%
1	G	5037	44% 27% • 27%
2	B	108	60% 38% ••
2	D	108	61% 37% ••
2	F	108	63% 35% ••
2	H	108	64% 34% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 111000 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	C	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	E	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		
1	G	3660	Total	C	N	O	S	0	0
			26917	17107	4682	4971	157		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	D	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	F	107	Total	C	N	O	S	0	0
			832	527	146	155	4		
2	H	107	Total	C	N	O	S	0	0
			832	527	146	155	4		

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

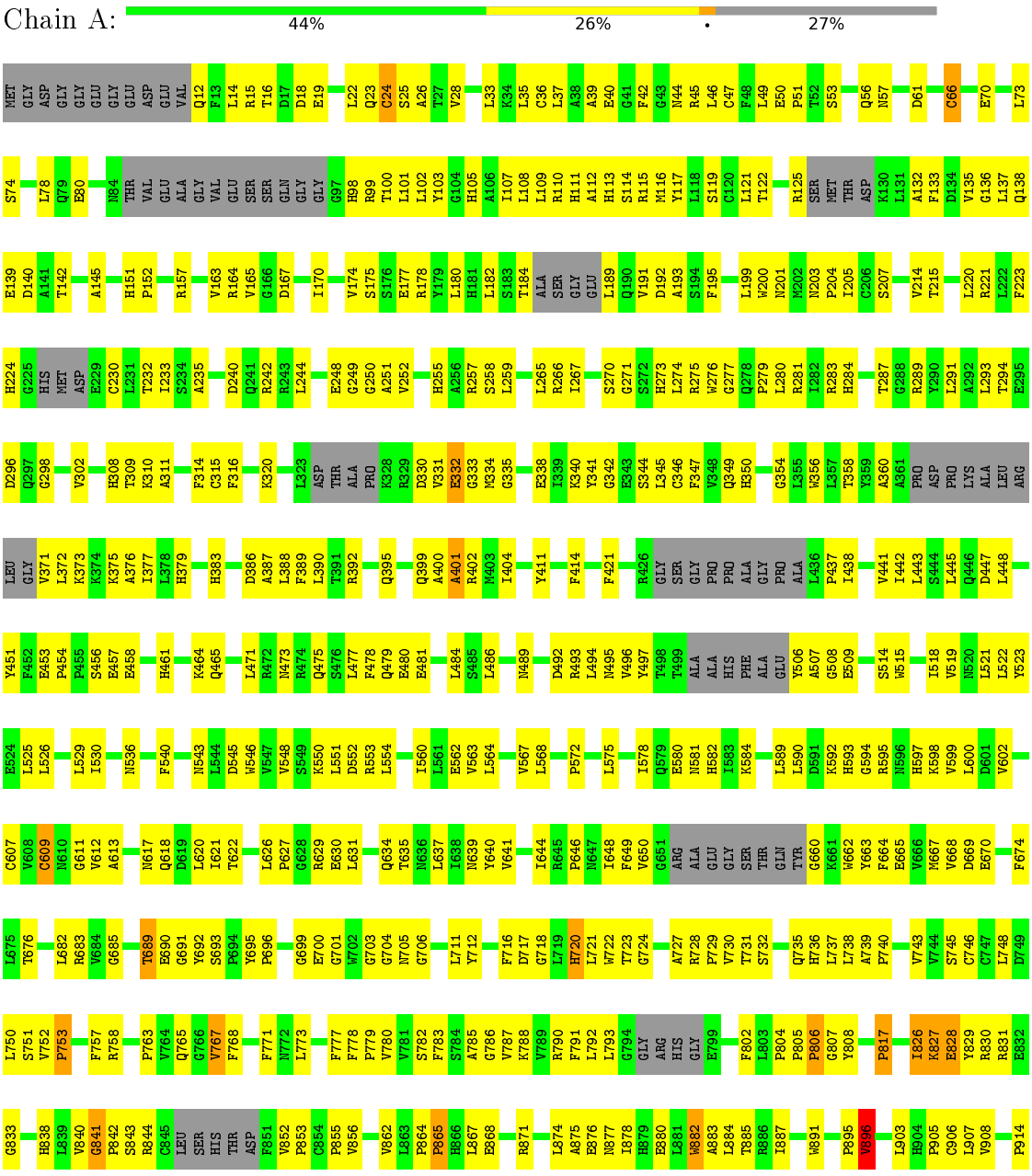
Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

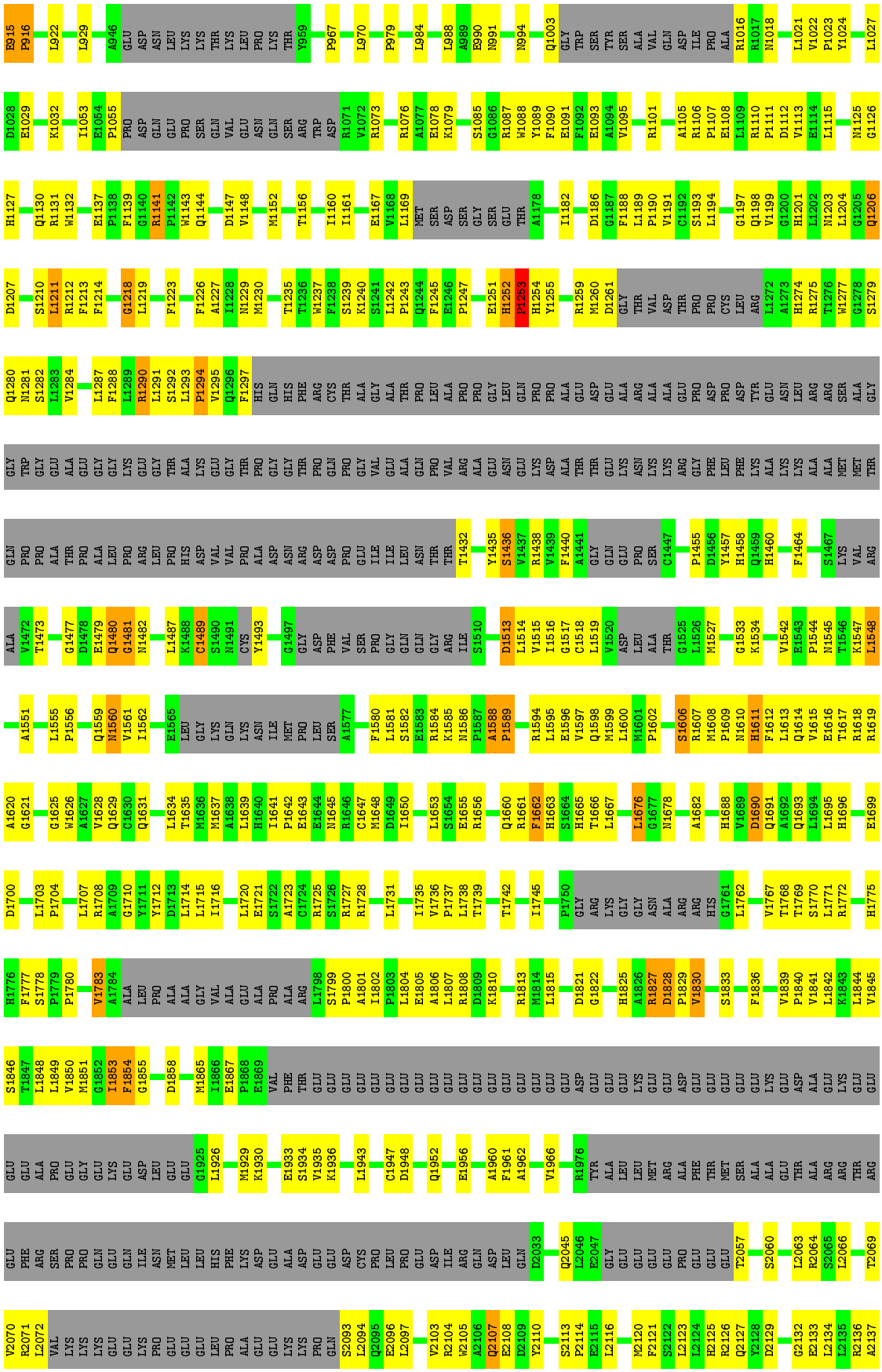
3 Residue-property plots (i)

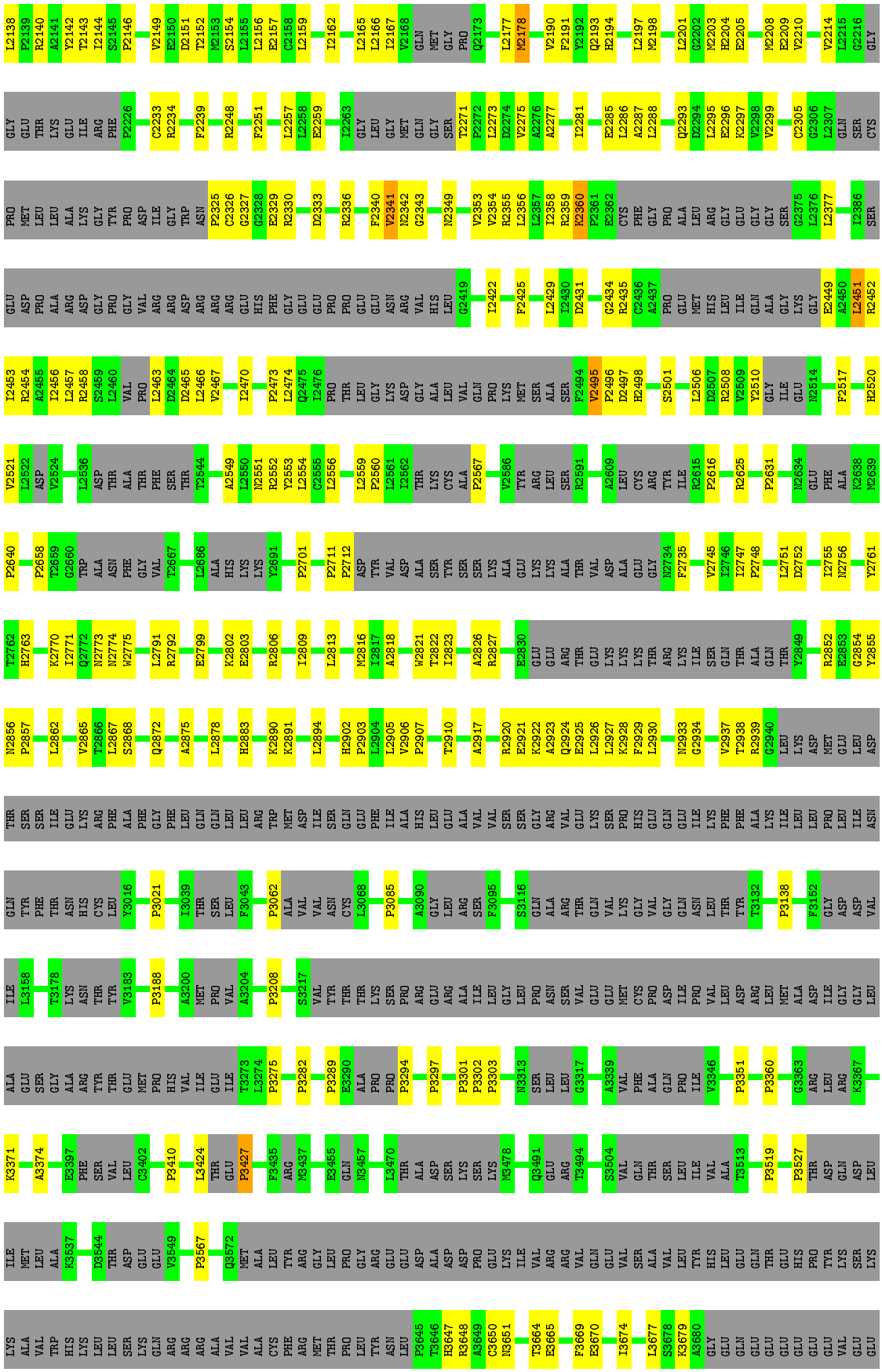
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. 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.

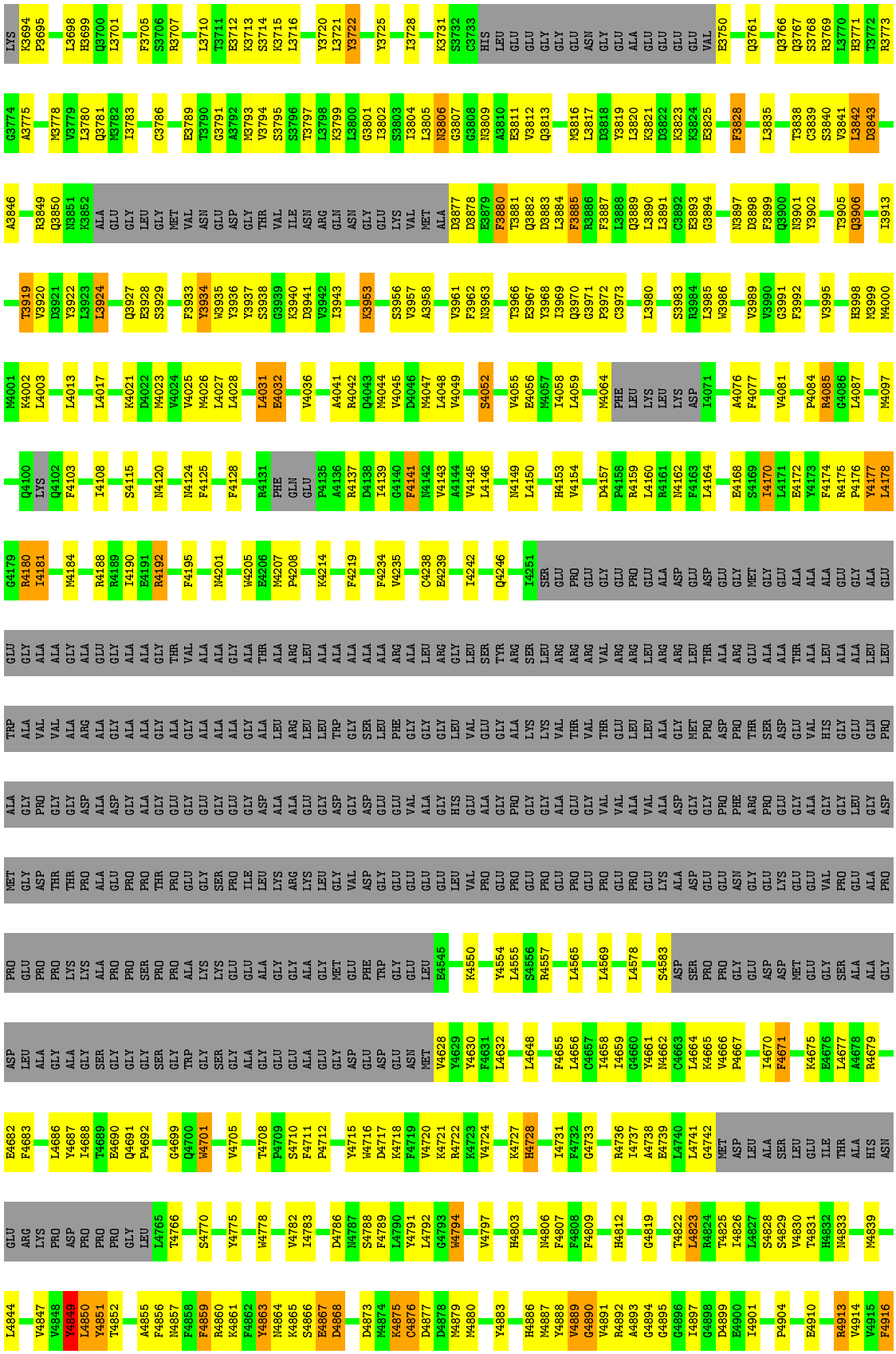
- Molecule 1: Ryanodine receptor 1

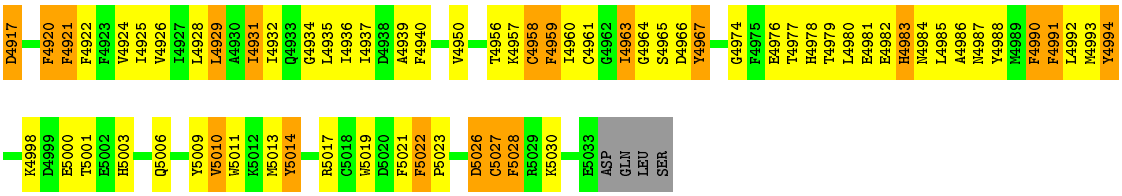
Chain A:





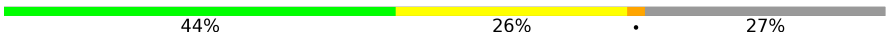


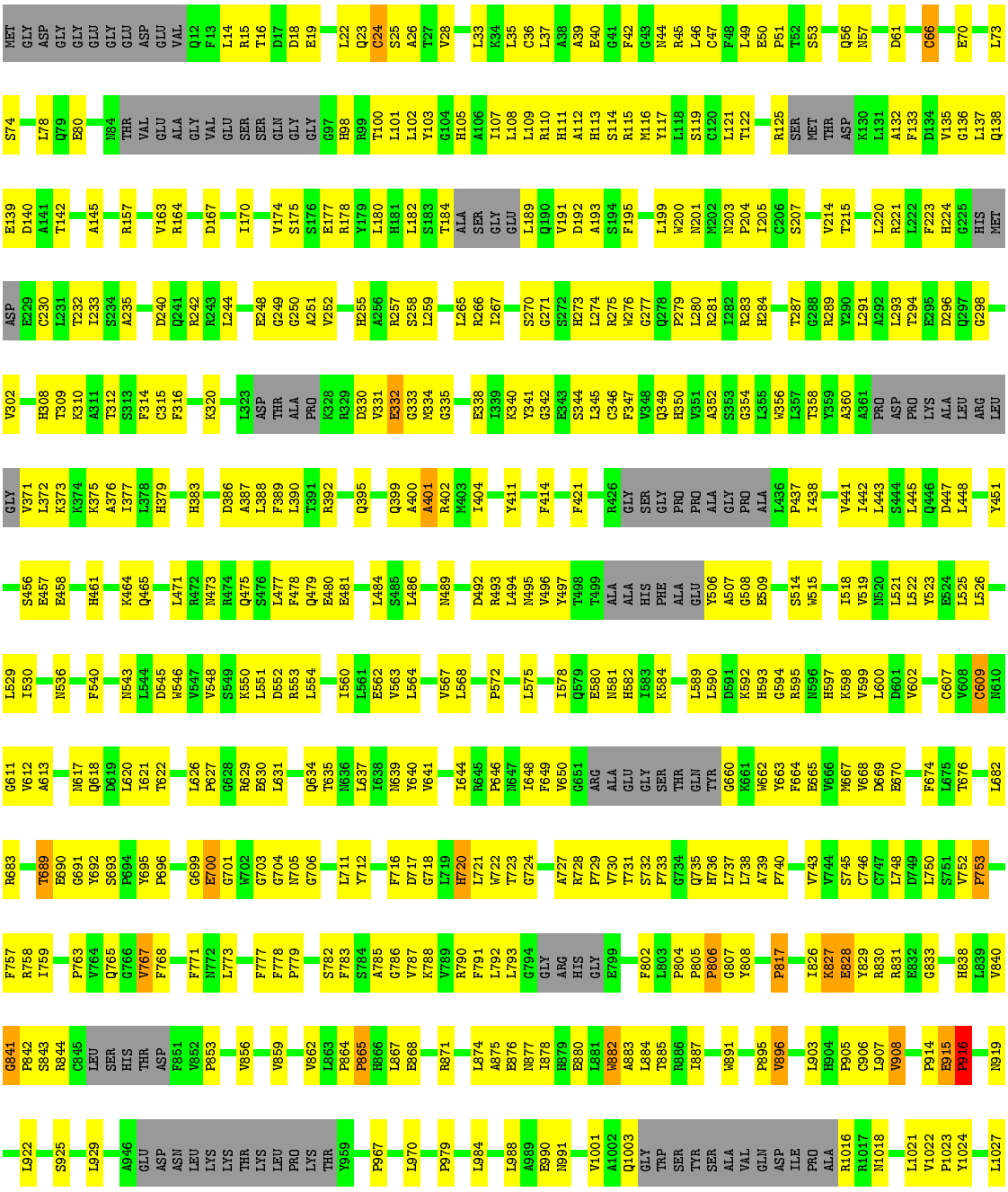


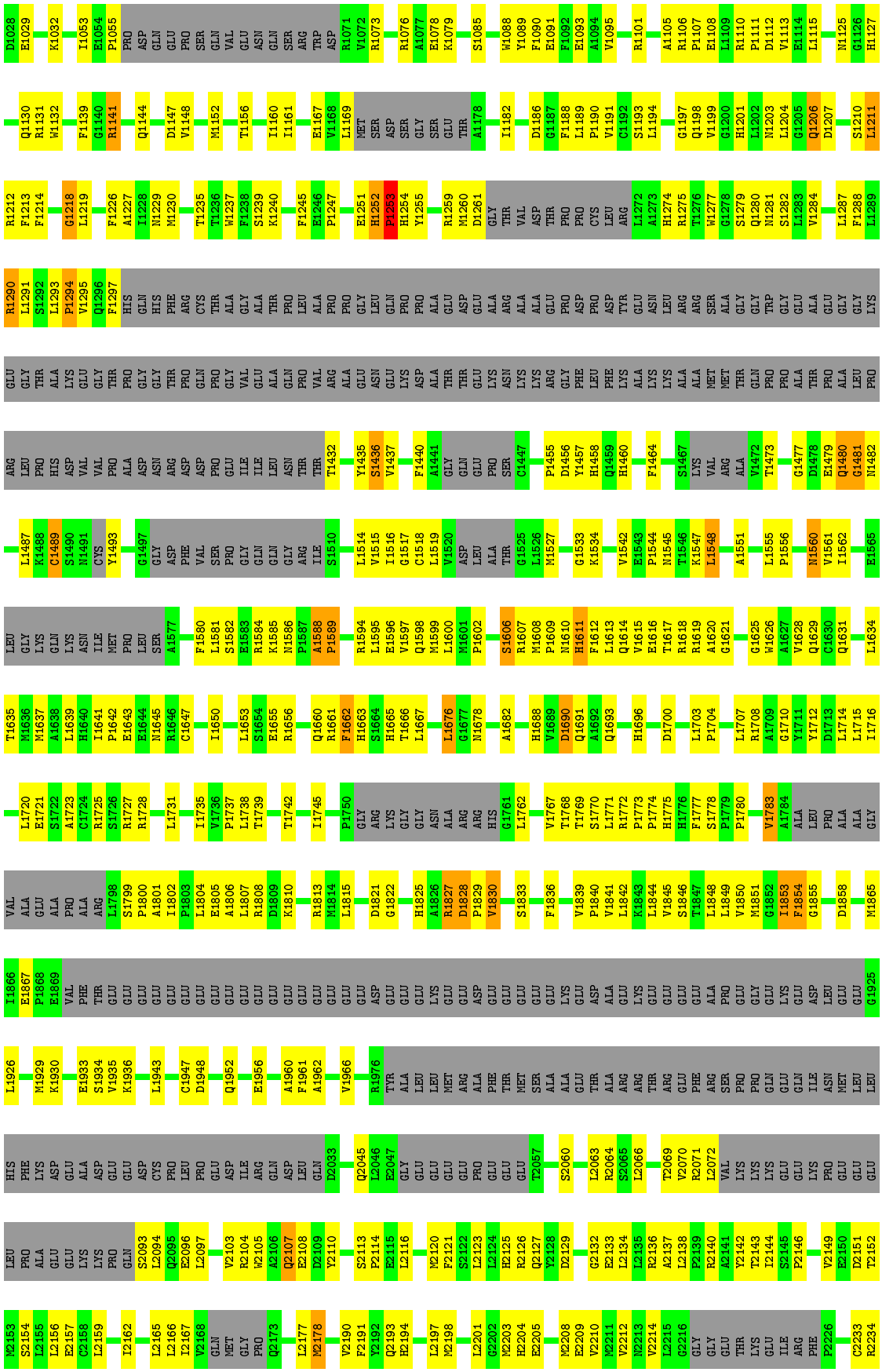


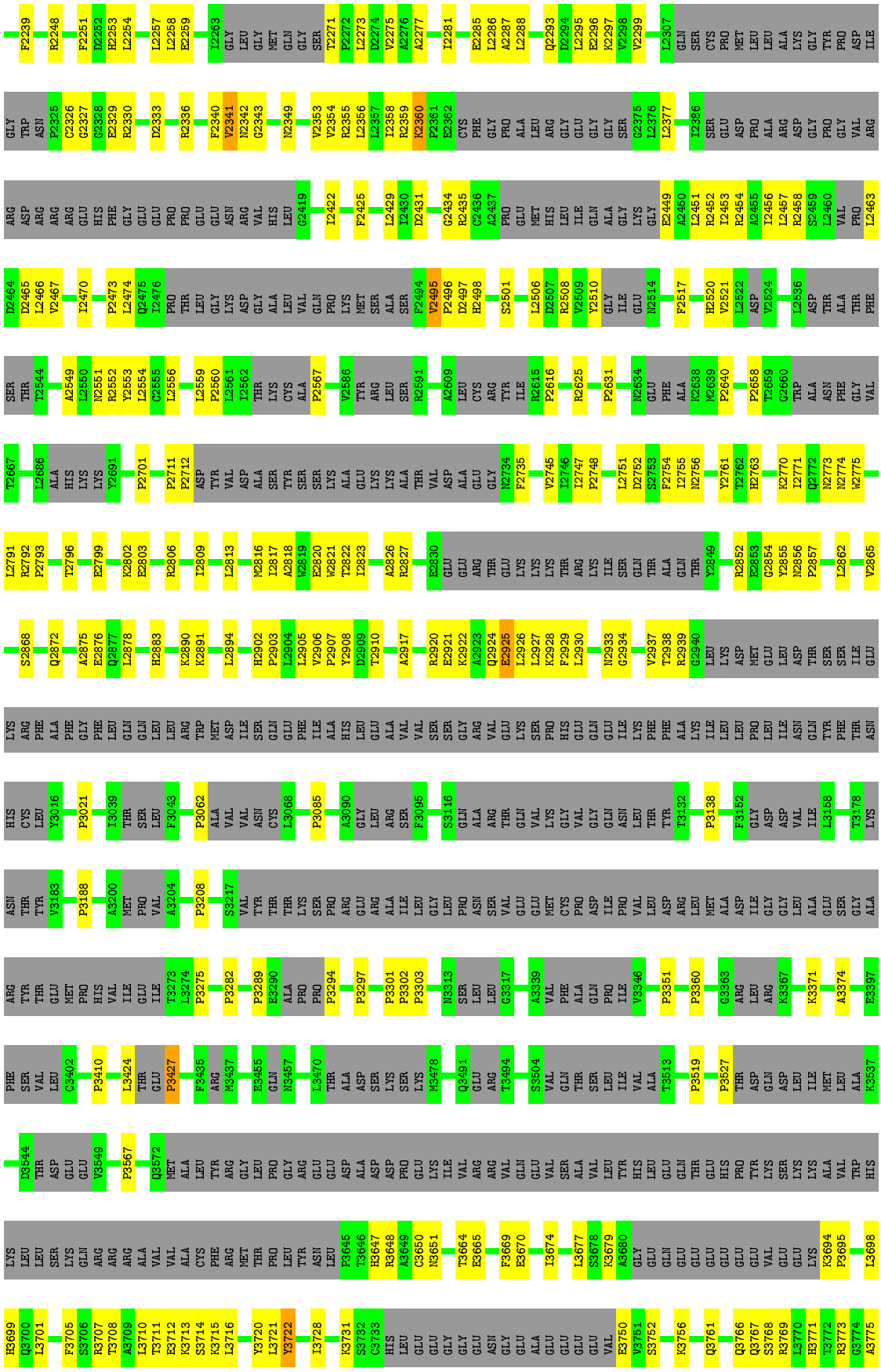
• Molecule 1: Ryanodine receptor 1

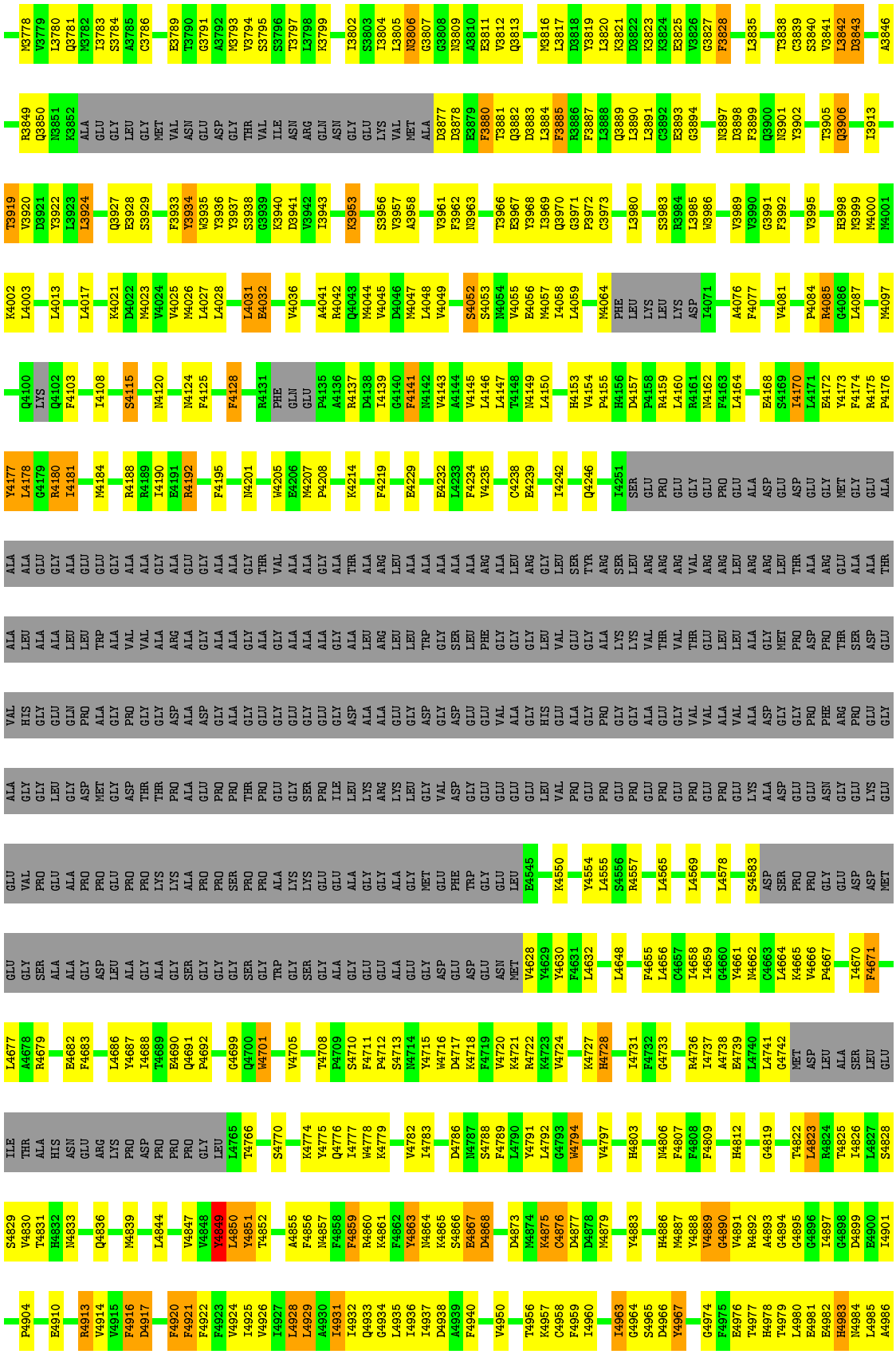
Chain C:





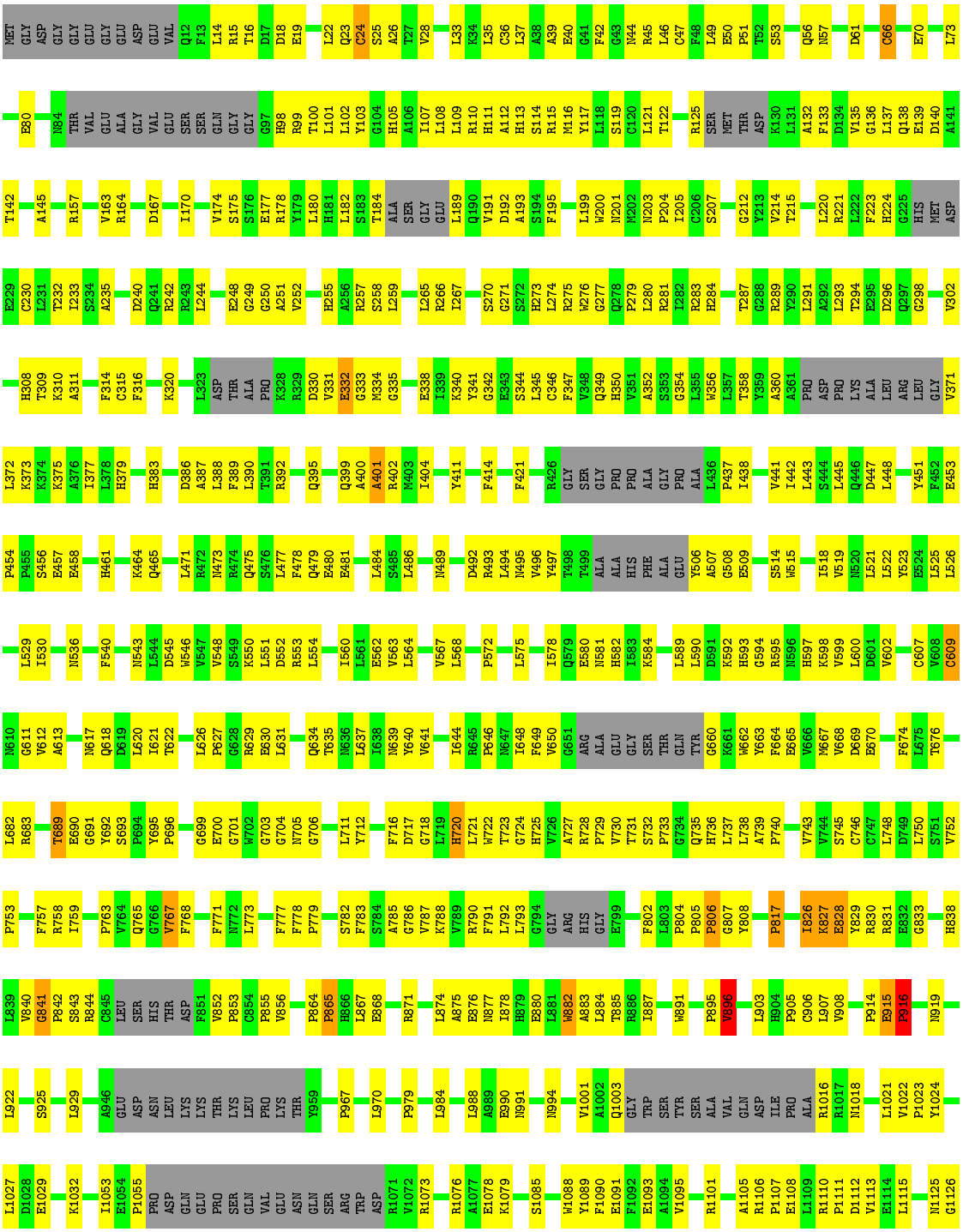


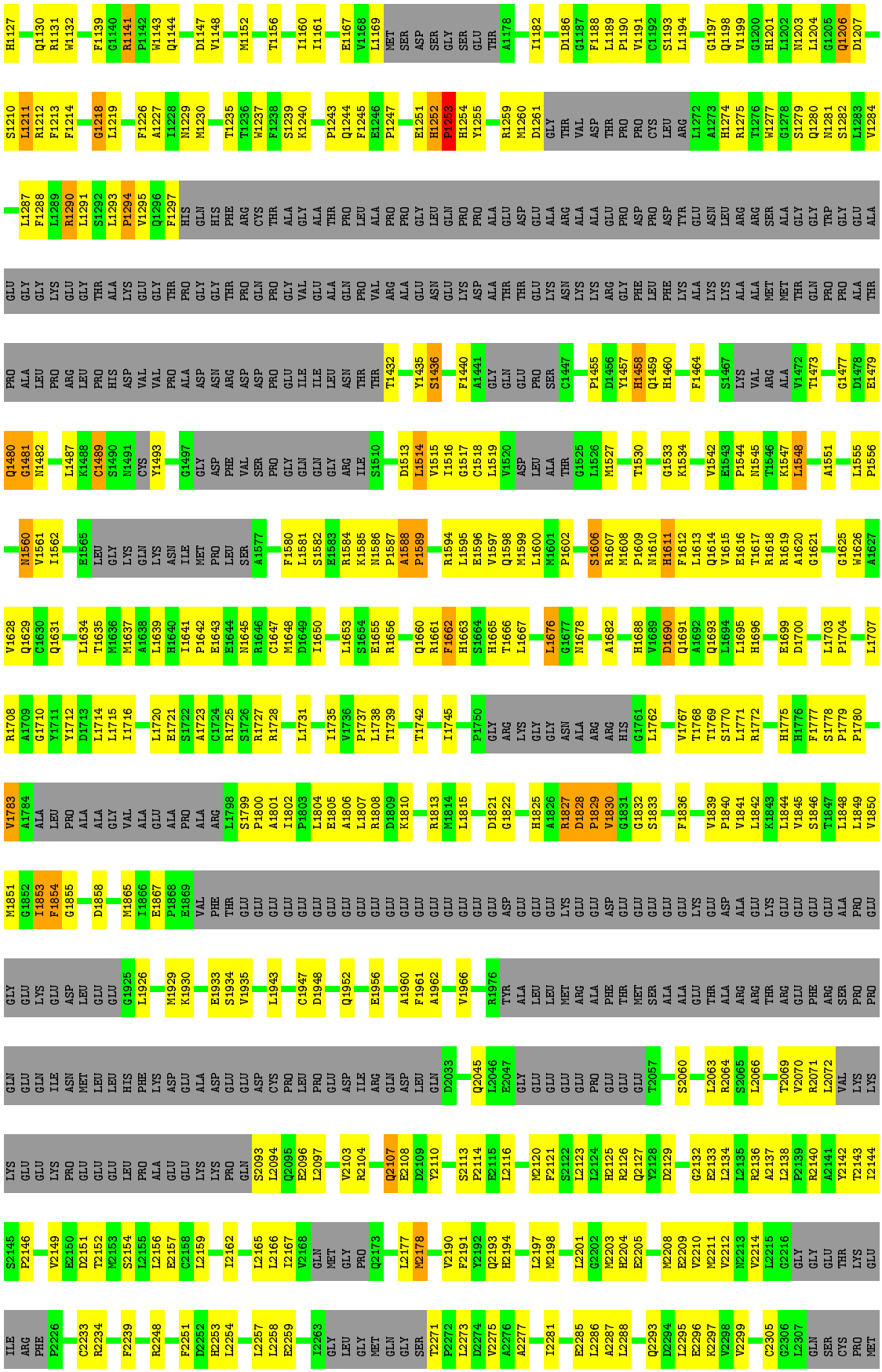


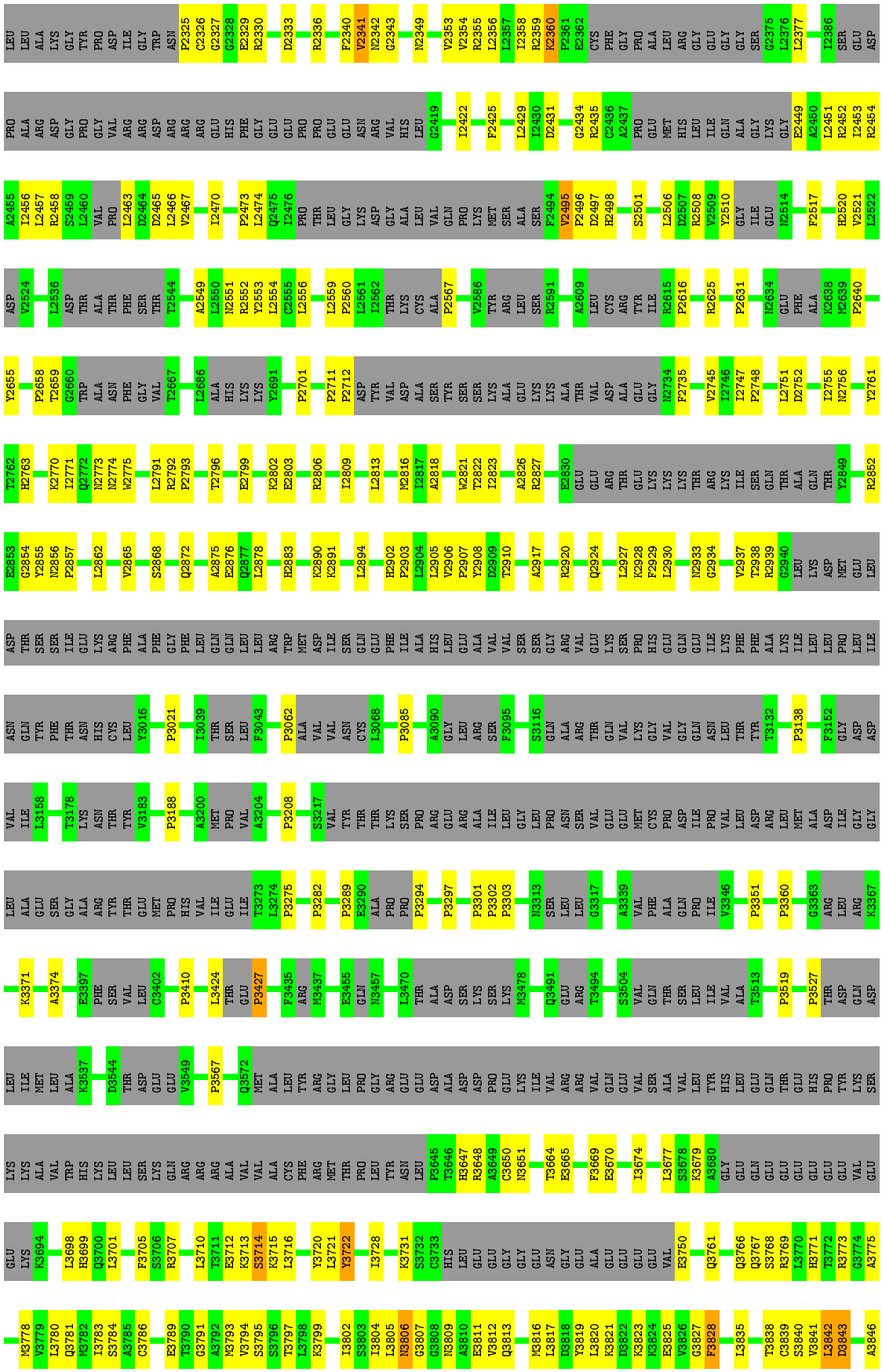


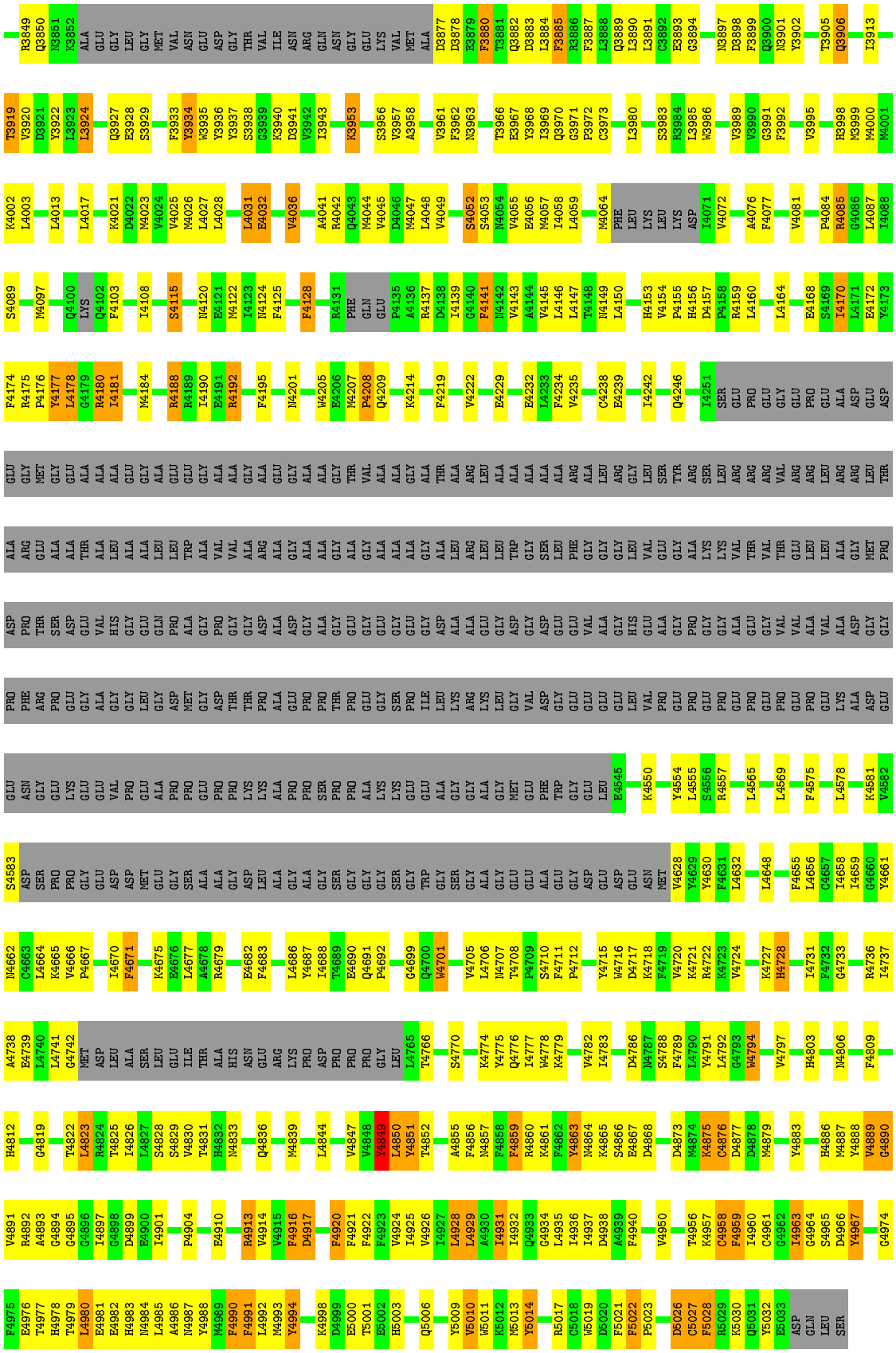
- Molecule 1: Ryanodine receptor 1

Chain E:



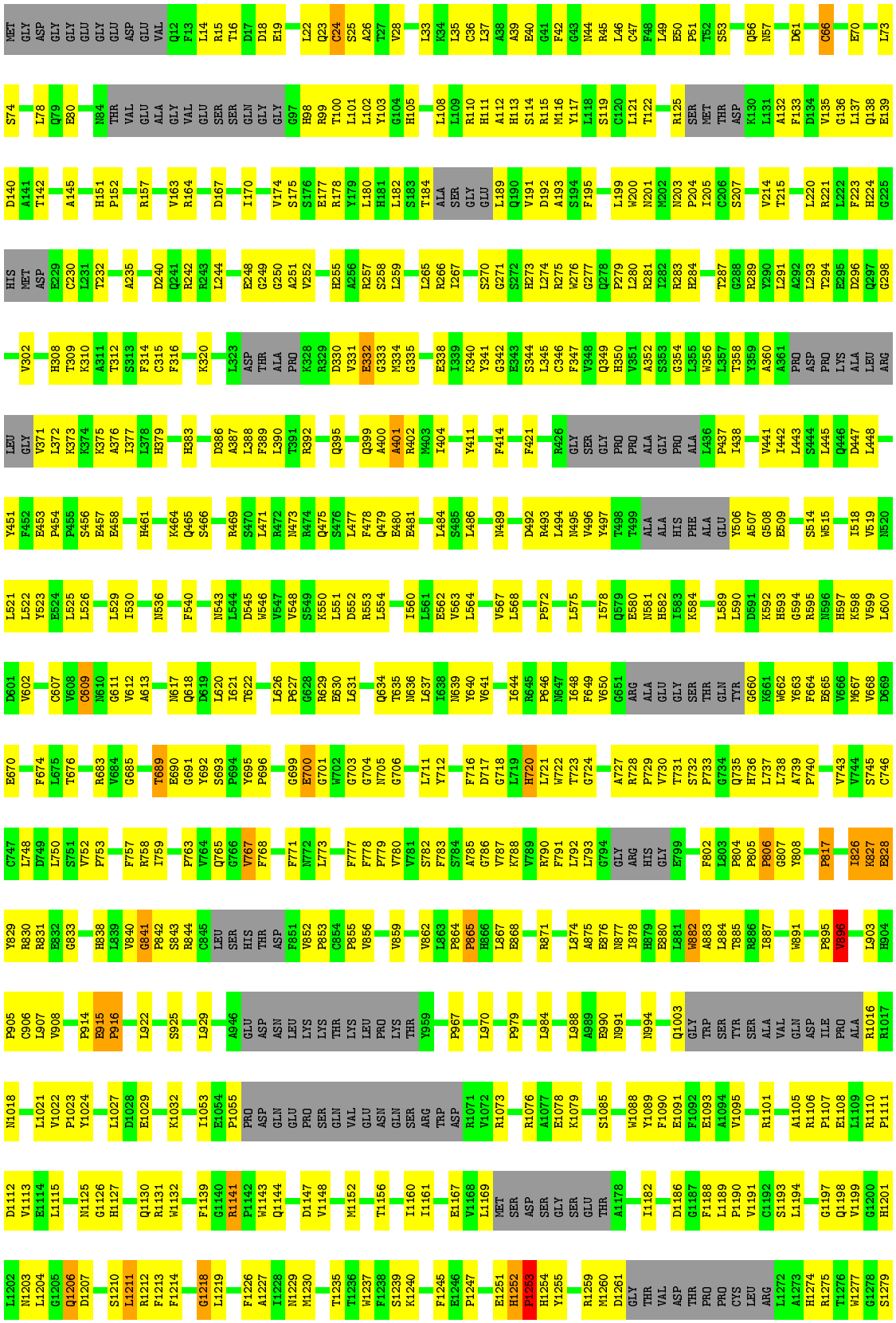


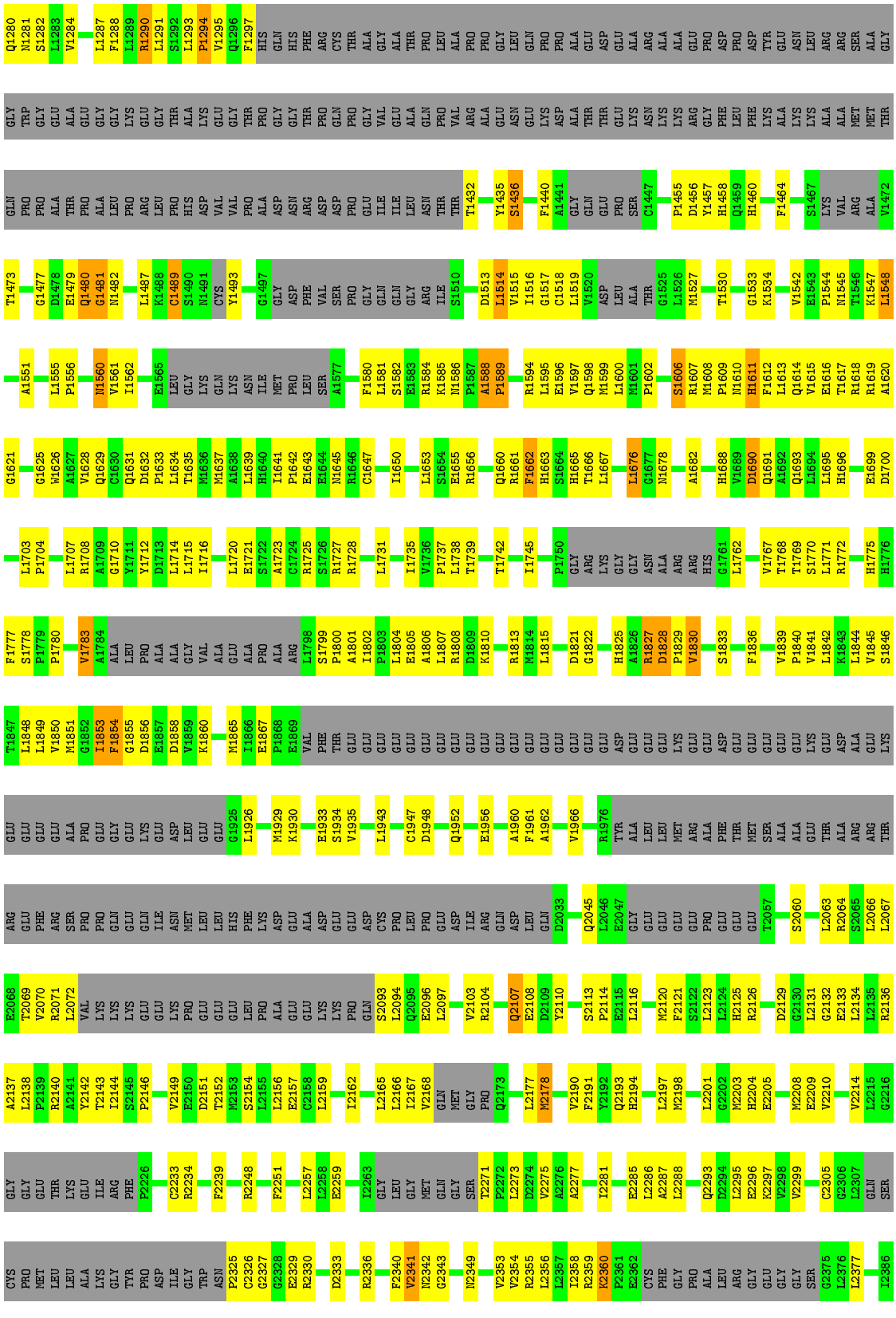


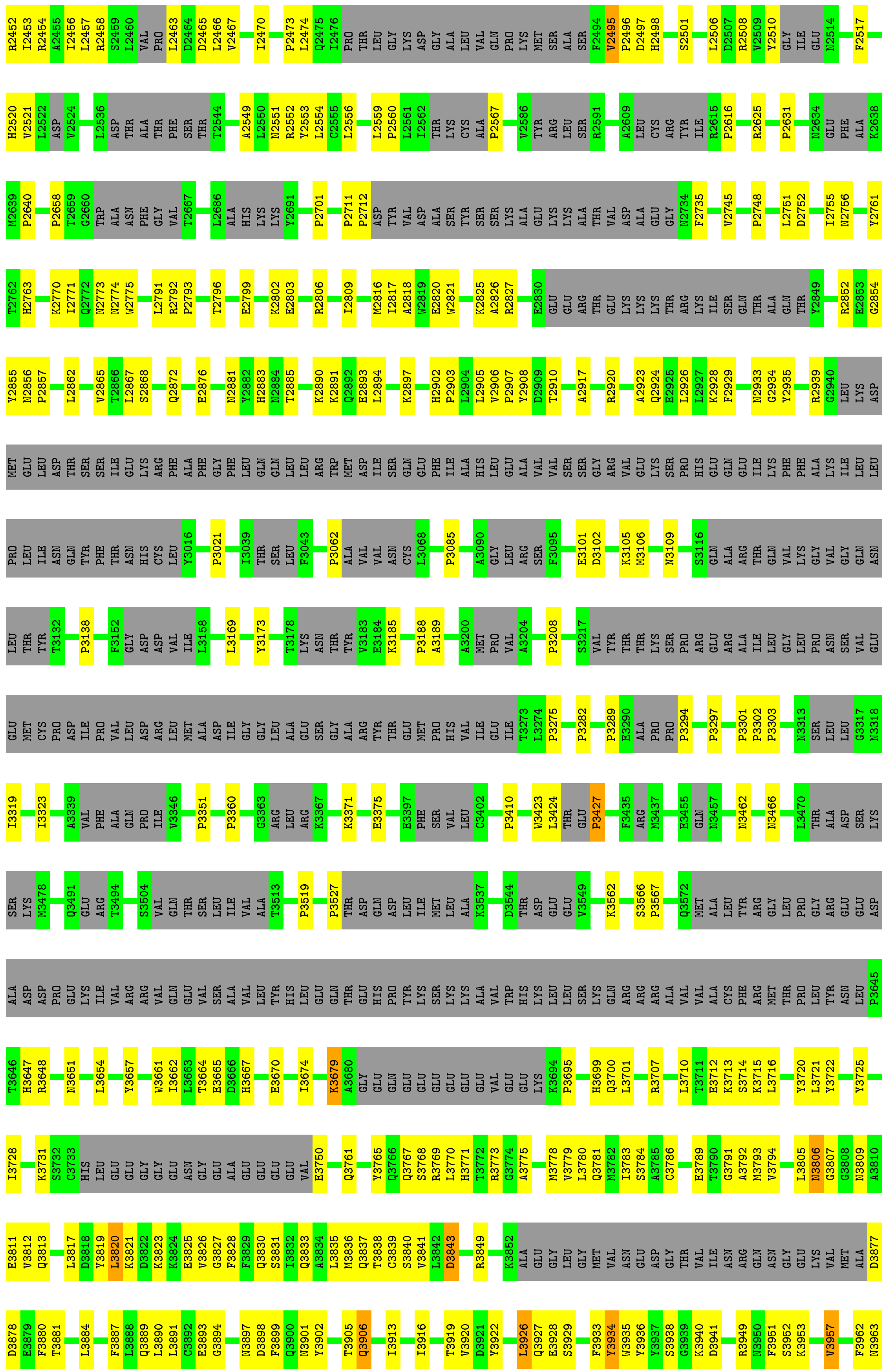


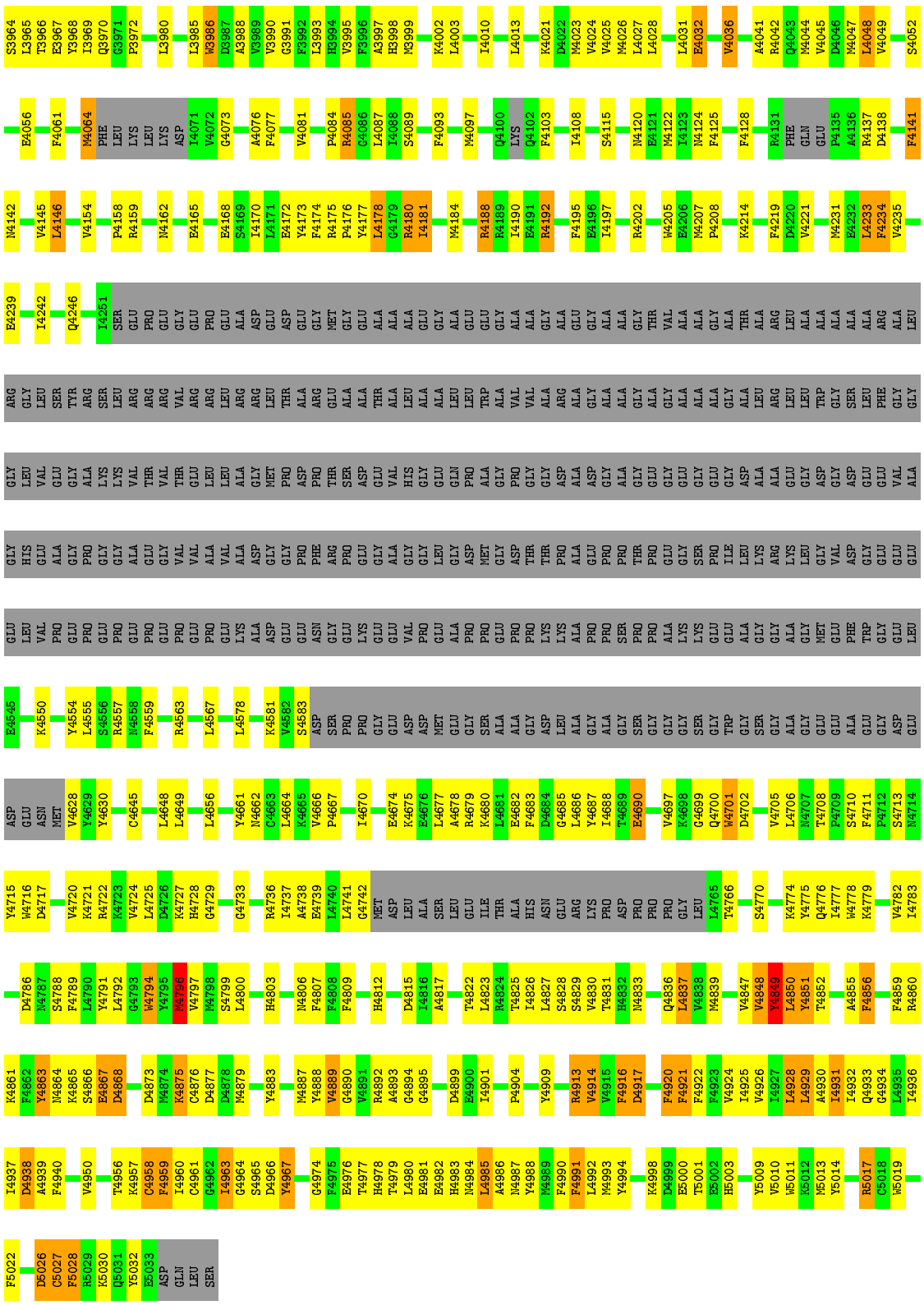
- Molecule 1: Ryanodine receptor 1

Chain G:



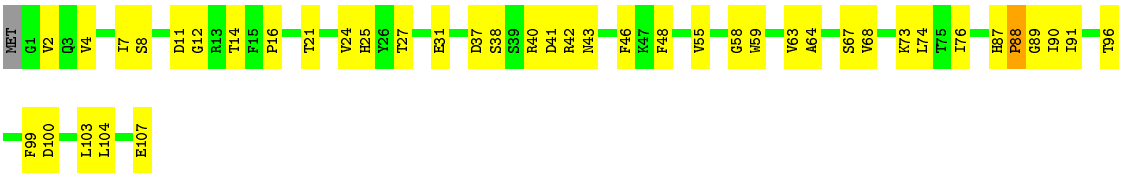



R2452 I2453 R2454 A2455 I2456 L2457 R2458 S2459 L2460 VAL PRO L2463 D2464 D2465 L2466 V2467 I2470 P2473 L2474 Q2475 I2476 PRO THR LEU GLY LYS ASP GLY ALA LEU VAL GLN PRO LYS MET SER ALA SER F2494 V2495 P2496 D2497 H2498 S2501 L2506 D2507 R2508 V2509 Y2510 GLY ILE GLU N2514 F2517
H2520 V2521 L2522 ASP V2524 L2536 ASP THR ALA THR PHE SER THR T2544 A2549 L2550 N2551 R2552 Y2553 L2554 C2555 L2556 L2559 P2560 L2561 I2562 THR LYS CYS ALA P2567 V2586 TYR ARG LEU SER R2591 A2609 LEU CYS ARG TYR ILE R2615 P2616 R2625 P2631 N2634 GLU PHE ALA K2638
M2639 P2640 P2658 T2659 G2660 TRP ALA ASN PHE GLY VAL T2667 L2686 ALA HIS LYS LYS Y2691 P2701 P2711 P2712 ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 V2745 P2748 L2751 D2752 I2755 N2756 Y2761
T2762 H2763 K2770 I2771 Q2772 N2773 N2774 W2775 L2791 R2792 P2793 T2796 E2799 K2802 E2803 R2806 I2809 M2816 I2817 A2818 W2819 E2820 W2821 K2825 A2826 R2827 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR Y2849 R2852 E2853 G2854
Y2855 N2856 P2857 L2862 V2865 T2866 L2867 S2868 Q2872 E2876 N2881 Y2882 H2883 N2884 T2885 K2890 K2891 Q2892 E2893 L2894 K2897 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 A2917 R2920 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 N2933 G2934 Y2935 R2939 G2940 LEU LYS ASP
MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU ILE LYS PHE PHE ALA LYS ILE LEU LEU
PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU Y3016 P3021 I3039 THR SER LEU F3043 P3062 ALA VAL VAL ASN CYS L3068 P3085 A3090 GLY LEU ARG SER F3095 E3101 D3102 K3105 M3106 N3109 S3116 GLN ALA ARG THR GLN VAL LYS GLY VAL GLY GLN ASN
LEU THR TYR T3132 P3138 F3152 GLY ASP ASP VAL ILE L3158 L3169 Y3173 T3178 LYS ASN THR TYR V3183 E3184 K3185 P3188 A3189 A3200 MET PRO VAL A3204 P3208 S3217 VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU
GLU MET CYS PRO ASP ILE PRO VAL LEU ASP ARG LEU MET ALA ASP ILE GLY GLY LEU ALA GLU SER GLY ALA ARG TYR THR GLU MET PRO HIS VAL ILE GLU ILE T3273 L3274 P3275 P3282 P3289 E3290 ALA PRO PRO P3294 P3297 P3301 P3302 P3303 N3313 SER LEU LEU G3317 N3318
I3319 I3323 A3339 VAL PHE ALA GLN PRO ILE V3346 P3351 P3360 G3363 ARG LEU ARG K3367 K3371 E3375 E3397 PHE SER VAL LEU C3402 P3410 W3423 L3424 THR GLU P3427 F3435 ARG M3437 E3455 GLN N3457 N3462 N3466 L3470 THR ALA ASP SER LYS
SER LYS M3478 Q3491 GLU ARG T3494 S3504 VAL GLN THR SER LEU ILE VAL ALA T3513 P3519 P3527 THR ASP GLN ASP LEU ILE MET LEU ALA K3537 D3544 THR ASP GLU GLU V3549 K3562 S3566 P3567 Q3572 MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP
ALA ASP ASP PRO GLU LYS ILE VAL ARG ARG VAL GLN GLU VAL SER ALA VAL LEU TYR HIS LEU GLU GLN THR GLU HIS PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET THR PRO LEU TYR ASN LEU P3645
T3646 H3647 R3648 N3651 L3654 Y3657 W3661 I3662 L3663 T3664 E3665 D3666 H3667 E3670 I3674 K3679 A3680 GLY GLU GLN GLU GLU GLU GLU GLU GLU VAL GLU LYS K3694 P3695 H3699 Q3700 L3701 R3707 L3710 T3711 E3712 K3713 S3714 K3715 L3716 Y3720 L3721 Y3722 Y3725
I3728 K3731 S3732 C3733 HIS LEU GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 Q3761 Y3765 Q3766 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 M3778 V3779 L3780 Q3781 M3782 I3783 S3784 A3785 C3786 E3789 T3790 G3791 A3792 M3793 V3794 L3805 N3806 G3807 G3808 N3809 A3810
E3811 V3812 Q3813 L3817 D3818 Y3819 L3820 K3821 D3822 K3823 K3824 E3825 V3826 G3827 F3828 F3829 Q3830 S3831 I3832 Q3833 A3834 L3835 M3836 Q3837 T3838 C3839 S3840 V3841 L3842 D3843 R3849 K3852 ALA GLU GLY LEU GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY GLU LYS VAL MET ALA D3877
D3878 E3879 F3880 T3881 L3884 F3887 L3888 Q3889 L3890 L3891 C3892 E3893 G3894 N3897 D3898 F3899 Q3900 N3901 Y3902 T3905 Q3906 I3913 I3916 T3919 V3920 D3921 Y3922 L3926 Q3927 E3928 S3929 F3933 Y3934 W3935 Y3936 Y3937 S3938 G3939 K3940 D3941 R3949 N3950 F3951 S3952 K3953 V3957 F3962 N3963



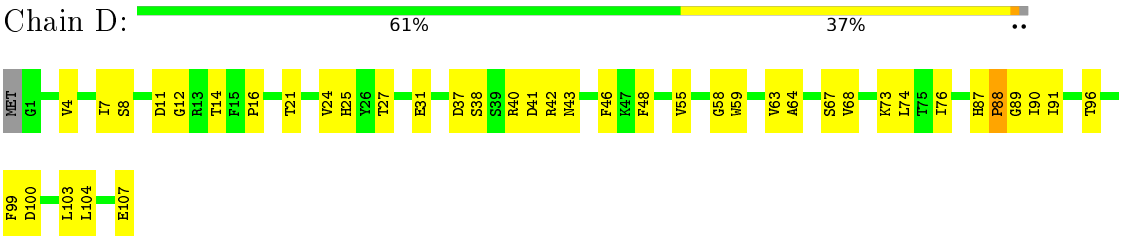
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain B:



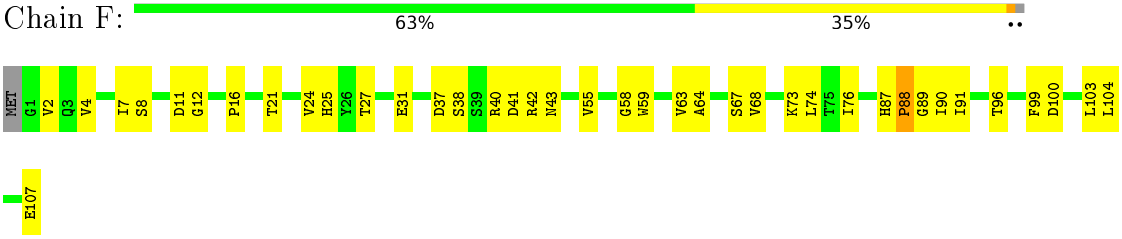
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain D:



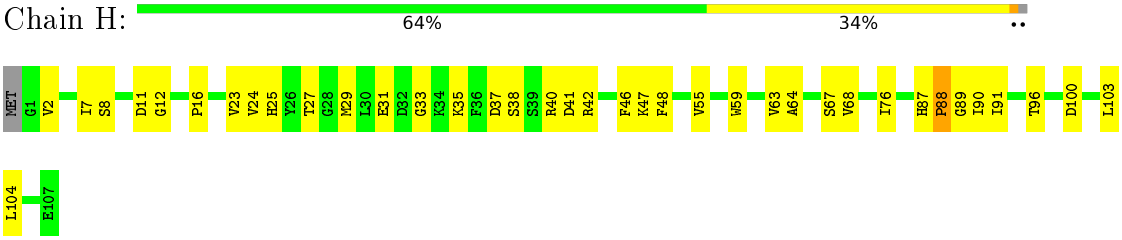
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	47000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.93	55/27385 (0.2%)	0.86	90/37104 (0.2%)
1	C	0.93	56/27385 (0.2%)	0.87	92/37104 (0.2%)
1	E	0.93	53/27385 (0.2%)	0.86	91/37104 (0.2%)
1	G	0.93	55/27385 (0.2%)	0.85	90/37104 (0.2%)
2	B	0.58	0/851	0.67	0/1146
2	D	0.58	0/851	0.67	0/1146
2	F	0.58	0/851	0.67	0/1146
2	H	0.60	0/851	0.67	0/1146
All	All	0.92	219/112944 (0.2%)	0.86	363/153000 (0.2%)

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
1	A	0	19
1	C	0	19
1	E	0	19
1	G	0	19
All	All	0	76

The worst 5 of 219 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4988	TYR	CG-CD2	-12.12	1.23	1.39
1	A	5014	TYR	CG-CD1	-11.55	1.24	1.39
1	E	5014	TYR	CG-CD1	-11.43	1.24	1.39
1	C	3922	TYR	CE1-CZ	-11.19	1.24	1.38
1	E	3922	TYR	CE1-CZ	-11.12	1.24	1.38

The worst 5 of 363 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	4128	PHE	CB-CG-CD2	-10.00	113.80	120.80
1	E	4128	PHE	CB-CG-CD2	-9.73	113.99	120.80
1	C	4128	PHE	CB-CG-CD2	-9.69	114.02	120.80
1	A	4128	PHE	CB-CG-CD2	-9.62	114.07	120.80
1	E	4064	MET	CG-SD-CE	8.87	114.39	100.20

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1252	HIS	Peptide
1	A	1253	PRO	Peptide
1	A	1464	PHE	Mainchain
1	A	332	GLU	Mainchain,Peptide
1	A	841	GLY	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	26917	0	24461	1094	0
1	C	26917	0	24461	1105	0
1	E	26917	0	24461	1108	0
1	G	26917	0	24461	1100	0
2	B	832	0	831	38	0
2	D	832	0	831	37	0
2	F	832	0	831	36	0
2	H	832	0	831	34	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111000	0	101168	4395	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 21.

The worst 5 of 4395 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)
1:E:4826:ILE:CG2	1:G:4931:ILE:HD11	1.79	1.10
1:A:4879:MET:SD	1:G:4578:LEU:HA	1.92	1.10
1:A:4826:ILE:CG2	1:C:4931:ILE:HD11	1.86	1.05
1:E:4578:LEU:HA	1:G:4879:MET:SD	1.99	1.03
1:C:4826:ILE:CG2	1:E:4931:ILE:HD11	1.91	1.00

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	3496/5037 (69%)	3173 (91%)	220 (6%)	103 (3%)	6	45
1	C	3496/5037 (69%)	3169 (91%)	223 (6%)	104 (3%)	5	45
1	E	3496/5037 (69%)	3169 (91%)	223 (6%)	104 (3%)	5	45
1	G	3496/5037 (69%)	3169 (91%)	226 (6%)	101 (3%)	6	45
2	B	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	19	65
2	D	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	19	65
2	F	105/108 (97%)	92 (88%)	12 (11%)	1 (1%)	19	65
2	H	105/108 (97%)	89 (85%)	15 (14%)	1 (1%)	19	65
All	All	14404/20580 (70%)	13045 (91%)	943 (6%)	416 (3%)	9	45

5 of 416 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	689	THR
1	A	720	HIS
1	A	806	PRO

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Mol	Chain	Res	Type
1	A	916	PRO
1	A	1253	PRO

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	2500/4276 (58%)	2486 (99%)	14 (1%)	90	95
1	C	2501/4276 (58%)	2487 (99%)	14 (1%)	90	95
1	E	2502/4276 (58%)	2486 (99%)	16 (1%)	90	95
1	G	2501/4276 (58%)	2482 (99%)	19 (1%)	86	93
2	B	89/90 (99%)	89 (100%)	0	100	100
2	D	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10360/17464 (59%)	10297 (99%)	63 (1%)	91	95

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	806	PRO
1	E	979	PRO
1	G	1934	SER
1	E	852	VAL
1	E	885	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3700	GLN
1	E	1127	HIS
1	G	2247	GLN

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Mol	Chain	Res	Type
1	C	3813	GLN
1	E	203	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.