wwPDB EM Validation Summary Report

Oct 5, 2024 – 10:52 AM EDT

PDB ID	:	5TB0
EMDB ID	:	EMD-8391
Title	:	Structure of rabbit RyR1 (EGTA-only 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:

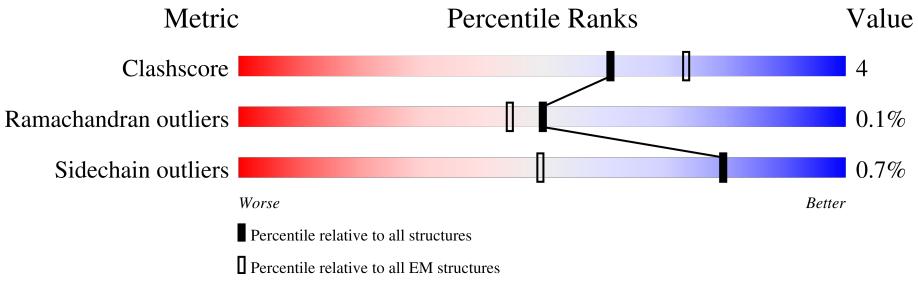
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	55% 91% 8% ·
1	F	108	55% 90% 9% ·
1	H	108	52% 91% 8% ·
1	J	108	54% 90% 9% ·
2	B	4416	52% 85% 10% 5%
2	E	4416	52% 85% 10% 5%
2	G	4416	51% 85% 10% 5%
2	I	4416	52% 85% 10% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 121272 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	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		

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

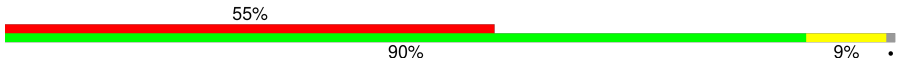
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

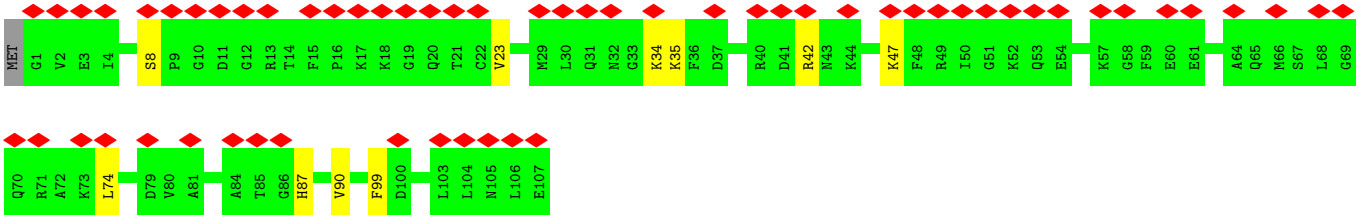
3 Residue-property plots (i)

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

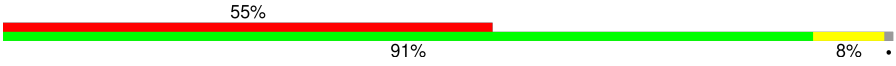
Chain F:

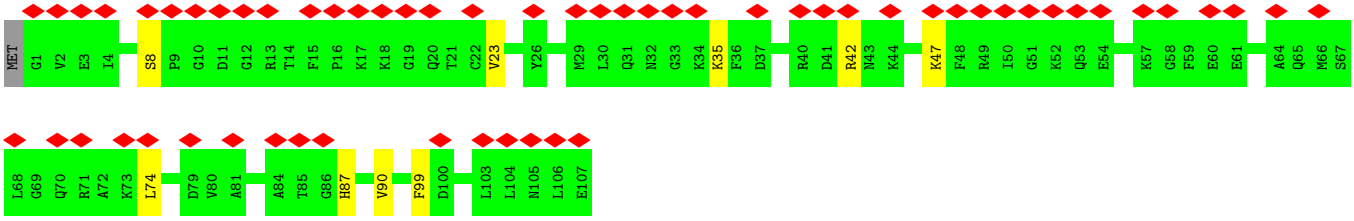




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

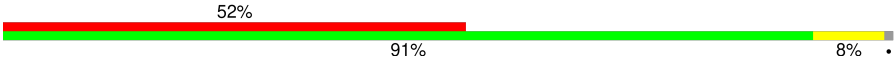
Chain A:

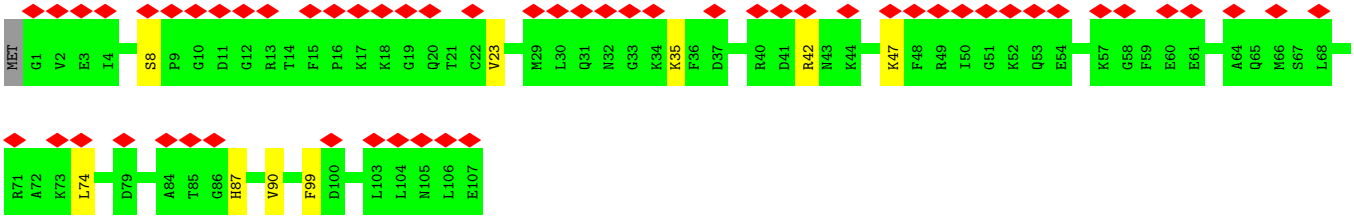




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

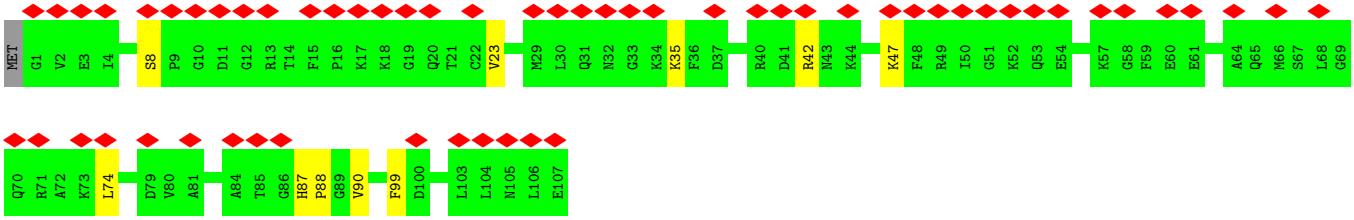
Chain H:





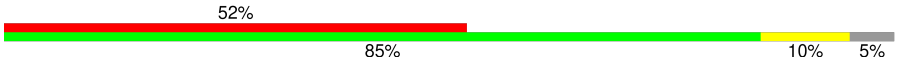
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

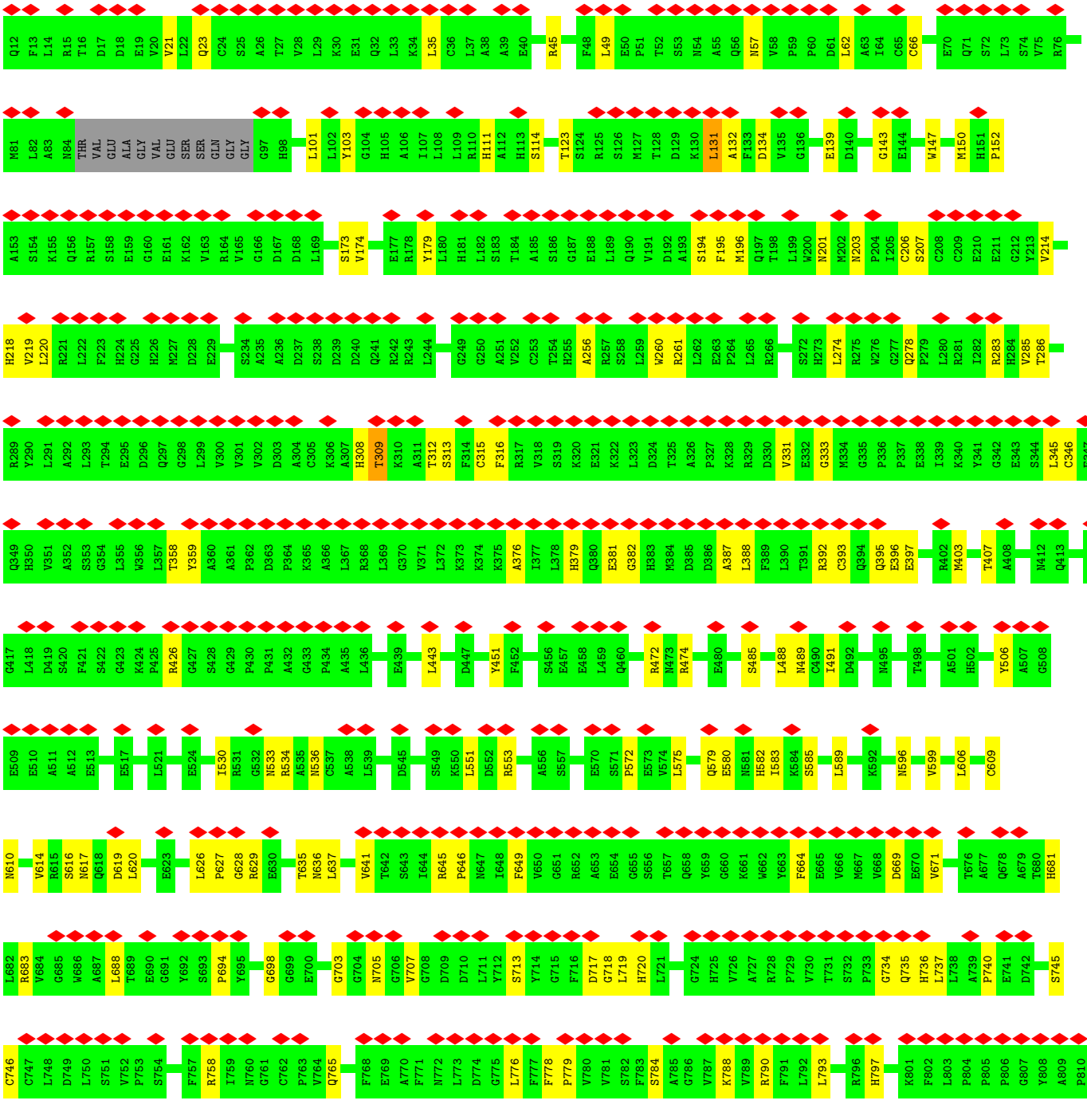
Chain J:

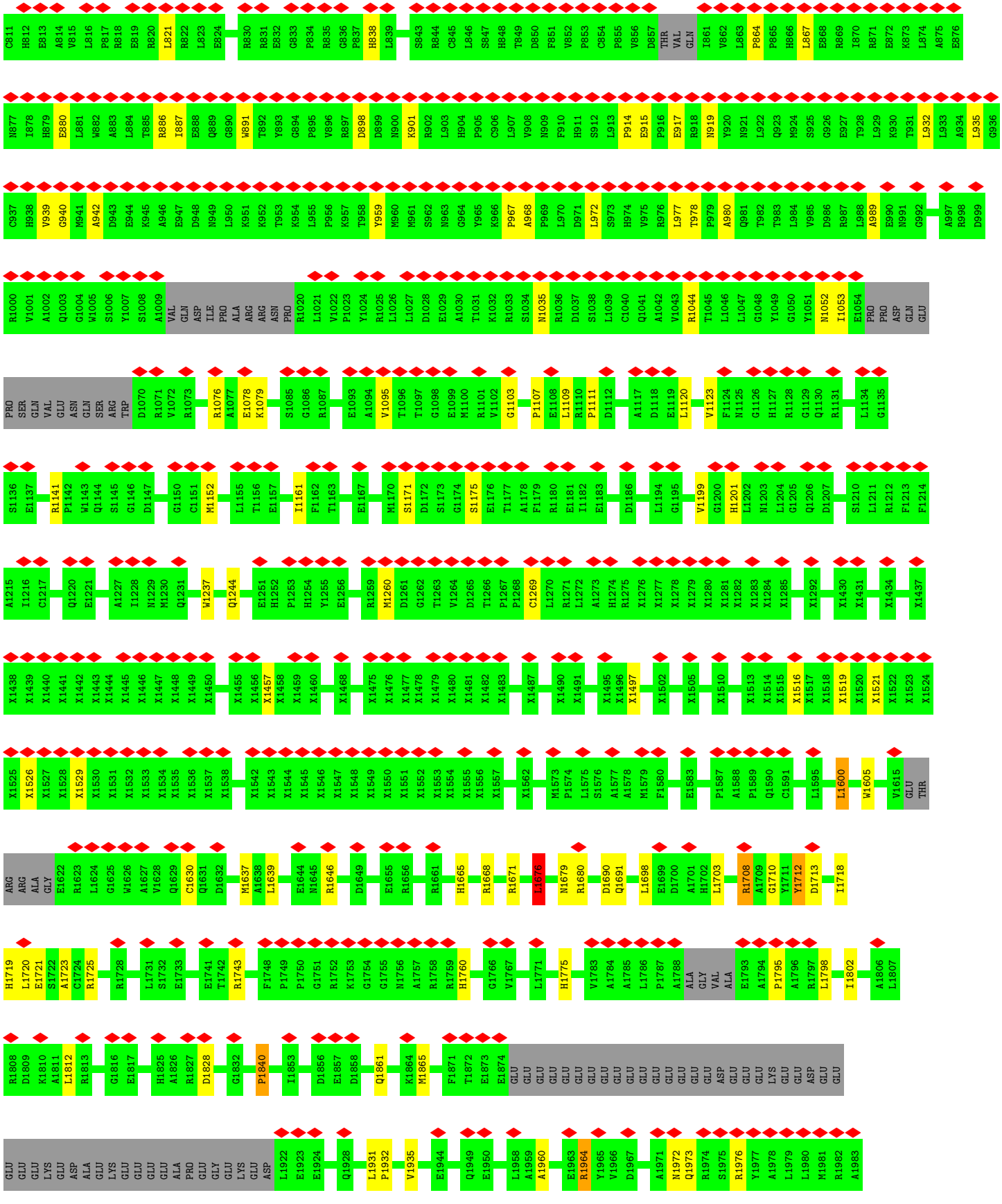


• Molecule 2: Ryanodine receptor 1

Chain B:



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R1000 V1001 A1002 Q1003 G1004 W1005 S1006 Y1007 S1008 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 P1023 Y1024 R1025 L1026 L1027 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU
PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 R1076 A1077 E1078 K1079 S1085 G1086 R1087 E1093 A1094 V1095 T1096 T1097 G1098 E1099 M1100 R1101 V1102 G1103 P1107 E1108 L1109 R1110 P1111 D1112 A1117 D1118 E1119 L1120 V1123 F1124 N1125 G1126 H1127 R1128 G1129 Q1130 R1131 L1134 G1135
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ARG ARG ALA GLY E1622 R1623 L1624 G1625 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 M1637 A1638 L1639 E1644 N1645 R1646 D1649 E1655 R1656 R1661 H1665 R1668 R1671 L1676 N1679 R1680 D1690 Q1691 L1698 E1699 D1700 A1701 H1702 L1703 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718
H1719 L1720 E1721 S1722 A1723 C1724 R1725 R1728 L1731 S1732 E1733 E1741 T1742 R1743 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1766 V1767 L1771 H1775 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798 I1802 A1806 L1807
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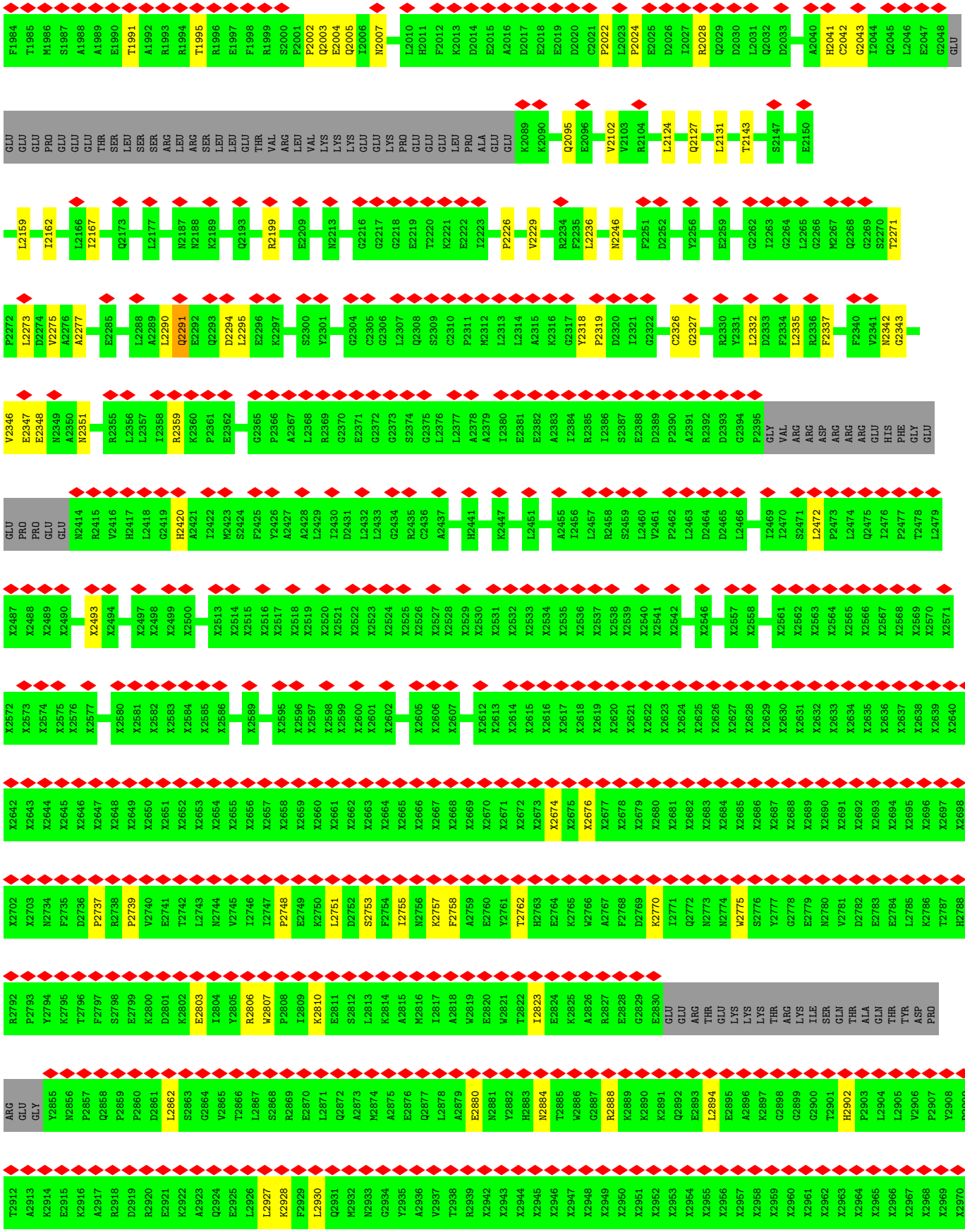
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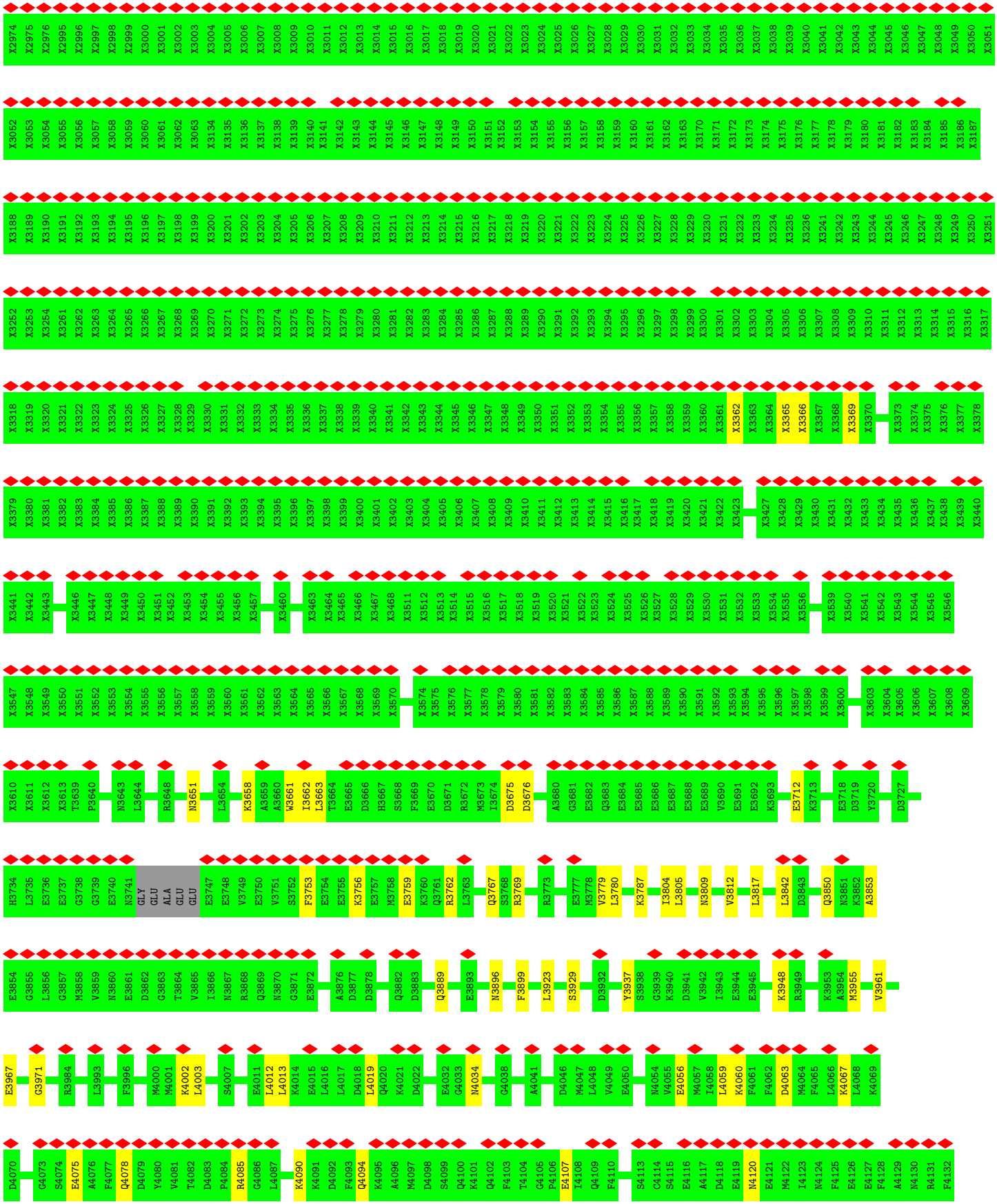
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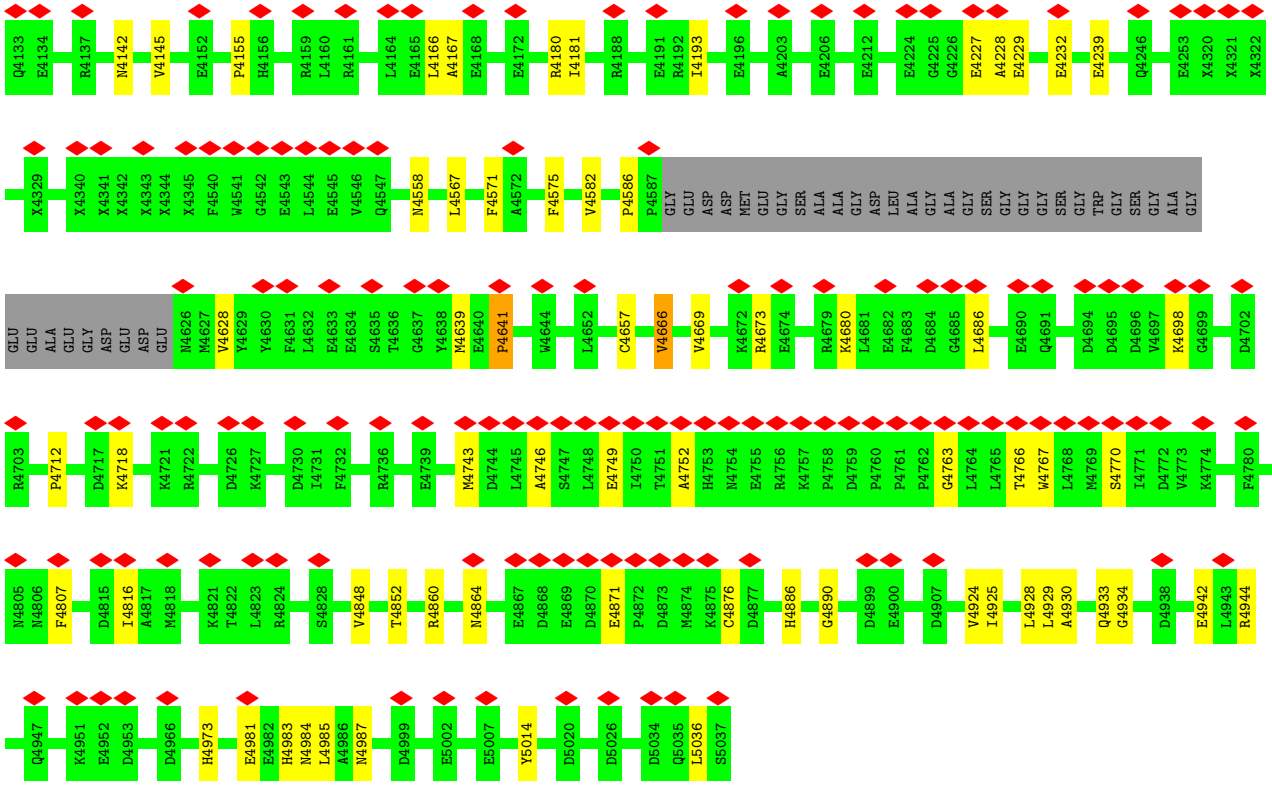

• Molecule 2: Ryanodine receptor 1

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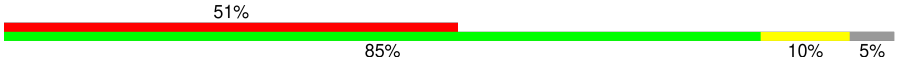

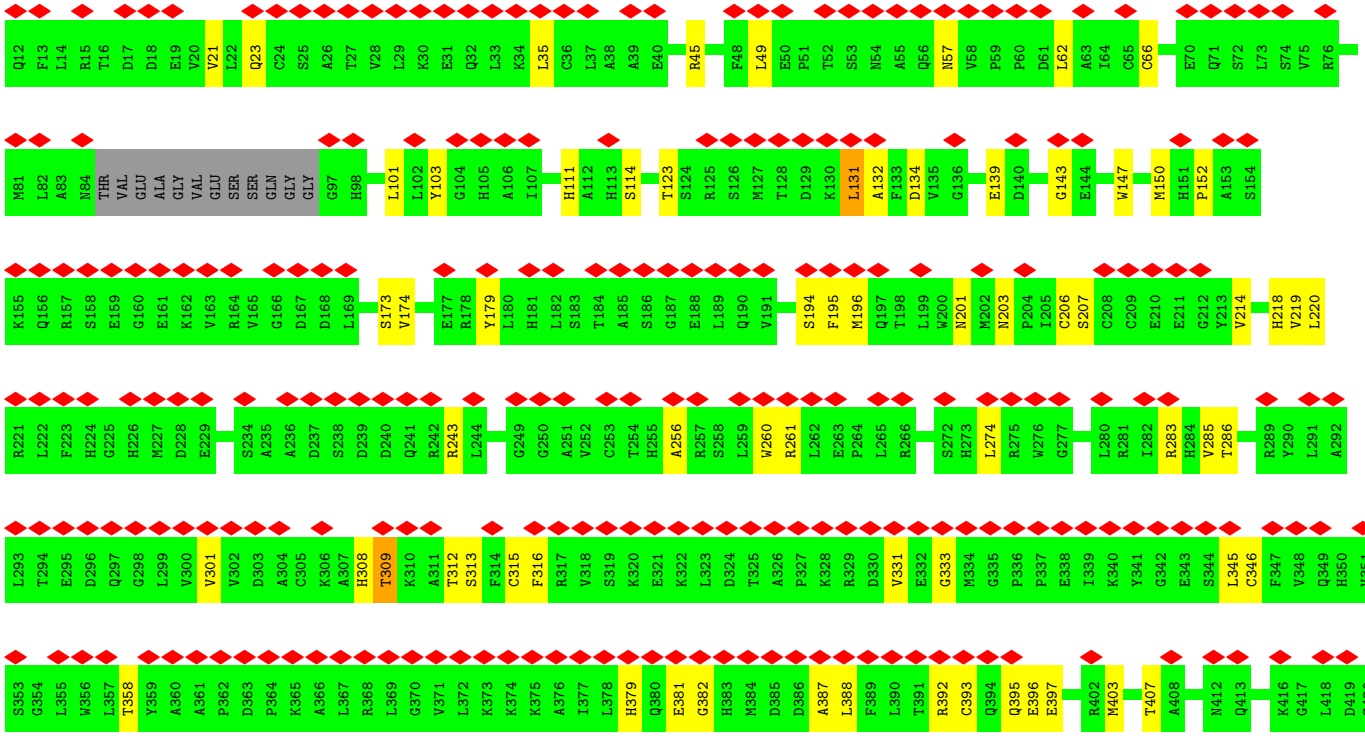

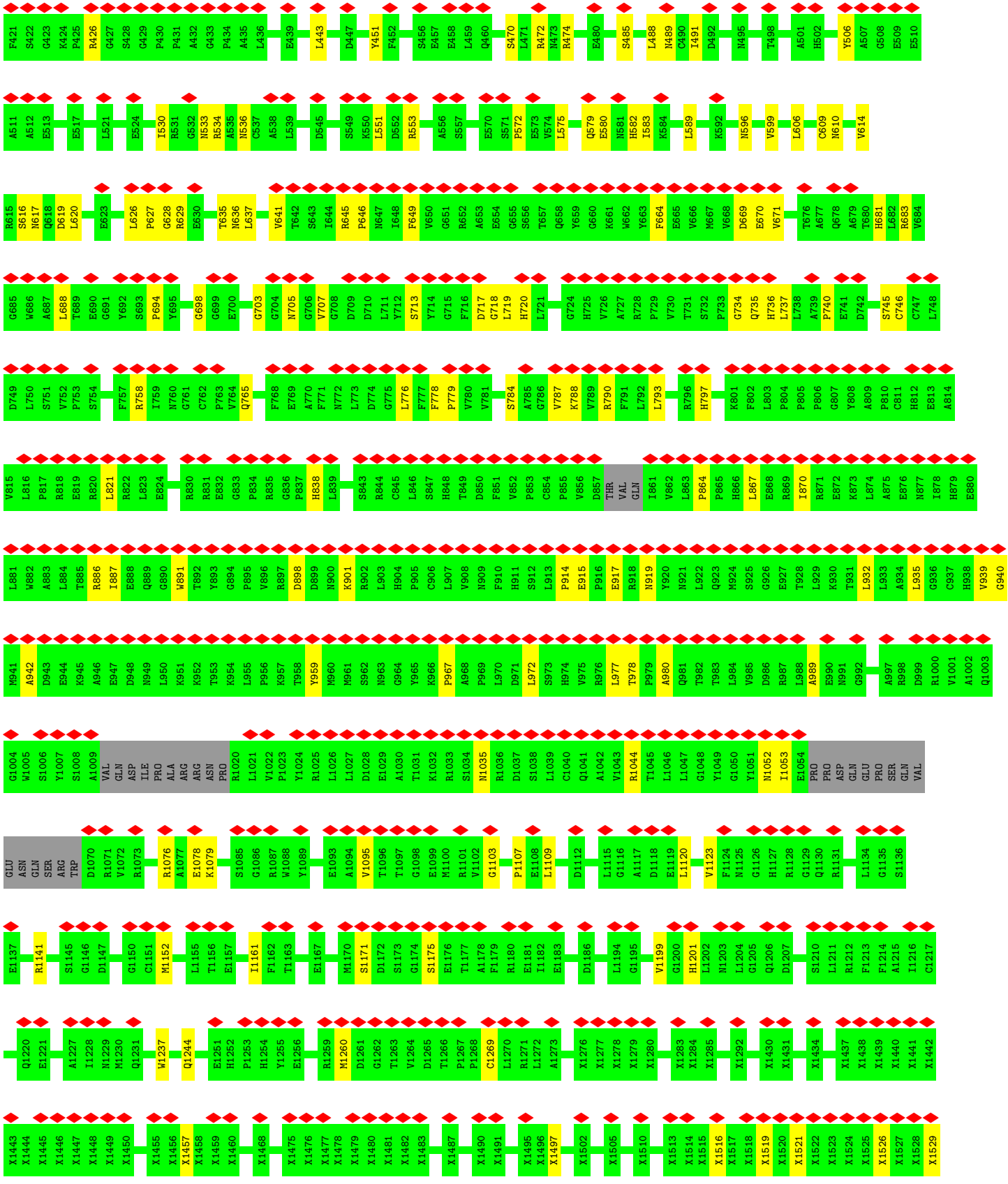
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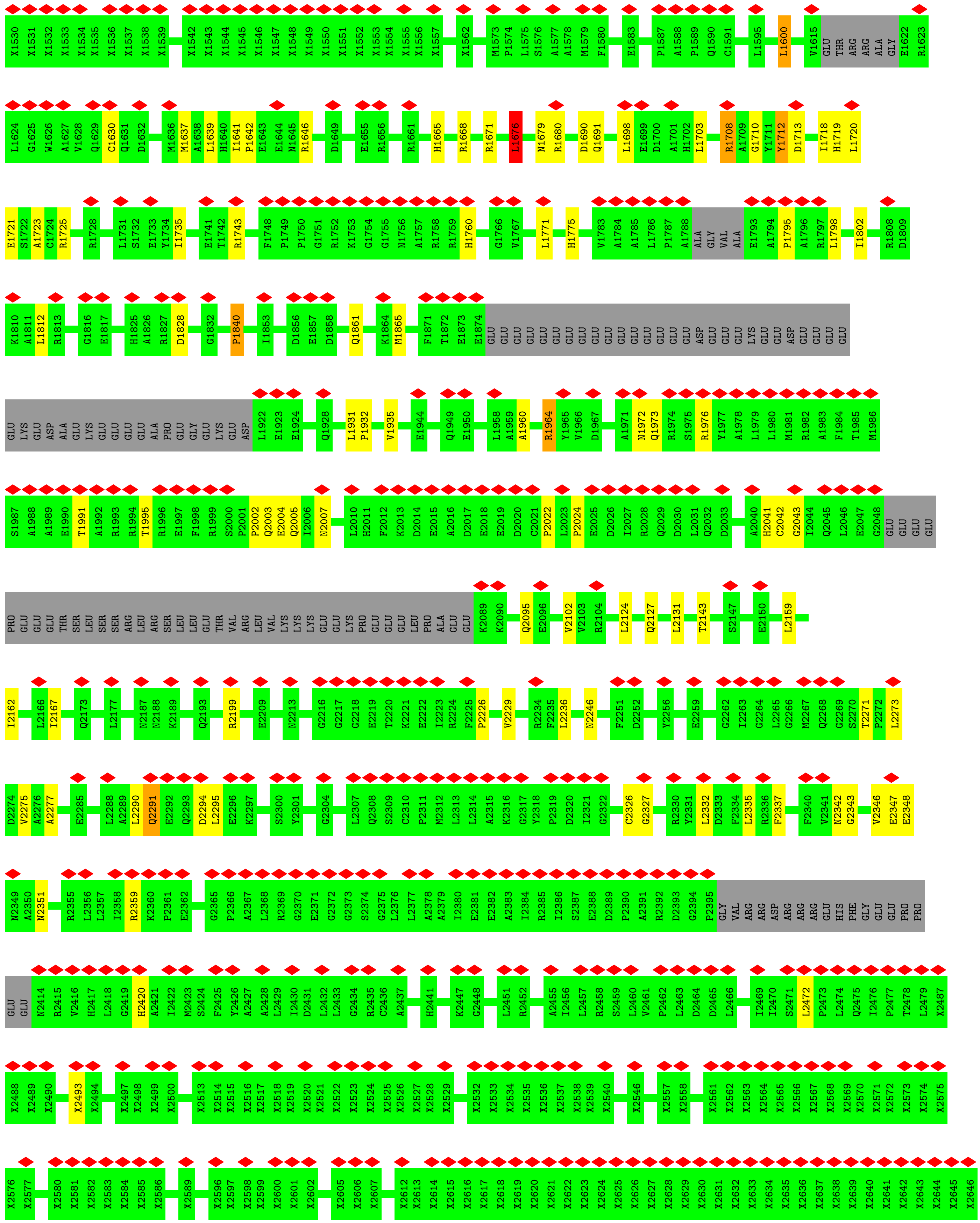
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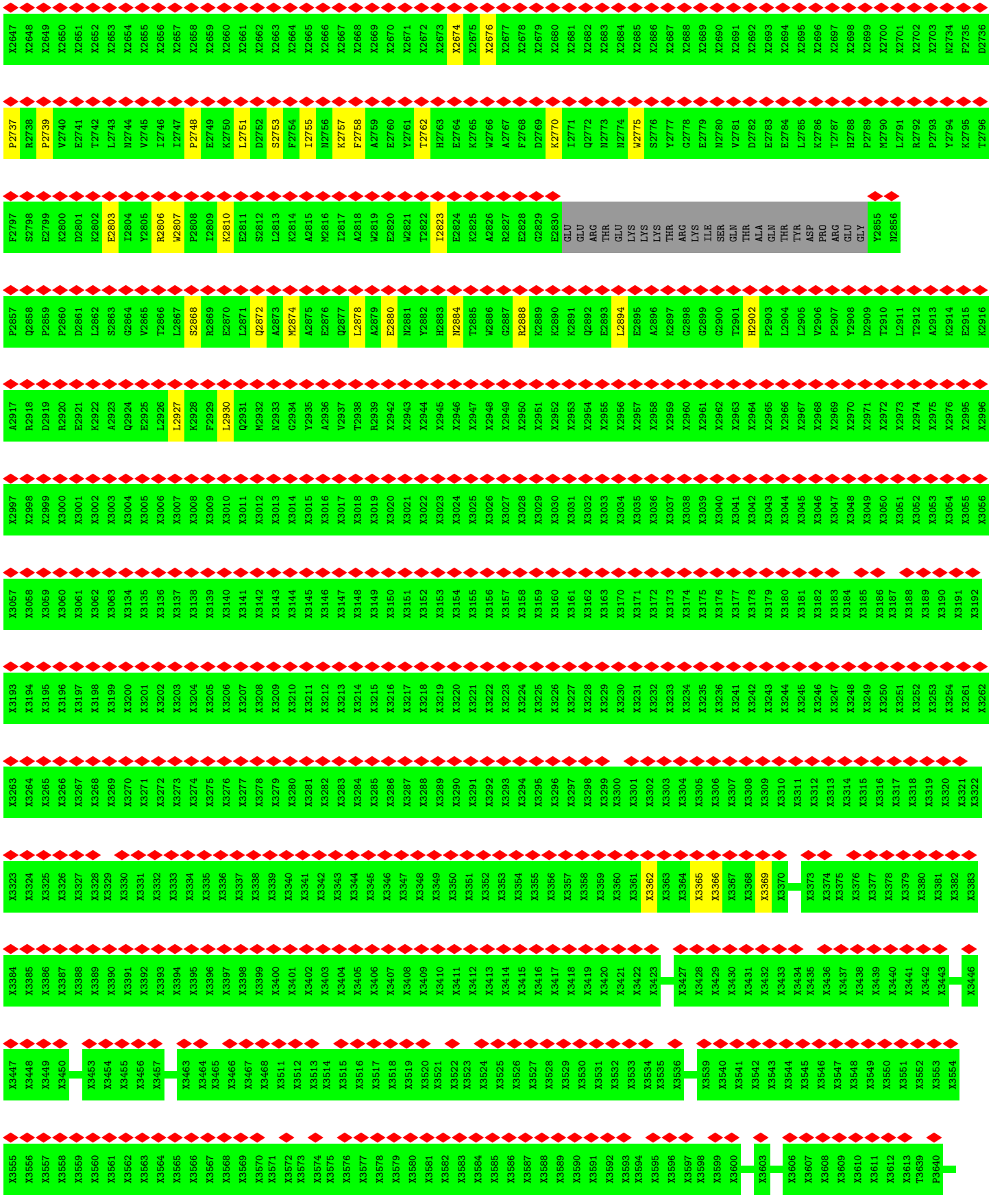
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• Molecule 2: Ryanodine receptor 1

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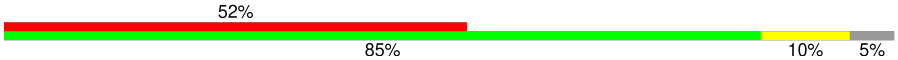

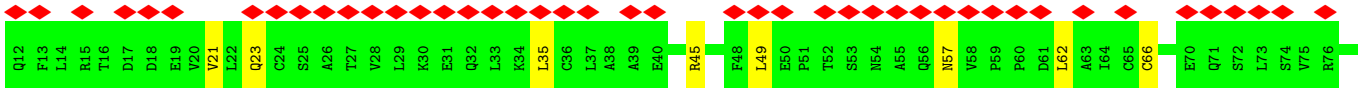

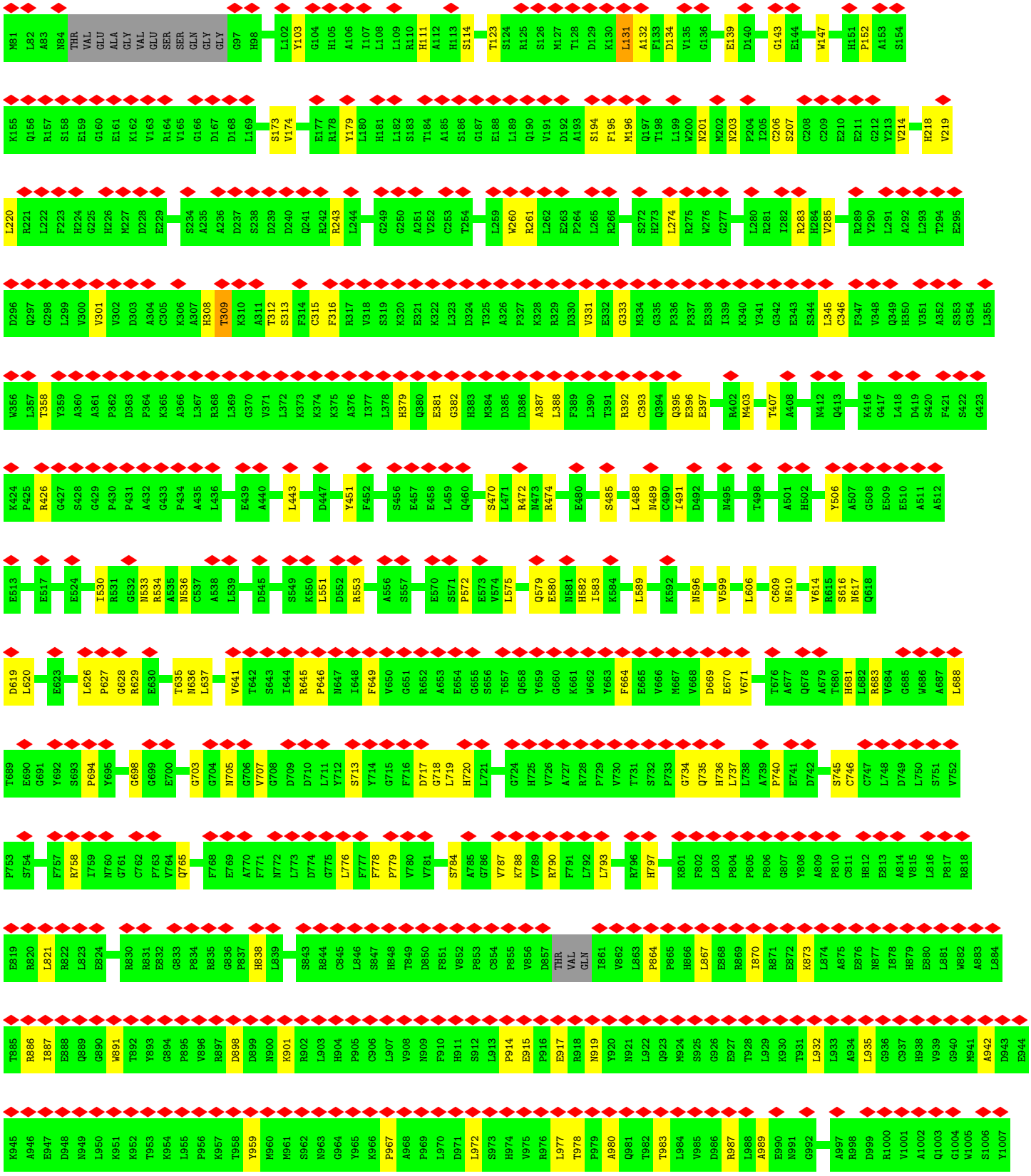
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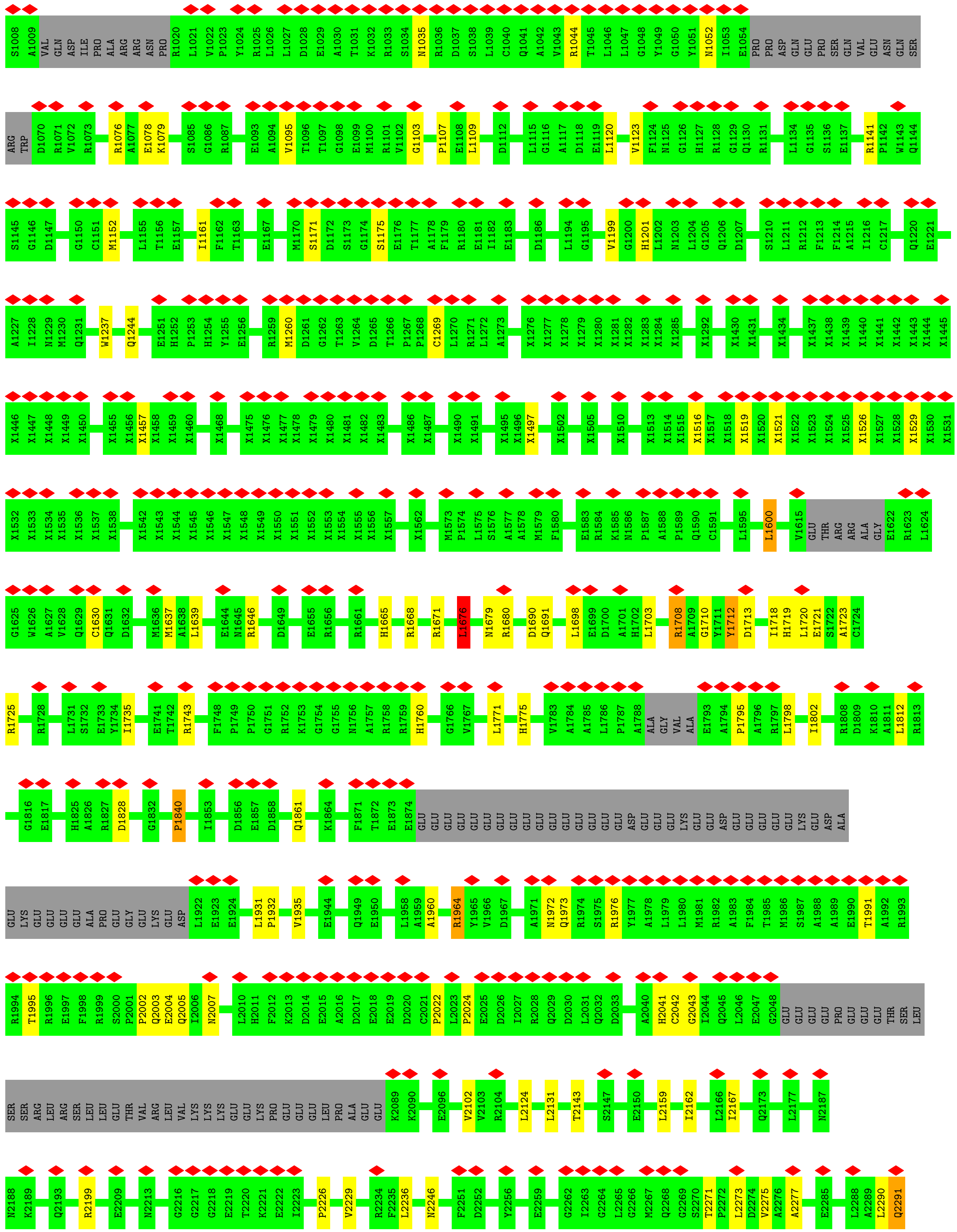
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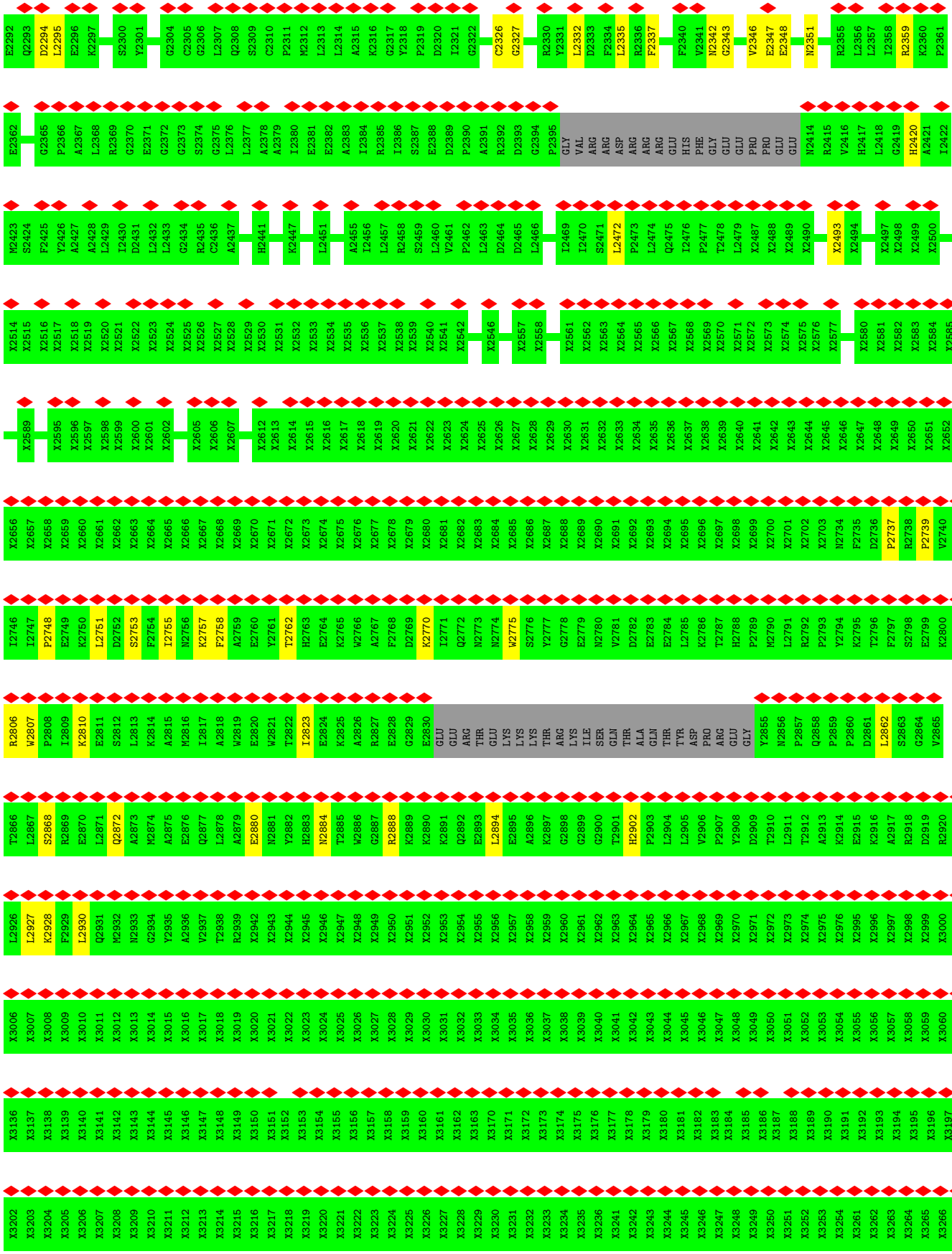
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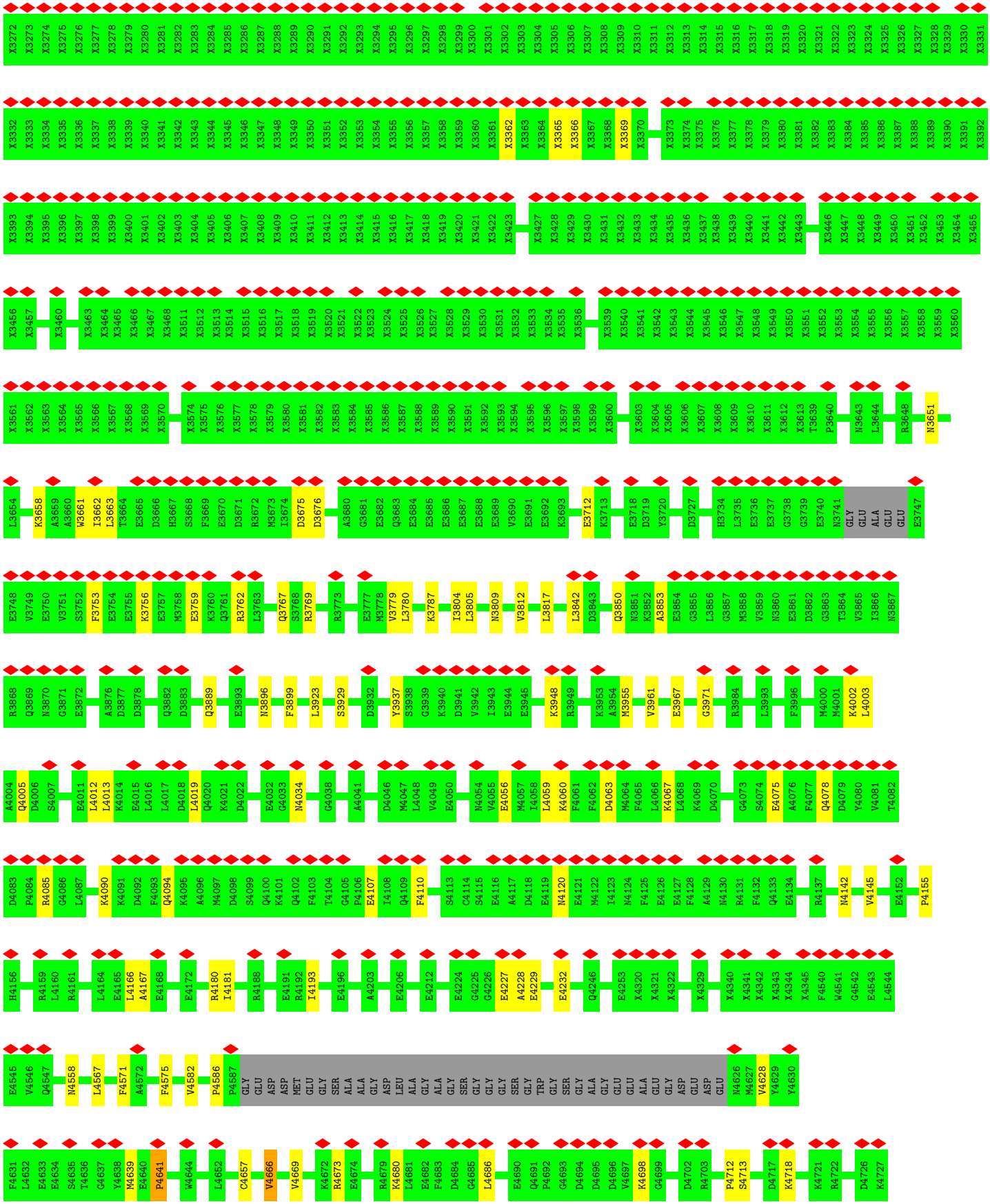
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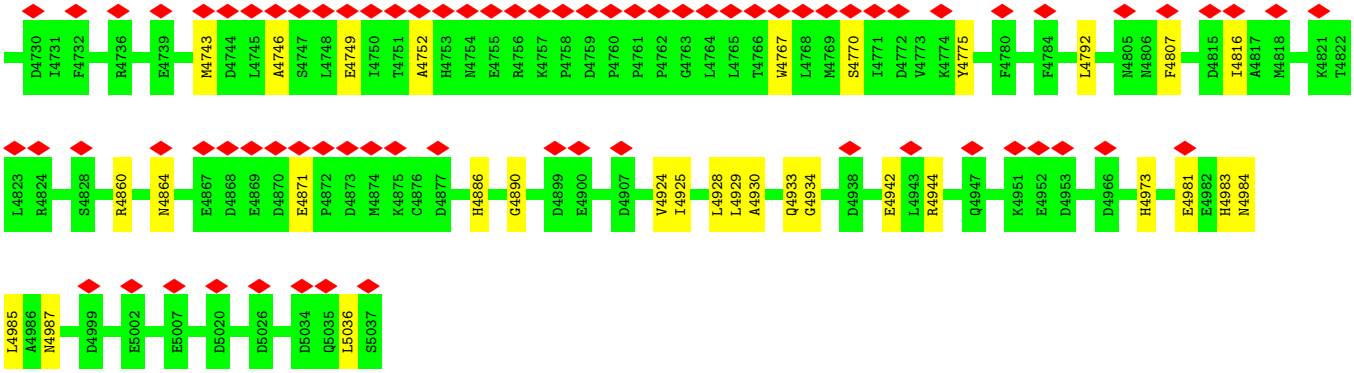

• Molecule 2: Ryanodine receptor 1

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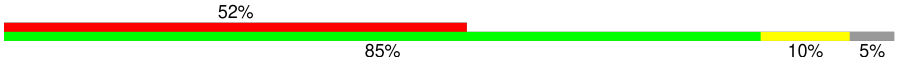

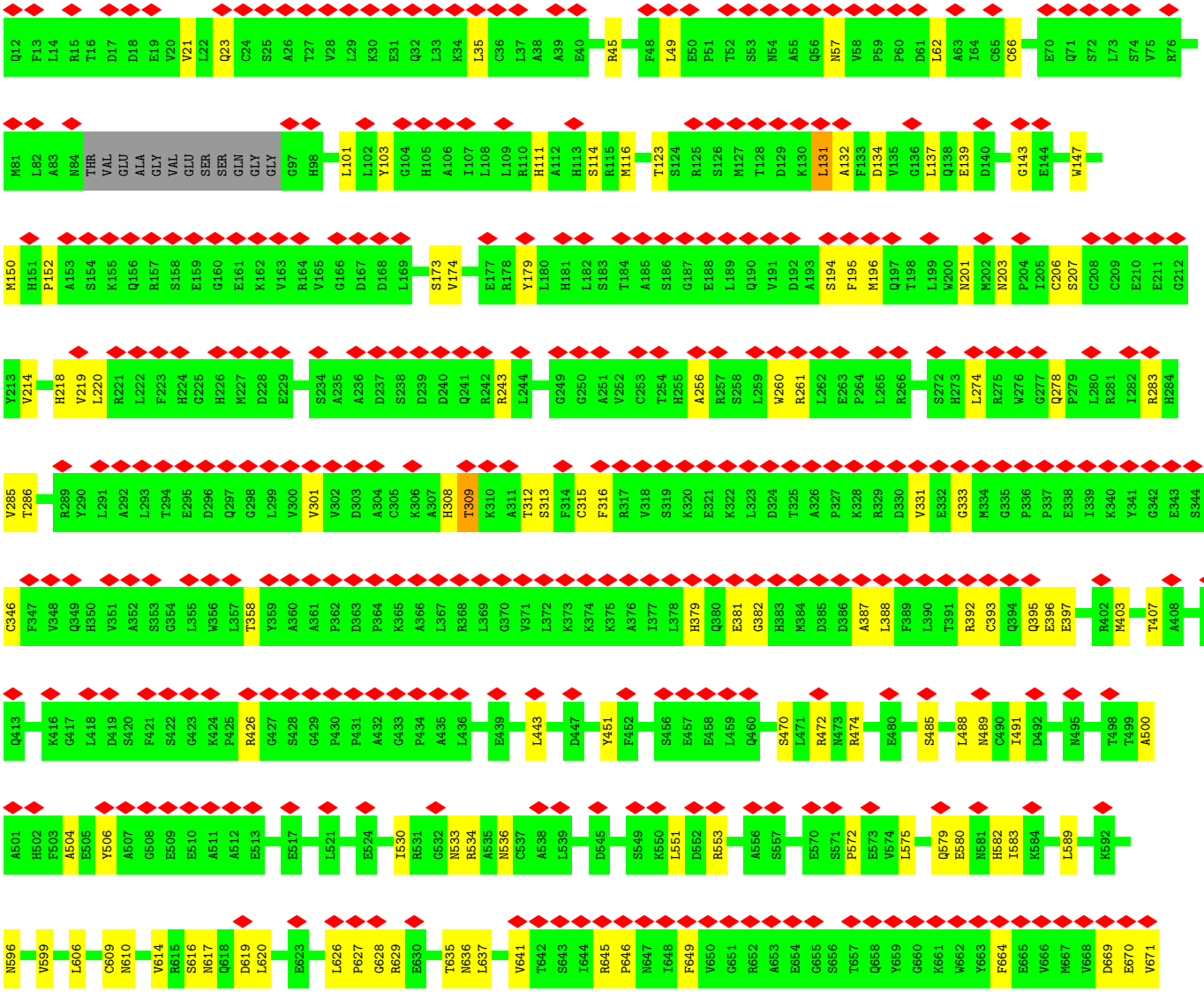

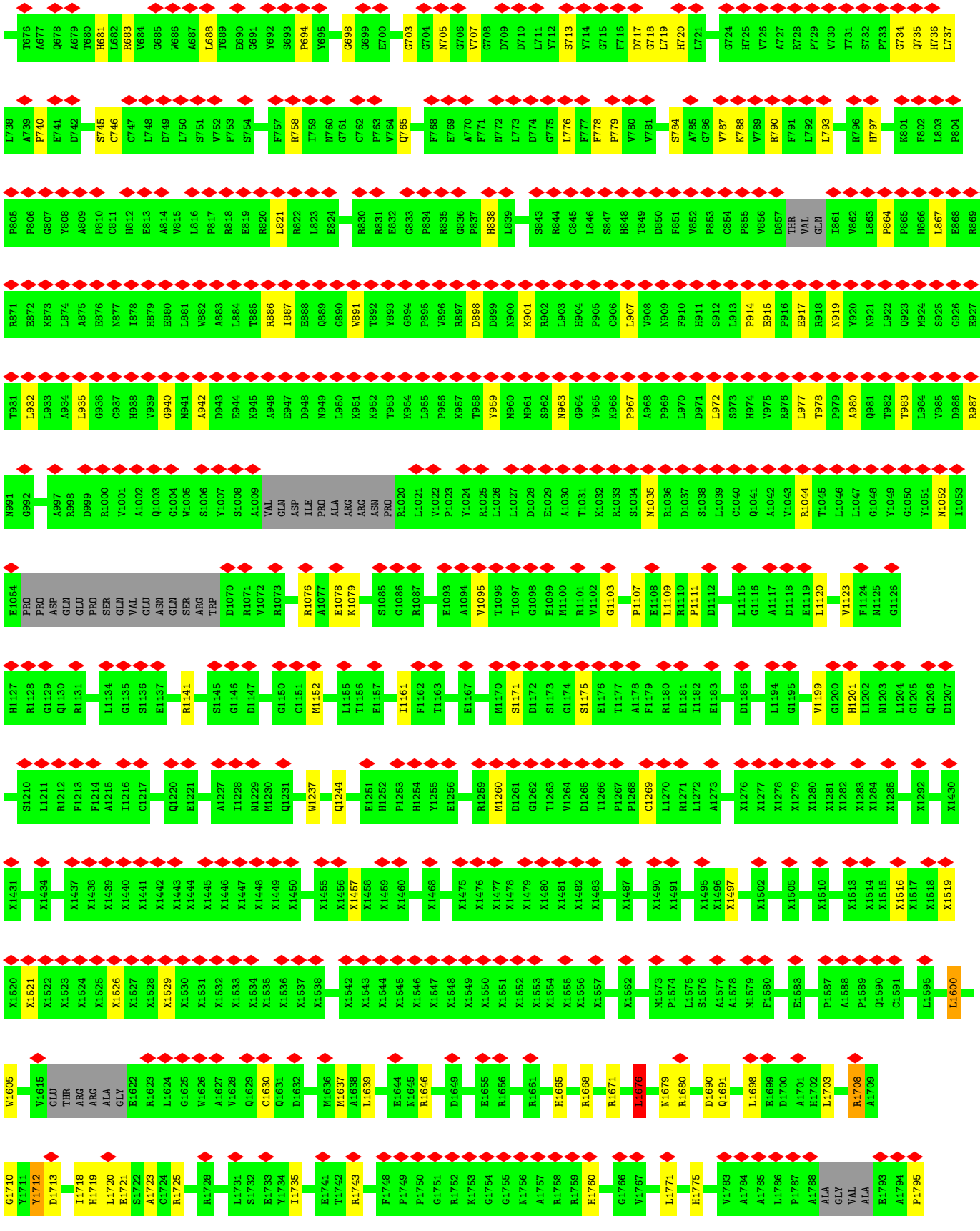
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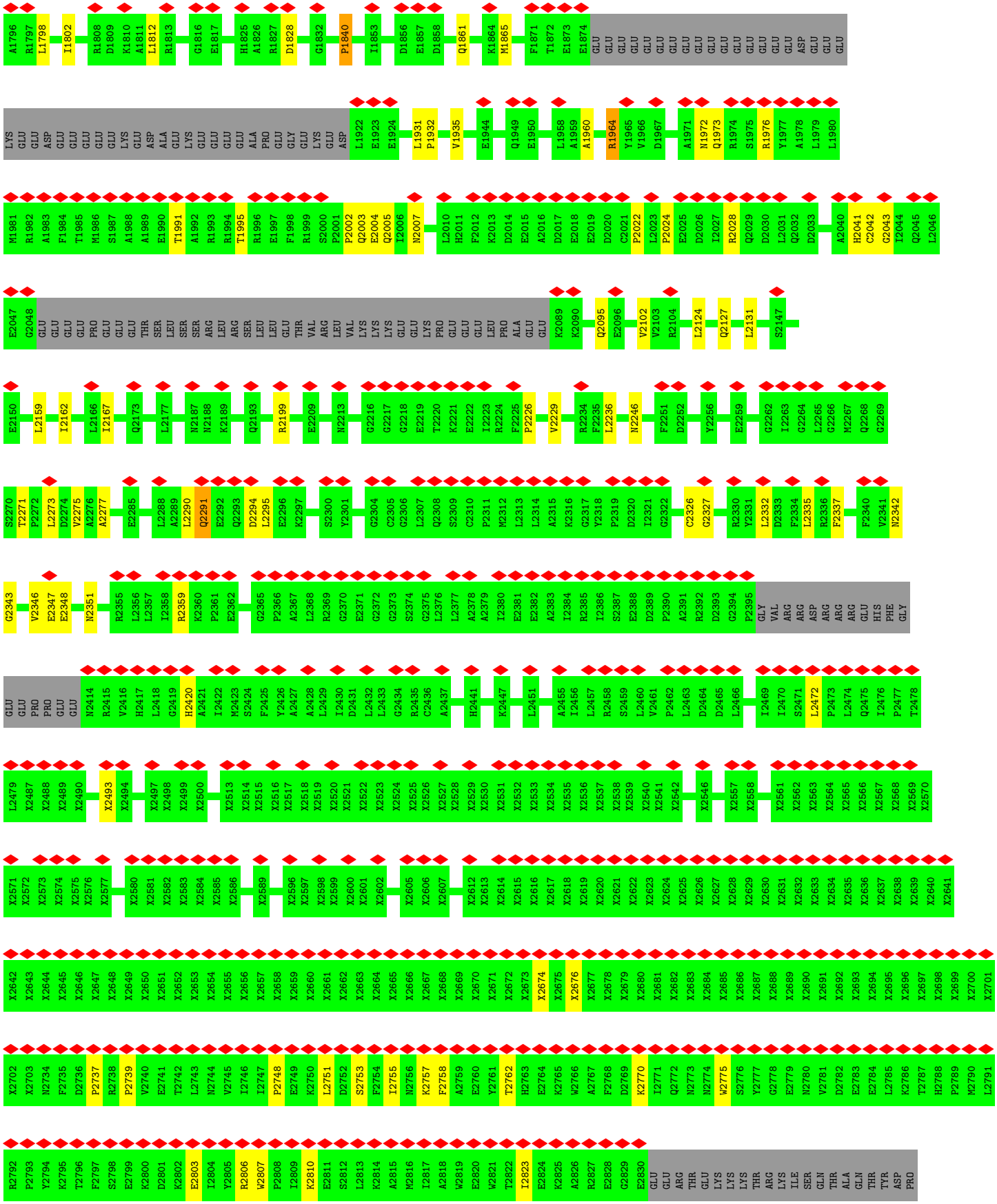
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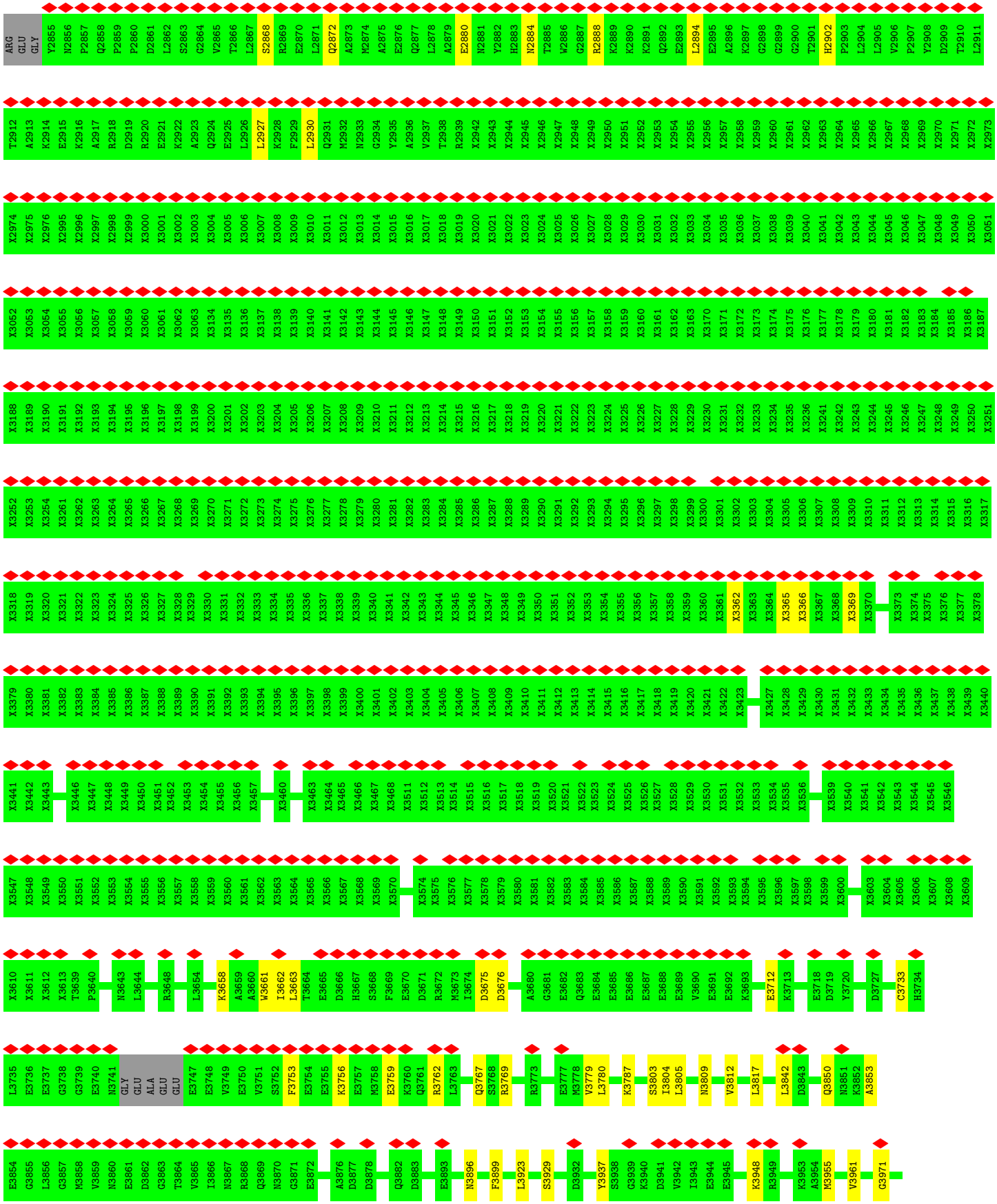
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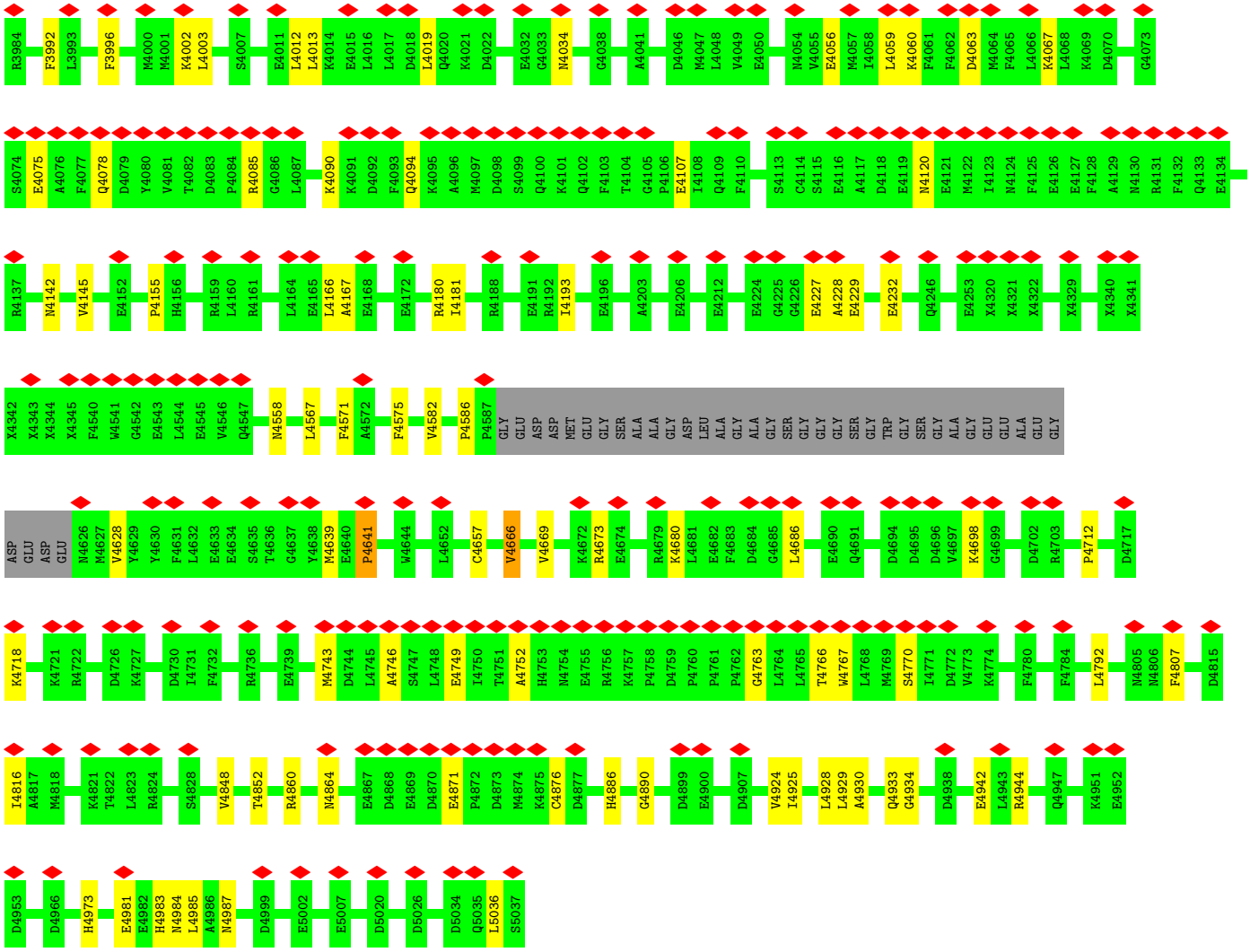
R3984 F3992 L3993 F3996 M4000 M4001 K4002 L4003 S4007 E4011 L4012 L4013 K4014 E4015 L4016 L4017 D4018 L4019 Q4020 K4021 D4022 E4032 G4033 M4034 G4038 A4041 D4046 M4047 L4048 V4049 E4050 M4054 V4055 E4056 M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 F4065 L4066 K4067 L4068 K4069 D4070 G4073
S4074 E4075 A4076 F4077 Q4078 D4079 Y4080 V4081 T4082 D4083 P4084 R4085 G4086 L4087 K4090 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 E4107 I4108 Q4109 F4110 S4113 C4114 S4115 E4116 A4117 D4118 E4119 N4120 E4121 M4122 I4123 N4124 F4125 E4126 E4127 F4128 A4129 N4130 R4131 F4132 Q4133 E4134
R4137 N4142 V4145 E4152 P4155 H4156 R4159 L4160 R4161 L4164 E4165 L4166 A4167 E4168 E4172 R4180 I4181 R4188 E4191 R4192 I4193 E4196 A4203 E4206 E4212 E4224 G4225 G4226 E4227 A4228 E4229 E4232 Q4246 E4253 X4320 X4321 X4322 X4329 X4340 X4341
X4342 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547 N4558 L4567 F4571 A4572 F4575 V4582 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY
ASP GLU ASP GLU N4626 M4627 V4628 Y4629 Y4630 F4631 L4632 E4633 E4634 S4635 T4636 G4637 Y4638 M4639 E4640 P4641 W4644 L4652 C4657 V4666 V4669 K4672 R4673 E4674 R4679 K4680 L4681 E4682 F4683 D4684 G4685 L4686 E4690 Q4691 D4694 D4695 D4696 V4697 K4698 G4699 D4702 R4703 P4712 D4717
K4718 K4721 R4722 D4726 K4727 D4730 I4731 F4732 R4736 E4739 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 K4774 F4780 F4784 L4792 N4805 N4806 F4807 D4815
I4816 A4817 M4818 K4821 T4822 L4823 R4824 S4828 V4848 T4852 R4860 N4864 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876 D4877 H4886 G4890 D4899 E4900 D4907 V4924 I4925 L4928 L4929 A4930 Q4933 G4934 D4938 E4942 L4943 R4944 Q4947 K4951 E4952
D4953 D4966 H4973 E4981 E4982 H4983 N4984 L4985 A4986 N4987 D4999 E5002 E5007 D5020 D5026 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	0.081	Depositor
Minimum map value	-0.049	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.32	0/25428	0.56	9/34534 (0.0%)
2	E	0.32	0/25428	0.56	9/34534 (0.0%)
2	G	0.32	0/25428	0.56	9/34534 (0.0%)
2	I	0.32	0/25428	0.56	9/34534 (0.0%)
All	All	0.32	0/105048	0.56	36/142628 (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
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.74	135.39	115.30
2	B	131	LEU	CA-CB-CG	8.73	135.38	115.30
2	I	131	LEU	CA-CB-CG	8.72	135.36	115.30
2	E	131	LEU	CA-CB-CG	8.72	135.36	115.30
2	I	1676	LEU	CA-CB-CG	6.26	129.70	115.30

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	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	6	0
1	H	818	0	824	5	0
1	J	818	0	824	6	0
2	B	29499	0	24749	236	0
2	E	29499	0	24750	227	0
2	G	29499	0	24749	236	0
2	I	29499	0	24749	237	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
All	All	121272	0	102293	929	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 4.

The worst 5 of 929 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.55	0.72
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.55	0.71
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.55	0.71
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.55	0.71
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.62	0.65

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%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4416 (73%)	2874 (89%)	357 (11%)	4 (0%)	48	83
2	E	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	48	83
2	G	3235/4416 (73%)	2875 (89%)	356 (11%)	4 (0%)	48	83
2	I	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	48	83
All	All	13360/18096 (74%)	11875 (89%)	1469 (11%)	16 (0%)	50	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	B	1932	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	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%)	81 87
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	81 87
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	81 87
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	81 87
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	80 87

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

Mol	Chain	Res	Type
2	I	1600	LEU
2	I	1964	ARG
2	I	4085	ARG
2	G	1676	LEU
2	G	1600	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	582	HIS
2	E	4120	ASN
2	E	1598	GLN
2	E	2005	GLN
2	I	111	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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	G	14
2	E	14
2	I	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	73.03
1	G	4345:UNK	C	4540:PHE	N	73.03
1	E	4345:UNK	C	4540:PHE	N	73.03
1	I	4345:UNK	C	4540:PHE	N	73.03

Continued on next page...

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	46.34

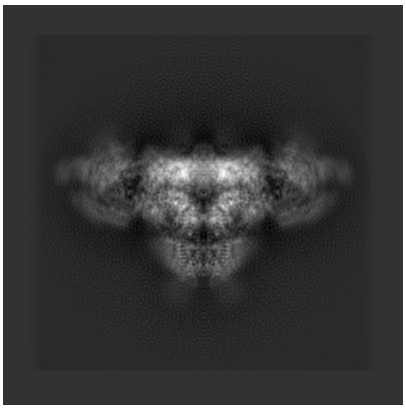
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8391. These allow visual inspection of the internal detail of the map and identification of artifacts.

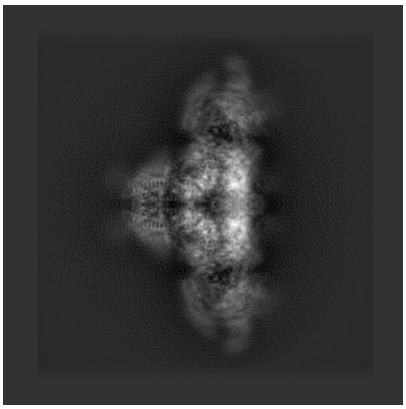
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

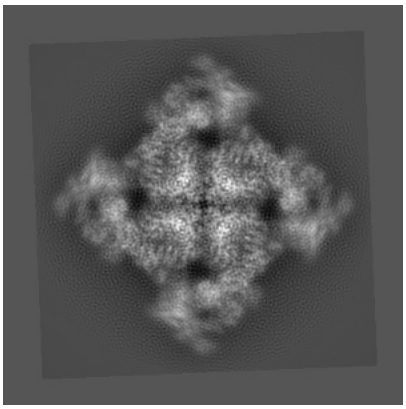
6.1.1 Primary map



X

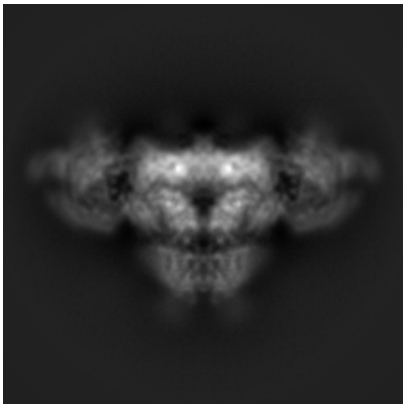


Y

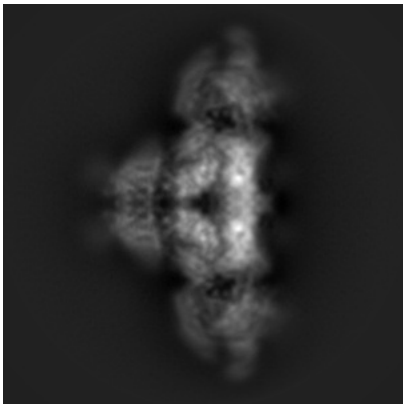


Z

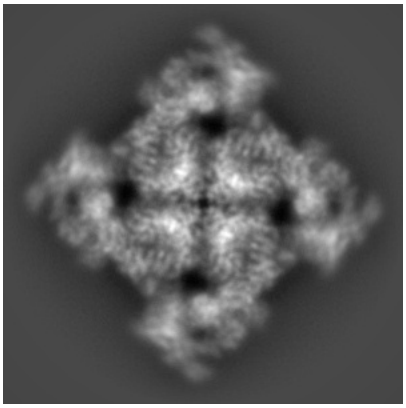
6.1.2 Raw map



X



Y



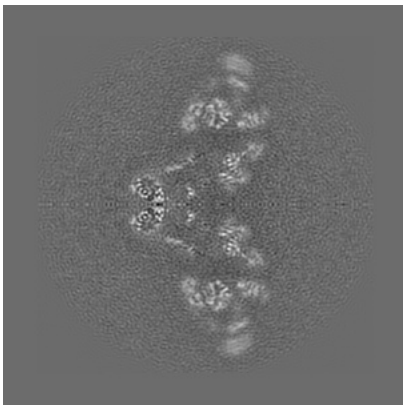
Z

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

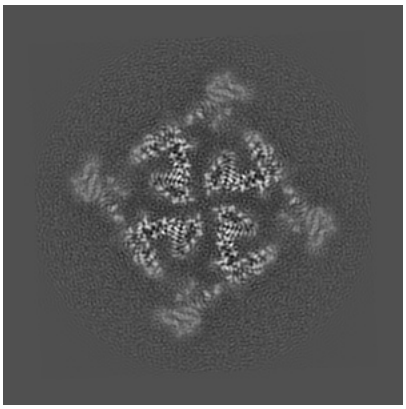
6.2 Central slices (i)

6.2.1 Primary map

X Index: 200

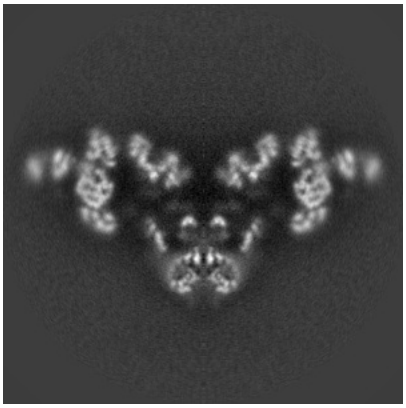


Y Index: 200

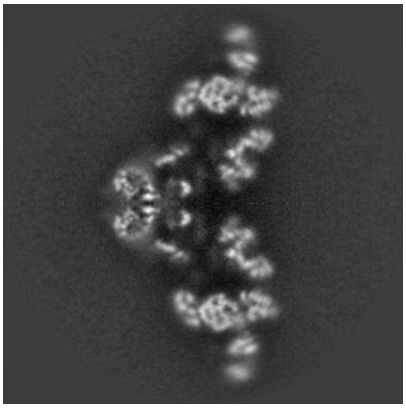


Z Index: 200

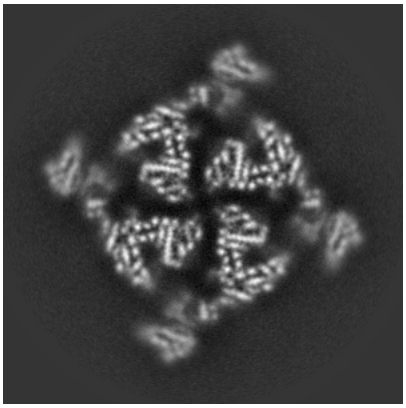
6.2.2 Raw map



X Index: 168



Y Index: 168

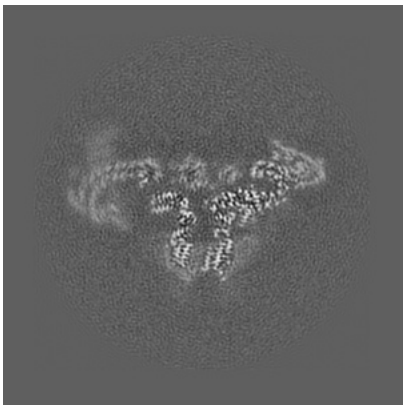


Z Index: 168

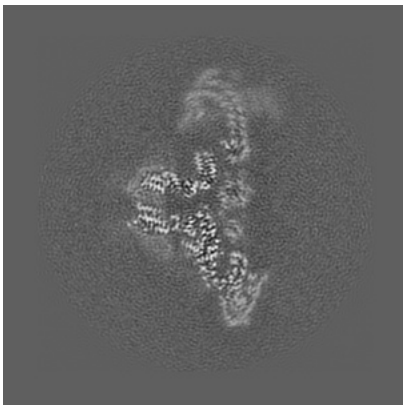
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

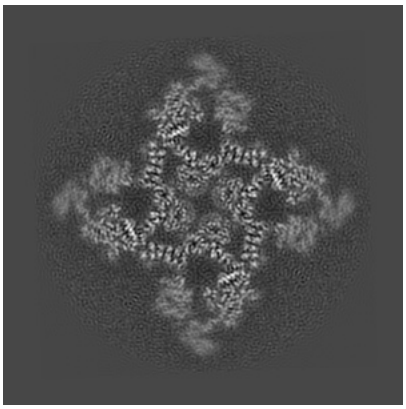
6.3.1 Primary map



X Index: 176

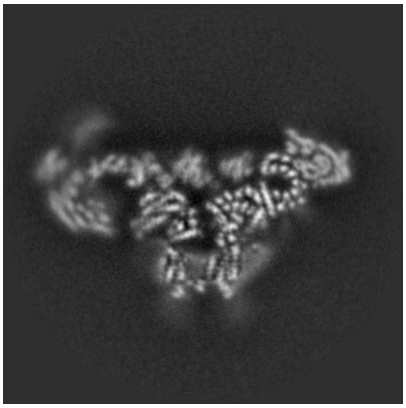


Y Index: 176

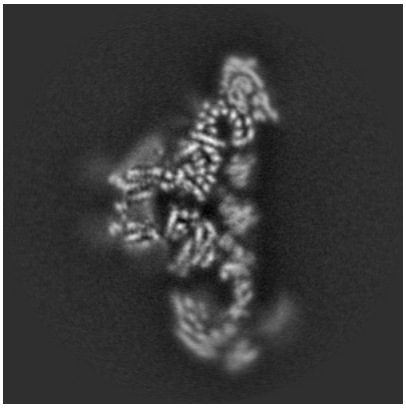


Z Index: 228

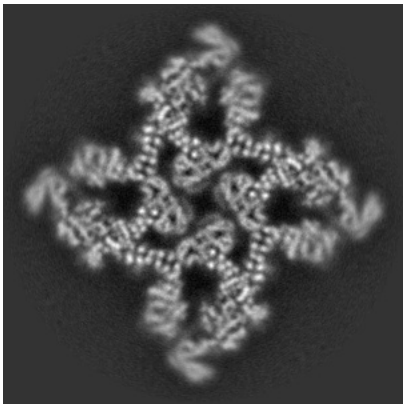
6.3.2 Raw map



X Index: 147



Y Index: 189

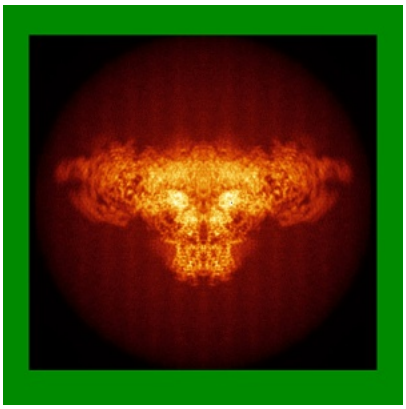


Z Index: 196

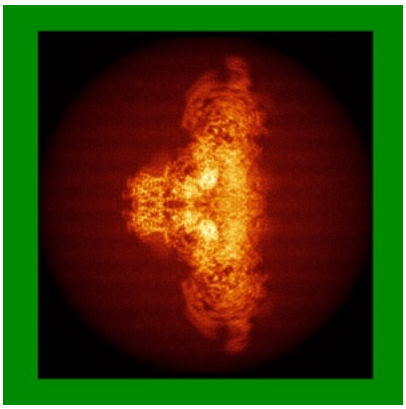
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

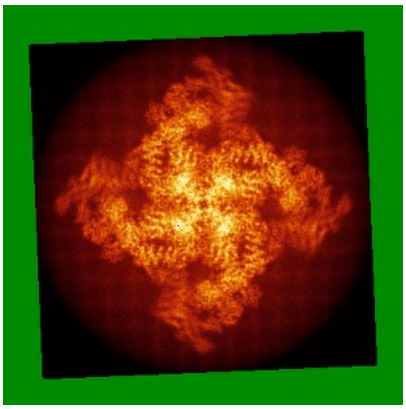
6.4.1 Primary map



X



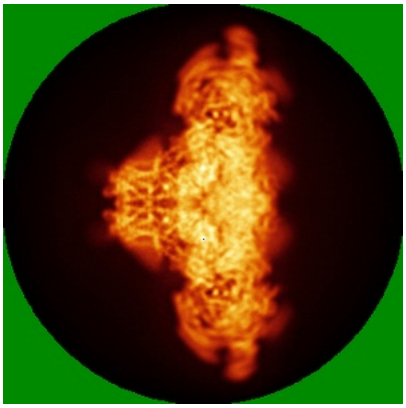
Y



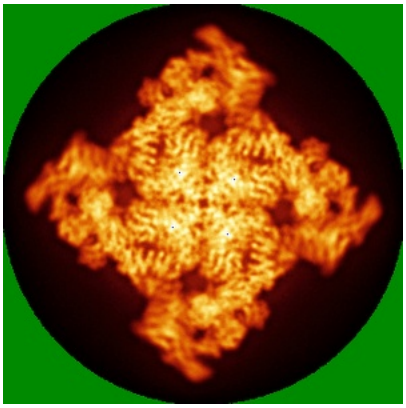
Z

6.4.2 Raw map

X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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.

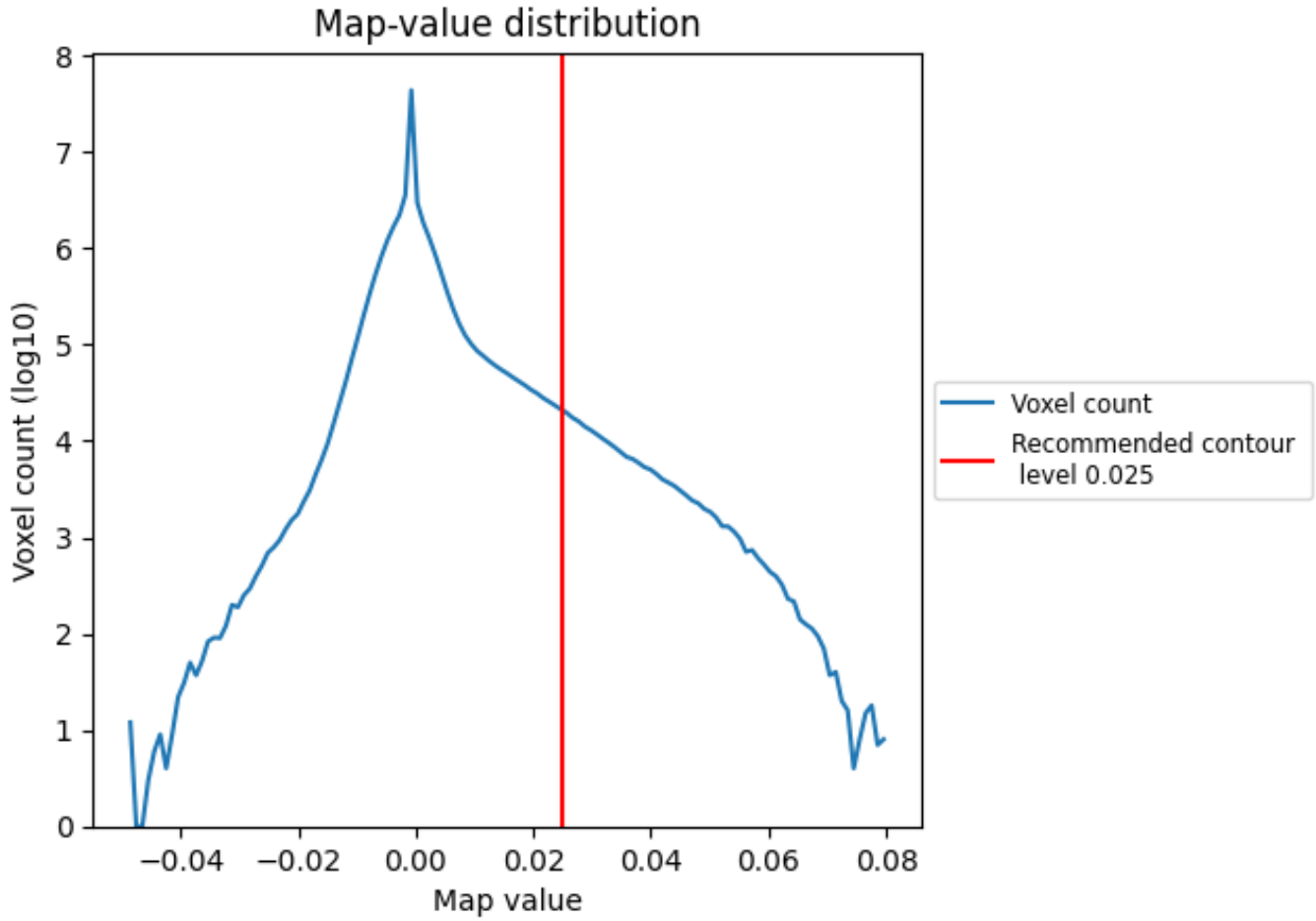
6.6 Mask visualisation (i)

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

7 Map analysis

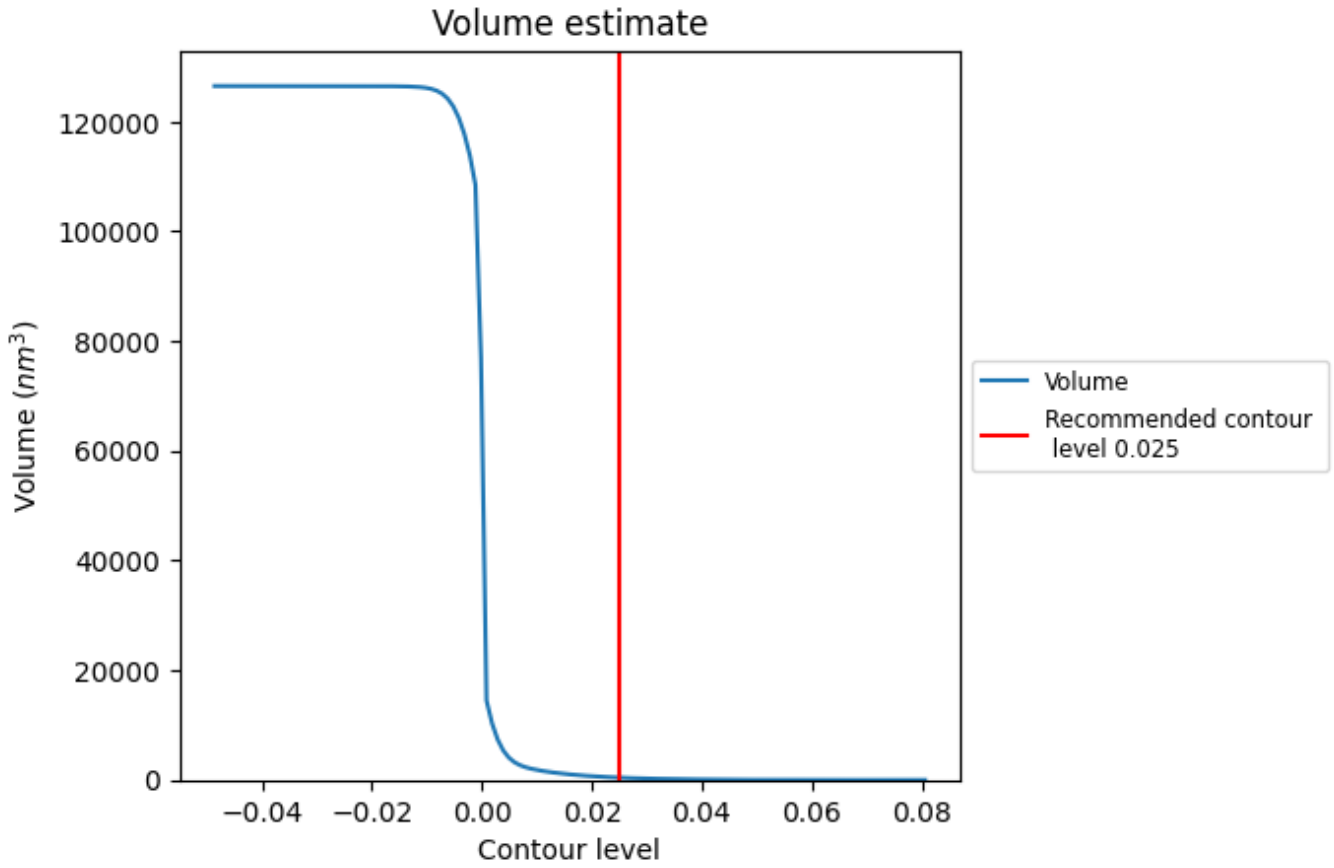
This section contains the results of statistical analysis of the map.

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.

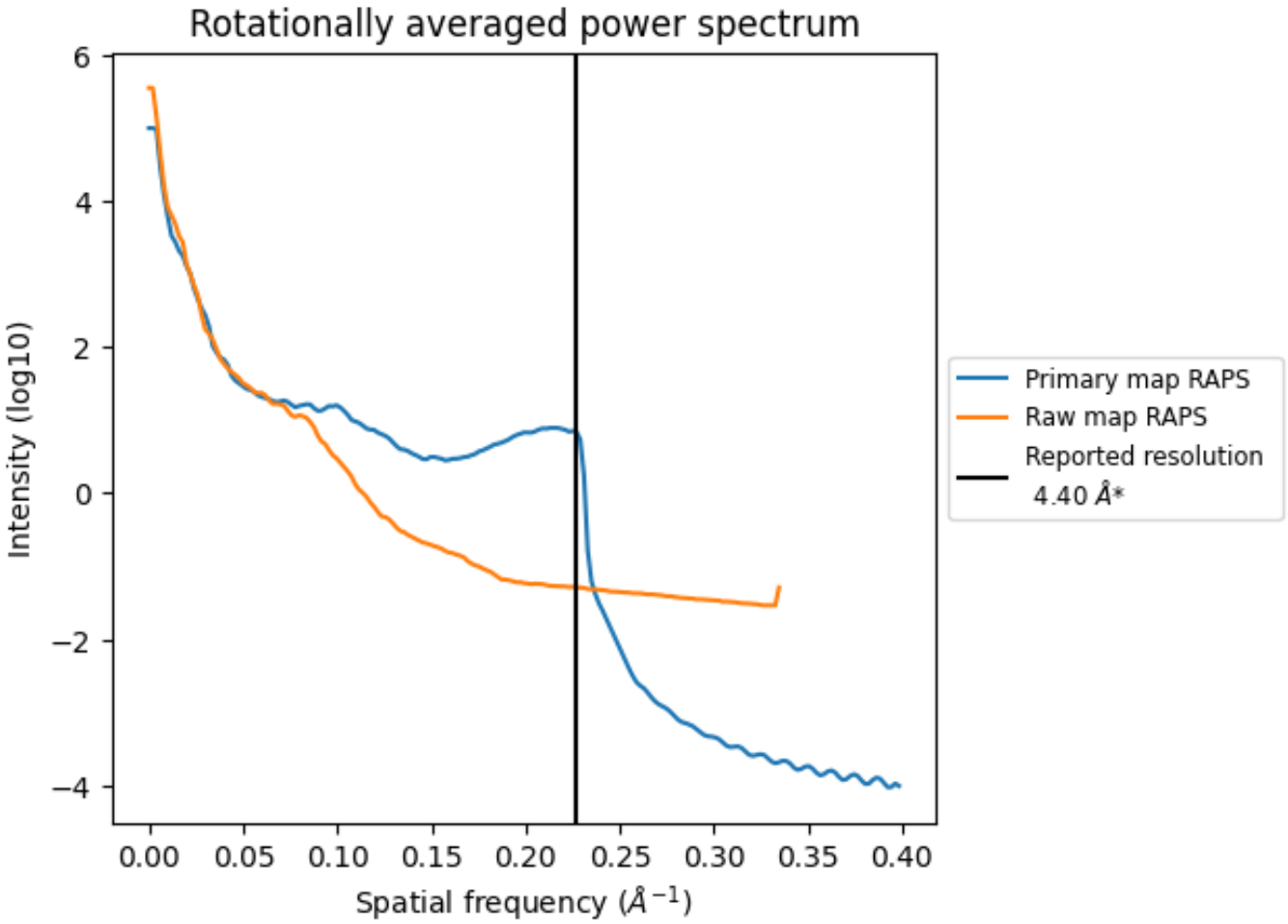
7.2 Volume estimate (i)



The volume at the recommended contour level is 422 nm^3; this corresponds to an approximate mass of 381 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)

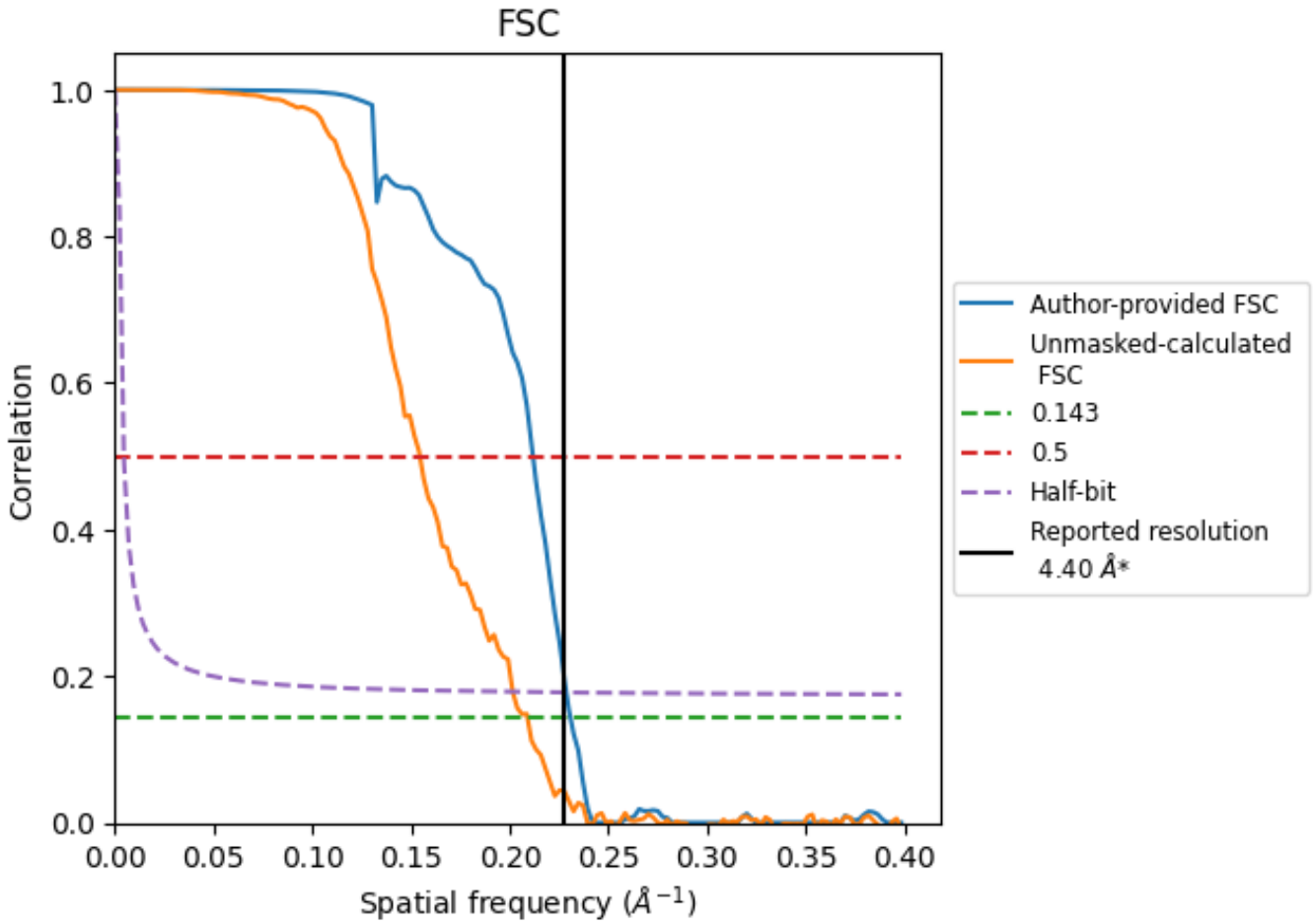


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

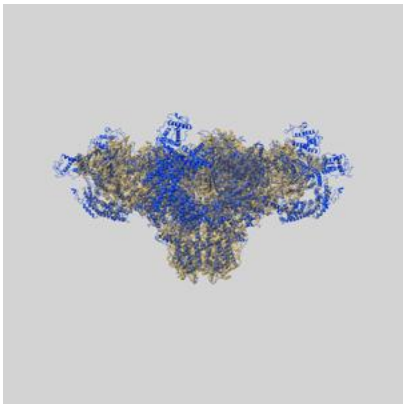
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.33	4.72	4.37
Unmasked-calculated*	4.78	6.47	4.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

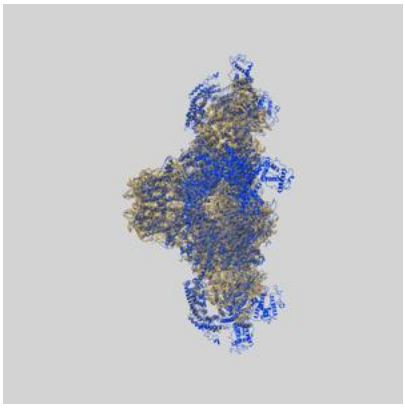
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8391 and PDB model 5TB0. Per-residue inclusion information can be found in section 3 on page 4.

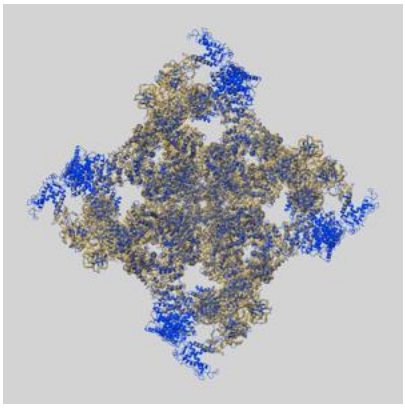
9.1 Map-model overlay



X



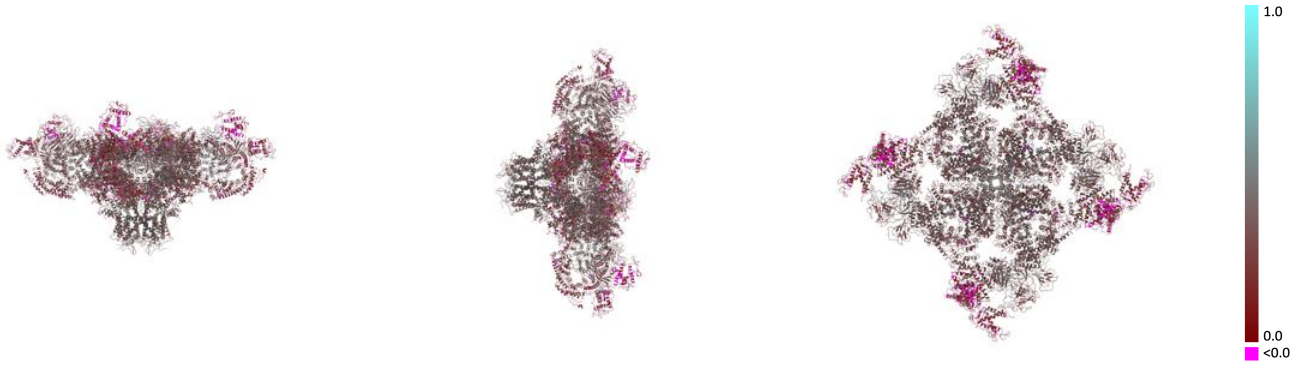
Y



Z

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

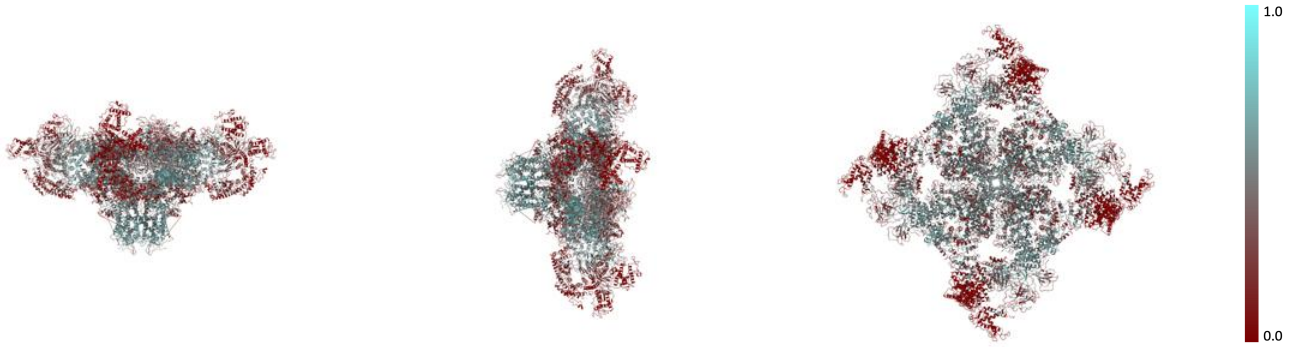
9.2 Q-score mapped to coordinate model



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.

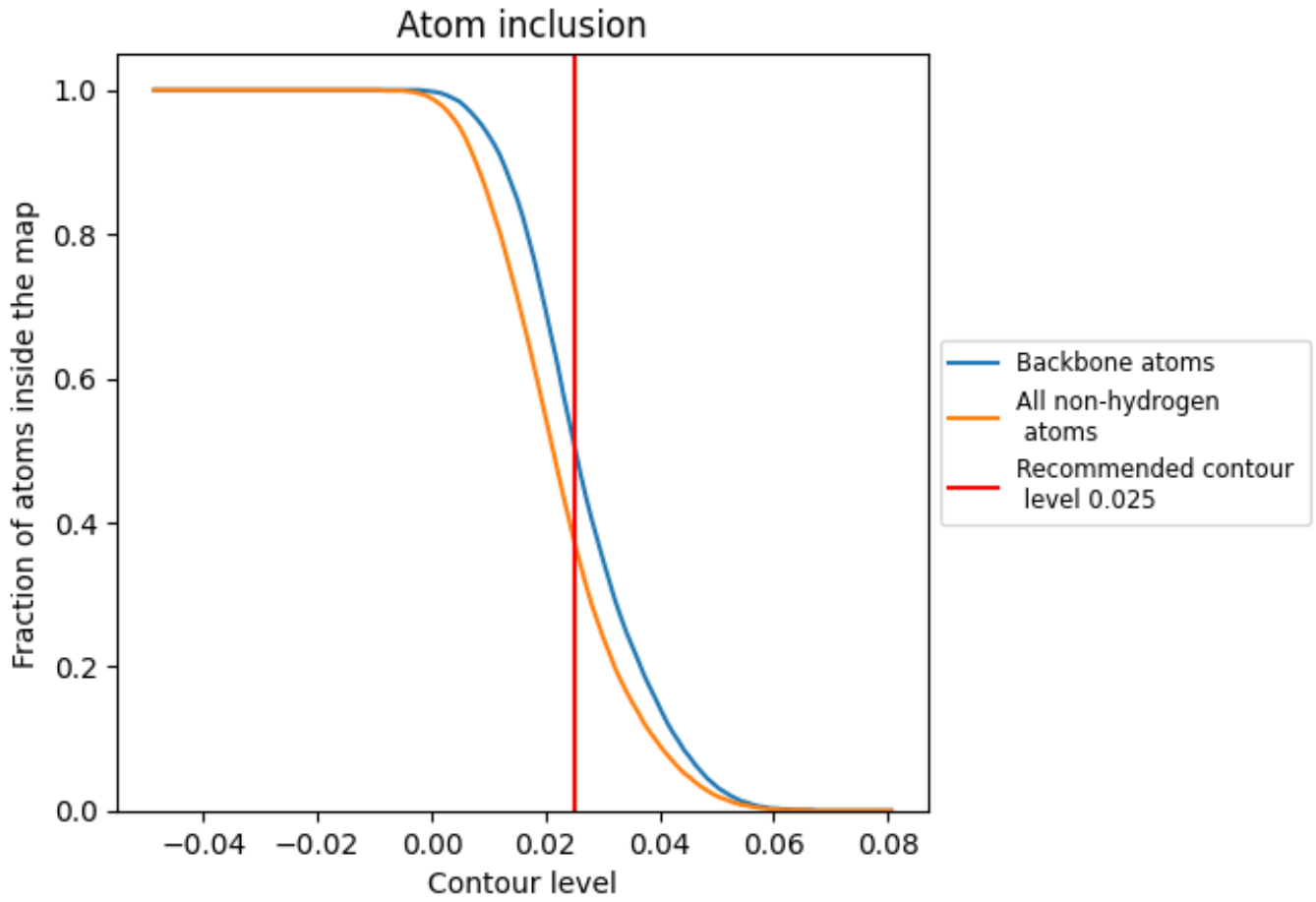
9.3 Atom inclusion mapped to coordinate model



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 37% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3740	0.3120
A	0.3810	0.3450
B	0.3750	0.3110
E	0.3730	0.3110
F	0.3780	0.3490
G	0.3740	0.3110
H	0.3810	0.3480
I	0.3740	0.3110
J	0.3800	0.3450