wwPDB EM Validation Summary Report

Oct 5, 2024 – 10:54 AM EDT

PDB ID	:	5T9S
EMDB ID	:	EMD-8375
Title	:	Structure of rabbit RyR1 (Ca2+-only dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	4.20 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:

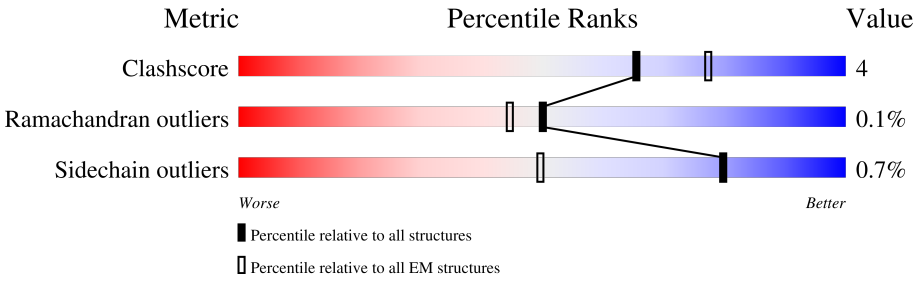
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 4.20 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	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	36% 84% 15%
1	F	108	36% 83% 16%
1	H	108	35% 84% 15%
1	J	108	34% 84% 15%
2	B	4676	31% 80% 8% 11%
2	E	4676	32% 80% 8% 11%
2	G	4676	32% 81% 8% 11%
2	I	4676	32% 81% 8% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	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	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- 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	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

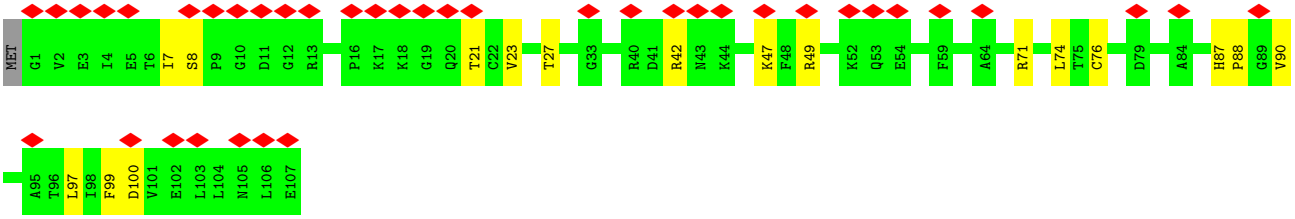
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0

3 Residue-property plots (i)

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

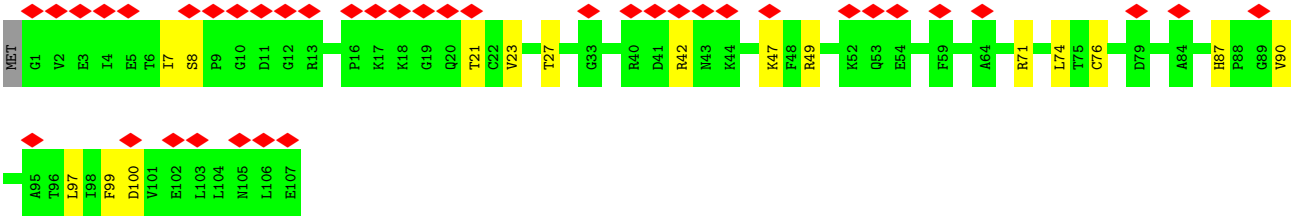
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



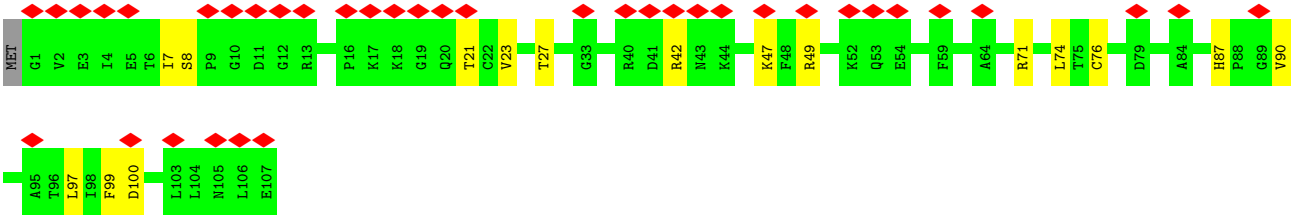
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



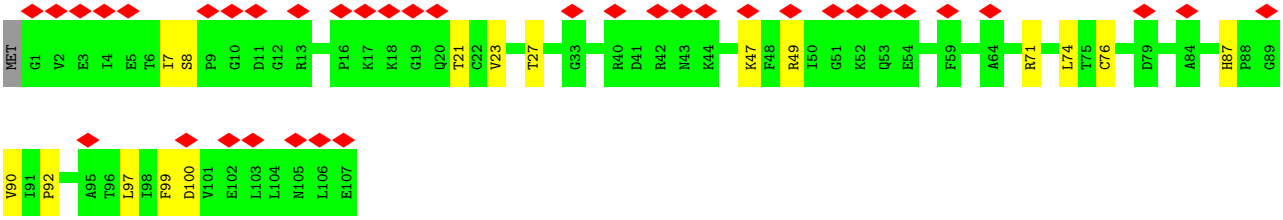
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



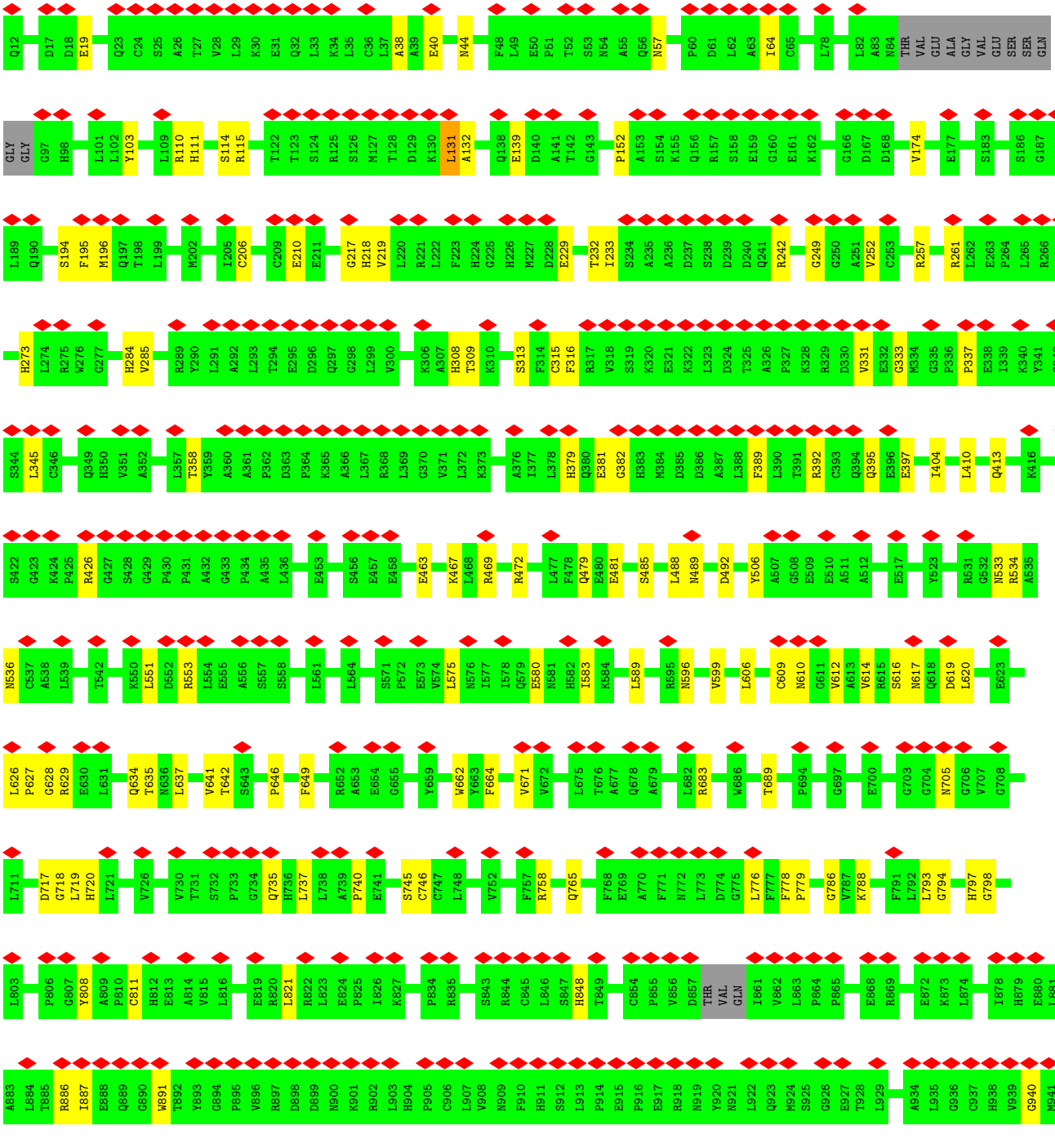
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

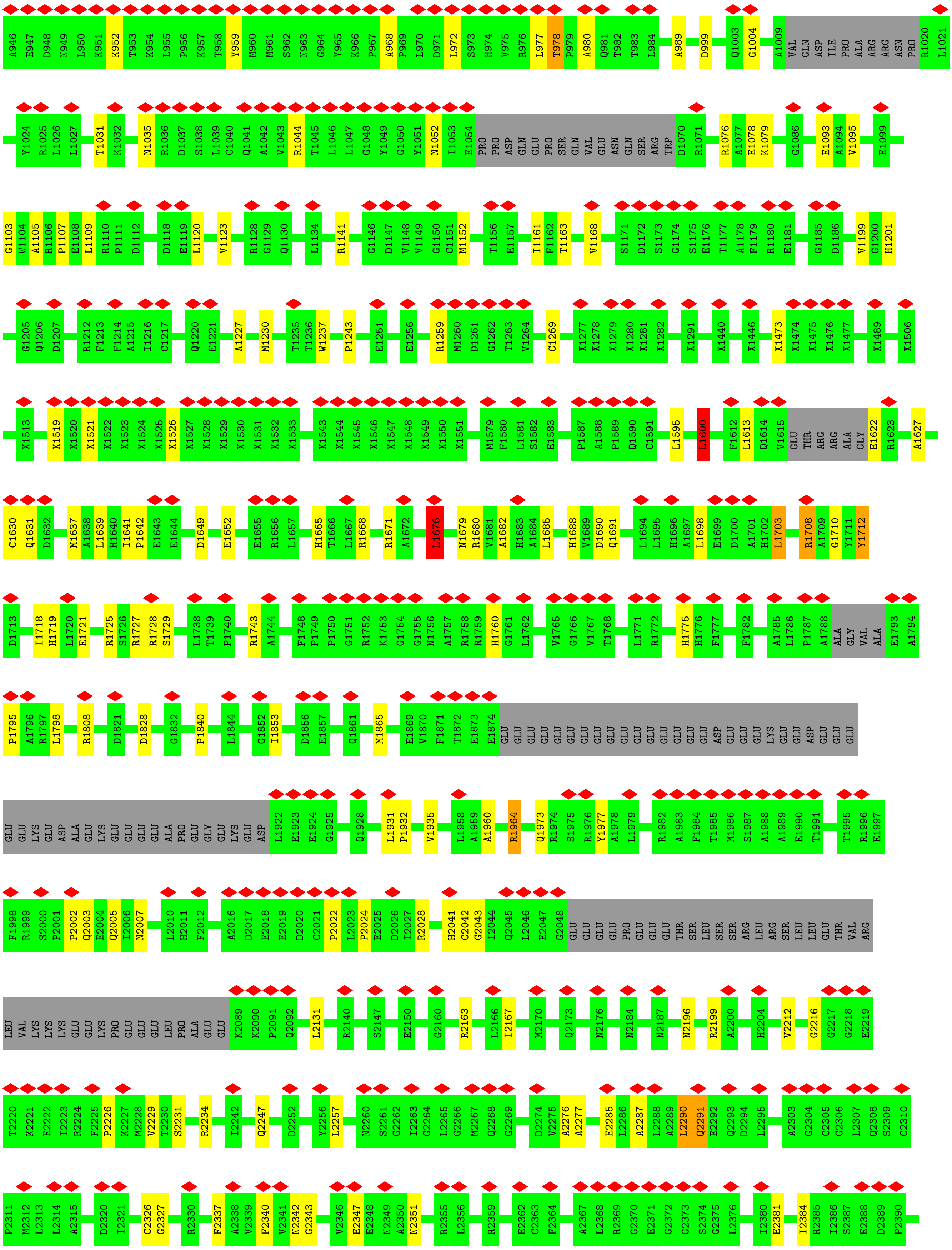
Chain J:



• Molecule 2: Ryanodine receptor 1

Chain B:

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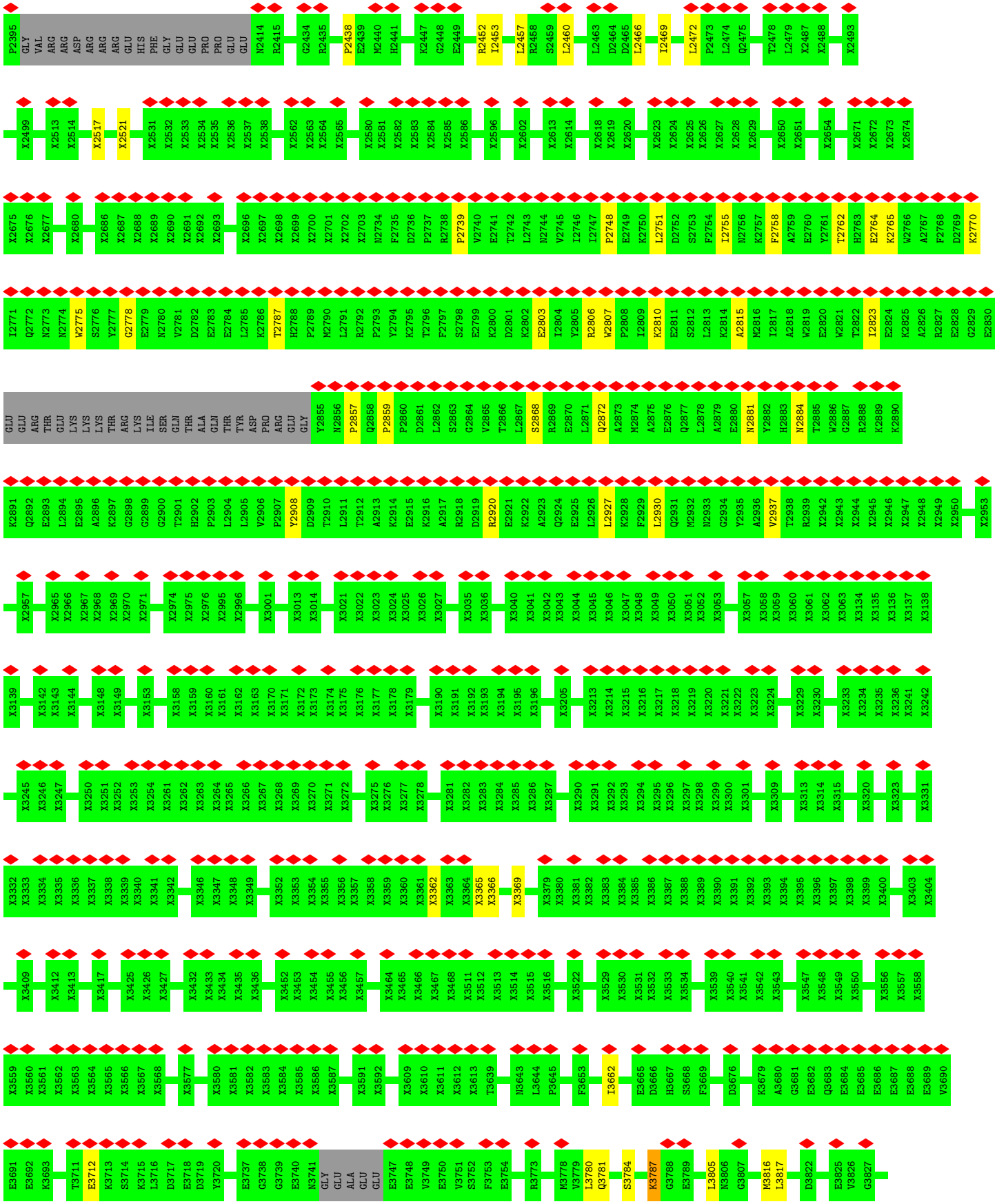
Y1024 R1025 L1026 L1027 T1031 K1032 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 V1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 R1076 A1077 E1078 K1079 G1086 E1093 A1094 V1095 E1099
G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 D1118 E1119 L1120 V1123 R1128 G1129 Q1130 L1134 R1141 G1146 D1147 V1148 V1149 G1150 C1151 M1152 T1156 E1157 I1161 F1162 T1163 V1168 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 G1185 D1186 V1199 G1200 H1201
G1205 Q1206 D1207 R1212 F1213 F1214 A1215 I1216 C1217 Q1220 E1221 A1227 M1230 T1235 T1236 W1237 P1243 E1251 E1256 R1259 M1260 D1261 G1262 T1263 V1264 C1269 X1277 X1278 X1279 X1280 X1281 X1282 X1291 X1440 X1446 X1473 X1474 X1475 X1476 X1477 X1489 X1506
X1513 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1532 X1533 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 X1551 M1579 F1580 L1581 S1582 E1583 P1587 A1588 P1589 Q1590 C1591 L1595 L1600 F1612 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 A1627
C1630 Q1631 D1632 M1637 A1638 L1639 H1640 I1641 P1642 E1643 E1644 D1649 E1652 E1655 R1656 L1657 H1665 T1666 L1667 R1668 R1671 A1672 L1676 N1679 R1680 V1681 A1682 H1683 A1684 L1685 H1688 V1689 D1690 Q1691 L1694 L1695 H1696 A1697 L1698 E1699 D1700 A1701 H1702 L1703 R1708 A1709 G1710 Y1711 Y1712
D1713 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 S1729 L1738 T1739 P1740 R1743 A1744 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1761 L1762 V1765 G1766 V1767 T1768 L1771 R1772 H1775 H1776 F1777 F1782 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794
P1795 A1796 R1797 L1798 R1808 D1821 D1828 G1832 P1840 L1844 G1852 I1853 D1856 E1857 Q1861 M1865 E1869 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU
GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 Q1928 L1931 P1932 V1935 L1958 A1959 A1960 R1964 Q1973 R1974 S1975 R1976 Y1977 A1978 L1979 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 T1995 R1996 E1997
F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006 N2007 L2010 H2011 F2012 A2016 D2017 E2018 E2019 D2020 C2021 P2022 L2023 P2024 E2025 D2026 I2027 R2028 H2041 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG
LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 K2090 P2091 Q2092 L2131 R2140 S2147 E2150 G2160 R2163 L2166 I2167 M2170 Q2173 N2176 N2184 N2187 N2196 R2199 A2200 H2204 V2212 G2216 G2217 G2218 E2219
T2220 K2221 E2222 I2223 R2224 F2225 P2226 K2227 M2228 V2229 T2230 S2231 R2234 I2242 Q2247 D2252 Y2256 L2257 N2260 S2261 G2262 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 D2274 V2275 A2276 A2277 E2285 L2286 A2287 L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295 A2303 G2304 C2305 G2306 L2307 Q2308 S2309 C2310
P2311 M2312 L2313 L2314 A2315 D2320 I2321 C2326 G2327 R2330 F2337 A2338 V2339 F2340 V2341 N2342 G2343 V2346 E2347 E2348 N2349 A2350 N2351 R2355 L2356 R2359 E2362 C2363 F2364 A2367 L2368 R2369 G2370 E2371 G2372 G2373 S2374 G2375 L2376 I2380 E2381 I2384 R2385 I2386 S2387 E2388 D2389 P2390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X2499 X2513 X2514 X2517 X2521 X2531 X2532 X2533 X2534 X2535 X2536 X2537 X2538 X2562 X2563 X2564 X2565 X2580 X2581 X2582 X2583 X2584 X2585 X2586 X2596 X2602 X2613 X2614 X2618 X2619 X2620 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2650 X2651 X2654 X2671 X2672 X2673 X2674
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I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 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 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890
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X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3346 X3347 X3348 X3349 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3369 X3379 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3403 X3404
X3409 X3412 X3413 X3417 X3425 X3426 X3427 X3432 X3433 X3434 X3435 X3436 X3452 X3453 X3454 X3455 X3456 X3457 X3464 X3465 X3466 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3522 X3529 X3530 X3531 X3532 X3533 X3534 X3539 X3540 X3541 X3542 X3543 X3547 X3548 X3549 X3550 X3556 X3557 X3558
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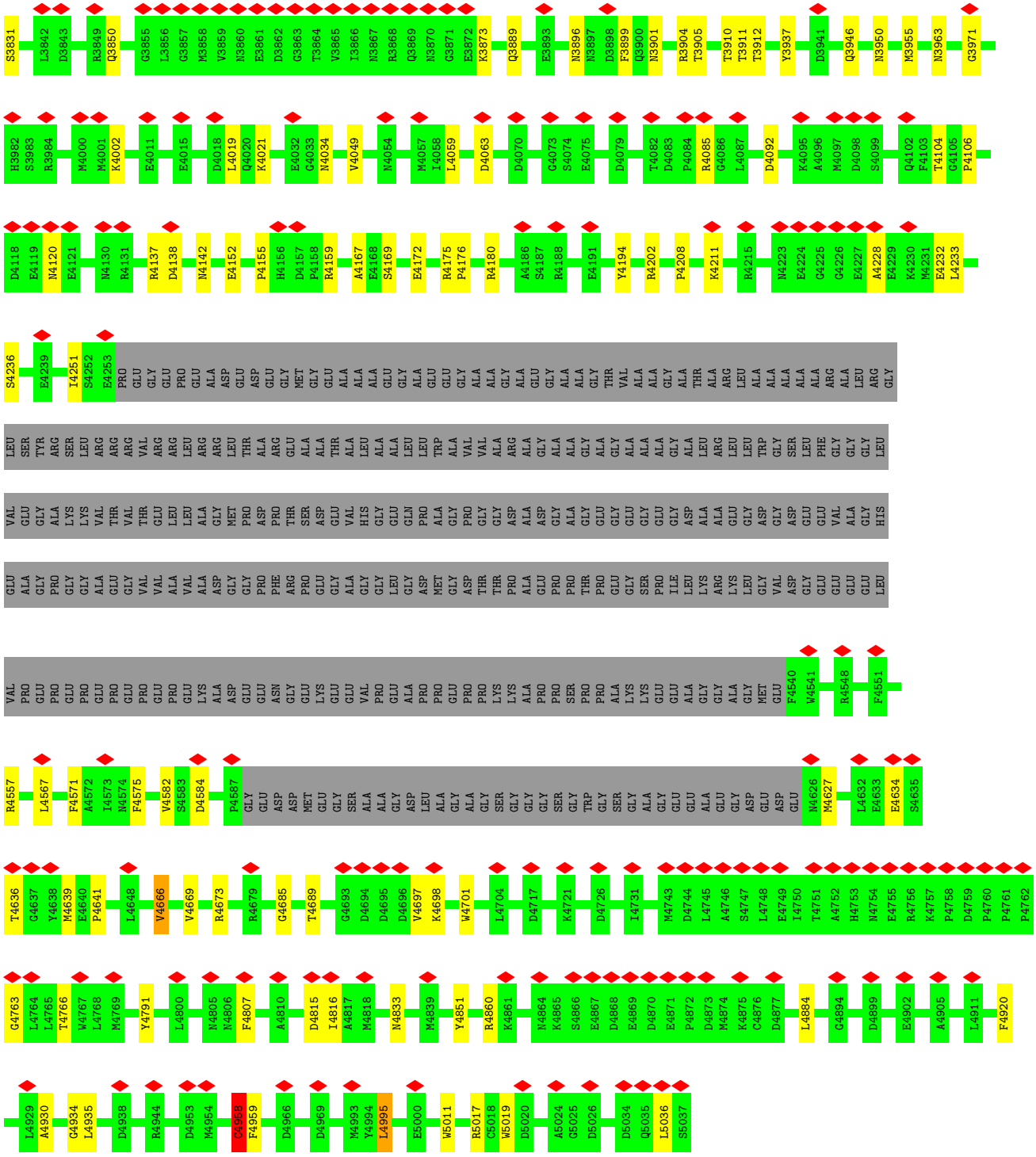
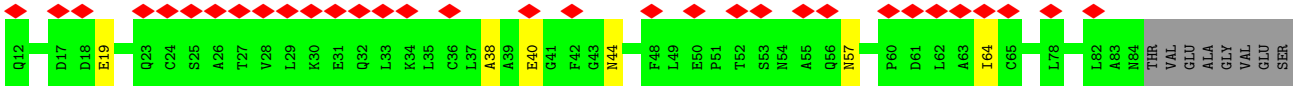
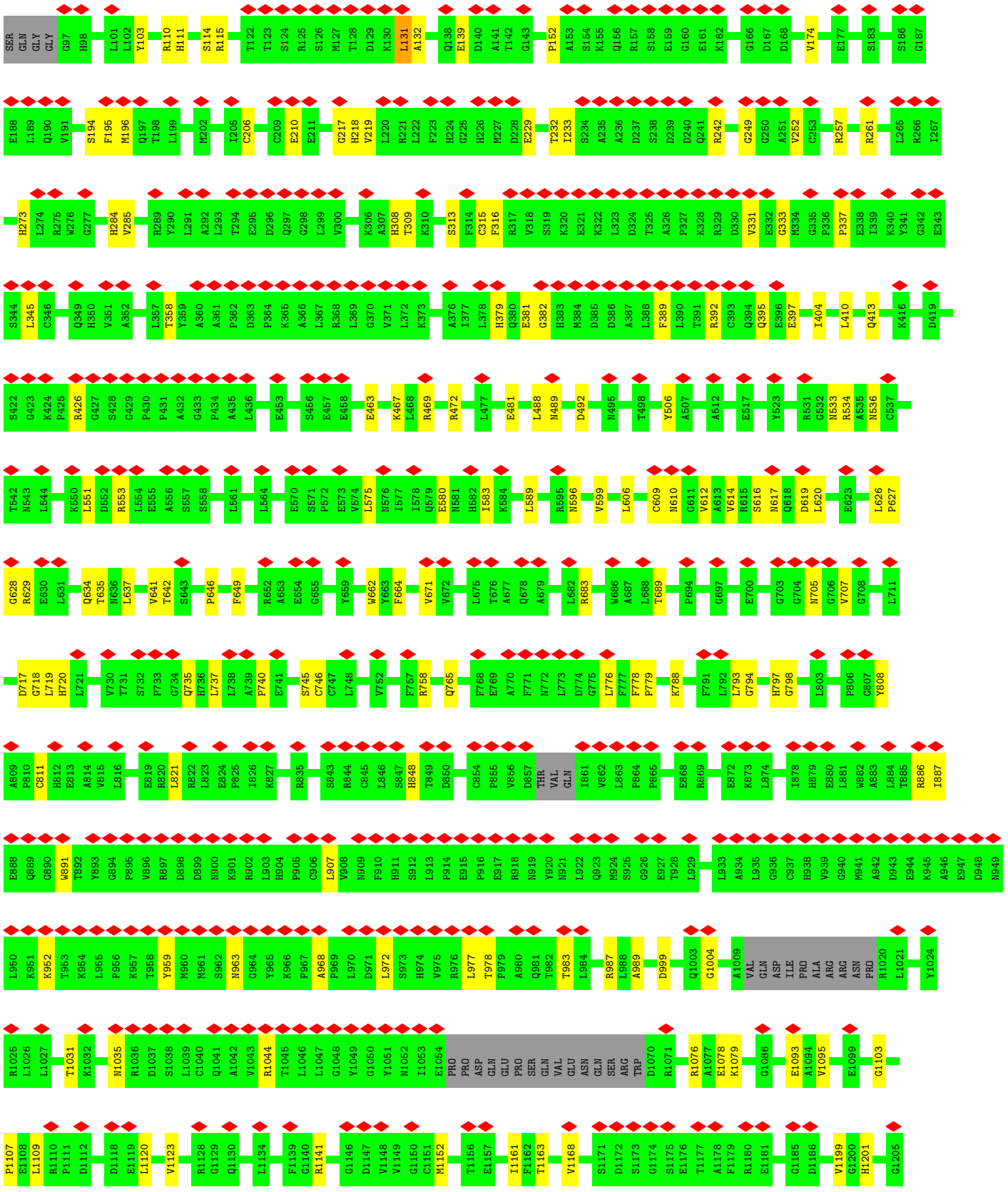
E3691 E3692 K3693 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754 R3773 M3778 Y3779 L3780 Q3781 S3784 K3787 G3788 E3789 L3805 N3806 G3807 M3816 L3817 D3822 E3825 V3826 G3827



• Molecule 2: Ryanodine receptor 1

Chain E:

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E188 L189 Q190 V191 S194 F195 M196 Q197 T198 L199 M202 I205 C206 C209 E210 E211 G217 H218 V219 L220 R221 L222 F223 H224 G225 H226 M227 D228 E229 T232 I233 S234 A235 A236 D237 S238 D239 D240 Q241 R242 G249 G250 A251 V252 C253 R257 R261 L265 R266 I267
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S422 G423 K424 P425 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 L436 E453 S456 E457 E458 E463 K467 L468 R469 R472 L477 E481 L488 N489 D492 N495 T498 Y506 A507 A512 E517 Y523 R531 G532 N533 R534 A535 N536 C537
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D717 G718 L719 H720 L721 V730 T731 S732 P733 G734 Q735 H736 L737 L738 A739 P740 E741 S745 C746 C747 L748 V752 F757 R758 Q765 F768 E769 A770 F771 N772 L773 D774 G775 L776 F777 F778 P779 K788 F791 L792 L793 G794 H797 G798 L803 P806 G807 Y808
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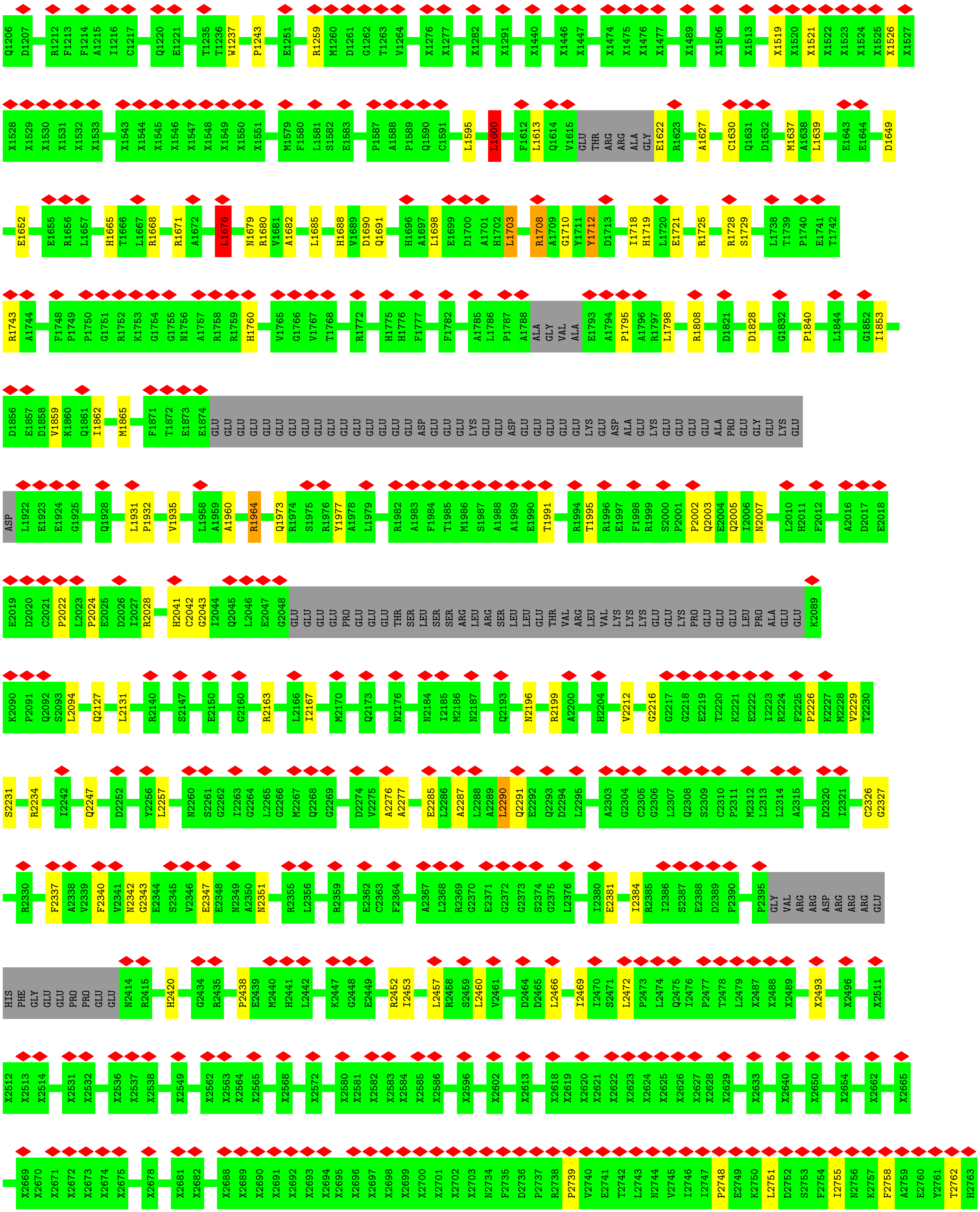
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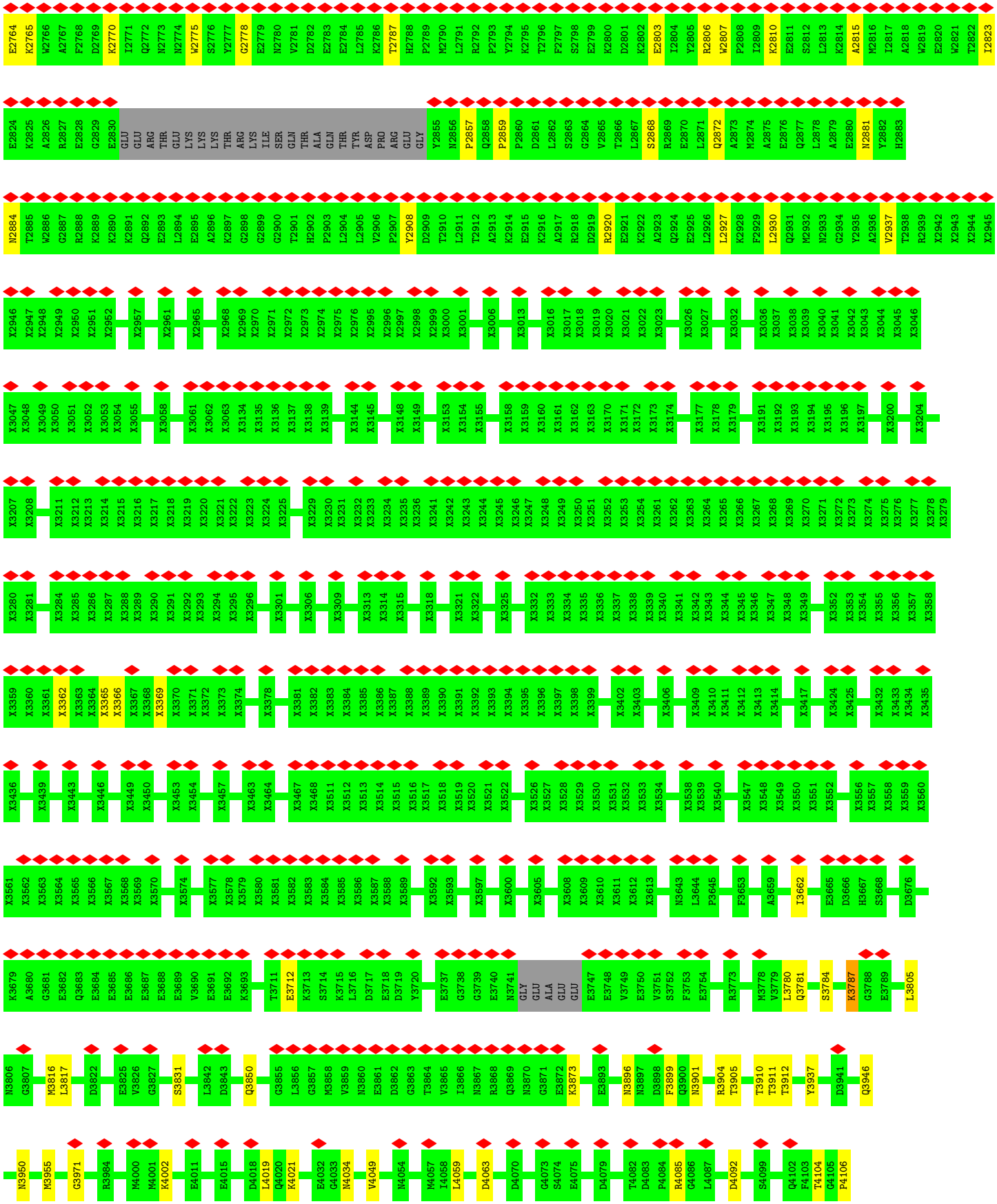
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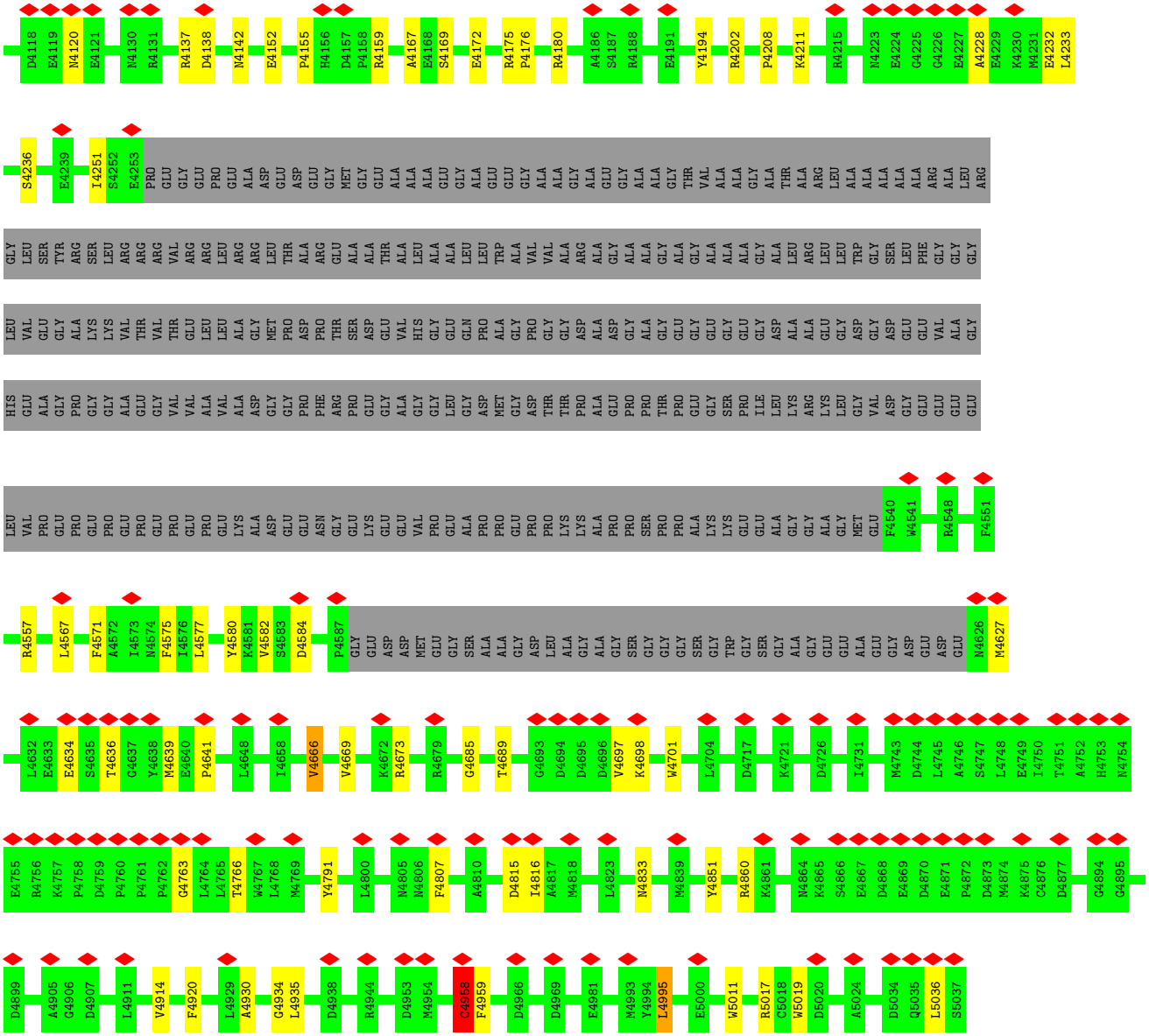

• Molecule 2: Ryanodine receptor 1

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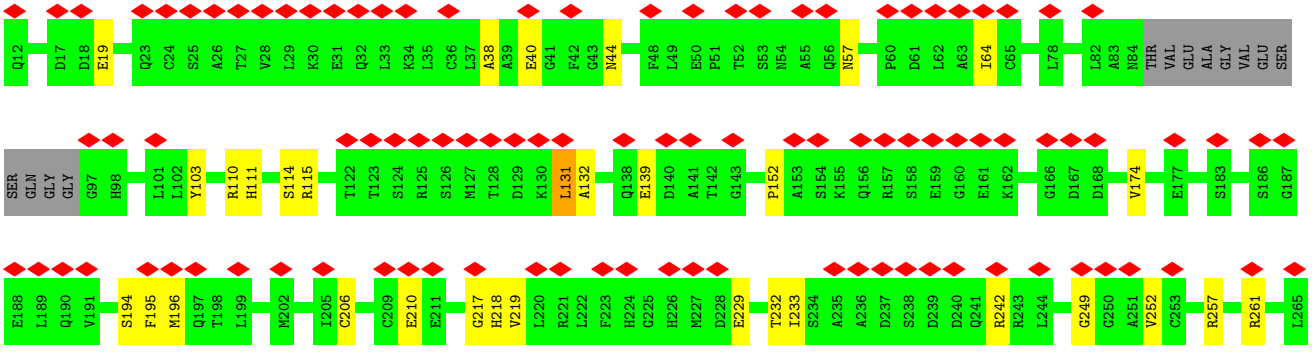

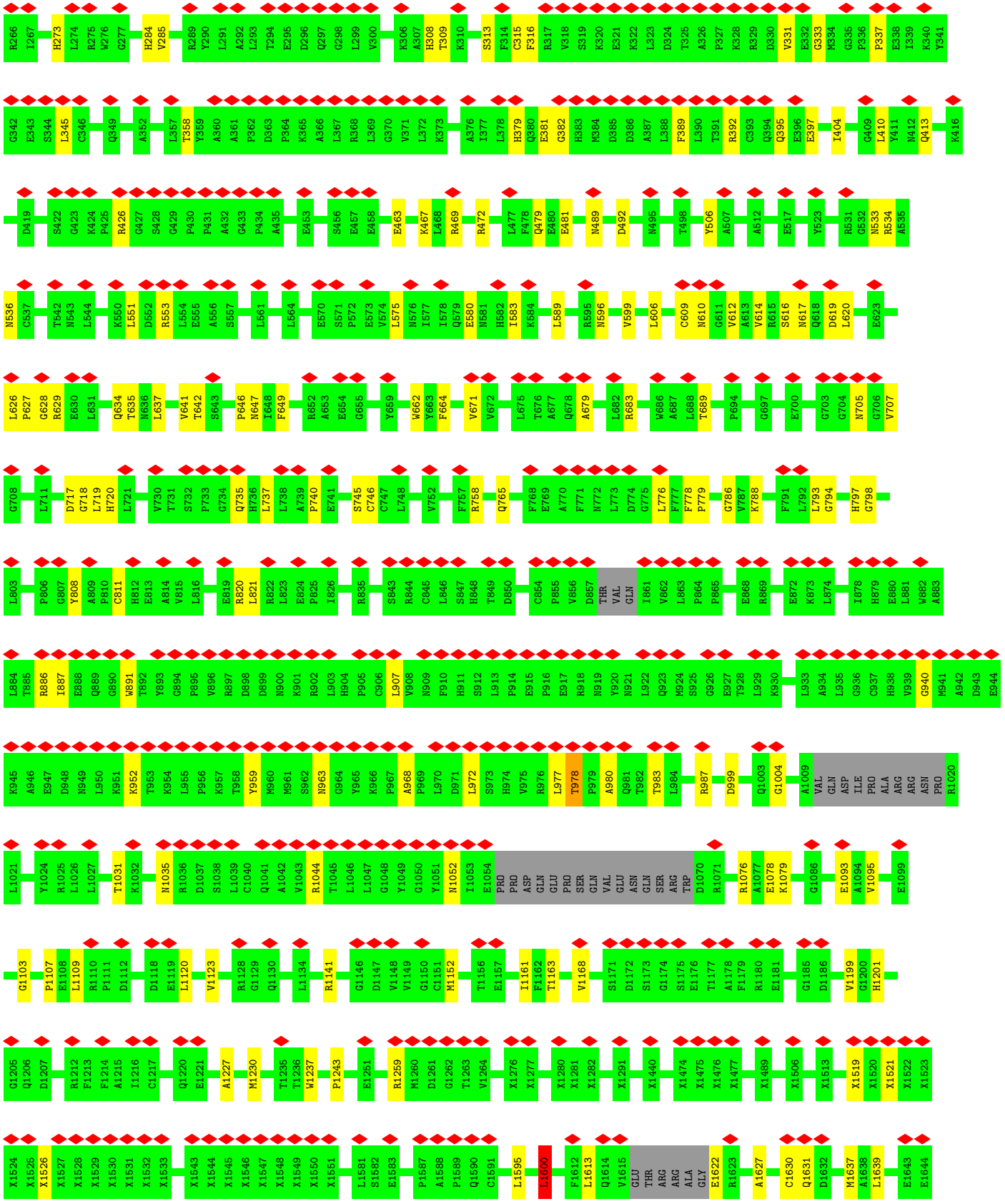
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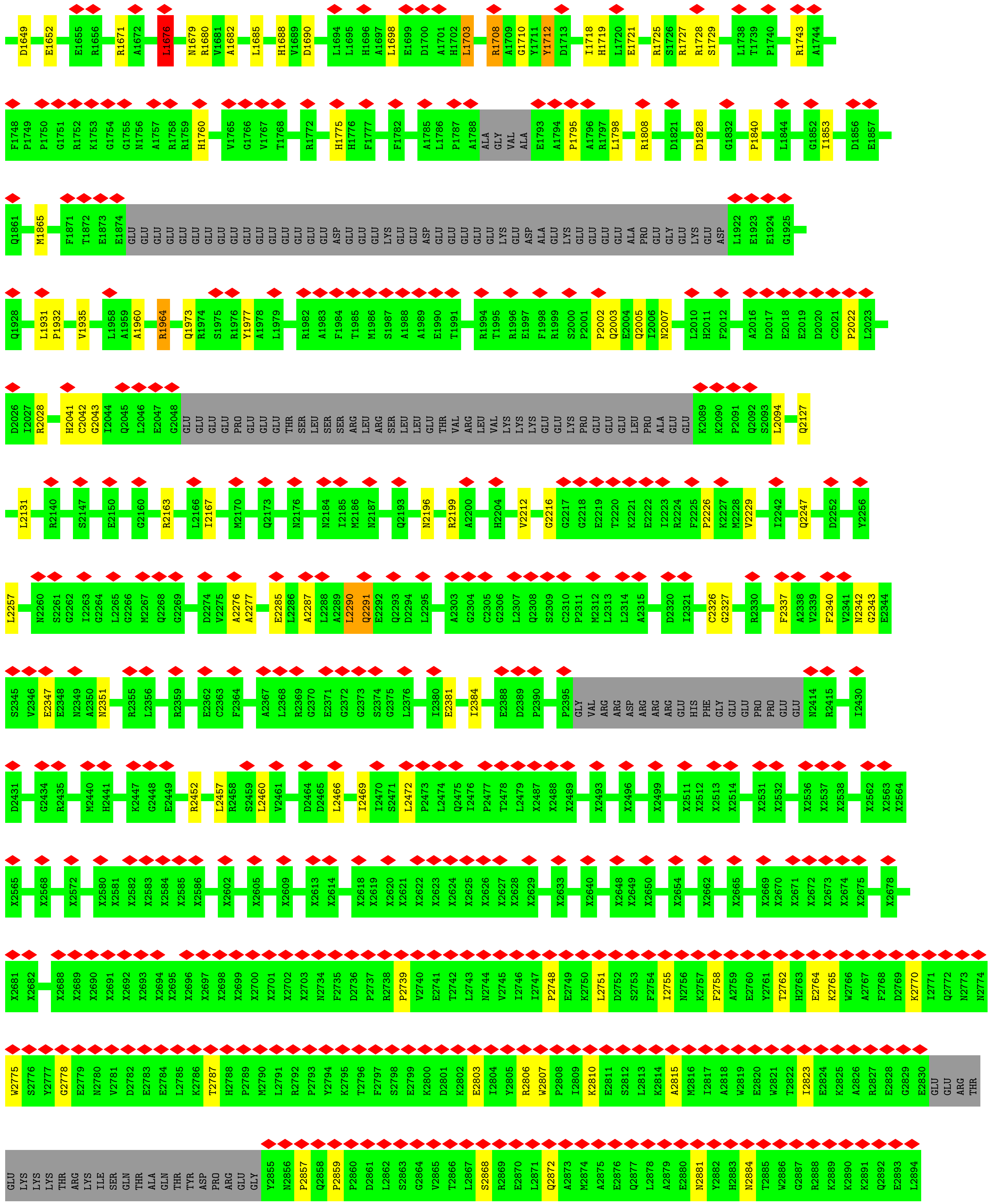
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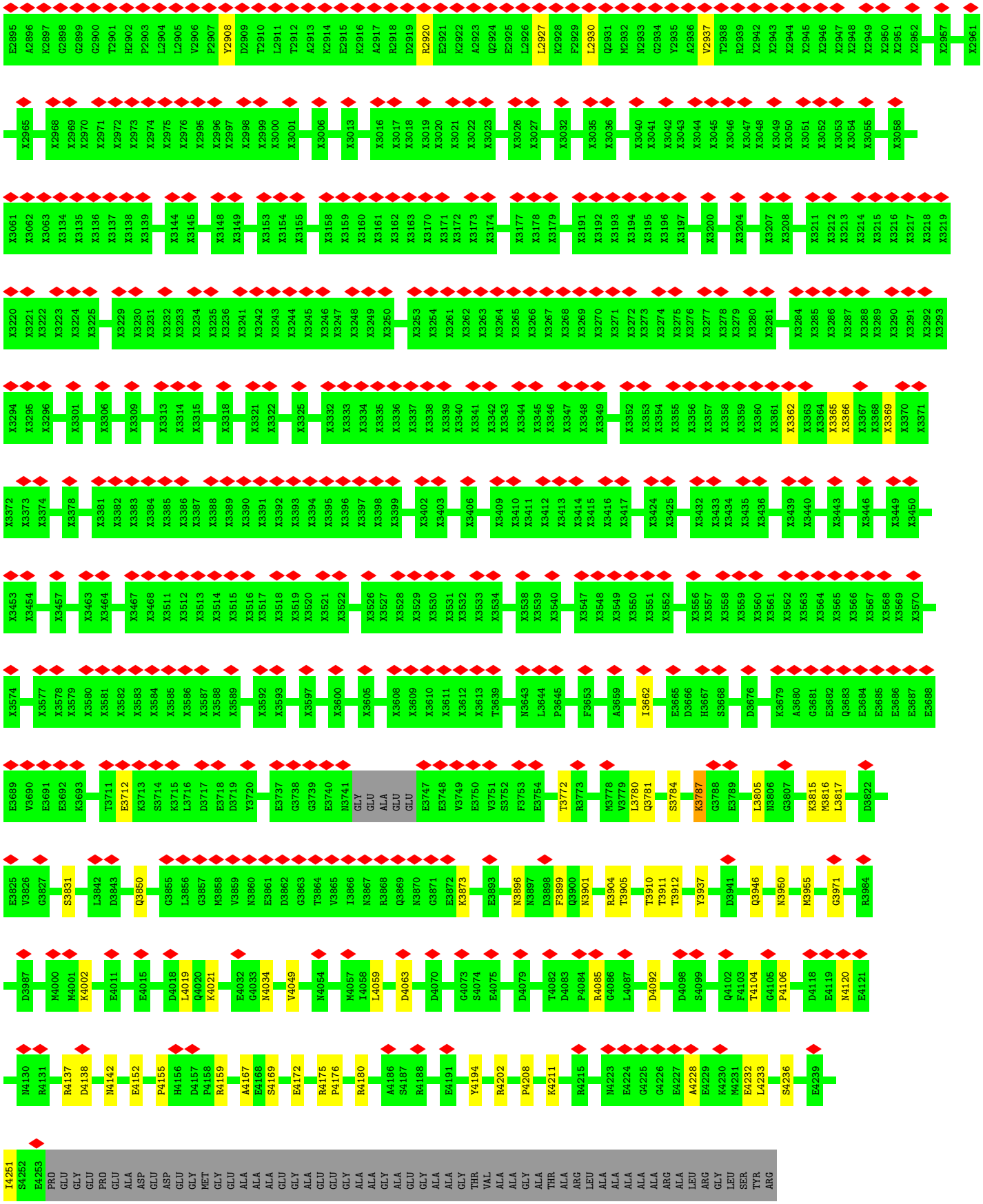
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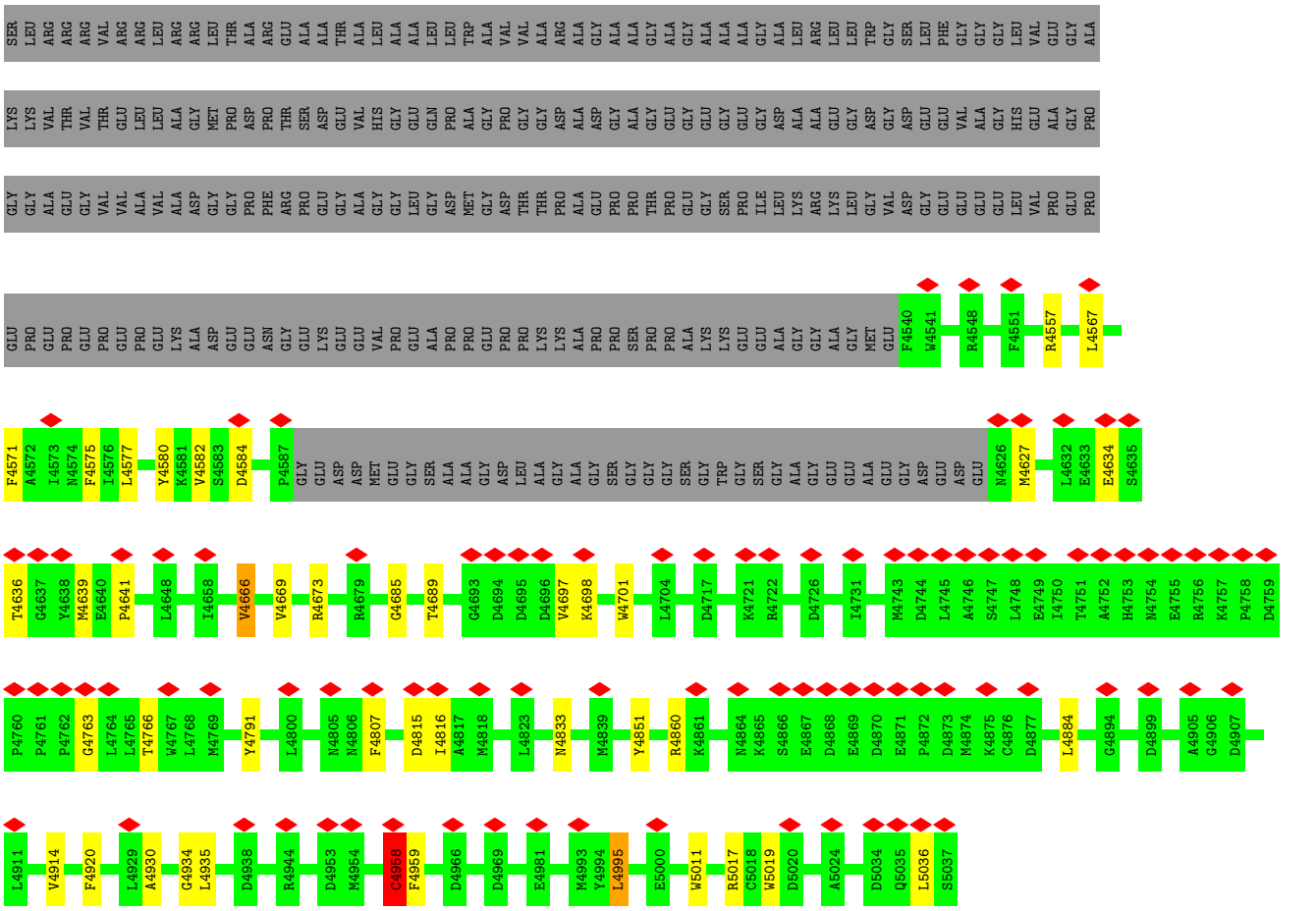

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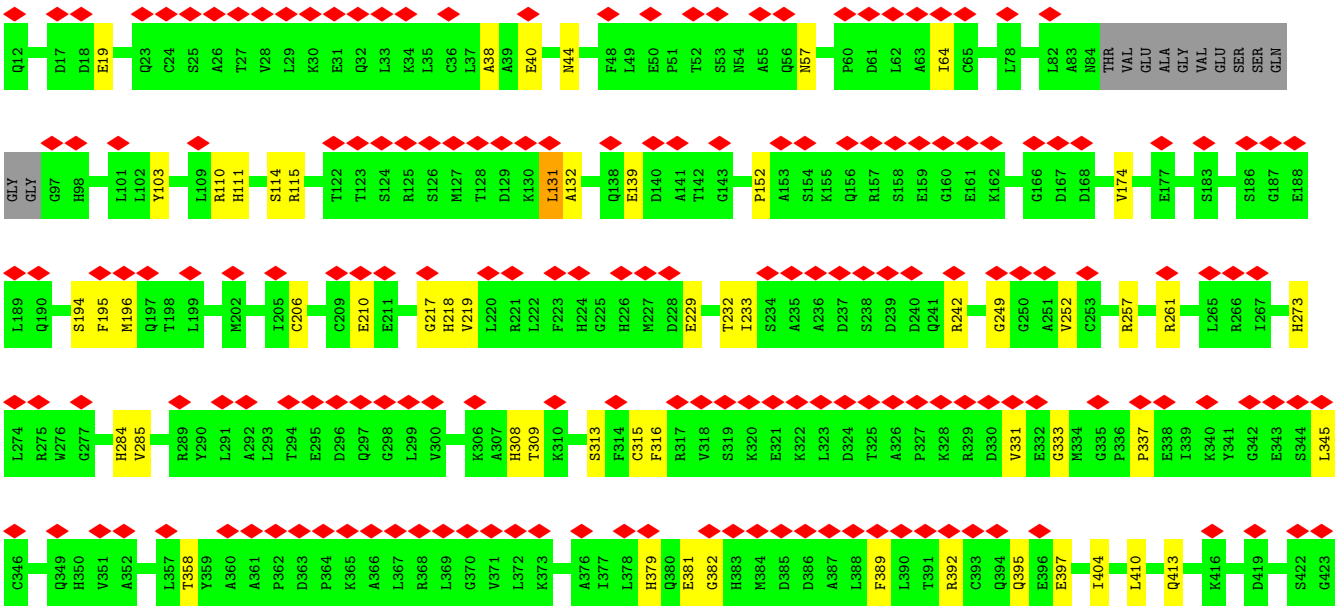

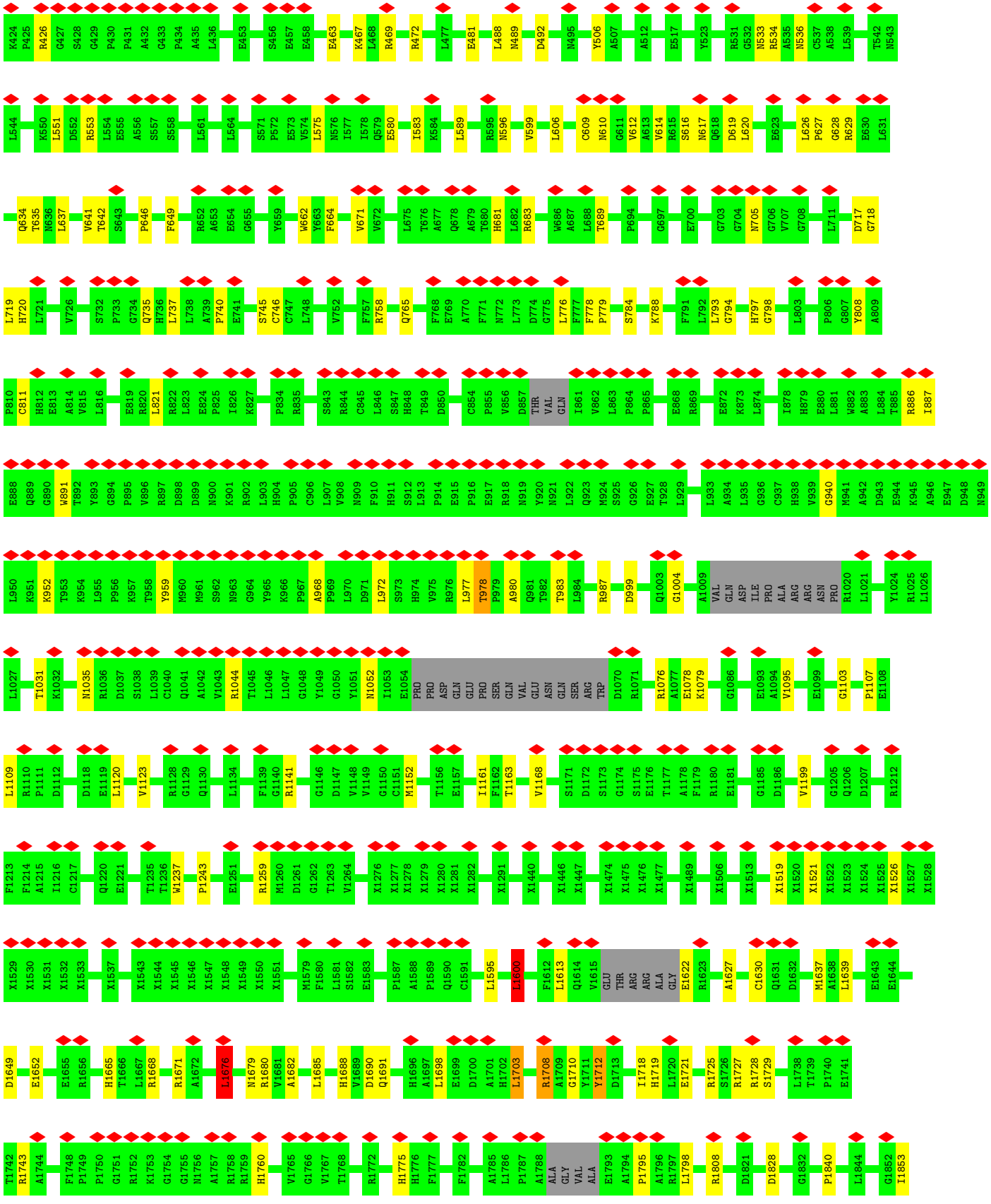
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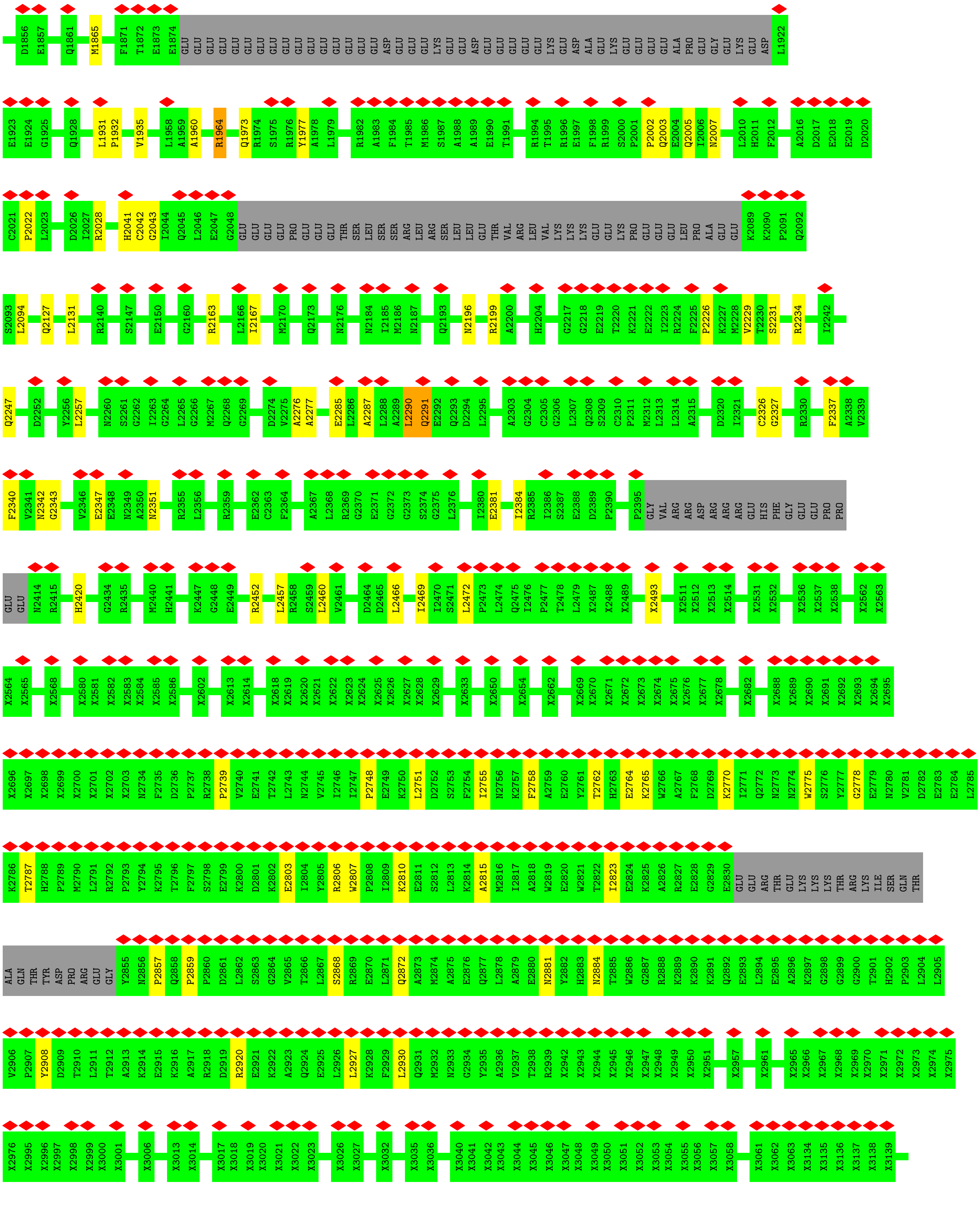
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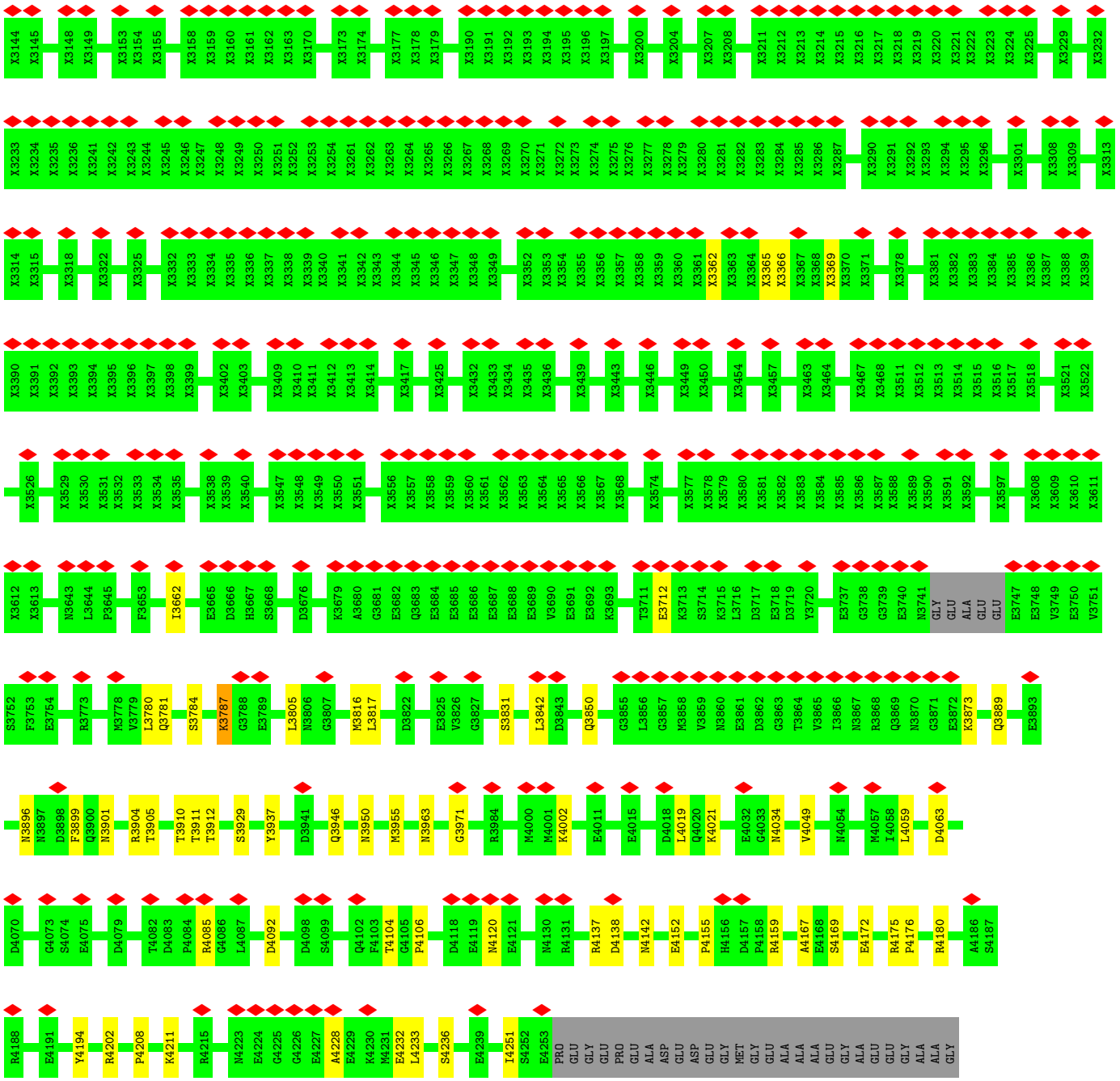
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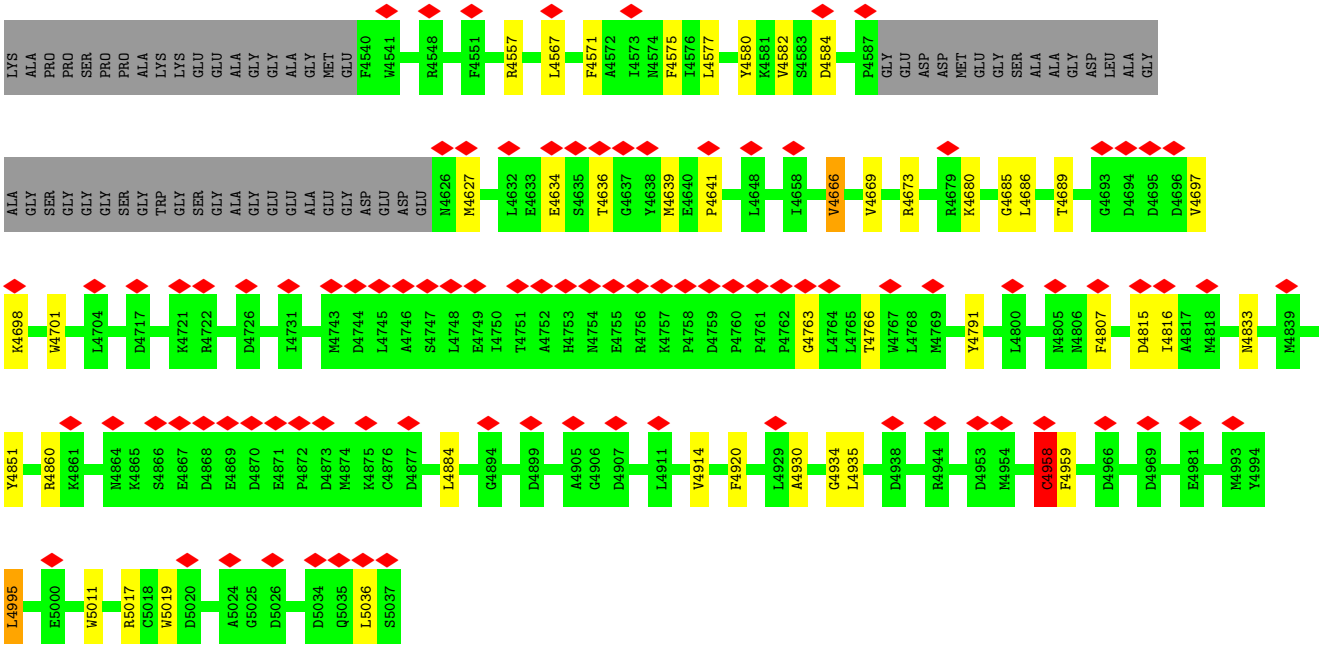
D4070 G4073 S4074 E4075 D4079 T4082 D4083 P4084 R4085 G4086 L4087 D4092 D4098 S4099 Q4102 F4103 T4104 G4105 P4106 D4118 E4119 N4120 E4121 N4130 R4131 R4137 D4138 N4142 E4152 P4155 H4156 D4157 P4158 R4159 A4167 E4168 S4169 E4172 R4175 P4176 R4180 A4186 S4187
R4188 E4191 Y4194 R4202 P4208 K4211 R4215 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4232 L4233 S4236 E4239 I4251 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ASP GLU GLU GLY ALA ALA GLY
ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ARG ARG LEU ALA ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU LEU ALA ALA LEU LEU TRP ALA VAL ALA
ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA GLY ALA LEU LEU TRP GLY SER LEU PHE GLY GLY GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY
ASP ALA ASP GLY ALA ALA GLY GLU GLY GLU GLY GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY GLU GLU VAL GLY GLY VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR
PRO ALA GLU PRO PRO THR PRO GLU GLY GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS


LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 R4548 F4551 R4557 L4567 F4571 A4572 I4573 N4574 F4575 I4576 L4577 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 ASP GLU N4626 M4627 L4632 E4633 E4634 S4635 T4636 G4637 Y4638 M4639 E4640 P4641 L4648 I4658 V4666 V4669 R4673 R4679 K4680 G4685 L4686 T4689 G4693 D4694 D4695 D4696 V4697
K4698 W4701 L4704 D4717 K4721 R4722 D4726 I4731 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 Y4791 L4800 N4805 N4806 F4807 D4815 I4816 A4817 M4818 N4833 M4839
Y4851 R4860 K4861 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876 D4877 L4884 G4894 D4899 A4905 G4906 D4907 L4911 V4914 F4920 L4929 A4930 G4934 L4935 D4938 R4944 D4953 M4954 C4958 F4959 D4966 D4969 E4981 M4993 Y4994
L4995 E5000 W5011 R5017 C5018 W5019 D5020 A5024 G5025 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	0.141	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

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	0.51	0/1123
1	F	0.31	0/834	0.51	0/1123
1	H	0.30	0/834	0.51	0/1123
1	J	0.31	0/834	0.51	0/1123
2	B	0.30	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.30	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	24/142628 (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	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	68

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.13	134.00	115.30
2	E	131	LEU	CA-CB-CG	8.11	133.96	115.30
2	I	131	LEU	CA-CB-CG	8.11	133.96	115.30
2	B	131	LEU	CA-CB-CG	8.10	133.94	115.30
2	E	1600	LEU	CA-CB-CG	7.05	131.51	115.30

There are no chirality outliers.

5 of 68 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	8	0
1	F	818	0	824	9	0
1	H	818	0	824	8	0
1	J	818	0	824	9	0
2	B	29369	0	24721	212	0
2	E	29369	0	24721	206	0
2	G	29369	0	24719	205	0
2	I	29369	0	24721	208	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102178	849	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 849 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.78	0.66
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.78	0.66
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.78	0.66
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.78	0.65
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.77	0.64

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	3235/4676 (69%)	2894 (90%)	336 (10%)	5 (0%)	44	77
2	E	3235/4676 (69%)	2896 (90%)	334 (10%)	5 (0%)	44	77
2	G	3235/4676 (69%)	2894 (90%)	336 (10%)	5 (0%)	44	77
2	I	3235/4676 (69%)	2895 (90%)	335 (10%)	5 (0%)	44	77
All	All	13360/19136 (70%)	11959 (90%)	1381 (10%)	20 (0%)	50	82

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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Mol	Chain	Res	Type
2	E	1708	ARG
2	I	1708	ARG
2	G	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	2493/3202 (78%)	2475 (99%)	18 (1%)	81	86
2	E	2493/3202 (78%)	2475 (99%)	18 (1%)	81	86
2	G	2493/3202 (78%)	2475 (99%)	18 (1%)	81	86
2	I	2493/3202 (78%)	2475 (99%)	18 (1%)	81	86
All	All	10324/13164 (78%)	10252 (99%)	72 (1%)	80	86

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	978	THR
2	G	4995	LEU
2	G	1141	ARG
2	G	3805	LEU
2	E	1600	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	4054	ASN

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Mol	Chain	Res	Type
2	G	3896	ASN
2	I	413	GLN
2	G	3781	GLN
2	G	4553	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	12
2	G	12
2	I	12
2	E	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	44.23
1	G	3613:UNK	C	3639:THR	N	43.95
1	I	3613:UNK	C	3639:THR	N	43.88
1	E	3613:UNK	C	3639:THR	N	43.84
1	E	3163:UNK	C	3170:UNK	N	16.60

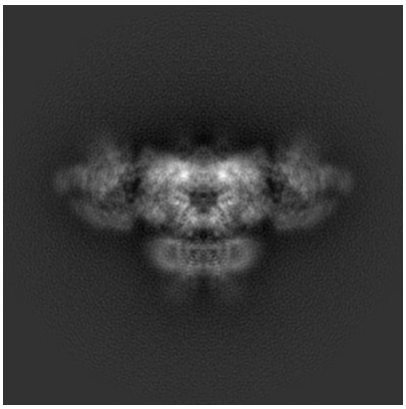
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8375. These allow visual inspection of the internal detail of the map and identification of artifacts.

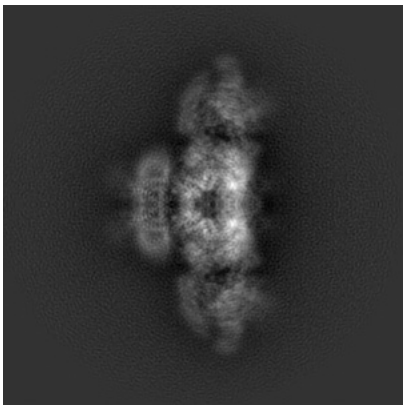
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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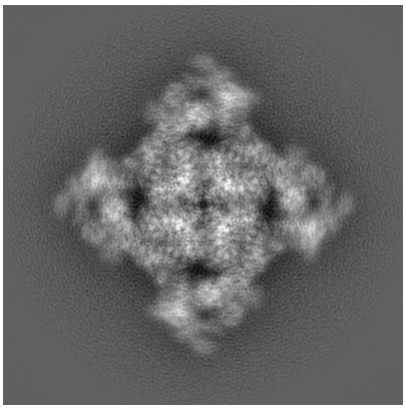
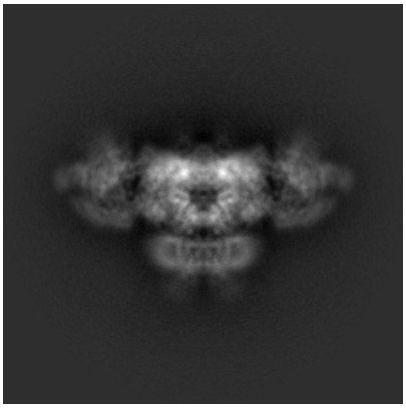


Z

6.1.2 Raw map



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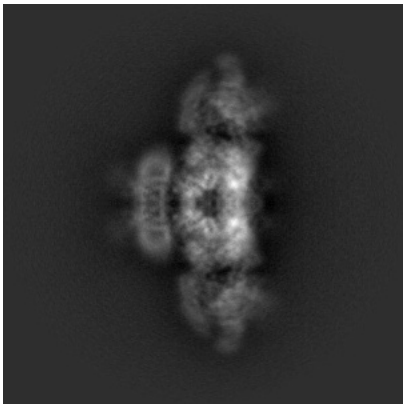
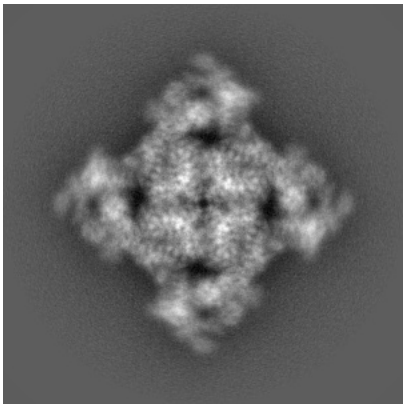


Y

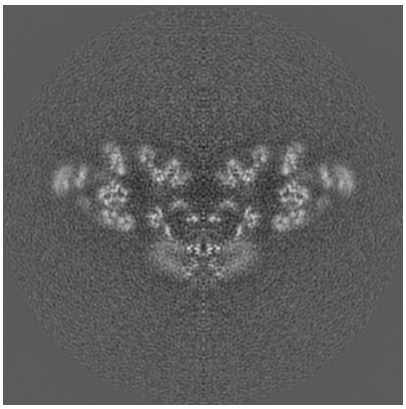


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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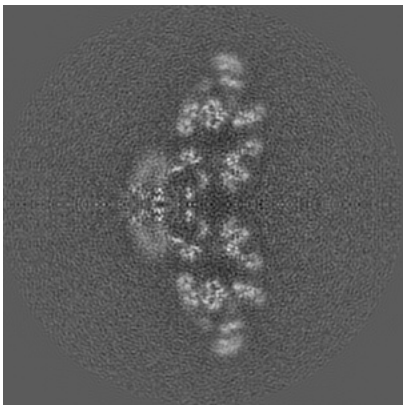
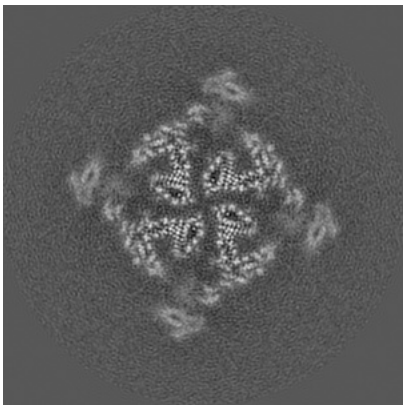
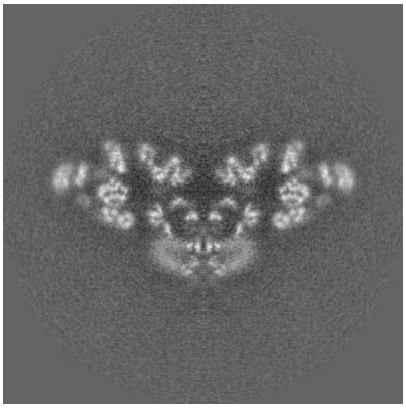


Y Index: 200



Z Index: 200

6.2.2 Raw map



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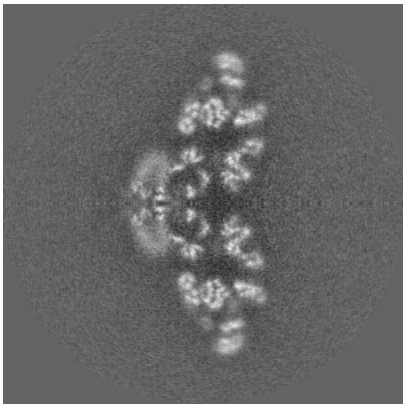

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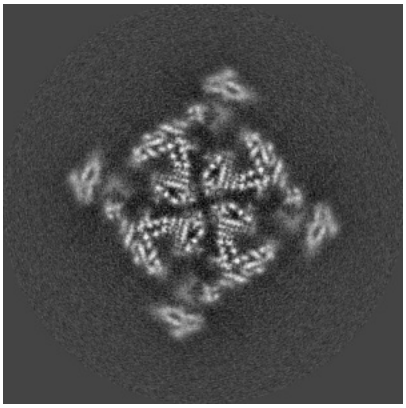
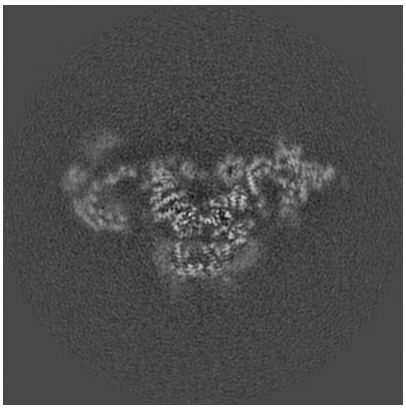


Z Index: 200

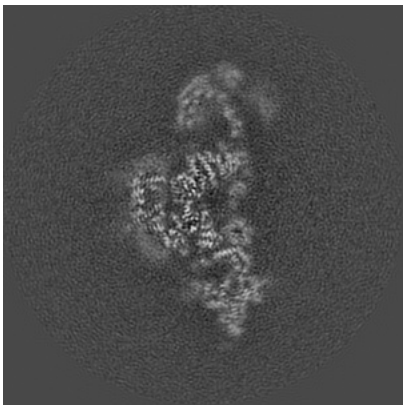
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

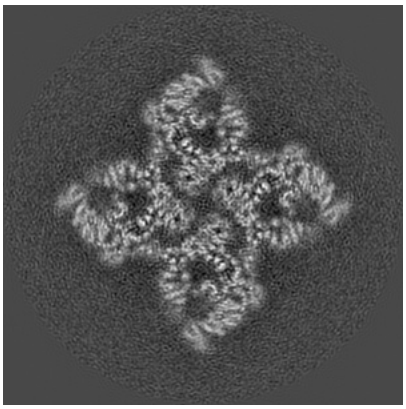
6.3.1 Primary map



X Index: 184

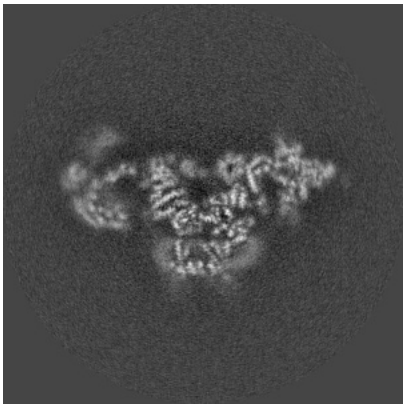


Y Index: 184

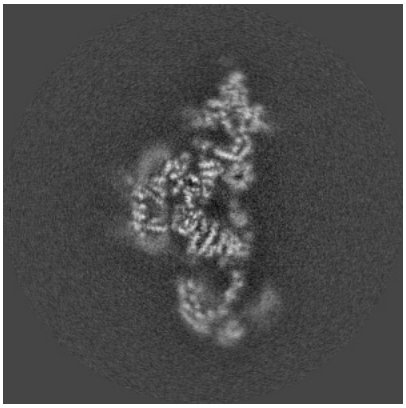


Z Index: 233

6.3.2 Raw map



X Index: 184



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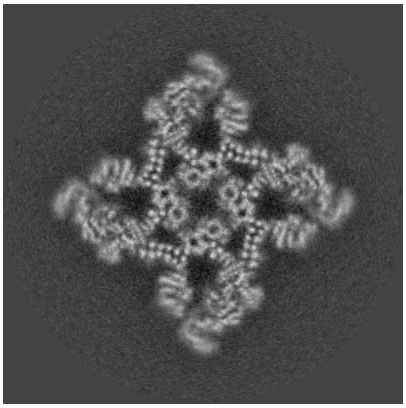
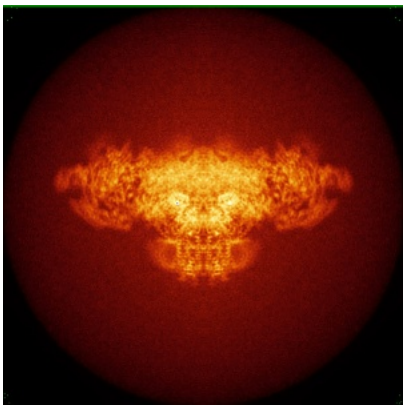


Z Index: 228

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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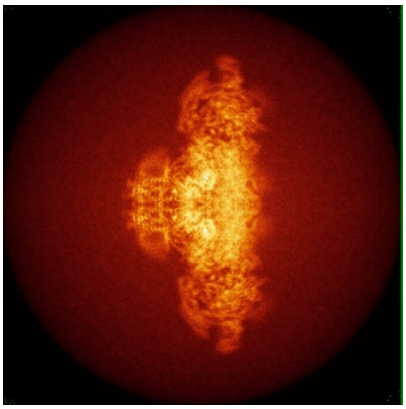
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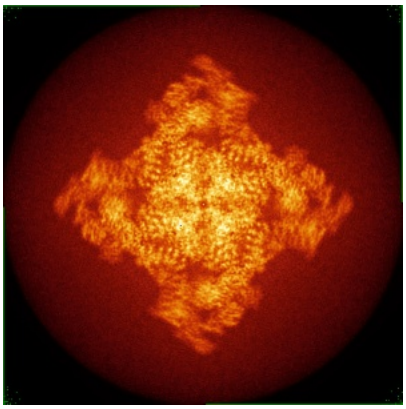
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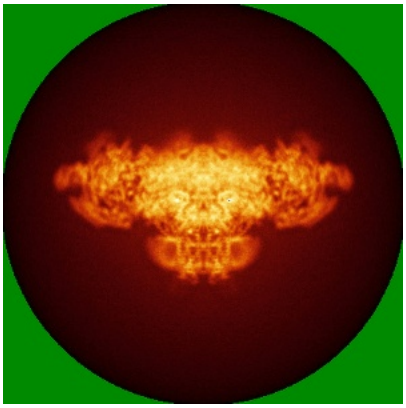
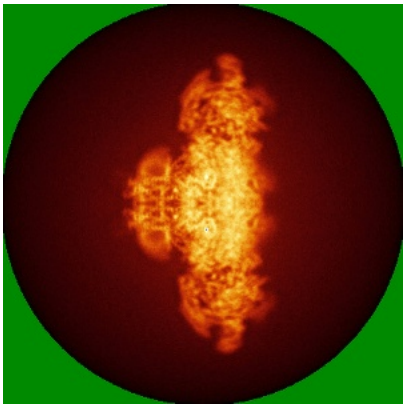
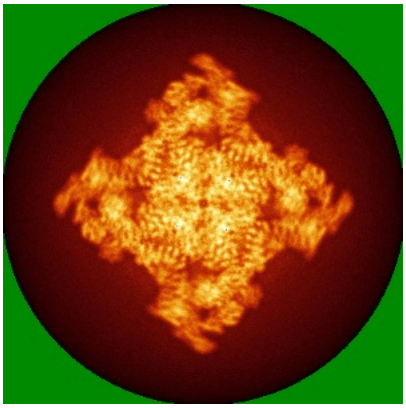
6.4.2 Raw map


X

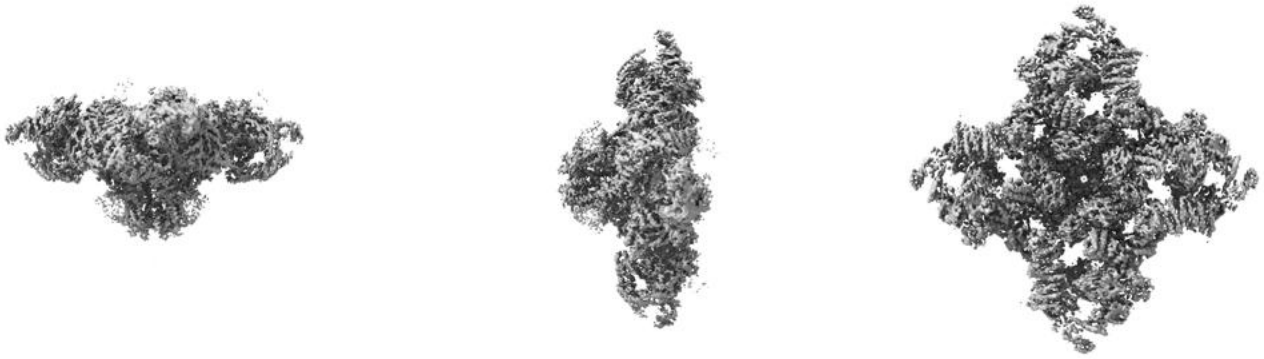

Y


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 0.04. 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.

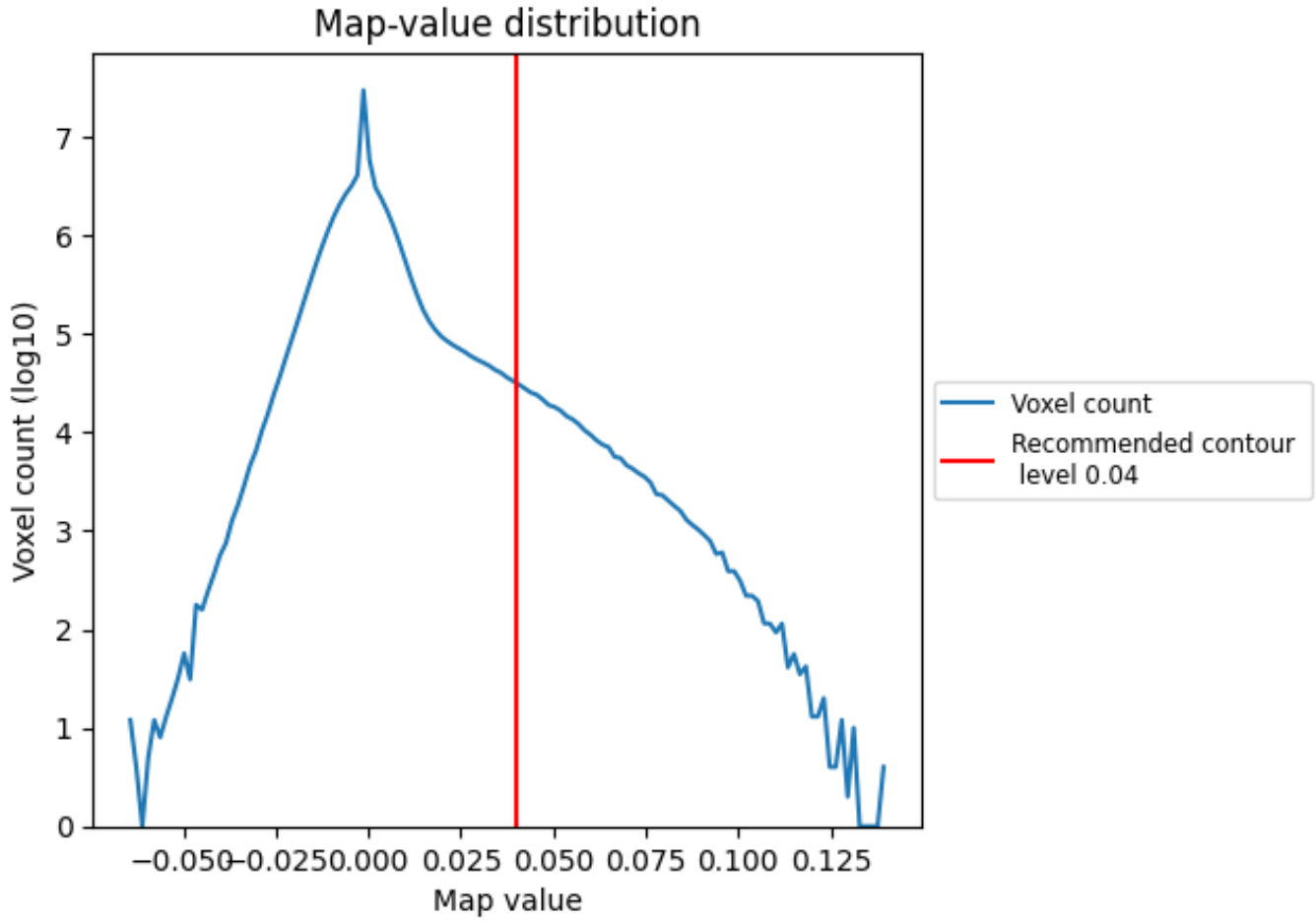
6.6 Mask visualisation (i)

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

7 Map analysis

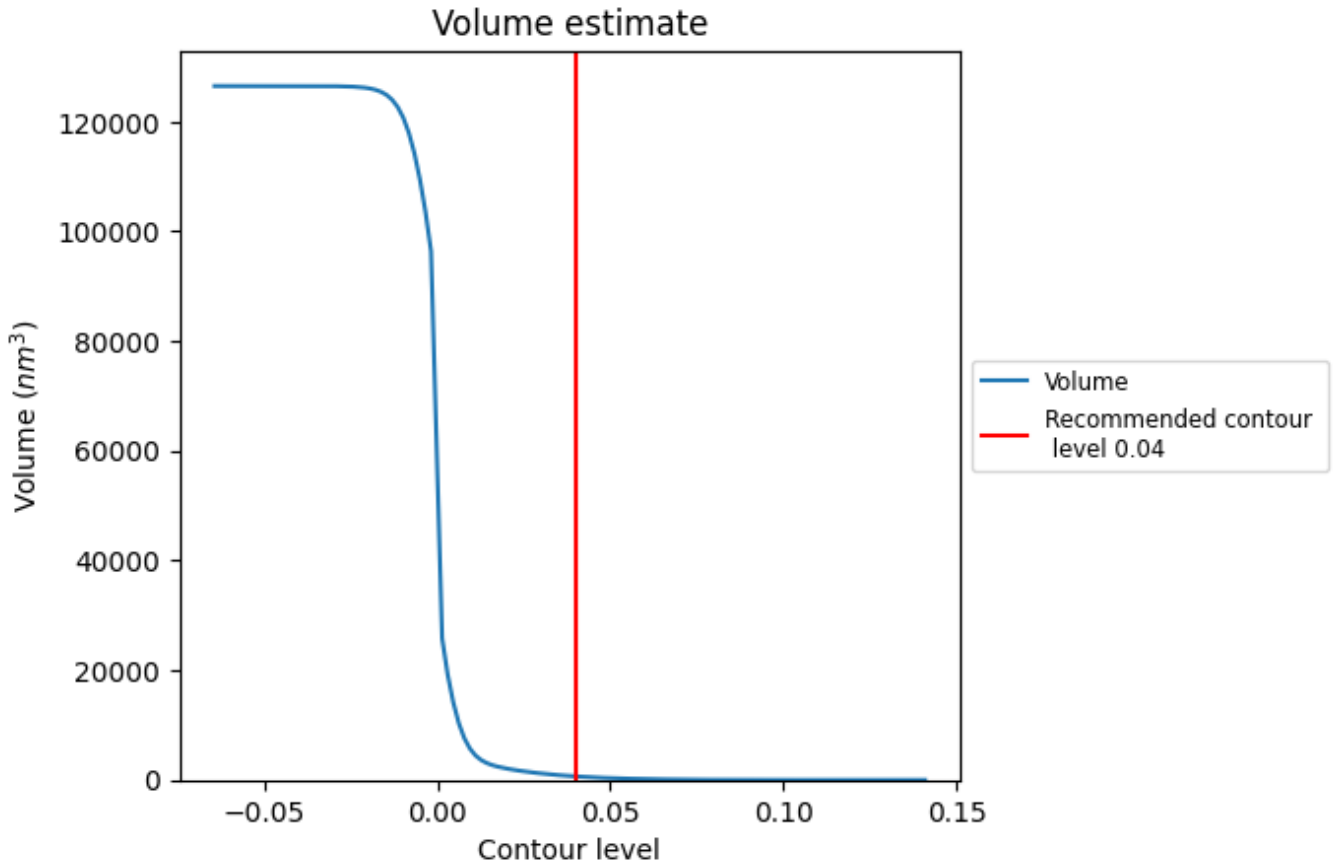
This section contains the results of statistical analysis of the map.

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.

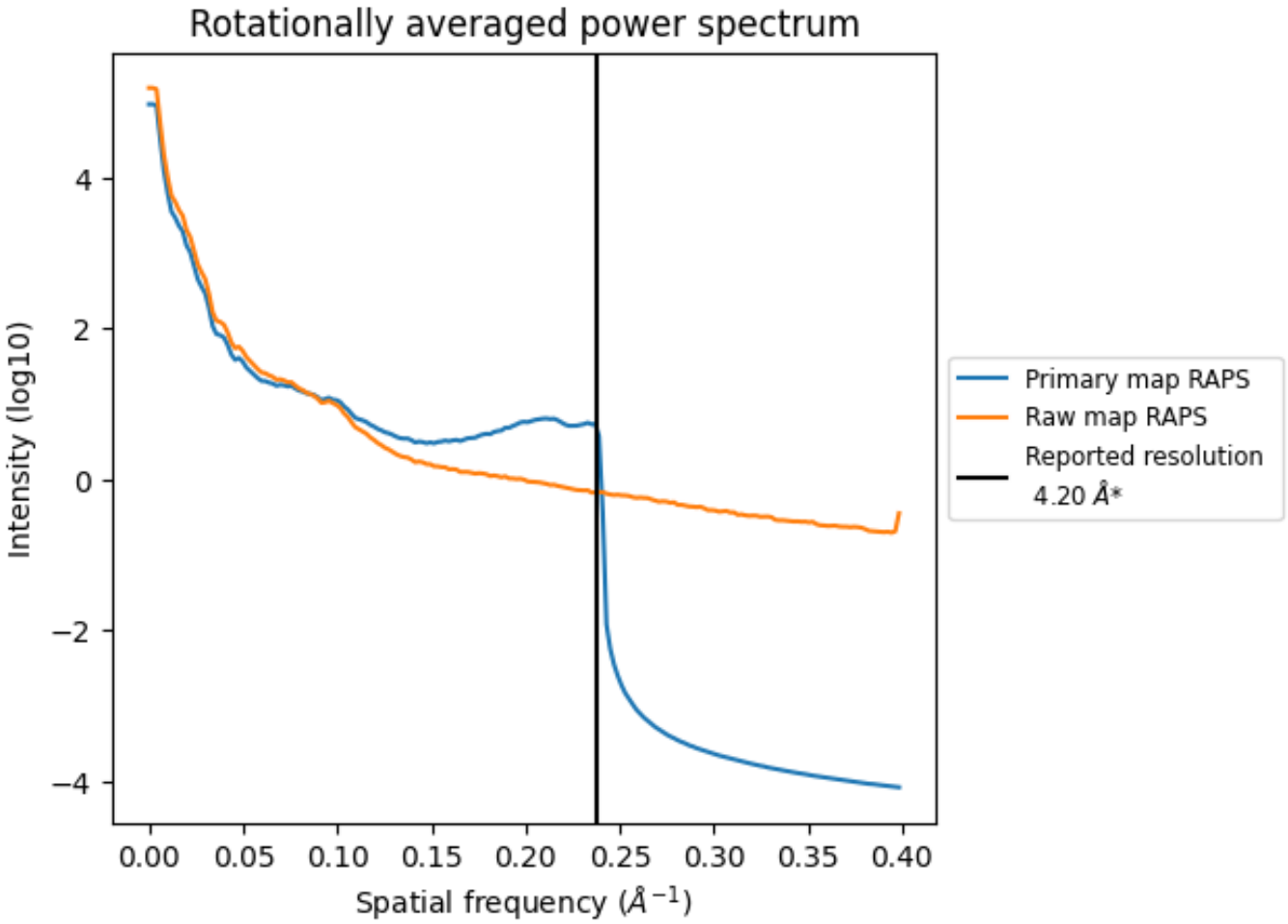
7.2 Volume estimate (i)



The volume at the recommended contour level is 651 nm^3; this corresponds to an approximate mass of 588 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)

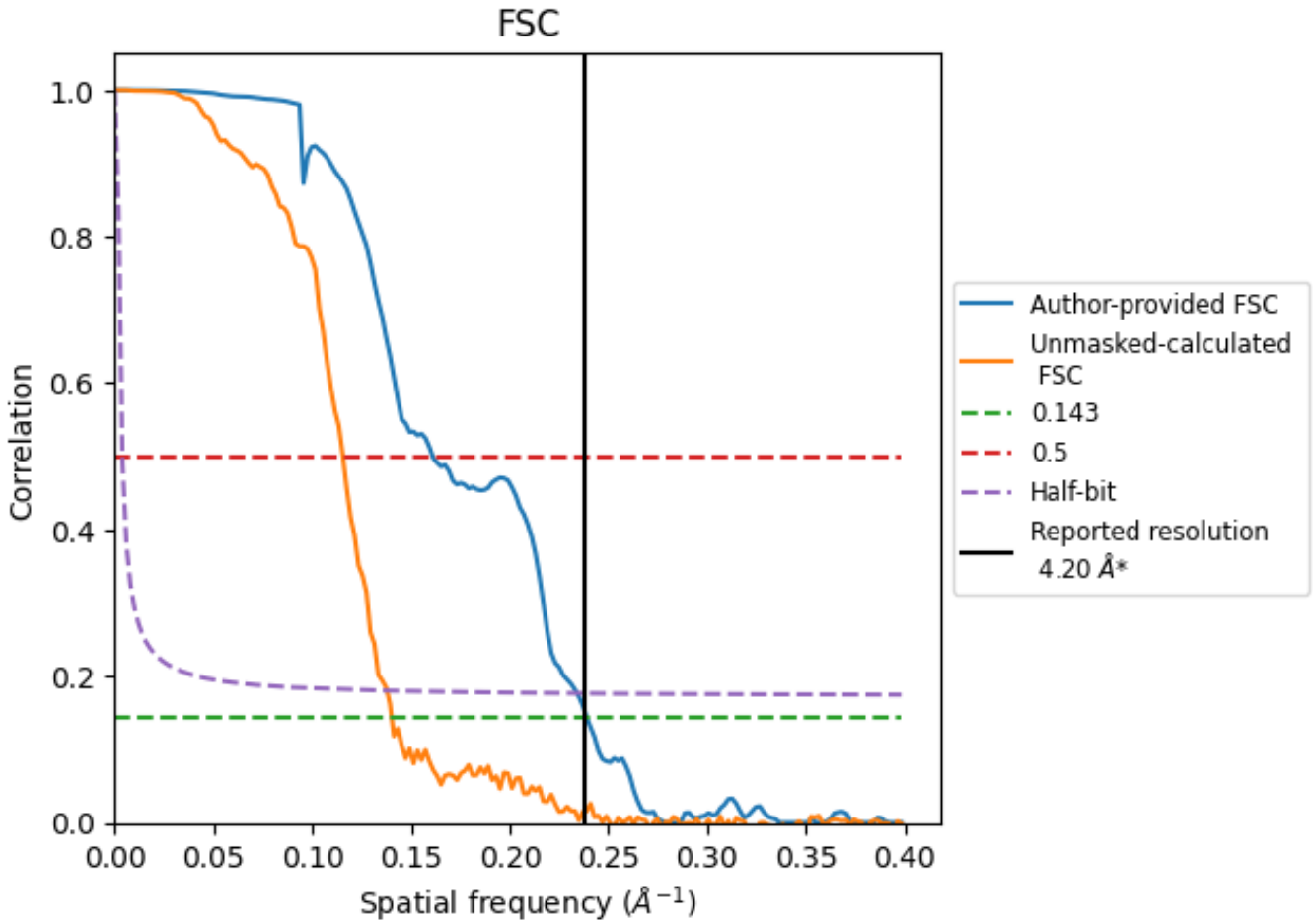


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

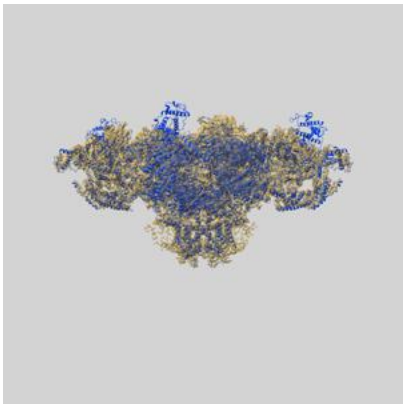
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.21	4.27
Unmasked-calculated*	7.13	8.65	7.26

*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 7.13 differs from the reported value 4.2 by more than 10 %

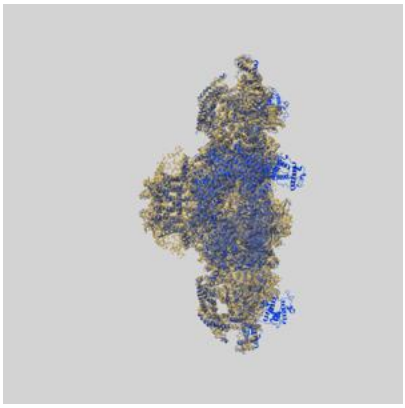
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8375 and PDB model 5T9S. Per-residue inclusion information can be found in section 3 on page 5.

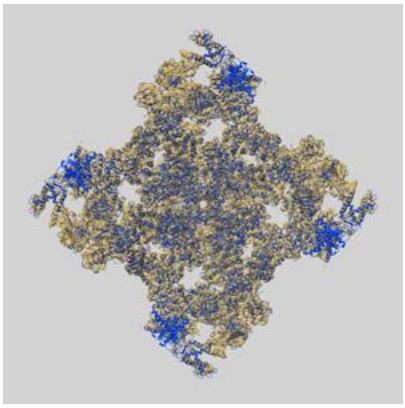
9.1 Map-model overlay



X



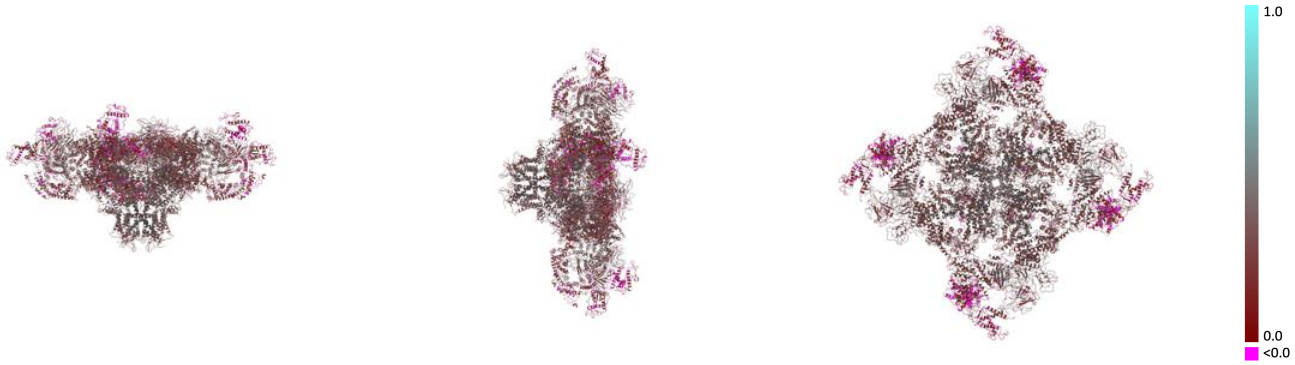
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

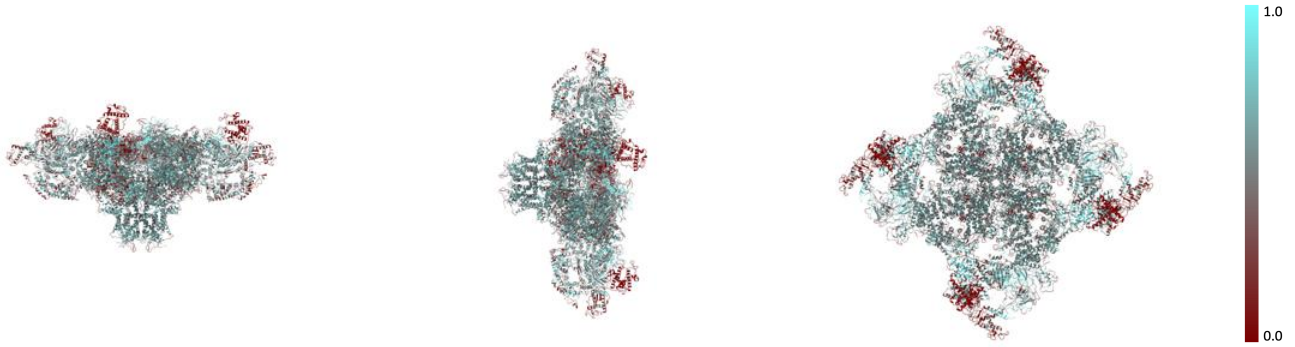
9.2 Q-score mapped to coordinate model



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.

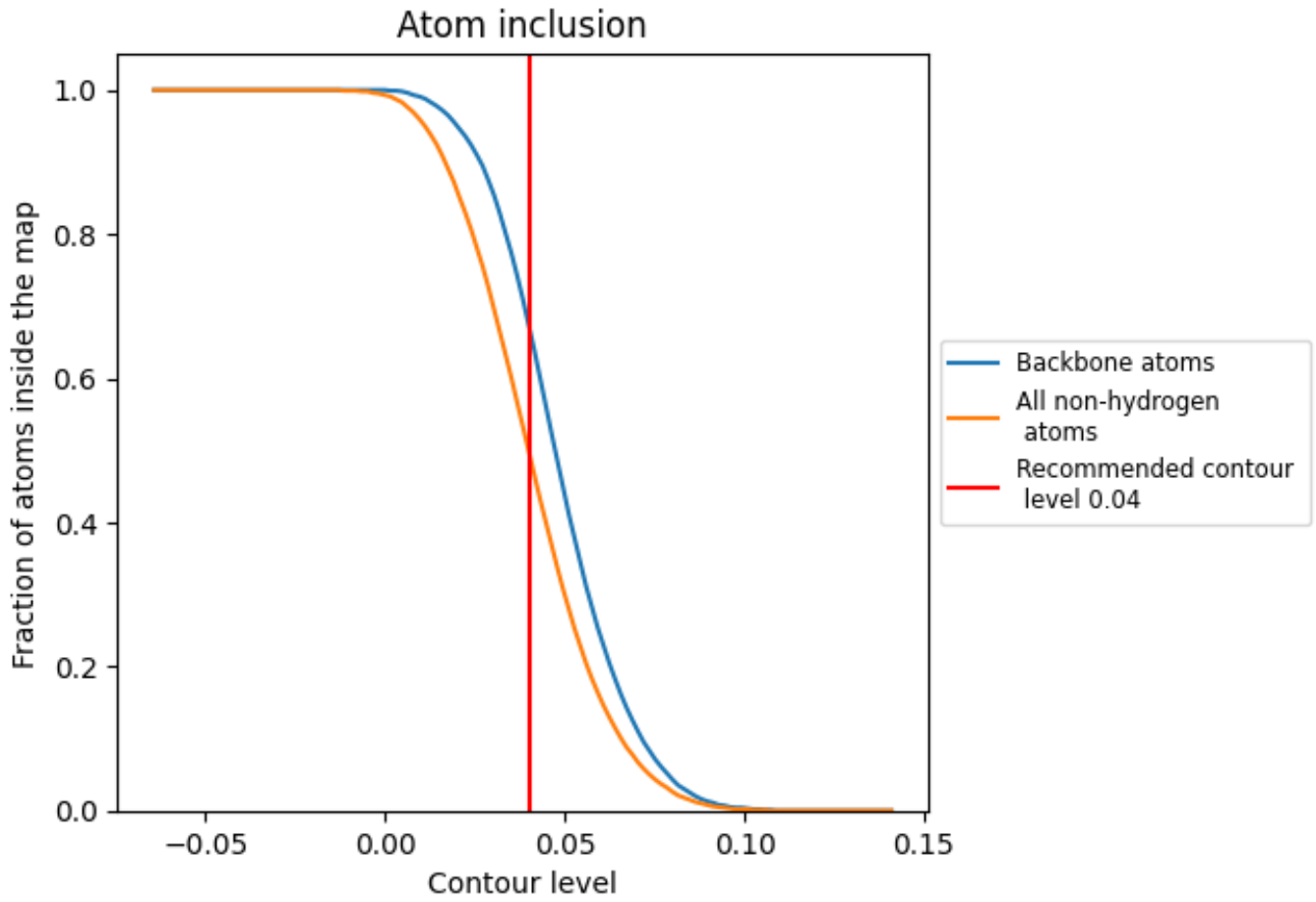
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4980	0.2870
A	0.4780	0.3000
B	0.5030	0.2900
E	0.4950	0.2850
F	0.4780	0.3050
G	0.5000	0.2870
H	0.4840	0.3060
I	0.4950	0.2850
J	0.4840	0.2990