wwPDB EM Validation Summary Report

Nov 20, 2022 – 08:38 AM EST

PDB ID	:	7M6L
EMDB ID	:	EMD-23699
Title	:	High resolution structure of the membrane embedded skeletal muscle ryanodine receptor
Authors	:	Melville, Z.; Kim, K.; Clarke, O.B.; Marks, A.R.
Deposited on	:	2021-03-25
Resolution	:	3.98 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

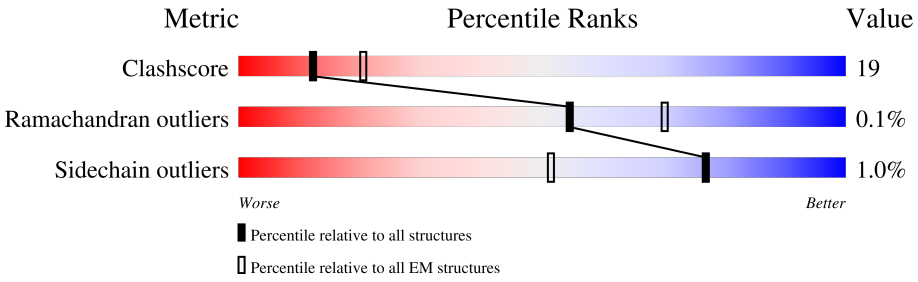
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.98 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	F	108	65% 30%
1	H	108	66% 29%
1	J	108	67% 28%
1	O	108	67% 28%
2	A	5037	18% 53% 32% 15%
2	B	5037	18% 53% 32% 15%
2	G	5037	18% 53% 32% 15%
2	I	5037	18% 53% 32% 15%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 140412 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.

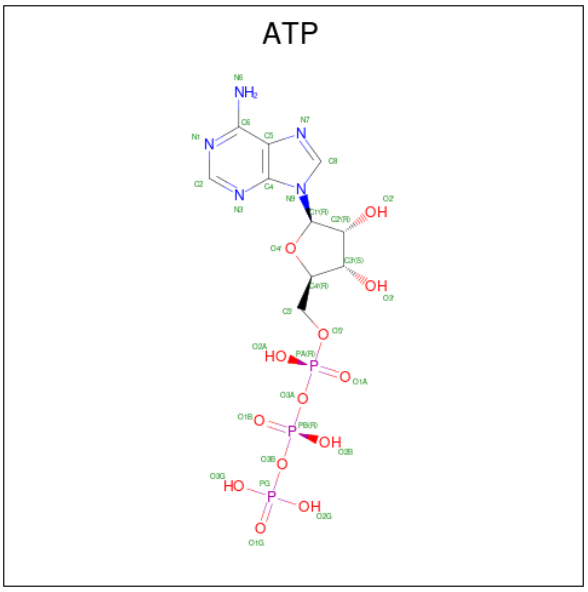
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	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		
1	O	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	A	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	G	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	B	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		
2	I	4299	Total	C	N	O	S	3	0
			34238	21819	5882	6302	235		

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



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

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

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

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

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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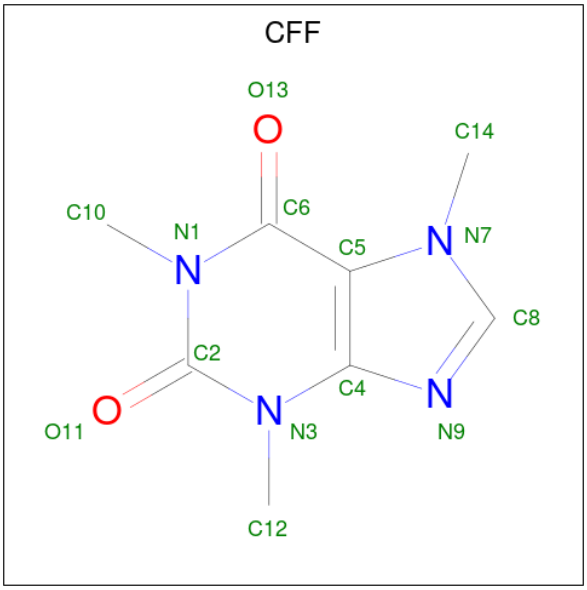
Mol	Chain	Residues	Atoms	AltConf
5	G	1	Total Zn 1 1	0
5	B	1	Total Zn 1 1	0
5	I	1	Total Zn 1 1	0

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



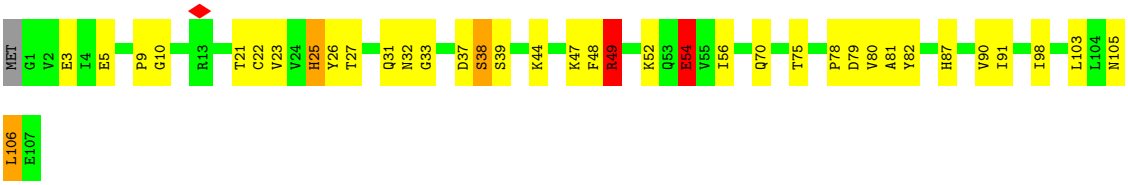
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 14 8 4 2	0
6	G	1	Total C N O 14 8 4 2	0
6	B	1	Total C N O 14 8 4 2	0
6	I	1	Total C N O 14 8 4 2	0

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.

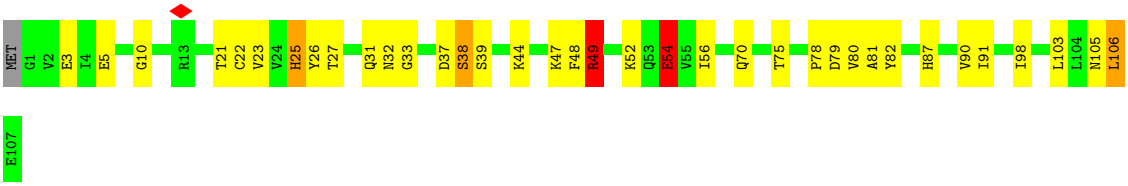
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



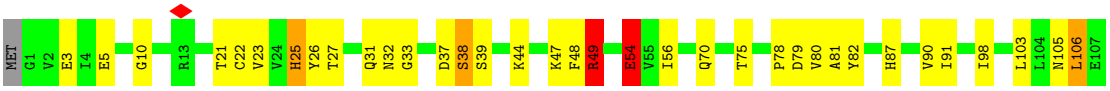
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



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

Chain J:

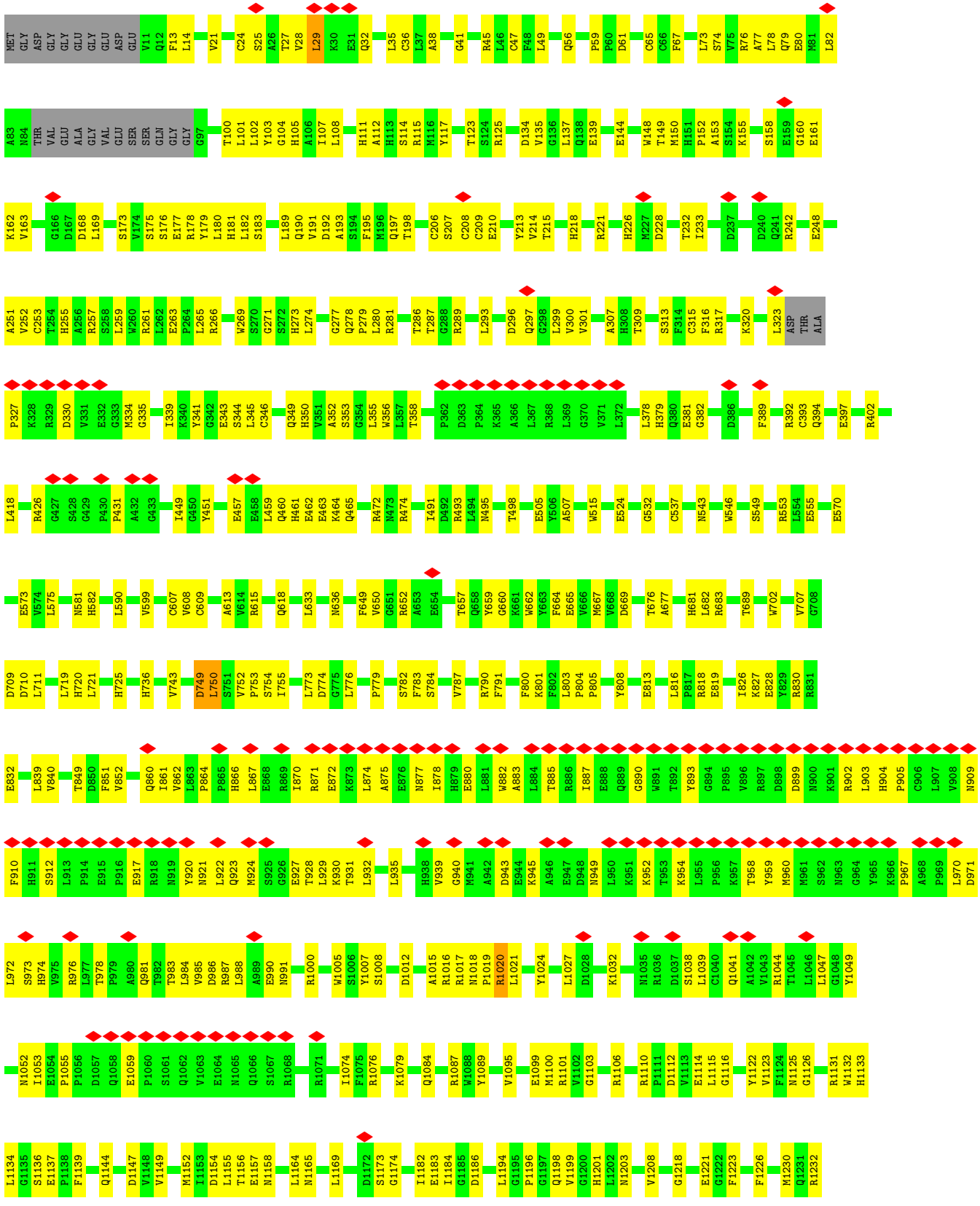


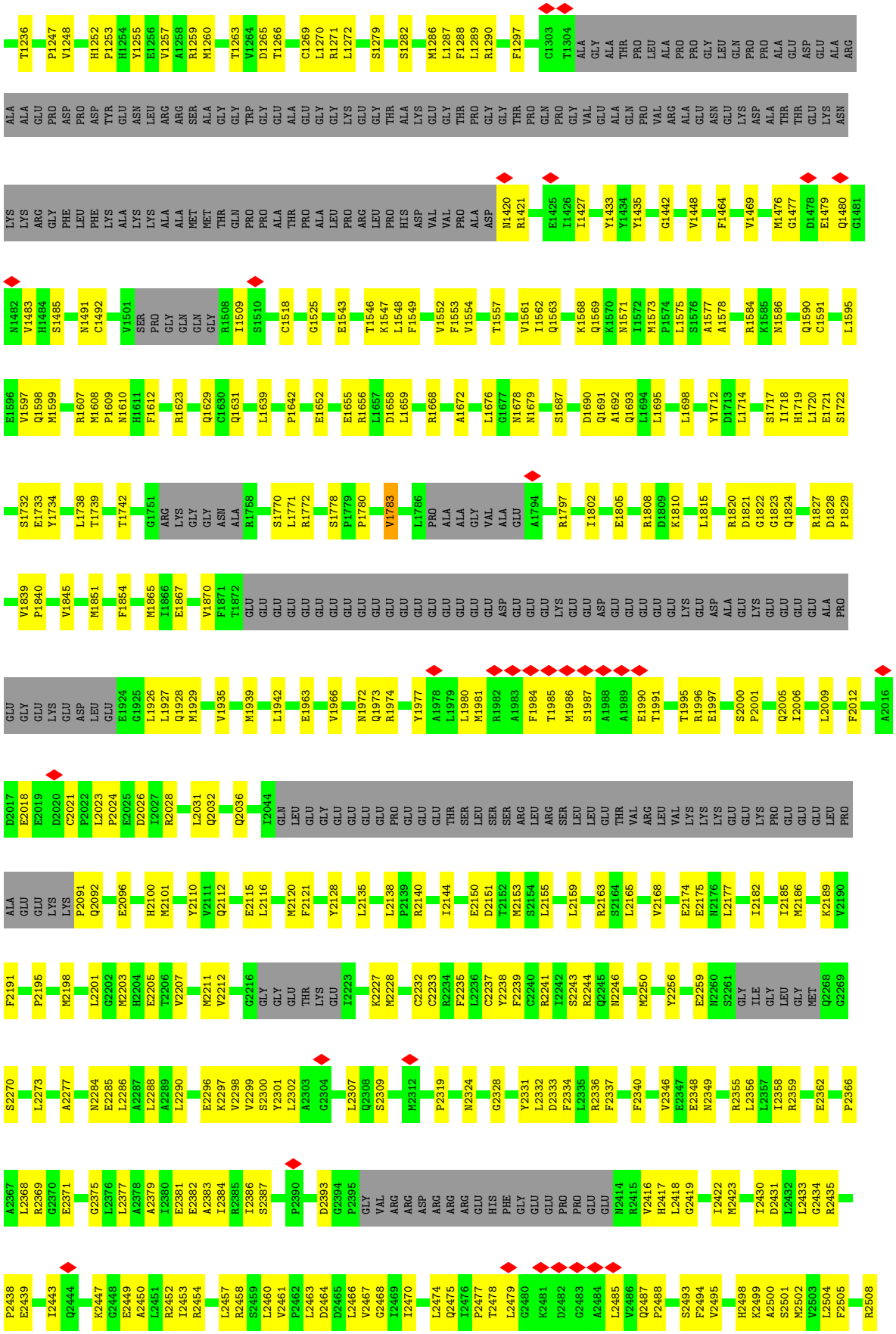
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain O:

• Molecule 2: Ryanodine receptor 1

Chain A:

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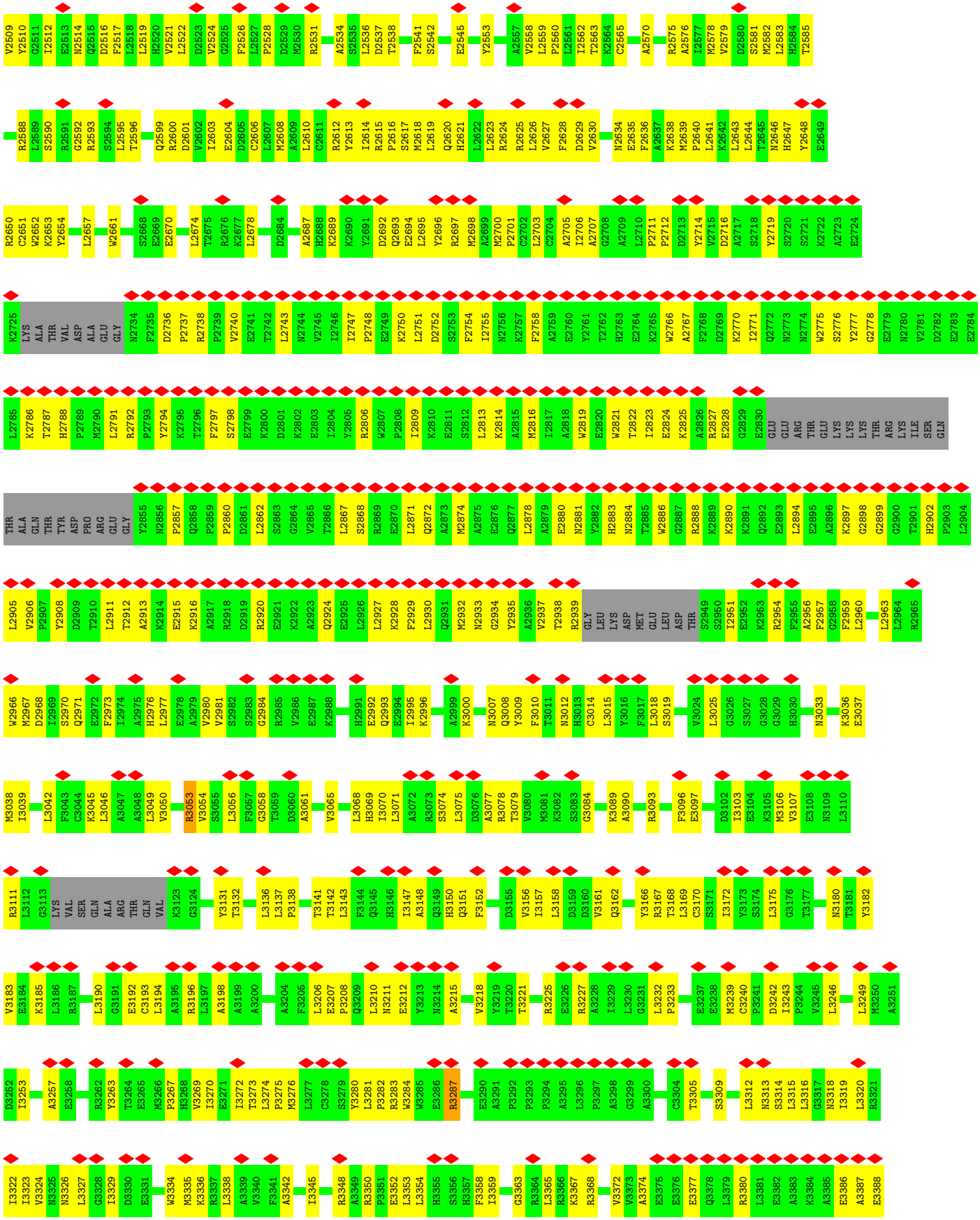
ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN
LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 E1425 I1426 I1427 Y1433 Y1434 Y1435 G1442 V1448 F1464 V1469 M1476 G1477 D1478 E1479 Q1480 G1481
N1482 V1483 H1484 S1485 N1491 C1492 V1501 SER PRO GLY GLN GLN GLY R1508 I1509 S1510 C1518 G1525 E1543 T1546 K1547 L1548 F1549 V1552 F1553 V1554 T1557 V1561 I1562 Q1563 K1568 Q1569 K1570 N1571 I1572 M1573 P1574 L1575 S1576 A1577 A1578 R1584 K1585 N1586 Q1590 C1591 L1595
E1596 V1597 Q1598 M1599 R1607 M1608 P1609 N1610 H1611 F1612 R1623 Q1629 C1630 Q1631 L1639 P1642 E1652 E1655 R1656 L1657 D1658 L1659 R1668 A1672 L1676 G1677 N1678 N1679 S1687 D1690 Q1691 A1692 Q1693 L1694 L1695 L1698 Y1712 D1713 L1714 S1717 I1718 H1719 L1720 E1721 S1722
S1732 E1733 Y1734 L1738 T1739 T1742 G1751 ARG LYS GLY GLY ASN ALA R1758 S1770 L1771 R1772 S1778 P1779 P1780 V1783 L1786 PRO ALA ALA GLY VAL ALA GLU A1794 R1797 I1802 E1805 R1808 D1809 K1810 L1815 R1820 D1821 G1822 G1823 Q1824 R1827 D1828 P1829
V1839 P1840 V1845 M1851 F1854 M1865 I1866 E1867 V1870 F1871 T1872 GLU GLU 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 LEU GLU E1924 G1925 L1926 L1927 Q1928 M1929 V1935 M1939 L1942 E1963 V1966 N1972 Q1973 R1974 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 T1995 R1996 E1997 S2000 P2001 Q2005 I2006 L2009 F2012 A2016
D2017 E2018 E2019 D2020 C2021 P2022 L2023 P2024 E2025 D2026 I2027 R2028 L2031 Q2032 Q2036 I2044 GLN LEU GLU GLY 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 LYS LYS P2091 Q2092 E2096 H2100 M2101 Y2110 V2111 Q2112 E2115 L2116 M2120 F2121 Y2128 L2135 L2138 P2139 R2140 I2144 E2150 D2151 T2152 M2153 S2154 L2155 L2159 R2163 S2164 L2165 V2168 E2174 E2175 N2176 L2177 I2182 I2185 M2186 K2189 V2190
F2191 P2195 M2198 L2201 G2202 M2203 H2204 E2205 T2206 V2207 M2211 V2212 G2216 GLY GLY GLU THR LYS GLU I2223 K2227 M2228 C2232 C2233 R2234 F2235 L2236 C2237 Y2238 F2239 C2240 R2241 I2242 S2243 R2244 Q2245 N2246 M2250 Y2256 E2259 N2260 S2261 GLY ILE GLY LEU GLY MET Q2268 G2269
S2270 L2273 A2277 N2284 E2285 L2286 A2287 L2288 A2289 L2290 E2296 K2297 V2298 V2299 S2300 Y2301 L2302 A2303 G2304 L2307 Q2308 S2309 M2312 P2319 N2324 G2328 Y2331 L2332 D2333 F2334 L2335 R2336 F2337 F2340 V2346 E2347 E2348 N2349 R2355 L2356 L2357 I2358 R2359 E2362 P2366
A2367 L2368 R2369 G2370 E2371 G2375 L2376 L2377 A2378 A2379 I2380 E2381 E2382 A2383 I2384 R2385 I2386 S2387 P2390 D2393 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 H2417 L2418 G2419 I2422 M2423 I2430 D2431 L2432 L2433 G2434 R2435
P2438 E2439 I2443 Q2444 K2447 G2448 E2449 A2450 L2451 R2452 I2453 R2454 L2457 R2458 S2459 L2460 V2461 P2462 L2463 D2464 D2465 L2466 V2467 G2468 I2469 I2470 L2474 Q2475 I2476 P2477 T2478 L2479 G2480 K2481 D2482 G2483 A2484 L2485 V2486 Q2487 P2488 S2493 F2494 V2495 H2498 K2499 A2500 S2501 M2502 V2503 L2504 F2505 R2508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R2588 L2589 S2590 R2591 G2592 R2593 S2594 L2595 T2596 Q2599 R2600 D2601 V2602 I2603 E2604 D2605 C2606 L2607 M2608 A2609 L2610 C2611 R2612 Y2613 I2614 R2615 P2616 S2617 M2618 L2619 Q2620 H2621 L2622 L2623 R2624 R2625 L2626 V2627 F2628 D2629 V2630 N2634 E2635 F2636 A2637 K2638 M2639 P2640 L2641 K2642 L2643 L2644 T2645 N2646 H2647 Y2648 E2649
R2650 C2651 W2652 K2653 Y2654 L2657 W2661 S2668 E2669 E2670 L2674 T2675 R2676 K2677 L2678 D2684 A2687 H2688 K2689 K2690 Y2691 D2692 Q2693 E2694 L2695 Y2696 R2697 M2698 A2699 M2700 P2701 C2702 L2703 C2704 A2705 I2706 A2707 G2708 A2709 L2710 P2711 P2712 D2713 Y2714 V2715 D2716 A2717 S2718 Y2719 S2720 S2721 K2722 A2723 E2724
K2725 LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 P2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784
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W2966 M2967 D2968 I2969 S2970 Q2971 E2972 F2973 I2974 A2975 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 H2991 E2992 Q2993 E2994 I2995 K2996 A2999 K3000 N3007 Q3008 Y3009 F3010 T3011 N3012 H3013 C3014 L3015 Y3016 F3017 L3018 S3019 V3024 L3025 G3026 S3027 G3028 G3029 H3030 N3033 K3036 E3037
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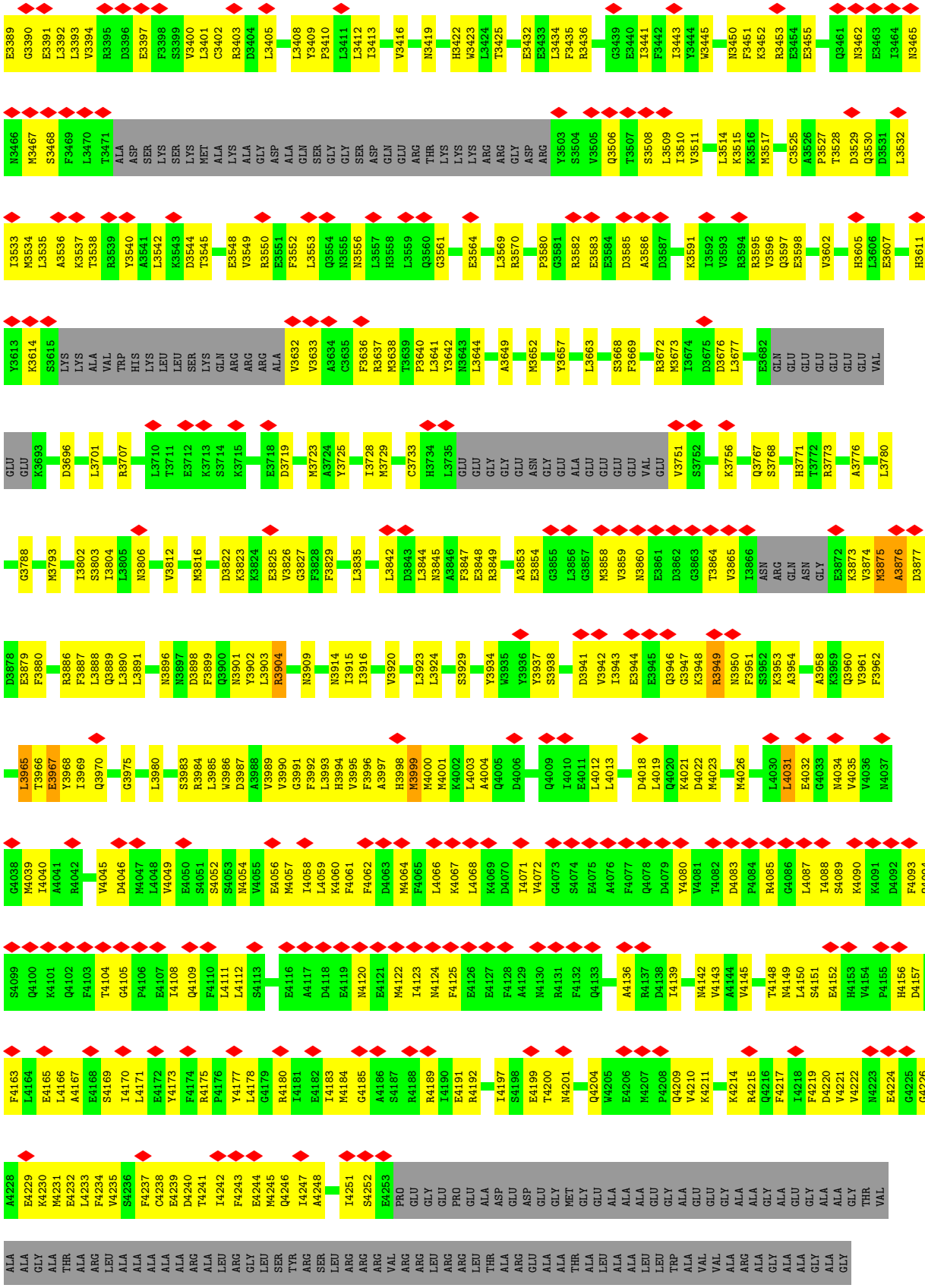
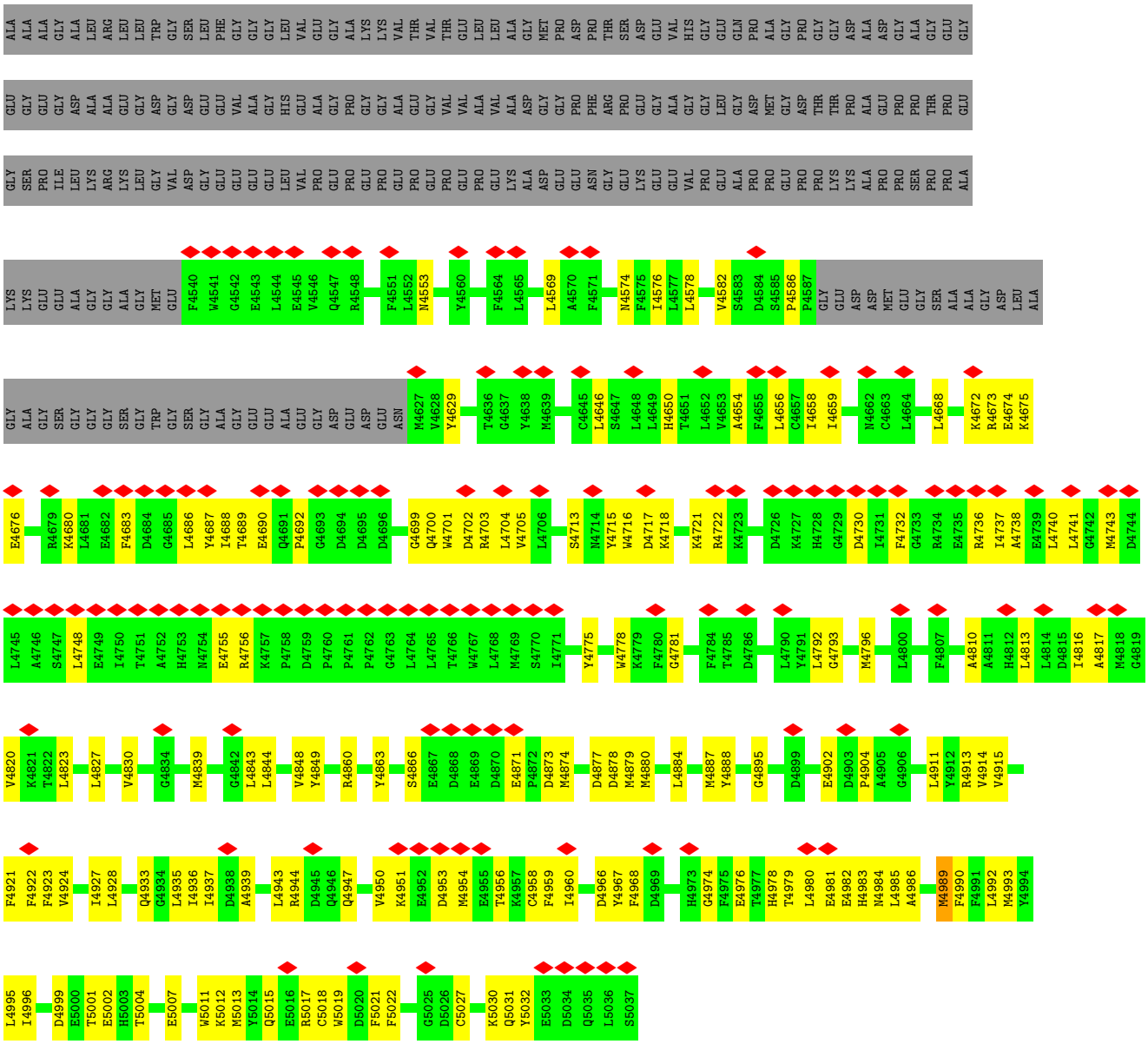
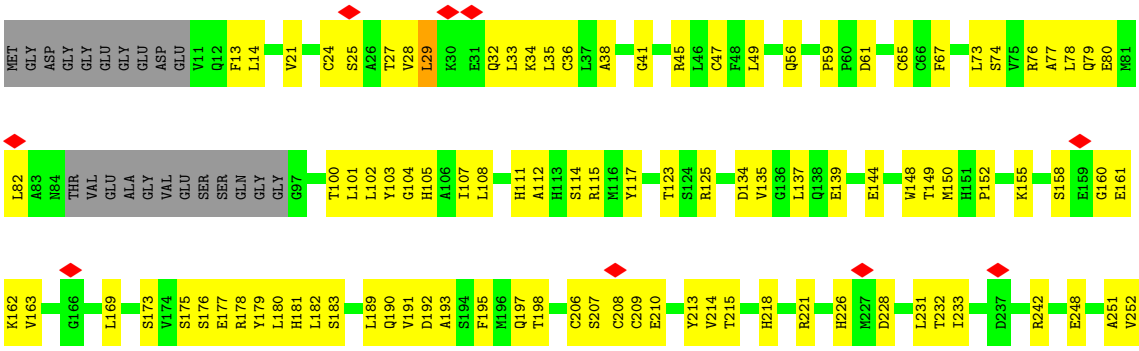
V3183 E3184 K3185 L3186 R3187 L3190 G3191 E3192 C3193 L3194 A3195 R3196 L3197 A3198 A3199 A3200 A3204 F3205 L3206 E3207 P3208 Q3209 L3210 N3211 E3212 Y3213 N3214 A3215 V3218 Y3219 T3220 T3221 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 E3237 E3238 M3239 C3240 P3241 D3242 I3243 P3244 V3245 L3246 L3249 M3250 A3251
D3262 I3263 A3257 E3258 R3262 Y3263 T3264 E3265 M3266 P3267 H3268 V3269 I3270 E3271 I3272 T3273 L3274 P3275 M3276 L3277 C3278 S3279 Y3280 L3281 P3282 R3283 W3284 W3285 E3286 R3287 E3290 A3291 P3292 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 C3304 T3305 S3309 L3312 N3313 S3314 L3315 L3316 G3317 N3318 I3319 L3320 R3321
I3322 I3323 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 W3334 M3335 K3336 R3337 L3338 A3339 V3340 F3341 A3342 I3345 R3348 A3349 R3350 P3351 E3352 L3353 L3354 H3355 S3356 H3357 F3358 I3359 G3363 R3364 L3365 R3366 K3367 R3368 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388

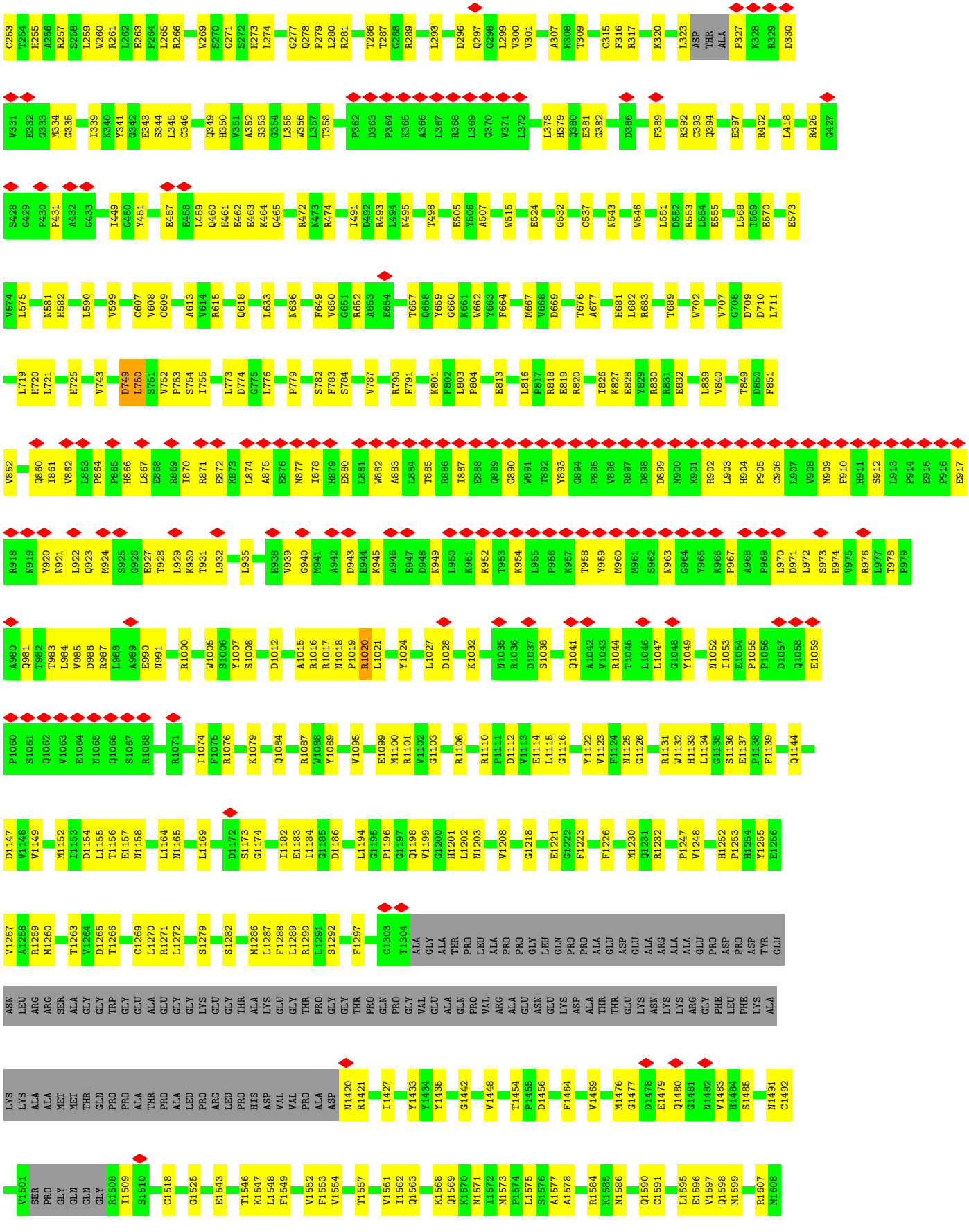




• Molecule 2: Ryanodine receptor 1

Chain G:

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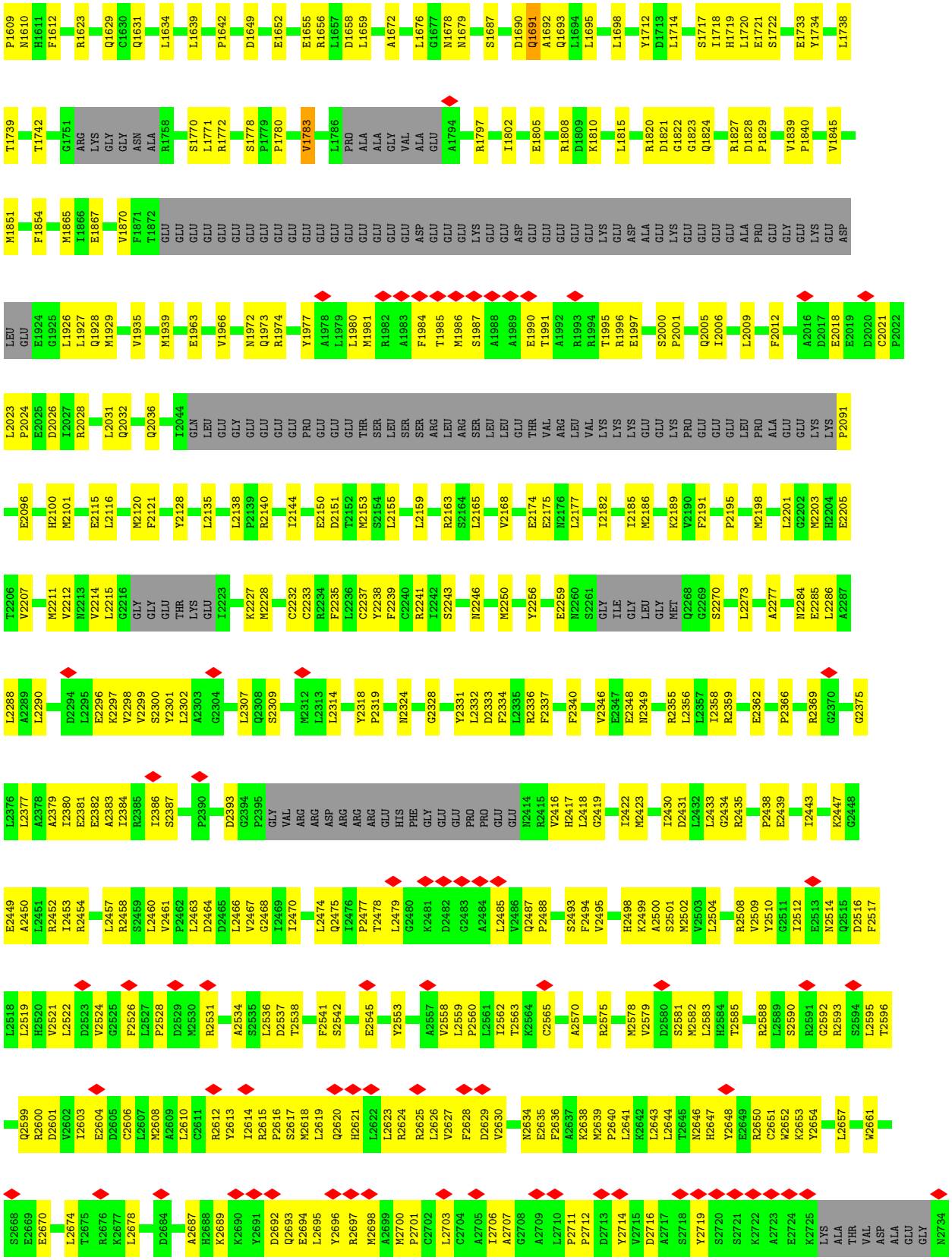

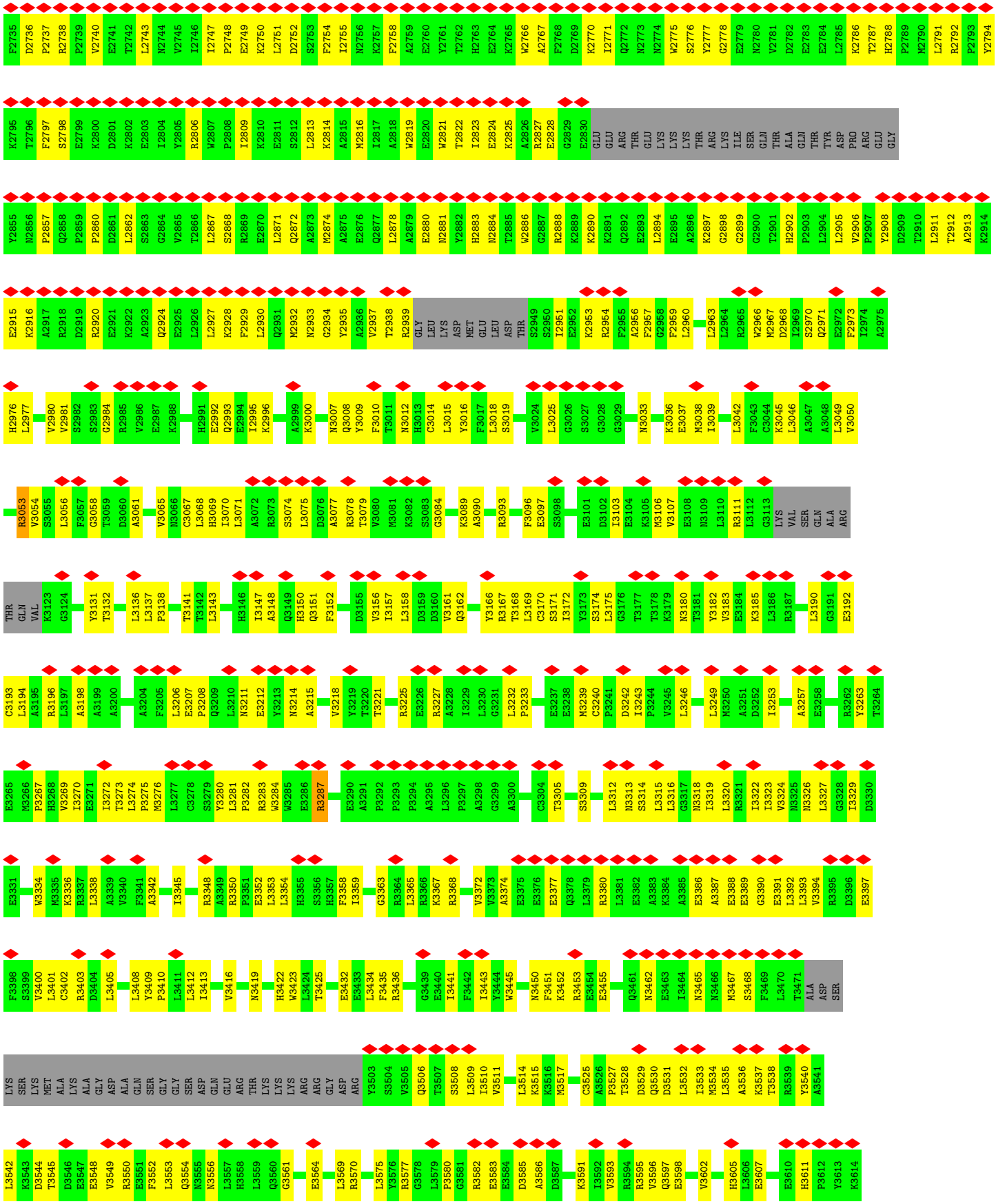
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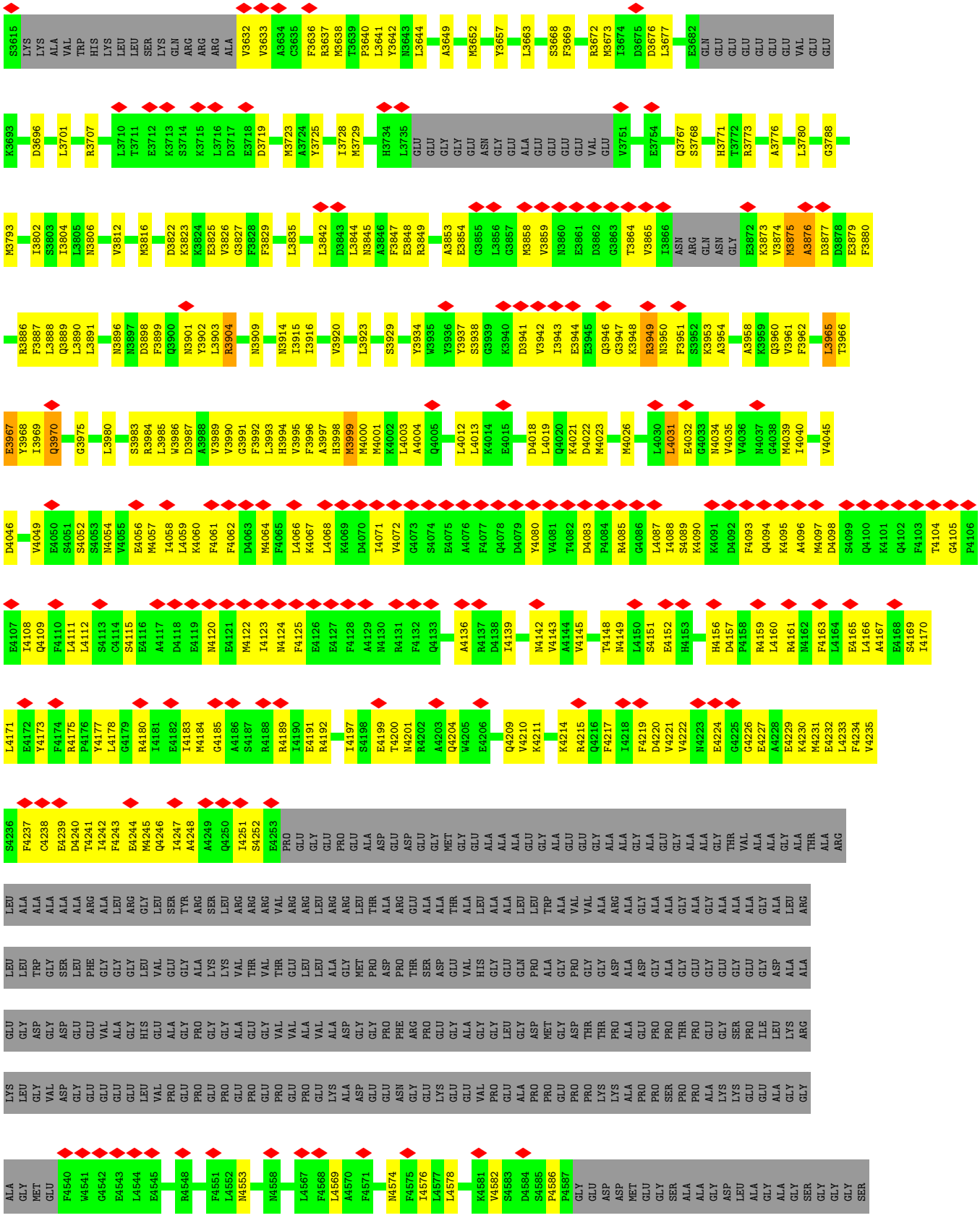
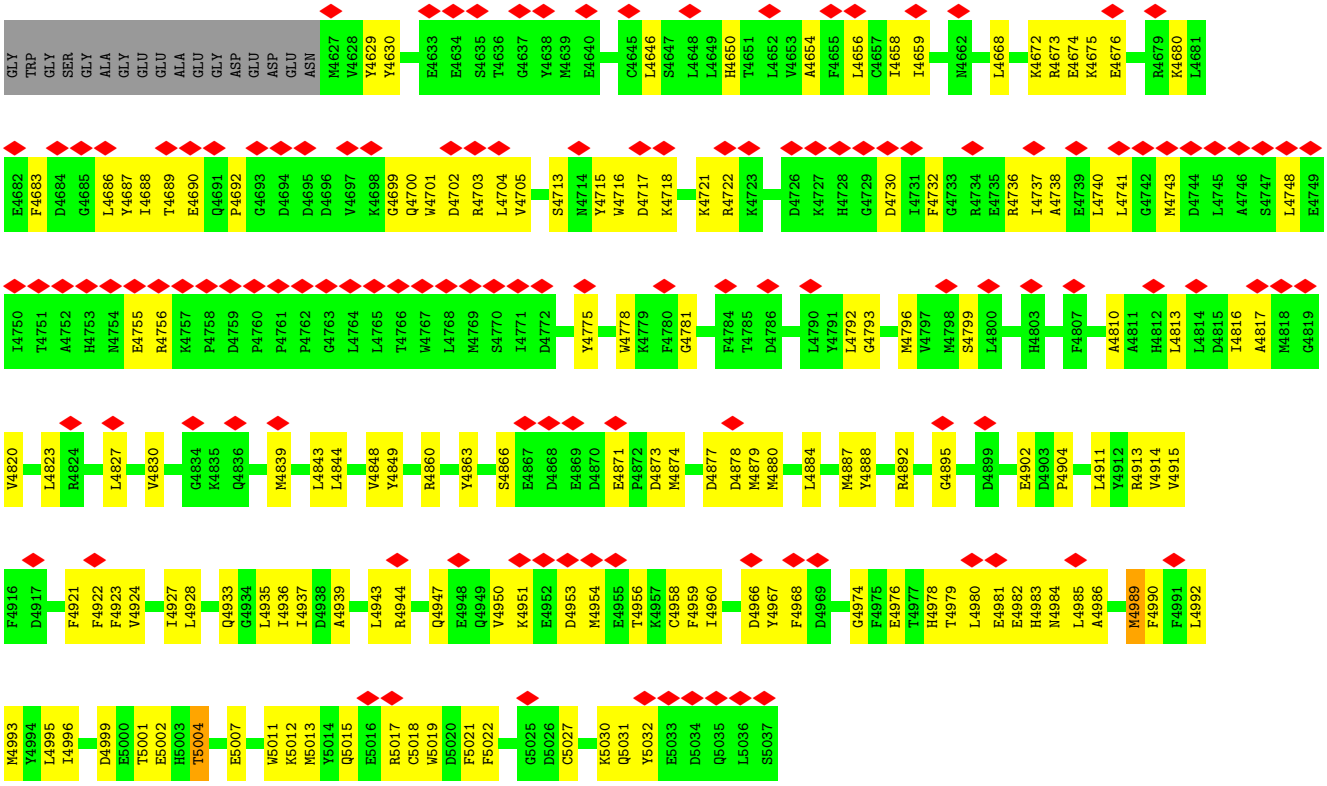
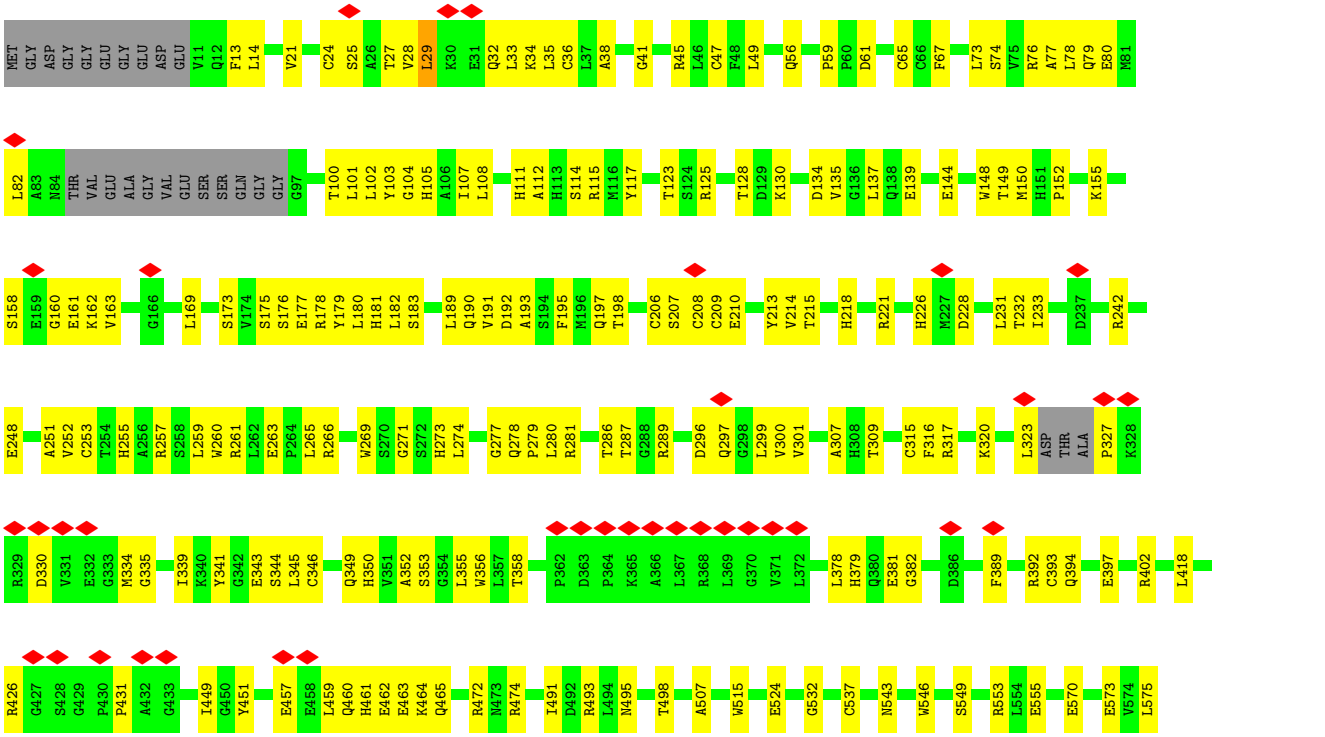
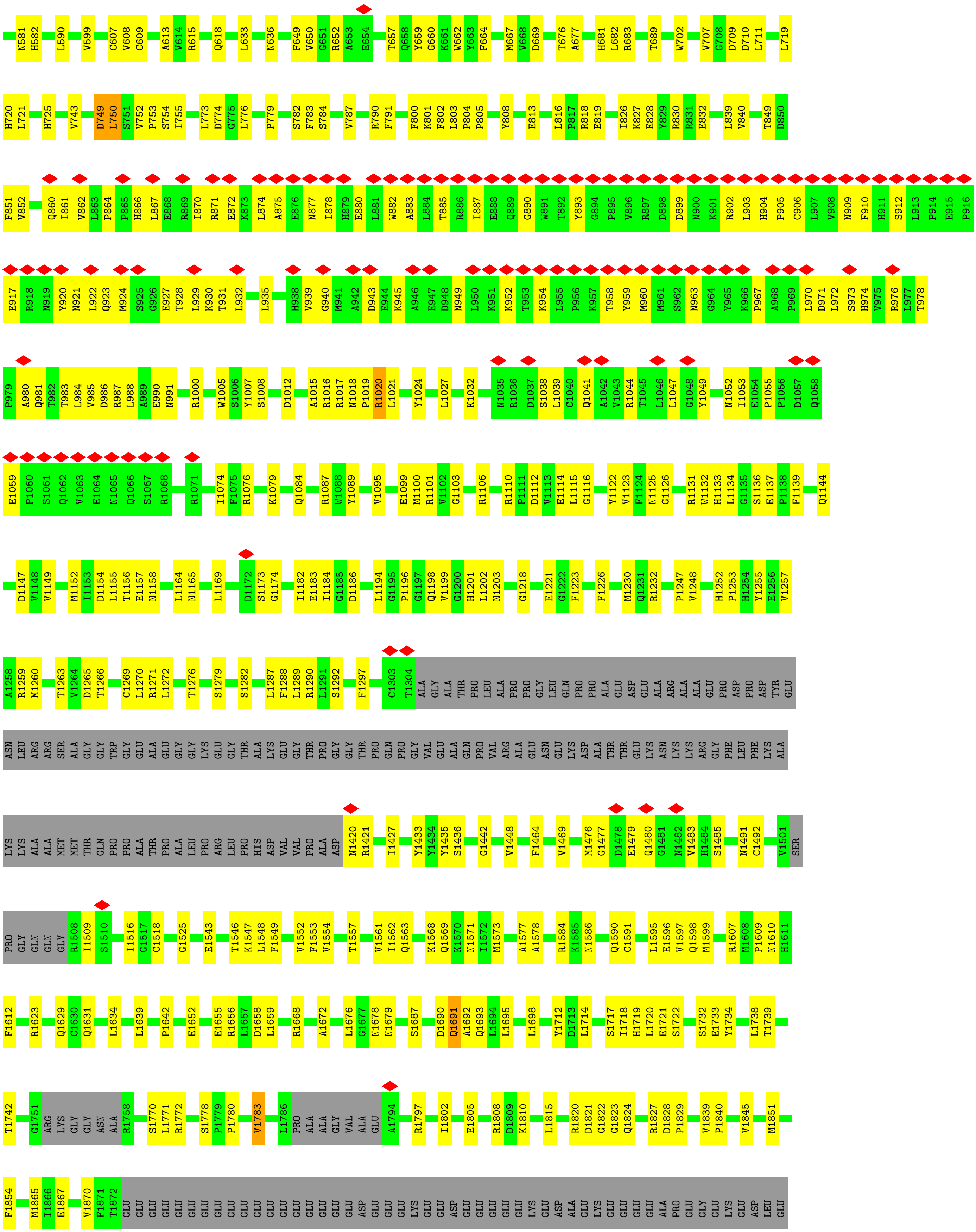




• Molecule 2: Ryanodine receptor 1

Chain B:

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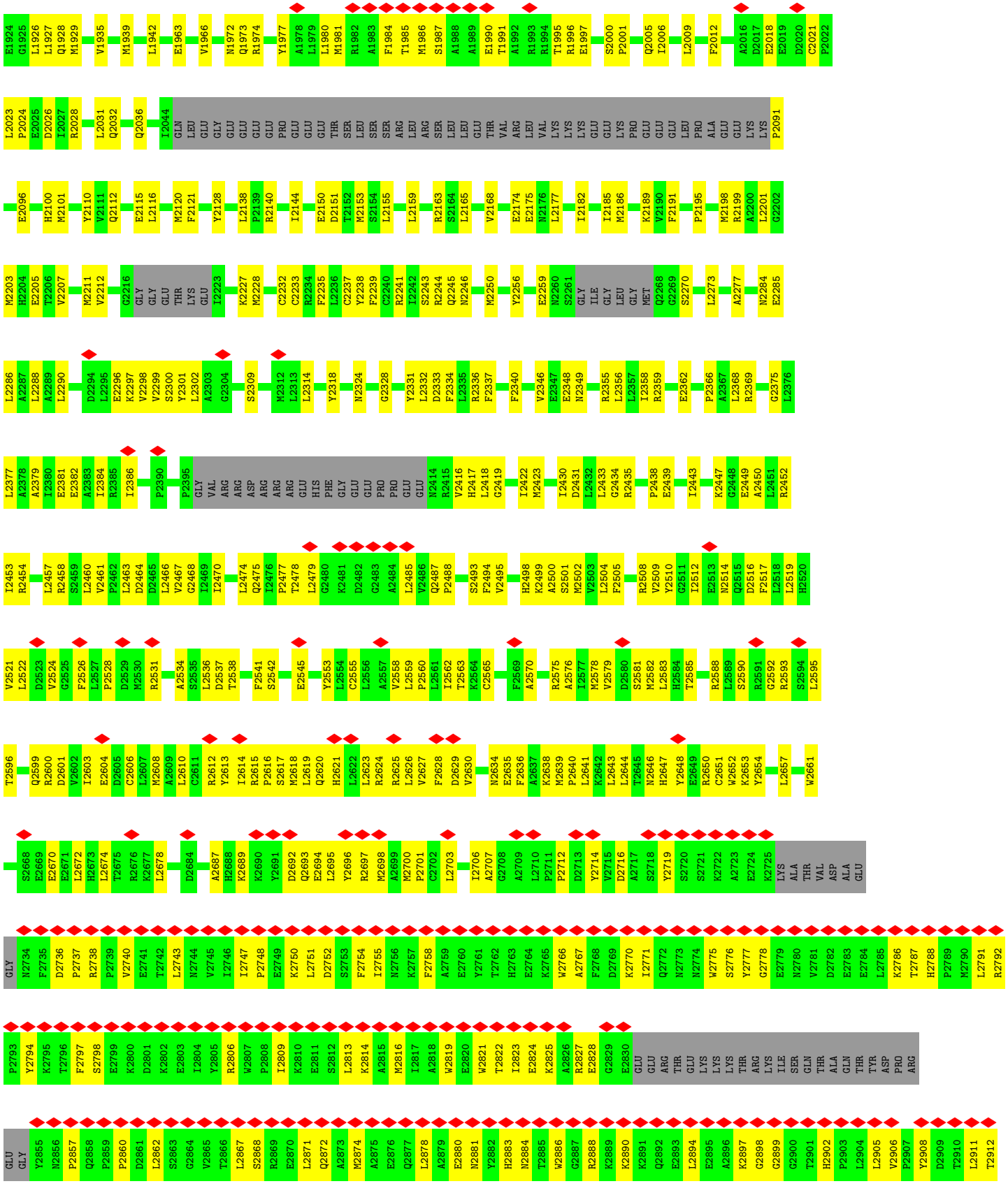
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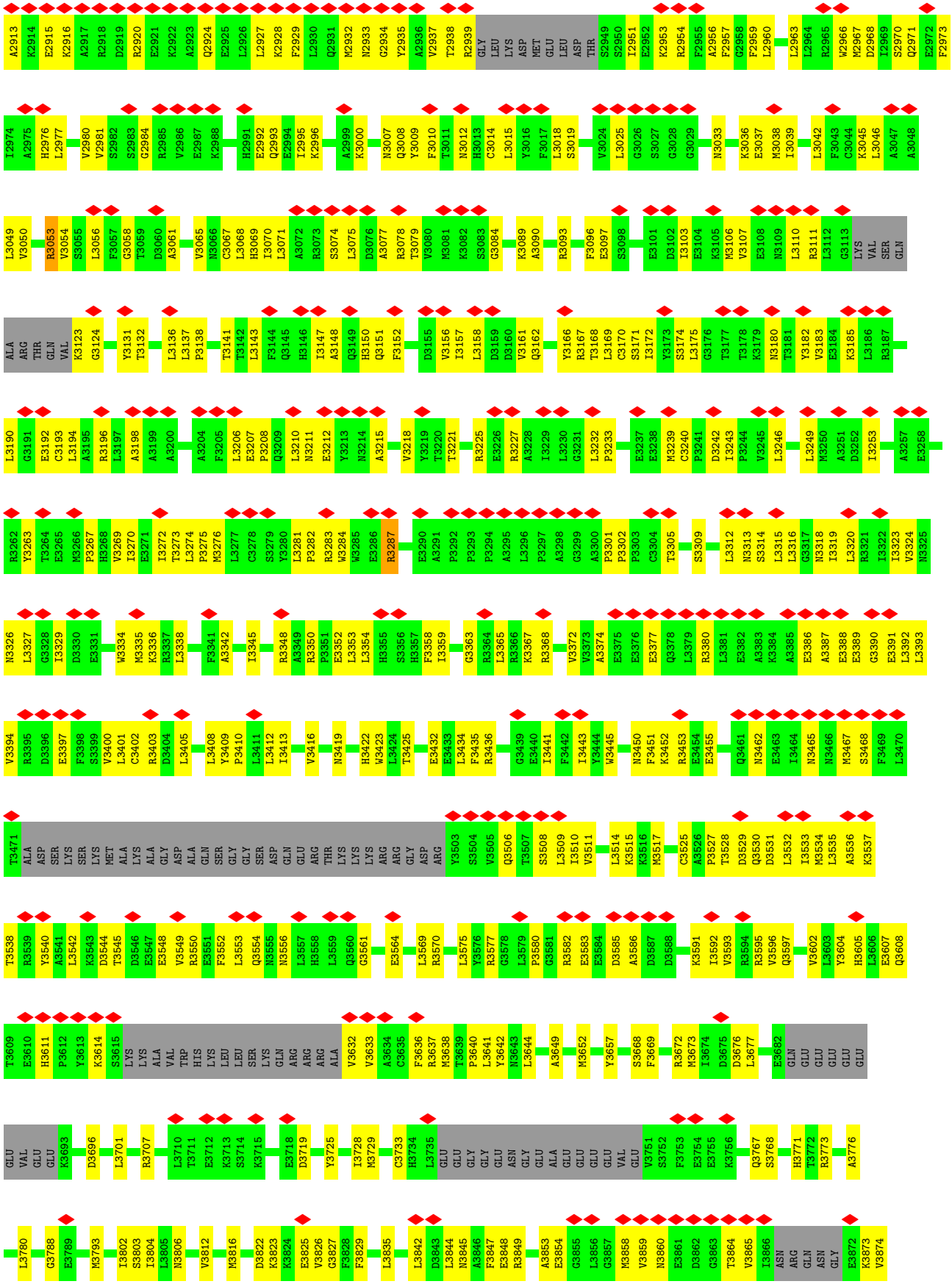
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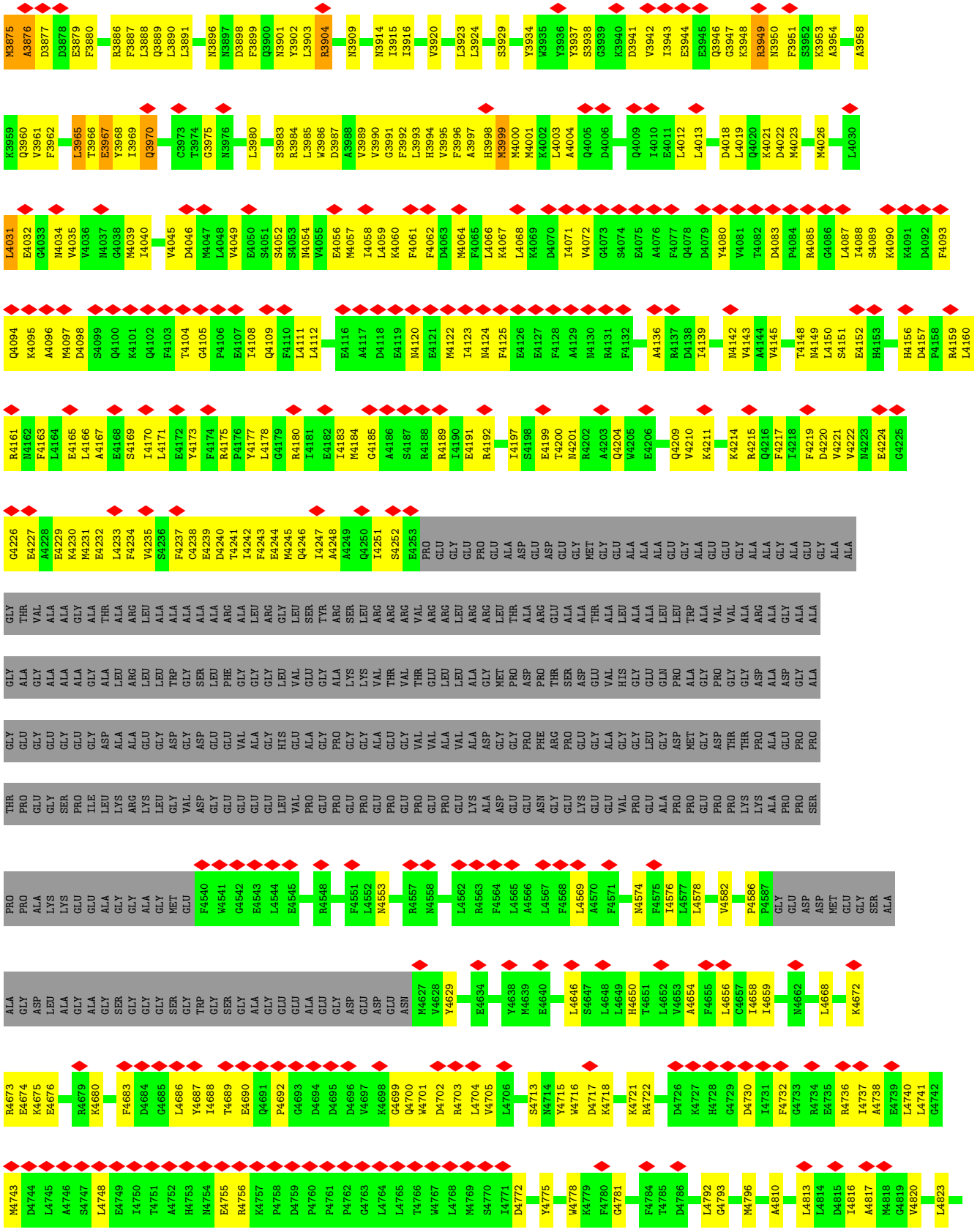
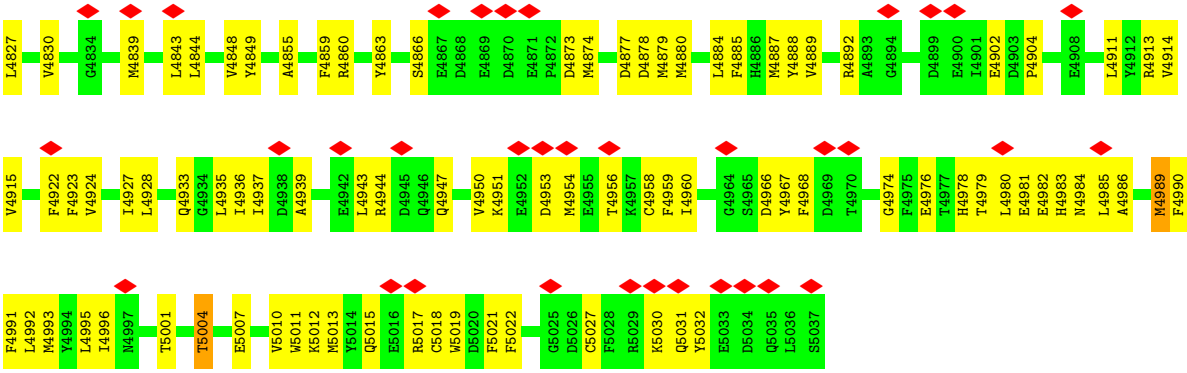
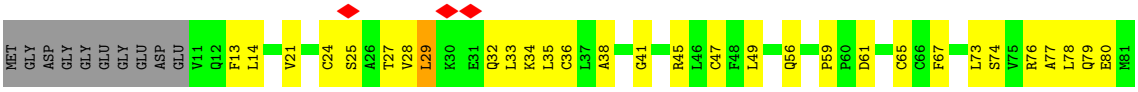
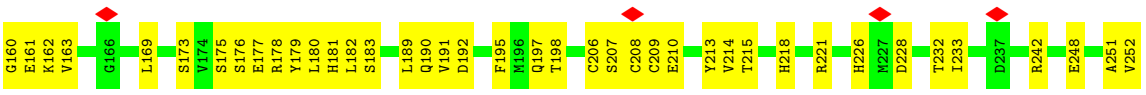


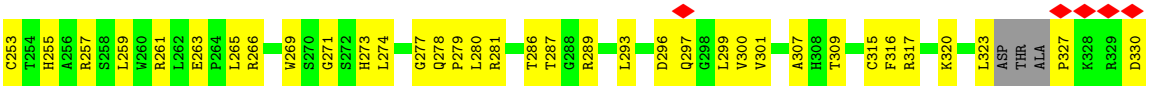


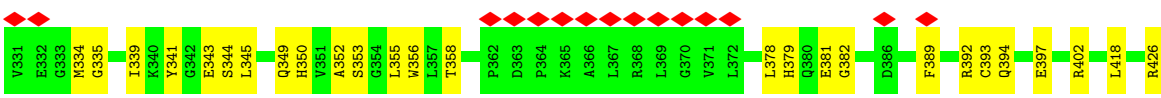
• Molecule 2: Ryanodine receptor 1

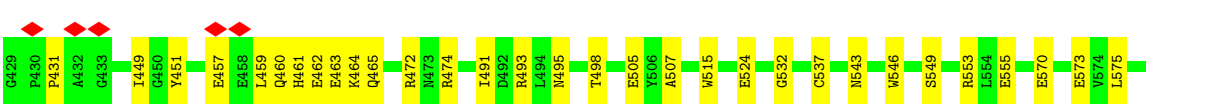
Chain I:

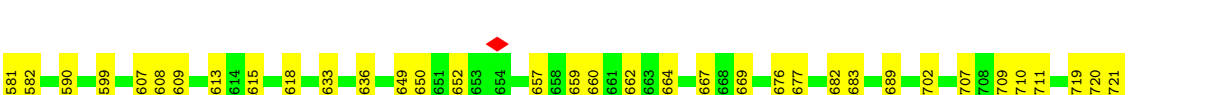


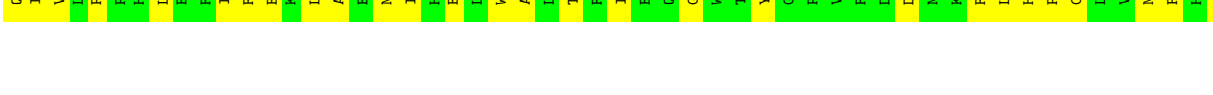


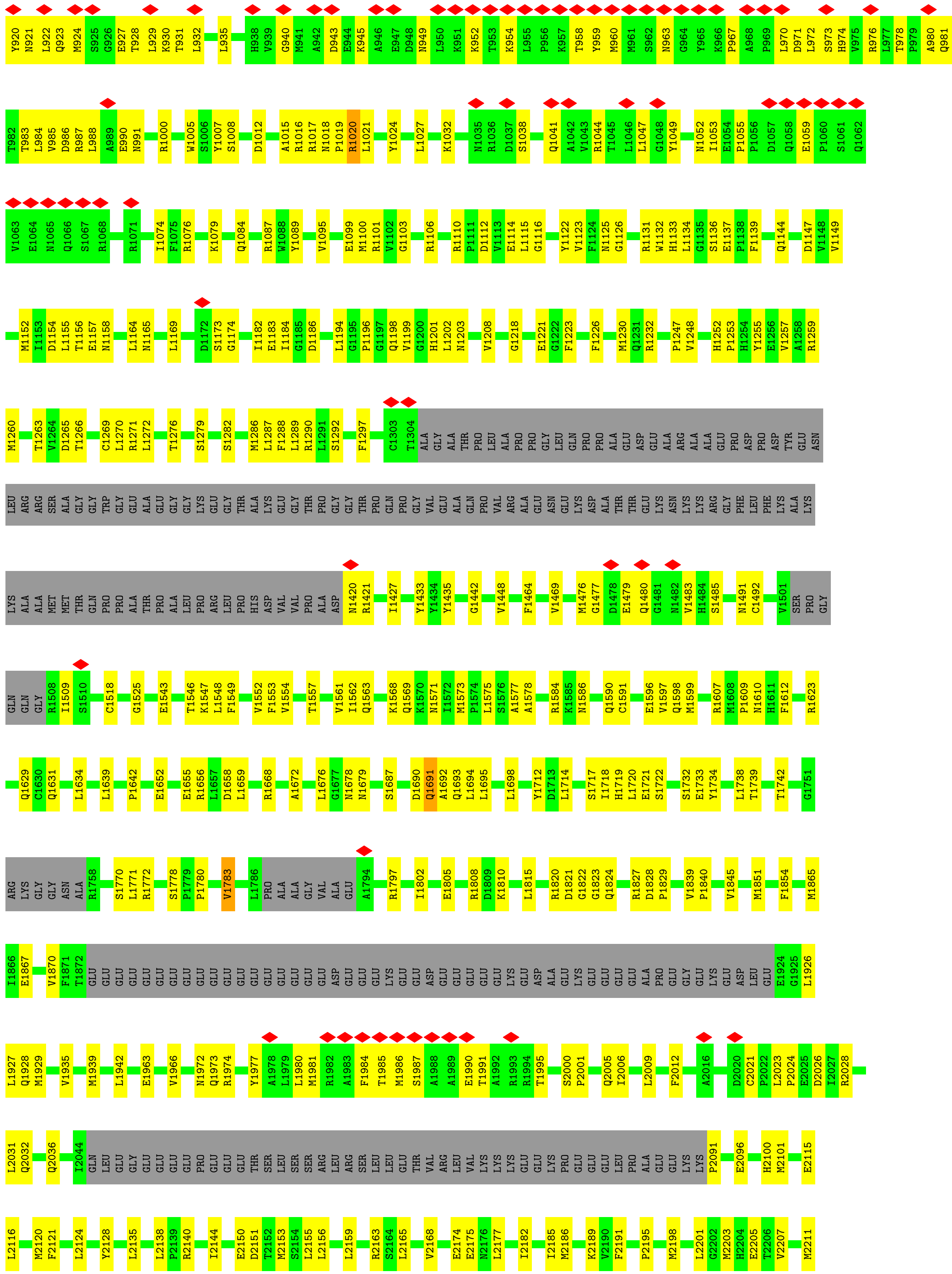








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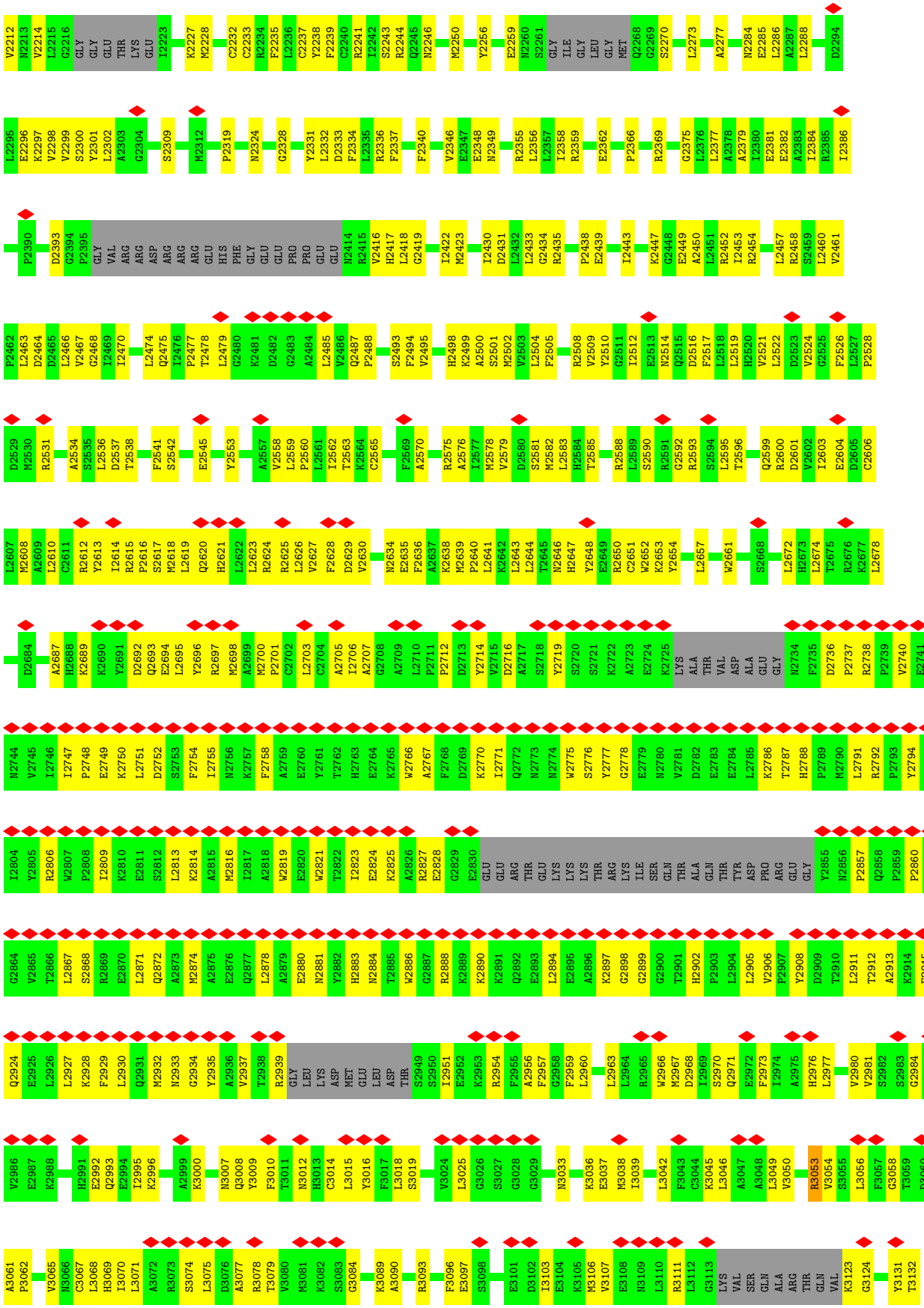
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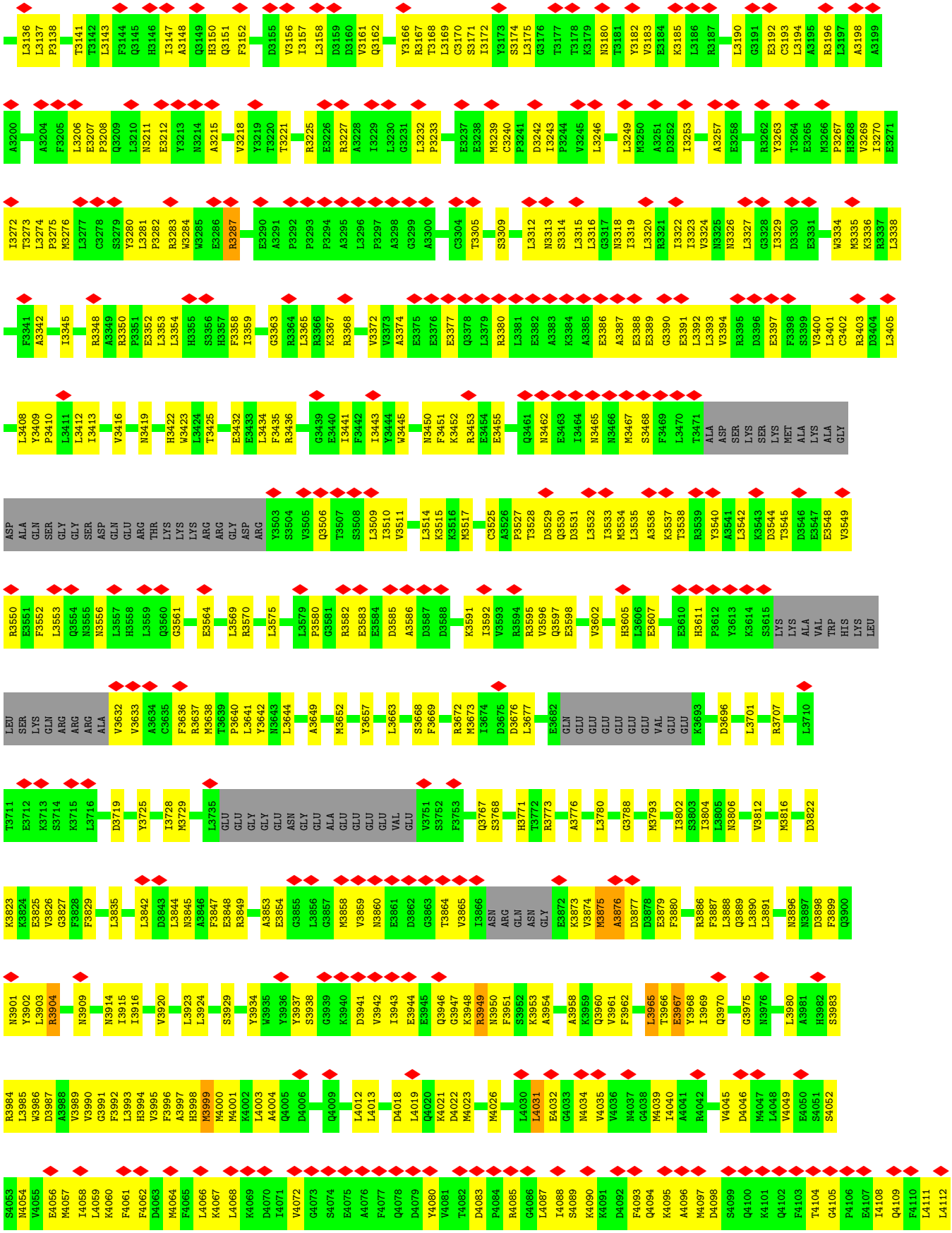

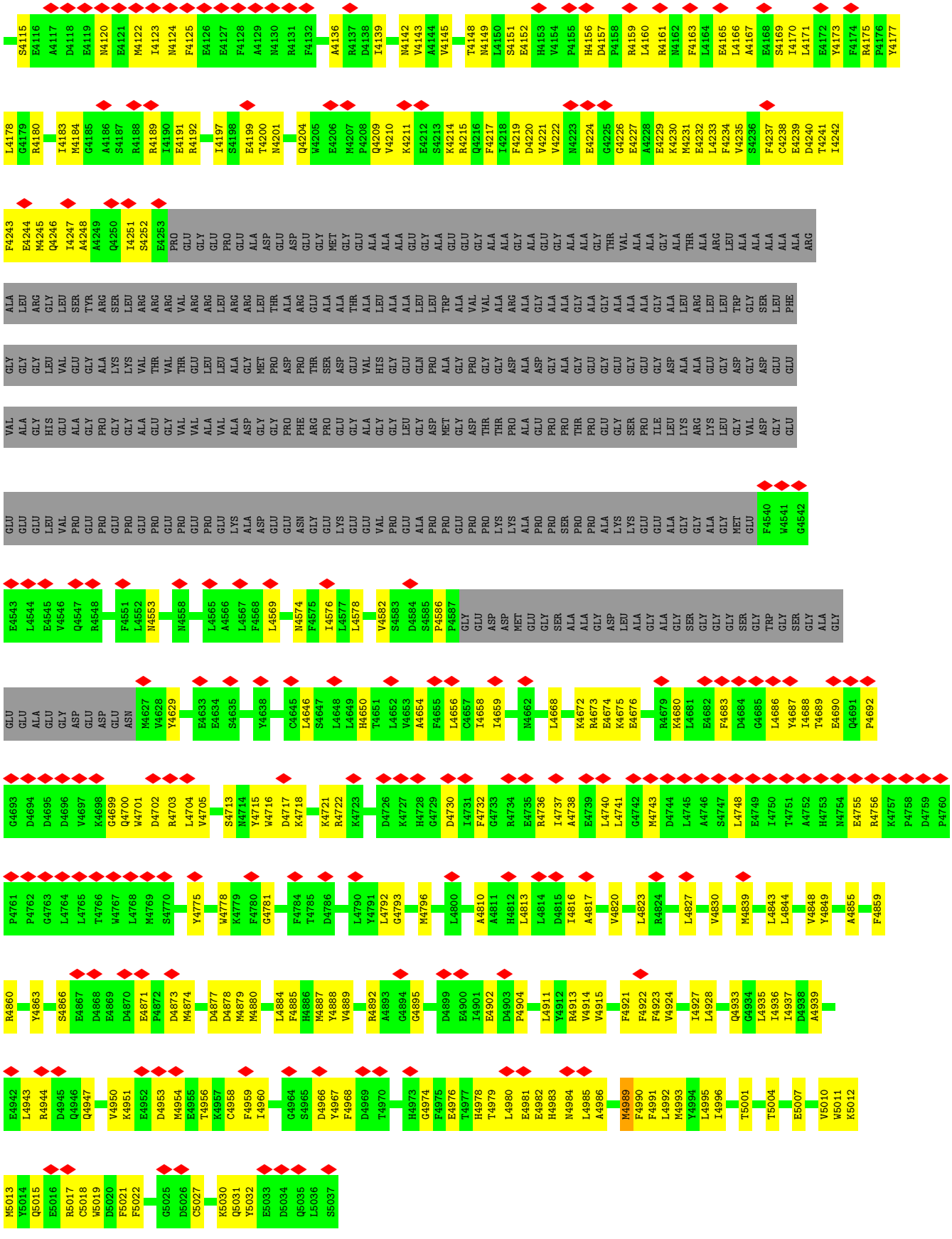
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L4178 G4179 R4180 I4183 M4184 G4185 A4186 S4187 R4188 R4189 I4190 E4191 R4192 I4197 S4198 E4199 T4200 N4201 Q4204 W4205 E4206 M4207 P4208 Q4209 V4210 K4211 E4212 S4213 K4214 R4215 Q4216 F4217 I4218 F4219 D4220 V4221 V4222 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4232 L4233 F4234 V4235 S4236 F4237 C4238 E4239 D4240 T4241 I4242
F4243 E4244 M4245 Q4246 I4247 A4248 A4249 Q4250 I4251 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA ALA GLY GLU GLU GLY ALA ALA GLY THR VAL ALA ALA ALA GLY ALA ALA GLY GLY ARG LEU ALA ALA ALA
ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA ALA LEU LEU LEU TRP ALA VAL VAL ALA ARG ALA ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE
GLY GLY GLY LEU VAL GLU 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 GLY GLU GLY GLY GLU GLY GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU
VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY 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 LEU VAL PRO GLU PRO PRO GLU PRO GLU PRO PRO GLU PRO GLU 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 GLY ALA GLY MET GLU F4540 W4541 G4542
E4543 L4544 E4545 V4546 Q4547 R4548 F4551 L4552 N4553 N4558 L4565 A4566 L4567 F4568 L4569 N4574 F4575 I4576 L4577 L4578 V4582 S4583 D4584 S4585 P4586 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 ASN M4627 V4628 Y4629 E4633 E4634 S4635 Y4638 C4645 L4646 S4647 L4648 L4649 H4650 T4651 L4652 V4653 A4654 F4655 L4656 C4657 I4658 I4659 N4662 L4668 K4672 R4673 E4674 K4675 E4676 R4679 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692
G4693 D4694 D4695 D4696 V4697 K4698 G4699 Q4700 W4701 D4702 R4703 L4704 V4705 S4713 N4714 Y4715 W4716 D4717 K4718 K4721 R4722 K4723 D4726 K4727 H4728 G4729 D4730 I4731 F4732 G4733 R4734 E4735 R4736 I4737 A4738 E4739 L4740 L4741 G4742 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760
P4761 P4762 G4763 L4764 L4765 T4766 W4767 K4768 M4769 S4770 Y4775 W4778 K4779 F4780 G4781 F4784 T4785 D4786 L4790 Y4791 L4792 G4793 M4796 L4800 A4810 A4811 H4812 L4813 L4814 D4815 I4816 A4817 V4820 L4823 R4824 L4827 V4830 M4839 L4843 L4844 V4848 Y4849 A4855 F4859
R4860 Y4863 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 D4877 D4878 M4879 M4880 L4884 F4885 H4886 M4887 Y4888 V4889 R4892 A4893 G4894 G4895 D4899 E4900 I4901 E4902 D4903 P4904 L4911 Y4912 R4913 V4914 V4915 F4921 F4922 F4923 V4924 I4927 L4928 Q4933 G4934 L4935 I4936 I4937 D4938 A4939
E4942 L4943 R4944 D4945 Q4946 Q4947 V4950 K4951 E4952 D4953 M4954 E4955 T4956 K4957 C4958 F4959 I4960 G4964 S4965 D4966 Y4967 F4968 D4969 T4970 H4973 G4974 F4975 E4976 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 M4989 F4990 F4991 L4992 M4993 Y4994 L4995 I4996 T5001 T5004 E5007 V5010 W5011 K5012
M5013 Y5014 Q5015 E5016 R5017 C5018 W5019 D5020 F5021 F5022 G5025 D5026 C5027 K5030 Q5031 Y5032 E5033 D5034 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	31599	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58.34	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.771	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.106	Depositor
Map size (Å)	425.472, 425.472, 425.472	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.831, 0.831, 0.831	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, CFF, 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	F	0.72	1/834 (0.1%)	0.76	3/1123 (0.3%)
1	H	0.73	1/834 (0.1%)	0.76	3/1123 (0.3%)
1	J	0.73	1/834 (0.1%)	0.76	3/1123 (0.3%)
1	O	0.72	1/834 (0.1%)	0.76	3/1123 (0.3%)
2	A	0.40	0/35023	0.51	6/47448 (0.0%)
2	B	0.40	0/35023	0.51	6/47448 (0.0%)
2	G	0.40	0/35023	0.51	6/47448 (0.0%)
2	I	0.40	0/35023	0.51	6/47448 (0.0%)
All	All	0.41	4/143428 (0.0%)	0.52	36/194284 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	39	SER	CA-CB	-5.12	1.45	1.52
1	J	39	SER	CA-CB	-5.11	1.45	1.52
1	F	39	SER	CA-CB	-5.08	1.45	1.52
1	O	39	SER	CA-CB	-5.06	1.45	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	752	VAL	C-N-CA	-9.43	82.41	122.00
2	G	752	VAL	C-N-CA	-9.42	82.42	122.00
2	B	752	VAL	C-N-CA	-9.42	82.42	122.00
2	I	752	VAL	C-N-CA	-9.42	82.42	122.00
2	B	752	VAL	N-CA-C	-7.32	91.23	111.00

There are no chirality outliers.

There are no planarity outliers.

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	F	818	0	824	25	0
1	H	818	0	824	24	0
1	J	818	0	824	23	0
1	O	818	0	824	23	0
2	A	34238	0	33844	1330	0
2	B	34238	0	33844	1337	0
2	G	34238	0	33844	1326	0
2	I	34238	0	33844	1329	0
3	A	31	0	12	5	0
3	B	31	0	12	5	0
3	G	31	0	12	6	0
3	I	31	0	12	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	A	14	0	10	2	0
6	B	14	0	10	2	0
6	G	14	0	10	2	0
6	I	14	0	10	2	0
All	All	140412	0	138760	5318	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 19.

The worst 5 of 5318 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4983:HIS:HB2	3:G:5301:ATP:HN62	1.25	1.01
2:A:4880:MET:SD	2:G:4578:LEU:O	2.19	1.00
2:A:4983:HIS:HB2	3:A:5301:ATP:HN62	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4983:HIS:HB2	3:I:5301:ATP:HN62	1.25	0.99
2:A:4935:LEU:CD2	2:G:4944:ARG:NH2	2.27	0.98

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	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	O	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	A	4256/5037 (84%)	3938 (92%)	314 (7%)	4 (0%)	51	83
2	B	4256/5037 (84%)	3936 (92%)	316 (7%)	4 (0%)	51	83
2	G	4256/5037 (84%)	3939 (93%)	313 (7%)	4 (0%)	51	83
2	I	4256/5037 (84%)	3940 (93%)	312 (7%)	4 (0%)	51	83
All	All	17444/20580 (85%)	16137 (92%)	1291 (7%)	16 (0%)	54	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	3876	ALA
2	G	3876	ALA
2	B	3876	ALA
2	I	3876	ALA
2	A	1783	VAL

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	F	88/89 (99%)	79 (90%)	9 (10%)	7 28
1	H	88/89 (99%)	79 (90%)	9 (10%)	7 28
1	J	88/89 (99%)	79 (90%)	9 (10%)	7 28
1	O	88/89 (99%)	79 (90%)	9 (10%)	7 28
2	A	3732/4276 (87%)	3702 (99%)	30 (1%)	81 88
2	B	3732/4276 (87%)	3702 (99%)	30 (1%)	81 88
2	G	3732/4276 (87%)	3702 (99%)	30 (1%)	81 88
2	I	3732/4276 (87%)	3702 (99%)	30 (1%)	81 88
All	All	15280/17460 (88%)	15124 (99%)	156 (1%)	77 85

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3904	ARG
2	I	3874	VAL
2	B	3967	GLU
2	I	877	ASN
2	I	3969	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	495	ASN
2	I	4946	GLN
2	B	3313	ASN
2	I	4109	GLN
2	I	3313	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	A	5301	-	26,33,33	0.84	0	31,52,52	1.63	5 (16%)
3	ATP	G	5301	-	26,33,33	0.84	0	31,52,52	1.63	5 (16%)
3	ATP	B	5301	-	26,33,33	0.84	0	31,52,52	1.62	5 (16%)
6	CFF	B	5304	-	8,15,15	2.54	4 (50%)	8,23,23	1.53	1 (12%)
6	CFF	G	5304	-	8,15,15	2.55	4 (50%)	8,23,23	1.54	1 (12%)
3	ATP	I	5301	-	26,33,33	0.83	0	31,52,52	1.63	5 (16%)
6	CFF	A	5304	-	8,15,15	2.54	4 (50%)	8,23,23	1.53	1 (12%)
6	CFF	I	5304	-	8,15,15	2.55	4 (50%)	8,23,23	1.53	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	5301	-	-	5/18/38/38	0/3/3/3
3	ATP	G	5301	-	-	5/18/38/38	0/3/3/3
3	ATP	B	5301	-	-	5/18/38/38	0/3/3/3
6	CFF	B	5304	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CFF	G	5304	-	-	-	0/2/2/2
3	ATP	I	5301	-	-	5/18/38/38	0/3/3/3
6	CFF	A	5304	-	-	-	0/2/2/2
6	CFF	I	5304	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5304	CFF	C5-C4	-4.57	1.33	1.39
6	I	5304	CFF	C5-C4	-4.55	1.33	1.39
6	A	5304	CFF	C5-C4	-4.55	1.33	1.39
6	G	5304	CFF	C5-C4	-4.53	1.33	1.39
6	G	5304	CFF	C6-N1	-4.25	1.32	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5301	ATP	PB-O3B-PG	-3.95	119.27	132.83
3	A	5301	ATP	PB-O3B-PG	-3.95	119.28	132.83
3	G	5301	ATP	PB-O3B-PG	-3.94	119.30	132.83
3	I	5301	ATP	PB-O3B-PG	-3.93	119.33	132.83
3	G	5301	ATP	PA-O3A-PB	-3.86	119.56	132.83

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	C5'-O5'-PA-O3A
3	A	5301	ATP	C3'-C4'-C5'-O5'
3	G	5301	ATP	C5'-O5'-PA-O3A
3	G	5301	ATP	C3'-C4'-C5'-O5'
3	B	5301	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5301	ATP	5	0
3	G	5301	ATP	6	0
3	B	5301	ATP	5	0
6	B	5304	CFF	2	0

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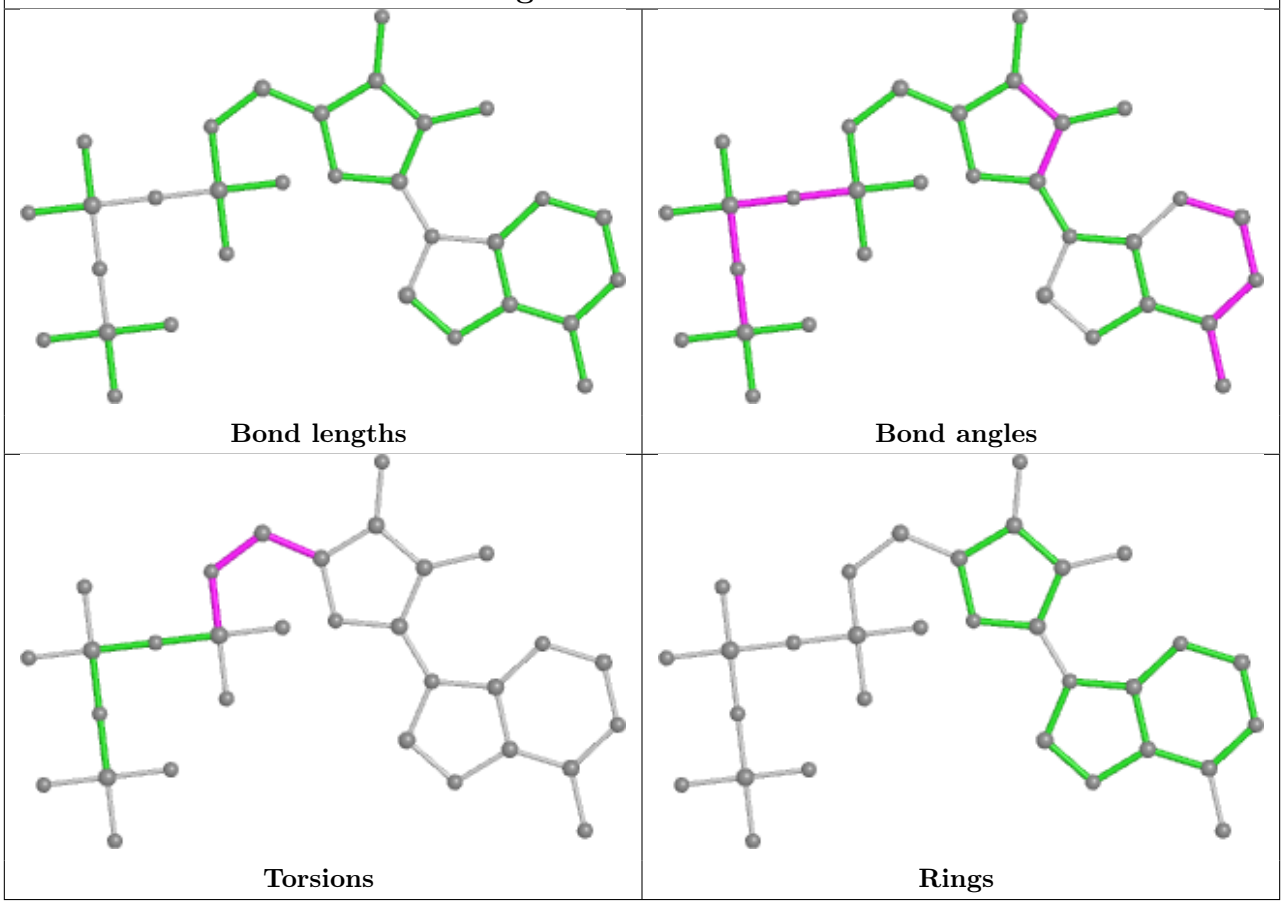
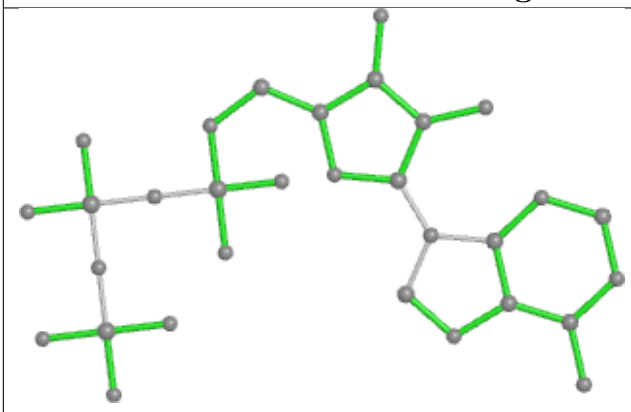
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	5304	CFF	2	0
3	I	5301	ATP	6	0
6	A	5304	CFF	2	0
6	I	5304	CFF	2	0

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

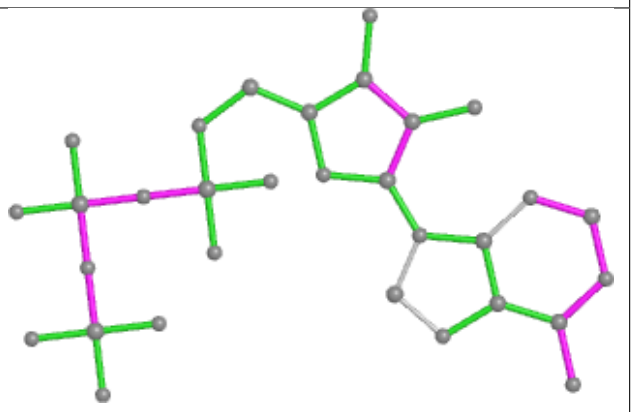
Ligand ATP A 5301



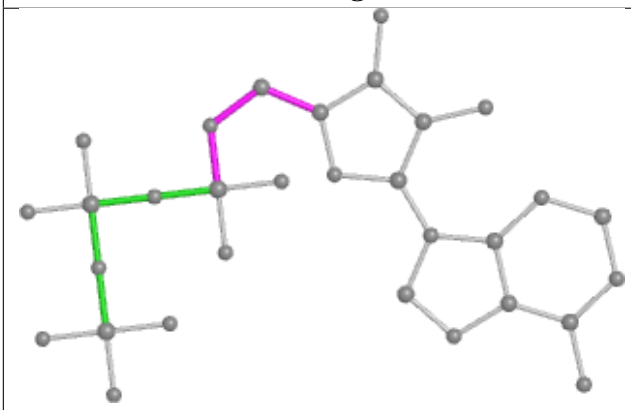
Ligand ATP G 5301



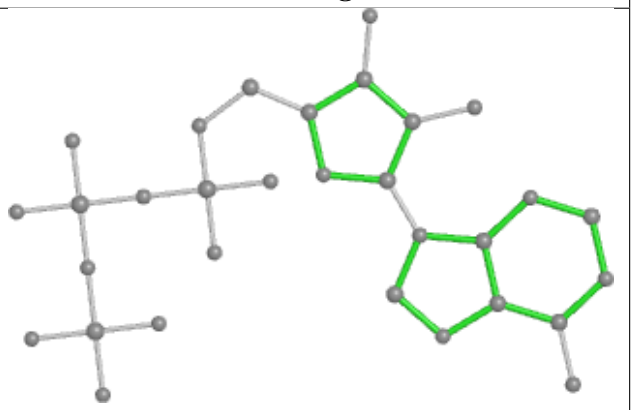
Bond lengths



Bond angles

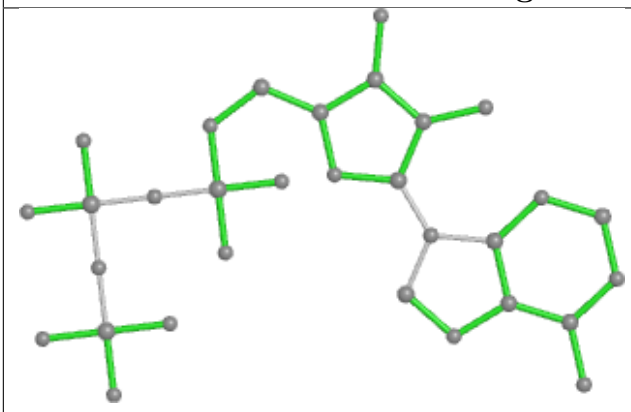


Torsions

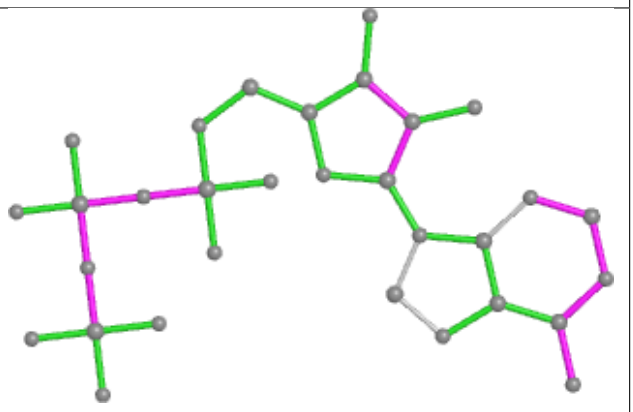


Rings

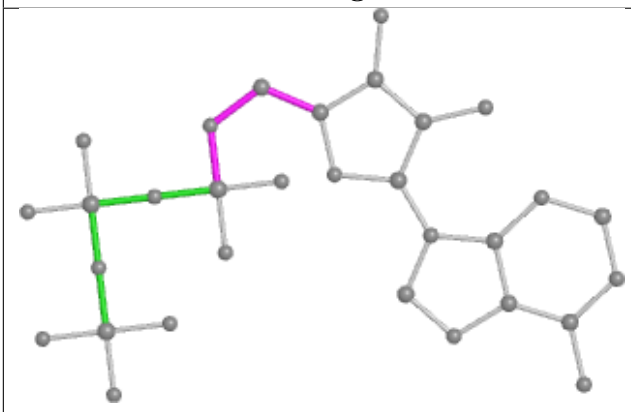
Ligand ATP B 5301



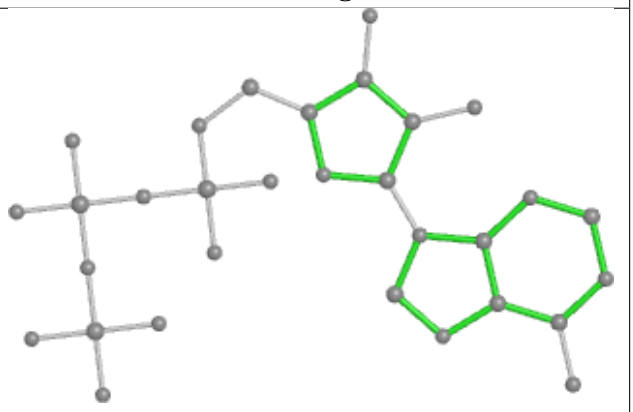
Bond lengths



Bond angles

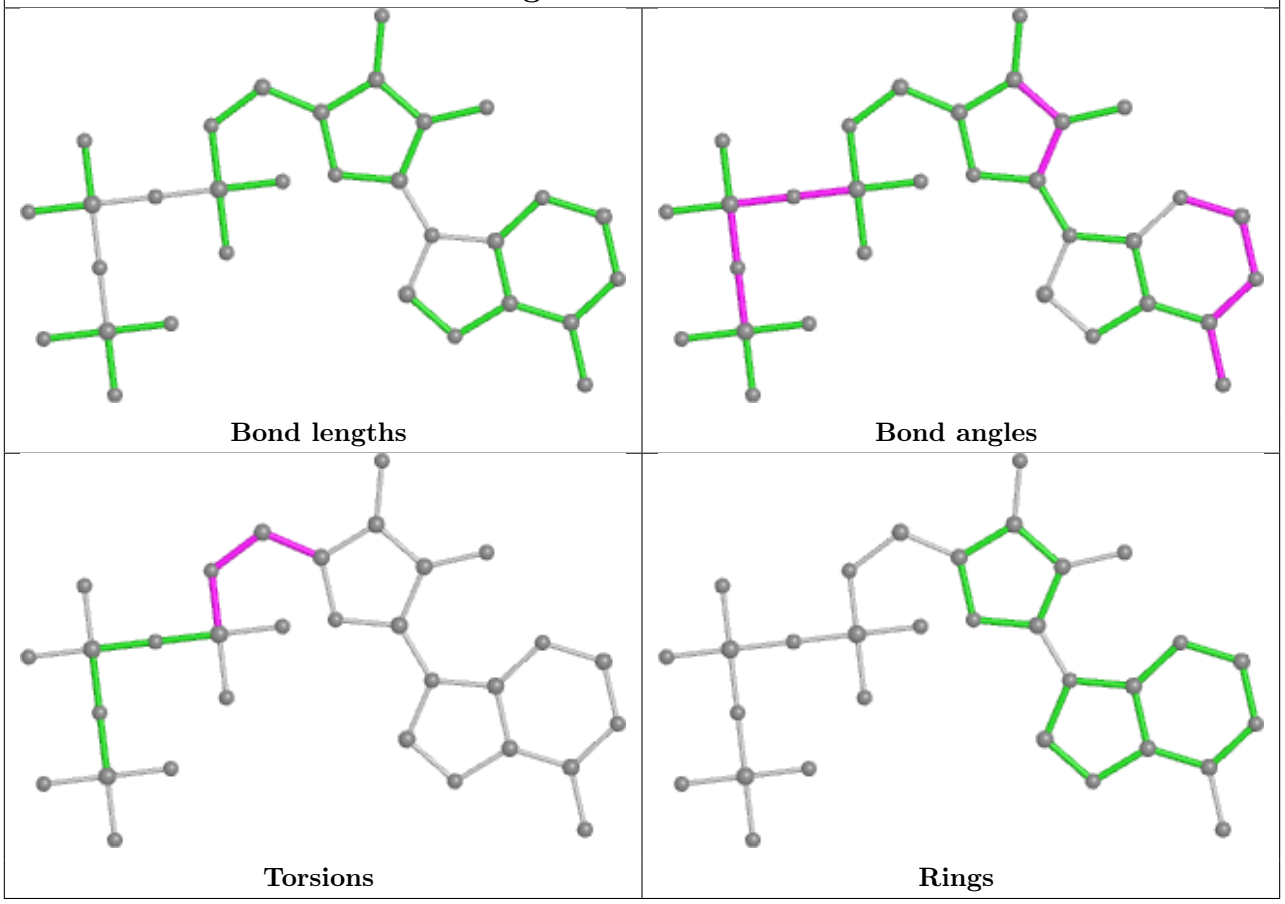


Torsions



Rings

Ligand ATP I 5301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

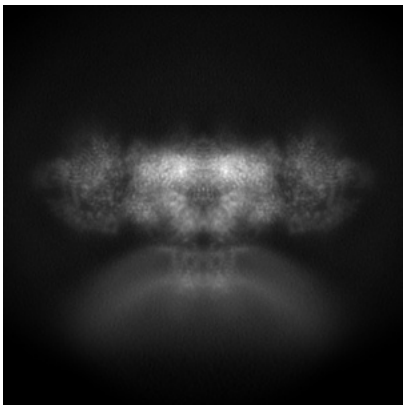
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23699. These allow visual inspection of the internal detail of the map and identification of artifacts.

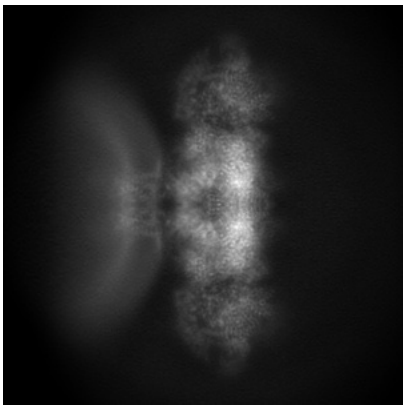
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

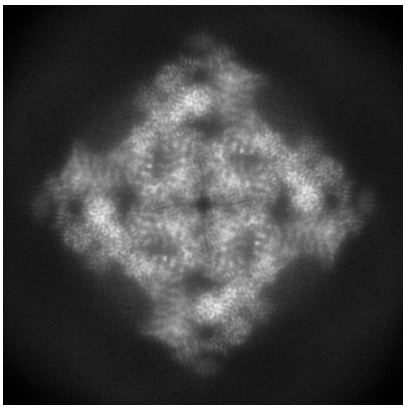
6.1.1 Primary map



X

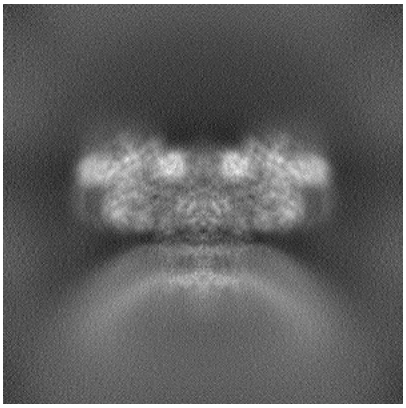


Y

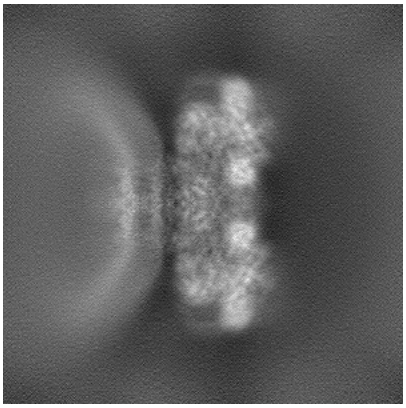


Z

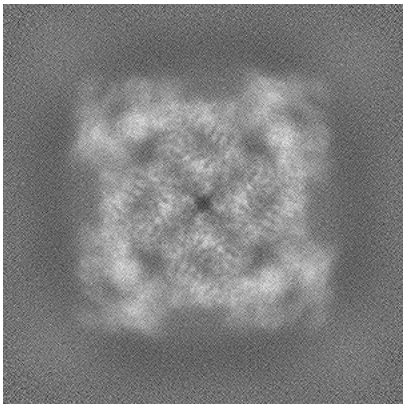
6.1.2 Raw map



X



Y

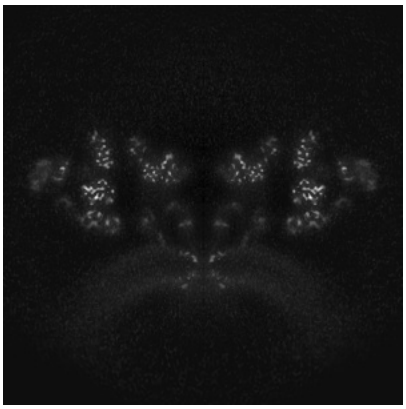


Z

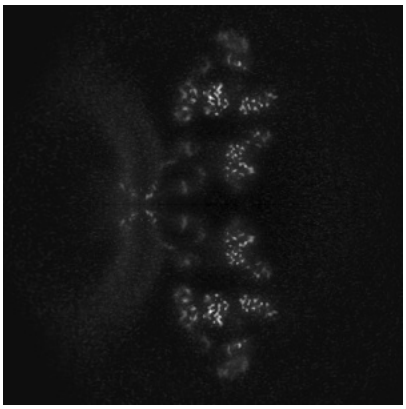
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

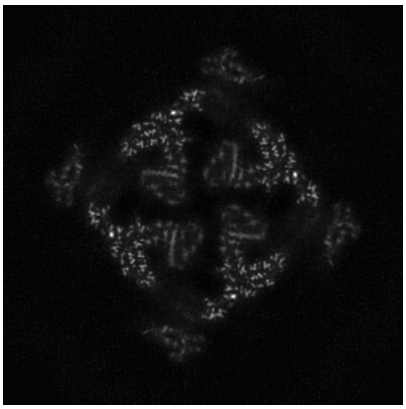
6.2.1 Primary map



X Index: 256

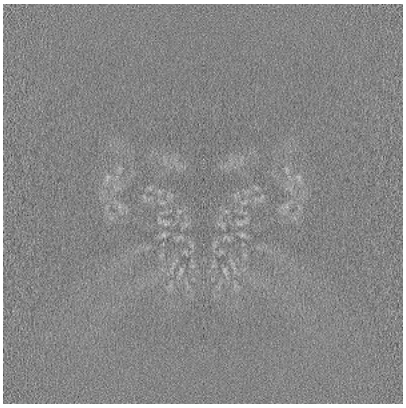


Y Index: 256

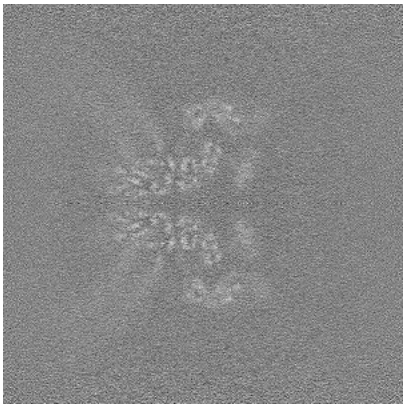


Z Index: 256

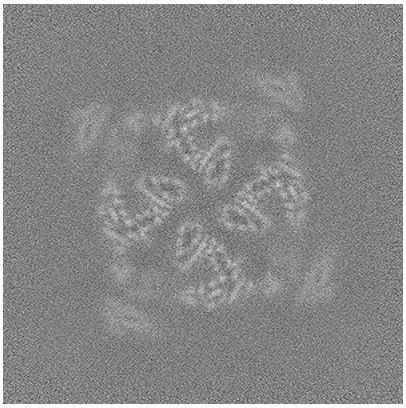
6.2.2 Raw map



X Index: 256



Y Index: 256

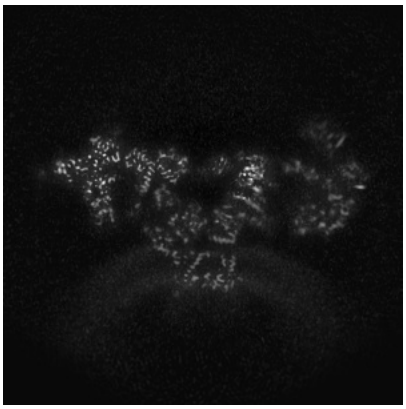


Z Index: 256

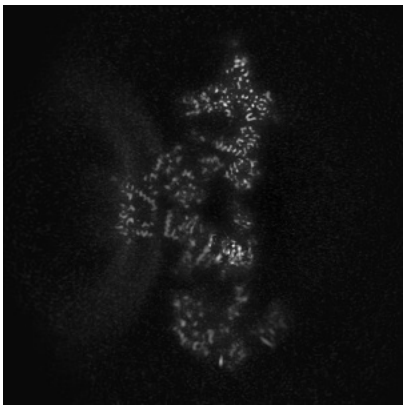
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

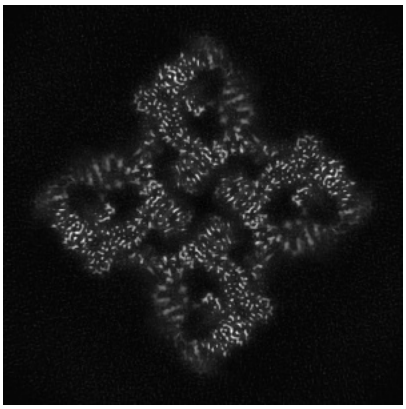
6.3.1 Primary map



X Index: 279

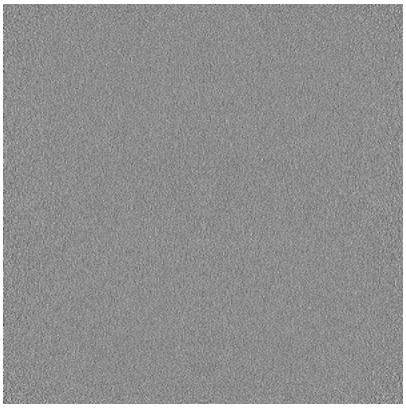


Y Index: 279

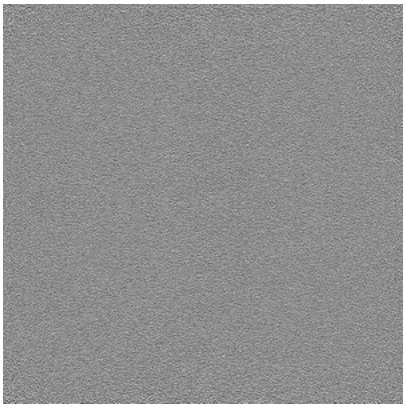


Z Index: 304

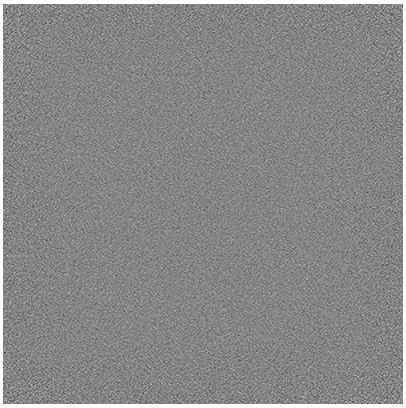
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

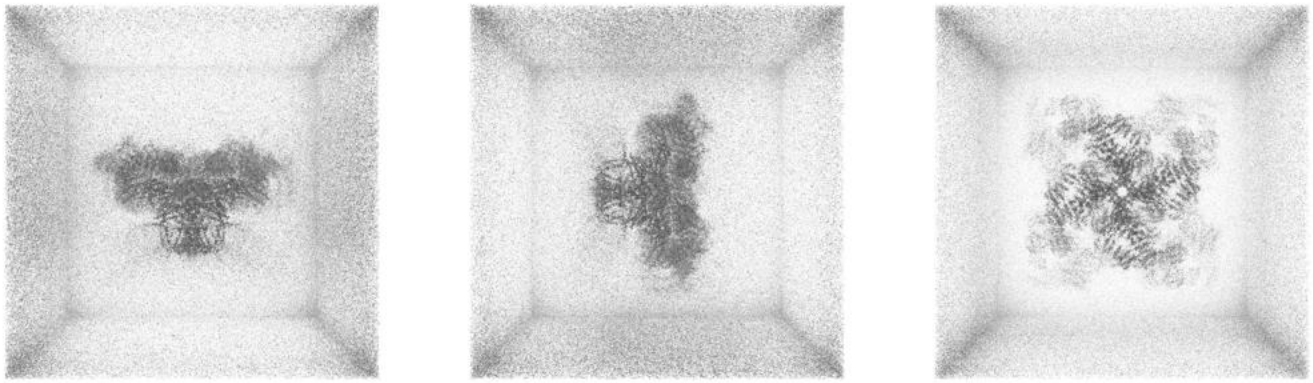
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.106. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

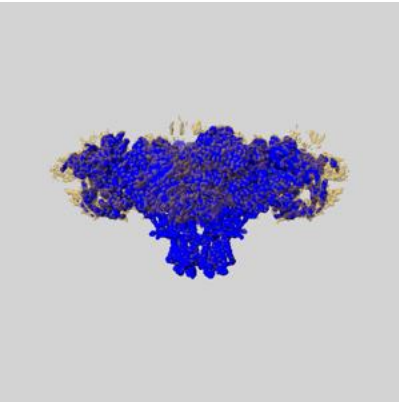
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

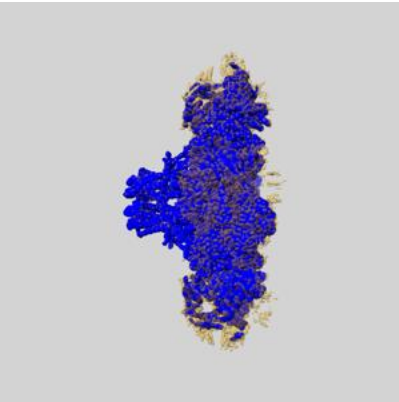
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

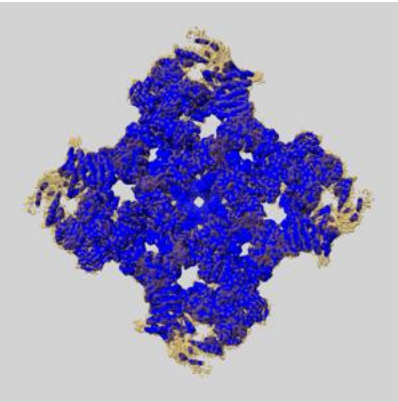
6.5.1 emd_23699_msk_1.map (i)



X



Y

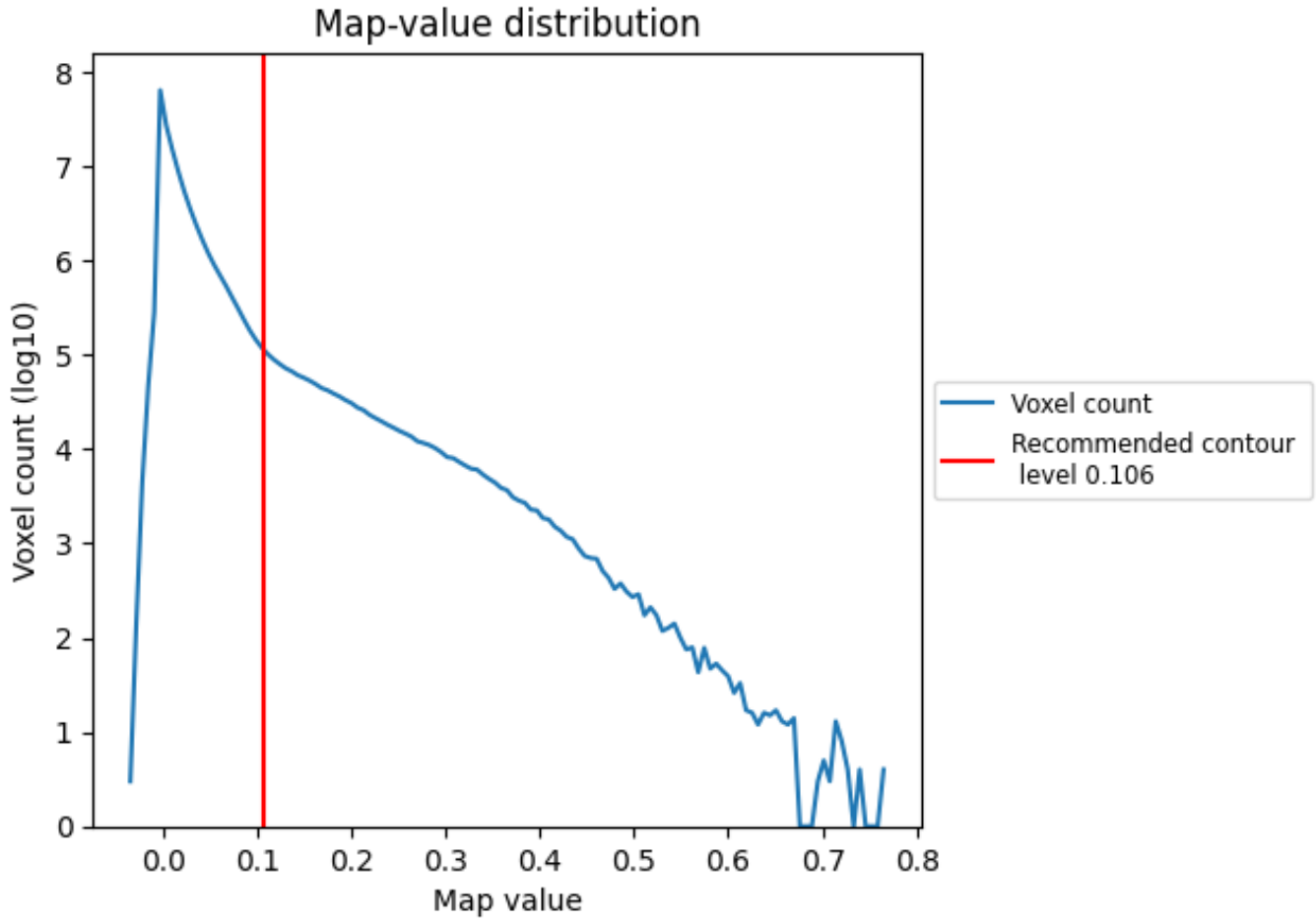


Z

7 Map analysis

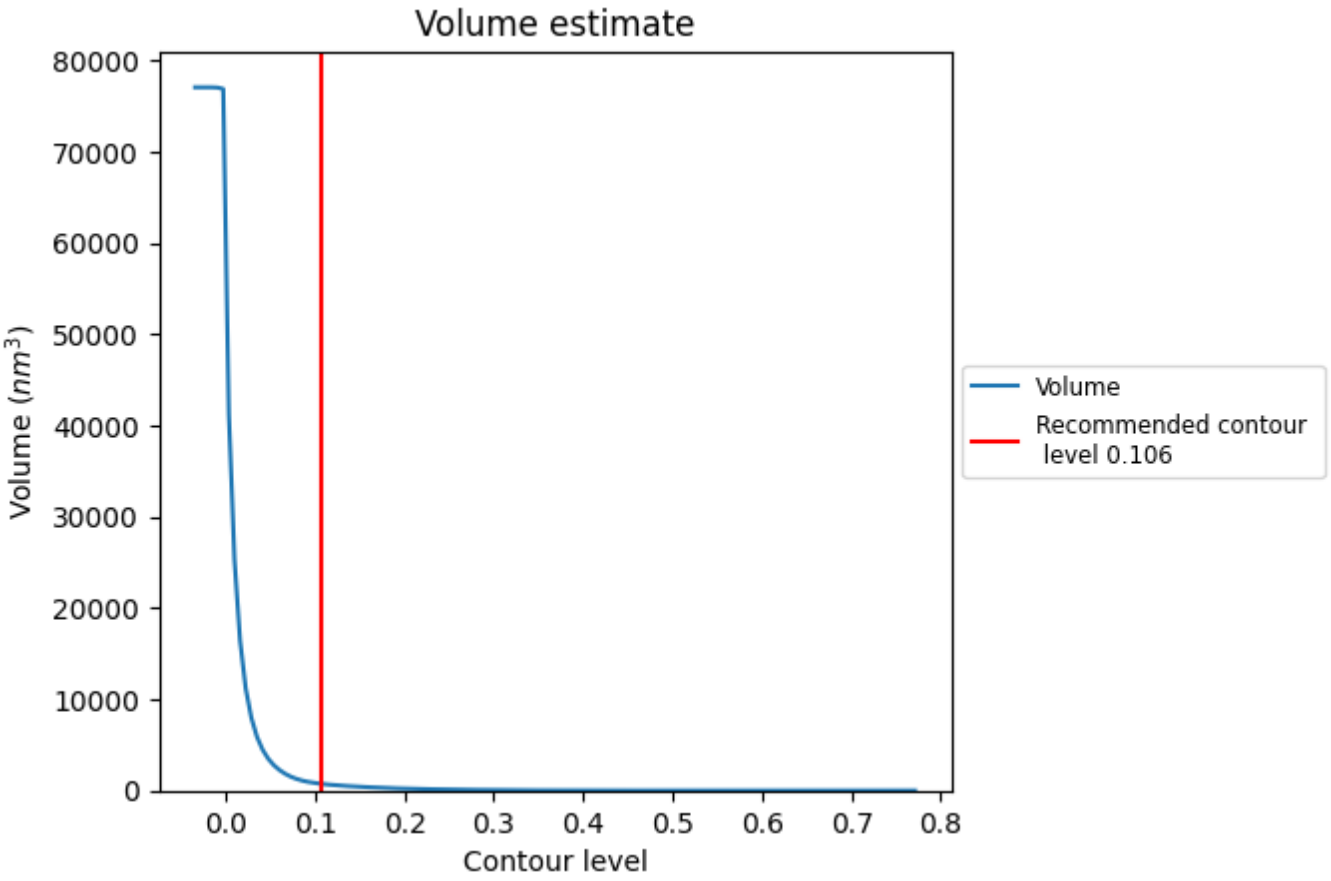
This section contains the results of statistical analysis of the map.

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.

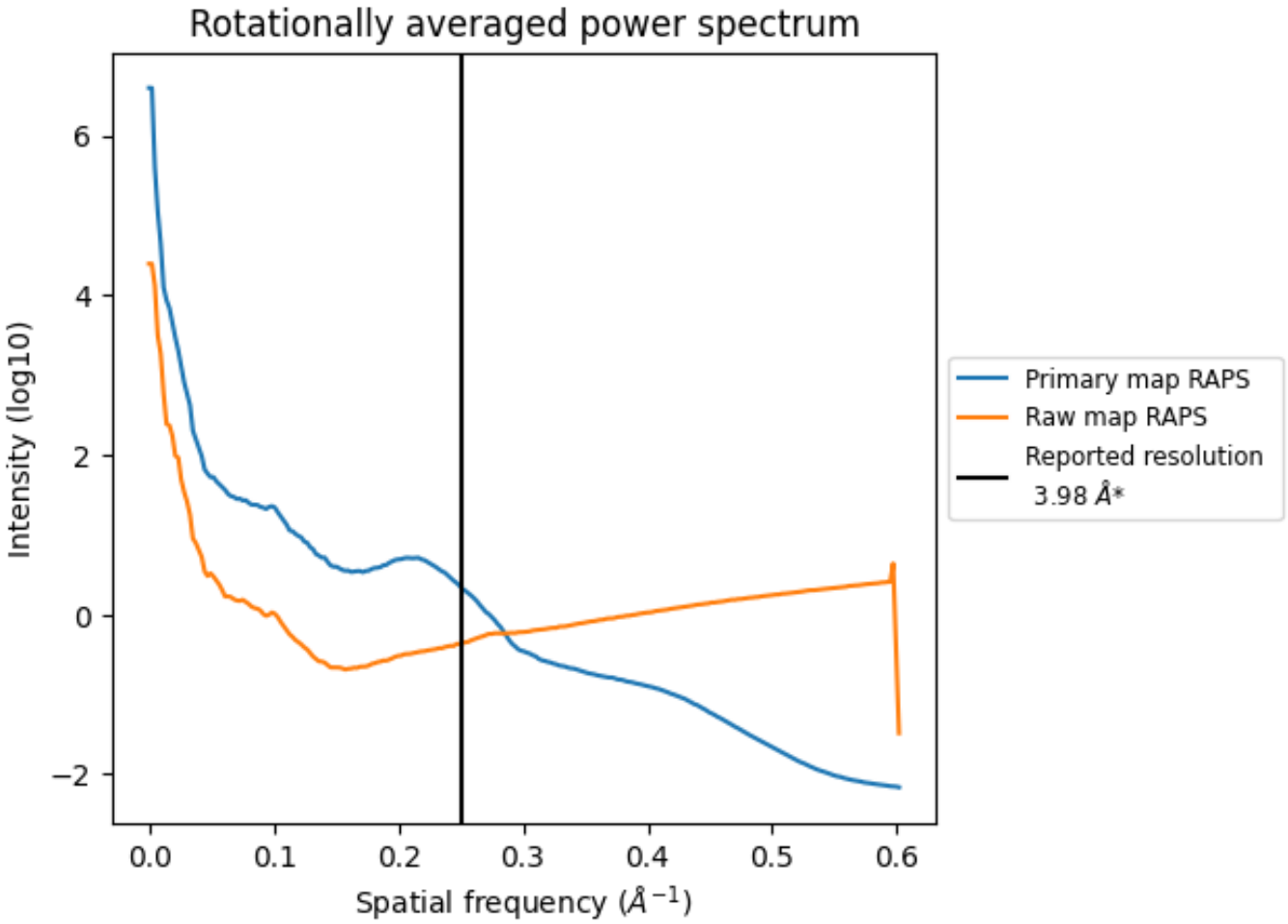
7.2 Volume estimate



The volume at the recommended contour level is 747 nm^3; this corresponds to an approximate mass of 675 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)

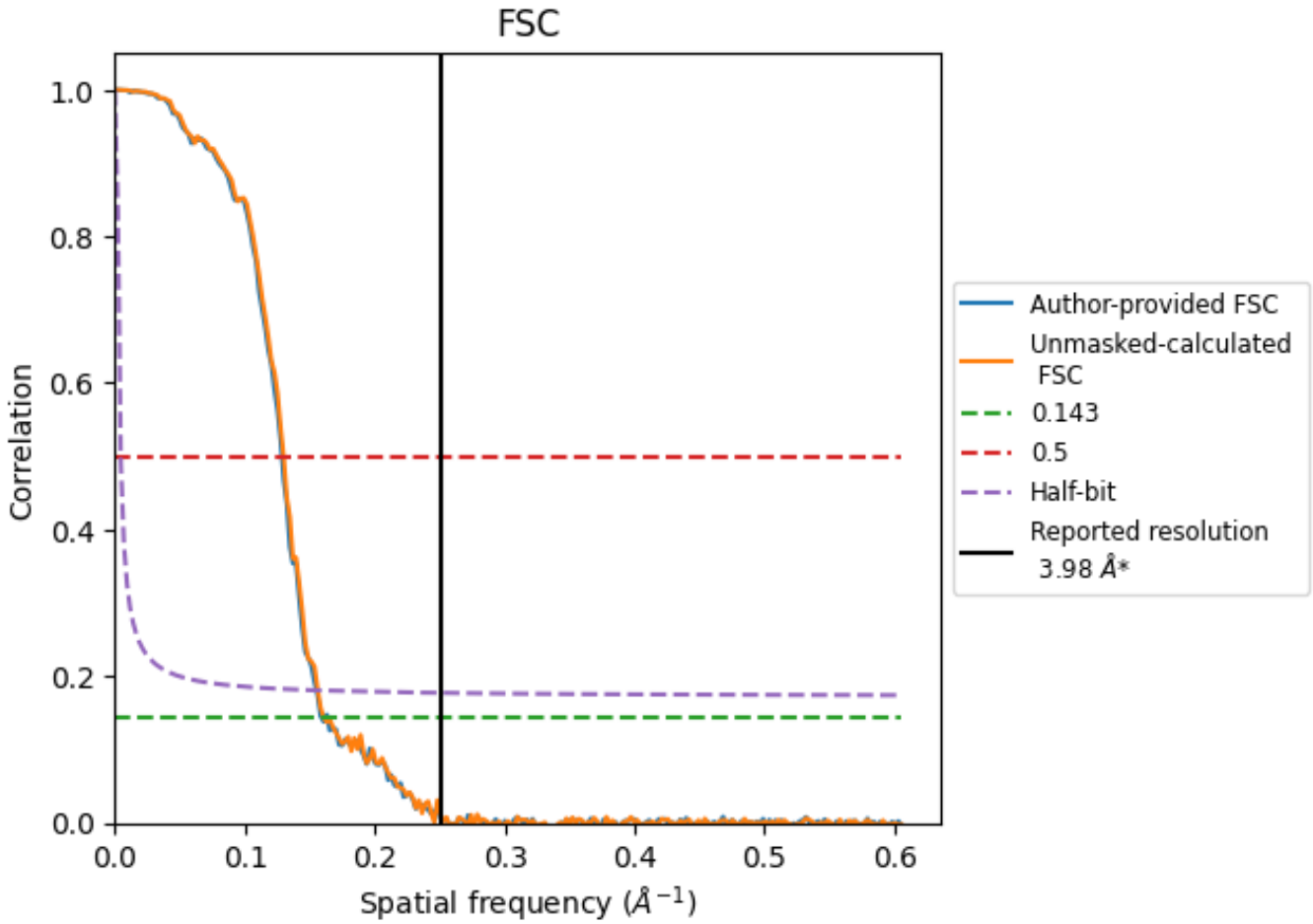


*Reported resolution corresponds to spatial frequency of 0.251 Å^{-1}

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 0.251 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	6.28	7.78	6.44
Unmasked-calculated*	6.22	7.70	6.40

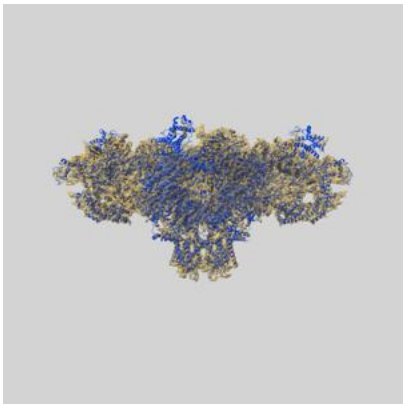
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.28 differs from the reported value 3.98 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.22 differs from the reported value 3.98 by more than 10 %

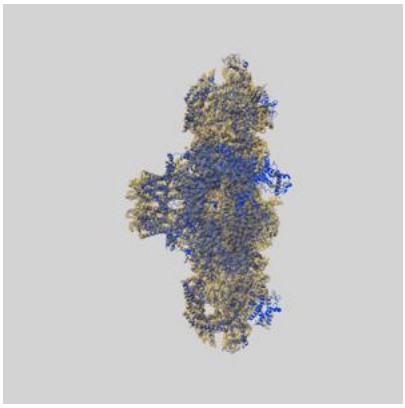
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23699 and PDB model 7M6L. Per-residue inclusion information can be found in section 3 on page 6.

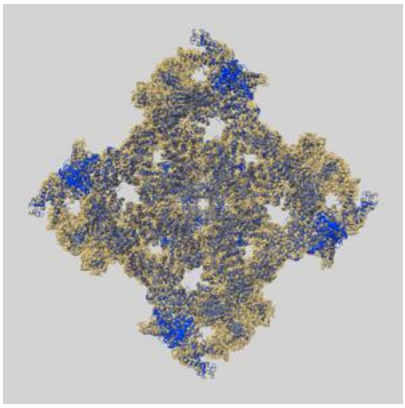
9.1 Map-model overlay



X



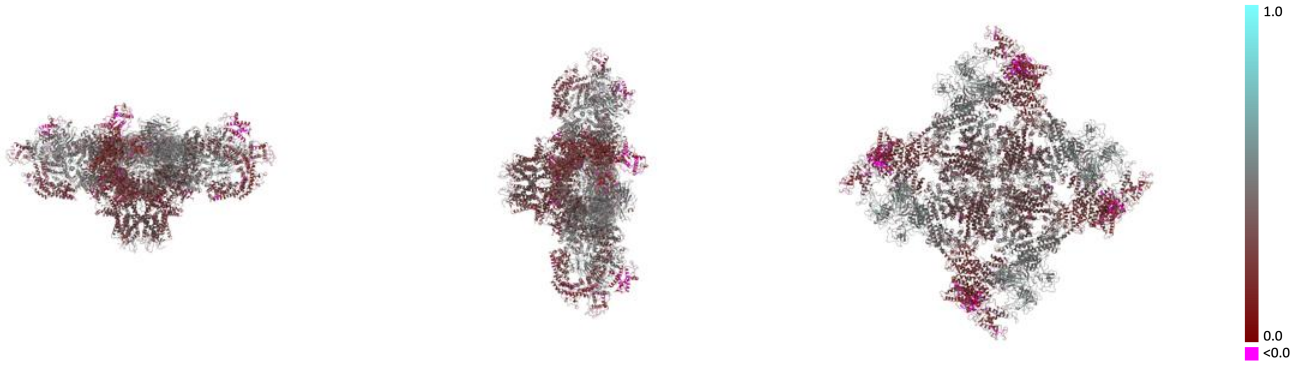
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.106 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.

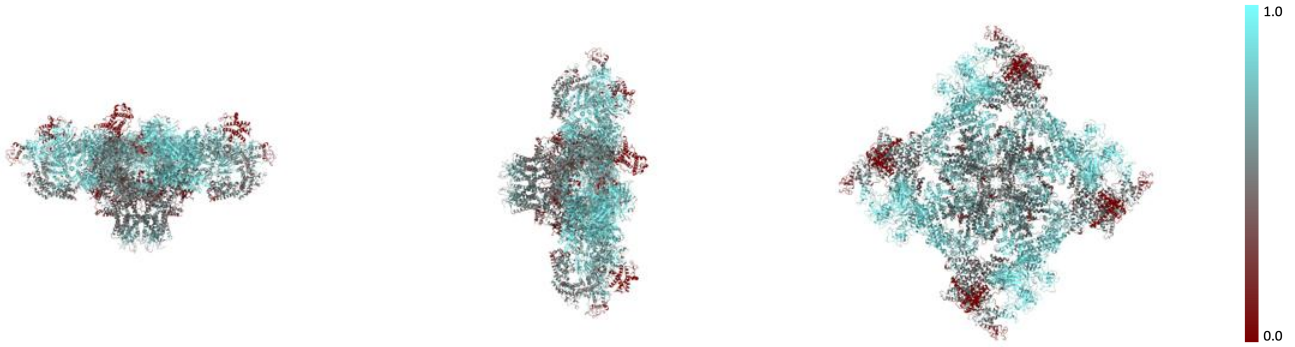
9.2 Q-score mapped to coordinate model



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.

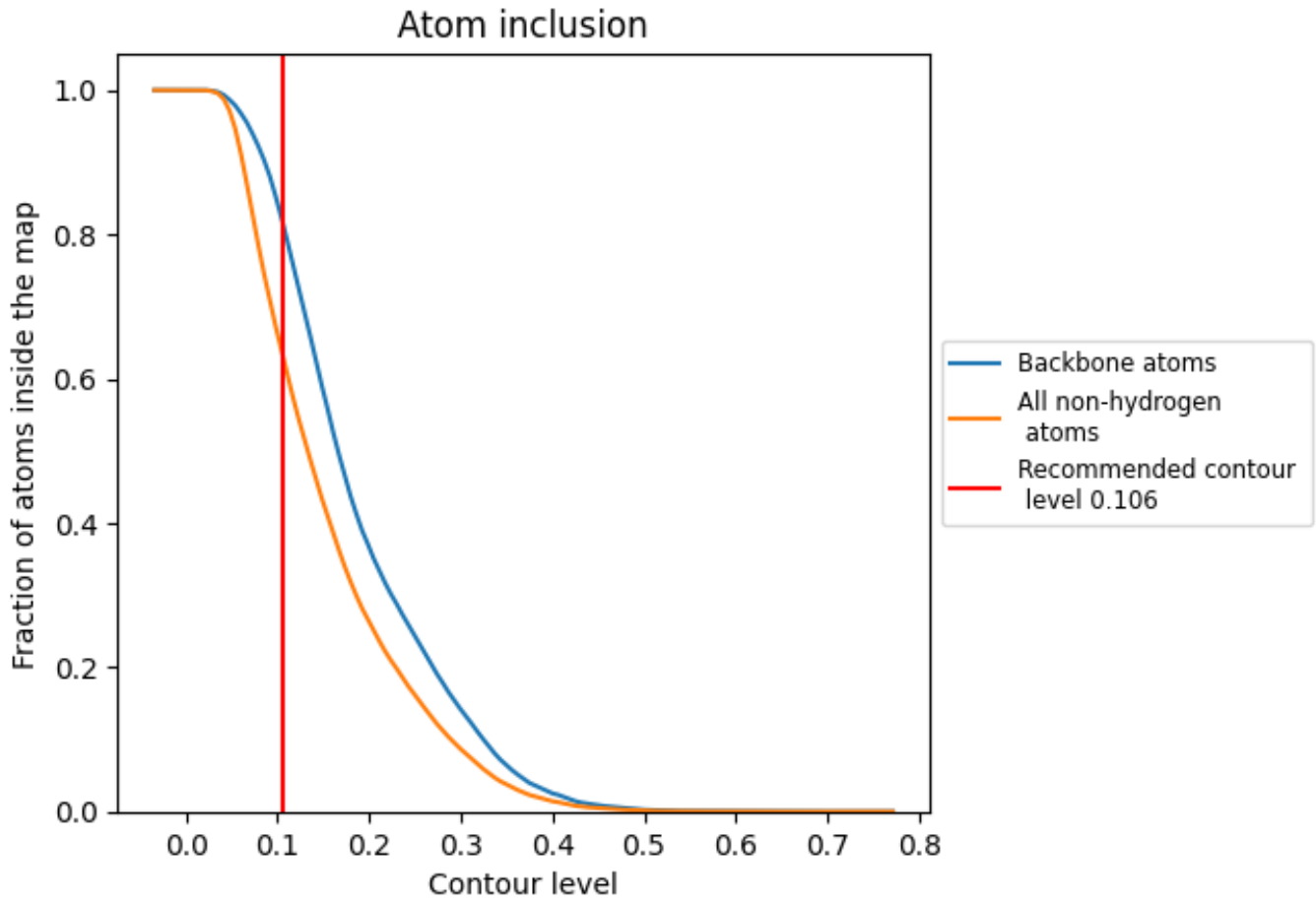
9.3 Atom inclusion mapped to coordinate model



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 (0.106).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 63% 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 (0.106) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6299	0.3560
A	0.6279	0.3600
B	0.6243	0.3500
F	0.8114	0.4790
G	0.6246	0.3500
H	0.8002	0.4790
I	0.6256	0.3500
J	0.8102	0.4780
O	0.8089	0.4800