wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Mar 2, 2017 – 12:38 pm GMT

PDB ID	:	5GKZ
EMDB ID:	:	EMD-9519
Title	:	Structure of RyR1 in a closed state (C3 conformer)
Authors	:	Bai, X.C.; Yan, Z.; Wu, J.P.; Yan, N.
Deposited on	:	2016-07-07
Resolution	:	4.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

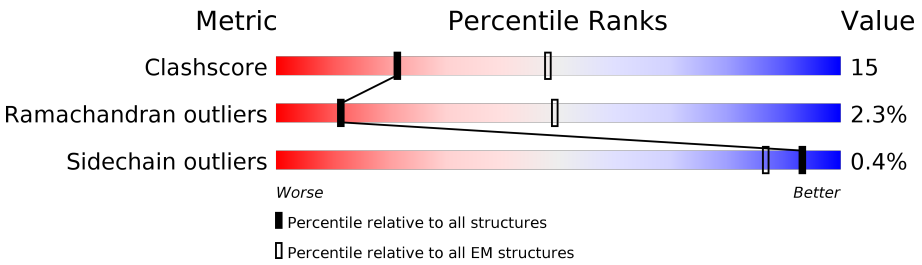
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc29047

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 4.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	5037	49% 22% • 27%
1	C	5037	48% 23% • 27%
1	E	5037	48% 23% • 27%
1	G	5037	49% 22% • 27%
2	B	108	67% 32% •
2	D	108	65% 34% •
2	F	108	68% 31% •
2	H	108	69% 30% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 111000 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ryanodine receptor 1.

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

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

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

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

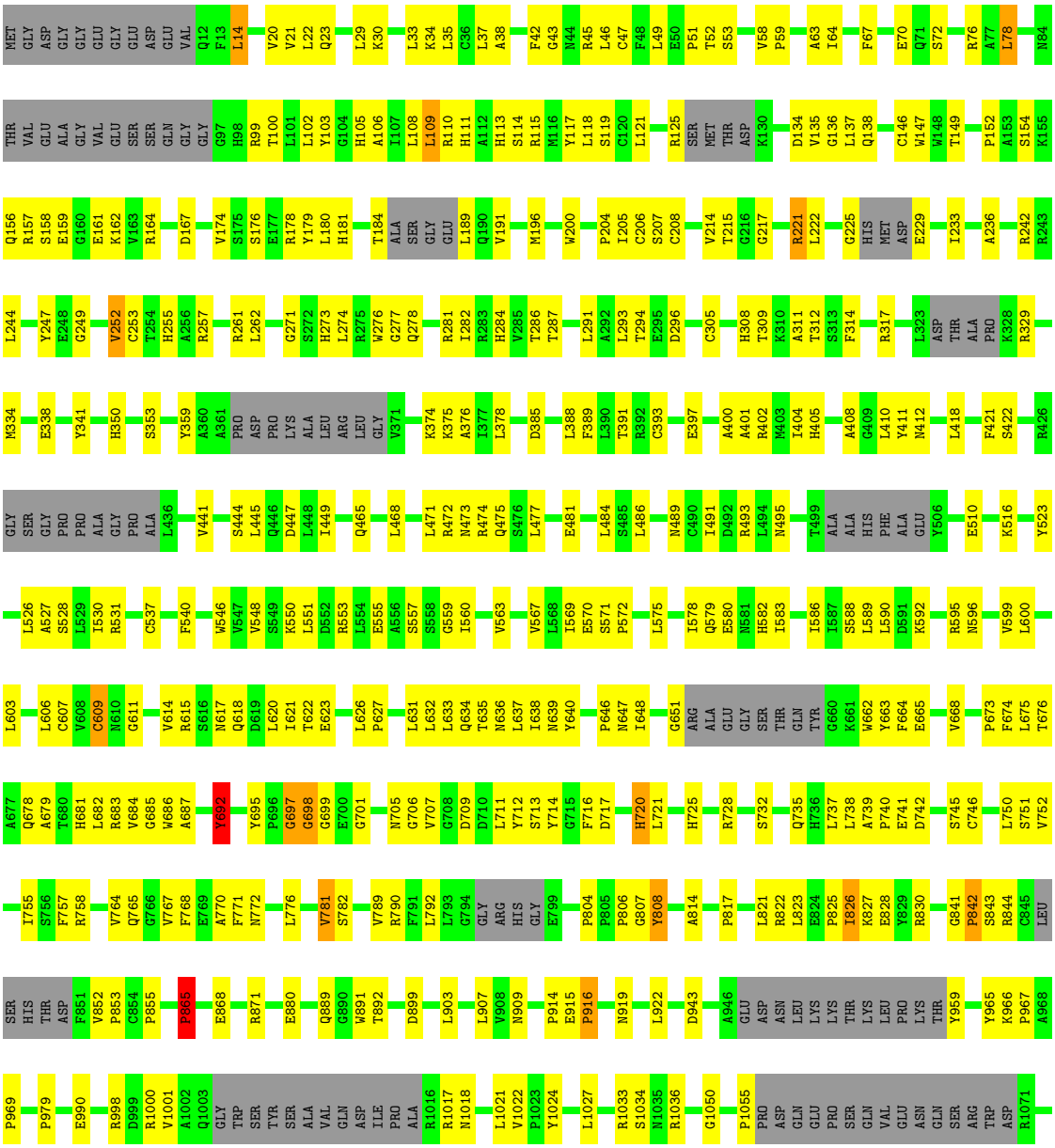
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	G	1	1	1	0
3	A	1	1	1	0
3	C	1	1	1	0
3	E	1	1	1	0

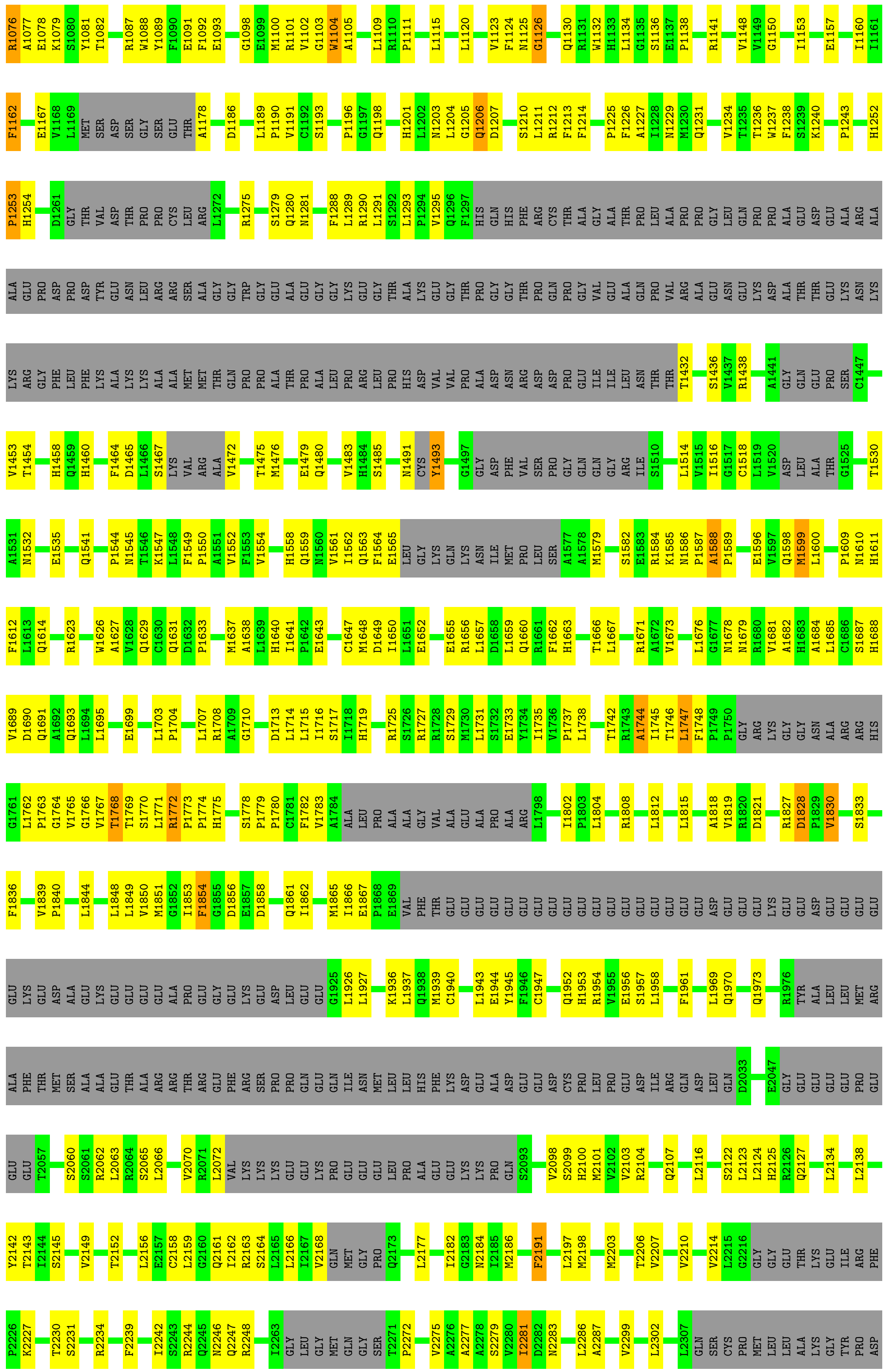
3 Residue-property plots (i)

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

- Molecule 1: Ryanodine receptor 1

Chain A: 49% 22% • 27%

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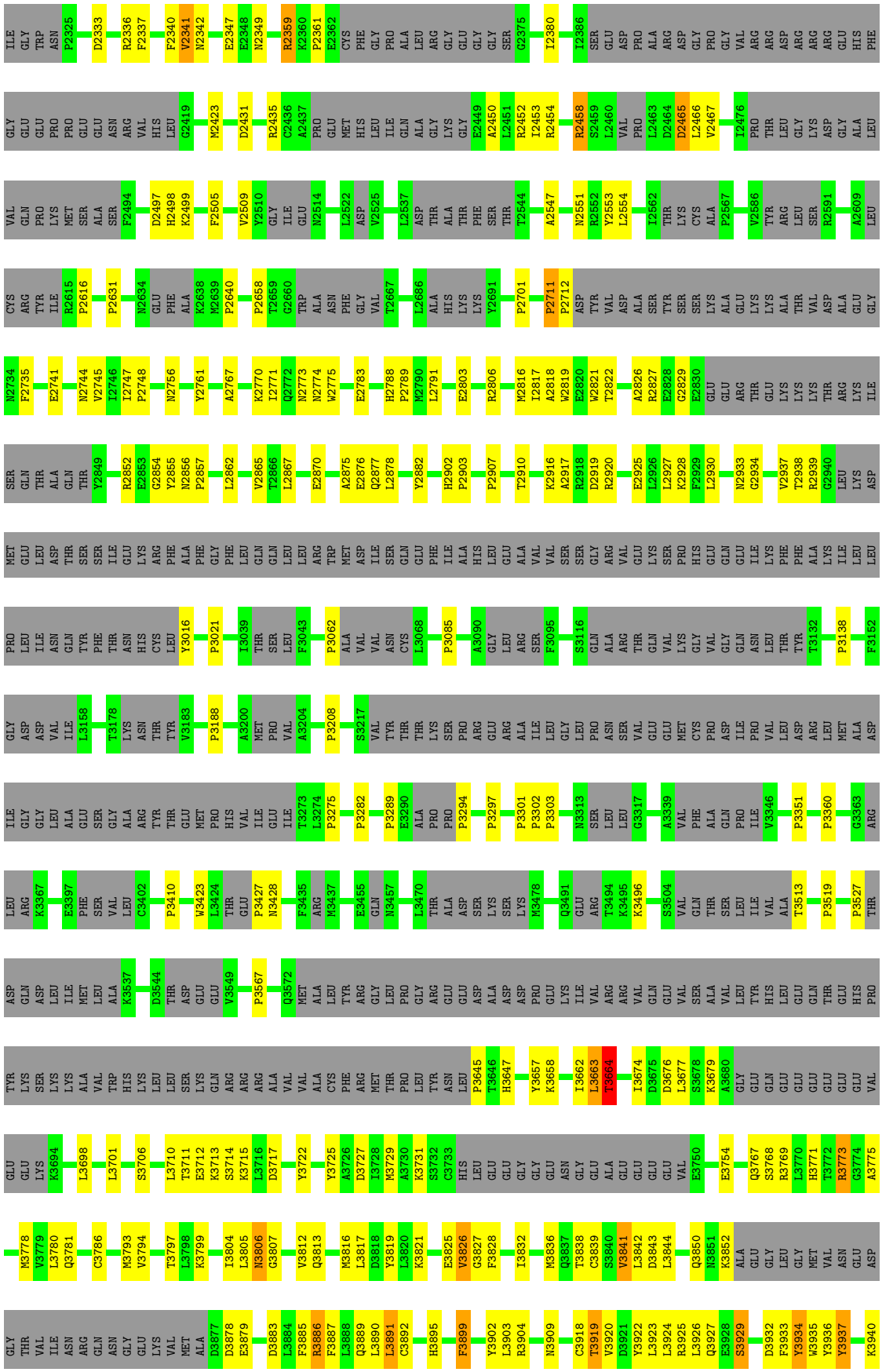
F1162 E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 D1186 L1189 P1190 V1191 C1192 S1193 P1196 G1197 Q1198 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 P1225 F1226 A1227 I1228 N1229 M1230 Q1231 V1234 T1235 T1236 W1237 F1238 S1239 K1240 P1243 H1252
P1253 H1254 D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272 R1275 S1279 Q1280 N1281 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG 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 PRO 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 LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO GLU ILE ILE LEU ASN THR THR T1432 S1436 V1437 R1438 A1441 GLY GLN GLU PRO SER C1447
V1453 T1454 H1458 Q1459 H1460 F1464 D1465 L1466 S1467 LYS VAL ARG ALA V1472 T1475 M1476 E1479 Q1480 V1483 H1484 S1485 N1491 CYS Y1493 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG ILE S1510 L1514 V1515 I1516 G1517 C1518 L1519 V1520 ASP LEU ALA THR G1525 T1530
A1531 N1532 E1535 Q1541 P1544 N1545 T1546 K1547 L1548 F1549 P1550 A1551 V1552 F1553 V1554 H1558 Q1559 N1560 V1561 I1562 Q1563 F1564 E1565 LEU GLY LYS GLN LYS ASN ILE MET PRO LEU SER A1577 A1578 M1579 S1582 E1583 R1584 K1585 N1586 P1587 A1588 P1589 E1596 V1597 Q1598 M1599 L1600 P1609 N1610 H1611
F1612 L1613 Q1614 R1623 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 H1640 I1641 P1642 E1643 C1647 M1648 D1649 I1650 L1651 E1652 E1655 R1656 L1657 D1658 L1659 Q1660 R1661 F1662 H1663 T1666 L1667 R1671 A1672 V1673 L1676 G1677 N1678 N1679 R1680 V1681 A1682 H1683 A1684 L1685 C1686 S1687 H1688
V1689 D1690 Q1691 A1692 Q1693 L1694 L1695 E1699 L1703 P1704 L1707 R1708 A1709 G1710 D1713 L1714 L1715 I1716 S1717 I1718 H1719 R1725 S1726 R1727 R1728 S1729 M1730 L1731 S1732 E1733 Y1734 I1735 V1736 P1737 L1738 T1742 R1743 A1744 I1745 T1746 L1747 F1748 P1749 P1750 GLY ARG LYS GLY GLY ASN ALA ARG ARG HIS
G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 P1773 P1774 H1775 S1778 P1779 P1780 C1781 F1782 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 I1802 P1803 L1804 R1808 L1812 L1815 A1818 V1819 R1820 D1821 R1827 D1828 P1829 V1830 S1833
F1836 V1839 P1840 L1844 L1848 L1849 V1850 M1851 G1852 I1853 F1854 G1855 D1856 E1857 D1858 Q1861 I1862 M1865 I1866 E1867 P1868 E1869 VAL PHE THR 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 GLU G1925 L1926 L1927 K1936 L1937 Q1938 M1939 C1940 L1943 E1944 Y1945 F1946 C1947 Q1952 H1953 R1954 V1955 E1956 S1957 L1958 F1961 L1969 Q1970 Q1973 R1976 TYR ALA LEU LEU MET ARG
ALA PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU ALA ASP GLU GLU ASP CYS PRO LEU PRO GLU ASP ILE ARG GLN ASP LEU GLN D2033 E2047 GLY GLU GLU GLU GLU PRO GLU
GLU GLU T2057 S2060 S2061 R2062 L2063 R2064 S2065 L2066 V2070 R2071 L2072 VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN S2093 V2098 S2099 H2100 M2101 V2102 V2103 R2104 Q2107 L2116 S2122 L2123 L2124 H2125 R2126 Q2127 L2134 L2138
Y2142 T2143 I2144 S2145 V2149 T2152 L2156 E2157 C2158 L2159 G2160 Q2161 I2162 R2163 S2164 L2165 L2166 I2167 V2168 GLN MET GLY PRO Q2173 L2177 I2182 G2183 N2184 I2185 M2186 F2191 L2197 M2198 M2203 T2206 V2207 V2210 V2214 L2215 G2216 GLY GLY GLU THR LYS GLU ILE ARG PHE
P2226 K2227 T2230 S2231 R2234 F2239 I2242 S2243 R2244 Q2245 N2246 Q2247 R2248 I2263 GLY LEU GLY MET GLN GLN SER T2271 P2272 V2275 A2276 A2277 A2278 S2279 V2280 I2281 D2282 N2283 L2286 A2287 V2299 L2302 L2307 GLN SER CYS PRO MET LEU LEU ALA LYS GLY TYR PRO ASP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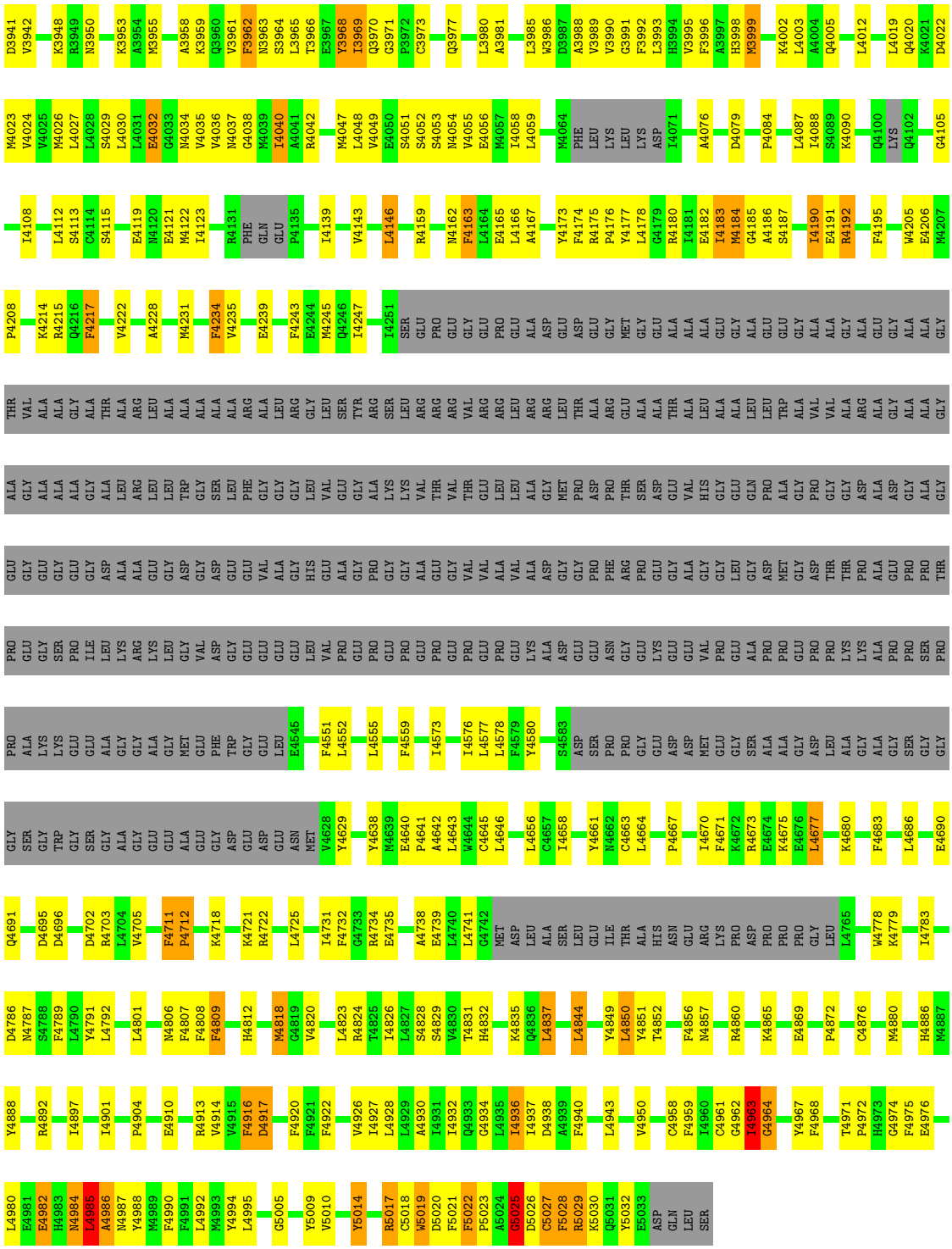
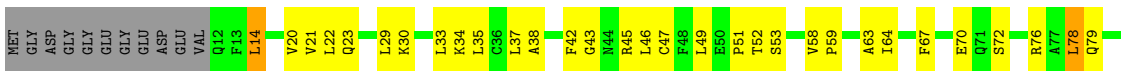
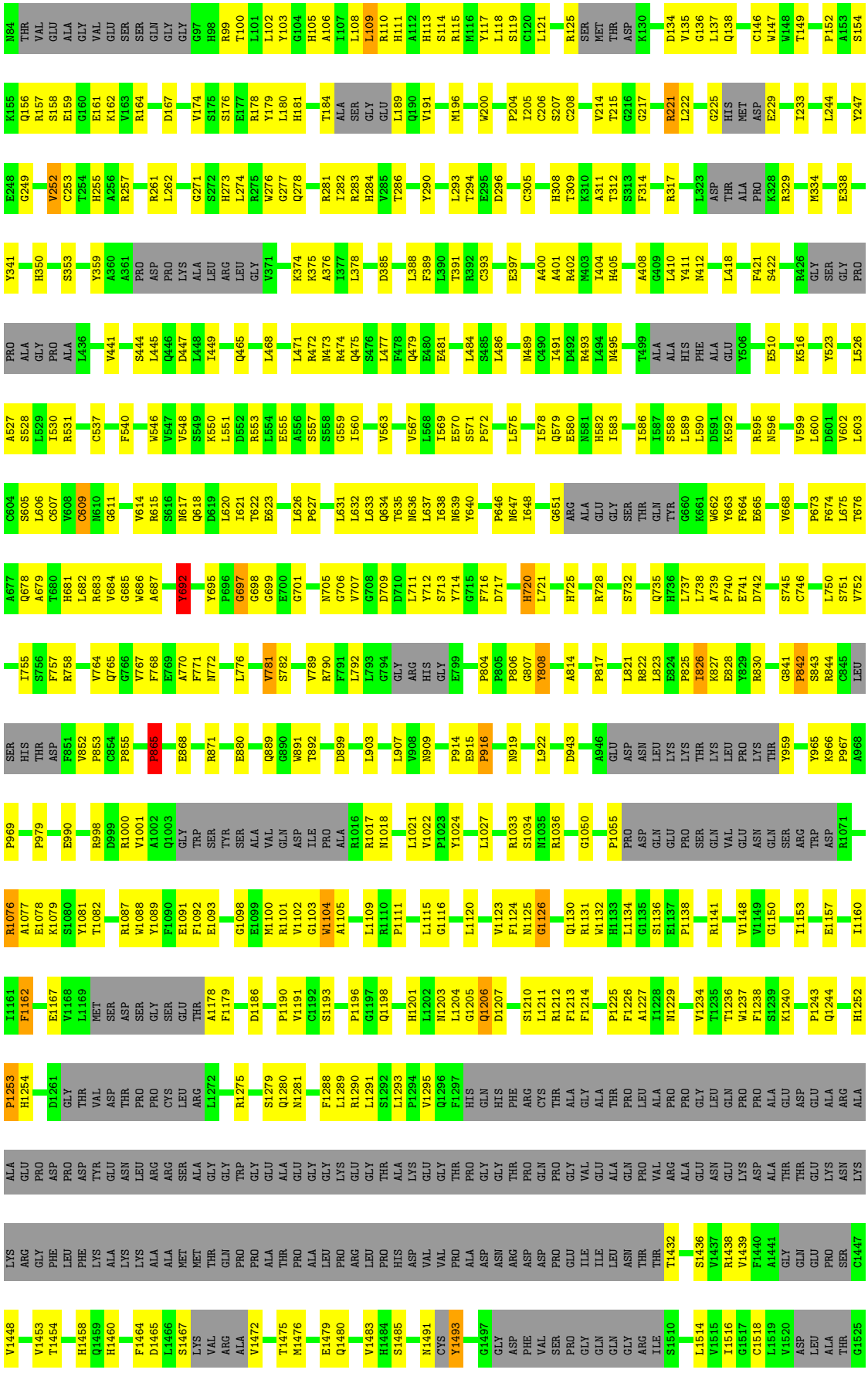
GLU GLU LYS K3694 L3698 L3701 S3706 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 Y3722 Y3725 A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733 HIS LEU GLU GLU GLY GLY GLU ASN GLY GLU GLU GLU VAL E3750 E3754 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775
TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA LEU CYS PHE ARG MET THR PRO LEU TYR ASN LEU P3645 T3646 H3647 Y3657 K3658 I3662 L3663 T3664 I3674 D3675 D3676 L3677 S3678 K3679 A3680 GLY GLU GLN GLU GLU GLU GLU VAL
ASP GLN ASP LEU ILE MET LEU ALA K3537 D3544 THR ASP GLU GLU V3549 P3567 Q3572 MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP ASP PRO GLU LYS ILE VAL ARG ARG VAL GLN GLU GLU GLU THR GLU HIS PRO
LEU ARG K3367 E3397 PHE SER VAL LEU C3402 P3410 W3423 L3424 THR GLU P3427 N3428 F3435 ARG M3437 E3455 GLN N3457 L3470 THR ALA ASP SER LYS SER LYS M3478 Q3491 GLU ARG T3494 K3495 K3496 S3504 VAL GLN THR SER LEU ILE VAL ALA T3513 P3519 P3527 THR
ILE GLY GLY LEU ALA GLU SER GLY ALA ARG TYR THR GLU MET PRO HIS VAL ILE GLU ILE T3273 L3274 P3275 P3282 P3289 E3290 ALA PRO PRO P3294 P3297 P3301 P3302 P3303 N3313 SER LEU LEU G3317 A3339 VAL PHE ALA GLN PRO ILE V3346 P3351 P3360 G3363 ARG
GLY ASP ASP VAL ILE L3158 T3178 LYS ASN THR TYR V3183 P3188 A3200 MET PRO VAL A3204 P3208 S3217 VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL LEU LEU ASP ARG LEU MET ALA ASP
PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU Y3016 P3021 I3039 THR SER LEU F3043 P3062 ALA VAL VAL ASN CYS L3068 P3085 A3090 GLY LEU ARG SER F3095 S3116 GLN ALA ARG THR GLN VAL LYS SER PRO HIS GLU GLN GLU ILE LYS PHE THR TYR T3132 P3138 F3152
MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU ILE LYS PHE PHE ALA LYS ILE LEU LEU
SER GLN THR ALA GLN THR Y2849 R2852 E2853 G2854 Y2855 N2856 P2857 L2862 V2865 T2866 L2867 E2870 A2875 E2876 Q2877 L2878 Y2882 H2902 P2903 P2907 T2910 K2916 A2917 R2918 D2919 R2920 E2925 L2926 L2927 K2928 F2929 L2930 N2933 G2934 V2937 T2938 R2939 G2940 LEU LYS ASP
N2734 F2735 E2741 N2744 V2745 I2746 I2747 P2748 N2756 Y2761 A2767 K2770 I2771 Q2772 N2773 N2774 W2775 E2783 H2788 P2789 M2790 L2791 E2803 R2806 M2816 I2817 A2818 W2819 E2820 W2821 T2822 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE
CYS ARG TYR ILE R2615 P2616 P2631 N2634 GLU PHE ALA K2638 M2639 P2640 P2658 T2659 G2660 TRP ALA ASN PHE GLY VAL T2667 L2686 ALA HIS LYS LYS Y2691 P2701 P2711 P2712 ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY
VAL GLN PRO LYS MET SER ALA SER F2494 D2497 H2498 K2499 F2505 V2509 Y2510 GLY ILE GLU N2514 L2522 ASP V2525 L2537 ASP THR ALA THR PHE SER THR T2544 A2547 N2551 R2552 Y2553 L2554 I2562 THR LYS CYS ALA P2567 V2586 TYR ARG LEU SER R2591 A2609 LEU
GLY GLU GLU PRO PRO GLU GLU ASN ARG VAL HIS LEU G2419 M2423 D2431 R2435 C2436 A2437 PRU GLU MET HIS LEU ILE GLN ALA GLY LYS GLY E2449 A2450 L2451 R2452 I2453 R2454 R2458 S2459 L2460 VAL PRO L2463 D2464 D2465 L2466 V2467 I2476 PRO THR LEU GLY LYS ASP GLY ALA LEU
ILE GLY TRP ASN P2325 D2333 R2336 F2337 F2340 V2341 N2342 E2347 E2348 N2349 R2359 K2360 P2361 E2362 CYS PHE GLY PRO ALA ARG ASP GLY PRO GLY VAL ARG ASP ARG ARG ARG GLU HIS PHE



- Molecule 1: Ryanodine receptor 1

Chain C:

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GLY PRO D1261 E1167 E1078 E990 THR A679 F757 L606 L529 GLY V252 R157 VAL
PHE ASP GLY V1168 K1079 R998 T680 R758 C607 1530 PRO C253 S158 GLU
LEU PRO THR L1169 S1080 D999 H681 V608 R531 ALA T254 E159 ALA
PHE ASP VAL MET Y1081 R1000 L682 C609 L436 H255 G160 GLY
LYS TYR ASP SER T1082 V1001 R683 N610 C537 Y359 E161 VAL
LYS ALA GLU ASP R1087 D999 V684 G611 V441 A256 K162 GLU
LYS LYS ASN THR W1088 R1000 G685 F540 A360 R257 V163 SER
LYS LYS LEU PRO Y1089 V1001 W686 V614 S444 A361 R164 SER
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MET MET ARG PRO E1091 Q1003 Y692 S616 L445 ASP V174 GLY
THR THR SER ARG F1092 GLY Y695 N617 W547 PRO Q446 S175 GLY
GLN ALA GLY GLU E1093 TRP P696 Q618 V548 LYS D447 S176 H98
PRO GLY GLY THR A1178 SER G697 D619 S549 ALA L448 E177 R99
PRO TRP GLY A1098 F1179 TYR G698 L620 K550 LEU I449 R178 T100
PRO GLU ALA R1275 D1186 SER G699 I621 L551 ARG Q465 Y179 L101
ALA ALA THR E1099 ALA E700 T622 D552 LEU L180 L102
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LEU GLY GLY F1288 S1193 G1103 ILE G706 L631 A556 K374 ALA A106
LYS VAL GLY L1289 P1196 W1104 PRO V707 L632 S557 K375 SER I107
GLU PRO GLU L1290 G1197 A1105 ALA G708 L633 S558 A376 MET L108
GLY ASN LYS L1291 Q1198 R1016 D709 Q634 C559 I377 THR L109
THR LEU GLU S1292 H1201 L1109 R1017 D710 T635 1560 L378 ASP R110
ALA LEU LYS L1293 P1111 R1110 N1018 L711 N636 V563 D385 K130 H111
LYS ARG ASP P1294 L1202 L1115 L1021 Y712 L637 V567 L388 A112
GLU ASP GLY V1295 N1203 G1116 V1022 S713 1568 F389 D134 H113
GLY VAL GLU Q1296 L1204 P1023 P914 Y714 1569 L390 V135 S114
THR VAL GLY F1297 G1205 Y1024 E915 G715 E570 T391 G136 R115
PRO PRO THR HIS Q1206 L1120 L1027 P916 F716 S571 R392 L137 M116
GLN PRO GLN D1207 V1123 R1033 P804 D717 P572 C393 Q138 Y117
GLY ALA GLY HIS S1210 F1124 N919 P805 L575 E397 C146 L118
ASP ALA THR PHE L1211 N1125 L922 P806 H720 W147 S119
ARG ALA PRO ARG R1212 N1034 G807 L721 E397 W148 C120
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PRO GLN THR PRO F1214 R1036 D943 A814 G651 P673 P152
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ASN PRO THR PRO L1134 ASP R822 GLY ASP
THR VAL PRO LEU G1135 ASN Q735 SER
THR VAL ARG ALA I1228 S1136 LEU L823 THR H736 GLN
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L1514 GLU ASN V1234 PRO LYS P825 L738 G660
V1515 ASN GLU T1235 SER THR I826 K661
I1516 GLU LYS T1236 GLN LYS A739 W662
G1517 LYS ASP W1237 VAL K827 P740 Y663
C1518 ASP ALA F1238 LEU E828 E741 F664
L1519 ALA THR S1239 GLU PRO Y829 D742 E665
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ASP THR GLU P1243 GLU THR Y959 C746 P673
LEU GLU LYS Q1244 ALA G841 L750 P674
ALA LYS ASN E1157 ARG P842 S751 L675
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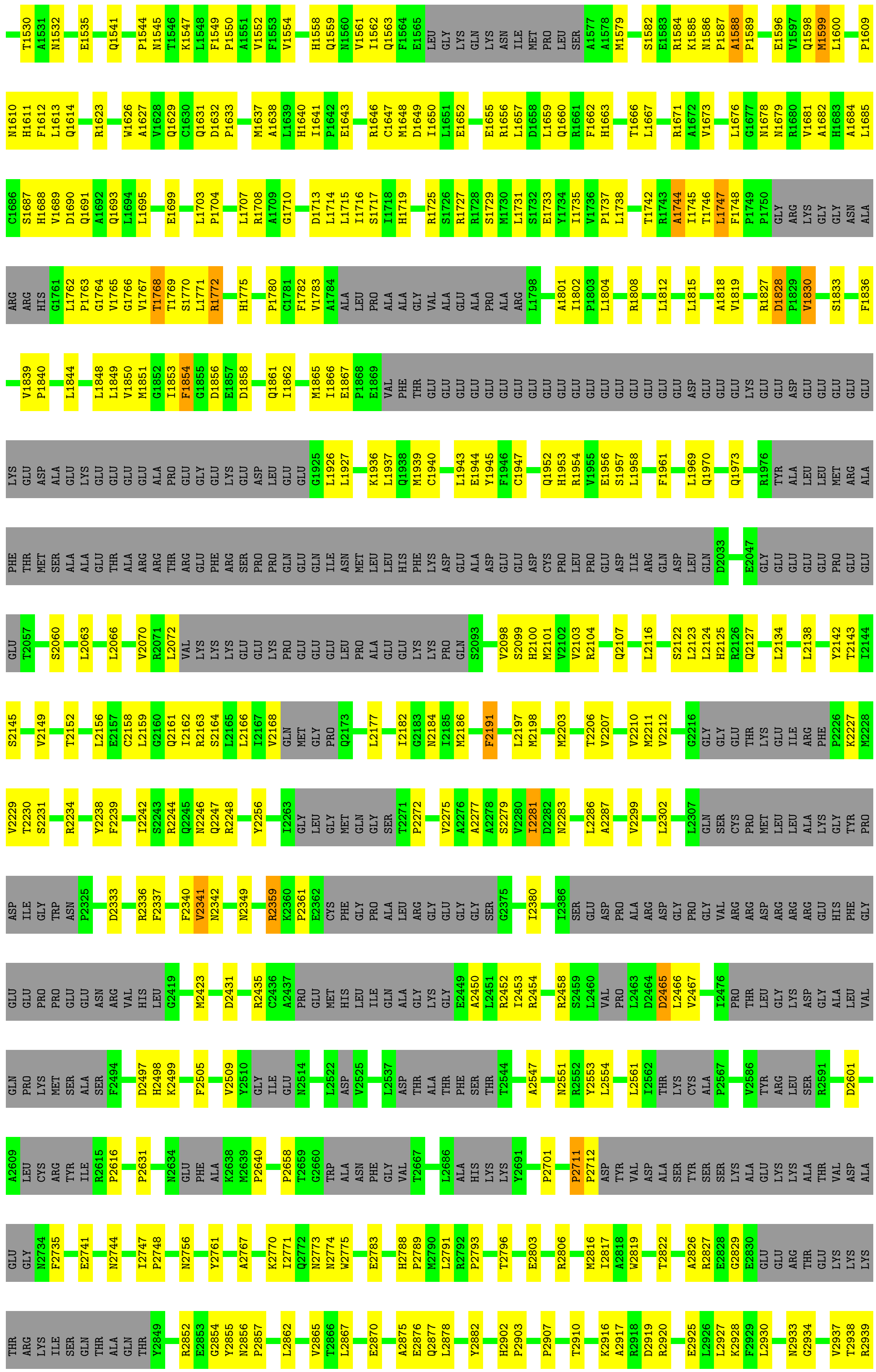
LEU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N1610 H1611 F1612 L1613 Q1614 R1623 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 H1640 I1641 P1642 E1643 R1646 C1647 M1648 D1649 I1650 L1651 E1652 E1655 R1656 L1657 D1658 L1659 Q1660 R1661 F1662 H1663 T1666 L1667 R1671 A1672 V1673 L1676 G1677 N1678 N1679 R1680 V1681 A1682 H1683 A1684 L1685
C1686 S1687 H1688 V1689 D1690 Q1691 A1692 Q1693 L1694 L1695 E1699 L1703 P1704 L1707 R1708 A1709 G1710 D1713 L1714 L1715 I1716 S1717 I1718 H1719 R1725 S1726 R1727 R1728 S1729 M1730 L1731 S1732 E1733 Y1734 I1735 V1736 P1737 L1738 T1742 R1743 A1744 I1745 T1746 L1747 F1748 P1749 P1750 GLY ARG LYS GLY GLY ASN ALA
ARG ARG HIS G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 H1775 P1780 C1781 F1782 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 A1801 I1802 P1803 L1804 R1808 L1812 L1815 A1818 V1819 R1827 D1828 P1829 V1830 S1833 F1836
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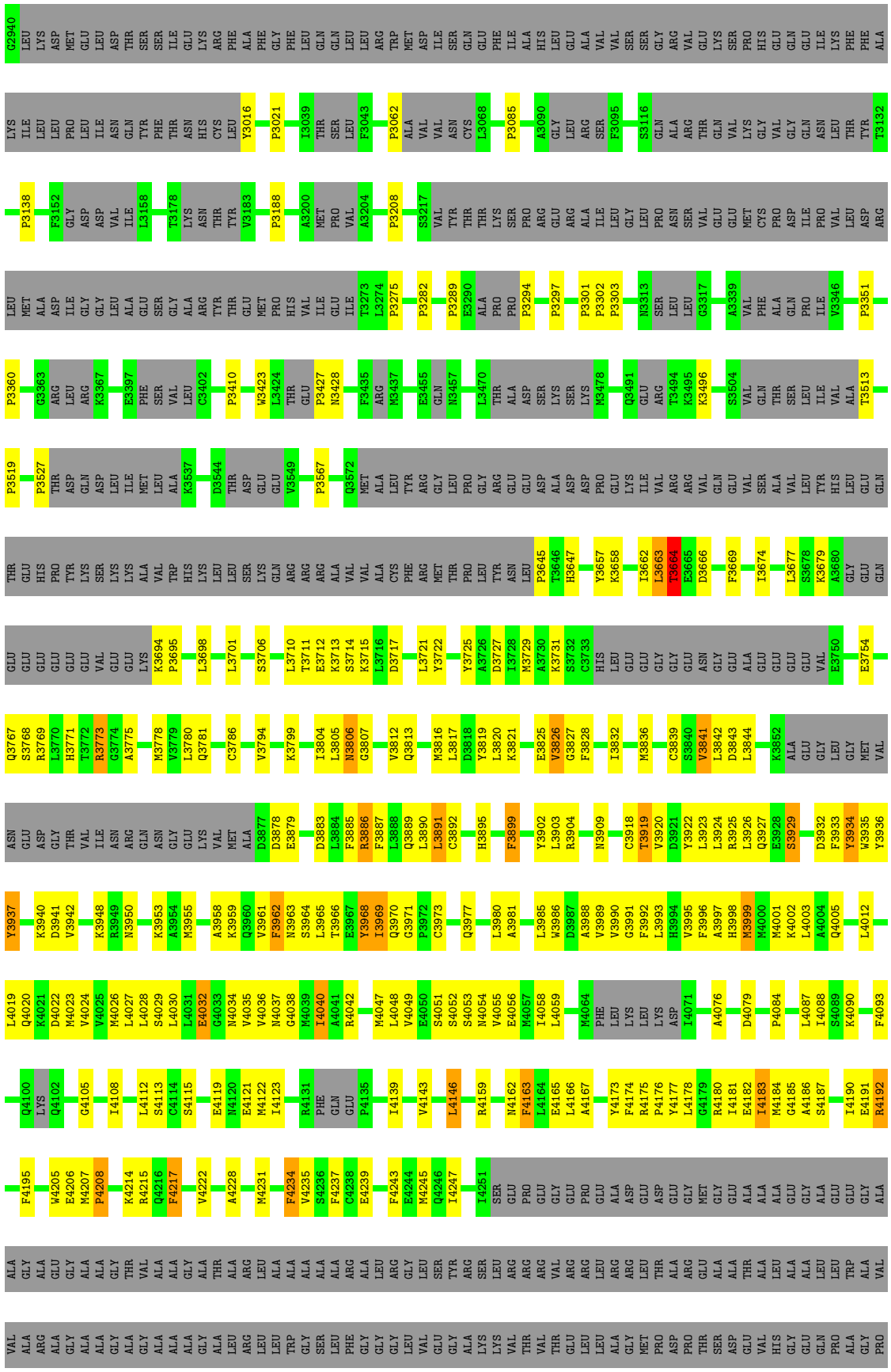
LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU GLU GLU G1925 L1926 L1927 K1936 L1937 Q1938 M1939 C1940 L1943 E1944 Y1945 F1946 C1947 Q1952 H1953 R1954 V1955 E1956 S1957 L1958 F1961 L1969 Q1970 Q1973 R1976 TYR ALA LEU LEU MET ARG ALA
PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU ALA ASP GLU GLU ASP CYS PRO LEU PRO GLU ASP ILE ARG GLN ASP LEU GLN D2033 E2047 GLY GLU GLU GLU GLU PRO GLU GLU
GLU T2057 S2060 L2063 L2066 V2070 R2071 L2072 VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN S2093 V2098 S2099 H2100 M2101 V2102 V2103 R2104 Q2107 L2116 S2122 L2123 L2124 H2125 R2126 Q2127 L2134 L2138 Y2142 T2143 I2144
S2145 V2149 T2152 L2156 E2157 C2158 L2159 G2160 Q2161 I2162 R2163 S2164 L2165 L2166 I2167 V2168 GLN MET GLY PRO Q2173 L2177 I2182 G2183 N2184 I2185 M2186 F2191 L2197 M2198 M2203 T2206 V2207 V2210 M2211 V2212 G2216 GLY GLY GLU THR LYS GLU ILE ARG PHE P2226 K2227 M2228
V2229 T2230 S2231 R2234 Y2238 F2239 I2242 S2243 R2244 Q2245 N2246 Q2247 R2248 Y2256 I2263 GLY LEU GLY MET GLN GLY SER T2271 P2272 V2275 A2276 A2277 A2278 S2279 V2280 I2281 D2282 N2283 L2286 A2287 V2299 L2302 L2307 GLN SER CYS PRO MET LEU LEU ALA LYS GLY TYR PRO
ASP ILE GLY TRP ASN P2325 D2333 R2336 F2337 F2340 V2341 N2342 N2349 R2359 K2360 P2361 E2362 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY SER G2375 I2380 I2386 SER GLU ASP PRO ALA ARG ASP GLY PRO GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY
GLU GLU PRO PRO GLU GLU ASN ARG VAL HIS LEU G2419 M2423 D2431 R2435 C2436 A2437 PRO GLU MET HIS LEU ILE GLN ALA GLY LYS GLY E2449 A2450 L2451 R2452 I2453 R2454 R2458 S2459 L2460 VAL PRO L2463 D2464 D2465 L2466 V2467 I2476 PRO THR LEU GLY LYS ASP GLY ALA LEU VAL
GLN PRO LYS MET SER ALA SER F2494 D2497 H2498 K2499 F2505 V2509 Y2510 GLY ILE GLU N2514 L2522 ASP V2525 L2537 ASP THR ALA THR PHE SER THR T2544 A2547 N2551 R2552 Y2553 L2554 L2561 I2562 THR LYS CYS ALA P2567 V2586 TYR ARG LEU SER R2591 D2601
A2609 LEU CYS ARG TYR ILE R2615 P2616 P2631 N2634 GLU PHE ALA K2638 M2639 P2640 P2658 T2659 G2660 TRP ALA ASN PHE GLY VAL T2667 L2686 ALA HIS LYS LYS Y2691 P2701 P2711 P2712 ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA
GLU GLY N2734 F2735 E2741 N2744 I2747 P2748 N2756 Y2761 A2767 K2770 I2771 Q2772 N2773 N2774 W2775 E2783 H2788 P2789 M2790 L2791 R2792 P2793 T2796 E2803 R2806 M2816 I2817 A2818 W2819 T2822 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS
THR ARG LYS ILE SER GLN THR ALA GLN THR Y2849 R2852 E2853 G2854 Y2855 N2856 P2857 L2862 V2865 T2866 L2867 E2870 A2875 E2876 Q2877 L2878 Y2882 H2902 P2903 P2907 T2910 K2916 A2917 R2918 D2919 R2920 E2925 L2926 L2927 K2928 F2929 L2930 N2933 G2934 V2937 T2938 R2939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ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG ARG VAL ARG ARG ARG ALA LEU ARG ALA GLU GLU ALA ALA ASP GLU LEU ASP GLU ALA ALA GLU GLY ALA GLU LEU LEU THR ALA VAL
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L4019 Q4020 K4021 D4022 M4023 V4024 V4025 M4026 L4027 L4028 S4029 L4030 L4031 E4032 G4033 N4034 V4035 V4036 N4037 G4038 M4039 I4040 A4041 R4042 M4047 L4048 V4049 E4050 S4051 S4052 S4053 N4054 V4055 E4056 M4057 I4058 L4059 M4064 PHE LEU LYS LEU LYS ASP I4071 A4076 D4079 P4084 G4084 L4087 I4088 S4089 K4090 F4093
Y3937 K3940 D3941 V3942 K3948 R3949 N3950 K3953 A3954 M3955 A3958 K3959 Q3960 V3961 F3962 N3963 S3964 L3965 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 Q3977 L3980 A3981 L3985 W3986 D3987 A3988 V3989 V3990 G3991 F3992 L3993 H3994 V3995 F3996 A3997 H3998 M3999 M4000 M4001 K4002 L4003 A4004 Q4005 L4012
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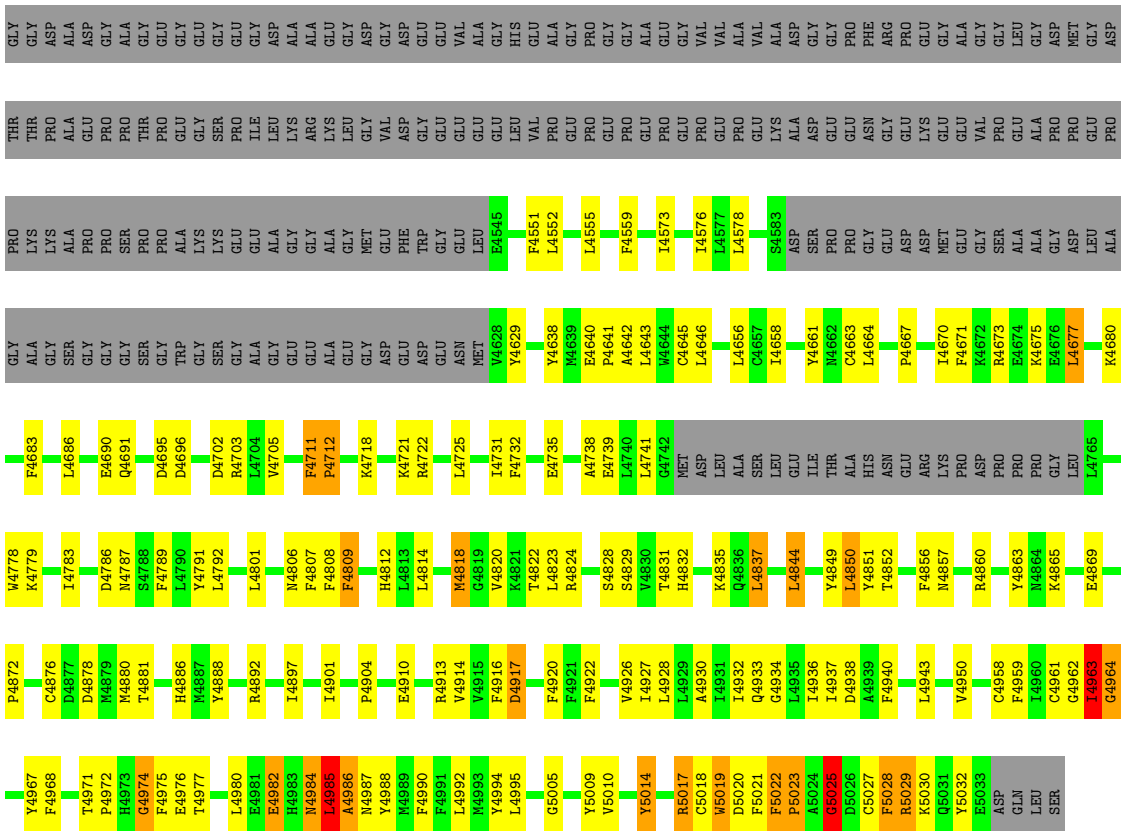
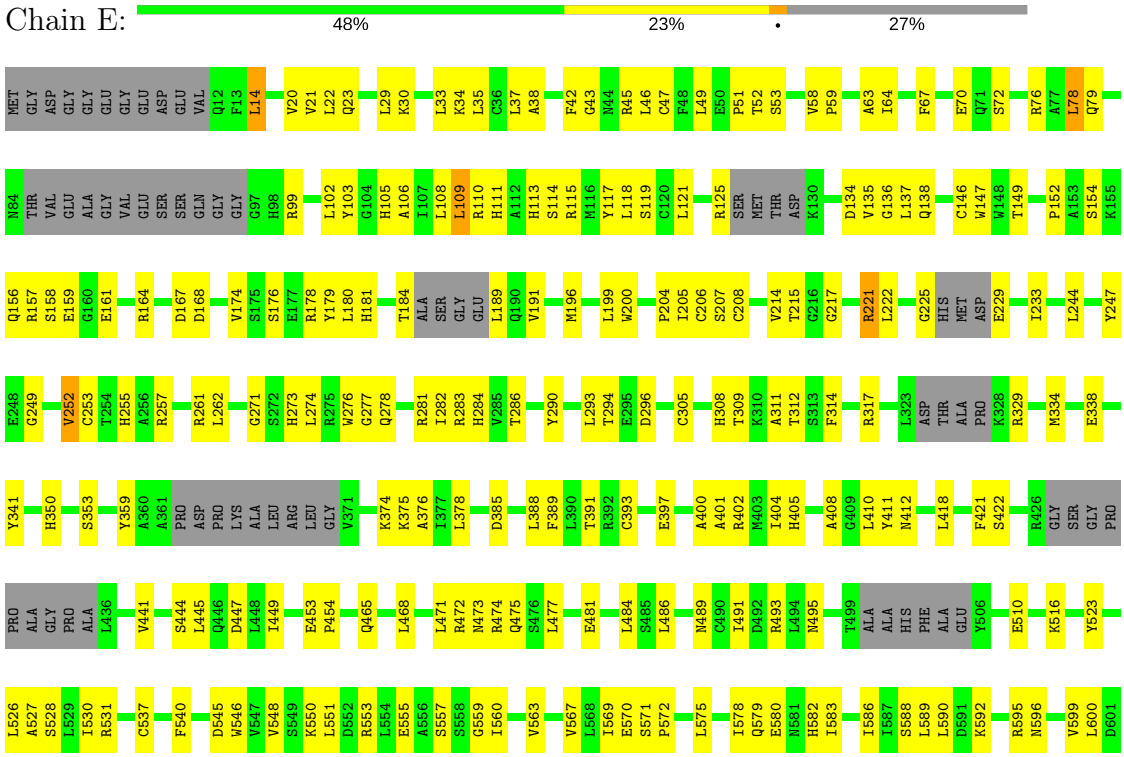
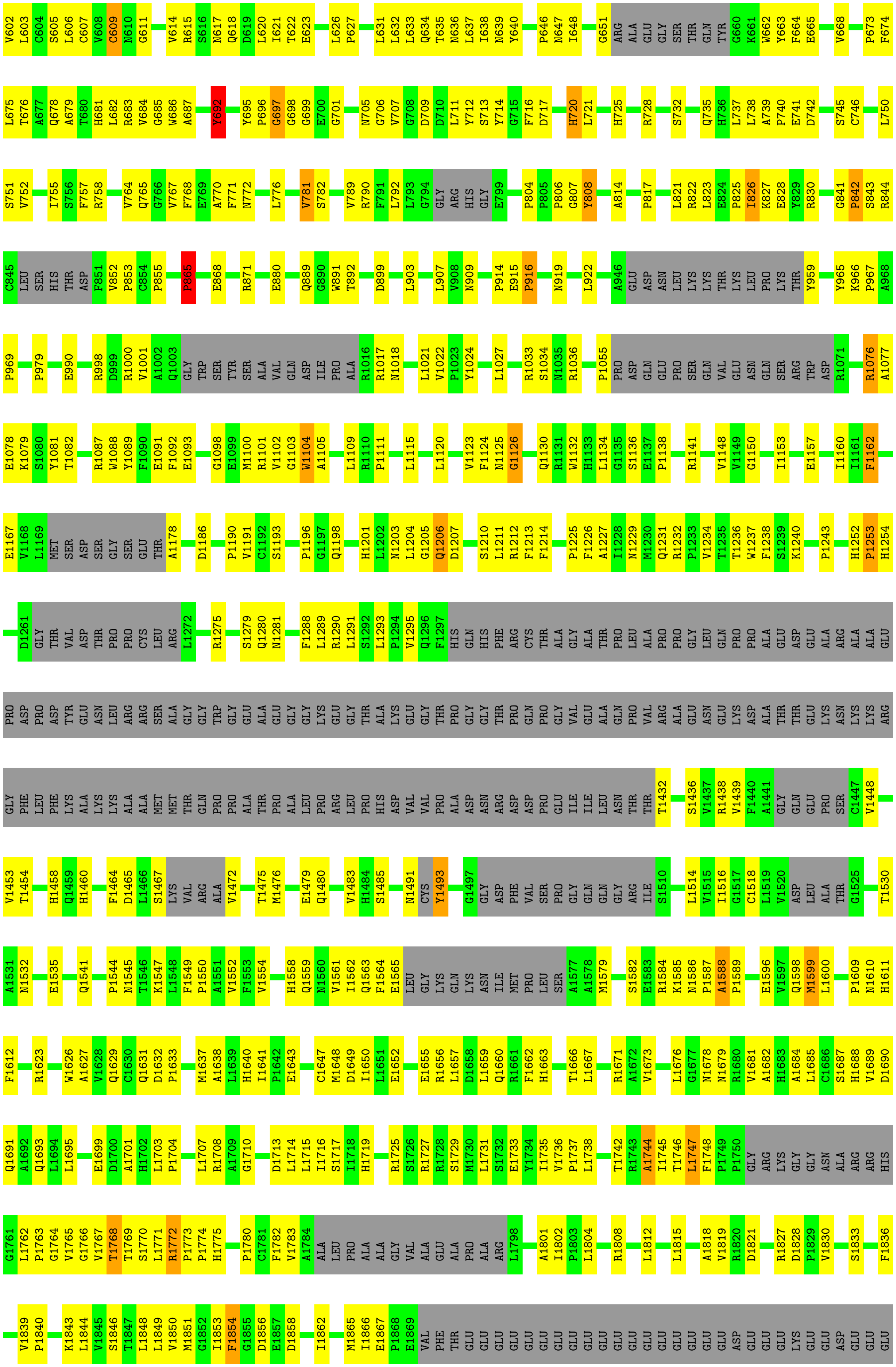
Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 M3778 V3779 L3780 Q3781 C3786 V3794 K3799 I3804 L3805 N3806 G3807 V3812 Q3813 M3816 L3817 D3818 Y3819 L3820 K3821 E3825 V3826 G3827 F3828 I3832 M3836 C3839 S3840 V3841 L3842 D3843 L3844 K3852 ALA GLU GLY LEU GLY MET VAL
GLU GLU GLU GLU GLU VAL GLU GLU LYS K3694 P3695 L3698 L3701 S3706 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 L3721 Y3722 Y3725 A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733 HIS LEU GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 E3754
THR GLU HIS PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA ALA VAL VAL ALA CYS PHE ARG MET THR PRO LEU TYR ASN LEU P3645 T3646 H3647 Y3657 K3658 I3662 L3663 T3664 E3665 D3666 F3669 I3674 L3677 S3678 K3679 A3680 GLY GLU GLN
P3519 P3527 THR ASP GLN ASP LEU ILE MET LEU ALA K3537 D3544 THR ASP GLU GLU V3549 P3567 Q3572 MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ALA ASP ASP PRO GLU LYS ILE VAL ARG ARG SER ALA VAL LEU TYR HIS LEU GLU GLN
P3360 G3363 ARG LEU ARG K3367 E3397 PHE SER VAL LEU C3402 P3410 W3423 L3424 THR GLU P3427 N3428 F3435 ARG M3437 E3455 GLN N3457 L3470 THR ALA ASP SER LYS SER LYS M3478 Q3491 GLU ARG T3494 K3495 K3496 S3504 VAL GLN THR SER LEU ILE VAL ALA T3513
LEU MET ALA ASP ILE GLY GLY LEU ALA ILE GLU MET PRO HIS VAL ILE GLU ILE T3273 L3274 P3275 P3282 P3289 E3290 ALA PRO PRO P3294 P3297 P3301 P3302 P3303 N3313 SER LEU LEU G3317 A3339 VAL PHE ALA GLN PRO ILE V3346 P3351
P3138 F3152 GLY ASP ASP VAL ILE L3158 T3178 LYS ASN THR TYR V3183 P3188 A3200 MET PRO VAL A3204 P3208 S3217 VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL LEU ASP ARG
LYS ILE LEU LEU PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU Y3016 P3021 I3039 THR SER LEU F3043 P3062 ALA VAL VAL ASN CYS L3068 P3085 A3090 GLY LEU ARG SER F3095 S3116 GLN ALA ARG THR GLN VAL LYS GLY VAL GLY GLN ASN LEU THR TYR T3132
G2940 LEU LYS ASP MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU ILE LYS PHE PHE ALA



- Molecule 1: Ryanodine receptor 1

Chain E:

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L675 T676 A677 Q678 A679 T680 H681 L682 R683 V684 G685 W686 A687 Y692 Y695 P696 G697 G698 G699 E700 G701 N705 G706 V707 G708 D709 D710 L711 Y712 S713 Y714 G715 F716 D717 H720 L721 H725 R728 S732 Q735 H736 L737 L738 A739 P740 E741 D742 S745 C746 L750
S751 V752 I755 S756 F757 R758 V764 Q765 G766 V767 F768 E769 A770 F771 N772 L776 V781 S782 V789 R790 F791 L792 L793 G794 GLY ARG HIS GLY E799 P804 P805 P806 G807 Y808 A814 P817 L821 R822 L823 E824 P825 I826 K827 E828 Y829 R830 G841 P842 S843 R844
C845 LEU SER HIS THR ASP F851 V852 P853 C854 P855 P865 E868 R871 E880 Q889 G890 W891 T892 D899 L903 L907 V908 N909 P914 E915 P916 N919 L922 A946 GLU ASP ASN LEU LYS LYS THR LYS LEU PRO LYS THR Y959 Y965 K966 P967 A968
P969 P979 E990 R998 D999 R1000 V1001 A1002 Q1003 GLY TRP SER TYR SER ALA VAL GLN ASP ILE PRO ALA R1016 R1017 N1018 L1021 V1022 P1023 Y1024 L1027 R1033 S1034 N1035 R1036 P1055 PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP ASP R1071 R1076 A1077
E1078 K1079 S1080 Y1081 T1082 R1087 W1088 Y1089 F1090 E1091 F1092 E1093 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 L1109 R1110 P1111 L1115 L1120 V1123 F1124 N1125 G1126 Q1130 R1131 W1132 H1133 L1134 G1135 S1136 E1137 P1138 R1141 V1148 V1149 G1150 I1153 E1157 I1160 I1161 F1162
E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 D1186 P1190 V1191 C1192 S1193 P1196 G1197 Q1198 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 P1225 F1226 A1227 I1228 N1229 M1230 Q1231 R1232 P1233 V1234 T1235 T1236 W1237 F1238 S1239 K1240 P1243 H1252 P1253 H1254
D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272 R1275 S1279 Q1280 N1281 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG 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 PRO 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 LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO GLU ILE ILE LEU ASN THR THR T1432 S1436 V1437 R1438 V1439 F1440 A1441 GLY GLN GLU PRO SER C1447 V1448
V1453 T1454 H1458 Q1459 H1460 F1464 D1465 L1466 S1467 LYS VAL ARG ALA V1472 T1475 M1476 E1479 Q1480 V1483 H1484 S1485 N1491 CYS Y1493 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG ILE S1510 L1514 V1515 I1516 G1517 C1518 L1519 V1520 ASP LEU ALA THR G1525 T1530
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G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 P1773 P1774 H1775 P1780 C1781 F1782 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 A1801 I1802 P1803 L1804 R1808 L1812 L1815 A1818 V1819 R1820 D1821 R1827 D1828 P1829 V1830 S1833 F1836
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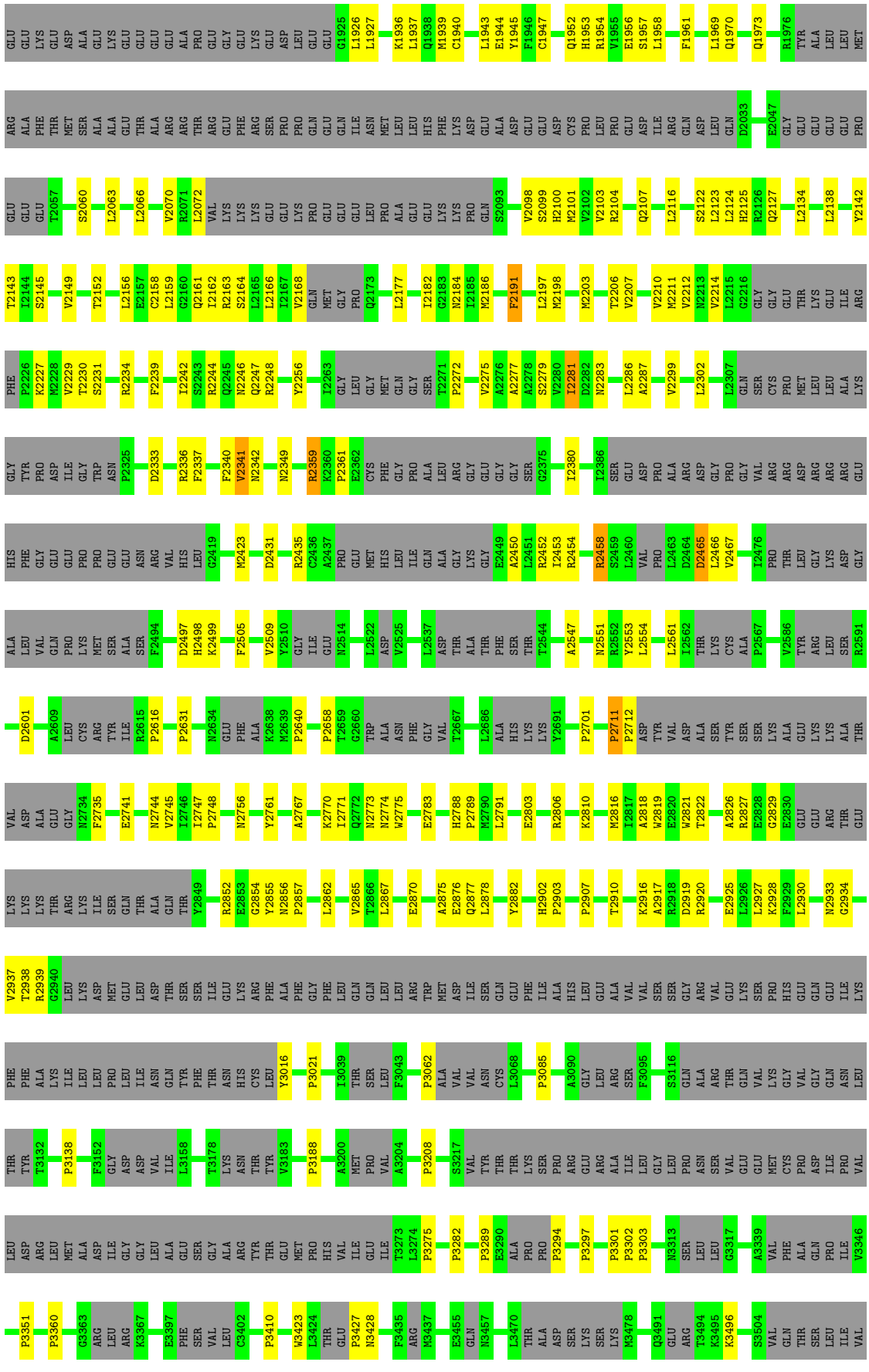

WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM

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Q4691	GLY	PRO	PRO	GLY	ALA	ALA	P4208	G4105	Q4020	K3940	ASP	T3772	GLU	GLN	
	SER	SER	PRO	ALA	ALA	ALA			K4021	D3941	GLY	R3773	GLU	THR	P3519
D4695	GLY	PRO	THR	GLY	GLY	GLY	K4214	I4108	D4022	V3942	THR	G3774	GLU	GLU	
D4696	TRP	PRO	PRO	GLU	ALA	THR	R4215		M4023	I3943	VAL	A3775	VAL	HIS	P3527
	GLY	ALA	GLU	GLY	GLY	VAL	Q4216	L4112	V4024		ILE		GLU	PRO	THR
D4702	SER	LYS	GLY	GLU	ALA	ALA	F4217	S4113	V4025	K3948	ASN	M3778	GLU	TYR	ASP
R4703	GLY	LYS	SER	GLY	ALA	ALA		C4114	M4026	R3949	ARG	V3779	LYS	LYS	GLN
L4704	ALA	GLU	PRO	GLU	ALA	GLY	V4221	S4115	L4027	N3950	GLN	L3780	K3694	SER	ASP
V4705	GLY	GLU	ILE	GLY	GLY	ALA	V4222		L4028		ASN	Q3781		LYS	LEU
	GLU	ALA	LEU	ASP	ALA	THR		E4119	S4029	K3953	GLY		L3698	LYS	ILE
T4708	GLU	GLY	LYS	ALA	LEU	ALA	A4228		L4030	A3954	GLU	C3786		ALA	MET
P4709	ALA	GLY	ARG	ALA	ARG	ARG	E4229	M4122	L4031	M3955	LYS		L3701	VAL	LEU
S4710	GLU	ALA	LYS	GLU	LEU	LEU	K4230	I4123	E4032		VAL	M3793		TRP	ALA
F4711	GLY	GLY	LEU	GLY	LEU	ALA	M4231		G4033	A3958	MET	V3794	S3706	HIS	K3537
P4712	ASP	MET	GLY	ASP	TRP	ALA	E4232	R4131	N4034	K3959	ALA			LYS	
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K4718	ASP	PHE	ASP	ASP	SER	ALA	F4234	GLN	V4036	V3961	D3878	L3798	T3711	LEU	THR
	GLU	TRP	GLY	GLU	LEU	ALA	V4235	GLU	N4037	F3962	E3879	K3799	E3712	SER	ASP
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	V4628	LEU	GLU	ALA	GLY	LEU		I4139	I4040	L3965	L3884	L3805	K3715	ARG	V3549
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I4731	Y4638	L4552	VAL	GLU	VAL	LEU	M4245			Y3968	F3887			ALA	
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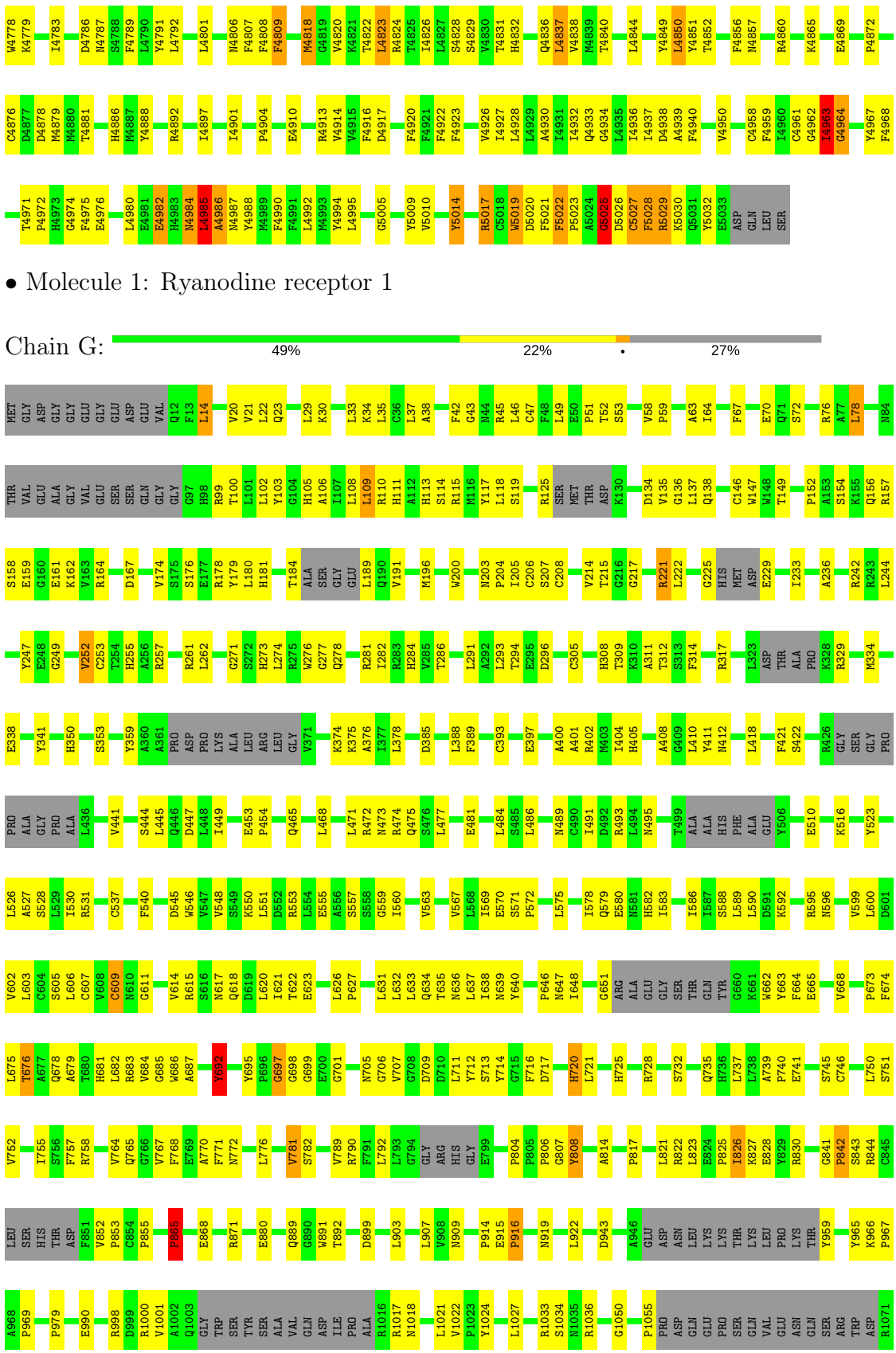
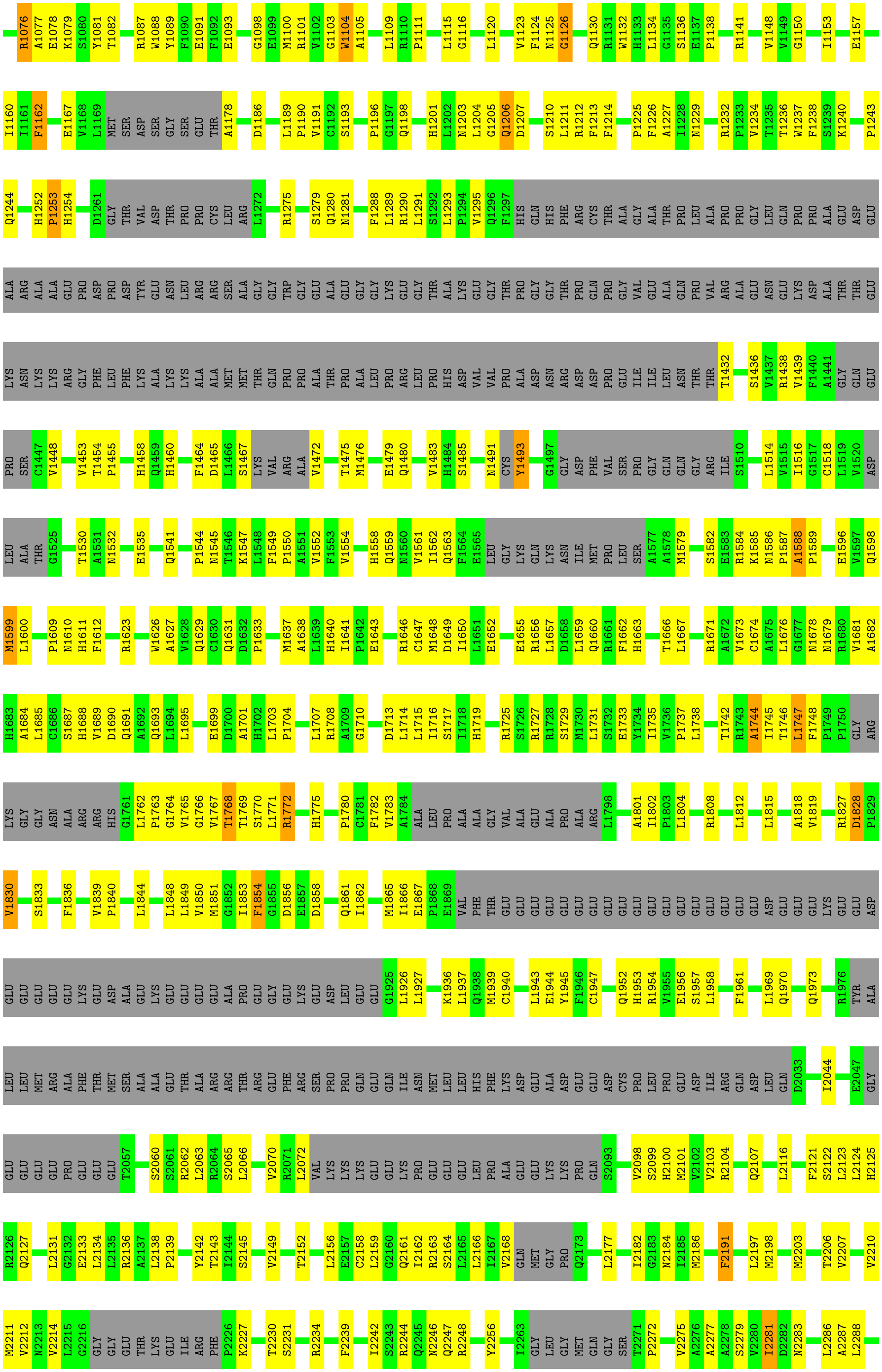
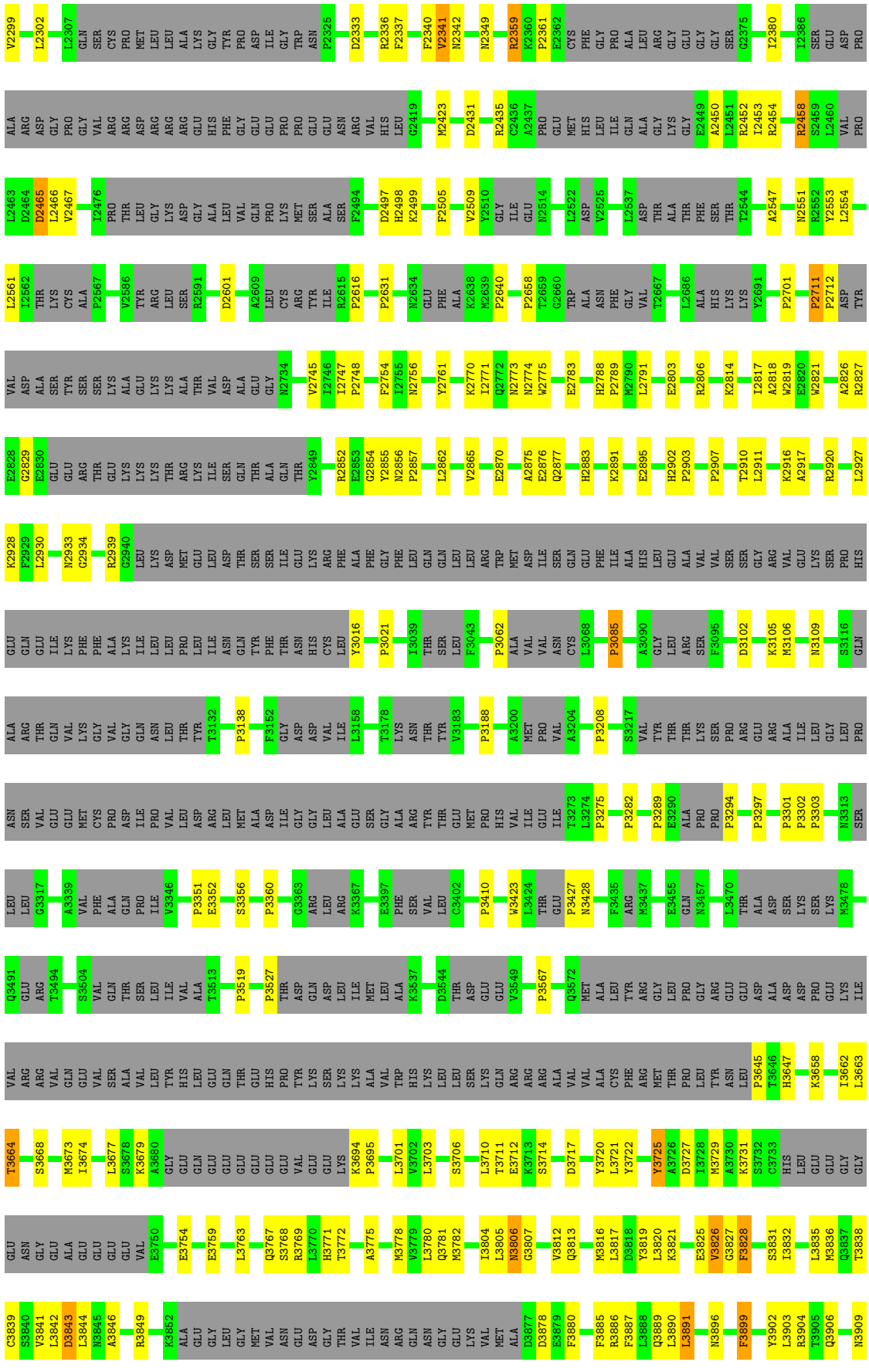
R4734	P4641		PRO	PRO	ALA	ARG		R4159	V4049	G3971	L3890		Y3725	ALA	ALA
E4735	A4642	F4559	GLU	GLY	LYS	SER	I4251		E4050	P3972	L3891	M3816	A3726	CYS	LEU
	L4643		PRO	GLY	LYS	LEU	SER	N4162	S4051	C3973	C3892	L3817	D3727	PHE	TYR
A4738	W4644	I4573	GLU	ALA	VAL	ARG	GLU	F4163	S4052			D3818	I3728	ARG	ARG
E4739	C4645		PRO	GLU	THR	ARG	PRO	L4164	S4053	L3980	H3895	Y3819	M3729	MET	GLY
L4740	L4646	I4576	GLU	GLY	VAL	ARG	GLU	E4165	N4054	A3981		L3820	A3730	THR	LEU
L4741		L4577	PRO	VAL	THR	VAL	GLY	L4166	V4055		F3899	K3821	K3731	PRO	PRO
G4742	L4656	L4578	GLU	VAL	GLU	ARG	GLU	A4167	E4056	L3985			S3732	LEU	GLY
MET	C4657		PRO	ALA	LEU	ARG	PRO		M4057	W3986	Y3902	E3825	C3733	TYR	ARG
ASP	I4658	S4583	GLU	VAL	LEU	LEU	GLU	Y4173	I4058	D3987	L3903	V3826	HIS	ASN	GLU
LEU		ASP	LYS	ALA	ALA	ARG	ALA	F4174	L4059	A3988	R3904	G3827	LEU	LEU	GLU
ALA	Y4661	SER	ALA	ASP	GLY	ARG	ASP	R4175		V3989		F3828	GLU	P3645	ASP
SER	N4662	PRO	ASP	GLY	MET	LEU	GLU	P4176	M4064	V3990	N3909		GLU	T3646	ALA
LEU	C4663	PRO	GLU	GLY	PRO	THR	ASP	Y4177	PHE	G3991		I3832	GLY	H3647	ASP
GLU	L4664	GLY	GLU	PRO	ASP	ALA	GLU	L4178	LEU	F3992	C3918		GLY		ASP
ILE		GLU	ASN	PHE	PRO	ARG	GLY	G4179	LYS	L3993	T3919	M3836	GLU	Y3657	PRO
THR	P4667	ASP	GLY	ARG	THR	GLU	MET	R4180	LEU	H3994	V3920		ASN	K3658	GLU
ALA		ASP	GLU	PRO	SER	ALA	GLY	I4181	LYS	V3995	D3921	C3839	GLY		LYS
HIS	I4670	MET	LYS	GLU	ASP	ALA	GLU	E4182	ASP	F3996	Y3922	S3840	GLU	I3662	ILE
ASN	F4671	GLU	GLU	GLY	GLU	THR	ALA	I4183	I4071	A3997	L3923	V3841	ALA	L3663	VAL
GLU	K4672	GLY	GLU	ALA	VAL	ALA	ALA	M4184		H3998	L3924	L3842	GLU	T3664	ARG
ARG	R4673	SER	VAL	GLY	HIS	LEU	ALA	G4185	A4076	M3999	R3925	D3843	GLU		ARG
LYS	E4674	ALA	PRO	GLY	GLY	ALA	GLU	A4186		M4000	L3926	L3844	GLU	I3674	VAL
PRO	K4675	ALA	GLU	LEU	GLU	ALA	GLY	S4187	D4079	M4001	Q3927		GLU		GLN
ASP	E4676	GLY	ALA	GLY	GLN	LEU	ALA			K4002	E3928	K3852	VAL	L3677	GLU
PRO	L4677	ASP	PRO	ASP	PRO	LEU	GLU	I4190	P4084	L4003	S3929	ALA	E3750	S3678	VAL
PRO		LEU	PRO	MET	ALA	TRP	GLU	E4191		A4004		GLU		K3679	SER
PRO	K4680	ALA	GLU	GLY	GLY	ALA	GLY	R4192	L4087	Q4005	D3932	GLY	E3754	A3680	ALA
GLY		GLY	PRO	ASP	PRO	VAL	ALA		I4088		F3933	LEU		GLY	VAL
LEU	F4683	ALA	PRO	THR	GLY	VAL	ALA	F4195		Q4009	Y3934	GLY	Q3767	GLU	LEU
L4765		GLY	LYS	THR	GLY	ALA	GLY		Q4100		W3935	MET	S3768	GLN	TYR
	L4686	SER	LYS	PRO	ASP	ARG	ALA	W4205	LYS	L4012	Y3936	VAL	R3769	GLU	HIS



- Molecule 1: Ryanodine receptor 1

Chain G: 49% 22% • 27%


R1076 A1077 E1078 K1079 S1080 Y1081 T1082 R1087 W1088 Y1089 F1090 E1091 F1092 E1093 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 L1109 R1110 P1111 L1115 G1116 L1120 V1123 F1124 N1125 G1126 Q1130 R1131 W1132 H1133 L1134 G1135 S1136 E1137 P1138 R1141 V1148 V1149 G1150 I1153 E1157
I1160 I1161 F1162 E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 D1186 L1189 P1190 V1191 C1192 S1193 P1196 G1197 Q1198 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 P1225 F1226 A1227 I1228 N1229 R1232 P1233 V1234 T1235 T1236 W1237 F1238 S1239 K1240 P1243
Q1244 H1252 P1253 H1254 D1261 GLY THR VAL ASP THR PRO PRO CYS LEU ARG L1272 R1275 S1279 Q1280 N1281 F1288 L1289 R1290 L1291 S1292 L1293 P1294 V1295 Q1296 F1297 HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU
ALA ARG 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 PRO 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 LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO GLU ILE ILE LEU ASN THR THR T1432 S1436 V1437 R1438 V1439 F1440 A1441 GLY GLN GLU
PRO SER C1447 V1448 V1453 T1454 P1455 H1458 Q1459 H1460 F1464 D1465 L1466 S1467 LYS VAL ARG ALA V1472 T1475 M1476 E1479 Q1480 V1483 H1484 S1485 N1491 CYS Y1493 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG ILE S1510 L1514 V1515 I1516 G1517 C1518 L1519 V1520 ASP
LEU ALA THR G1525 T1530 A1531 N1532 E1535 Q1541 P1544 N1545 T1546 K1547 L1548 F1549 P1550 A1551 V1552 F1553 V1554 H1558 Q1559 N1560 V1561 I1562 Q1563 F1564 E1565 LEU GLY LYS GLN LYS ASN ILE MET PRO LEU SER A1577 A1578 M1579 S1582 E1583 R1584 K1585 N1586 P1587 A1588 P1589 E1596 V1597 Q1598
M1599 L1600 P1609 N1610 H1611 F1612 R1623 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 L1640 I1641 P1642 E1643 R1646 C1647 M1648 D1649 I1650 L1651 E1652 E1655 R1656 L1657 D1658 L1659 Q1660 R1661 F1662 H1663 T1666 L1667 R1671 A1672 V1673 C1674 A1675 L1676 G1677 N1678 N1679 R1680 V1681 A1682
H1683 A1684 L1685 C1686 S1687 H1688 V1689 D1690 Q1691 A1692 Q1693 L1694 L1695 E1699 D1700 A1701 H1702 L1703 P1704 L1707 R1708 A1709 G1710 D1713 L1714 L1715 I1716 S1717 I1718 H1719 R1725 S1726 R1727 R1728 S1729 M1730 L1731 S1732 E1733 Y1734 I1735 V1736 P1737 L1738 T1742 R1743 A1744 I1745 T1746 L1747 F1748 P1749 P1750 GLY ARG
LYS GLY GLY ASN ALA ARG HIS G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 T1769 S1770 L1771 R1772 H1775 P1780 C1781 F1782 V1783 A1784 ALA LEU PRO ALA ALA GLY VAL ALA GLU ALA PRO ALA ARG L1798 A1801 I1802 P1803 L1804 R1808 L1812 L1815 A1818 V1819 R1827 D1828 P1829
V1830 S1833 F1836 V1839 P1840 L1844 L1848 L1849 V1850 M1851 G1852 I1853 F1854 G1855 D1856 E1857 D1858 Q1861 I1862 M1865 I1866 E1867 P1868 E1869 VAL PHE THR 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 GLU G1925 L1926 L1927 K1936 L1937 Q1938 M1939 C1940 L1943 E1944 Y1945 F1946 C1947 Q1952 H1953 R1954 V1955 E1956 S1957 L1958 F1961 L1969 Q1970 Q1973 R1976 TYR ALA
LEU LEU MET ARG ALA PHE THR MET SER ALA ALA GLU THR ALA ARG ARG THR ARG GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU HIS PHE LYS ASP GLU ALA ASP GLU GLU ASP CYS PRO LEU PRO GLU ASP ILE ARG GLN ASP LEU GLN D2033 I2044 E2047 GLY
GLU GLU GLU GLU PRO GLU GLU GLU T2057 S2060 S2061 R2062 L2063 R2064 S2065 L2066 V2070 R2071 L2072 VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU LYS LYS PRO GLN S2093 V2098 S2099 H2100 M2101 V2102 V2103 R2104 Q2107 L2116 F2121 S2122 L2123 L2124 H2125
R2126 Q2127 L2131 G2132 E2133 L2134 L2135 R2136 A2137 L2138 P2139 Y2142 T2143 I2144 S2145 V2149 T2152 L2156 E2157 C2158 L2159 G2160 Q2161 I2162 R2163 S2164 L2165 L2166 I2167 V2168 GLN MET GLY PRO Q2173 L2177 I2182 G2183 N2184 I2185 M2186 F2191 L2197 M2198 M2203 T2206 V2207 V2210
M2211 V2212 N2213 V2214 L2215 G2216 GLY GLY GLU THR LYS GLU ILE ARG PHE P2226 K2227 T2230 S2231 R2234 F2239 I2242 S2243 R2244 Q2245 N2246 Q2247 R2248 Y2256 I2263 GLY LEU GLY MET GLN GLY SER T2271 P2272 V2275 A2276 A2277 A2278 S2279 V2280 I2281 D2282 N2283 L2286 A2287 L2288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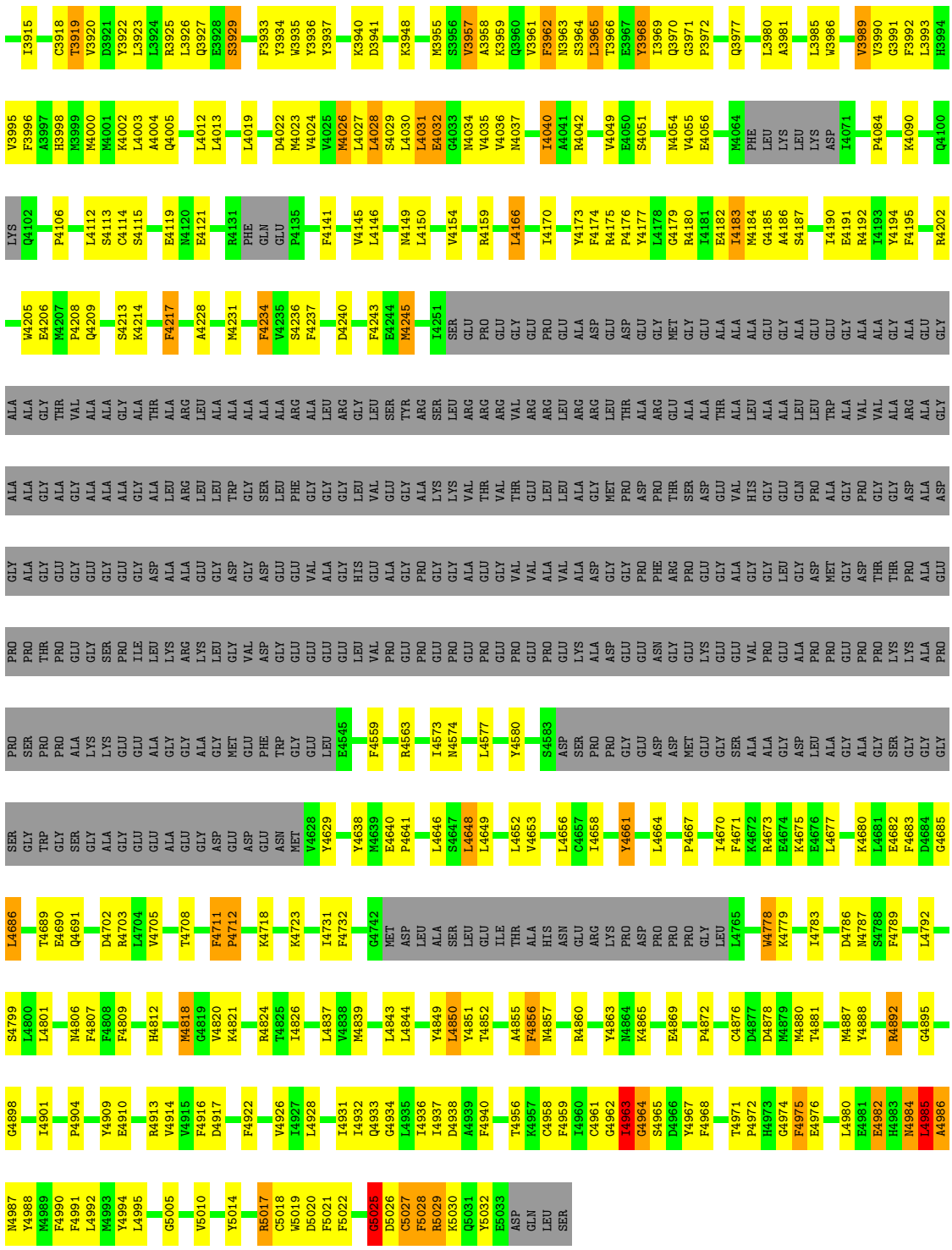
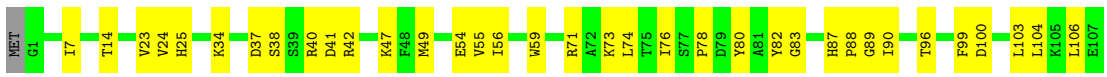
ALA ARG ASP GLY PRO GLY VAL ARG ARG ASP ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU GLU ASN ARG VAL HIS LEU G2419 M2423 D2431 R2435 C2436 A2437 PRO GLU MET HIS LEU ILE GLN ALA GLY LYS GLY E2449 A2450 L2451 R2452 I2453 R2454 R2458 S2459 L2460 VAL PRO
L2463 D2464 D2465 L2466 V2467 I2476 PRO THR LEU GLY LYS ASP GLY ALA LEU VAL GLN PRO LYS MET SER ALA SER F2494 D2497 H2498 K2499 F2505 V2509 Y2510 GLY ILE GLU N2514 L2522 ASP V2525 L2537 ASP THR ALA THR PHE SER THR T2544 A2547 N2551 R2552 Y2553 L2554
L2561 I2562 THR LYS CYS ALA P2567 V2586 TYR ARG LEU SER R2591 D2601 A2609 LEU CYS ARG TYR ILE R2615 P2616 P2631 N2634 GLU PHE ALA K2638 M2639 P2640 P2658 T2659 G2660 TRP ALA ASN PHE GLY VAL T2667 L2686 ALA HIS LYS LYS Y2691 P2701 P2711 P2712 ASP TYR
VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 V2745 I2746 I2747 P2748 F2754 I2755 N2756 Y2761 K2770 I2771 Q2772 N2773 N2774 W2775 E2783 H2788 P2789 M2790 L2791 E2803 R2806 K2814 I2817 A2818 W2819 E2820 W2821 A2826 R2827
E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR Y2849 R2852 E2853 G2854 Y2855 N2856 P2857 L2862 V2865 E2870 A2875 A2876 Q2877 H2883 K2891 E2895 H2902 P2903 P2907 T2910 L2911 K2916 A2917 R2920 L2927
K2928 F2929 L2930 N2933 G2934 R2939 G2940 LEU LYS ASP MET GLU LEU ASP THR SER SER ILE GLU LYS ARG PHE ALA PHE PHE GLY PHE LEU GLN GLN LEU LEU ARG TRP MET ASP ILE SER GLN GLU PHE ILE ALA HIS LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS
GLU GLN GLU ILE LYS PHE PHE ALA LYS ILE LEU LEU PRO LEU ILE ASN GLN TYR PHE THR ASN HIS CYS LEU Y3016 P3021 I3039 THR SER LEU F3043 P3062 ALA VAL VAL ASN CYS L3068 P3085 A3090 GLY LEU ARG SER F3095 D3102 K3105 M3106 N3109 S3116 GLN
ALA ARG THR GLN VAL LYS GLY VAL GLY GLN ASN LEU THR TYR T3132 P3138 F3152 GLY ASP ASP VAL ILE L3158 T3178 LYS ASN THR TYR V3183 P3188 A3200 MET PRO VAL A3204 P3208 S3217 VAL TYR THR THR LYS SER PRO ARG GLU ARG ALA ILE LEU GLY LEU PRO
ASN SER VAL GLU GLU MET CYS PRO ASP ILE PRO VAL LEU ASP ARG LEU MET ALA ASP ILE GLY GLY LEU ALA GLU SER GLY ALA ARG TYR THR GLU MET PRO HIS VAL ILE GLU ILE T3273 L3274 P3275 P3282 P3289 E3290 ALA PRO PRO P3294 P3297 P3301 P3302 P3303 N3313 SER
LEU LEU G3317 A3339 VAL PHE ALA GLN PRO ILE V3346 P3351 E3352 S3356 P3360 G3363 ARG LEU ARG K3367 E3397 PHE SER VAL LEU C3402 P3410 W3423 L3424 THR GLU F3435 ARG M3437 E3455 GLN N3457 L3470 THR ALA ASP SER LYS SER LYS M3478
Q3491 GLU ARG T3494 S3504 VAL GLN THR SER LEU ILE VAL ALA T3513 P3519 P3527 THR ASP GLN ASP LEU ILE MET LEU ALA K3537 D3544 THR ASP GLU GLU V3549 P3567 Q3572 MET ALA LEU TYR ARG GLY LEU PRO GLY ARG GLU GLU ASP ASP ALA ASP ASP PRO GLU LYS ILE
VAL ARG ARG VAL GLN GLU VAL SER ALA VAL LEU TYR HIS LEU GLU GLN THR GLU HIS PRO TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET THR PRO LEU TYR ASN LEU P3645 T3646 H3647 K3658 I3662 L3663
T3664 S3668 M3673 I3674 L3677 S3678 K3679 A3680 GLY GLU GLN GLU GLU GLU GLU GLU VAL GLU GLU LYS K3694 P3695 L3701 V3702 L3703 S3706 L3710 T3711 E3712 K3713 S3714 D3717 Y3720 L3721 Y3722 Y3725 A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733 HIS LEU GLU GLY GLY
GLU ASN GLY GLU ALA GLU GLU GLU VAL E3750 E3754 E3759 L3763 Q3767 S3768 R3769 L3770 H3771 T3772 A3775 M3778 V3779 L3780 Q3781 M3782 I3804 L3805 N3806 G3807 V3812 Q3813 M3816 L3817 D3818 Y3819 L3820 K3821 E3825 V3826 G3827 F3828 S3831 I3832 L3835 M3836 Q3837 T3838
C3839 S3840 V3841 L3842 D3843 L3844 N3845 A3846 R3849 K3852 ALA GLU GLY LEU GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY GLU LYS VAL MET ALA D3877 D3878 E3879 F3880 F3885 R3886 F3887 L3888 Q3889 L3890 L3891 N3896 F3899 Y3902 L3903 R3904 T3905 Q3906 N3909



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

Chain B: 67% 32%



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

Chain D: 65% 34%

MET G1 T6 I7 T14 V23 V24 H25 K34 D37 S38 S39 R40 D41 R42 K47 F48 M49 E54 V55 I56 W59 Q70 R71 A72 K73 L74 T75 I76 S77 P78 D79 Y80 A81 Y82 G83 H87 P88 G89 I90 T96 F99 D100 L103 L104 K105 L106

E107

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

Chain F: 68% 31%

MET G1 I7 T14 V23 V24 H25 K34 D37 S38 S39 R40 D41 R42 K47 E54 V55 I56 W59 R71 A72 K73 L74 T75 I76 S77 P78 D79 Y80 A81 Y82 G83 H87 P88 G89 I90 T96 F99 D100 L103 L104 K105 L106 E107

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

Chain H: 69% 30%

MET G1 V2 D11 T14 V23 V24 H25 D37 S38 S39 R40 D41 R42 F46 K47 V55 I56 W59 S67 V68 G69 Q70 R71 I76 Y82 H87 P88 G89 I90 F99 D100 V101 E102 L103 L104 K105 L106 E107

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	64000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.98	87/27385 (0.3%)	0.88	108/37104 (0.3%)
1	C	0.98	89/27385 (0.3%)	0.88	114/37104 (0.3%)
1	E	0.98	87/27385 (0.3%)	0.88	108/37104 (0.3%)
1	G	0.99	94/27385 (0.3%)	0.88	112/37104 (0.3%)
2	B	0.63	0/851	0.63	0/1146
2	D	0.63	0/851	0.63	0/1146
2	F	0.63	0/851	0.63	0/1146
2	H	0.63	0/851	0.62	0/1146
All	All	0.98	357/112944 (0.3%)	0.88	442/153000 (0.3%)

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	20
1	C	0	20
1	E	0	20
1	G	0	20
All	All	0	80

The worst 5 of 357 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4988	TYR	CG-CD2	-20.55	1.12	1.39
1	E	4988	TYR	CG-CD2	-19.42	1.14	1.39
1	C	4988	TYR	CG-CD2	-19.41	1.14	1.39
1	A	4988	TYR	CG-CD2	-19.37	1.14	1.39
1	G	4988	TYR	CE1-CZ	-17.94	1.15	1.38

The worst 5 of 442 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	5029	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	E	5029	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	E	4988	TYR	CB-CG-CD1	10.56	127.34	121.00
1	A	4988	TYR	CB-CG-CD1	10.55	127.33	121.00
1	C	4988	TYR	CB-CG-CD1	10.53	127.32	121.00

There are no chirality outliers.

5 of 80 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1464	PHE	Mainchain,Peptide
1	A	1465	ASP	Peptide
1	A	697	GLY	Mainchain,Peptide
1	A	807	GLY	Mainchain,Peptide
1	A	841	GLY	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26917	0	24461	801	0
1	C	26917	0	24461	789	0
1	E	26917	0	24461	787	0
1	G	26917	0	24461	770	0
2	B	832	0	831	34	0
2	D	832	0	831	35	0
2	F	832	0	831	33	0
2	H	832	0	831	28	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	111000	0	101168	3132	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 15.

The worst 5 of 3132 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1782:PHE:O	2:H:82:TYR:OH	1.75	1.03
1:A:1782:PHE:O	2:B:82:TYR:OH	1.76	1.03
1:A:4888:TYR:CD1	1:G:4914:VAL:HG23	1.95	1.02
1:C:1782:PHE:O	2:D:82:TYR:OH	1.78	1.01
1:E:1782:PHE:O	2:F:82:TYR:OH	1.77	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3496/5037 (69%)	3185 (91%)	227 (6%)	84 (2%)	7	45
1	C	3496/5037 (69%)	3185 (91%)	228 (6%)	83 (2%)	7	45
1	E	3496/5037 (69%)	3187 (91%)	226 (6%)	83 (2%)	7	45
1	G	3496/5037 (69%)	3192 (91%)	217 (6%)	87 (2%)	6	44
2	B	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	D	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
All	All	14404/20580 (70%)	13130 (91%)	937 (6%)	337 (2%)	11	46

5 of 337 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	GLY
1	A	915	GLU
1	A	916	PRO

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Mol	Chain	Res	Type
1	A	969	PRO
1	A	1589	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	2503/4276 (58%)	2493 (100%)	10 (0%)	93	96
1	C	2502/4276 (58%)	2492 (100%)	10 (0%)	93	96
1	E	2500/4276 (58%)	2491 (100%)	9 (0%)	93	96
1	G	2501/4276 (58%)	2489 (100%)	12 (0%)	91	96
2	B	89/90 (99%)	88 (99%)	1 (1%)	78	89
2	D	89/90 (99%)	88 (99%)	1 (1%)	78	89
2	F	89/90 (99%)	88 (99%)	1 (1%)	78	89
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10362/17464 (59%)	10318 (100%)	44 (0%)	93	96

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4850	LEU
1	E	914	PRO
1	G	4106	PRO
1	C	4972	PRO
1	E	806	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 208 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4223	ASN
1	E	596	ASN
1	G	3906	GLN

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Mol	Chain	Res	Type
1	C	4803	HIS
1	E	105	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.