wwPDB EM Map/Model Validation Report (i)

Sep 14, 2016 – 11:39 AM EDT

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

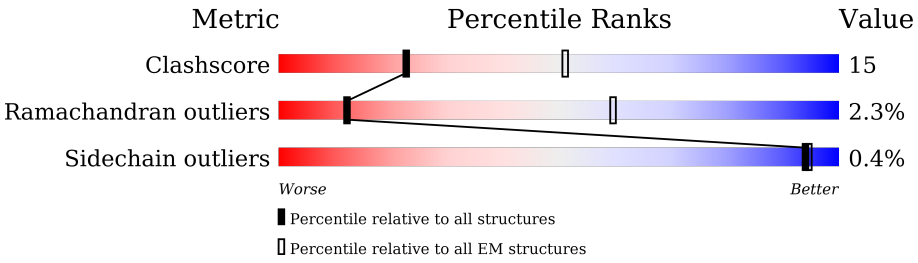
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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

Mol	Chain	Length	Quality of chain
1	A	5037	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

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

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

- Molecule 1 is a protein called Ryanodine receptor 1.

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

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

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

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

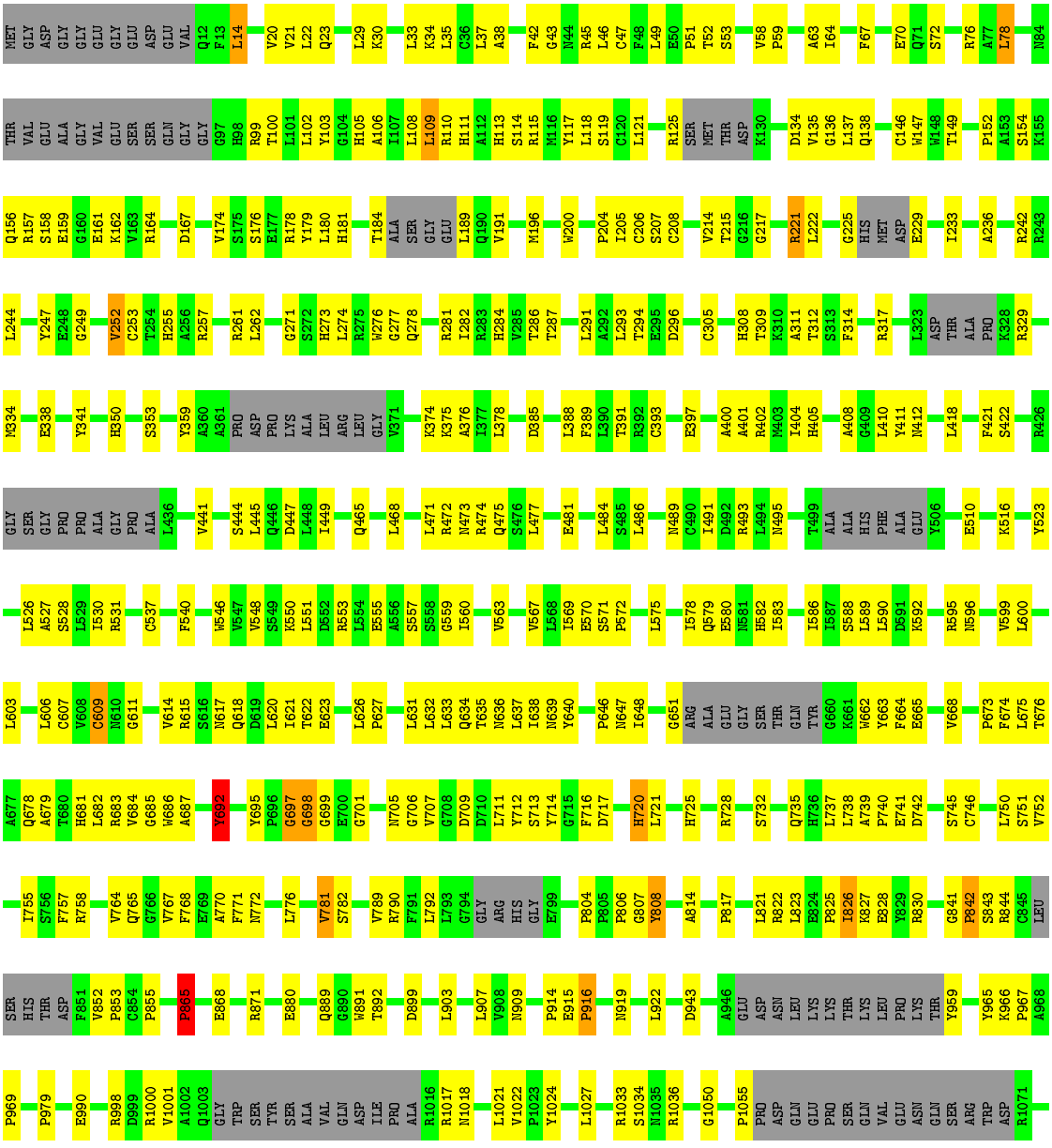
Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total 1	Zn 1	0
3	A	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	E	1	Total 1	Zn 1	0

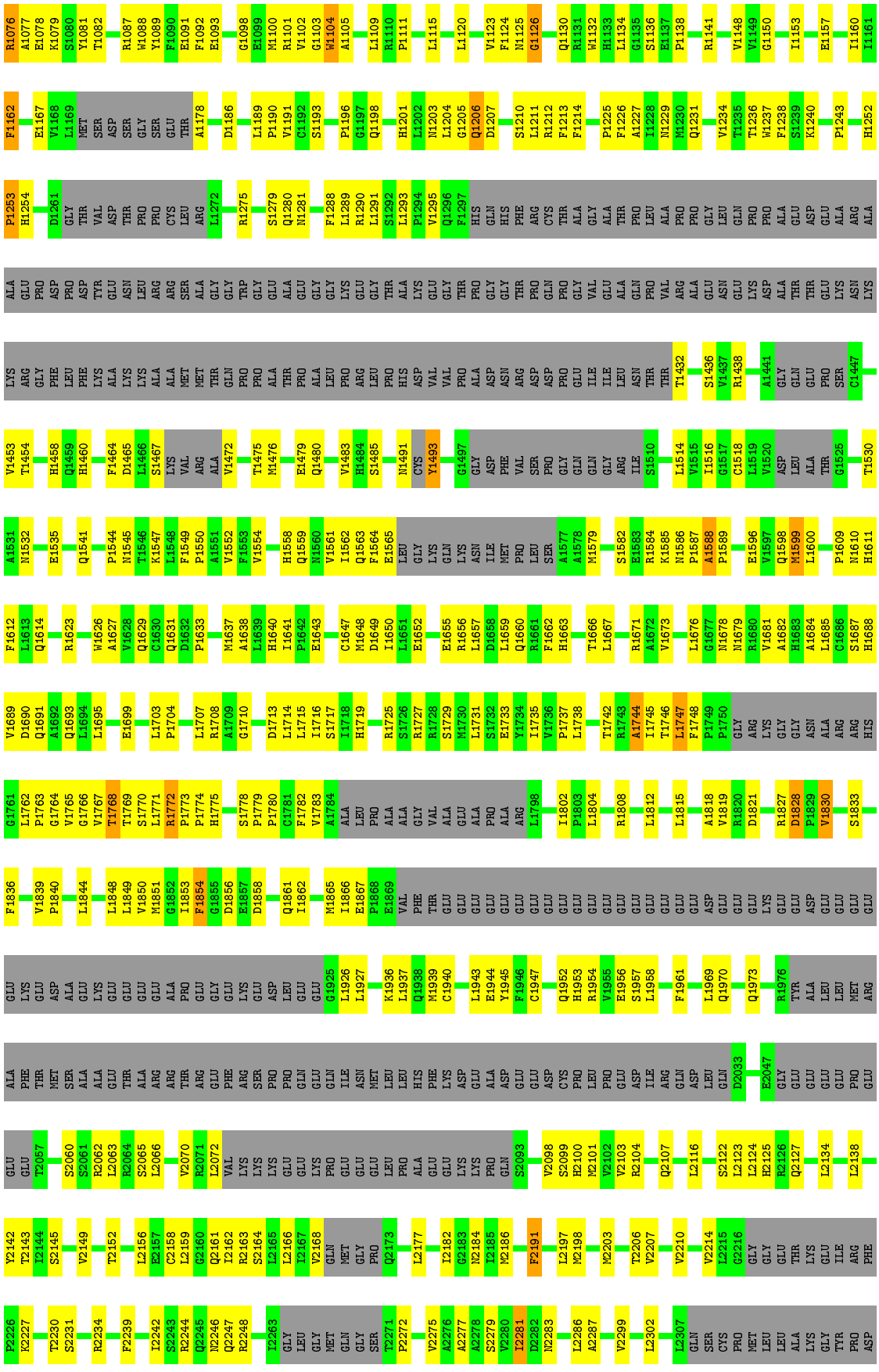
3 Residue-property plots (i)

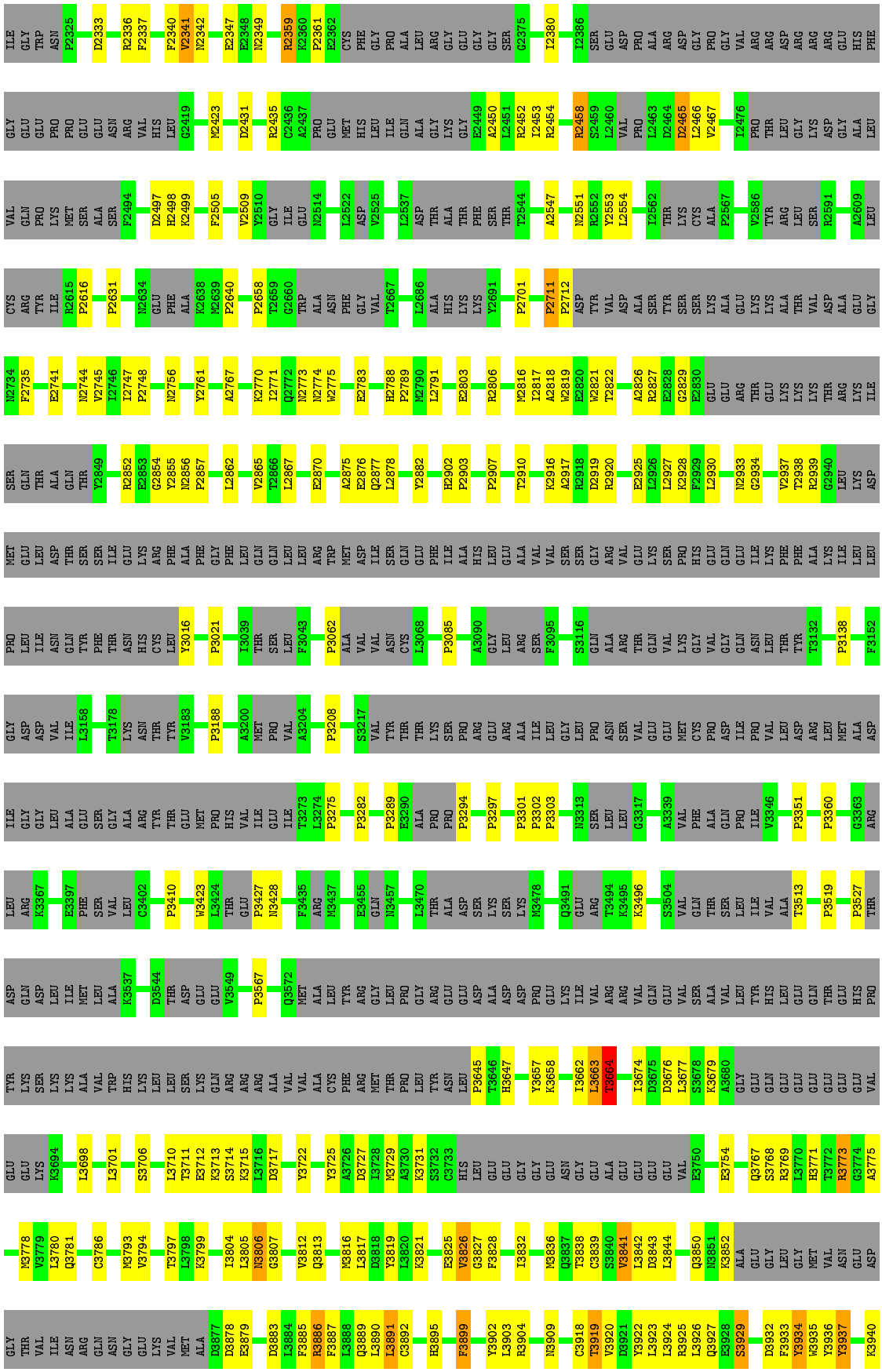
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

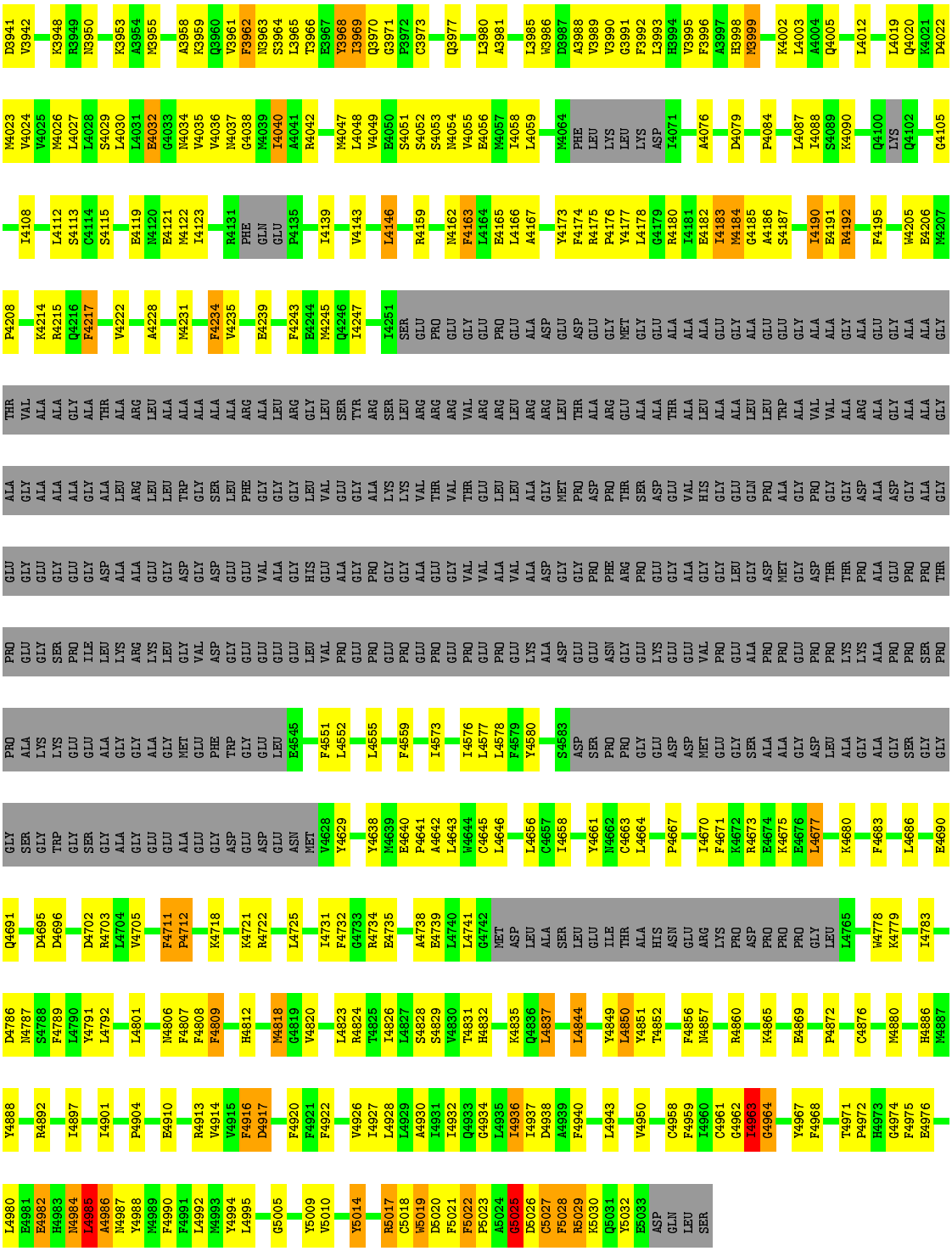
- Molecule 1: Ryanodine receptor 1

Chain A:



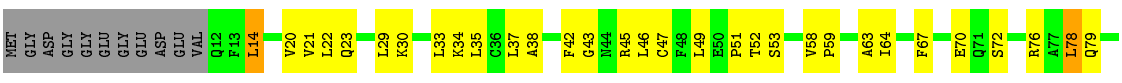


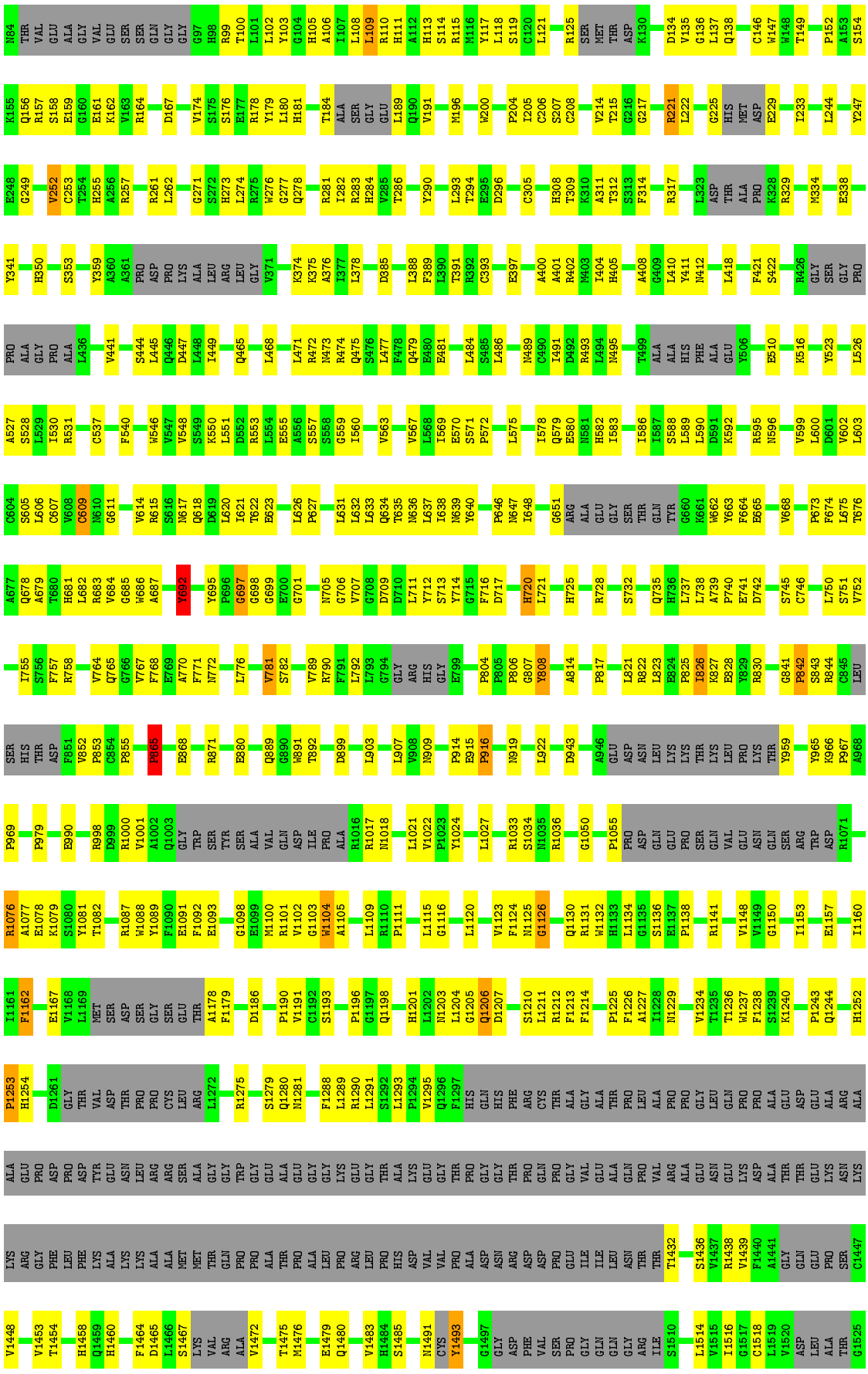


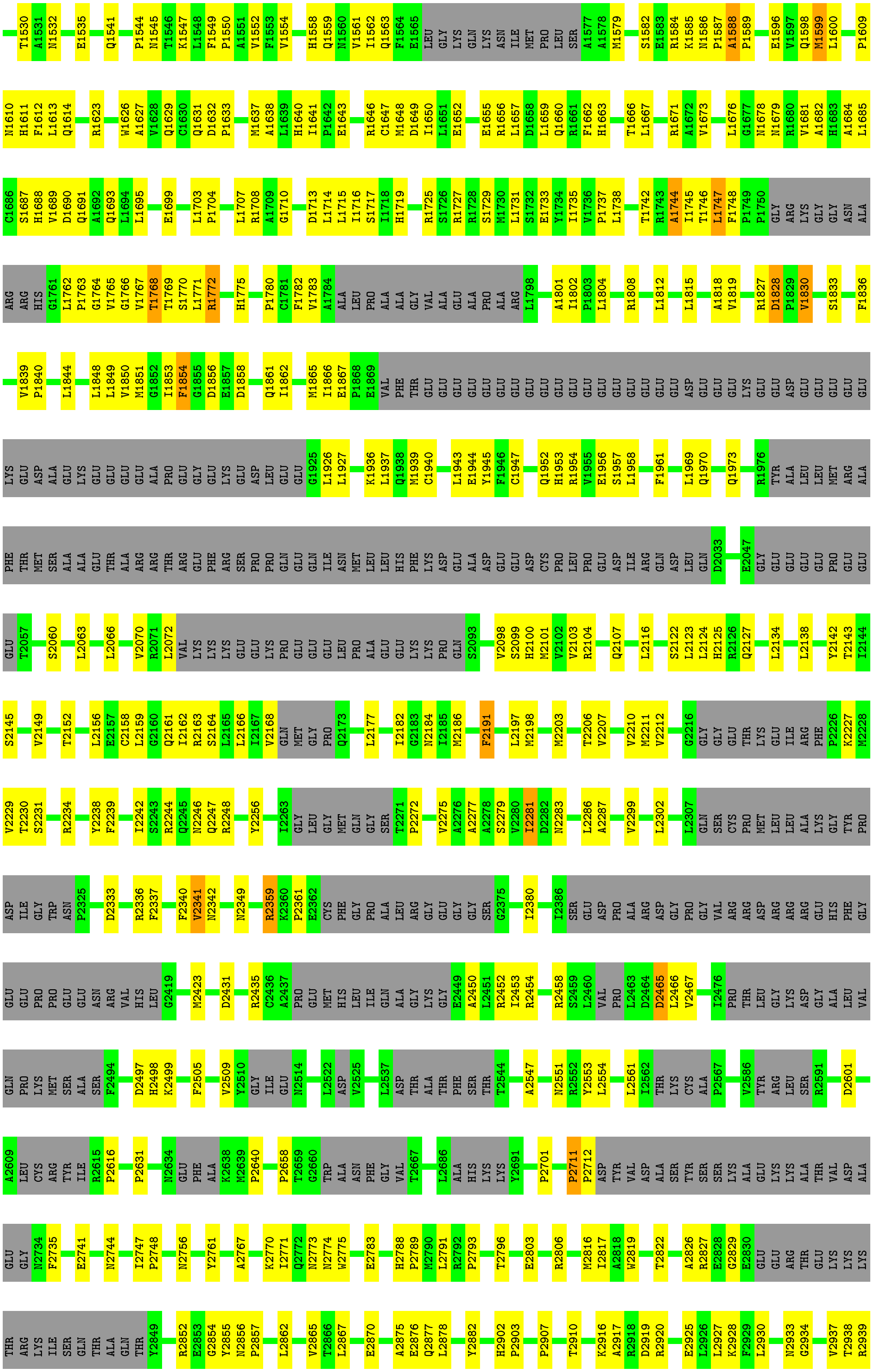


- Molecule 1: Ryanodine receptor 1

Chain C:



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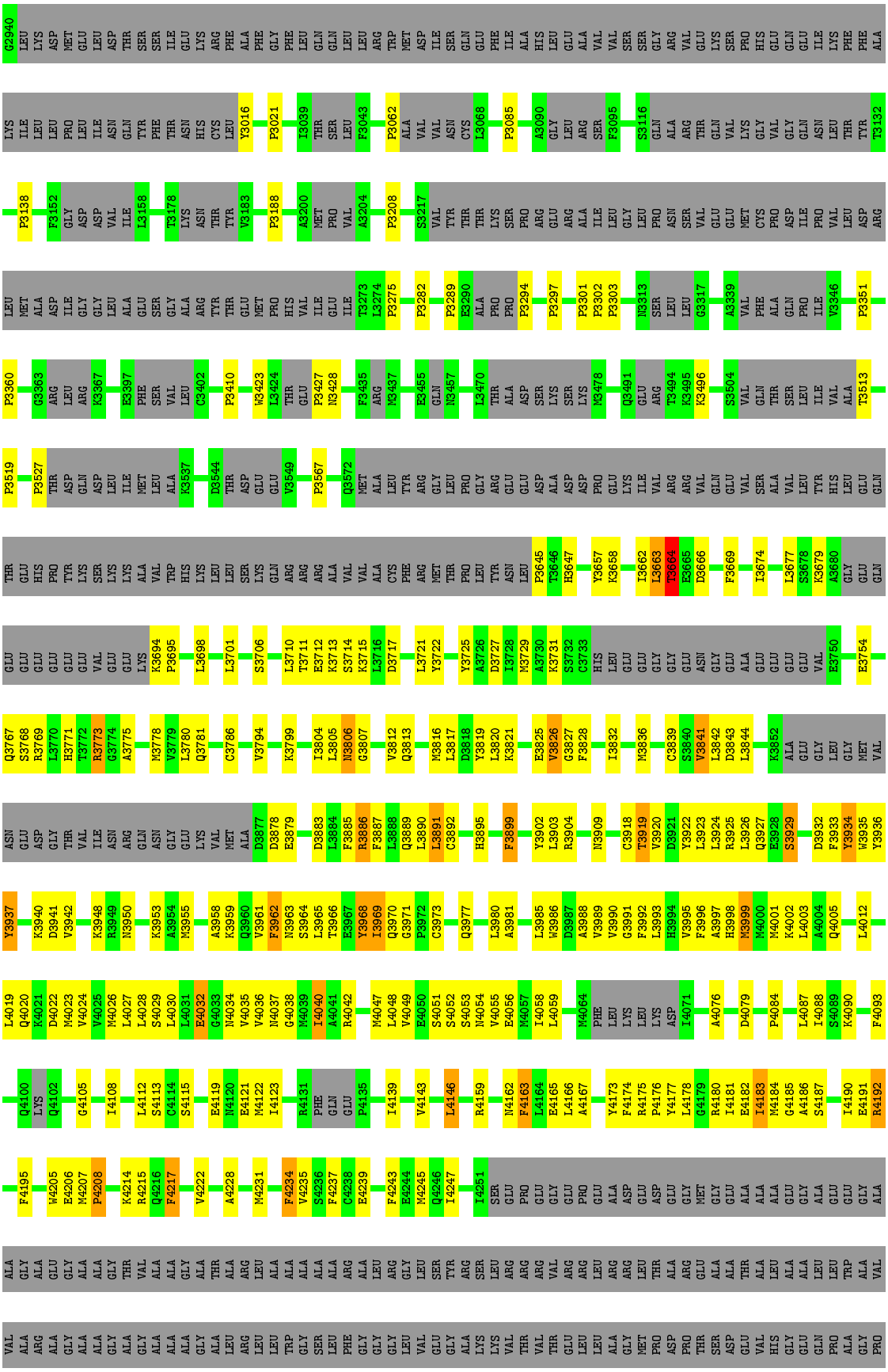
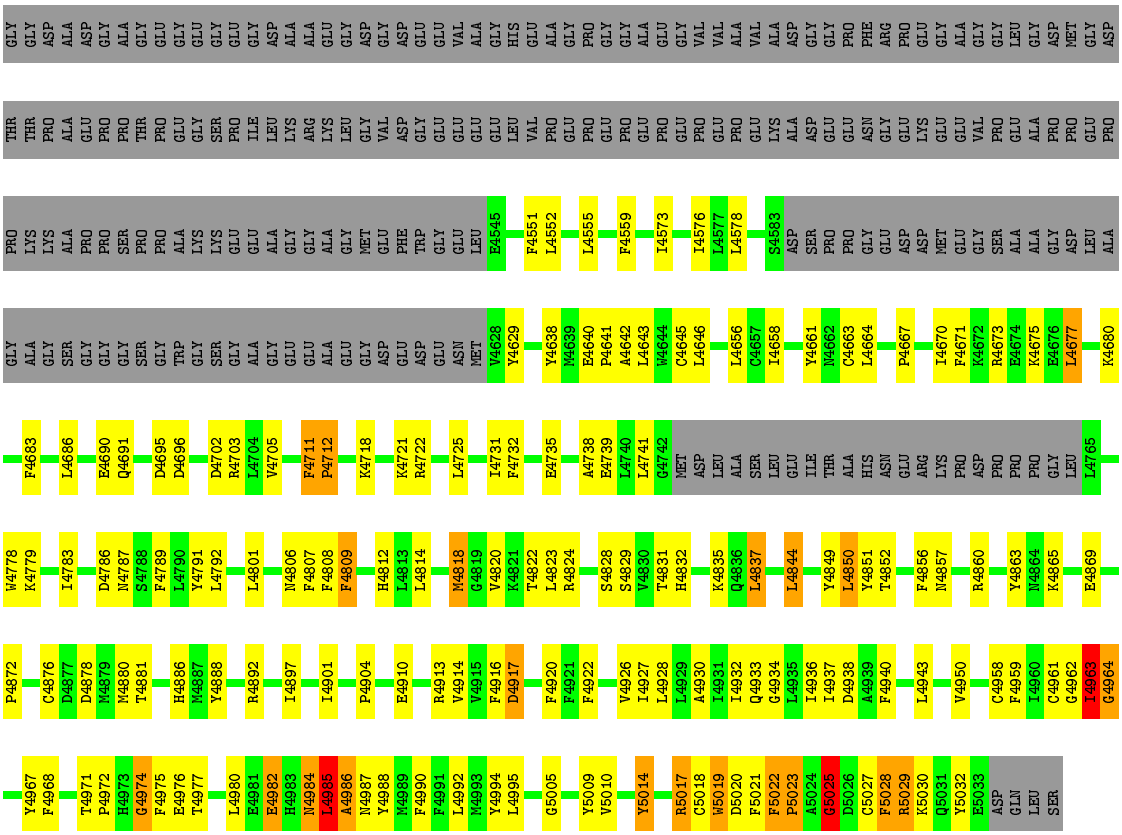
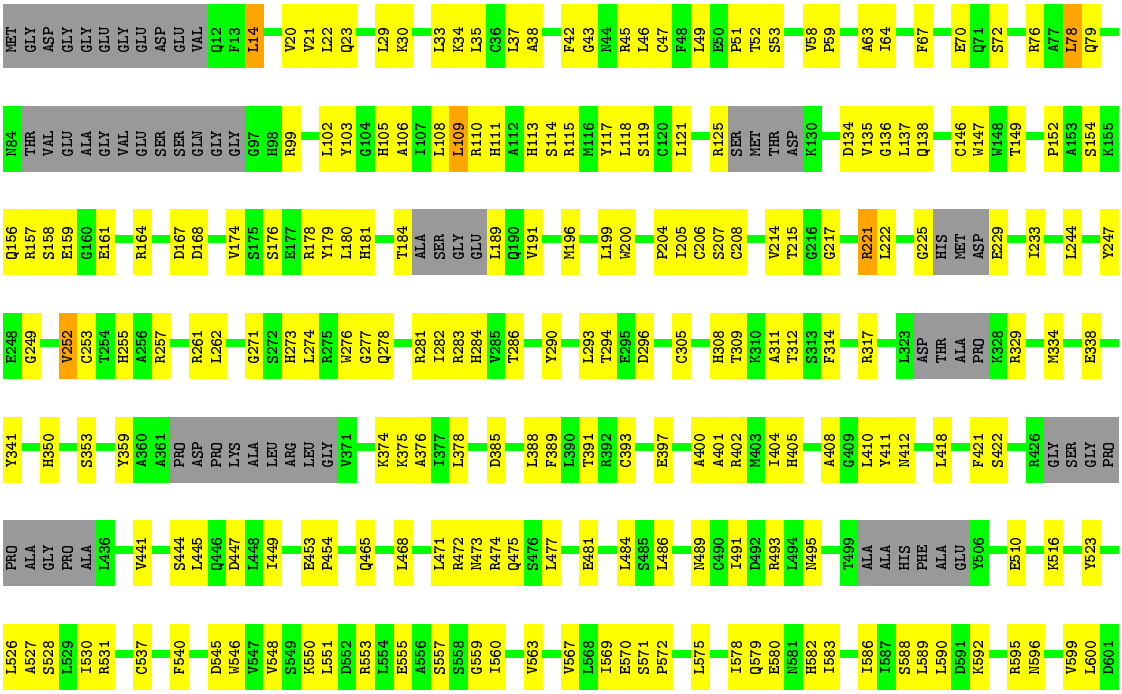
N1610 H1611 F1612 L1613 Q1614 R1623 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 M1637 A1638 L1639 H1640 I1641 P1642 E1643 R1646 C1647 M1648 D1649 I1650 L1651 E1652 E1655 R1656 L1657 D1658 L1659 Q1660 R1661 F1662 H1663 T1666 L1667 R1671 A1672 V1673 L1676 G1677 N1678 N1679 R1680 V1681 A1682 H1683 A1684 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
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 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

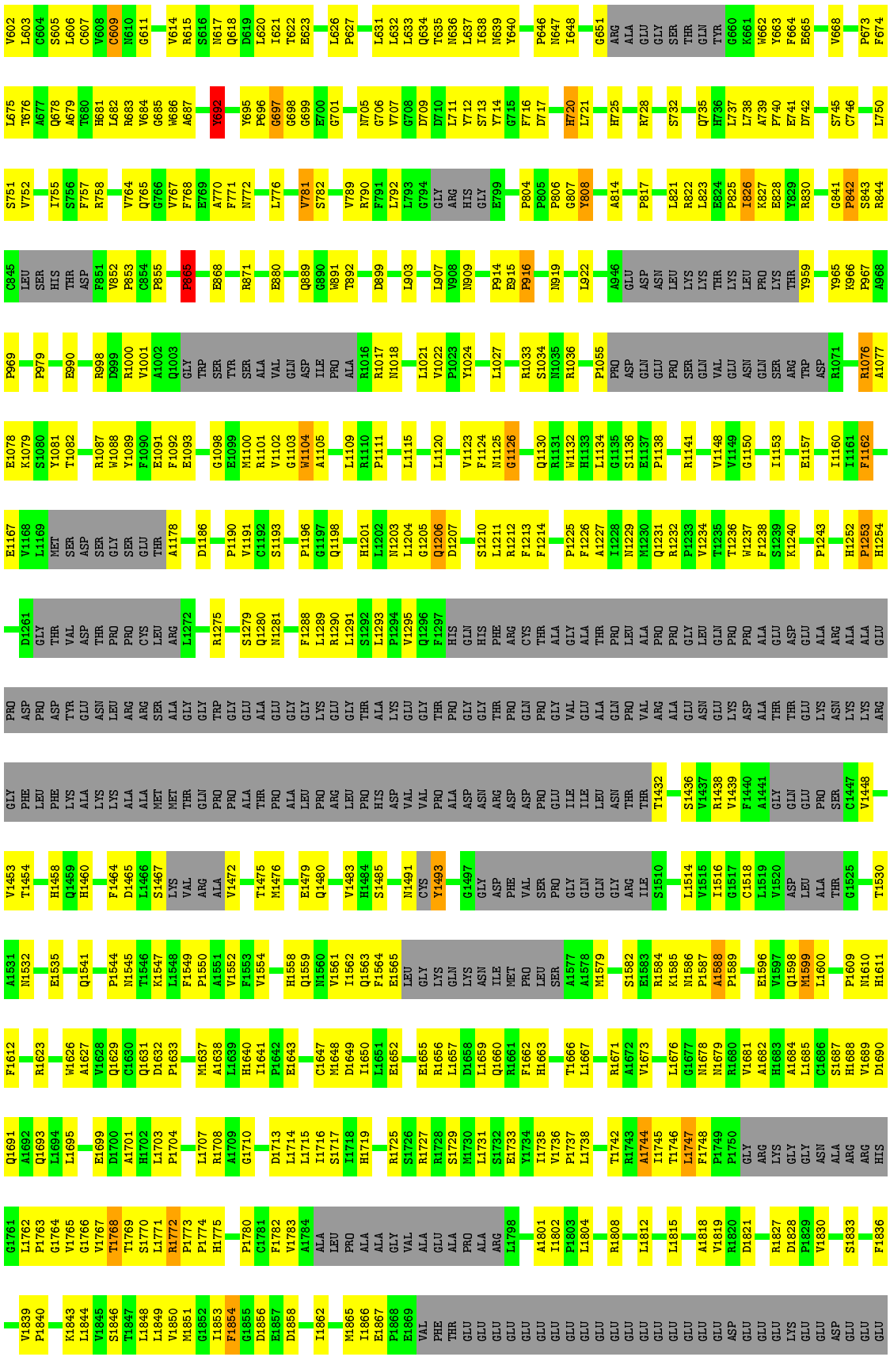


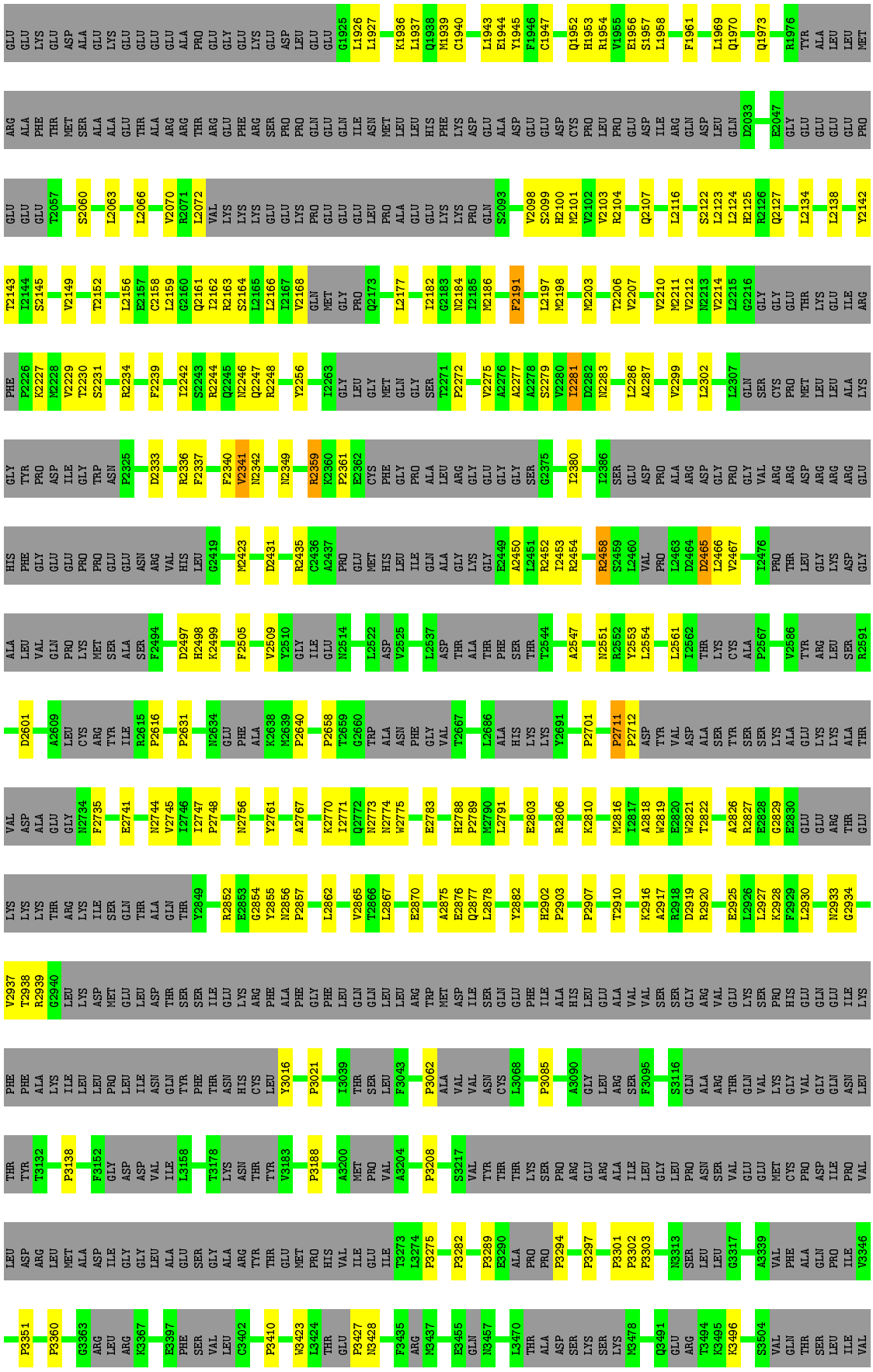


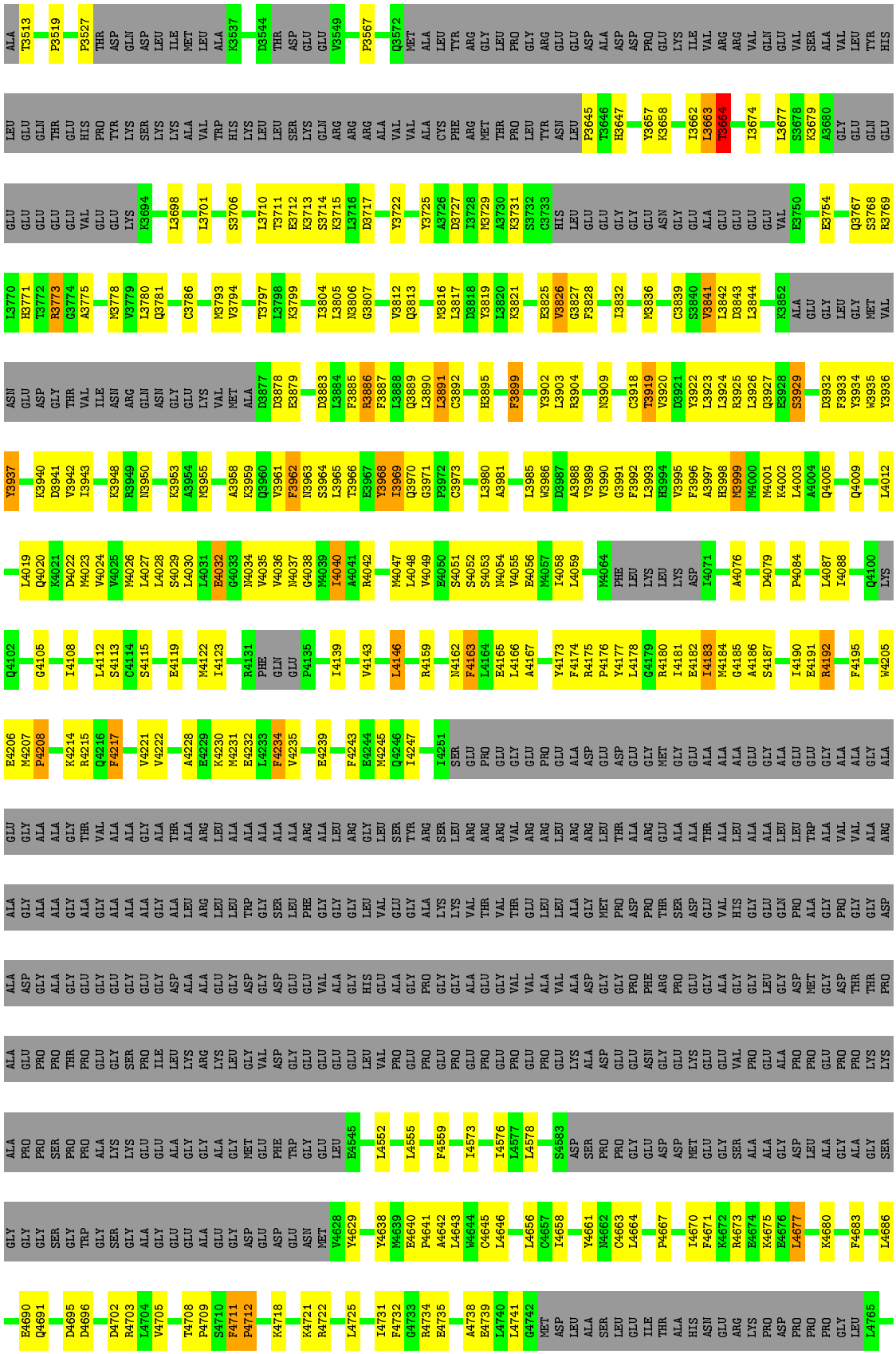
• Molecule 1: Ryanodine receptor 1

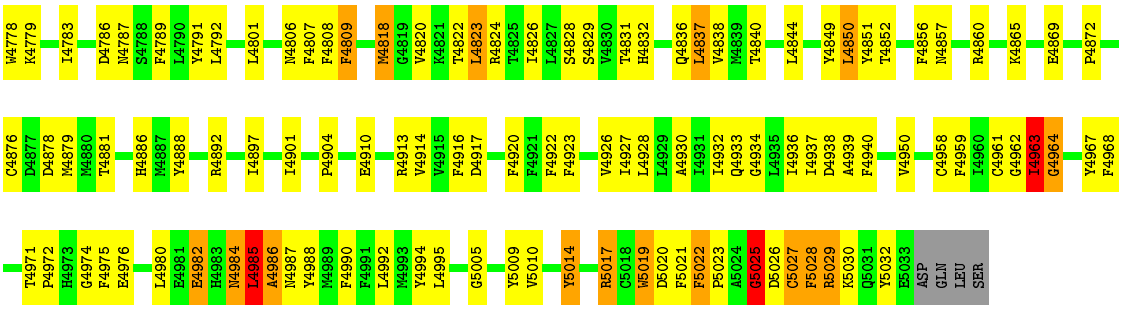
Chain E:

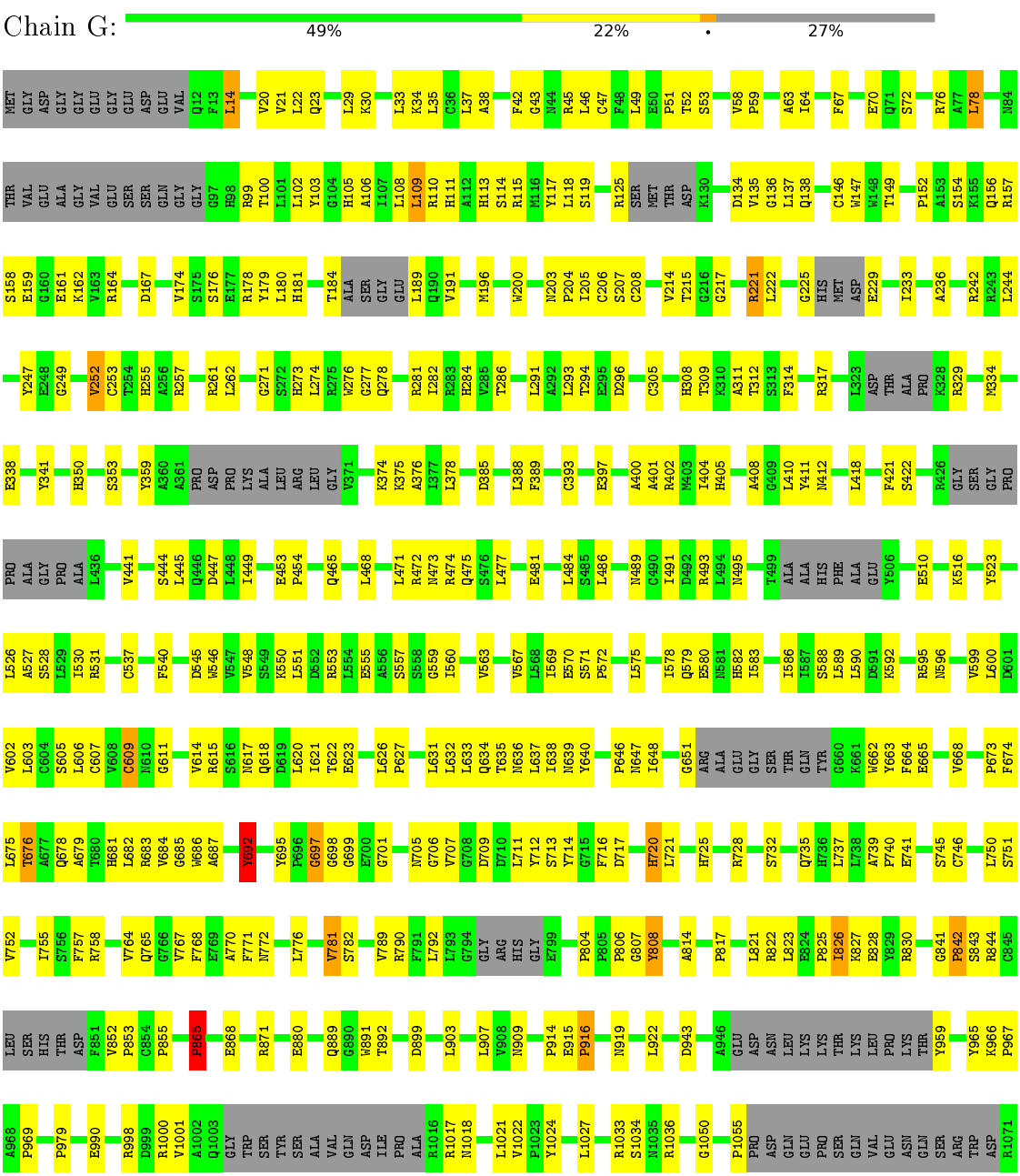






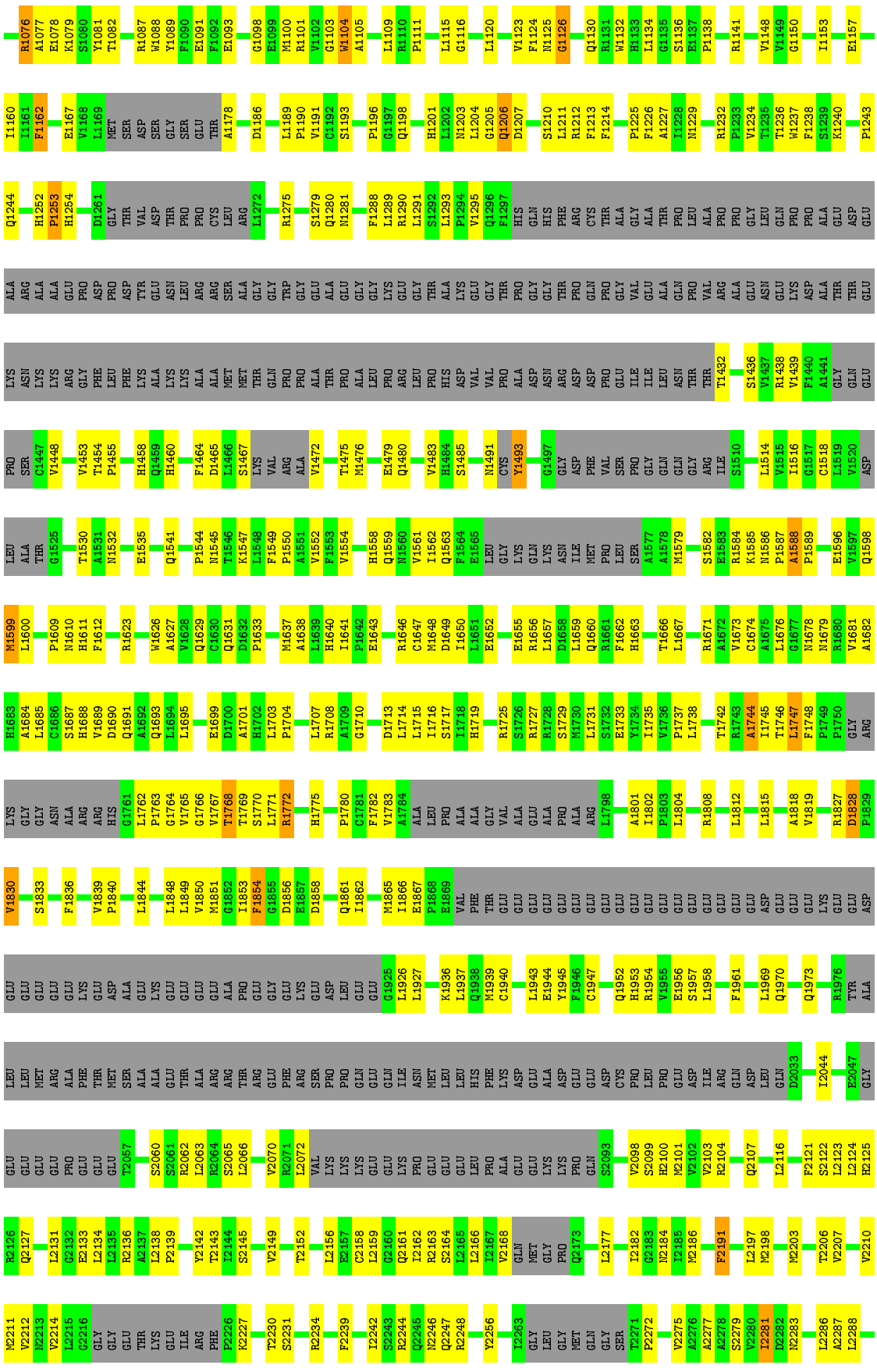






- Molecule 1: Ryanodine receptor 1

Chain G: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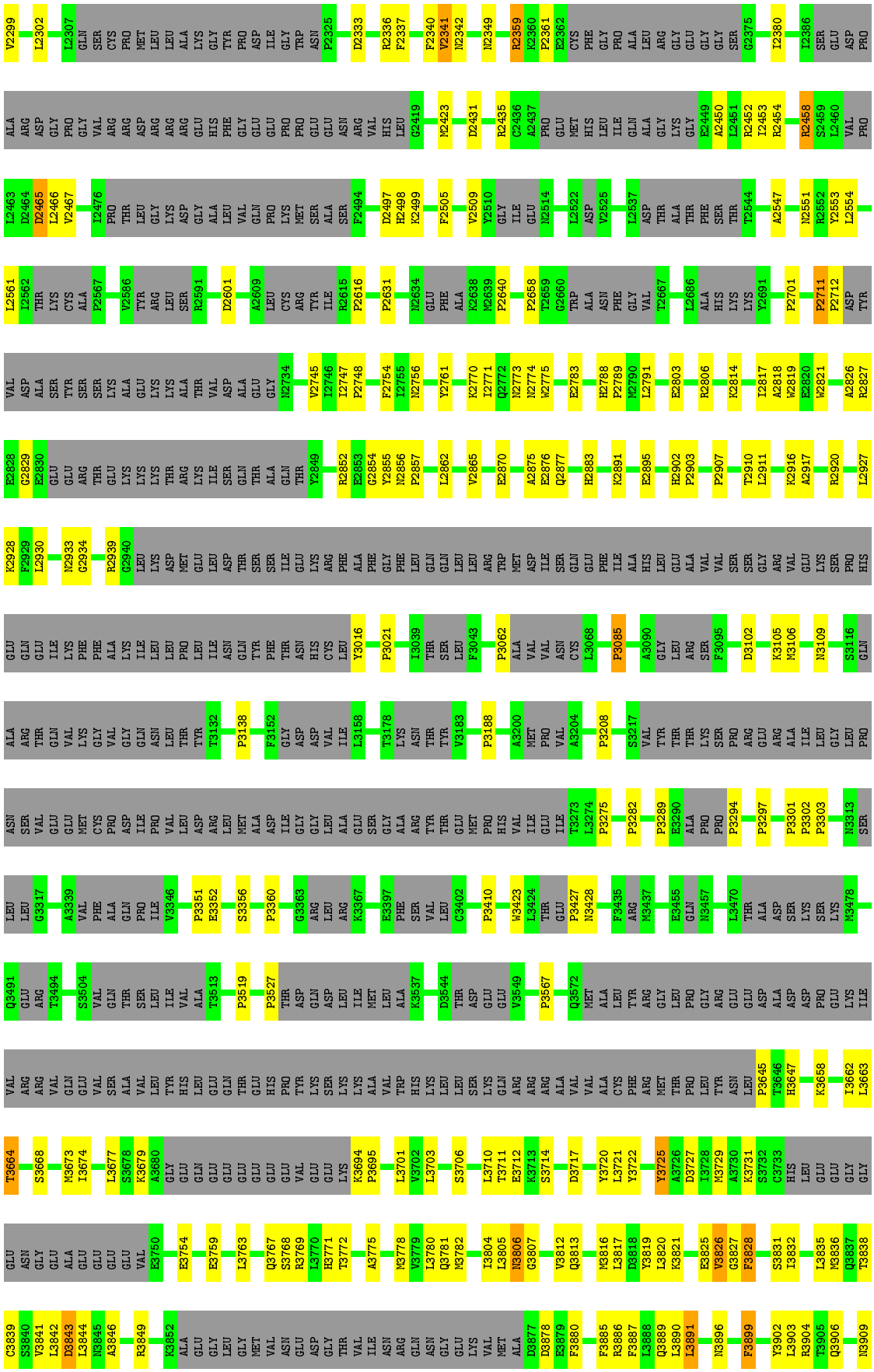
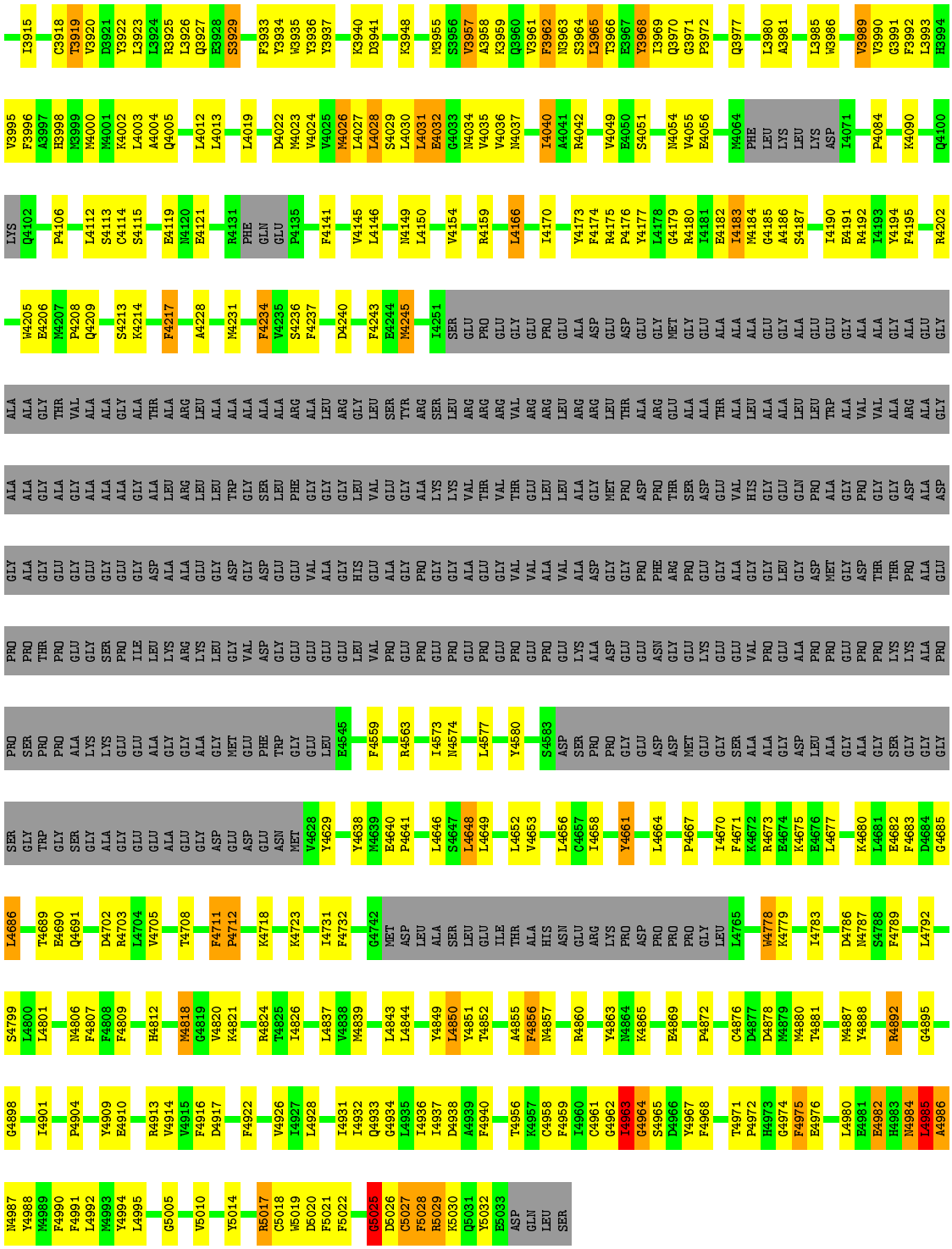
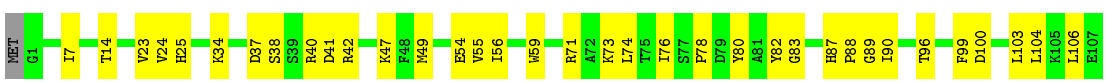
I1160 I1161 F1162 E1167 V1168 L1169 MET SER ASP SER GLY SER GLU THR A1178 D1186 L1189 P1190 V1191 C1192 S1193 P1196 G1197 Q1198 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 P1225 F1226 A1227 I1228 N1229 R1232 P1233 V1234 T1235 T1236 W1237 F1238 S1239 K1240 P1243
Q1244 H1252 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 ALA GLU ASP GLU
ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA 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 GLU
LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO LYS HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP PRO GLU ILE ILE LEU ALA GLN 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 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 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 H1709 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 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





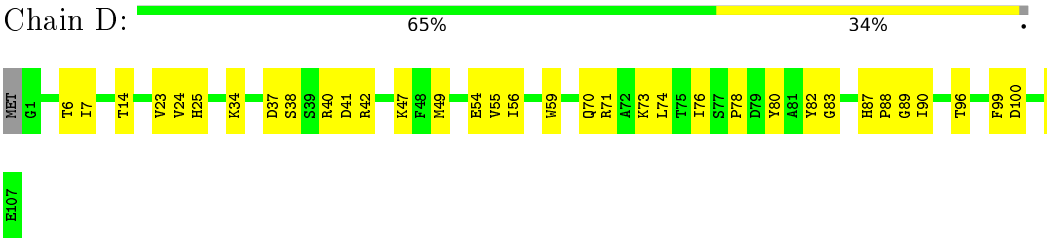
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain B:



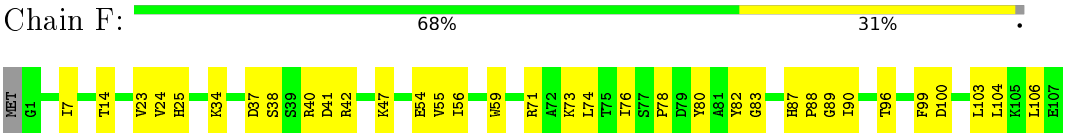
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain D:



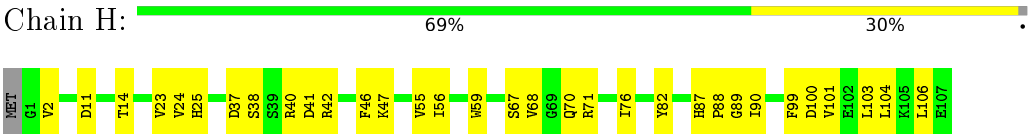
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	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 ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.98	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 50
1	C	3496/5037 (69%)	3185 (91%)	228 (6%)	83 (2%)	7 50
1	E	3496/5037 (69%)	3187 (91%)	226 (6%)	83 (2%)	7 50
1	G	3496/5037 (69%)	3192 (91%)	217 (6%)	87 (2%)	7 49
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%)	12 51

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	97
1	C	2502/4276 (58%)	2492 (100%)	10 (0%)	93	97
1	E	2500/4276 (58%)	2491 (100%)	9 (0%)	93	97
1	G	2501/4276 (58%)	2489 (100%)	12 (0%)	92	96
2	B	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	D	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	F	89/90 (99%)	88 (99%)	1 (1%)	80	91
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	10362/17464 (59%)	10318 (100%)	44 (0%)	94	97

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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.