wwPDB EM Validation Summary Report (i)

Mar 19, 2024 – 10:15 PM JST

PDB ID	:	6JIU
EMDB ID	:	EMD-9836
Title	:	Structure of RyR2 (F/A/C/L-Ca2+/Ca2+CaM dataset)
Authors	:	Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on	:	2019-02-23
Resolution	:	4.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

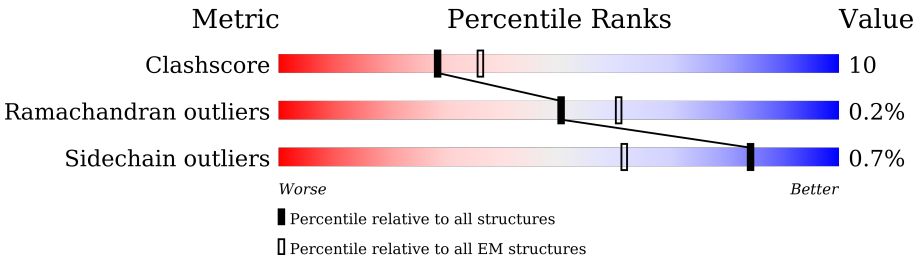
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	A	4968	6% 54% 16% 30%
1	D	4968	6% 54% 16% 30%
1	G	4968	6% 54% 16% 30%
1	J	4968	6% 54% 16% 30%
2	B	108	79% 19% ••
2	E	108	79% 19% ••
2	H	108	80% 19% ••
2	K	108	80% 19% ••

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Mol	Chain	Length	Quality of chain
3	C	149	42% 38% 7% 54%
3	F	149	42% 39% 7% 54%
3	I	149	42% 39% 7% 54%
3	L	149	42% 39% 7% 54%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 112212 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3496	26661	16986	4571	4947	157	0	0
1	D	3496	26661	16986	4571	4947	157	0	0
1	G	3496	26661	16986	4571	4947	157	0	0
1	J	3496	26661	16986	4571	4947	157	0	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	107	819	516	144	155	4	0	0
2	E	107	819	516	144	155	4	0	0
2	H	107	819	516	144	155	4	0	0
2	K	107	819	516	144	155	4	0	0

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	68	524	326	83	110	5	0	0
3	F	68	524	326	83	110	5	0	0
3	I	68	524	326	83	110	5	0	0
3	L	68	524	326	83	110	5	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

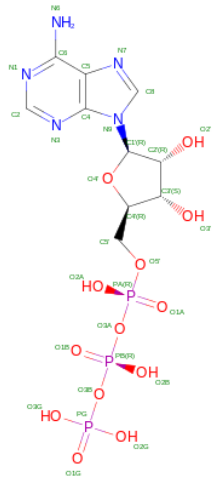
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	A	1	1	1	0
4	D	1	1	1	0
4	G	1	1	1	0
4	J	1	1	1	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	A	1	1	1	0
5	C	2	2	2	0
5	D	1	1	1	0
5	F	2	2	2	0
5	G	1	1	1	0
5	I	2	2	2	0
5	J	1	1	1	0
5	L	2	2	2	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

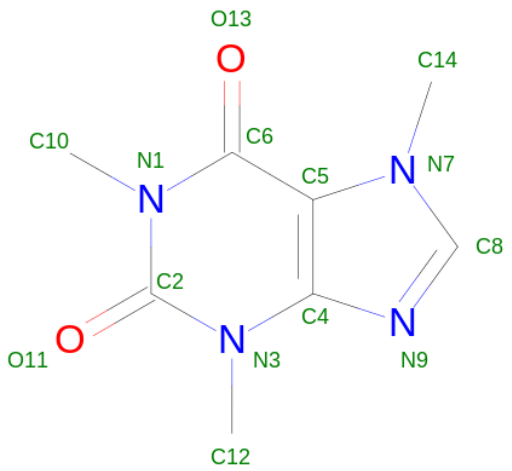
ATP



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).

CFF



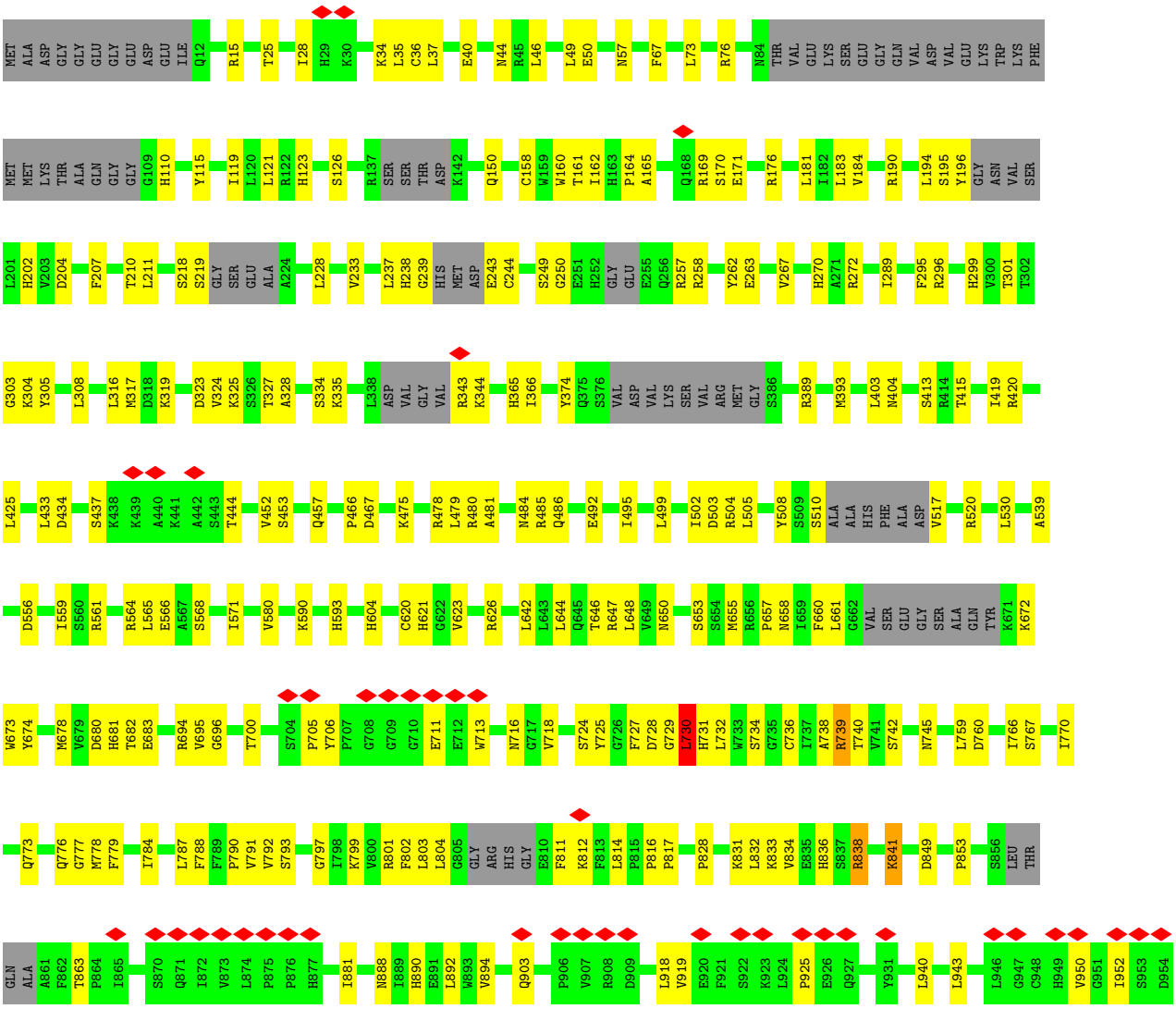
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	14	8	4	2	0
7	D	1	14	8	4	2	0
7	G	1	14	8	4	2	0
7	J	1	14	8	4	2	0

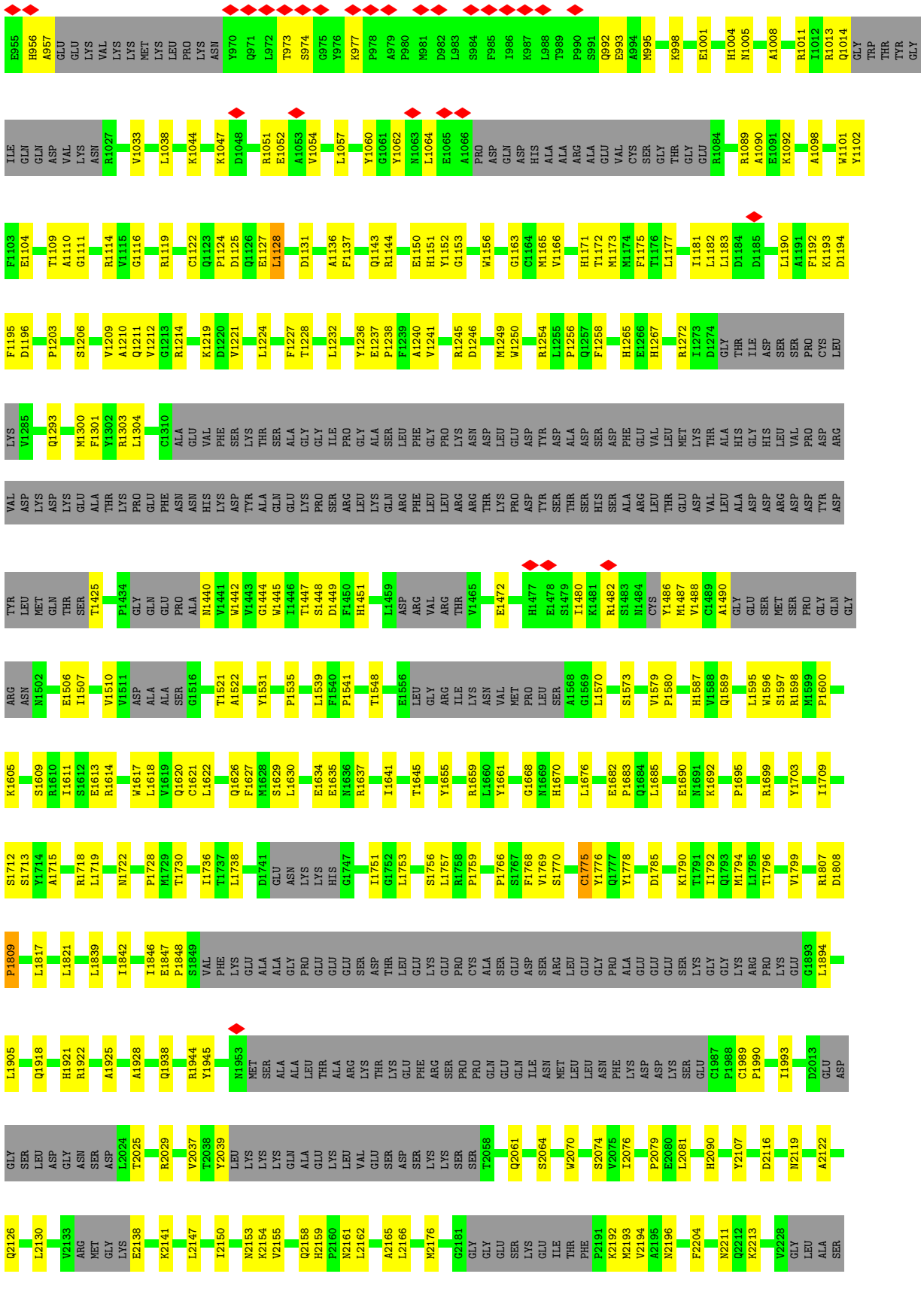
3 Residue-property plots (i)

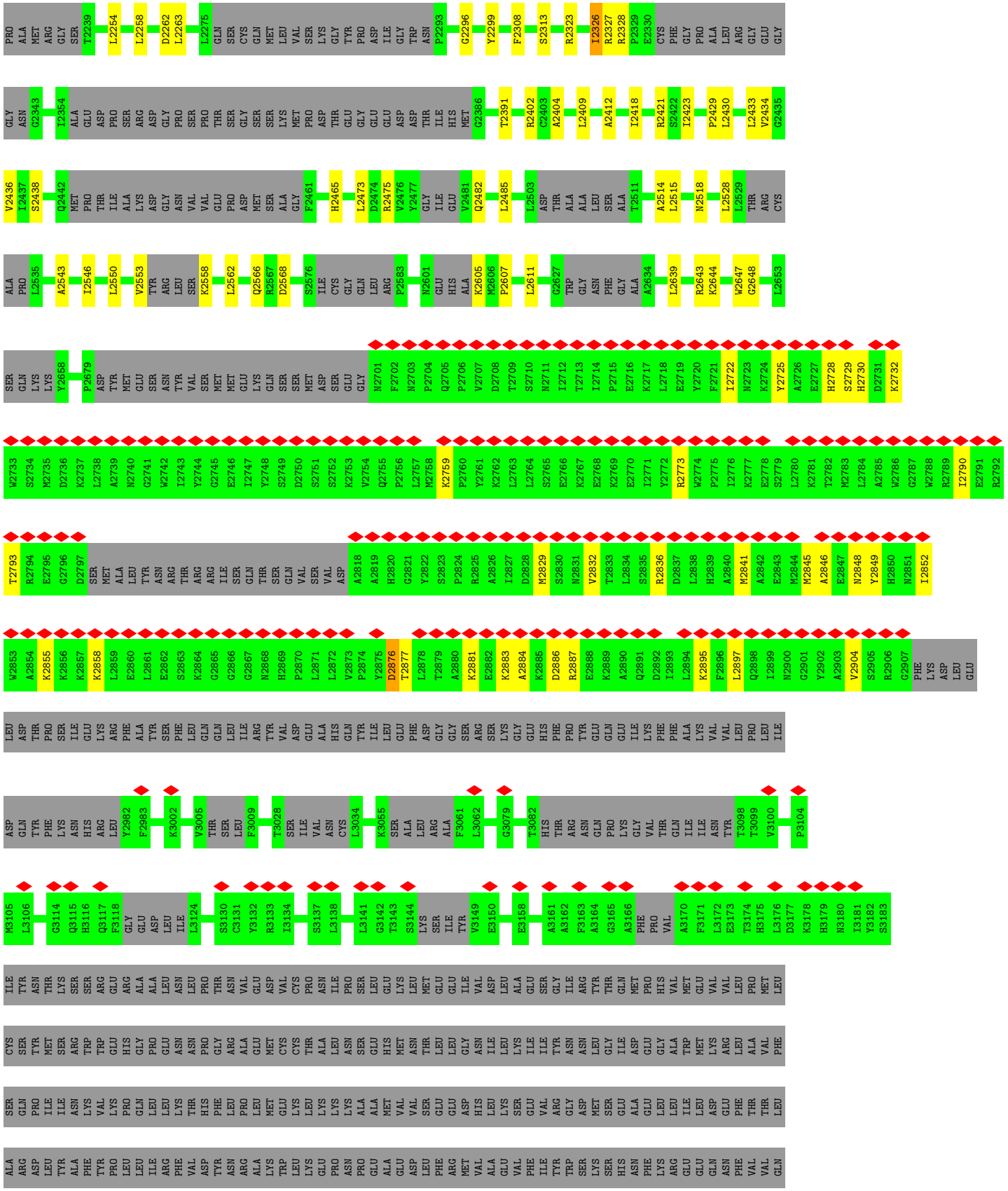
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

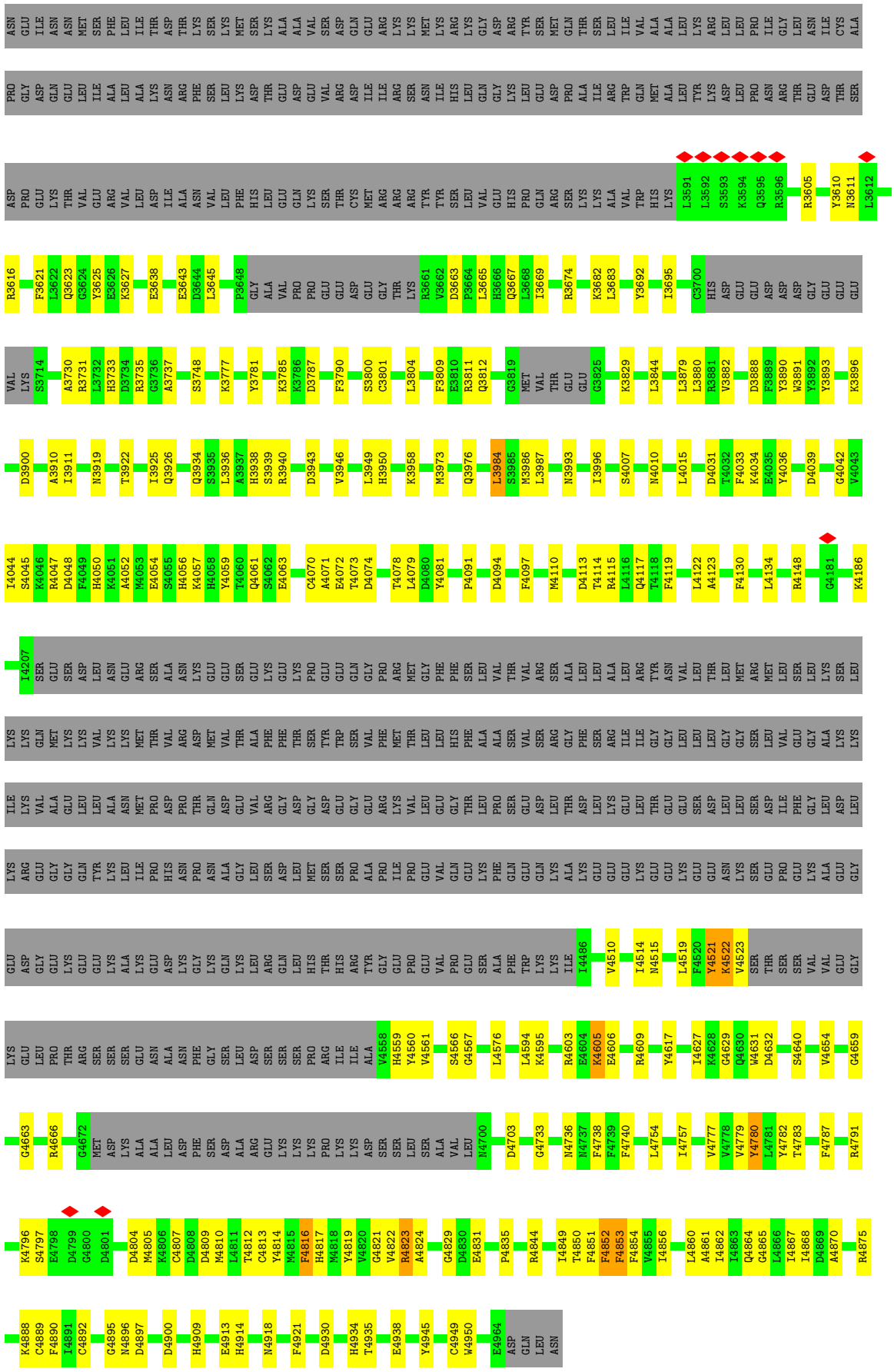
- Molecule 1: RyR2

Chain A: 6% 54% 16% 30%




E955 H956 A957 GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 K998 E1001 H1004 N1005 A1008 R1011 I1012 R1013 Q1014 GLY TRP THR TYR GLY
ILE GLN GLN ASP VAL LYS ASN R1027 V1033 L1038 K1044 K1047 D1048 R1051 E1052 A1053 V1054 L1057 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 PRO ASP GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 R1089 A1090 E1091 K1092 A1098 W1101 Y1102
F1103 E1104 T1109 A1110 G1111 R1114 Y1115 G1116 R1119 C1122 Q1123 P1124 D1125 Q1126 E1127 L1128 D1131 A1136 F1137 Q1143 R1144 E1150 H1151 Y1152 G1153 W1156 G1163 C1164 M1165 V1166 H1171 T1172 M1173 M1174 F1175 T1176 L1177 I1181 L1182 L1183 D1184 D1185 L1190 A1191 F1192 K1193 D1194
F1195 D1196 P1203 S1206 V1209 A1210 Q1211 V1212 G1213 R1214 K1219 D1220 V1221 L1224 F1227 T1228 L1232 Y1236 E1237 P1238 F1239 A1240 V1241 R1245 D1246 M1249 W1250 R1254 L1255 P1256 Q1257 F1258 H1265 E1266 H1267 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU
LYS V1285 Q1293 M1300 F1301 Y1302 R1303 L1304 C1310 ALA GLU VAL PHE SER LYS THR SER ALA GLY GLY ILE PRO GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG
VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ASP ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP
TYR LEU MET GLN THR SER T1425 P1434 GLY GLN GLU PRO ALA N1440 V1441 W1442 V1443 G1444 W1445 I1446 T1447 S1448 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 E1472 H1477 E1478 S1479 I1480 K1481 R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO GLY GLN GLY
ARG ASN N1502 E1506 I1507 V1510 V1511 ASP ALA ALA SER G1516 T1521 A1522 Y1531 P1535 L1539 F1540 P1541 T1548 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 L1570 S1573 V1579 P1580 H1587 V1588 Q1589 L1595 W1596 S1597 R1598 M1599 P1600
K1605 S1609 R1610 I1611 S1612 E1613 R1614 W1617 L1618 V1619 Q1620 C1621 L1622 Q1626 F1627 M1628 S1629 L1630 E1634 E1635 N1636 R1637 I1641 T1645 Y1655 R1659 L1660 Y1661 G1668 N1669 H1670 L1676 E1682 P1683 Q1684 L1685 E1690 N1691 K1692 P1695 R1699 Y1703 I1709
S1712 S1713 Y1714 A1715 R1718 L1719 N1722 P1728 M1729 T1730 I1736 T1737 L1738 D1741 GLU ASN LYS LYS HIS G1747 I1751 G1752 L1753 S1756 L1757 R1758 P1759 P1766 S1767 F1768 V1769 S1770 C1775 Y1776 Q1777 Y1778 D1785 K1790 T1791 I1792 Q1793 M1794 L1795 T1796 V1799 R1807 D1808
P1809 L1817 L1821 L1839 I1842 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP SER ARG LEU GLU GLY PRO ALA GLU GLU GLU SER LYS GLY GLY LYS ARG PRO LYS GLU G1893 L1894
L1905 Q1918 H1921 R1922 A1925 A1928 Q1938 R1944 Y1945 N1953 MET SER ALA ALA LEU THR ALA ARG LYS THR LYS GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU C1987 P1988 C1989 P1990 I1993 D2013 GLU ASP
GLY SER LEU ASP GLY ASN SER ASP L2024 T2025 R2029 V2037 T2038 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 Q2061 S2064 W2070 S2074 V2075 I2076 P2079 E2080 L2081 H2090 Y2107 D2116 N2119 A2122
Q2126 L2130 V2133 ARG MET GLY LYS E2138 K2141 L2147 I2150 N2153 K2154 V2155 Q2158 H2159 P2160 N2161 L2162 A2165 L2166 M2176 G2181 GLY GLY GLU SER LYS GLU ILE THR PHE P2191 K2192 M2193 V2194 A2195 N2196 F2204 N2211 Q2212 K2213 V2228 GLY LEU ALA SER


PRO ALA MET ARG GLY SER T2239 L2254 L2258 D2262 L2263 L2275 GLN SER CYS GLN MET LEU VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 G2296 Y2299 F2308 S2313 R2323 I2326 R2327 R2328 P2329 E2330 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY
GLY ASN G2343 I2354 ALA GLU ASP PRO SER ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS MET PRO ASP THR GLU GLY GLU GLU ASP ASP THR ILE HIS MET G2386 T2391 R2402 C2403 A2404 L2409 A2412 I2418 R2421 S2422 I2423 P2429 L2430 L2433 V2434 G2435
V2436 I2437 S2438 Q2442 MET PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 H2465 L2473 D2474 R2475 V2476 Y2477 GLY ILE GLU V2481 Q2482 L2485 L2503 ASP THR ALA ALA LEU SER ALA T2511 A2514 L2515 N2518 L2528 L2529 THR ARG CYS
ALA PRO L2535 A2543 I2546 L2550 V2553 TYR ARG LEU SER K2558 L2562 Q2566 R2567 D2568 S2576 ILE CYS GLY GLN LEU ARG P2583 N2601 GLU HIS ALA K2605 M2606 P2607 L2611 G2627 TRP GLY ASN PHE GLY ALA A2634 L2639 R2643 K2644 W2647 G2648 L2653
SER GLN LYS LYS Y2658 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725 A2726 E2727 H2728 S2729 H2730 D2731 K2732
W2733 S2734 M2735 D2736 K2737 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 W2788 R2789 I2790 E2791 R2792
T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852
W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 V2873 P2874 Y2875 D2876 T2877 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU GLU
LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE
ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 F2983 K3002 V3005 THR SER LEU F3009 T3028 SER ILE VAL ASN CYS L3034 K3055 SER ALA LEU ARG ALA F3061 L3062 G3079 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 P3104
M3105 L3106 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 S3130 C3131 Y3132 R3133 I3134 S3137 L3138 L3141 G3142 T3143 S3144 LYS SER ILE TYR V3149 E3150 E3158 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183
ILE TYR ASN THR LYS SER SER ARG GLU ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS ASN MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU
CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE
SER GLN PRO ILE ILE ASN LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU GLU LEU LEU ILE LEU LEU ASP GLU PHE THR THR LEU
ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU ASP LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN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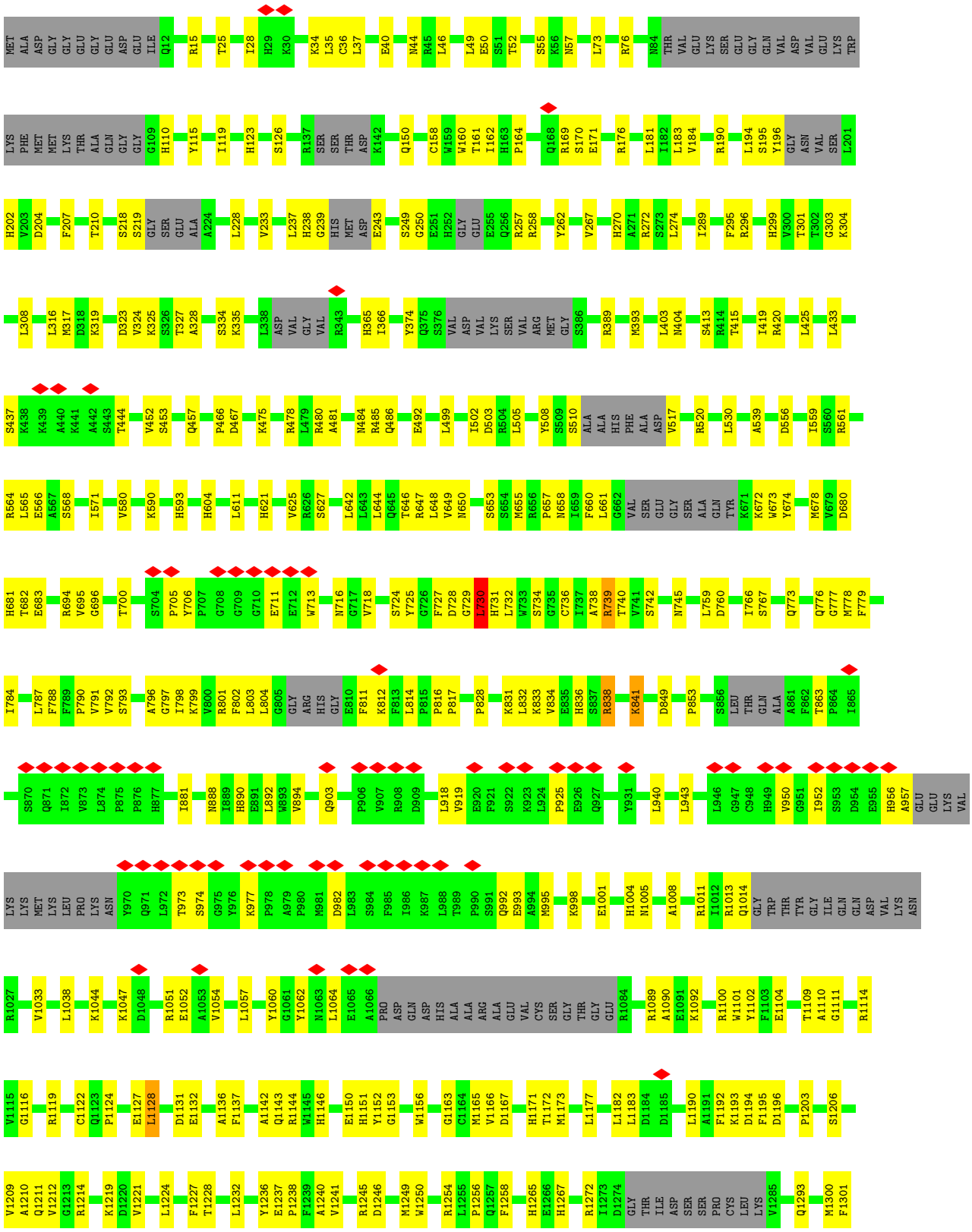
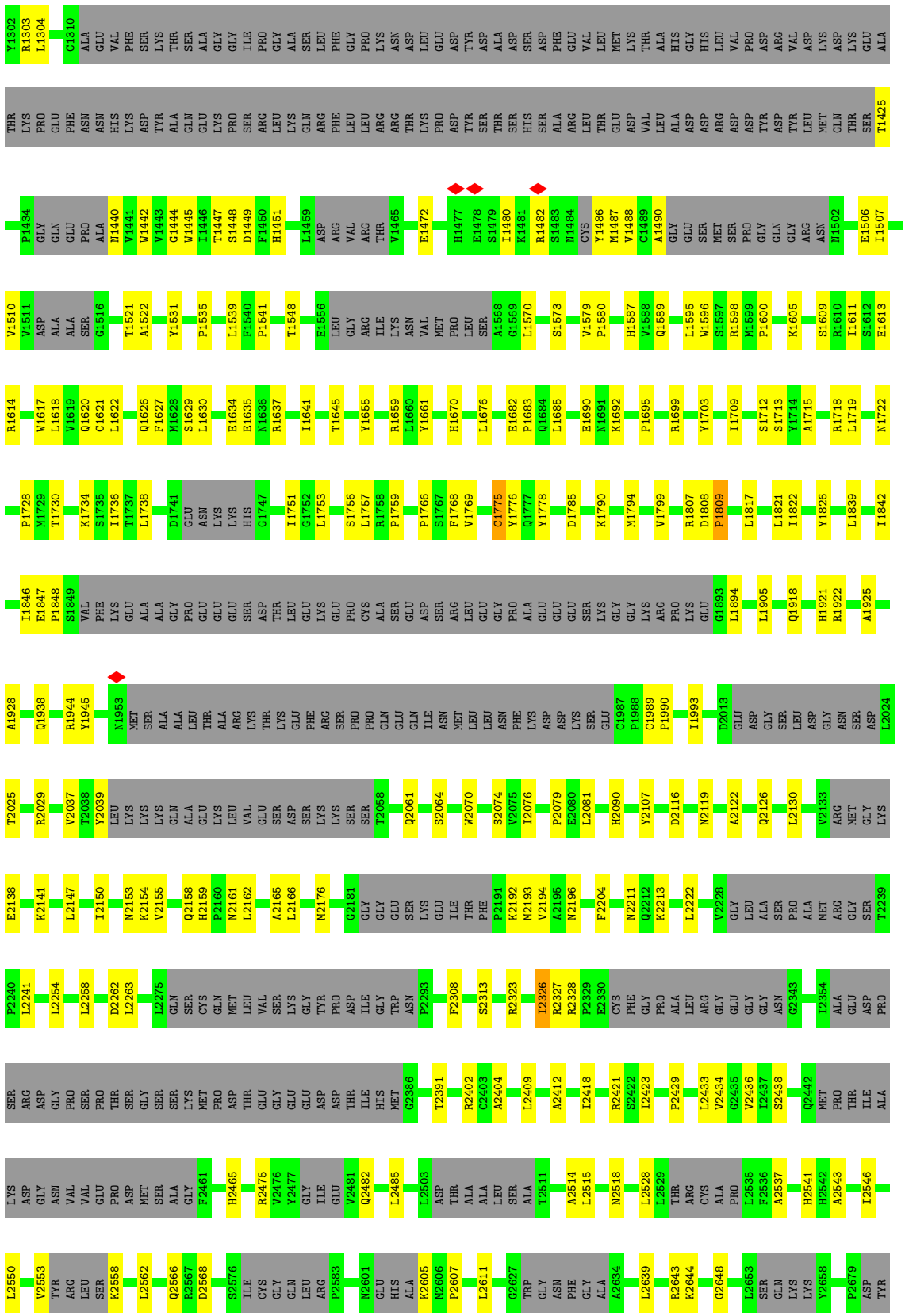
K4796 S4797 E4798 D4799 G4800 D4801 D4804 M4805 K4806 C4807 D4808 D4809 M4810 L4811 T4812 C4813 Y4814 M4815 F4816 H4817 M4818 Y4819 V4820 G4821 V4822 R4823 A4824 G4829 D4830 E4831 P4835 R4844 I4849 T4850 F4851 F4852 F4853 F4854 V4855 I4856 L4860 A4861 I4862 I4863 Q4864 G4865 L4866 I4867 I4868 D4869 A4870 R4875
G4663 R4666 G4672 N4700 D4703 G4733 N4736 N4737 F4738 F4739 F4740 L4754 I4757 V4777 V4778 V4779 Y4780 L4781 Y4782 T4783 F4787 R4791
LYS GLU LEU PRO THR ARG SER SER SER PRO ARG ILE ILE ALA V4558 H4559 Y4560 V4561 S4566 G4567 L4576 L4594 K4595 R4603 E4604 K4605 E4606 R4609 Y4617 I4627 K4628 G4629 Q4630 W4631 D4632 S4640 V4654 G4659
GLU ASP GLY GLU LYS GLU GLU LYS ALA LYS GLU ASP LYS GLY LYS GLN GLN LEU HIS THR HIS ARG TYR GLY LYS GLU VAL PRO GLU PRO GLU VAL GLN GLU LYS LYS LYS ILE I4486 V4510 I4514 N4515 L4519 F4520 Y4521 K4522 V4523 SER THR SER VAL VAL GLU GLY
LYS ARG GLU GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU LEU SER ASP GLY LEU ASP MET ASP SER SER PRO ALA PRO ILE PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS GLU GLU GLU LYS GLU GLU LYS LYS GLU GLU GLY
ILE LYS VAL ALA GLU LEU LEU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLY GLU GLY ARG LYS VAL LEU GLU GLY THR LEU ASP GLY LEU THR ASP LEU LYS GLU THR GLU LEU GLU GLU LEU GLU GLU GLU GLU GLU GLU LEU ASP LEU
LYS LYS GLN MET LYS LYS VAL LYS MET THR VAL ARG ASP MET VAL THR ALA PHE PHE THR SER TRP TRP SER VAL PHE MET THR LEU LEU HIS PHE ALA ALA SER VAL SER ARG GLY PHE SER ARG ILE ILE GLY GLY LEU LEU LEU GLY GLY GLY SER SER SER LYS LYS LYS
I4207 SER GLU SER ASP LEU ASN GLU ARG SER ALA ASN LYS GLU GLU LYS PRO GLU GLU GLN GLY PRO ARG MET GLY PHE PHE SER LEU LEU VAL THR VAL ARG SER ALA LEU LEU ALA LEU ARG TYR ASN VAL LEU THR LEU SER SER SER LEU LEU SER LEU LYS SER LEU
I4044 S4045 K4046 R4047 D4048 F4049 H4050 K4051 A4052 M4053 E4054 S4055 H4056 K4057 H4058 Y4059 T4060 Q4061 S4062 E4063 C4070 A4071 E4072 T4073 D4074 T4078 L4079 D4080 Y4081 P4091 D4094 F4097 M4110 D4113 T4114 R4115 L4116 Q4117 T4118 F4119 L4122 A4123 F4130 L4134 R4148 G4181 K4186
D3900 A3910 I3911 N3919 T3922 I3925 Q3926 Q3934 S3935 L3936 A3937 H3938 S3939 R3940 D3943 V3946 L3949 H3950 K3958 M3973 Q3976 L3984 S3985 M3986 L3987 N3993 I3996 S4007 N4010 L4015 D4031 T4032 F4033 K4034 E4035 Y4036 D4039 G4042 V4043
VAL LYS S3714 A3730 R3731 L3732 H3733 D3734 R3735 G3736 A3737 S3748 K3777 Y3781 K3785 K3786 D3787 F3790 S3800 C3801 L3804 F3809 E3810 R3811 Q3812 G3819 MET VAL THR GLU GLU G3825 K3829 L3844 L3879 L3880 R3881 Y3882 D3888 F3889 Y3890 W3891 Y3892 Y3893 K3896
R3616 F3621 L3622 Q3623 G3624 Y3625 E3626 K3627 E3638 E3643 D3644 L3645 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 V3662 D3663 P3664 L3665 H3666 Q3667 L3668 I3669 R3674 K3682 L3683 Y3692 I3695 C3700 HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU
ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLU GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLN LYS LYS ALA VAL TRP HIS LYS L3591 L3592 S3593 K3594 Q3595 R3596 R3605 Y3610 N3611 L3612
PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU GLN GLY LYS LEU GLU ASP PRO ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP THR SER
ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA

- Molecule 1: RyR2

Chain D: 6% 54% 16% 30%

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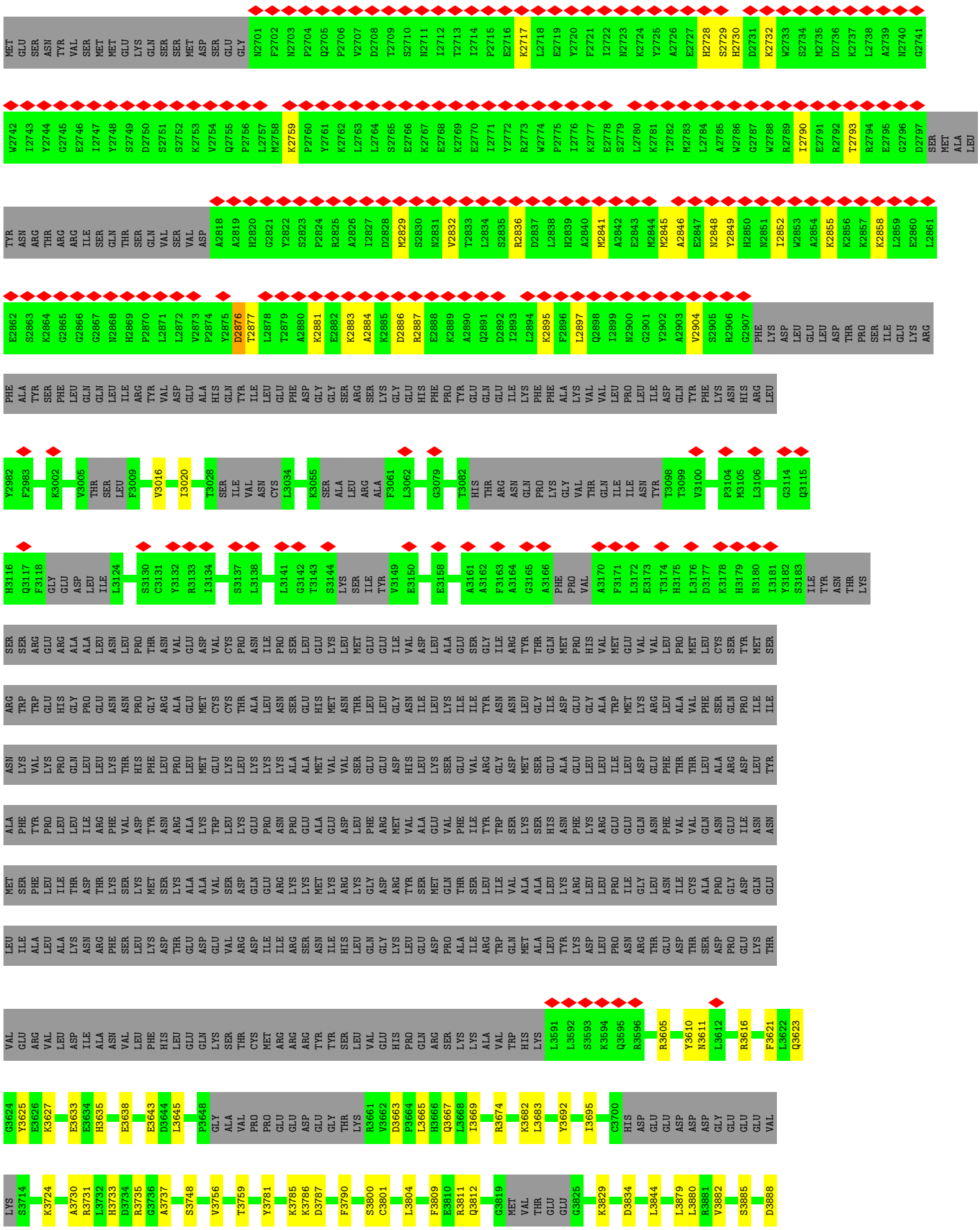
THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR ARG LEU MET GLN THR SER T1425
P1434 GLY GLN GLU PRO ALA N1440 V1441 W1442 V1443 G1444 W1445 I1446 T1447 S1448 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 E1472 H1477 E1478 S1479 I1480 K1481 R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO GLY GLN GLY ARG ASN N1502 E1506 I1507
V1510 V1511 ASP ALA ALA SER G1516 T1521 A1522 Y1531 P1535 L1539 F1540 P1541 T1548 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 L1570 S1573 V1579 P1580 H1587 V1588 Q1589 L1595 W1596 S1597 R1598 M1599 P1600 K1605 S1609 R1610 I1611 S1612 E1613
R1614 W1617 L1618 V1619 Q1620 C1621 L1622 Q1626 F1627 M1628 S1629 L1630 E1634 E1635 N1636 R1637 I1641 T1645 Y1655 R1659 L1660 Y1661 H1670 L1676 E1682 P1683 Q1684 L1685 E1690 N1691 K1692 P1695 R1699 Y1703 I1709 S1712 S1713 Y1714 A1715 R1718 L1719 N1722
P1728 M1729 T1730 K1734 S1735 I1736 T1737 L1738 D1741 GLU ASN LYS LYS HIS G1747 I1751 G1752 L1753 S1756 L1757 R1758 P1759 P1766 S1767 F1768 V1769 C1775 Y1776 Q1777 Y1778 D1785 K1790 M1794 V1799 R1807 D1808 P1809 L1817 L1821 I1822 Y1826 L1839 I1842
I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP SER ARG LEU GLU GLY PRO ALA GLU GLU GLU SER LYS GLY GLY LYS ARG PRO LYS GLU G1893 L1894 L1905 Q1918 H1921 R1922 A1925
A1928 Q1938 R1944 Y1945 N1953 MET SER ALA ALA LEU THR ALA ARG LYS THR LYS GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU LEU ASN PHE LYS ASP ASP LYS SER GLU C1987 P1988 C1989 P1990 I1993 D2013 GLU ASP GLY SER LEU ASP GLY ASN SER ASP L2024
T2025 R2029 V2037 T2038 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 Q2061 S2064 W2070 S2074 V2075 I2076 P2079 E2080 L2081 H2090 Y2107 D2116 N2119 A2122 Q2126 L2130 V2133 ARG MET GLY LYS
E2138 K2141 L2147 I2150 N2153 K2154 V2155 Q2158 H2159 P2160 N2161 L2162 A2165 L2166 M2176 G2181 GLY GLY GLU SER LYS GLU ILE THR PHE P2191 K2192 M2193 V2194 A2195 N2196 F2204 N2211 Q2212 K2213 L2222 V2228 GLY LEU ALA SER PRO ALA MET ARG GLY SER T2239
P2240 L2241 L2254 L2258 D2262 L2263 L2275 GLN SER CYS GLN MET LEU VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 F2308 S2313 R2323 I2326 R2327 R2328 P2329 E2330 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 I2354 ALA GLU ASP PRO
SER ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS MET PRO ASP THR GLU GLY GLU GLU ASP ASP THR ILE HIS MET G2386 T2391 R2402 C2403 A2404 L2409 A2412 I2418 R2421 S2422 I2423 P2429 L2433 V2434 G2435 V2436 I2437 S2438 Q2442 MET PRO THR ILE ALA
LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 H2465 R2475 V2476 Y2477 GLY ILE GLU V2481 Q2482 L2485 L2503 ASP THR ALA ALA LEU SER ALA T2511 A2514 L2515 N2518 L2528 L2529 THR ARG CYS ALA PRO L2535 F2536 A2537 H2541 H2542 A2543 I2546
L2550 V2553 TYR ARG LEU SER K2558 L2562 Q2566 R2567 D2568 S2576 ILE CYS GLY GLN LEU ARG P2583 N2601 GLU HIS ALA K2605 M2606 P2607 L2611 G2627 TRP GLY ASN PHE GLY ALA A2634 L2639 R2643 K2644 G2648 L2653 SER GLN LYS LYS Y2658 P2679 ASP TYR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W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785 W2786 G2787 W2788 R2789 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU
TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845 A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861
E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 V2873 P2874 Y2875 D2876 T2877 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU LEU GLU LEU ASP THR PRO SER ILE GLU LYS ARG
PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU
Y2982 F2983 K3002 V3005 THR SER LEU F3009 V3016 I3020 T3028 SER ILE VAL ASN CYS L3034 K3055 SER ALA LEU ARG ALA F3061 L3062 G3079 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 P3104 M3105 L3106 G3114 Q3115
H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 S3130 C3131 Y3132 R3133 I3134 S3137 L3138 L3141 G3142 T3143 S3144 LYS SER ILE TYR V3149 E3150 E3158 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS
SER SER ARG GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER
ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE
ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU LEU ALA ARG ASP LEU TYR
ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU ASP LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN
MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA SER ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER GLN THR SER LEU ILE VAL ALA ALA LEU LYS LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU
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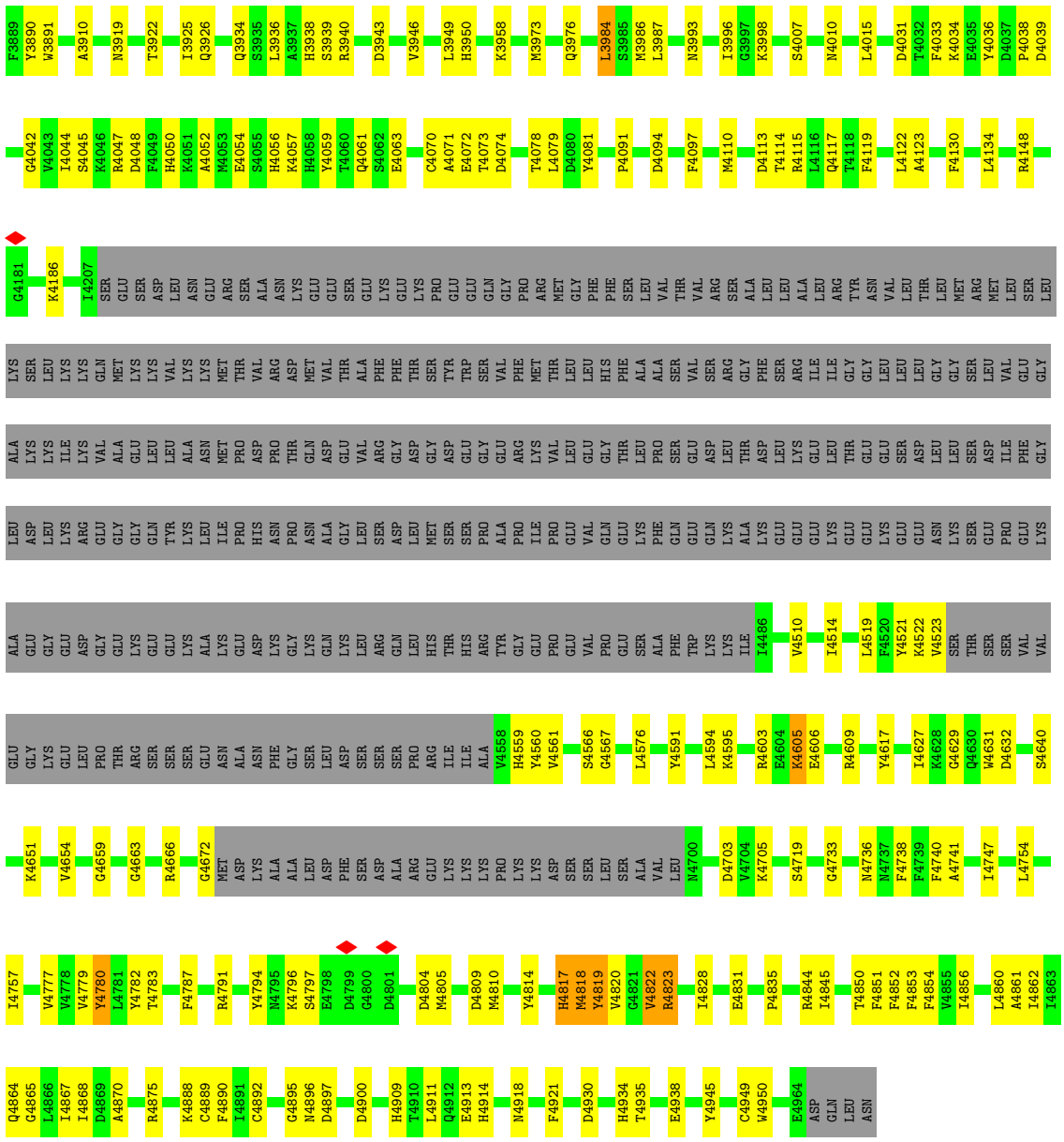
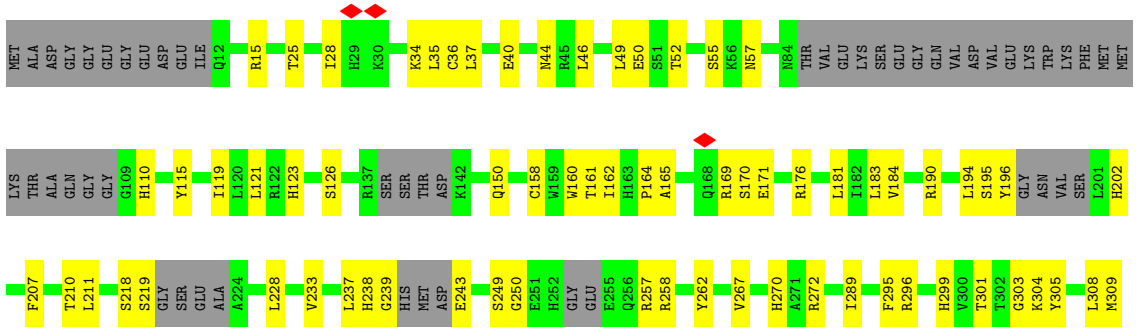
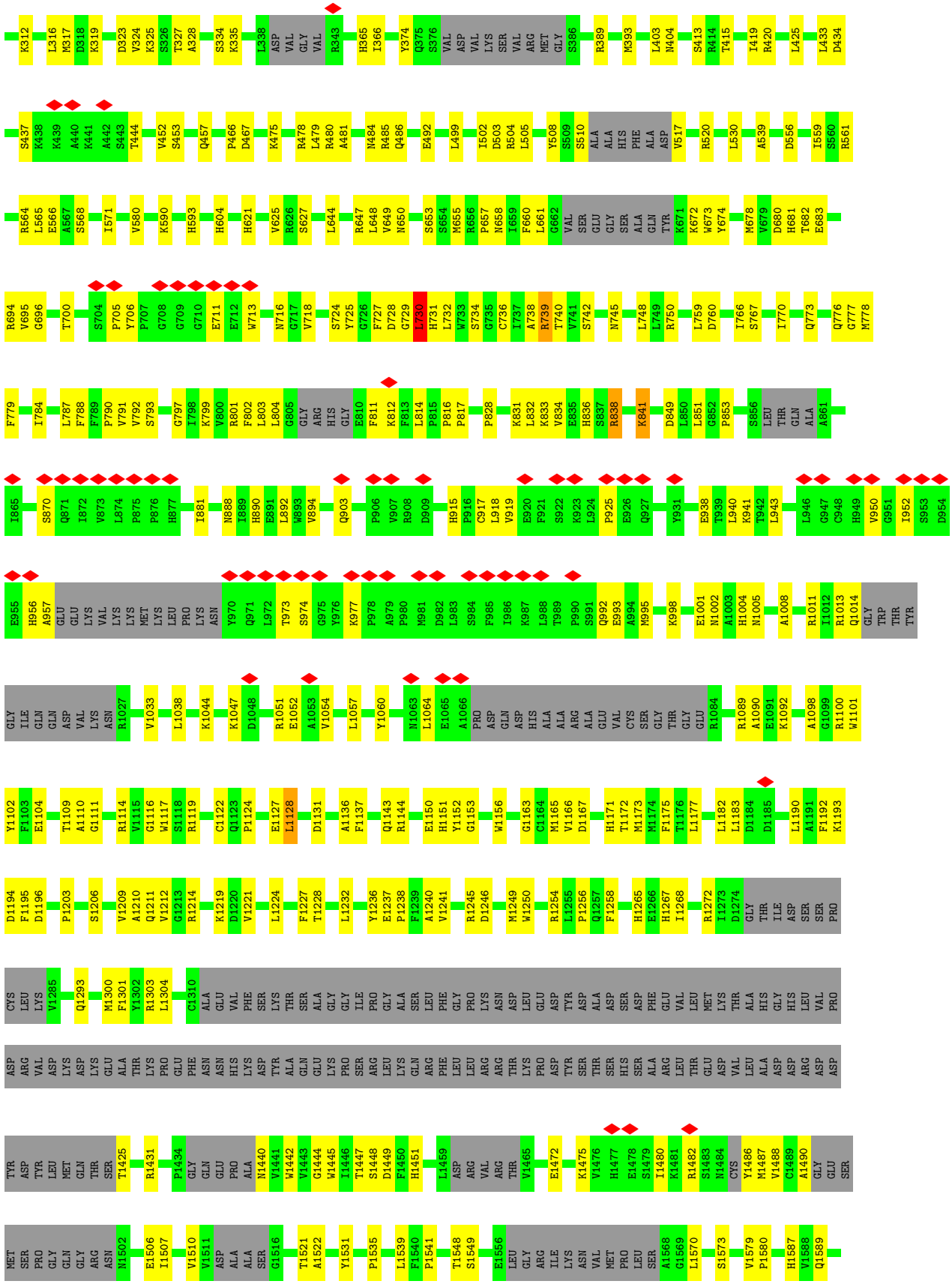
VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN GLY LYS SER THR CYS MET ARG ARG ARG TYR TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS L3591 L3592 S3593 K3594 Q3595 R3596 R3605 Y3610 N3611 L3612 R3616 F3621 L3622 Q3623
G3624 Y3625 E3626 K3627 E3633 E3634 H3635 E3638 E3643 D3644 L3645 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 V3662 D3663 P3664 L3665 H3666 Q3667 L3668 I3669 R3674 K3682 L3683 Y3692 I3695 C3700 HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU VAL
LYS S3714 K3724 A3730 R3731 L3732 H3733 D3734 R3735 G3736 A3737 S3748 V3756 T3759 Y3781 K3785 K3786 D3787 F3790 S3800 C3801 L3804 F3809 E3810 R3811 Q3812 G3819 MET VAL THR GLU GLU G3825 K3829 D3834 L3844 L3879 L3880 R3881 V3882 S3885 D3888



- Molecule 1: RyR2

Chain G:

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S437 K438 K439 A440 K441 A442 S443 T444 V452 S453 Q457 P466 D467 K475 R478 L479 R480 A481 N484 R485 Q486 E492 L499 I502 D503 R504 L505 Y508 S509 S510 ALA ALA HIS PHE ALA ASP V517 R520 L530 A539 D556 I559 S560 R561
R564 L565 E566 A567 S568 I571 V580 K590 H593 H604 H621 E625 R626 S627 L644 R647 L648 V649 N650 S653 S654 M655 R656 P657 N658 I659 F660 L661 G662 VAL SER GLU GLY SER ALA GLN TYR K671 K672 W673 Y674 M678 V679 D680 H681 T682 E683
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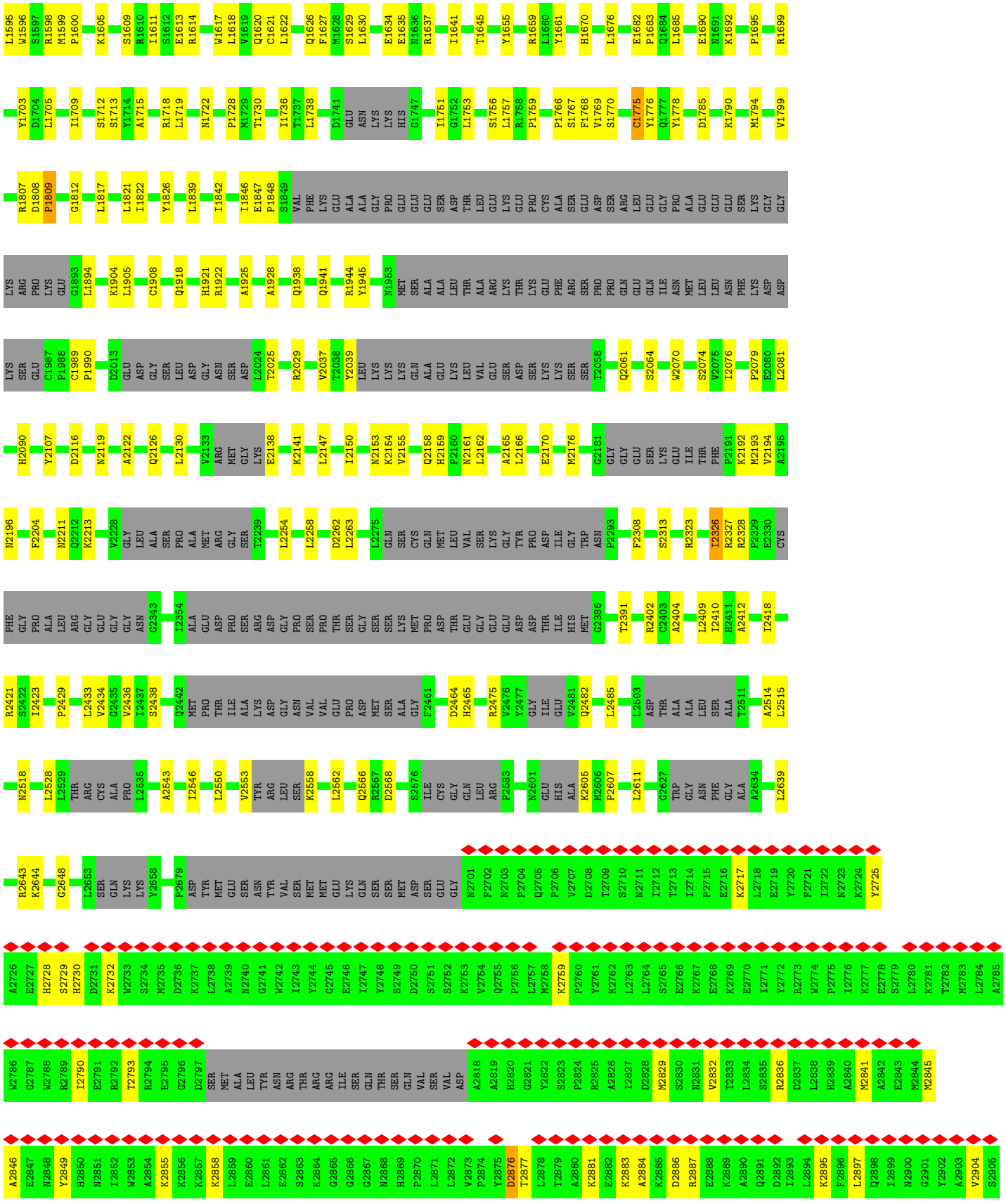
Y1102 F1103 E1104 T1109 A1110 G1111 R1114 V1115 G1116 W1117 S1118 R1119 C1122 Q1123 P1124 E1127 L1128 D1131 A1136 F1137 Q1143 R1144 E1150 H1151 Y1152 G1153 W1156 G1163 C1164 M1165 V1166 D1167 H1171 T1172 M1173 M1174 F1175 T1176 L1177 L1182 L1183 D1184 D1185 L1190 A1191 F1192 K1193
D1194 F1195 D1196 P1203 S1206 V1209 A1210 Q1211 V1212 G1213 R1214 K1219 D1220 V1221 L1224 F1227 T1228 L1232 Y1236 E1237 P1238 F1239 A1240 V1241 R1245 D1246 M1249 W1250 R1254 L1255 P1256 Q1257 F1258 H1265 E1266 H1267 I1268 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO
CYS LEU LYS V1285 Q1293 M1300 F1301 Y1302 R1303 L1304 C1310 ALA GLU VAL PHE SER LYS THR SER ALA GLY GLY ILE PRO GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO
ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP
TYR ASP TYR LEU MET GLN THR SER T1425 R1431 P1434 GLY GLN GLU PRO ALA N1440 V1441 W1442 V1443 G1444 W1445 I1446 T1447 S1448 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 E1472 K1475 V1476 H1477 E1478 S1479 I1480 K1481 R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER
MET SER PRO GLY GLN GLY ARG ASN N1502 E1506 I1507 V1510 V1511 ASP ALA ALA SER G1516 T1521 A1522 Y1531 P1535 L1539 F1540 P1541 T1548 S1549 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 L1570 S1573 V1579 P1580 H1587 V1588 Q1589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R1807 D1808 P1809 G1812 L1817 L1821 I1822 Y1826 L1839 I1842 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU ASP SER ARG LEU GLU GLU GLU SER LYS GLY GLY
LYS ARG PRO LYS GLU G1893 L1894 K1904 L1905 C1908 Q1918 H1921 R1922 A1925 A1928 Q1938 Q1941 R1944 Y1945 M1953 MET SER ALA ALA LEU THR ALA ARG LYS THR LYS GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP
LYS SER GLU C1987 P1988 C1989 P1990 D2013 GLU ASP GLY SER LEU ASP GLY ASN SER ASP L2024 T2025 R2029 V2037 T2038 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 Q2061 S2064 W2070 S2074 V2075 I2076 P2079 E2080 L2081
H2090 Y2107 D2116 N2119 A2122 Q2126 L2130 V2133 ARG MET GLY LYS E2138 K2141 L2147 I2150 N2153 K2154 V2155 Q2158 H2159 P2160 N2161 L2162 A2165 L2166 E2170 M2176 G2181 GLY GLY GLU SER LYS GLU ILE THR PHE P2191 K2192 M2193 V2194 A2195
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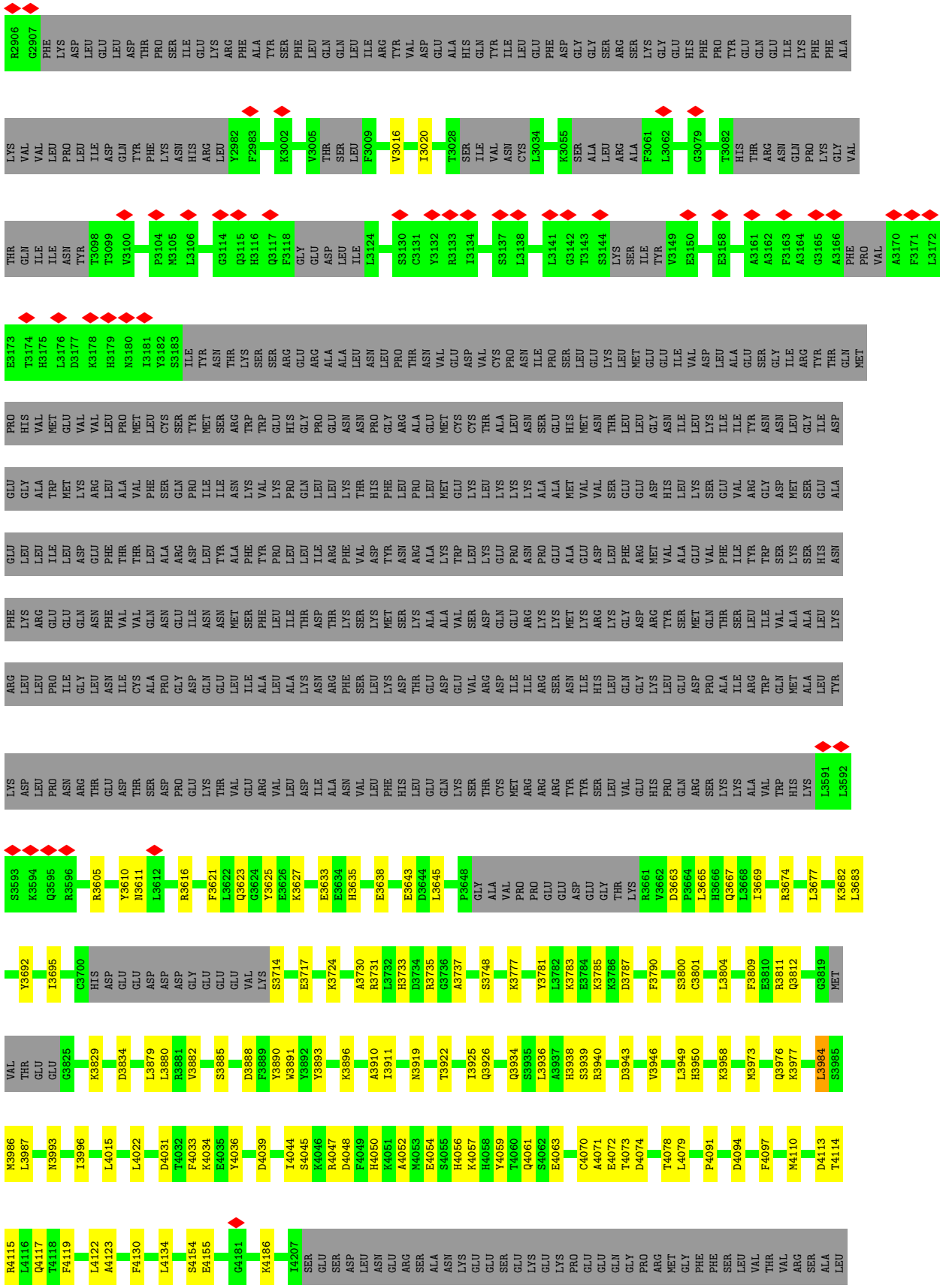
PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY GLY ASN G2343 I2354 ALA GLU ASP PRO SER ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS MET PRO ASP THR GLU GLY GLU GLU ASP ASP THR ILE HIS MET G2386 T2391 R2402 C2403 A2404 L2409 I2410 H2411 A2412 I2418
R2421 S2422 I2423 P2429 L2433 V2434 G2435 V2436 I2437 S2438 Q2442 MET PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 D2464 H2465 R2475 V2476 Y2477 GLY ILE GLU V2481 Q2482 L2485 L2503 ASP THR ALA ALA LEU SER ALA T2511 A2514 L2515
N2518 L2528 L2529 THR ARG CYS ALA PRO L2535 A2543 I2546 L2550 V2553 TYR ARG LEU SER K2558 L2562 Q2566 R2567 D2568 S2576 ILE CYS GLY GLN LEU ARG P2583 N2601 GLU HIS ALA K2605 M2606 P2607 L2611 G2627 TRP GLY ASN PHE GLY ALA A2634 L2639
R2643 K2644 G2648 L2653 SER GLN LYS LYS Y2658 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720 F2721 I2722 N2723 K2724 Y2725
A2726 E2727 H2728 S2729 H2730 D2731 K2732 W2733 S2734 M2735 D2736 K2737 L2738 A2739 N2740 G2741 W2742 I2743 Y2744 G2745 E2746 I2747 Y2748 S2749 D2750 S2751 S2752 K2753 V2754 Q2755 P2756 L2757 M2758 K2759 P2760 Y2761 K2762 L2763 L2764 S2765 E2766 K2767 E2768 K2769 E2770 I2771 Y2772 R2773 W2774 P2775 I2776 K2777 E2778 S2779 L2780 K2781 T2782 M2783 L2784 A2785
W2786 G2787 W2788 R2789 I2790 E2791 R2792 T2793 R2794 E2795 G2796 D2797 SER MET ALA LEU TYR ASN ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP A2818 A2819 H2820 G2821 Y2822 S2823 P2824 R2825 A2826 I2827 D2828 M2829 S2830 N2831 V2832 T2833 L2834 S2835 R2836 D2837 L2838 H2839 A2840 M2841 A2842 E2843 M2844 M2845
A2846 E2847 N2848 Y2849 H2850 N2851 I2852 W2853 A2854 K2855 K2856 K2857 K2858 L2859 E2860 L2861 E2862 S2863 K2864 G2865 G2866 G2867 N2868 H2869 P2870 L2871 L2872 V2873 P2874 Y2875 D2876 T2877 L2878 T2879 A2880 K2881 E2882 K2883 A2884 K2885 D2886 R2887 E2888 K2889 A2890 Q2891 D2892 I2893 L2894 K2895 F2896 L2897 Q2898 I2899 N2900 G2901 Y2902 A2903 V2904 S2905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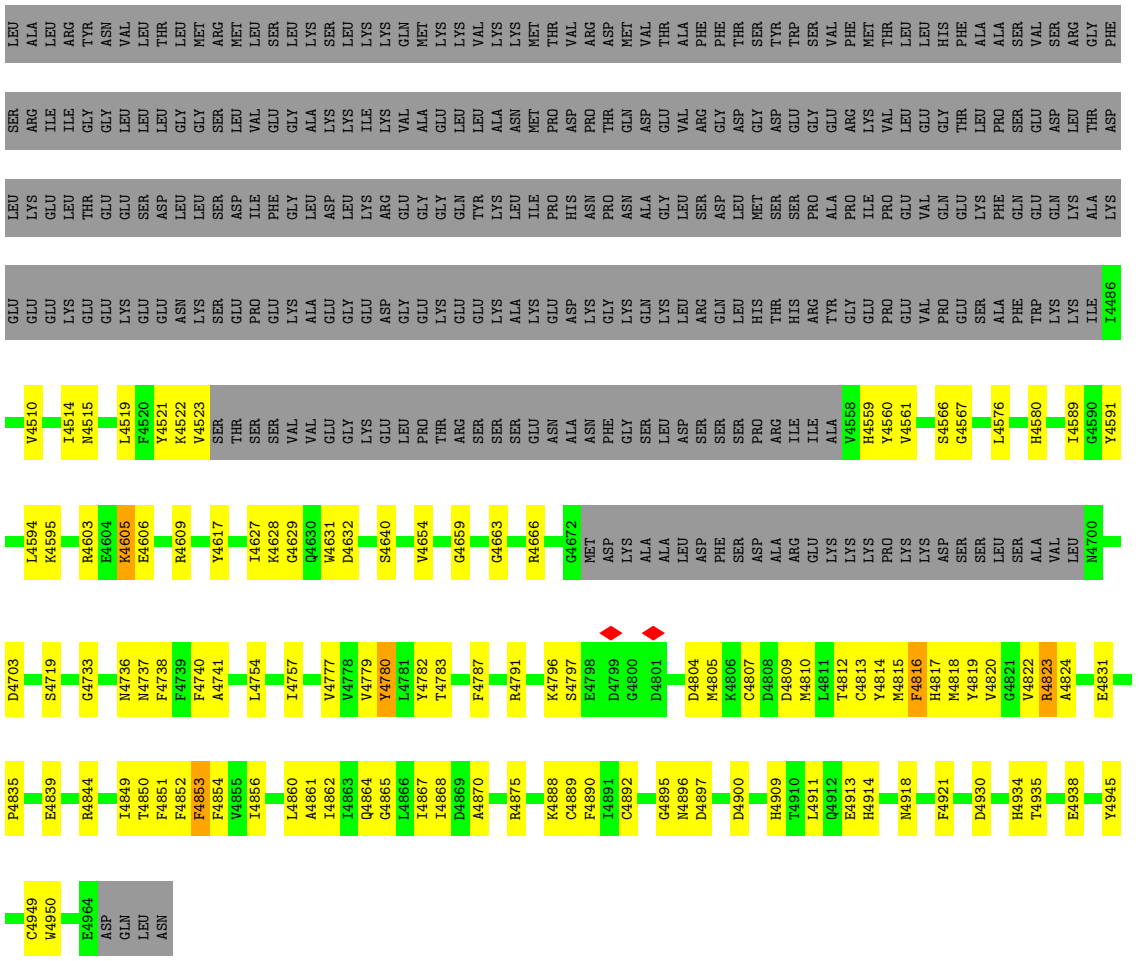
LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 F2983 K3002 V3005 THR SER LEU F3009 V3016 I3020 T3028 SER ILE VAL ASN CYS L3034 K3055 SER ALA LEU ARG ALA F3061 L3062 G3079 T3082 HIS THR ARG ASN GLN PRO LYS GLY VAL
THR GLN ILE ILE ASN TYR T3098 T3099 V3100 P3104 M3105 L3106 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 S3130 C3131 Y3132 R3133 I3134 S3137 L3138 L3141 G3142 T3143 S3144 LYS SER ILE TYR V3149 E3150 E3158 A3161 A3162 F3163 A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172
E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ARG TYR THR GLN MET
PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS ILE ILE TYR ASN ASN LEU GLY ILE ASP
GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LEU LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER GLU VAL ARG GLY ASP MET SER GLU ALA
GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU ALA MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN
PHE LYS ARG GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ASP GLN GLU ARG LYS LYS MET LYS ARG LYS GLY ASP ARG TYR SER MET GLN THR SER LEU ILE VAL ALA ALA LEU LYS
ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG SER ASN ILE HIS LEU LEU GLN GLY LEU GLU ASP PRO GLN ARG TRP GLN MET ALA LEU TYR
LYS ASP LEU PRO ASN ARG THR GLU ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS L3591 L3592
S3593 K3594 Q3595 R3596 R3605 Y3610 N3611 L3612 R3616 F3621 L3622 Q3623 G3624 Y3625 E3626 K3627 E3633 E3634 H3635 E3638 E3643 D3644 L3645 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU GLY THR LYS R3661 V3662 D3663 P3664 L3665 H3666 Q3667 L3668 I3669 R3674 L3677 K3682 L3683
Y3692 I3695 C3700 HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU VAL LYS S3714 E3717 K3724 A3730 R3731 L3732 H3733 D3734 R3735 G3736 A3737 S3748 K3777 Y3781 L3782 K3783 E3784 K3785 K3786 D3787 F3790 S3800 C3801 L3804 F3809 E3810 R3811 Q3812 G3819 MET
VAL THR GLU GLU G3825 K3829 D3834 L3879 L3880 R3881 V3882 S3885 D3888 F3889 Y3890 W3891 Y3892 Y3893 K3896 A3910 I3911 N3919 T3922 I3925 Q3926 Q3934 S3935 L3936 A3937 H3938 S3939 R3940 D3943 V3946 L3949 H3950 K3958 M3973 Q3976 K3977 L3984 S3985
M3986 L3987 N3993 I3996 L4015 L4022 D4031 T4032 F4033 K4034 E4035 Y4036 D4039 I4044 S4045 K4046 R4047 D4048 F4049 H4050 K4051 A4052 M4053 E4054 S4055 H4056 K4057 H4058 Y4059 T4060 Q4061 S4062 E4063 C4070 A4071 E4072 T4073 D4074 T4078 L4079 P4091 D4094 F4097 M4110 D4113 T4114
R4115 L4116 Q4117 T4118 F4119 L4122 A4123 F4130 L4134 S4154 E4155 G4181 K4186 I4207 SER GLU SER ASP LEU ASN GLU ARG SER ALA ASN LYS GLU GLU SER GLU LYS GLU LYS PRO GLU GLU GLN GLY PRO ARG MET GLY PHE PHE SER LEU VAL THR VAL ARG SER ALA LEU



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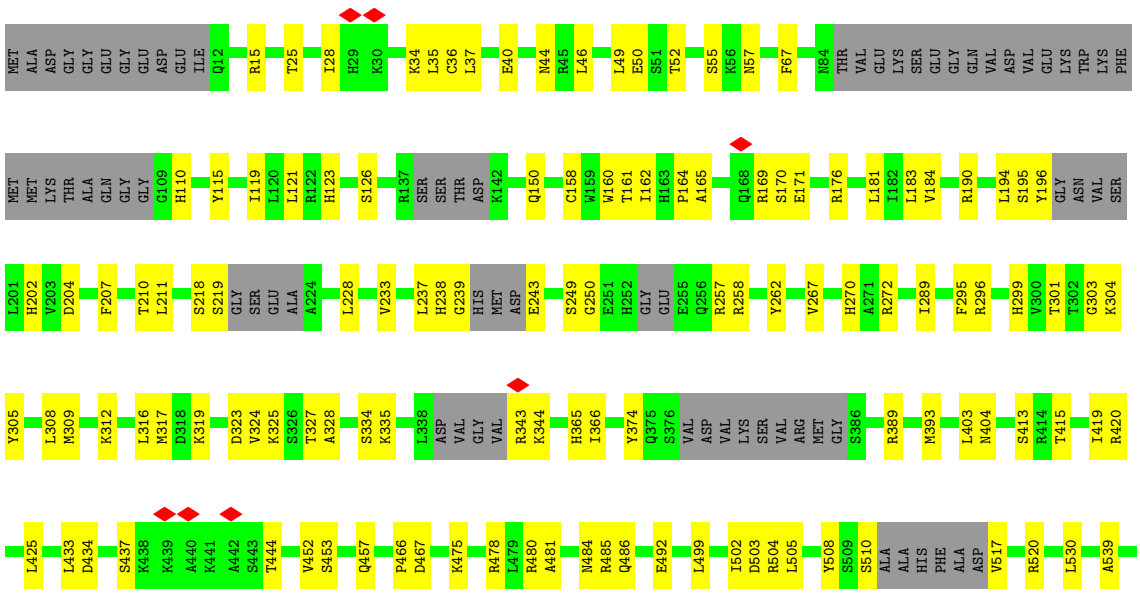

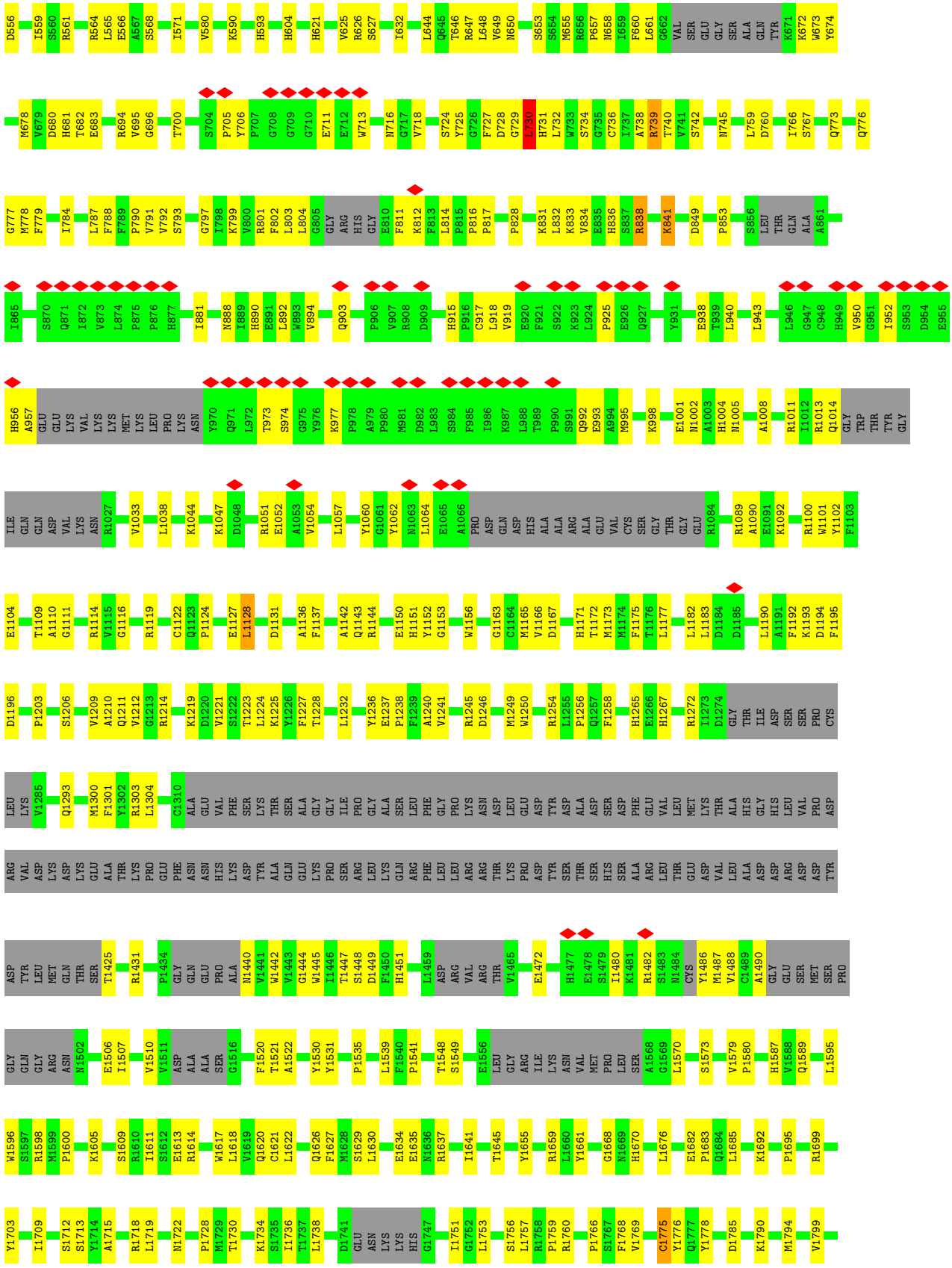
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M678 V679 D680 H681 T682 E683 R694 V695 G696 T700 S704 P705 Y706 P707 G708 G709 G710 E711 E712 W713 N716 G717 V718 S724 Y725 G726 F727 D728 G729 L730 H731 L732 W733 S734 G735 C736 I737 A738 R739 T740 V741 S742 N745 L759 D760 I766 S767 Q773 Q776
G777 M778 F779 I784 L787 F788 F789 P790 V791 V792 S793 G797 I798 K799 W800 R801 F802 L803 L804 G805 GLY ARG HIS GLY E810 F811 K812 F813 L814 P815 P816 P817 P828 K831 L832 K833 Y834 E835 H836 S837 R838 K841 D849 P853 S856 LEU THR GLN ALA A861
I865 S870 Q871 I872 V873 L874 P875 P876 H877 I881 N888 I889 H890 E891 L892 W893 V894 Q903 P906 V907 R908 D909 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 Y931 E938 T939 L940 L943 L946 G947 C948 H949 V950 G951 I952 S953 D954 E955
H956 A957 GLU GLU LYS VAL LYS LYS MET LYS LEU PRO LYS ASN Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 K998 E1001 N1002 A1003 H1004 N1005 A1008 R1011 I1012 R1013 Q1014 GLY TRP THR TYR GLY
ILE GLN GLN ASP VAL LYS ASN R1027 V1033 L1038 K1044 K1047 D1048 R1051 E1052 A1053 V1054 L1057 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 PRO ASP GLN ASP HIS ALA ALA ARG ALA GLU VAL CYS SER GLY THR GLY GLU R1084 R1089 A1090 E1091 K1092 R1100 W1101 Y1102 F1103
E1104 T1109 A1110 G1111 R1114 V1115 G1116 R1119 C1122 Q1123 P1124 E1127 L1128 D1131 A1136 F1137 A1142 Q1143 R1144 E1150 H1151 Y1152 G1153 W1156 G1163 C1164 M1165 V1166 D1167 H1171 T1172 M1173 M1174 F1175 T1176 L1177 L1182 L1183 D1184 D1185 L1190 A1191 F1192 K1193 D1194 F1195
D1196 P1203 S1206 V1209 A1210 Q1211 V1212 G1213 R1214 K1219 D1220 V1221 S1222 T1223 L1224 K1225 Y1226 F1227 T1228 L1232 Y1236 E1237 P1238 F1239 A1240 V1241 R1245 D1246 M1249 W1250 R1254 L1255 P1256 Q1257 F1258 H1265 E1266 H1267 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS
LEU LYS V1285 Q1293 M1300 F1301 Y1302 R1303 L1304 C1310 ALA GLU VAL PHE SER LYS THR SER ALA GLY GLY ILE PRO GLY ALA SER LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP
ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS HIS LYS ASP TYR ALA GLN GLU GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR
ASP TYR LEU MET GLN THR SER T1425 R1431 P1434 GLY GLN GLU PRO ALA N1440 V1441 W1442 V1443 G1444 W1445 I1446 T1447 S1448 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 E1472 H1477 E1478 S1479 I1480 K1481 R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO
GLY GLN GLY ARG ASN N1502 E1506 I1507 V1510 V1511 ASP ALA ALA SER G1516 F1520 T1521 A1522 Y1530 Y1531 P1535 L1539 F1540 P1541 T1548 S1549 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 G1569 L1570 S1573 V1579 P1580 H1587 V1588 Q1589 L1595
W1596 S1597 R1598 M1599 P1600 K1605 S1609 R1610 I1611 S1612 E1613 R1614 W1617 L1618 V1619 Q1620 C1621 L1622 Q1626 F1627 M1628 S1629 L1630 E1634 E1635 N1636 R1637 I1641 T1645 Y1655 R1659 L1660 Y1661 G1668 N1669 H1670 L1676 E1682 P1683 Q1684 L1685 K1692 P1695 R1699
Y1703 I1709 S1712 S1713 Y1714 A1715 R1718 L1719 N1722 P1728 M1729 T1730 K1734 S1735 I1736 T1737 L1738 D1741 GLU ASN LYS LYS HIS G1747 I1751 G1752 L1753 S1756 L1757 R1758 P1759 R1760 P1766 S1767 F1768 V1769 C1775 Y1776 Q1777 Y1778 D1785 K1790 M1794 V1799

R1807 D1808 P1809 L1817 L1821 L1828 L1839 I1842 I1846 E1847 P1848 S1849 VAL PHE LYS GLU ALA ALA GLY PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU PRO CYS ALA SER GLU GLU ASP SER ARG LEU GLU GLY PRO ALA GLU GLU GLU SER LYS GLY GLY LYS ARG PRO LYS

GLU G1893 L1894 L1905 Q1918 H1921 R1922 A1925 A1928 Q1938 Q1941 R1944 Y1945 N1953 MET SER ALA ALA LEU THR ALA ARG LYS THR LYS GLU PHE ARG SER PRO PRO GLN GLU GLN ILE ASN MET LEU LEU ASN PHE LYS ASP ASP LYS SER GLU C1987 P1988 C1989 P1990

D2013 GLU ASP GLY SER LEU ASP GLY ASN SER ASP L2024 T2025 R2029 V2037 T2038 Y2039 LEU LYS LYS LYS GLN ALA ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS LYS SER SER T2058 Q2061 S2064 W2070 S2074 V2075 I2076 P2079 E2080 L2081 H2090 Y2093 Y2107

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V2228 GLY LEU ALA SER PRO ALA MET ARG GLY SER T2239 L2254 L2258 D2262 L2263 L2275 GLN SER CYS GLN MET LEU VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 G2296 Y2299 F2308 S2313 R2323 I2326 R2327 R2328 P2329 E2330 CYS PHE GLY PRO

ALA LEU ARG GLY GLU GLY GLY ASN G2343 I2354 ALA GLU ASP PRO SER ARG ASP GLY PRO SER PRO THR SER GLY SER SER LYS MET PRO ASP THR GLU GLY GLU GLU ASP THR ILE HIS MET G2386 T2391 R2402 C2403 A2404 L2409 A2412 I2418 R2421 S2422 I2423 L2424

R2425 P2429 L2430 L2433 V2434 G2435 V2436 I2437 S2438 Q2442 MET PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 H2465 L2473 D2474 R2475 V2476 Y2477 GLY ILE GLU V2481 Q2482 L2485 L2503 ASP THR ALA ALA LEU SER ALA T2511 A2514 L2515

N2518 L2528 L2529 THR ARG CYS ALA PRO L2535 F2536 A2537 H2541 H2542 A2543 I2546 L2550 V2553 TYR ARG LEU SER K2558 L2562 Q2566 R2567 D2568 S2576 ILE CYS GLY GLN LEU ARG F2583 N2601 GLU HIS ALA K2605 M2606 P2607 L2611 G2627 TRP GLY ASN PHE GLY

ALA A2634 L2639 R2643 K2644 W2647 G2648 L2653 SER GLN LYS LYS Y2658 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 V2707 D2708 T2709 S2710 N2711 I2712 T2713 I2714 P2715 E2716 K2717 L2718 E2719 Y2720

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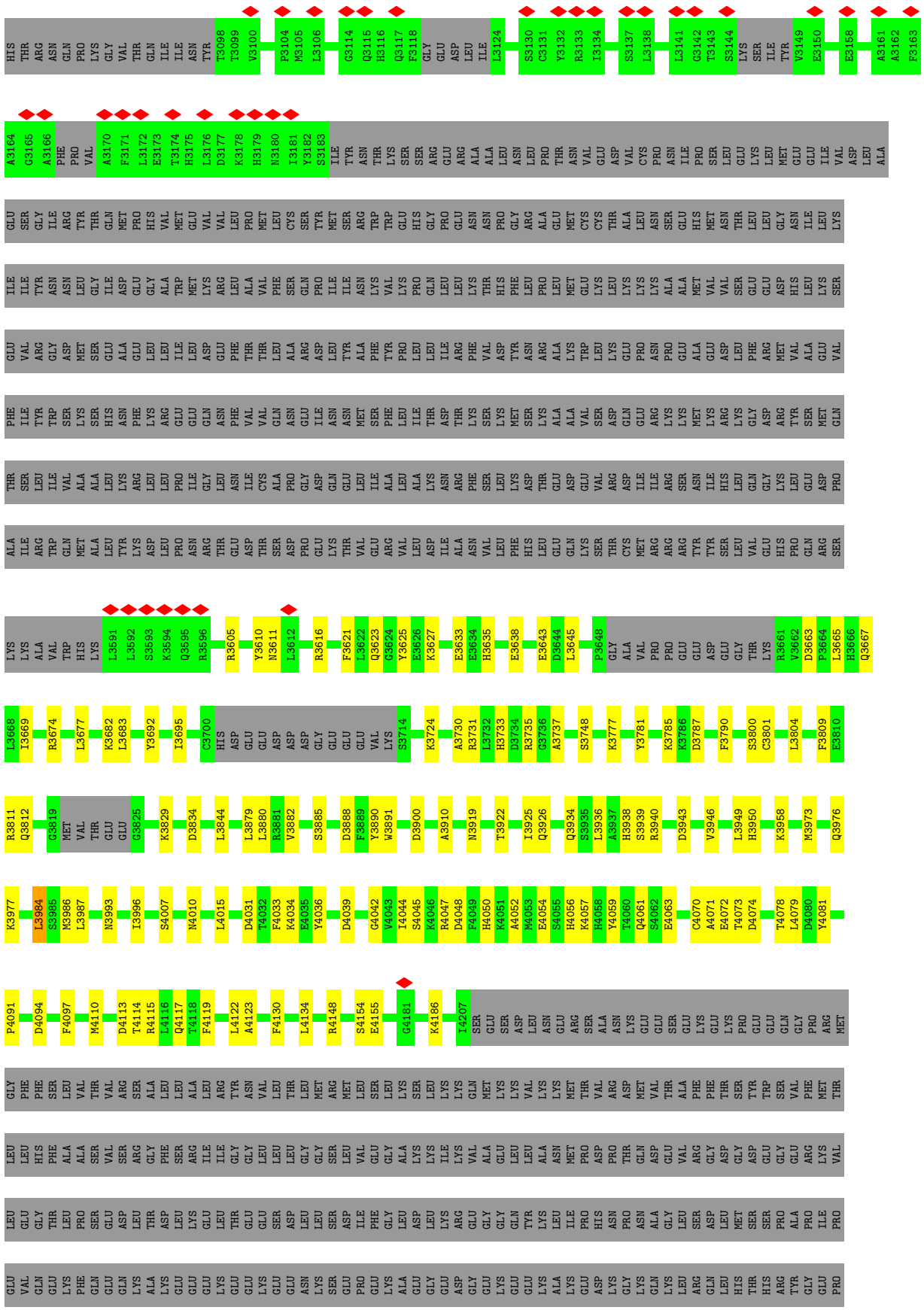
G2901 Y2902 A2903 V2904 S2905 R2906 G2907 PHE LYS ASP LEU GLU LEU ASP THR PRO SER ILE GLU LYS ARG PHE ALA TYR SER PHE LEU GLN GLN LEU ILE ARG TYR VAL ASP GLU ALA HIS GLN TYR ILE LEU GLU PHE ASP GLY GLY SER ARG SER LYS GLY GLU HIS PHE PRO TYR GLU GLN GLU

ILE LYS PHE PHE ALA LYS VAL VAL LEU PRO LEU ILE ASP GLN TYR PHE LYS ASN HIS ARG LEU Y2982 F2983 K3002 V3005 THR SER LEU F3009 V3016 I3020 T3028 SER ILE VAL ASN CYS L3034 K3055 SER ALA LEU ARG ALA F3061 L3062 D3068 T3072 G3079 T3082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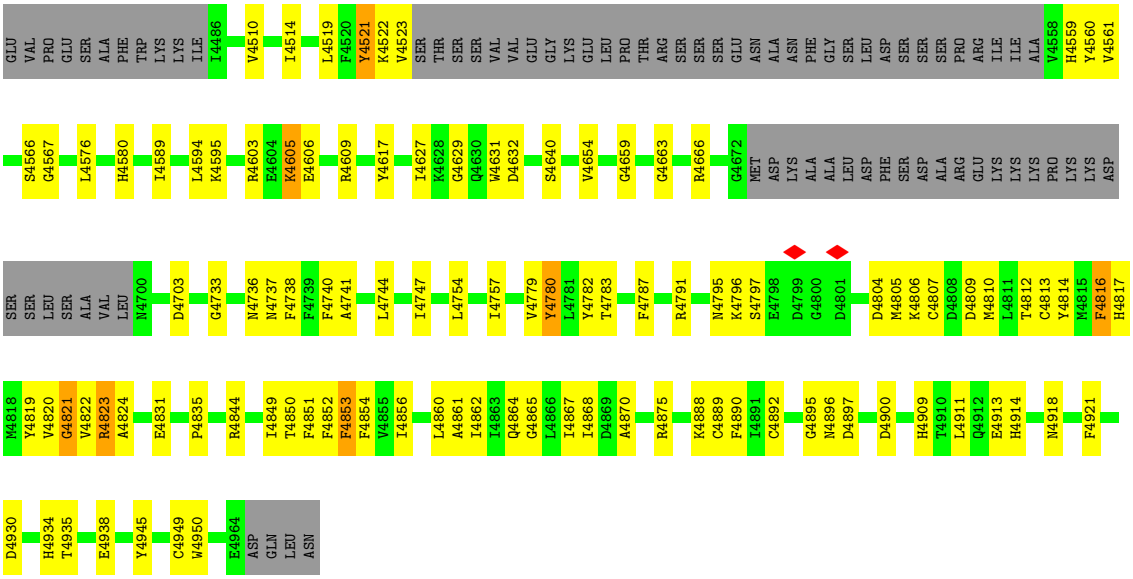
A3164 G3165 A3166 PHE PRO VAL A3170 F3171 L3172 E3173 T3174 H3175 L3176 D3177 K3178 H3179 N3180 I3181 Y3182 S3183 ILE TYR ASN THR LYS SER SER ARG GLU ARG ALA ALA LEU ASN LEU PRO THR ASN VAL GLU ASP VAL CYS PRO ASN ILE PRO SER LEU GLU LYS LEU MET GLU GLU ILE VAL ASP LEU ALA
GLU SER GLY ILE ARG TYR THR GLN MET PRO HIS VAL MET GLU VAL VAL LEU PRO MET LEU CYS SER TYR MET SER ARG TRP TRP GLU HIS GLY PRO GLU ASN ASN PRO GLY ARG ALA GLU MET CYS CYS THR ALA LEU ASN SER GLU HIS MET ASN THR LEU LEU GLY ASN ILE LEU LYS
ILE ILE TYR ASN ASN LEU GLY ILE ASP GLU GLY ALA TRP MET LYS ARG LEU ALA VAL PHE SER GLN PRO ILE ILE ASN ASN LYS VAL LYS PRO GLN LEU LEU LYS THR HIS PHE LEU PRO LEU MET GLU LYS LYS LYS LYS ALA ALA MET VAL VAL SER GLU GLU ASP HIS LEU LYS SER
GLU VAL ARG GLY ASP MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA ARG MET VAL ALA GLU VAL
PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG GLU GLN GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE ILE ILE SER LYS MET SER LYS ALA VAL SER ASP GLN GLU ARG LYS LYS GLY ASP ARG TYR SER MET GLN
THR SER LEU ILE VAL ALA ALA ALA LEU LYS ARG LEU LEU PRO ILE GLY LEU ASN ILE CYS ALA PRO GLY ASP GLN GLU LEU ILE ALA LEU ALA LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP GLU VAL ARG ASP ILE ILE ARG LEU LEU GLU ASP PRO
ALA ILE ARG TRP GLN MET ALA LEU TYR LYS ASP LEU PRO ASN ARG THR GLU ASP THR SER ASP PRO GLU LYS THR VAL GLU ARG VAL LEU ASP ILE ALA ASN VAL LEU PHE HIS LEU GLU GLN LYS SER THR CYS MET ARG ARG ARG TYR TYR SER LEU VAL GLU HIS PRO GLN ARG SER
LYS LYS ALA VAL TRP HIS LYS L3591 L3592 S3593 K3594 Q3595 R3596 R3605 Y3610 N3611 L3612 R3616 F3621 L3622 Q3623 G3624 Y3625 E3626 K3627 E3633 E3634 H3635 E3638 E3643 D3644 L3645 P3648 GLY ALA VAL PRO PRO GLU GLU ASP GLU THR LYS R3661 V3662 D3663 P3664 L3665 H3666 Q3667
L3668 I3669 R3674 L3677 K3682 L3683 Y3692 I3695 C3700 HIS ASP GLU GLU ASP ASP ASP GLY GLU GLU GLU VAL LYS S3714 K3724 A3730 R3731 L3732 H3733 D3734 R3735 G3736 A3737 S3748 K3777 Y3781 K3785 K3786 D3787 F3790 S3800 C3801 L3804 F3809 E3810
R3811 Q3812 G3819 MET VAL THR GLU GLU G3825 K3829 D3834 L3844 L3879 L3880 R3881 V3882 S3885 D3888 F3889 Y3890 W3891 D3900 A3910 N3919 T3922 I3925 Q3926 Q3934 S3935 L3936 A3937 H3938 S3939 R3940 D3943 V3946 L3949 H3950 K3958 M3973 Q3976
K3977 L3984 S3985 M3986 L3987 N3993 I3996 S4007 N4010 L4015 D4031 T4032 F4033 K4034 E4035 Y4036 D4039 G4042 V4043 I4044 S4045 K4046 R4047 D4048 F4049 H4050 K4051 A4052 M4053 E4054 S4055 H4056 K4057 H4058 Y4059 T4060 Q4061 S4062 E4063 C4070 A4071 E4072 T4073 D4074 T4078 L4079 D4080 Y4081
P4091 D4094 F4097 M4110 D4113 T4114 R4115 L4116 Q4117 T4118 F4119 L4122 A4123 F4130 L4134 R4148 S4154 E4155 G4181 K4186 I4207 SER GLU SER ASP LEU ASN GLU ARG SER ALA ASN LYS GLU GLU SER GLU LYS GLU LYS PRO GLU GLU GLN GLY PRO ARG MET
GLY PHE PHE SER LEU VAL THR VAL ARG SER ALA LEU LEU ALA LEU ARG TYR ASN VAL LEU THR LEU MET ARG MET LEU SER LEU LYS LYS VAL LYS LYS MET LYS SER LEU LYS LYS GLN MET MET LYS LYS VAL ALA MET THR VAL ARG ASP MET VAL THR ALA PHE PHE THR SER TYR TRP SER VAL PHE MET THR
LEU LEU HIS PHE ALA ALA SER ARG GLY PHE SER ARG ILE ILE GLY GLY LEU LEU SER ARG GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU ALA ASN ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLY GLY ASP GLU GLU GLN GLY GLU GLU ARG LYS VAL
LEU GLU GLY THR LEU PRO SER GLU ASP LEU THR GLU GLU SER ASP LEU LEU SER ASP ILE PHE GLY LEU ASP LEU GLY GLY GLN TYR LYS ARG GLU GLY GLN LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET SER SER PRO ALA GLU GLU ARG PRO ILE PRO
GLU VAL GLN GLU LYS PHE GLN GLU GLN LYS ALA LYS LYS GLU GLU LYS SER GLU PRO GLU LYS ALA GLU GLY GLU ASP GLY GLU LYS GLU LYS ALA ALA LYS GLU LYS SER GLU ASP LYS GLY GLN LYS LEU ARG GLN LEU HIS THR HIS ARG TYR GLY GLU ARG



- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

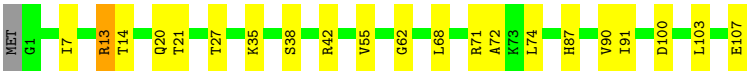
Chain B:

- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

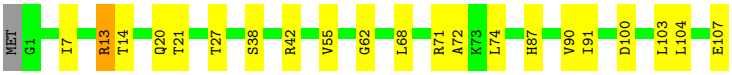
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



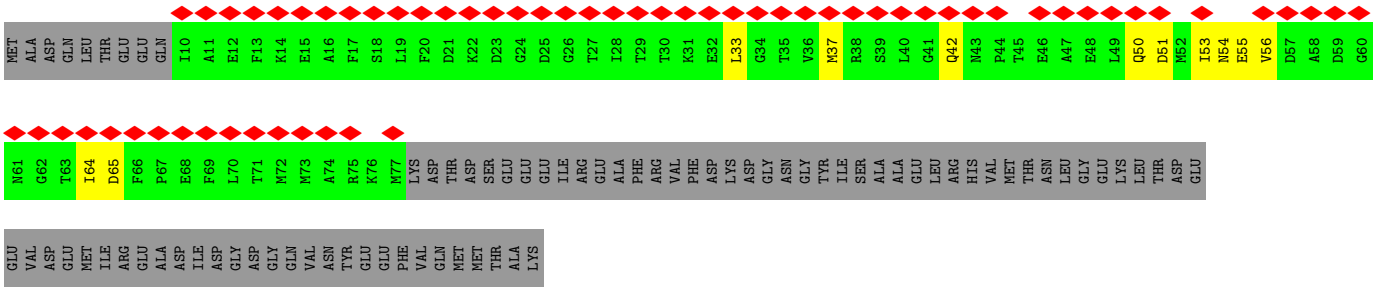
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:



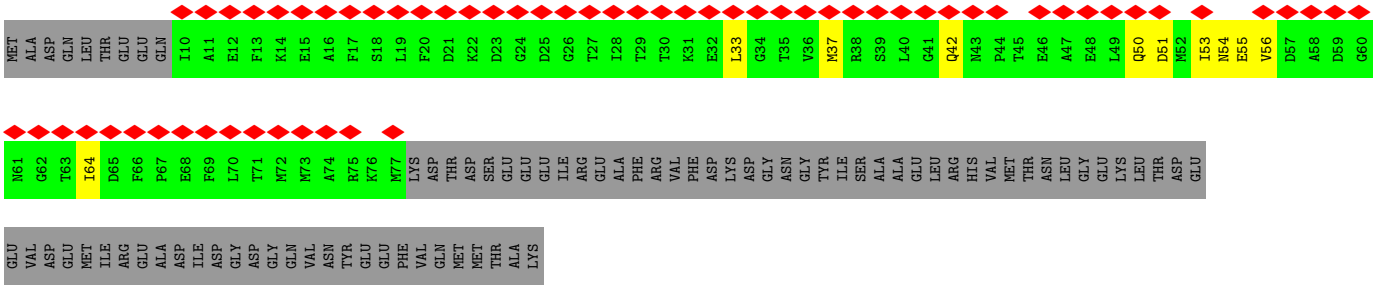
- Molecule 3: Calmodulin-1

Chain C:



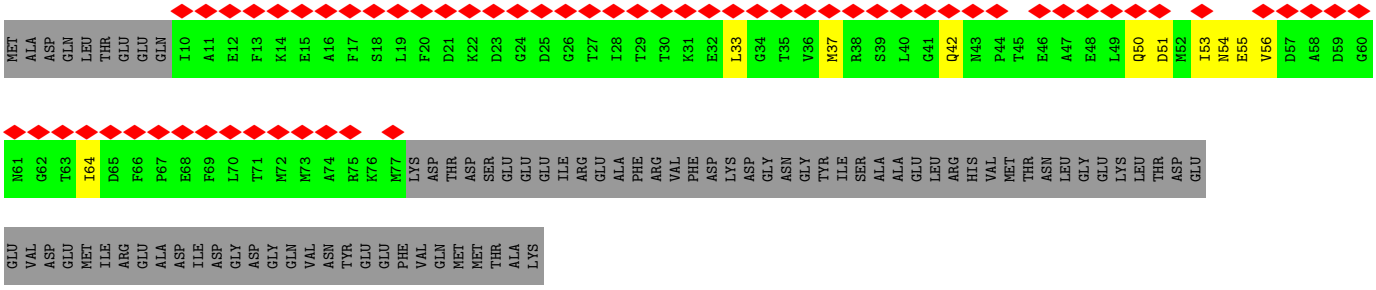
- Molecule 3: Calmodulin-1

Chain F:



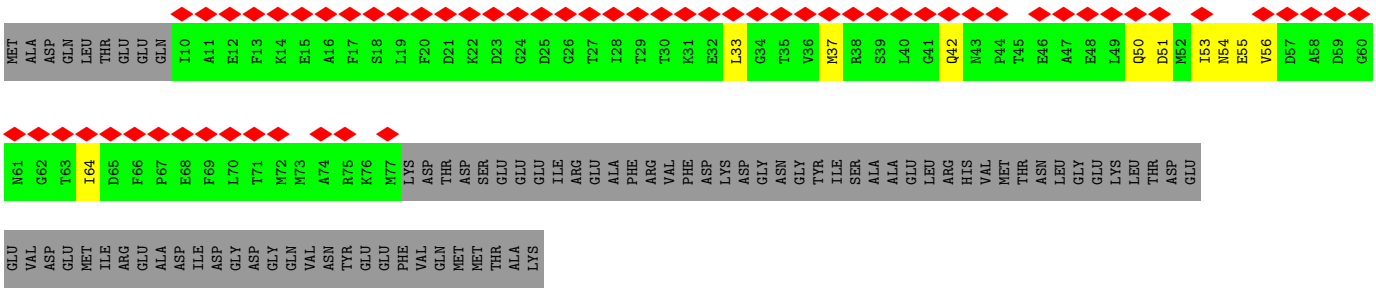
- Molecule 3: Calmodulin-1

Chain I:



- Molecule 3: Calmodulin-1

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	77092	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 ($e^-/Å^2$)	45.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	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, ATP, CA, CFF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.35	2/27161 (0.0%)	0.55	7/36737 (0.0%)
1	D	0.34	0/27161	0.55	9/36737 (0.0%)
1	G	0.34	0/27161	0.55	5/36737 (0.0%)
1	J	0.34	0/27161	0.55	6/36737 (0.0%)
2	B	0.33	0/835	0.53	0/1123
2	E	0.33	0/835	0.53	0/1123
2	H	0.33	0/835	0.53	0/1123
2	K	0.33	0/835	0.53	0/1123
3	C	0.29	0/530	0.49	0/711
3	F	0.29	0/530	0.49	0/711
3	I	0.29	0/530	0.49	0/711
3	L	0.29	0/530	0.49	0/711
All	All	0.34	2/114104 (0.0%)	0.55	27/154284 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23
1	D	0	23
1	G	0	23
1	J	0	23
All	All	0	92

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4521	TYR	N-CA	7.55	1.61	1.46
1	A	4522	LYS	CA-C	-6.22	1.36	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4823	ARG	N-CA-C	10.38	139.02	111.00
1	D	4823	ARG	CB-CA-C	-7.98	94.43	110.40
1	A	730	LEU	CA-CB-CG	6.89	131.16	115.30
1	D	730	LEU	CA-CB-CG	6.89	131.16	115.30
1	G	730	LEU	CA-CB-CG	6.89	131.16	115.30

There are no chirality outliers.

5 of 92 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	PHE	Peptide
1	A	728	ASP	Peptide
1	A	729	GLY	Peptide
1	A	739	ARG	Peptide
1	A	816	PRO	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	26661	0	25136	600	0
1	D	26661	0	25136	589	0
1	G	26661	0	25136	605	0
1	J	26661	0	25136	598	0
2	B	819	0	824	15	0
2	E	819	0	824	15	0
2	H	819	0	824	14	0
2	K	819	0	824	14	0
3	C	524	0	504	8	0
3	F	524	0	504	7	0
3	I	524	0	504	7	0
3	L	524	0	504	7	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0
5	J	1	0	0	0	0
5	L	2	0	0	0	0
6	A	31	0	12	0	0
6	D	31	0	12	0	0
6	G	31	0	12	0	0
6	J	31	0	12	0	0
7	A	14	0	10	1	0
7	D	14	0	10	1	0
7	G	14	0	10	1	0
7	J	14	0	10	1	0
All	All	112212	0	105944	2282	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 10.

The worst 5 of 2282 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:A:4852:PHE:CZ	1:D:4823:ARG:HA	1.59	1.37
1:G:4861:ALA:CB	1:J:4864:GLN:HE21	1.53	1.22
1:D:4861:ALA:CB	1:G:4864:GLN:HE21	1.52	1.22
1:A:4861:ALA:CB	1:D:4864:GLN:HE21	1.52	1.21
1:A:4782:TYR:CD2	1:A:4851:PHE:CD1	2.30	1.20

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	3374/4968 (68%)	3009 (89%)	357 (11%)	8 (0%)	47	80
1	D	3374/4968 (68%)	3012 (89%)	355 (10%)	7 (0%)	47	80
1	G	3374/4968 (68%)	3012 (89%)	354 (10%)	8 (0%)	47	80
1	J	3374/4968 (68%)	3010 (89%)	355 (10%)	9 (0%)	41	76
2	B	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	E	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	H	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	K	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
3	C	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
3	F	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
3	I	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	L	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
All	All	14180/20900 (68%)	12694 (90%)	1454 (10%)	32 (0%)	50	80

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4823	ARG
1	J	4823	ARG
1	G	4823	ARG
1	A	730	LEU
1	A	853	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	2672/4355 (61%)	2653 (99%)	19 (1%)	84	90
1	D	2671/4355 (61%)	2650 (99%)	21 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	2671/4355 (61%)	2651 (99%)	20 (1%)	84	90
1	J	2671/4355 (61%)	2653 (99%)	18 (1%)	84	90
2	B	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	E	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	H	88/89 (99%)	87 (99%)	1 (1%)	73	84
2	K	88/89 (99%)	87 (99%)	1 (1%)	73	84
3	C	57/127 (45%)	57 (100%)	0	100	100
3	F	57/127 (45%)	57 (100%)	0	100	100
3	I	57/127 (45%)	57 (100%)	0	100	100
3	L	57/127 (45%)	57 (100%)	0	100	100
All	All	11265/18284 (62%)	11183 (99%)	82 (1%)	84	90

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	4780	TYR
1	J	1683	PRO
1	G	4818	MET
1	J	841	LYS
1	J	2836	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 162 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	3993	ASN
1	J	2196	ASN
1	G	4864	GLN
1	J	604	HIS
1	J	3852	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 24 ligands modelled in this entry, 16 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	$\#\|Z\| > 2$
7	CFF	J	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	1 (12%)
6	ATP	G	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
7	CFF	A	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	1 (12%)
7	CFF	D	6003	-	8,15,15	2.60	4 (50%)	8,23,23	1.30	1 (12%)
7	CFF	G	6003	-	8,15,15	2.61	4 (50%)	8,23,23	1.31	1 (12%)
6	ATP	J	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
6	ATP	D	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)
6	ATP	A	6002	-	26,33,33	0.90	1 (3%)	31,52,52	1.46	5 (16%)

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
7	CFF	J	6003	-	-	-	0/2/2/2
6	ATP	G	6002	-	-	7/18/38/38	0/3/3/3
7	CFF	A	6003	-	-	-	0/2/2/2
7	CFF	D	6003	-	-	-	0/2/2/2
7	CFF	G	6003	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	J	6002	-	-	7/18/38/38	0/3/3/3
6	ATP	D	6002	-	-	7/18/38/38	0/3/3/3
6	ATP	A	6002	-	-	7/18/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	6003	CFF	C5-C4	-4.65	1.33	1.39
7	D	6003	CFF	C5-C4	-4.63	1.33	1.39
7	A	6003	CFF	C5-C4	-4.61	1.33	1.39
7	J	6003	CFF	C5-C4	-4.61	1.33	1.39
7	A	6003	CFF	C6-N1	-4.27	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})
6	A	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	D	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	G	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	J	6002	ATP	C3'-C2'-C1'	3.17	105.75	100.98
6	A	6002	ATP	PB-O3B-PG	-3.15	122.02	132.83

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C5'-O5'-PA-O3A
6	D	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C5'-O5'-PA-O3A
6	G	6002	ATP	C5'-O5'-PA-O2A

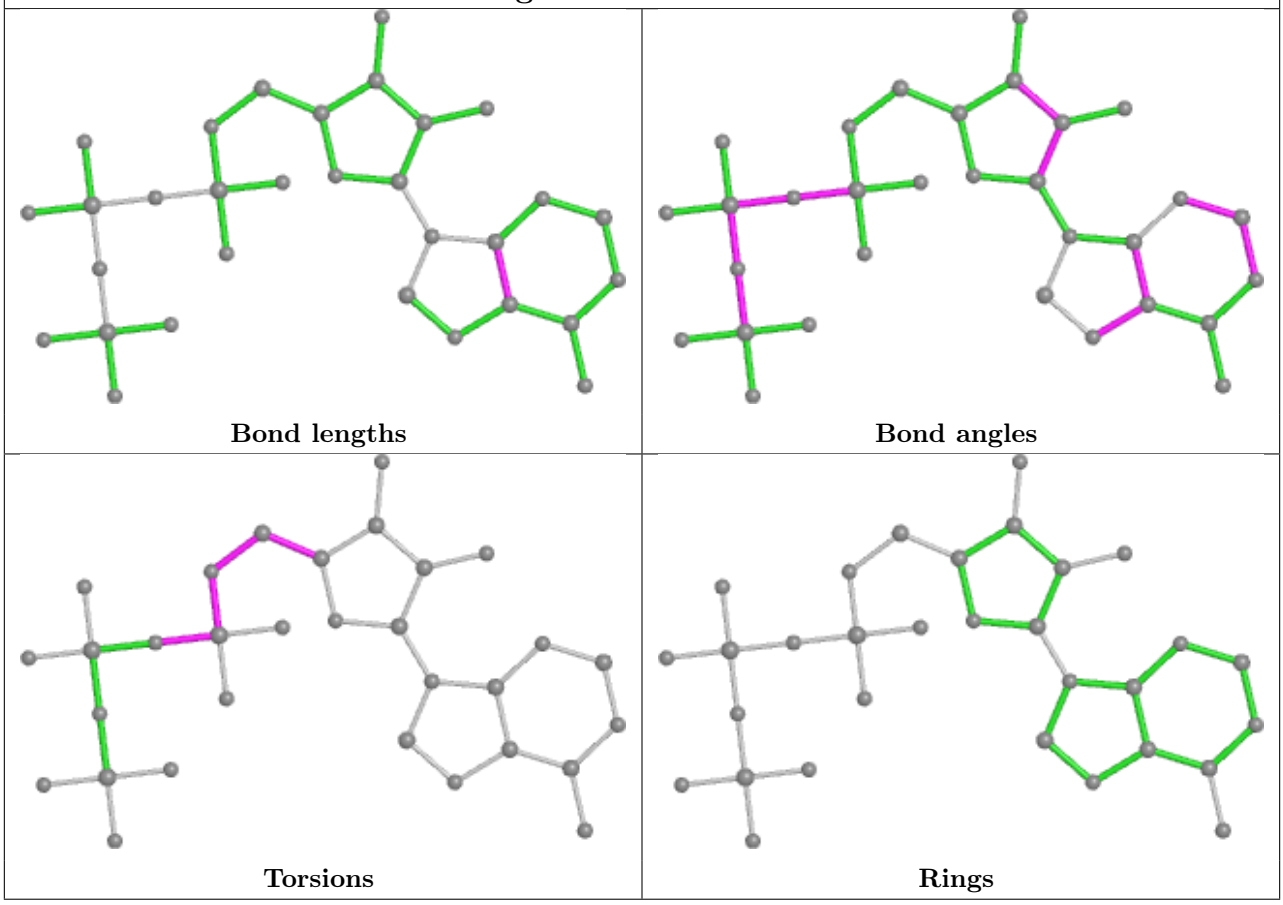
There are no ring outliers.

4 monomers are involved in 4 short contacts:

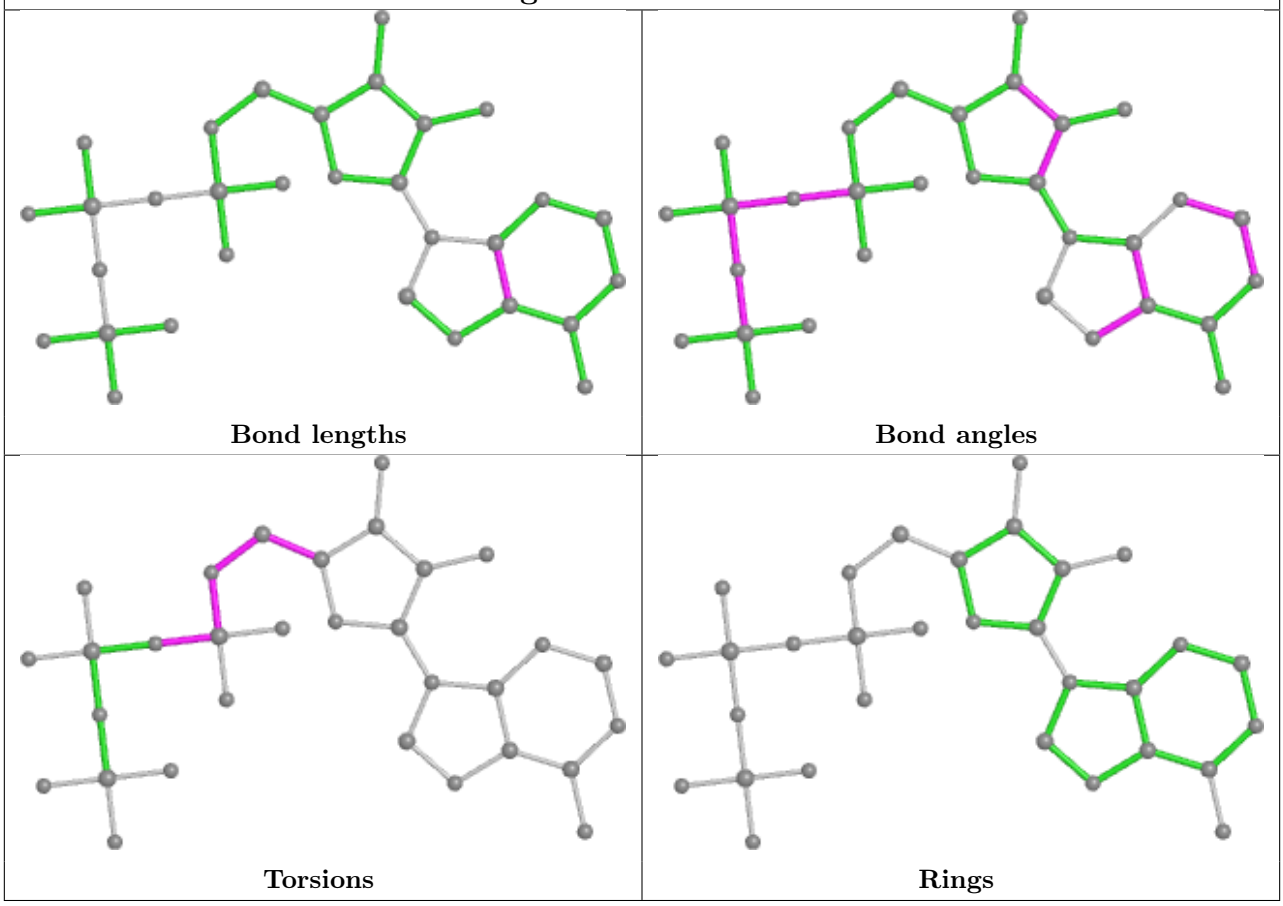
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	6003	CFF	1	0
7	A	6003	CFF	1	0
7	D	6003	CFF	1	0
7	G	6003	CFF	1	0

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.

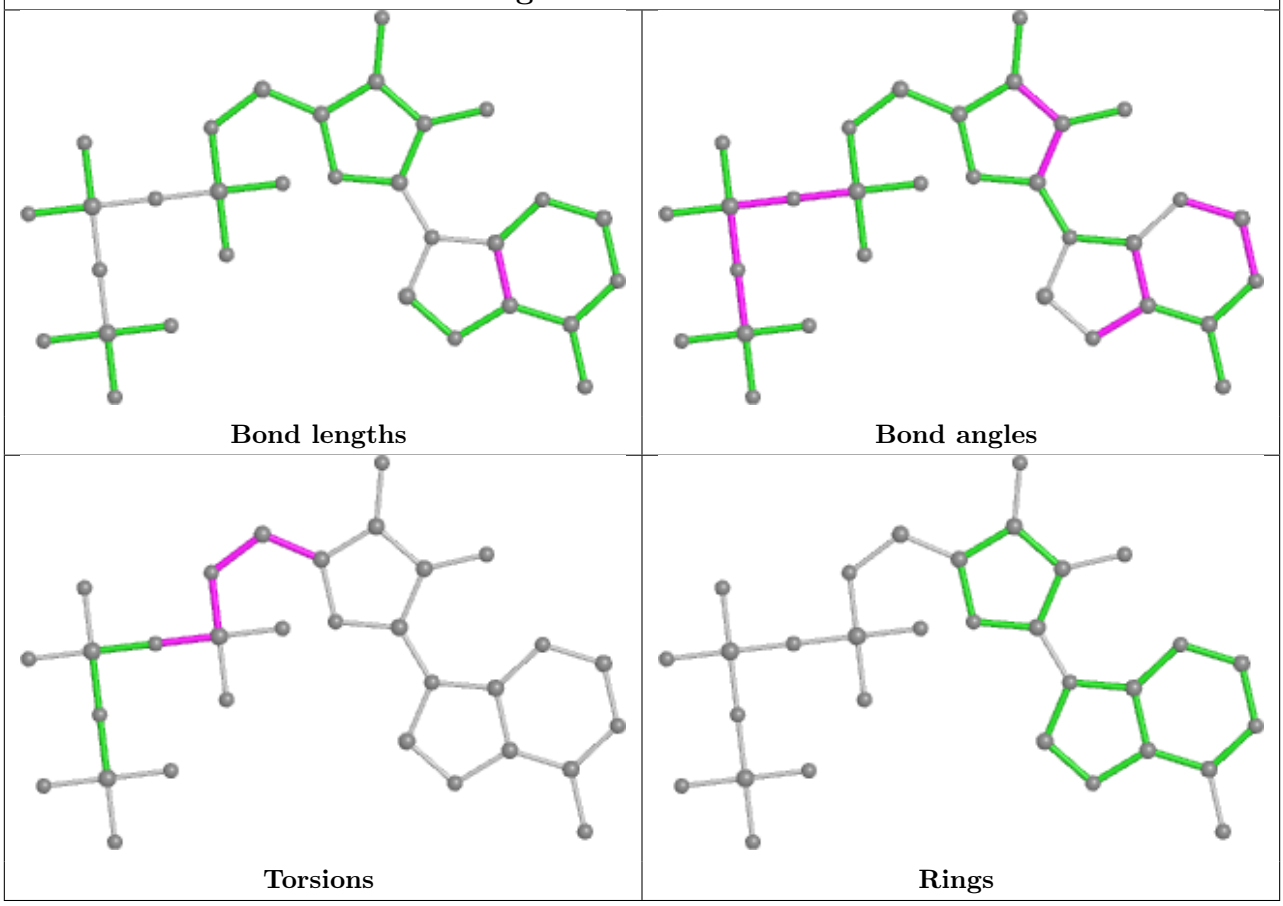
Ligand ATP G 6002



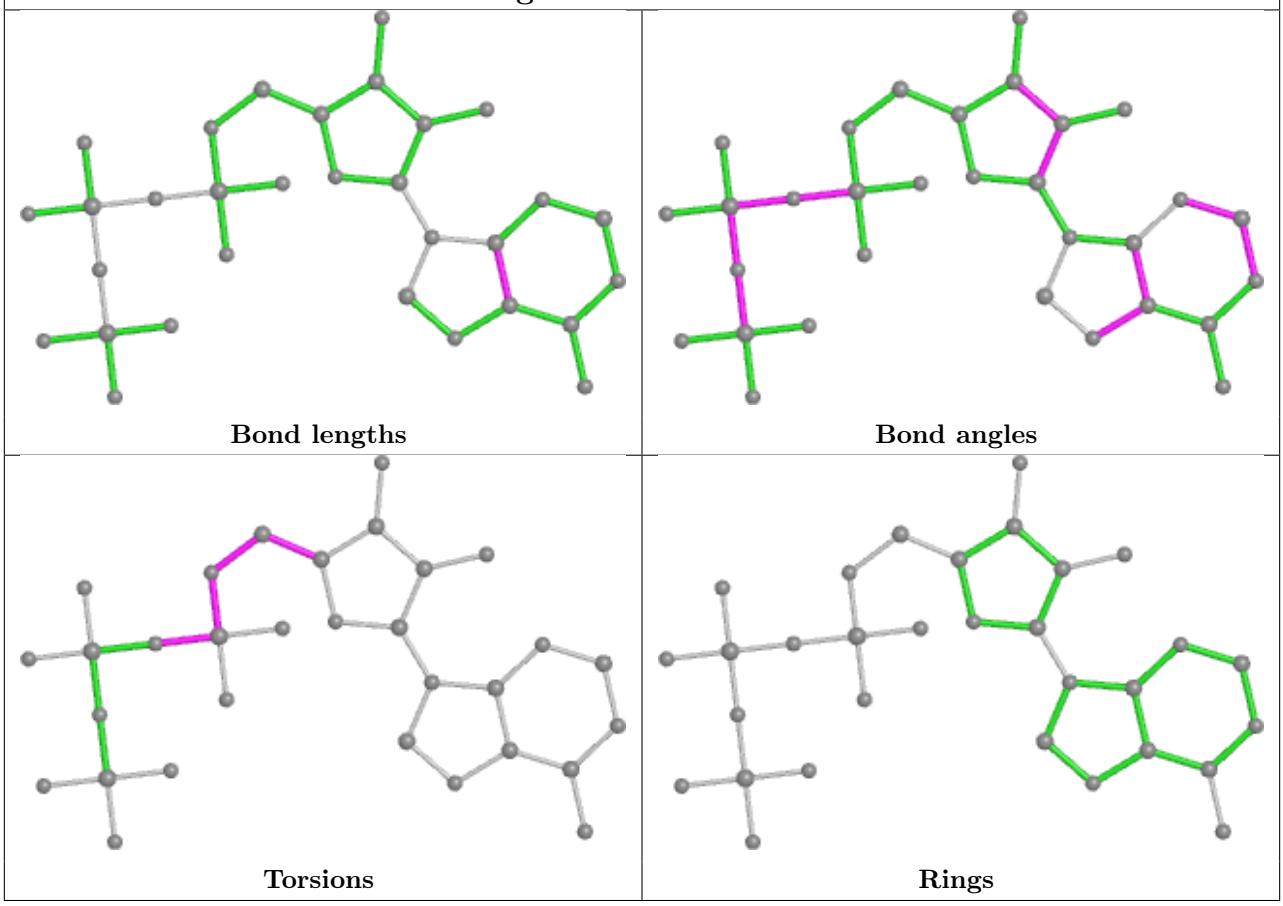
Ligand ATP J 6002



Ligand ATP D 6002



Ligand ATP A 6002



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.

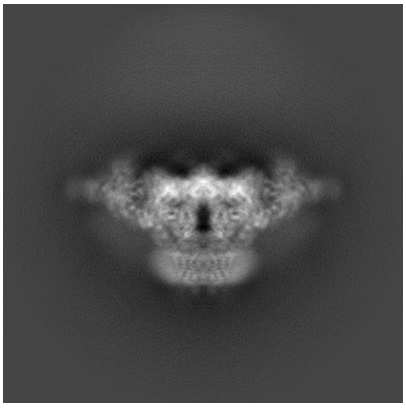
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9836. These allow visual inspection of the internal detail of the map and identification of artifacts.

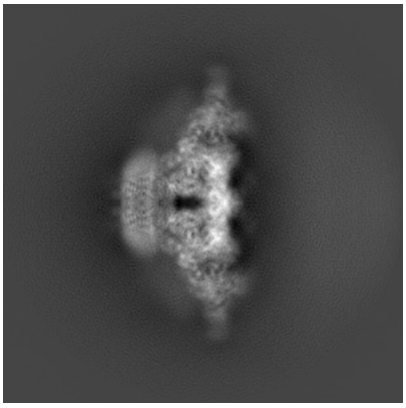
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

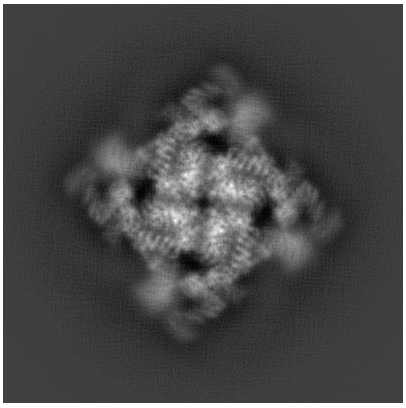
6.1.1 Primary map



X



Y

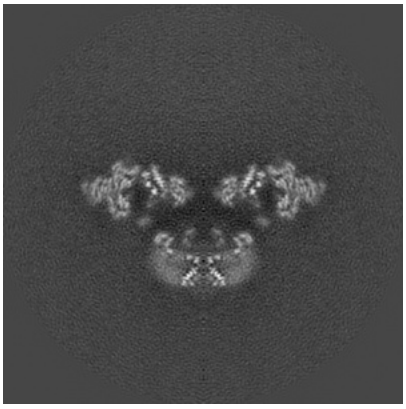


Z

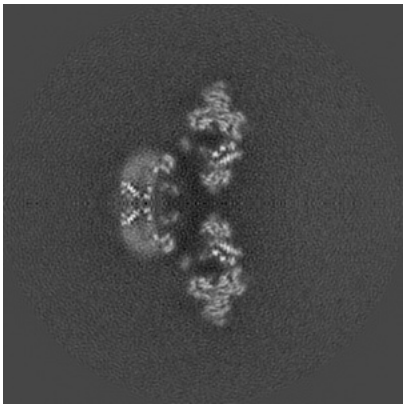
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

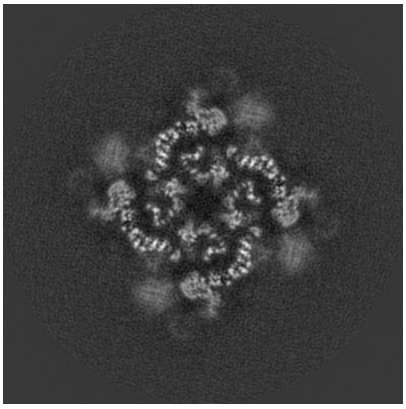
6.2.1 Primary map



X Index: 200



Y Index: 200

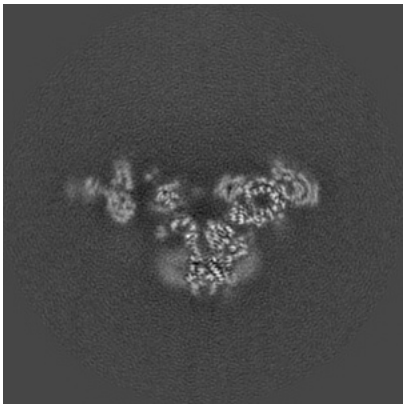


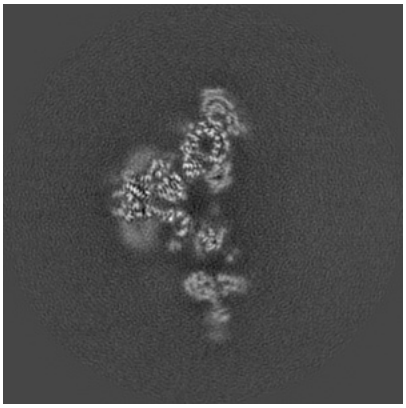
Z Index: 200

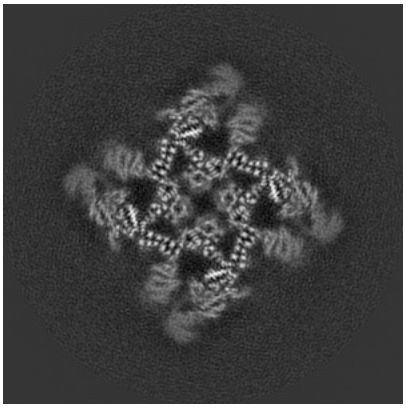
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 190

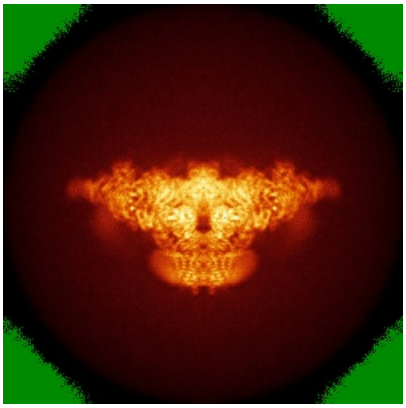

Y Index: 210

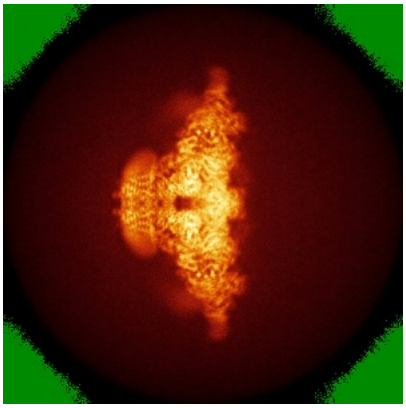

Z Index: 209

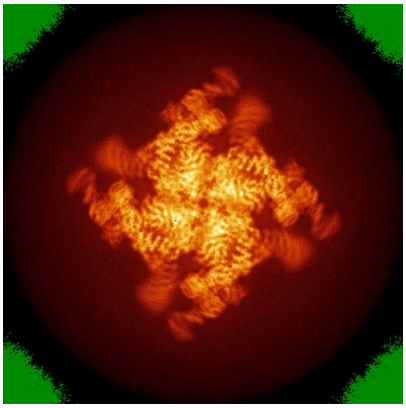
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

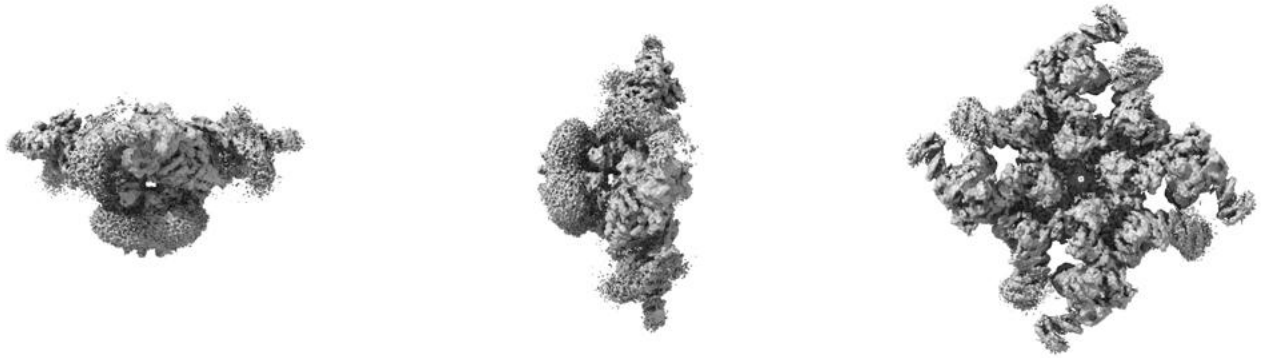

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

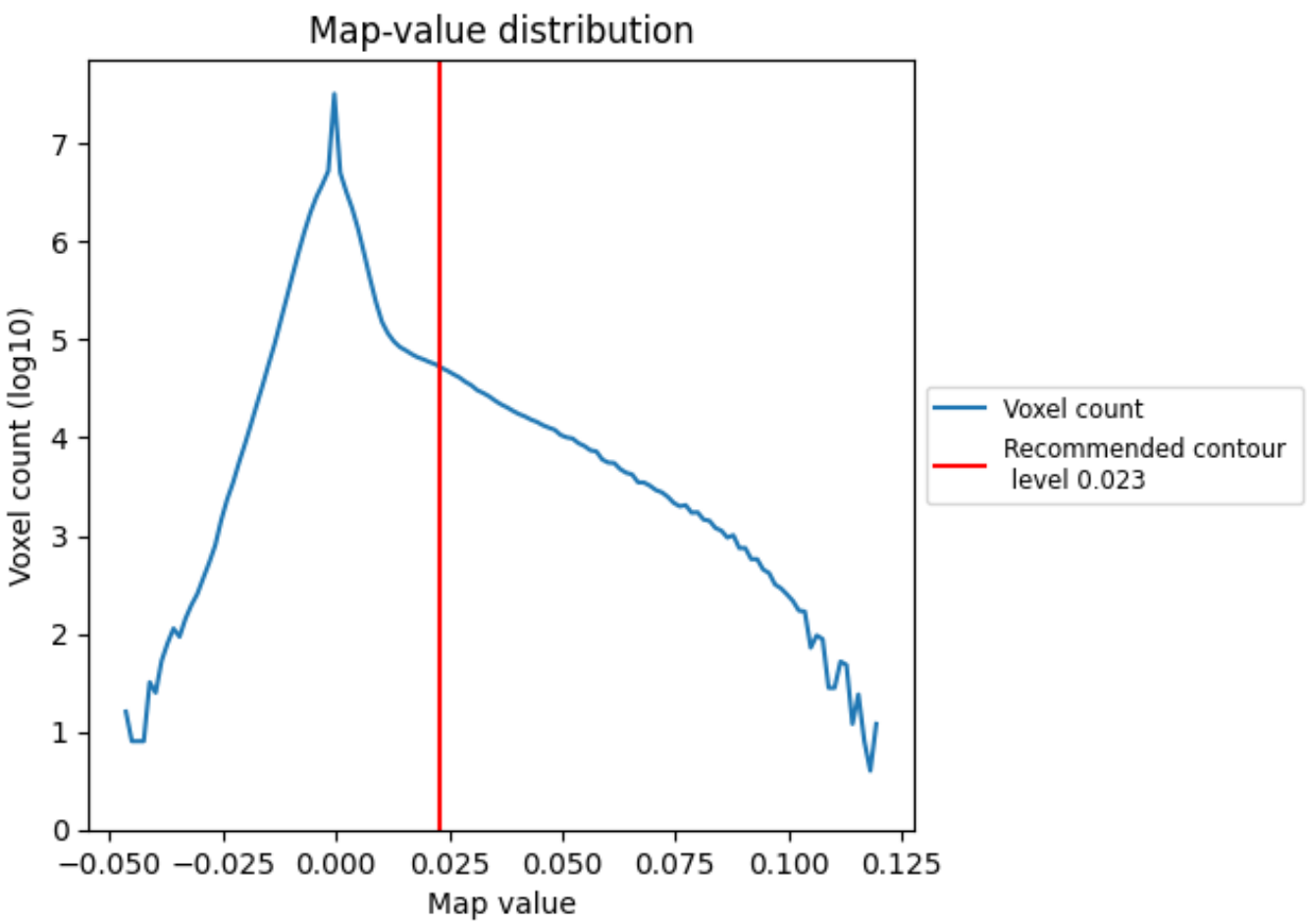
6.6 Mask visualisation (i)

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

7 Map analysis (i)

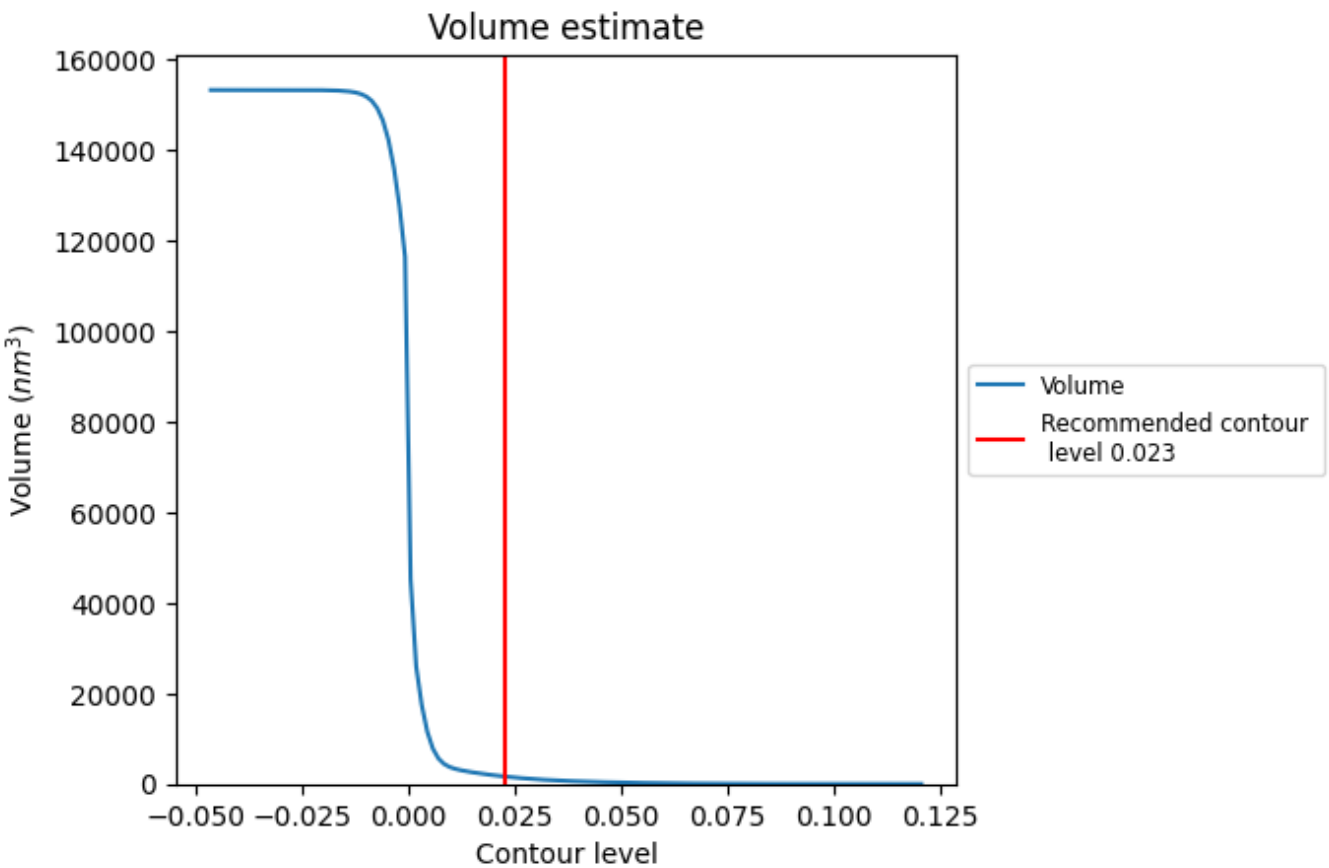
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

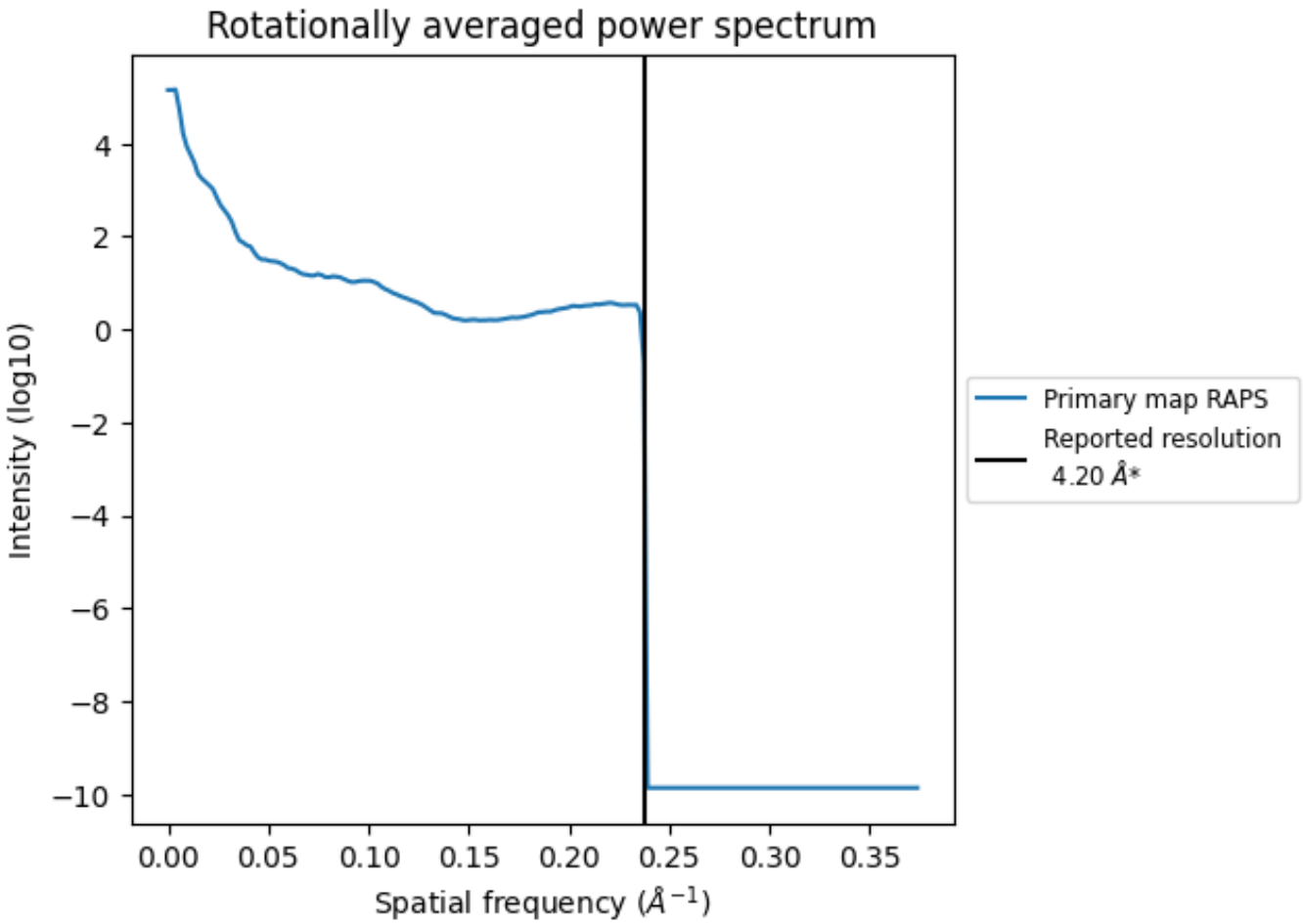
7.2 Volume estimate (i)



The volume at the recommended contour level is 1619 nm^3; this corresponds to an approximate mass of 1462 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

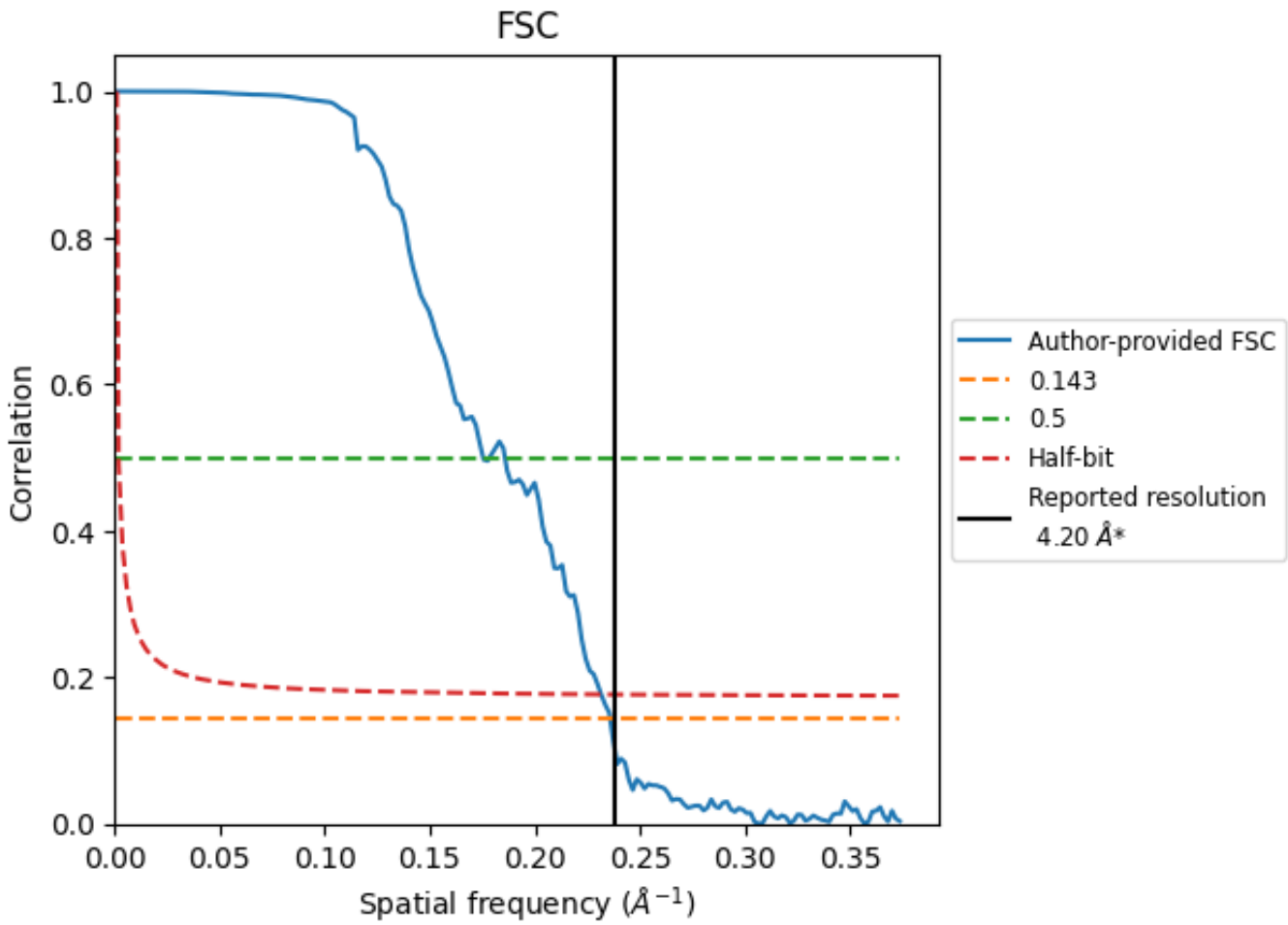


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



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

8.2 Resolution estimates (i)

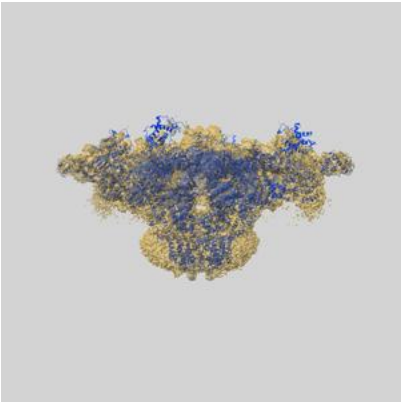
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.24	5.70	4.32
Unmasked-calculated*	-	-	-

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

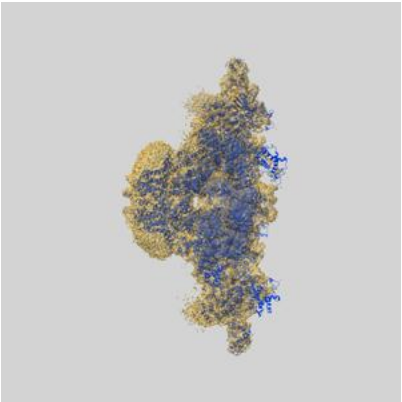
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9836 and PDB model 6JIU. Per-residue inclusion information can be found in section 3 on page 8.

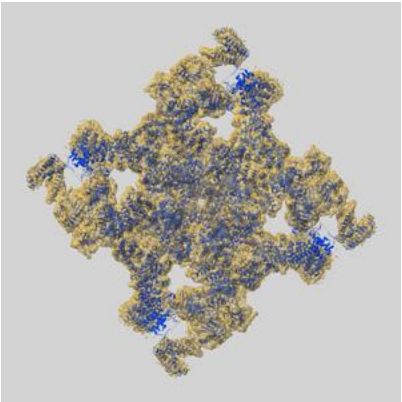
9.1 Map-model overlay (i)



X



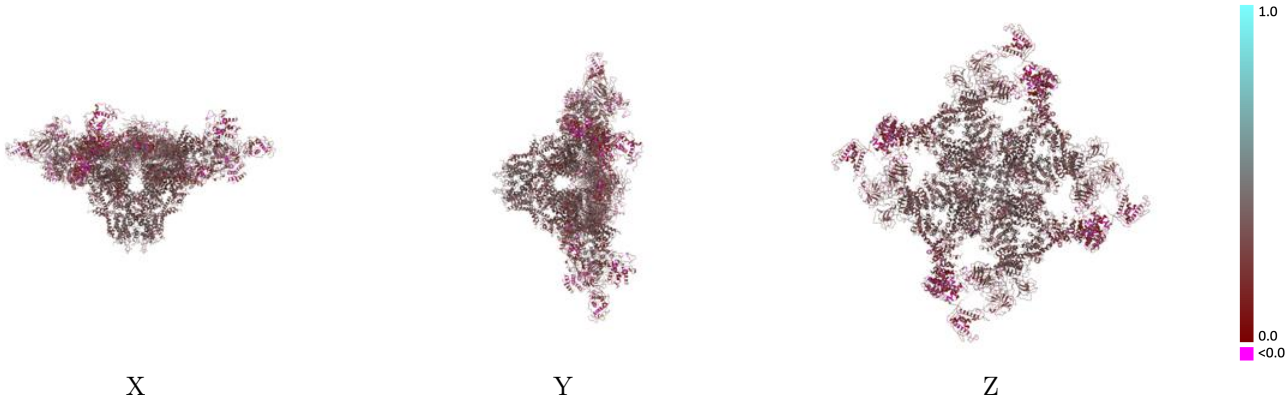
Y



Z

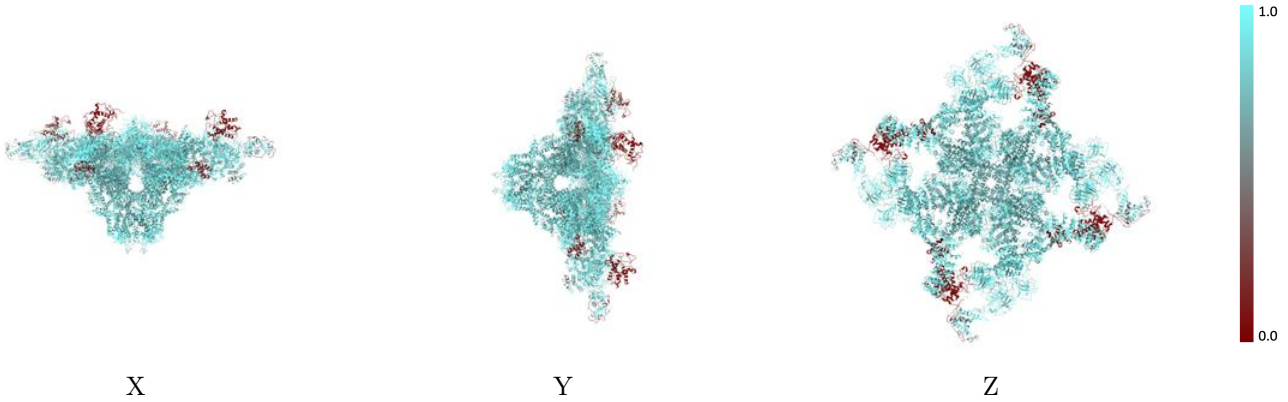
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



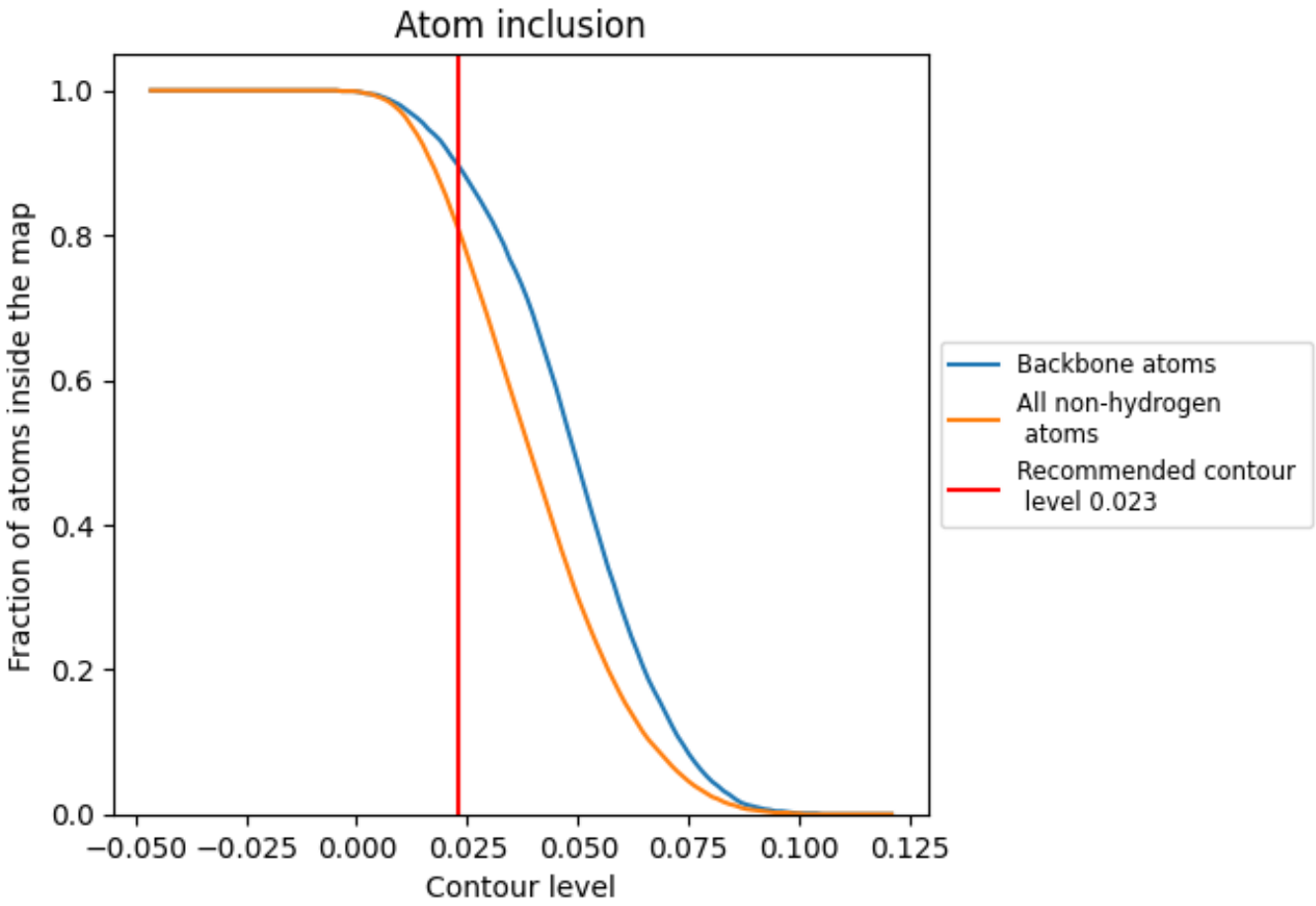
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (i)



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 (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.3030
A	0.8200	0.3050
B	0.8710	0.3450
C	0.1110	0.1780
D	0.8200	0.3050
E	0.8700	0.3430
F	0.1110	0.1750
G	0.8200	0.3040
H	0.8720	0.3420
I	0.1110	0.1790
J	0.8210	0.3040
K	0.8720	0.3420
L	0.1110	0.1800