wwPDB EM Validation Summary Report

Mar 19, 2024 – 11:01 PM JST

PDB ID	:	6JIY
EMDB ID	:	EMD-9837
Title	:	Structure of RyR2 (F/A/C/H-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	:	2019-02-24
Resolution	:	3.90 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 (i)) were used in the production of this report:

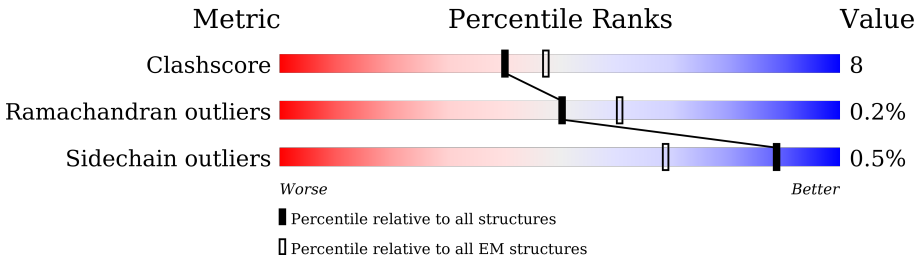
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	10% 59% 12% 29%
1	D	4968	10% 59% 12% 29%
1	G	4968	10% 59% 12% 29%
1	J	4968	10% 58% 12% 29%
2	B	108	81% 19%
2	E	108	84% 15%
2	H	108	84% 15%
2	K	108	82% 17%

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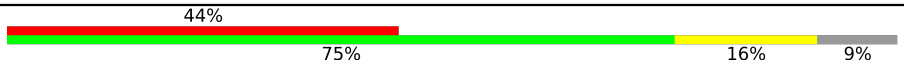
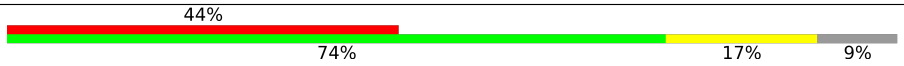
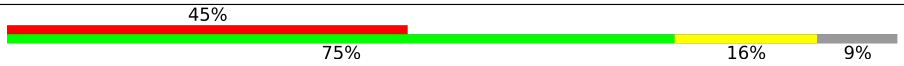
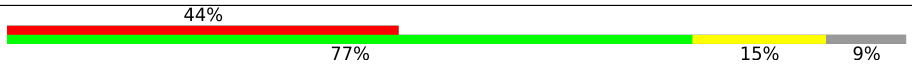
Mol	Chain	Length	Quality of chain
3	C	149	
3	F	149	
3	I	149	
3	L	149	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 115288 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
1	A	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	D	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	G	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	J	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		

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

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

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	F	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	I	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	L	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		

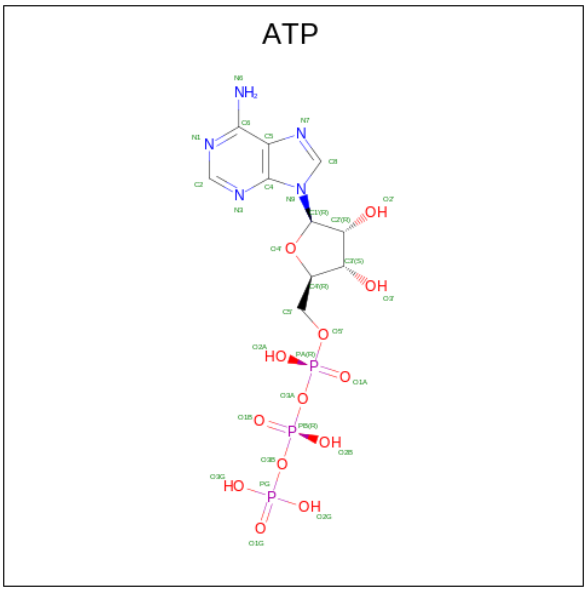
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

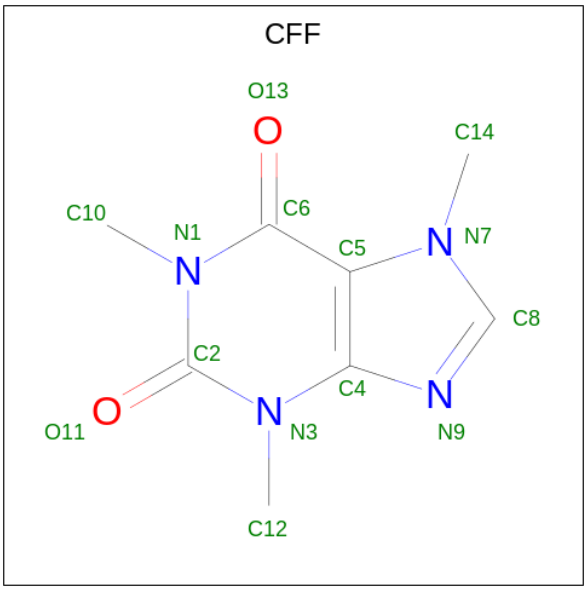
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Ca 1 1	0
5	C	4	Total Ca 4 4	0
5	D	1	Total Ca 1 1	0
5	F	4	Total Ca 4 4	0
5	G	1	Total Ca 1 1	0
5	I	4	Total Ca 4 4	0
5	J	1	Total Ca 1 1	0
5	L	4	Total Ca 4 4	0

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



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: $C_8H_{10}N_4O_2$).



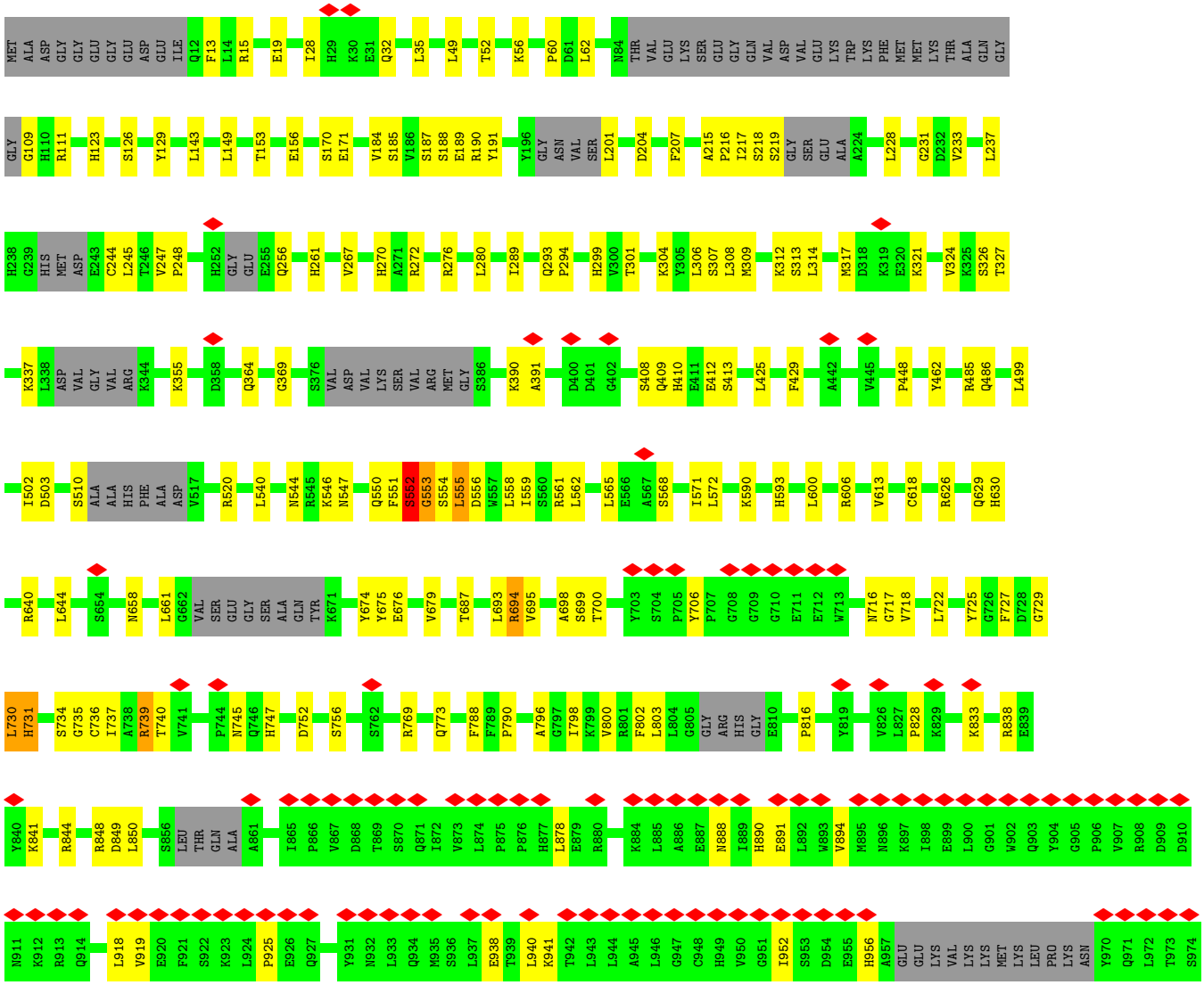
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	D	1	Total	C	N	O	0
			14	8	4	2	
7	G	1	Total	C	N	O	0
			14	8	4	2	
7	J	1	Total	C	N	O	0
			14	8	4	2	

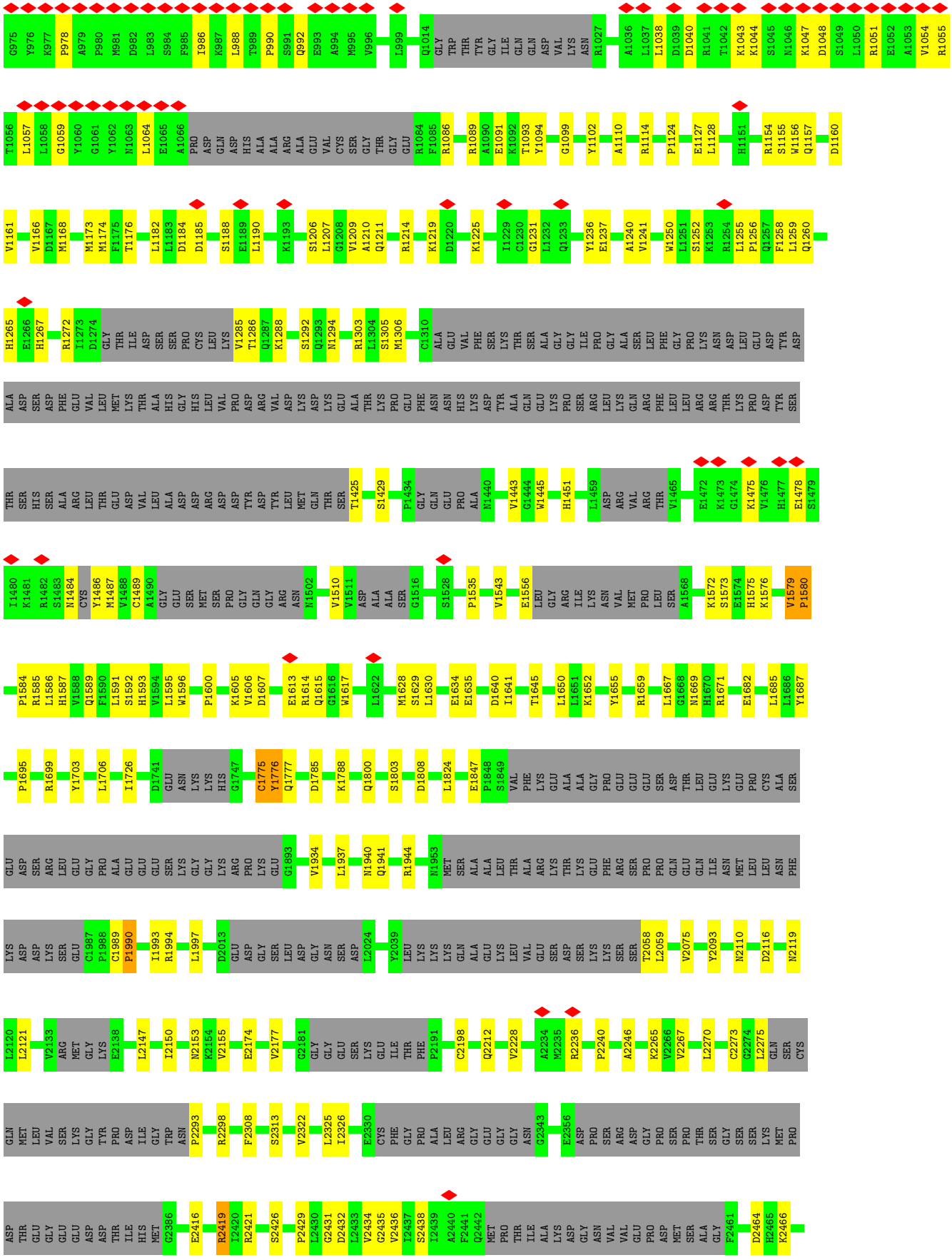
3 Residue-property plots (i)

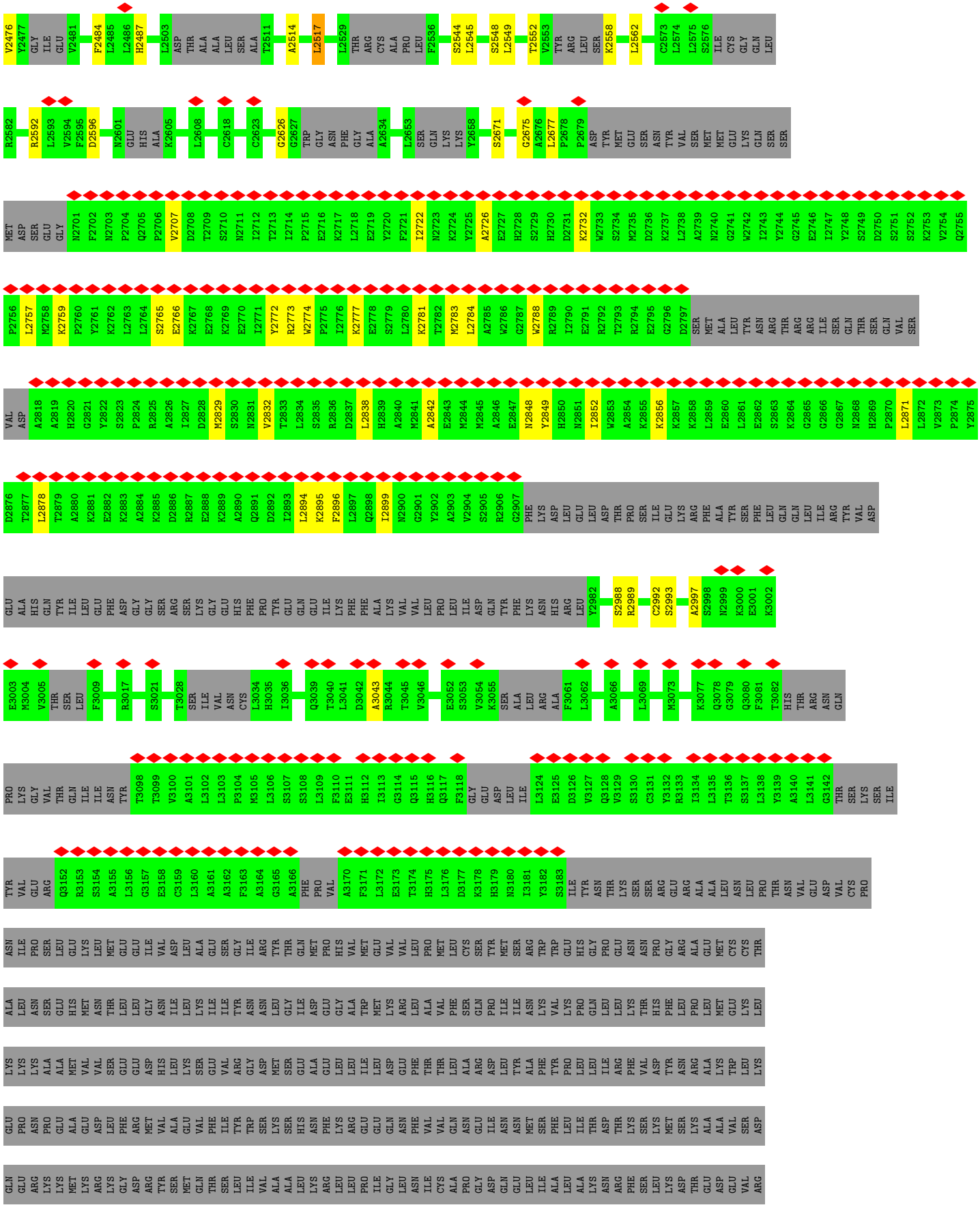
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

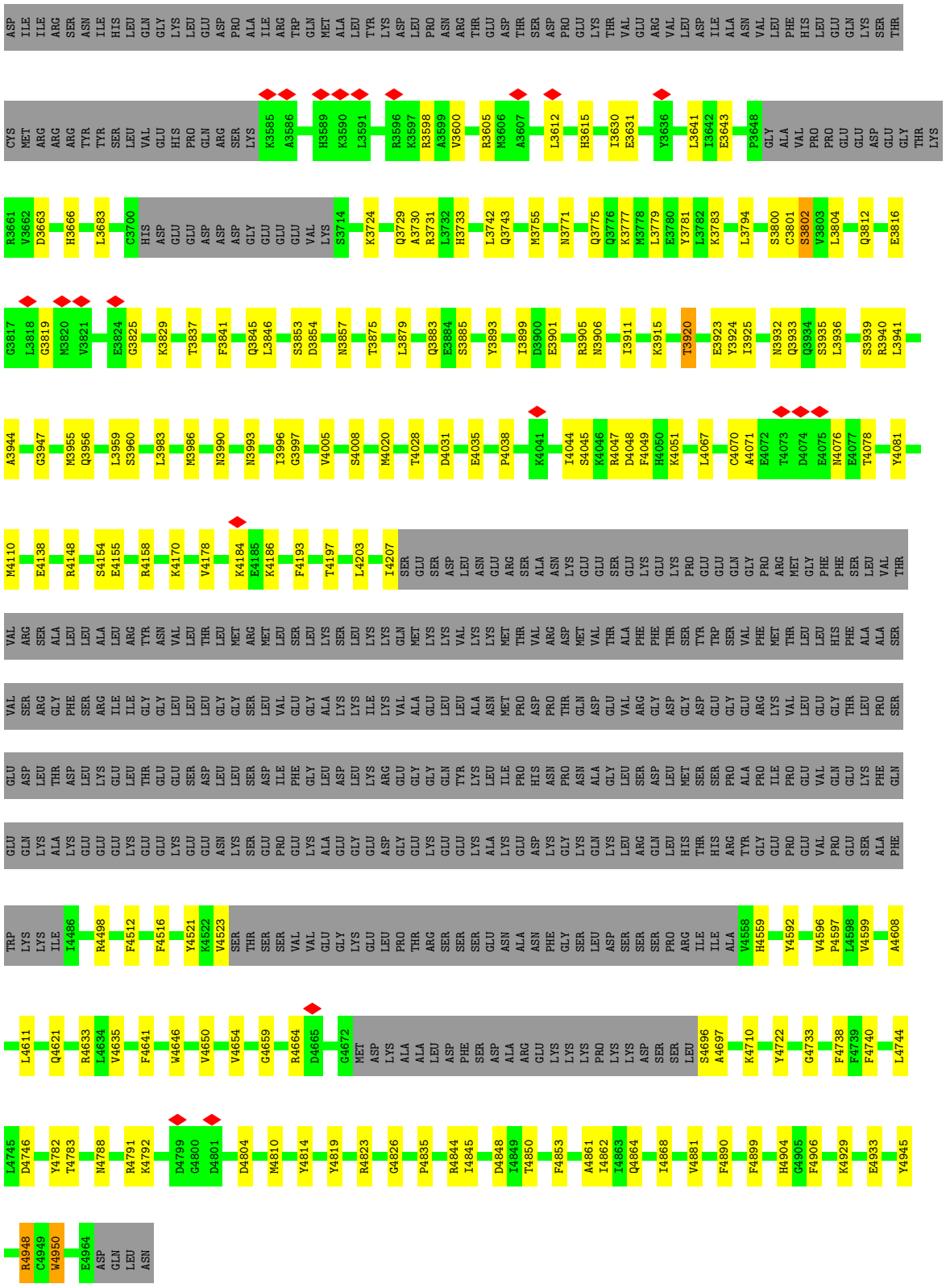
- Molecule 1: RyR2

Chain A:



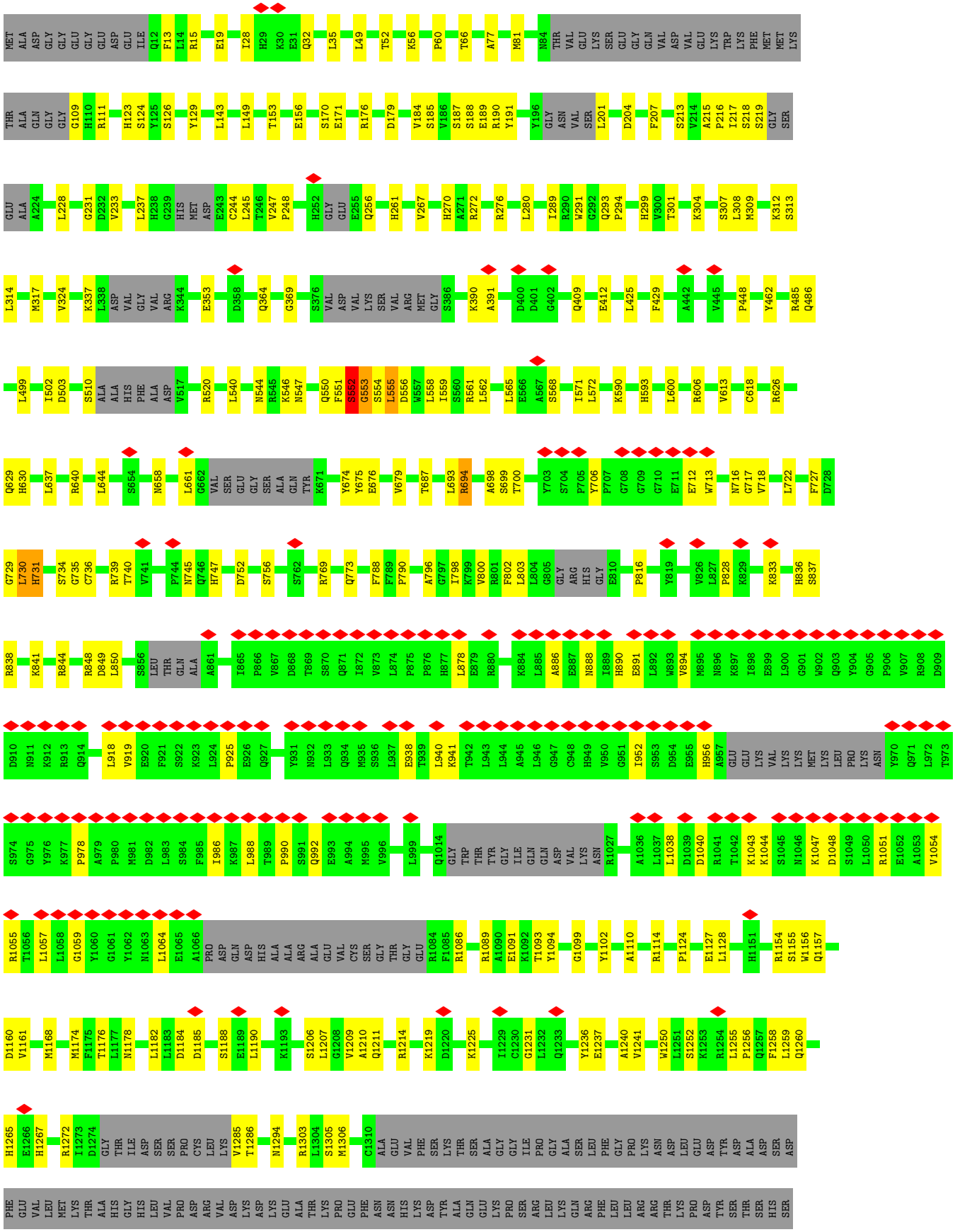

G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 E993 A994 M995 V996 L999 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 A1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055
T1056 L1057 L1058 G1059 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 F1085 R1086 R1089 A1090 E1091 K1092 T1093 Y1094 G1099 Y1102 A1110 R1114 P1124 E1127 L1128 H1151 R1154 S1155 W1156 Q1157 D1160
V1161 V1166 D1167 M1168 M1173 M1174 F1175 T1176 L1182 L1183 D1184 D1185 S1188 E1189 L1190 K1193 S1206 L1207 G1208 V1209 A1210 Q1211 R1214 K1219 D1220 K1225 I1229 C1230 G1231 L1232 Q1233 Y1236 E1237 A1240 V1241 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 F1258 L1259 Q1260
H1265 E1266 H1267 R1272 I1273 D1274 GLY THR ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 Q1287 K1288 S1292 Q1293 N1294 R1303 L1304 S1305 M1306 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 SER
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 VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR LEU MET GLN THR SER T1425 S1429 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 W1445 H1451 L1459 ASP ARG VAL ARG THR V1465 E1472 K1473 G1474 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 GLY ASN N1502 V1510 V1511 ASP ALA ALA SER G1516 S1528 P1535 V1543 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 K1572 S1573 E1574 H1575 K1576 V1579 P1580
P1584 R1585 L1586 H1587 V1588 Q1589 F1590 L1591 S1592 H1593 V1594 L1595 W1596 P1600 K1605 V1606 D1607 E1613 R1614 Q1615 G1616 W1617 L1622 M1628 S1629 L1630 E1634 E1635 D1640 I1641 T1645 L1650 L1651 K1652 Y1655 R1659 L1667 G1668 N1669 H1670 R1671 E1682 L1685 L1686 Y1687
P1695 R1699 Y1703 L1706 I1726 D1741 GLU ASN LYS LYS HIS G1747 C1775 Y1776 Q1777 D1785 K1788 Q1800 S1803 D1808 L1824 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 V1934 L1937 N1940 Q1941 R1944 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 R1994 L1997 D2013 GLU ASP GLY SER LEU ASP GLY ASN SER ASP L2024 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 L2059 V2075 Y2093 N2110 D2116 N2119
L2120 L2121 V2133 ARG MET GLY LYS E2138 L2147 I2150 N2153 K2154 V2155 E2174 V2177 G2181 GLY GLY GLU SER LYS GLU ILE THR PHE P2191 C2198 Q2212 V2228 A2234 M2235 R2236 P2240 A2246 K2265 V2266 V2267 L2270 C2273 G2274 L2275 GLN SER CYS
GLN MET LEU VAL SER LYS GLY TYR PRO ASP ILE GLY TRP ASN P2293 R2298 F2308 S2313 V2322 L2325 I2326 E2330 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 E2356 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 E2416 R2419 I2420 R2421 S2426 P2429 L2430 G2431 D2432 L2433 V2434 G2435 V2436 I2437 S2438 I2439 A2440 R2441 Q2442 MET PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 D2464 H2465 K2466

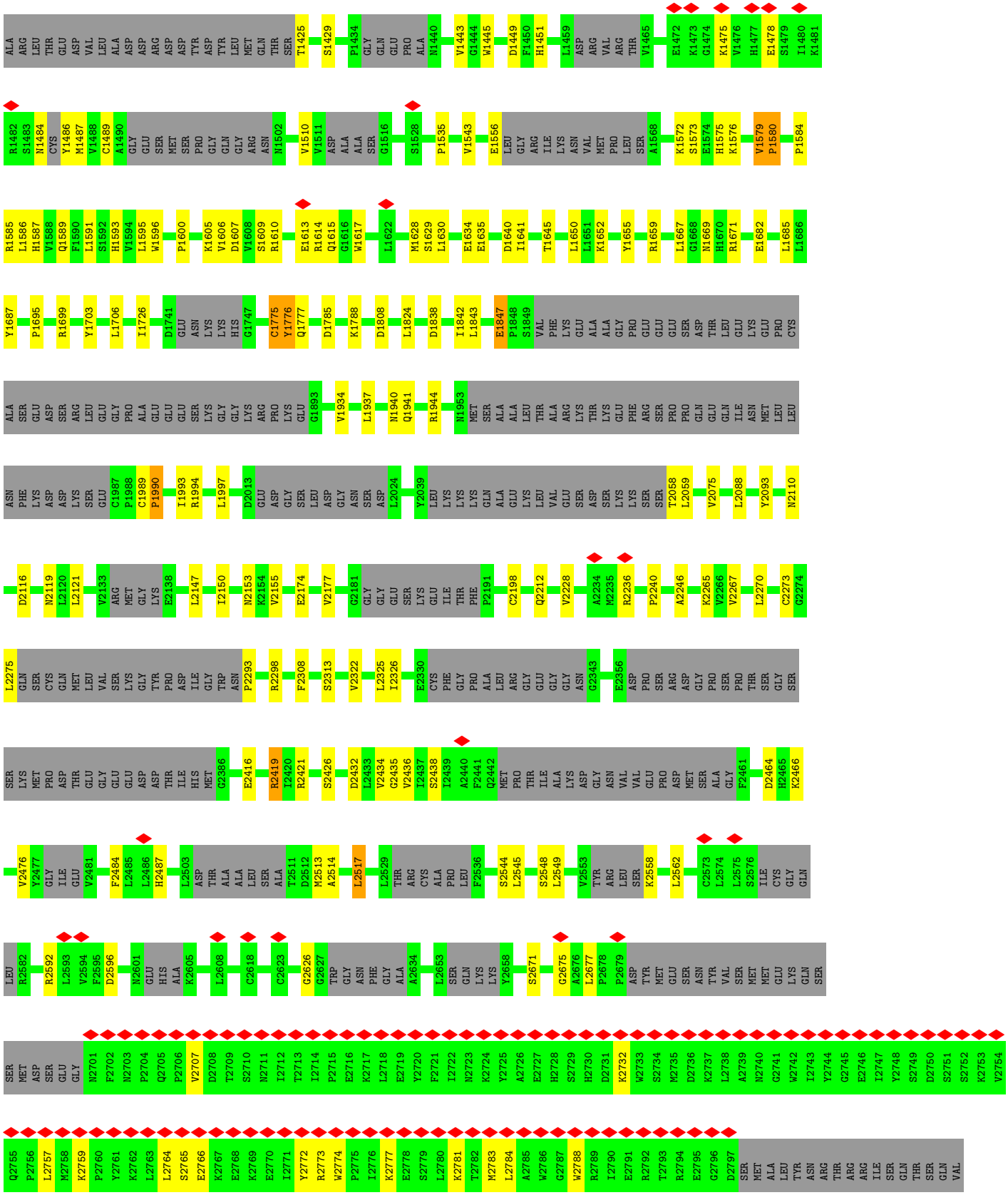


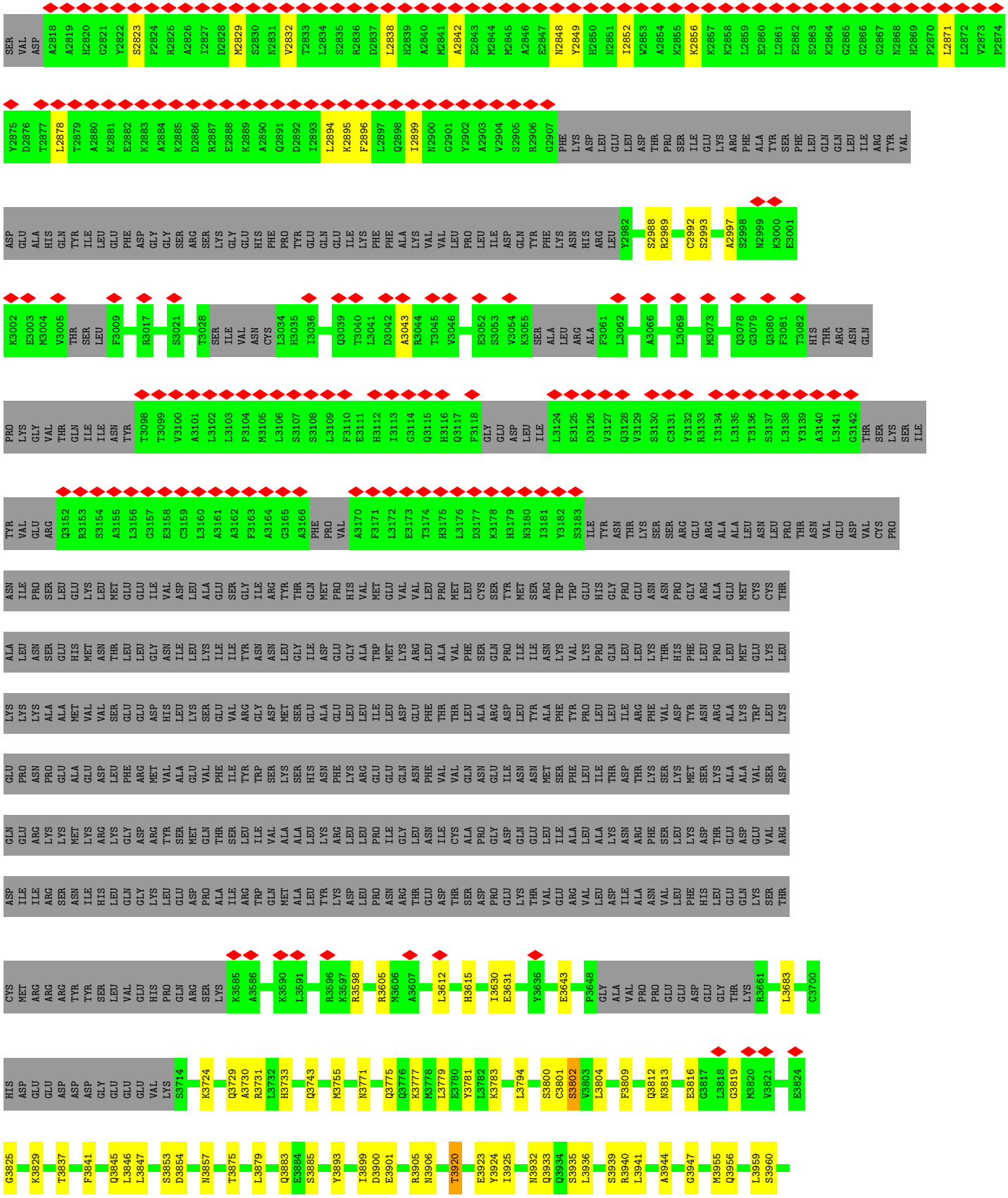


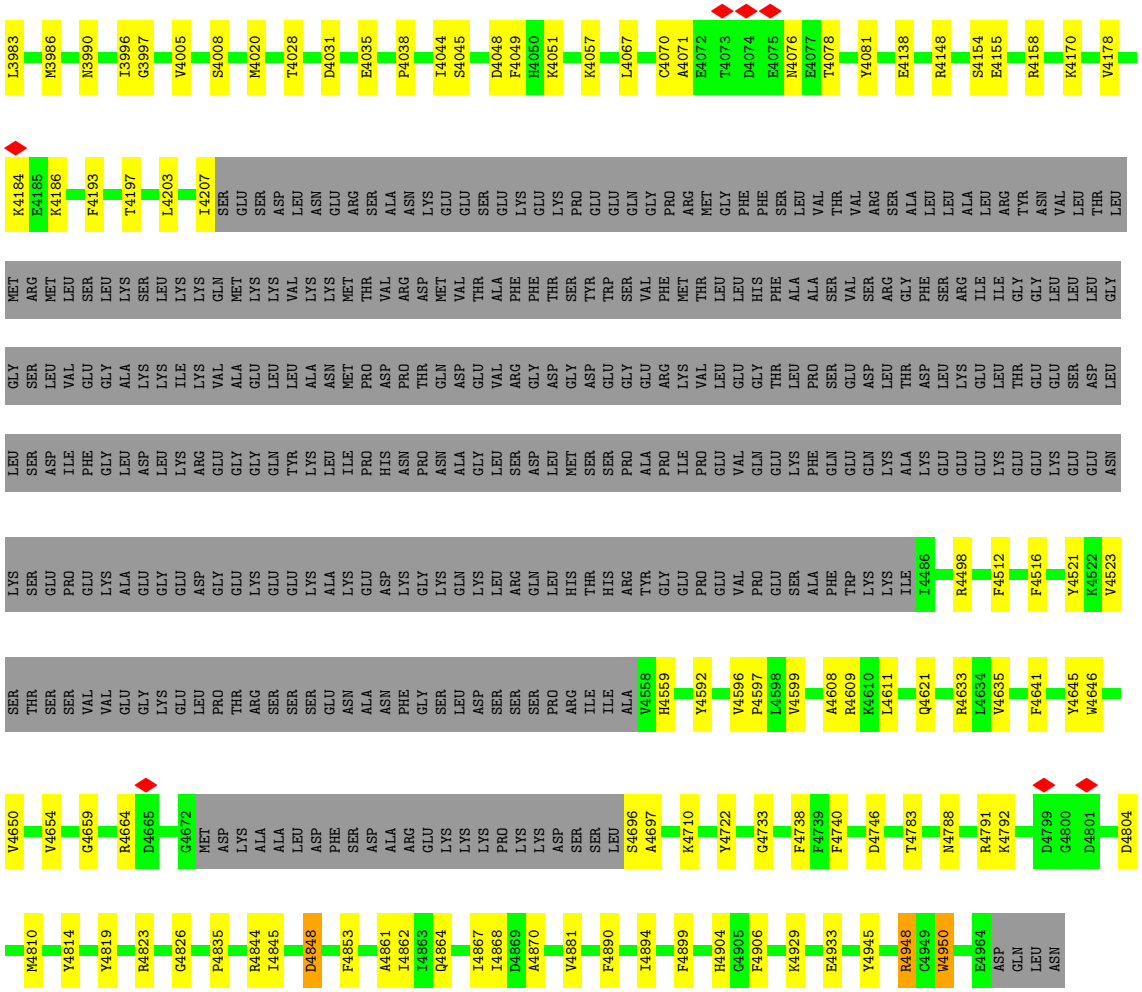
• Molecule 1: RyR2

Chain D:



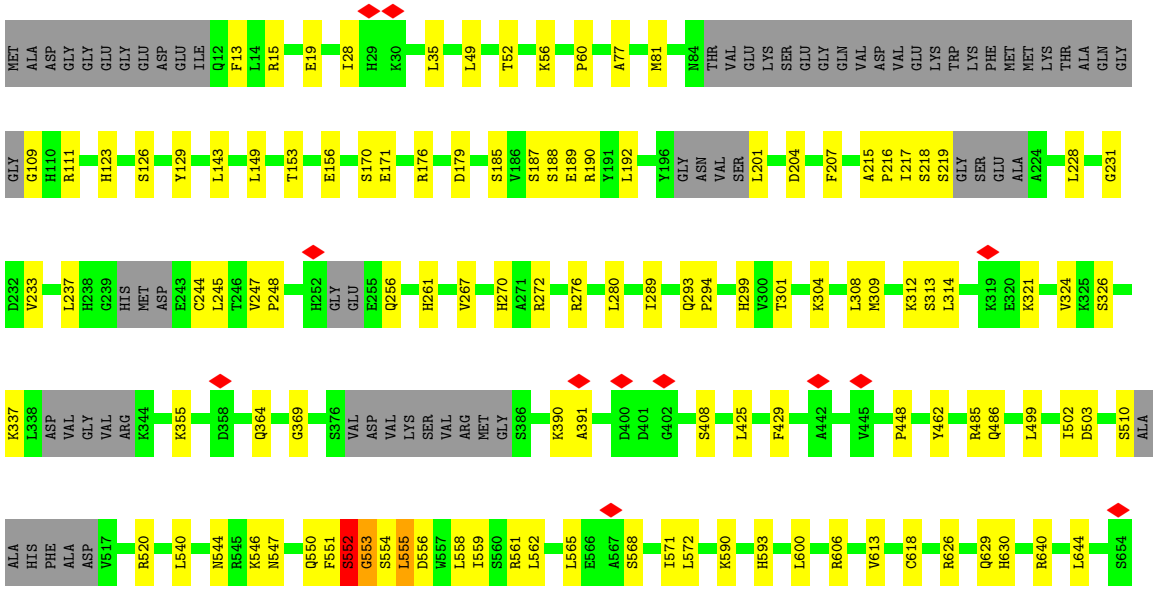

ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP ARG ASP ASP TYR ASP TYR LEU MET GLN THR SER T1425 S1429 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 W1445 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 E1472 K1473 G1474 K1475 V1476 H1477 E1478 S1479 I1480 K1481
R1482 S1483 N1484 CYS Y1486 M1487 V1488 C1489 A1490 GLY GLU SER MET SER PRO GLY GLN GLY ARG ASN N1502 V1510 V1511 ASP ALA ALA SER G1516 S1528 P1535 V1543 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 K1572 S1573 E1574 H1575 K1576 V1579 P1580 P1584
R1585 L1586 H1587 V1588 Q1589 F1590 L1591 S1592 H1593 V1594 L1595 W1596 P1600 K1605 V1606 D1607 V1608 S1609 R1610 E1613 R1614 Q1615 G1616 W1617 L1622 M1628 S1629 L1630 E1634 E1635 D1640 I1641 T1645 L1650 L1651 K1652 Y1655 R1659 L1667 C1668 N1669 H1670 R1671 E1682 L1685 L1686
Y1687 P1695 R1699 Y1703 L1706 I1726 D1741 GLU ASN LYS LYS HIS G1747 C1775 Y1776 Q1777 D1785 K1788 D1808 L1824 D1838 I1842 L1843 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 V1934 L1937 N1940 Q1941 R1944 N1953 MET SER ALA ALA LEU THR ALA ARG LYS THR LYS GLU PHE ARG SER PRO PRO GLN GLU GLN GLN ILE ASN MET LEU LEU
ASN PHE LYS ASP ASP LYS SER GLU C1987 P1988 C1989 P1990 I1993 R1994 L1997 D2013 GLU ASP GLY SER LEU ASP GLY ASN SER ASP L2024 Y2039 LEU LYS LYS LYS GLN ALA GLU LYS LEU VAL GLU SER ASP SER LYS LYS SER SER T2058 L2059 V2075 L2088 Y2093 N2110
D2116 N2119 L2120 L2121 V2133 ARG MET GLY LYS E2138 L2147 I2150 N2153 K2154 V2155 E2174 V2177 G2181 GLY GLY GLU SER LYS GLU ILE THR PHE P2191 C2198 Q2212 V2228 A2234 M2235 R2236 P2240 A2246 K2265 V2266 V2267 L2270 C2273 G2274
L2275 GLN SER CYS GLN MET LEU VAL SER LYS GLY GLY TYR PRO ASP ILE GLY TRP ASN P2293 R2298 F2308 S2313 V2322 L2325 I2326 E2330 CYS PHE GLY PRO ALA LEU ARG GLY GLU GLY GLY ASN G2343 E2356 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 E2416 R2419 I2420 R2421 S2426 D2432 L2433 V2434 G2435 V2436 I2437 S2438 I2439 A2440 F2441 Q2442 MET PRO THR ILE ALA LYS ASP GLY ASN VAL VAL GLU PRO ASP MET SER ALA GLY F2461 D2464 H2465 K2466
V2476 Y2477 GLY ILE GLU V2481 F2484 L2485 L2486 H2487 L2503 ASP THR ALA ALA LEU SER ALA T2511 D2512 M2513 A2514 L2517 L2529 THR ARG CYS ALA PRO LEU F2536 S2544 L2545 S2548 L2549 V2553 TYR ARG LEU SER K2558 L2562 C2573 L2574 L2575 S2576 ILE CYS GLY GLN
LEU R2582 R2592 L2593 V2594 F2595 D2596 N2601 GLU HIS ALA K2605 L2608 C2618 C2623 G2626 G2627 TRP GLY ASN PHE GLY ALA A2634 L2653 SER GLN LYS LYS Y2658 S2671 G2675 A2676 L2677 P2678 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

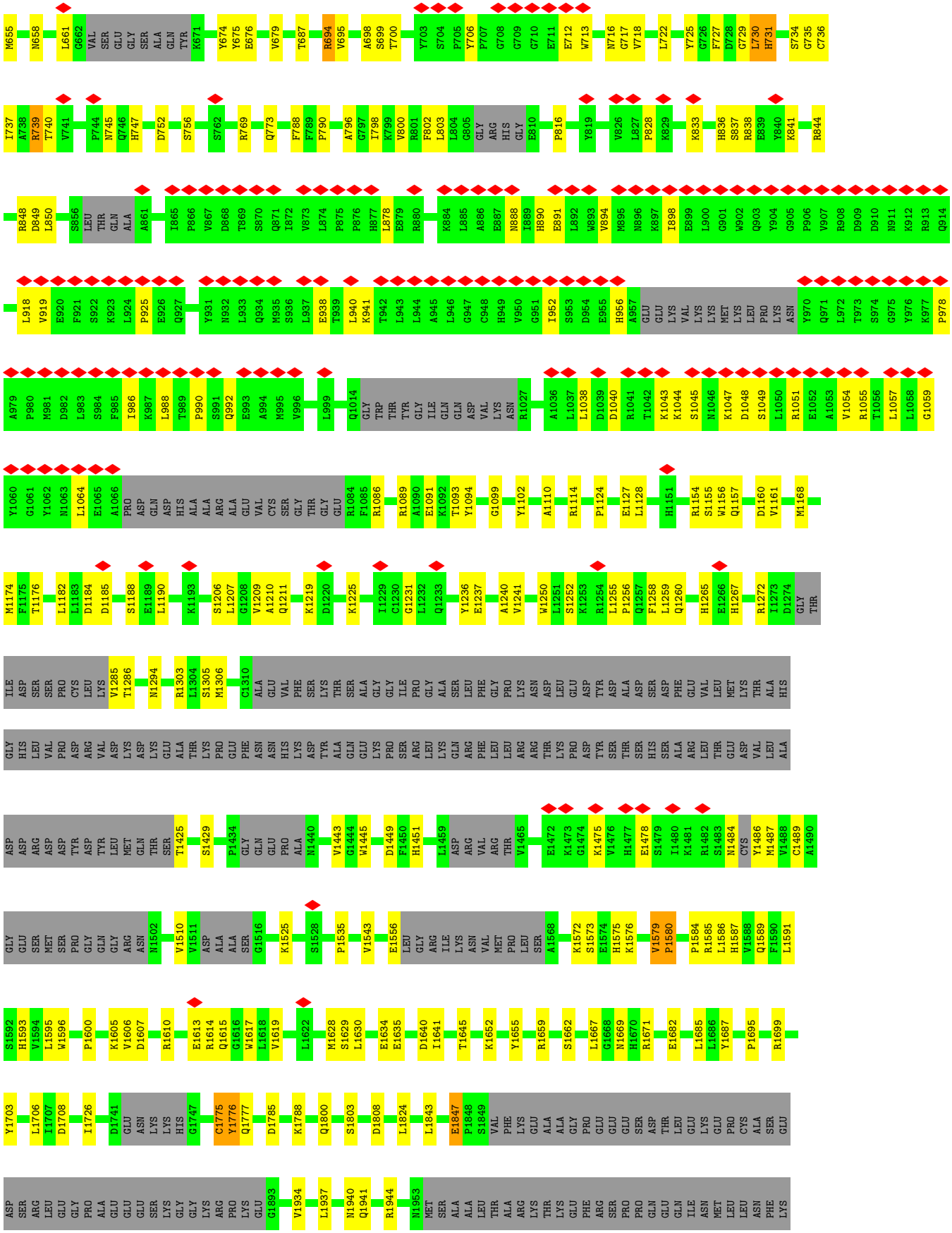


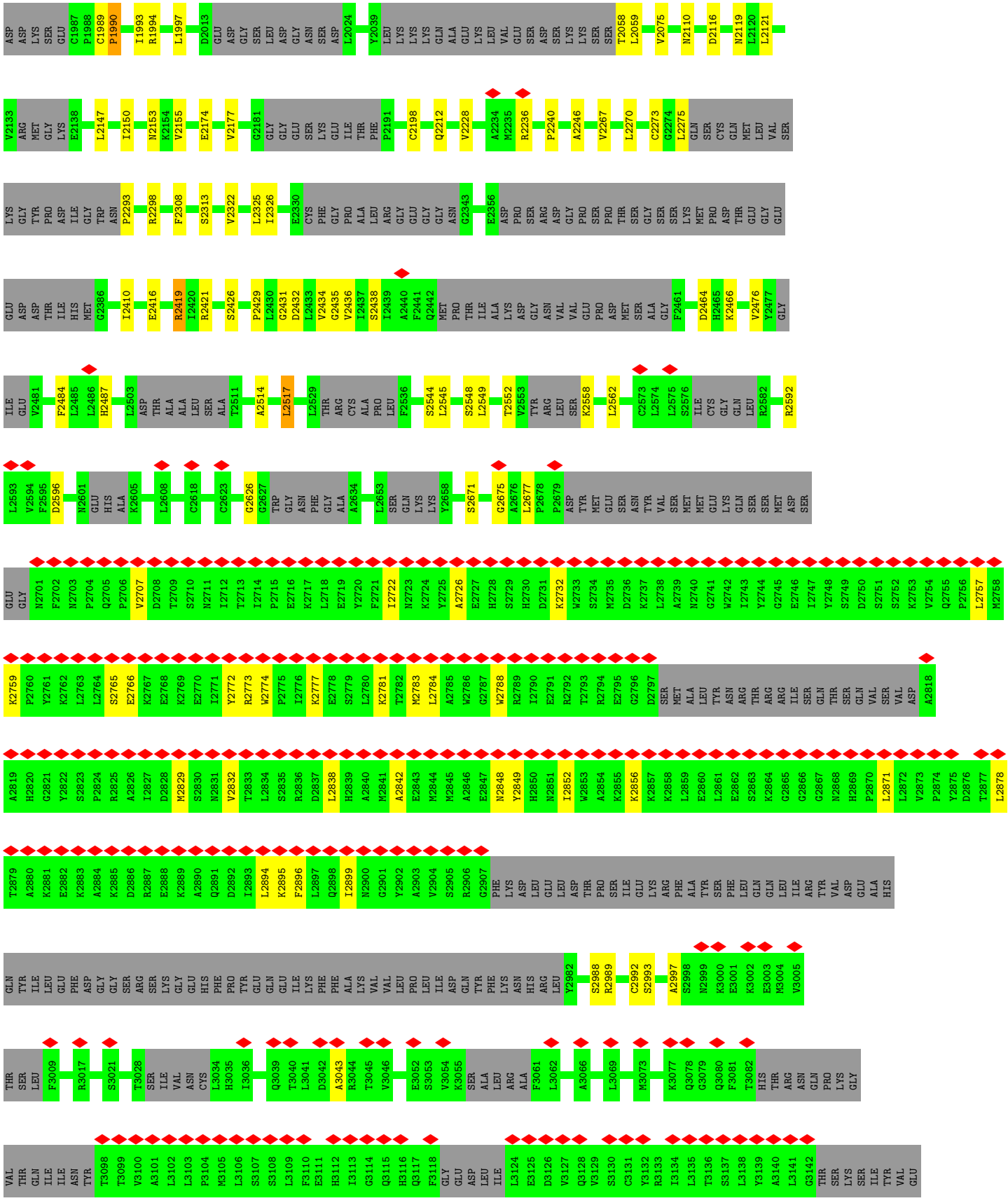


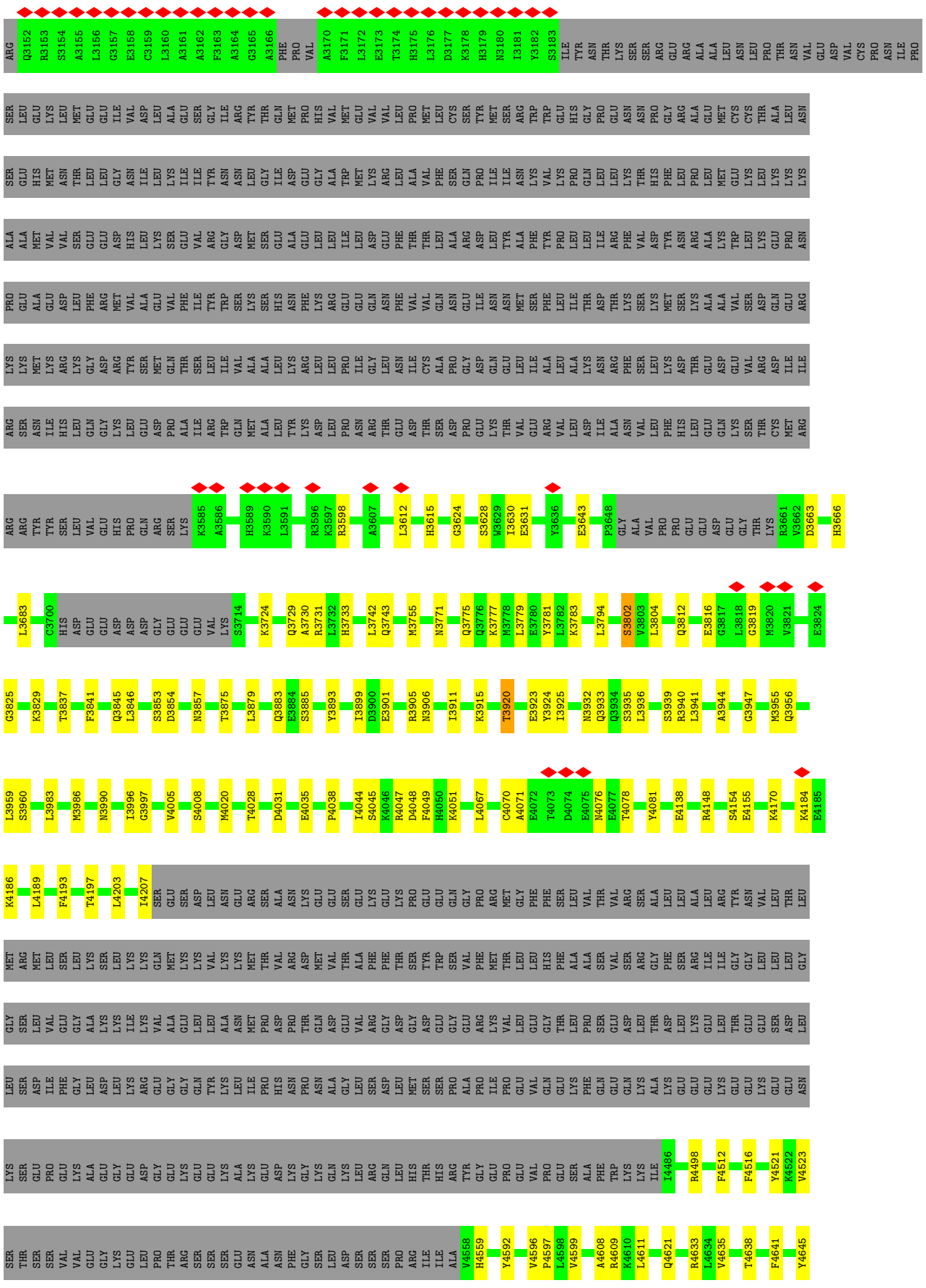
• Molecule 1: RyR2

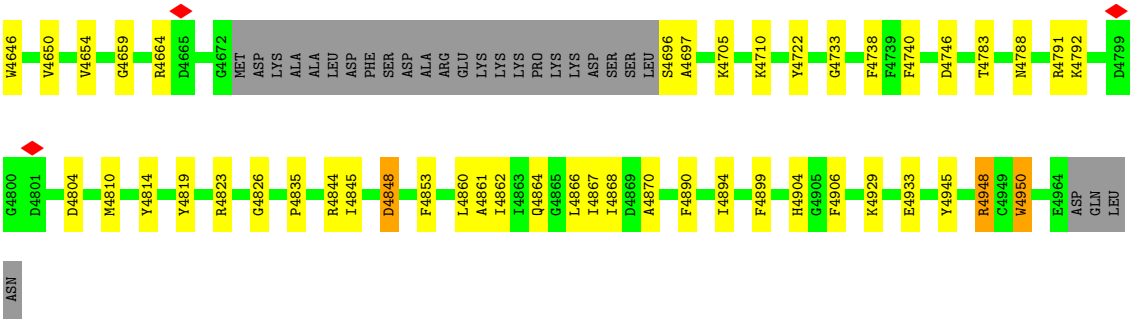
Chain G:




M655 N658 L661 G662 VAL SER GLU GLY SER ALA GLN TYR K671 Y674 Y675 E676 V679 T687 R694 V695 A698 S699 T700 Y703 S704 P705 Y706 P707 G708 G709 G710 E711 E712 W713 N716 G717 V718 L722 Y725 G726 F727 D728 G729 L730 H731 S734 G735 C736
I737 A738 R739 T740 V741 F744 N745 Q746 H747 D752 S756 S762 R769 Q773 F788 F789 F790 A796 G797 I798 K799 V800 R801 F802 L803 L804 G805 GLY ARG HIS GLY E810 P816 Y819 V826 L827 P828 K829 K833 H836 S837 R838 E839 Y840 K841 R844
R848 D849 L850 S856 LEU THR GLN ALA A861 I865 P866 V867 D868 T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 K884 L885 A886 E887 N888 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914
L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 Y931 N932 L933 Q934 M935 S936 L937 E938 T939 L940 K941 T942 L943 L944 A945 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 V996 L999 Q1014 GLY TRP THR TYR GLY ILE GLN GLN ASP VAL LYS ASN R1027 A1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059
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 F1085 R1086 R1089 A1090 E1091 K1092 T1093 Y1094 G1099 Y1102 A1110 R1114 P1124 E1127 L1128 H1151 R1154 S1155 W1156 Q1157 D1160 V1161 M1168
M1174 F1175 T1176 L1182 L1183 D1184 D1185 S1188 E1189 L1190 K1193 S1206 L1207 G1208 V1209 A1210 Q1211 K1219 D1220 K1225 I1229 C1230 G1231 L1232 Q1233 Y1236 E1237 A1240 V1241 W1250 L1251 S1252 K1253 R1254 L1255 P1256 Q1257 F1258 L1259 Q1260 H1265 E1266 H1267 R1272 I1273 D1274 GLY THR
ILE ASP SER SER PRO CYS LEU LYS V1285 T1286 N1294 R1303 L1304 S1305 M1306 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 HIS ALA
GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP 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 S1429 P1434 GLY GLN GLU PRO ALA N1440 V1443 G1444 W1445 D1449 F1450 H1451 L1459 ASP ARG VAL ARG THR V1465 E1472 K1473 G1474 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 V1510 V1511 ASP ALA ALA SER G1516 K1525 S1528 P1535 V1543 E1556 LEU GLY ARG ILE LYS ASN VAL MET PRO LEU SER A1568 K1572 S1573 E1574 H1575 K1576 V1579 P1580 P1584 R1585 L1586 H1587 V1588 Q1589 F1590 L1591
S1592 H1593 Y1594 L1595 W1596 P1600 K1605 V1606 D1607 R1610 E1613 R1614 Q1615 G1616 W1617 K1618 V1619 L1622 M1628 S1629 L1630 E1634 E1635 D1640 I1641 T1645 K1652 Y1655 R1659 S1662 L1667 G1668 N1669 H1670 R1671 E1682 L1685 L1686 Y1687 P1695 R1699
Y1703 L1706 I1707 D1708 I1726 D1741 GLU ASN LYS LYS HIS G1747 C1775 Y1776 Q1777 D1785 K1788 Q1800 S1803 D1808 L1824 L1843 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 SER LYS GLY GLY LYS ARG PRO LYS GLU G1893 V1934 L1937 N1940 Q1941 R1944 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

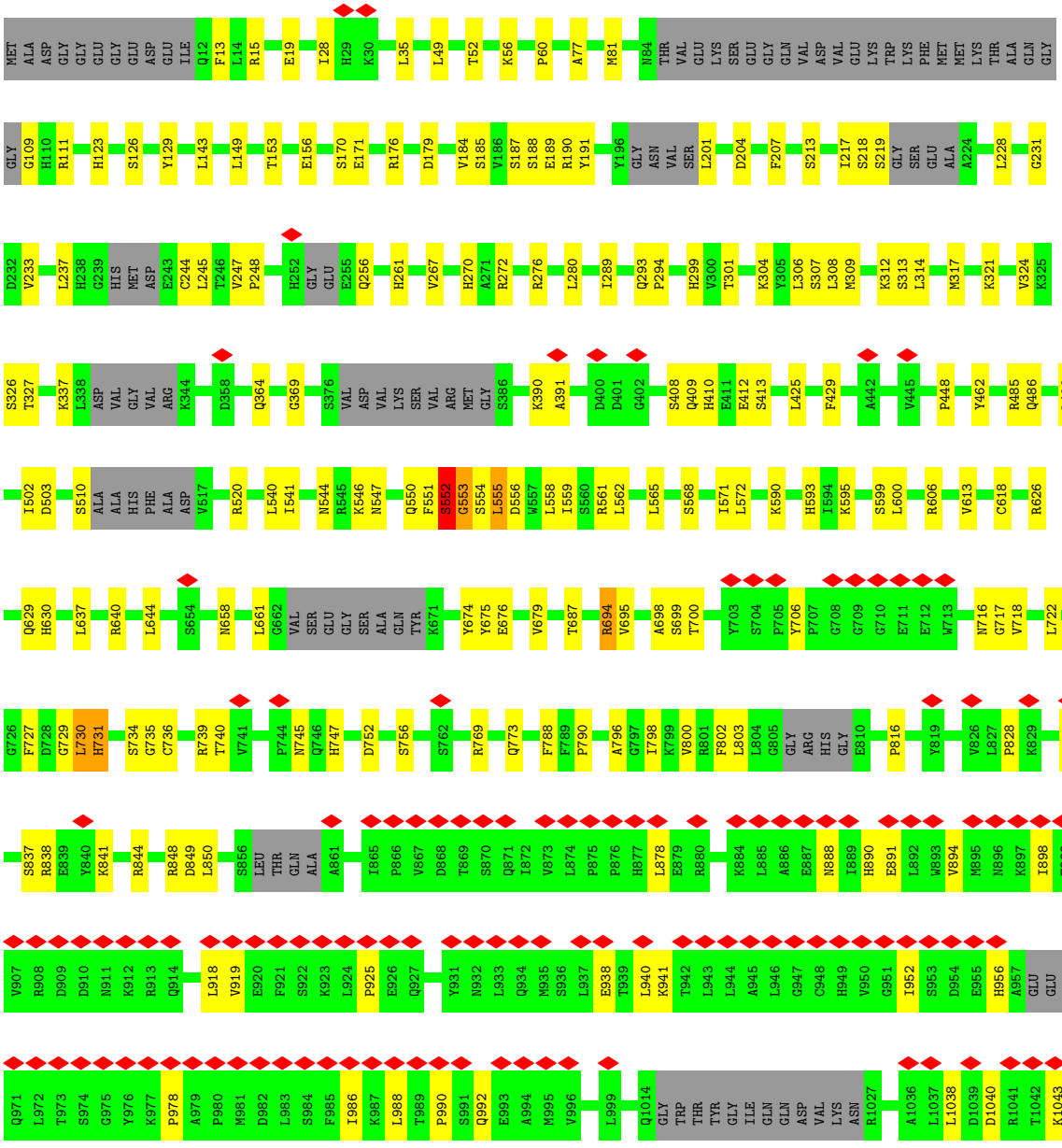


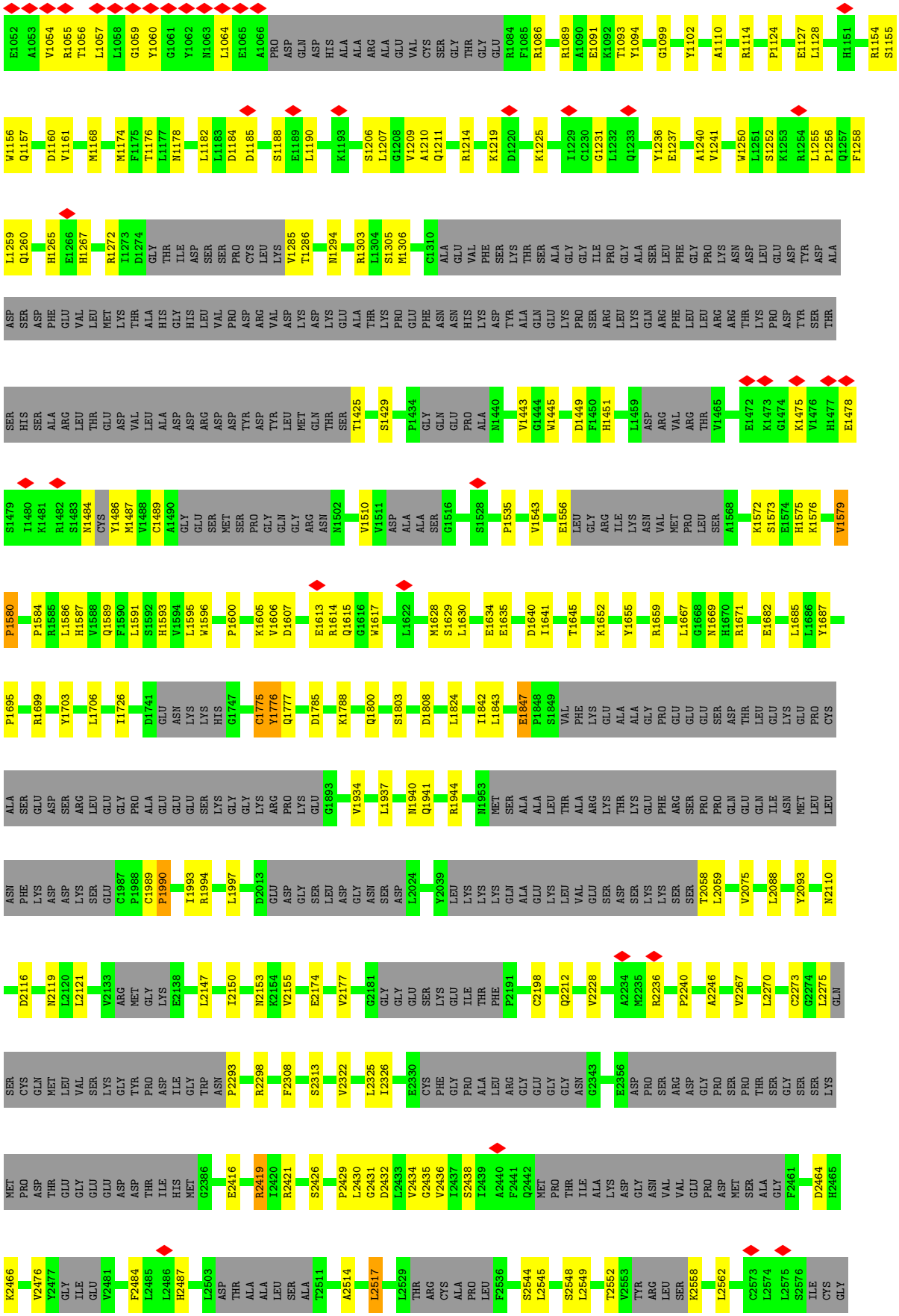


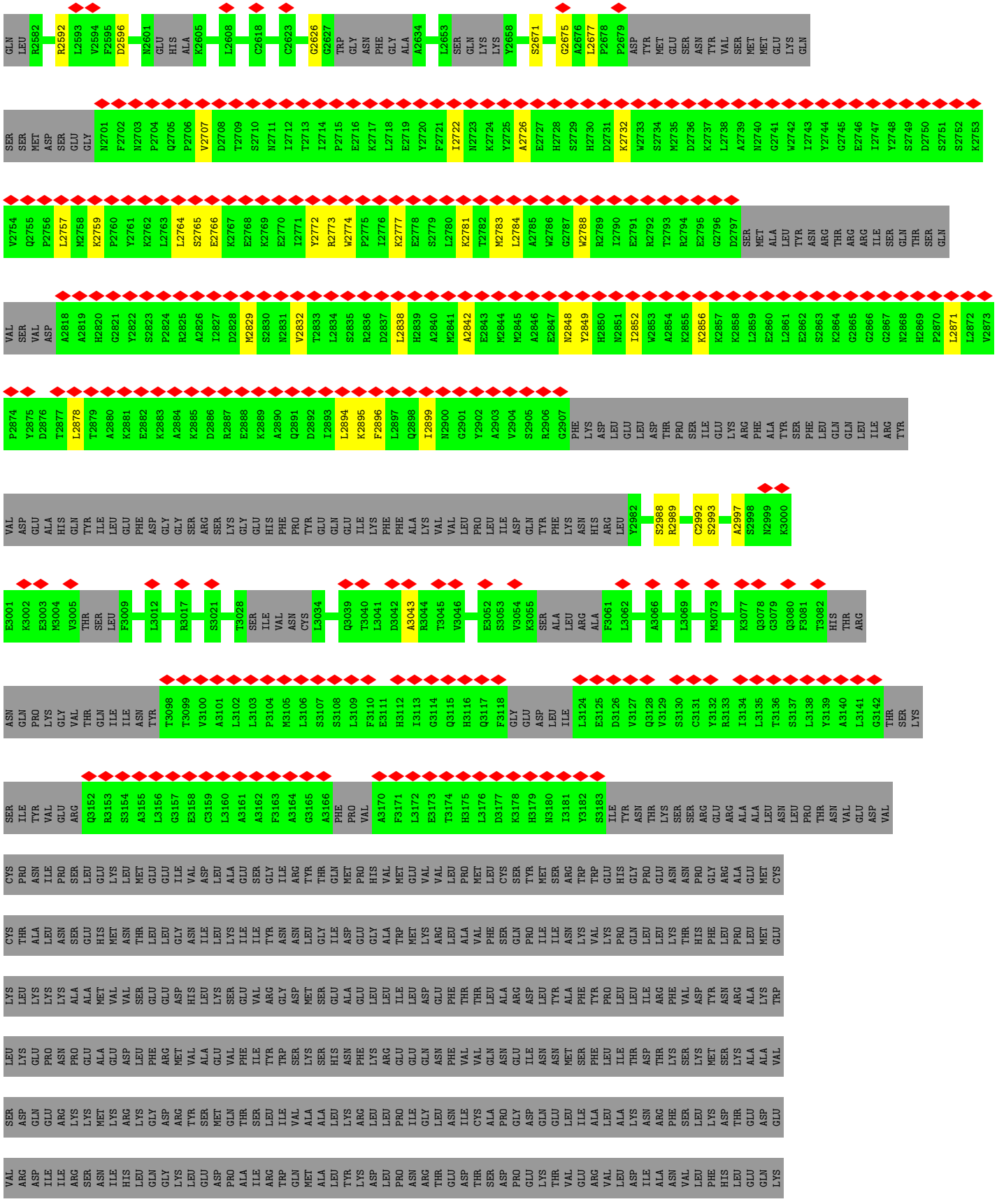


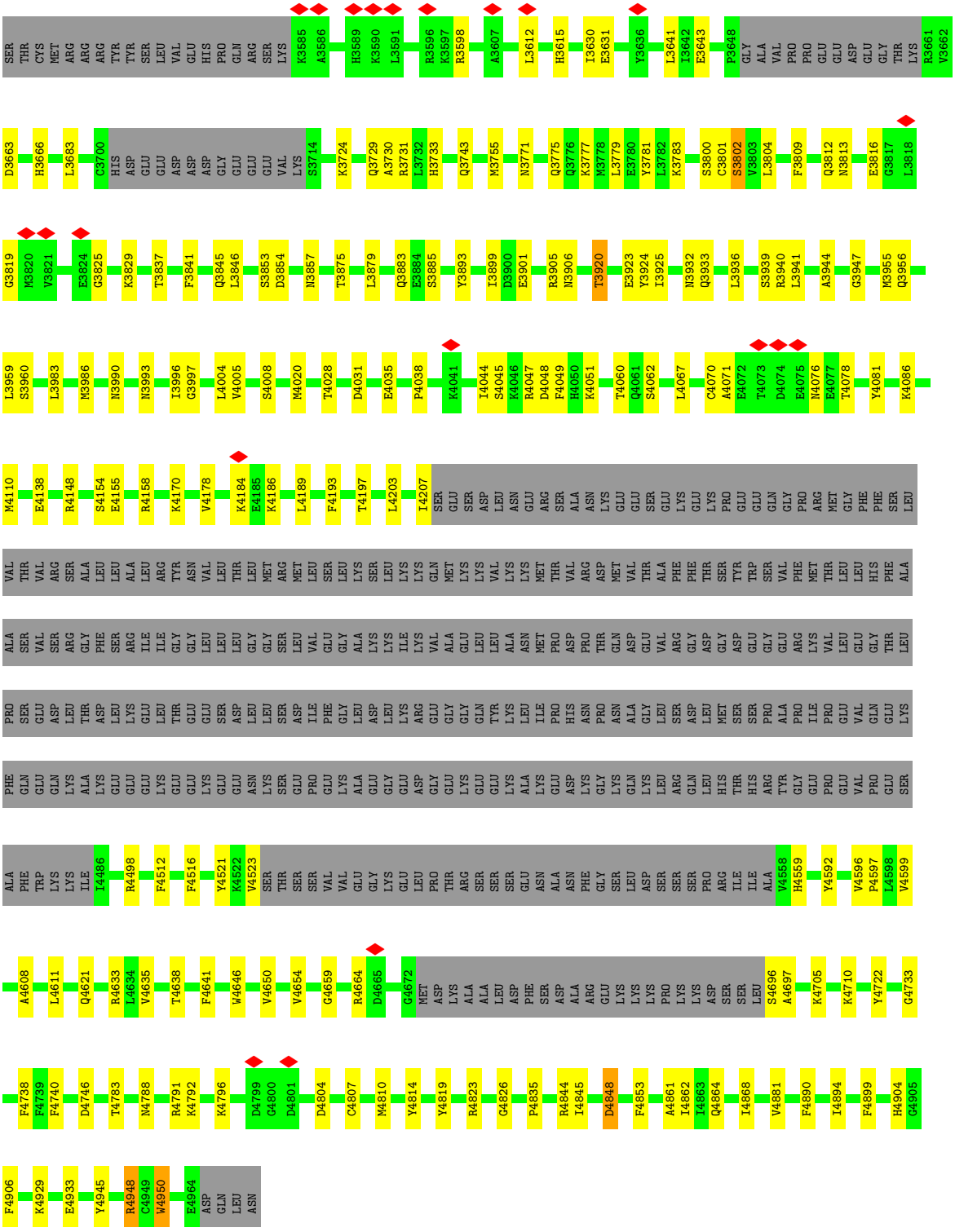
• Molecule 1: RyR2

Chain J:



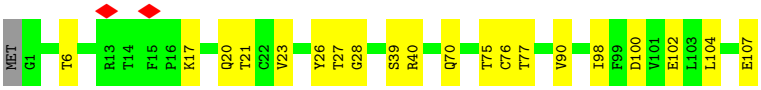



GLN LEU R2582 R2592 L2593 V2594 P2595 D2596 N2601 GLU HIS ALA K2605 L2608 C2618 C2623 G2626 G2627 TRP GLY ASN PHE GLY ALA A2634 L2653 SER GLN LYS LYS Y2658 S2671 G2675 A2676 L2677 P2679 ASP TYR MET GLU SER ASN TYR VAL SER MET MET GLU LYS GLN
SER SER MET ASP SER GLU GLY N2701 F2702 N2703 P2704 Q2705 P2706 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 S2988 R2989 C2992 S2993 A2997 S2998 N2999 K3000
E3001 K3002 E3003 M3004 V3005 THR SER LEU F3009 L3012 R3017 S3021 T3028 SER ILE VAL ASN CYS L3034 Q3039 T3040 L3041 D3042 A3043 R3044 T3045 V3046 E3052 S3053 V3054 K3055 SER ALA LEU ARG ALA F3061 L3062 A3066 L3069 M3073 K3077 Q3078 G3079 Q3080 F3081 T3082 HIS THR ARG
ASN GLN PRO LYS GLY VAL THR GLN ILE ILE ASN TYR T3098 T3099 V3100 A3101 L3102 L3103 P3104 M3105 L3106 S3107 S3108 L3109 F3110 E3111 H3112 I3113 G3114 Q3115 H3116 Q3117 F3118 GLY GLU ASP LEU ILE L3124 E3125 D3126 V3127 Q3128 V3129 S3130 C3131 Y3132 R3133 I3134 L3135 T3136 S3137 L3138 Y3139 A3140 L3141 G3142 THR SER LYS
SER ILE TYR VAL GLU ARG Q3152 R3153 S3154 A3155 L3156 G3157 E3158 C3159 L3160 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 MET GLU GLU ILE VAL ASP LEU ALA GLU SER GLY ILE ASP 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 ILE ARG GLY ASP MET 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 ASP LEU PHE PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER LYS SER HIS ASN PHE LYS ARG LEU LEU ARG GLU GLU GLN ASN PHE VAL VAL GLN ASN GLU ILE ASN ASN MET SER PHE LEU LEU ILE THR ASP THR LYS SER LYS MET SER LYS ALA ALA VAL
SER ASP GLN GLU ARG LYS LYS MET ALA LEU LYS ARG LEU LEU PRO ILE ASN ARG THR GLU ASP THR SER ALA PRO GLY ASP GLN GLU LEU LYS ASN ARG PHE SER LEU LYS ASP THR GLU ASP ASP
VAL ARG ASP ILE ILE ARG TRP GLN MET ALA 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



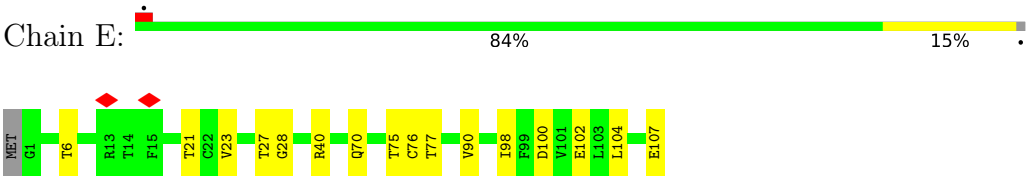
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B:



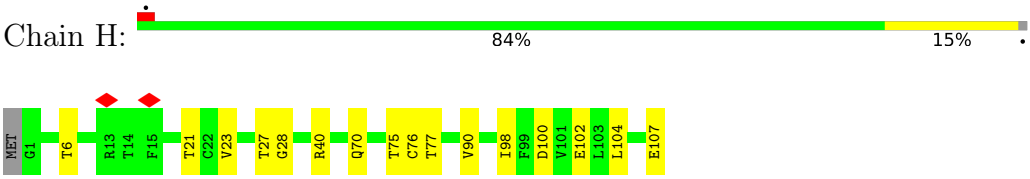
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



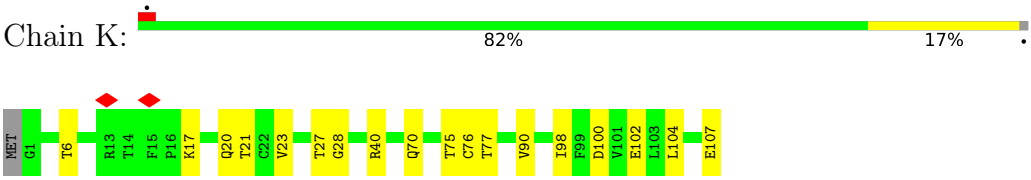
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



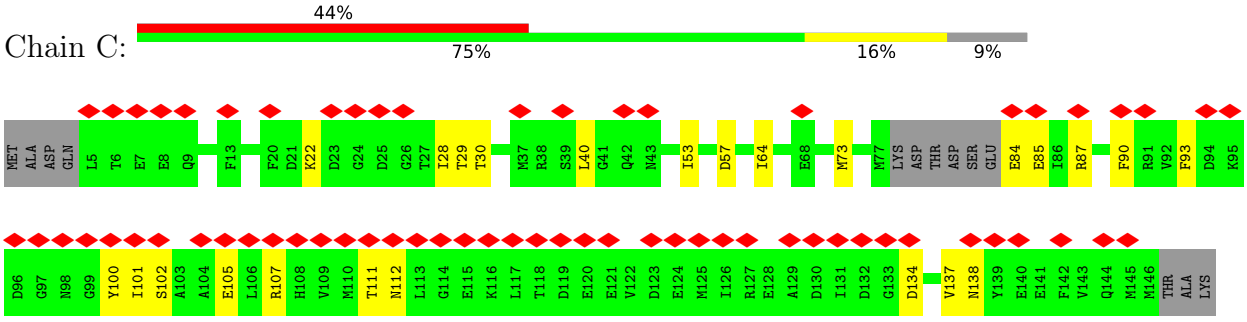
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:



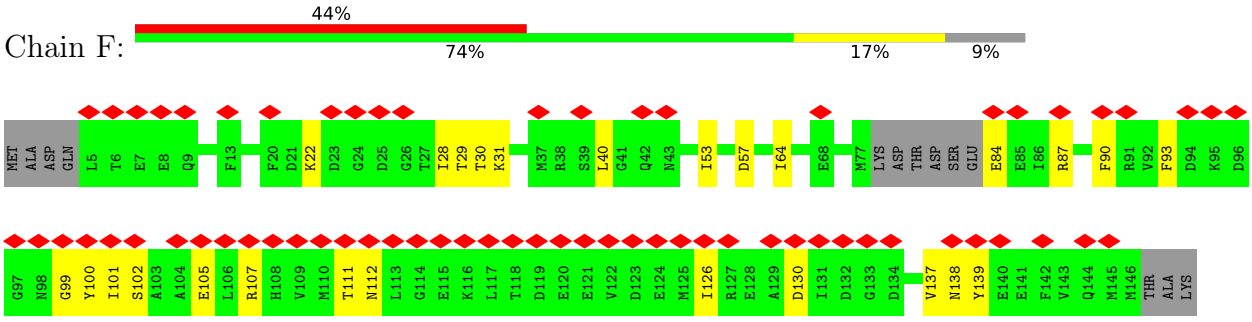
• Molecule 3: Calmodulin-1

Chain C:



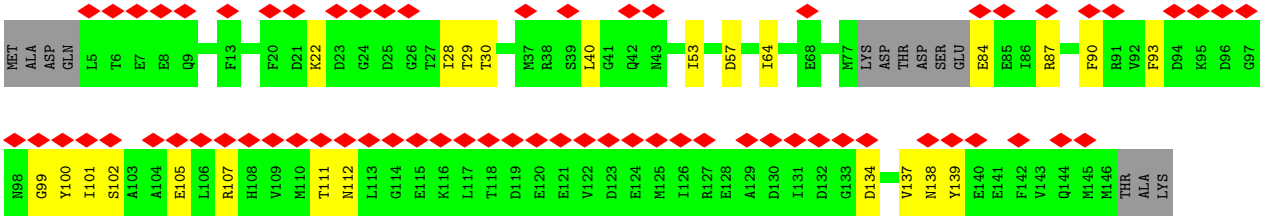
• Molecule 3: Calmodulin-1

Chain F:

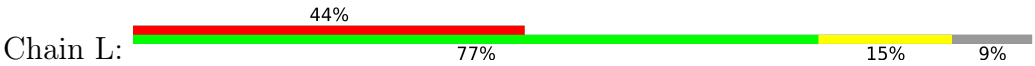


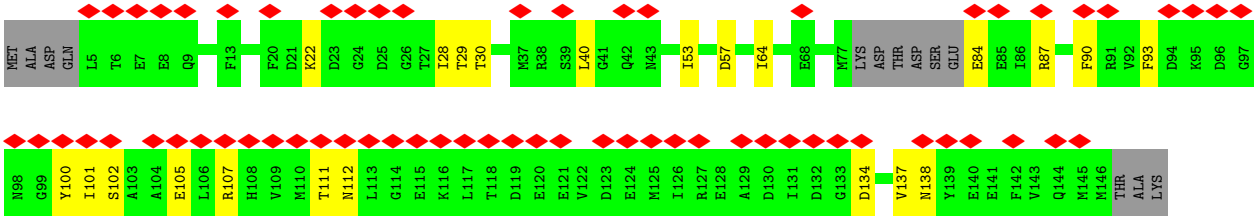
• Molecule 3: Calmodulin-1

Chain I:



• Molecule 3: Calmodulin-1





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	96158	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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: CA, ATP, CFF, 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	2/27385 (0.0%)	0.57	7/37042 (0.0%)
1	D	0.40	2/27385 (0.0%)	0.57	7/37042 (0.0%)
1	G	0.40	2/27385 (0.0%)	0.57	7/37042 (0.0%)
1	J	0.40	2/27385 (0.0%)	0.57	7/37042 (0.0%)
2	B	0.35	0/835	0.55	0/1123
2	E	0.35	0/835	0.55	0/1123
2	H	0.35	0/835	0.55	0/1123
2	K	0.35	0/835	0.55	0/1123
3	C	0.28	0/1086	0.48	0/1456
3	F	0.28	0/1086	0.48	0/1456
3	I	0.28	0/1086	0.48	0/1456
3	L	0.28	0/1086	0.48	0/1456
All	All	0.39	8/117224 (0.0%)	0.57	28/158484 (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	19
1	D	0	19
1	G	0	19
1	J	0	19
All	All	0	76

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4950	TRP	CB-CG	-6.13	1.39	1.50
1	G	4950	TRP	CB-CG	-6.13	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	4950	TRP	CB-CG	-6.13	1.39	1.50
1	D	4950	TRP	CB-CG	-6.09	1.39	1.50
1	G	2198	CYS	CB-SG	-5.54	1.72	1.81

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3612	LEU	CA-CB-CG	7.47	132.49	115.30
1	G	3612	LEU	CA-CB-CG	7.47	132.49	115.30
1	A	3612	LEU	CA-CB-CG	7.47	132.48	115.30
1	J	3612	LEU	CA-CB-CG	7.46	132.46	115.30
1	G	2517	LEU	CA-CB-CG	6.33	129.85	115.30

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	PHE	Peptide
1	A	552	SER	Peptide
1	A	729	GLY	Peptide
1	A	731	HIS	Peptide
1	A	739	ARG	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	26877	0	25382	455	0
1	D	26877	0	25382	463	0
1	G	26877	0	25382	458	0
1	J	26877	0	25382	454	0
2	B	819	0	824	11	0
2	E	819	0	824	9	0
2	H	819	0	824	9	0
2	K	819	0	824	11	0
3	C	1075	0	1011	16	0
3	F	1075	0	1011	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1075	0	1011	16	0
3	L	1075	0	1011	14	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
5	A	1	0	0	0	0
5	C	4	0	0	0	0
5	D	1	0	0	0	0
5	F	4	0	0	0	0
5	G	1	0	0	0	0
5	I	4	0	0	0	0
5	J	1	0	0	0	0
5	L	4	0	0	0	0
6	A	31	0	12	1	0
6	D	31	0	12	1	0
6	G	31	0	12	1	0
6	J	31	0	12	1	0
7	A	14	0	10	2	0
7	D	14	0	10	2	0
7	G	14	0	10	2	0
7	J	14	0	10	2	0
All	All	115288	0	108956	1705	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 8.

The worst 5 of 1705 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:4862:ILE:HG22	1:J:4868:ILE:CD1	1.57	1.35
1:A:4868:ILE:CD1	1:J:4862:ILE:HG22	1.58	1.34
1:D:4862:ILE:HG22	1:G:4868:ILE:CD1	1.59	1.30
1:A:4862:ILE:HG22	1:D:4868:ILE:CD1	1.60	1.30
1:G:4862:ILE:CG2	1:J:4868:ILE:HD13	1.64	1.28

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	3405/4968 (68%)	2973 (87%)	423 (12%)	9 (0%)	41	75
1	D	3405/4968 (68%)	2974 (87%)	422 (12%)	9 (0%)	41	75
1	G	3405/4968 (68%)	2973 (87%)	423 (12%)	9 (0%)	41	75
1	J	3405/4968 (68%)	2974 (87%)	422 (12%)	9 (0%)	41	75
2	B	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	E	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	H	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	K	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
3	C	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	F	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	I	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	L	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
All	All	14568/20900 (70%)	12750 (88%)	1782 (12%)	36 (0%)	50	79

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	553	GLY
1	A	1776	TYR
1	D	553	GLY
1	D	1776	TYR
1	G	553	GLY

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	2701/4355 (62%)	2687 (100%)	14 (0%)	88 93
1	D	2700/4355 (62%)	2685 (99%)	15 (1%)	86 91
1	G	2700/4355 (62%)	2685 (99%)	15 (1%)	86 91
1	J	2700/4355 (62%)	2685 (99%)	15 (1%)	86 91
2	B	88/89 (99%)	88 (100%)	0	100 100
2	E	88/89 (99%)	88 (100%)	0	100 100
2	H	88/89 (99%)	88 (100%)	0	100 100
2	K	88/89 (99%)	88 (100%)	0	100 100
3	C	116/127 (91%)	116 (100%)	0	100 100
3	F	116/127 (91%)	116 (100%)	0	100 100
3	I	116/127 (91%)	116 (100%)	0	100 100
3	L	116/127 (91%)	116 (100%)	0	100 100
All	All	11617/18284 (64%)	11558 (100%)	59 (0%)	89 93

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4853	PHE
1	J	3920	THR
1	G	1176	THR
1	J	3879	LEU
1	J	990	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	32	GLN
1	J	4076	ASN
1	J	544	ASN
1	J	1684	GLN
1	J	4937	GLN

5.3.3 RNA

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 32 ligands modelled in this entry, 24 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	$\#\|Z\| > 2$
6	ATP	J	6002	-	26,33,33	0.87	1 (3%)	31,52,52	1.55	5 (16%)
6	ATP	A	6002	-	26,33,33	0.87	1 (3%)	31,52,52	1.55	5 (16%)
7	CFF	G	6003	-	8,15,15	2.73	4 (50%)	8,23,23	1.20	1 (12%)
7	CFF	J	6003	-	8,15,15	2.74	4 (50%)	8,23,23	1.21	1 (12%)
7	CFF	A	6003	-	8,15,15	2.74	4 (50%)	8,23,23	1.21	1 (12%)
6	ATP	D	6002	-	26,33,33	0.87	0	31,52,52	1.55	5 (16%)
7	CFF	D	6003	-	8,15,15	2.74	4 (50%)	8,23,23	1.21	1 (12%)
6	ATP	G	6002	-	26,33,33	0.86	1 (3%)	31,52,52	1.55	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
6	ATP	J	6002	-	-	5/18/38/38	0/3/3/3
6	ATP	A	6002	-	-	5/18/38/38	0/3/3/3
7	CFF	G	6003	-	-	-	0/2/2/2
7	CFF	J	6003	-	-	-	0/2/2/2
7	CFF	A	6003	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	D	6002	-	-	5/18/38/38	0/3/3/3
7	CFF	D	6003	-	-	-	0/2/2/2
6	ATP	G	6002	-	-	5/18/38/38	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	6003	CFF	C5-C4	-4.77	1.33	1.39
7	D	6003	CFF	C5-C4	-4.77	1.33	1.39
7	J	6003	CFF	C5-C4	-4.77	1.33	1.39
7	G	6003	CFF	C6-N1	-4.74	1.31	1.38
7	A	6003	CFF	C6-N1	-4.73	1.31	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	6002	ATP	PB-O3B-PG	-3.84	119.66	132.83
6	A	6002	ATP	PB-O3B-PG	-3.84	119.66	132.83
6	G	6002	ATP	PB-O3B-PG	-3.84	119.66	132.83
6	J	6002	ATP	PB-O3B-PG	-3.83	119.67	132.83
6	J	6002	ATP	PA-O3A-PB	-3.57	120.59	132.83

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O1A
6	A	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C5'-O5'-PA-O1A
6	D	6002	ATP	C5'-O5'-PA-O2A
6	G	6002	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	6002	ATP	1	0
6	A	6002	ATP	1	0
7	G	6003	CFF	2	0
7	J	6003	CFF	2	0

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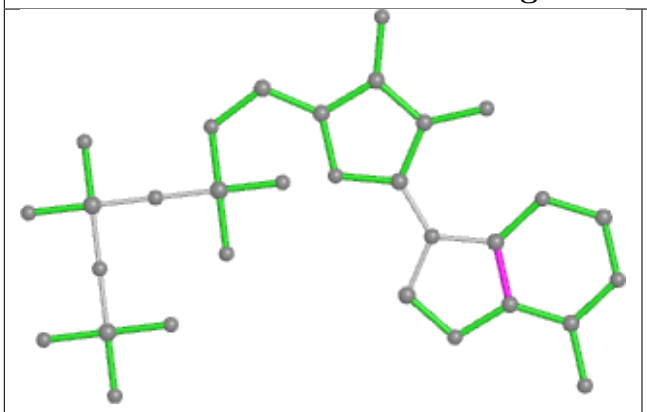
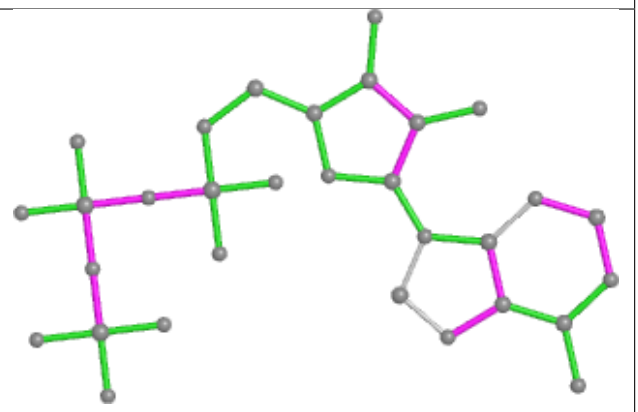
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	6003	CFF	2	0
6	D	6002	ATP	1	0
7	D	6003	CFF	2	0
6	G	6002	ATP	1	0

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.

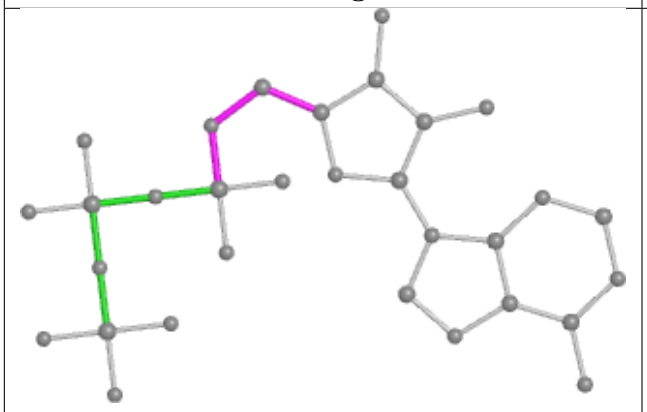
Ligand ATP J 6002



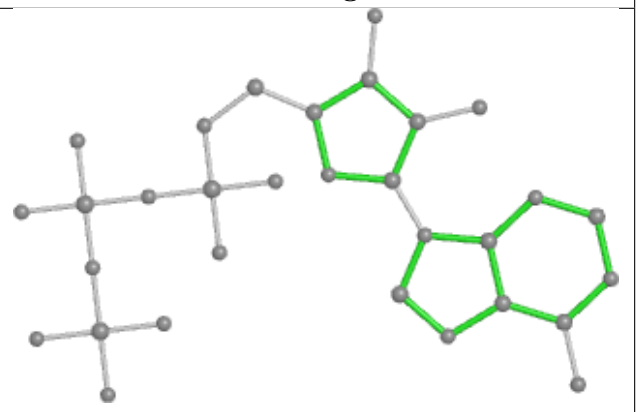
Bond lengths



Bond angles

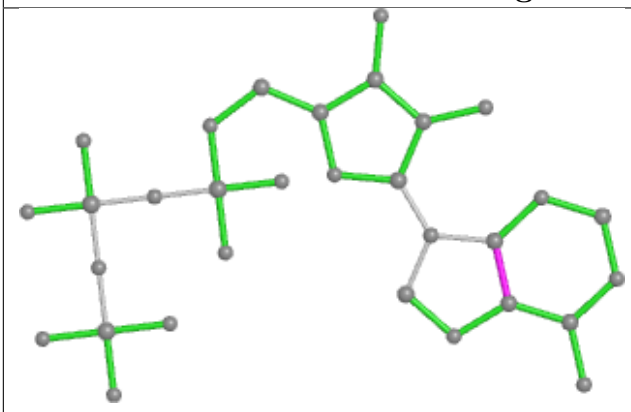


Torsions

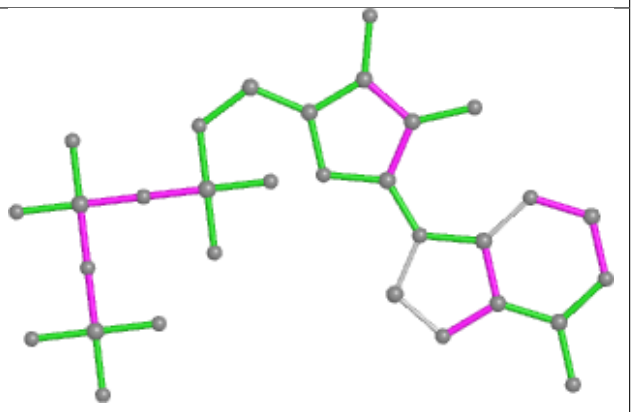


Rings

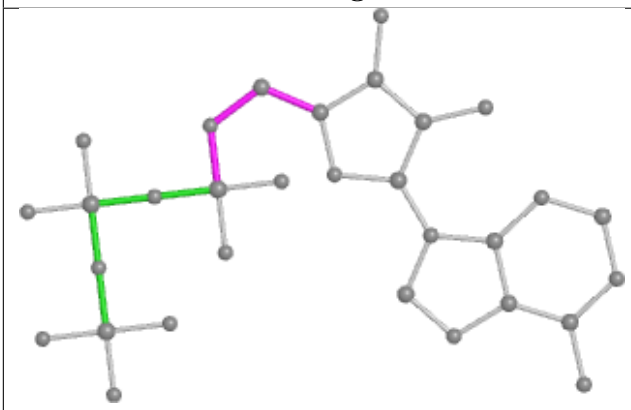
Ligand ATP A 6002



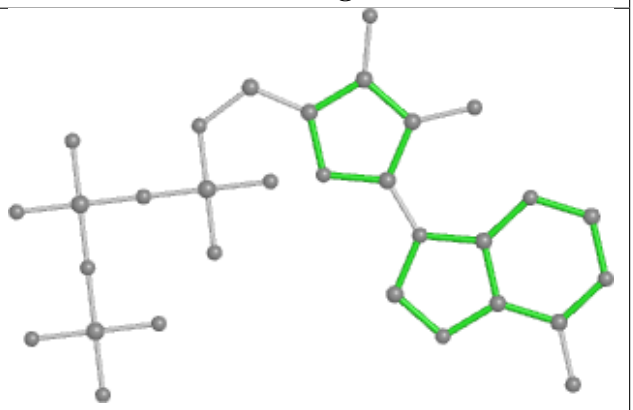
Bond lengths



Bond angles

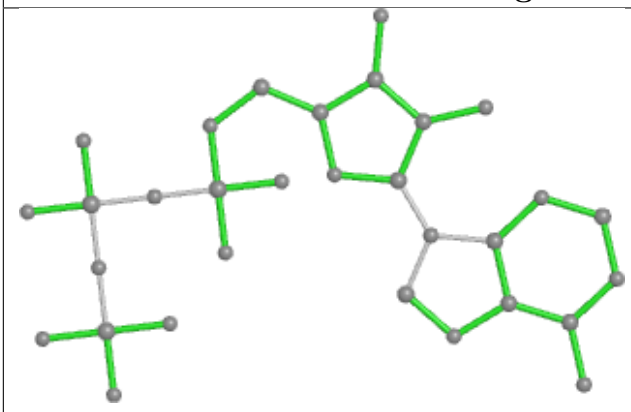


Torsions

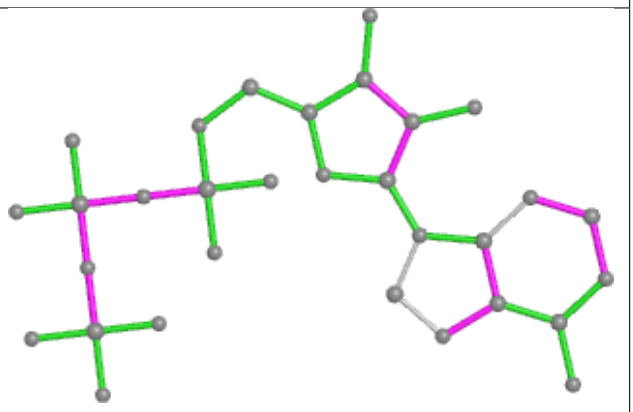


Rings

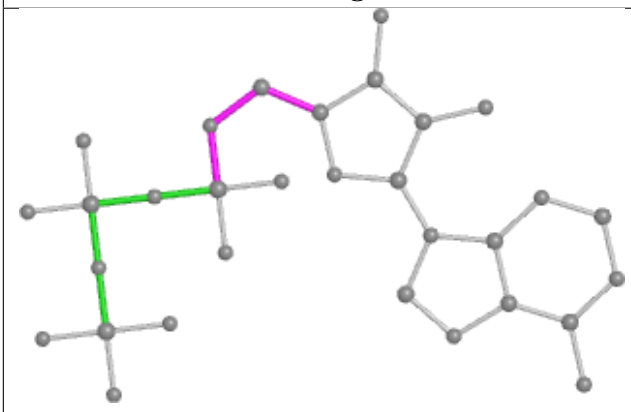
Ligand ATP D 6002



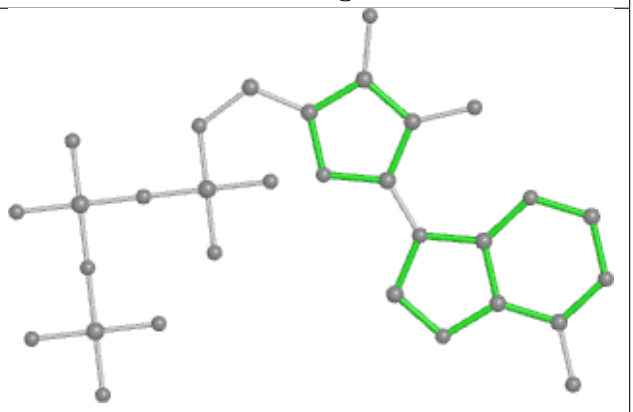
Bond lengths



Bond angles

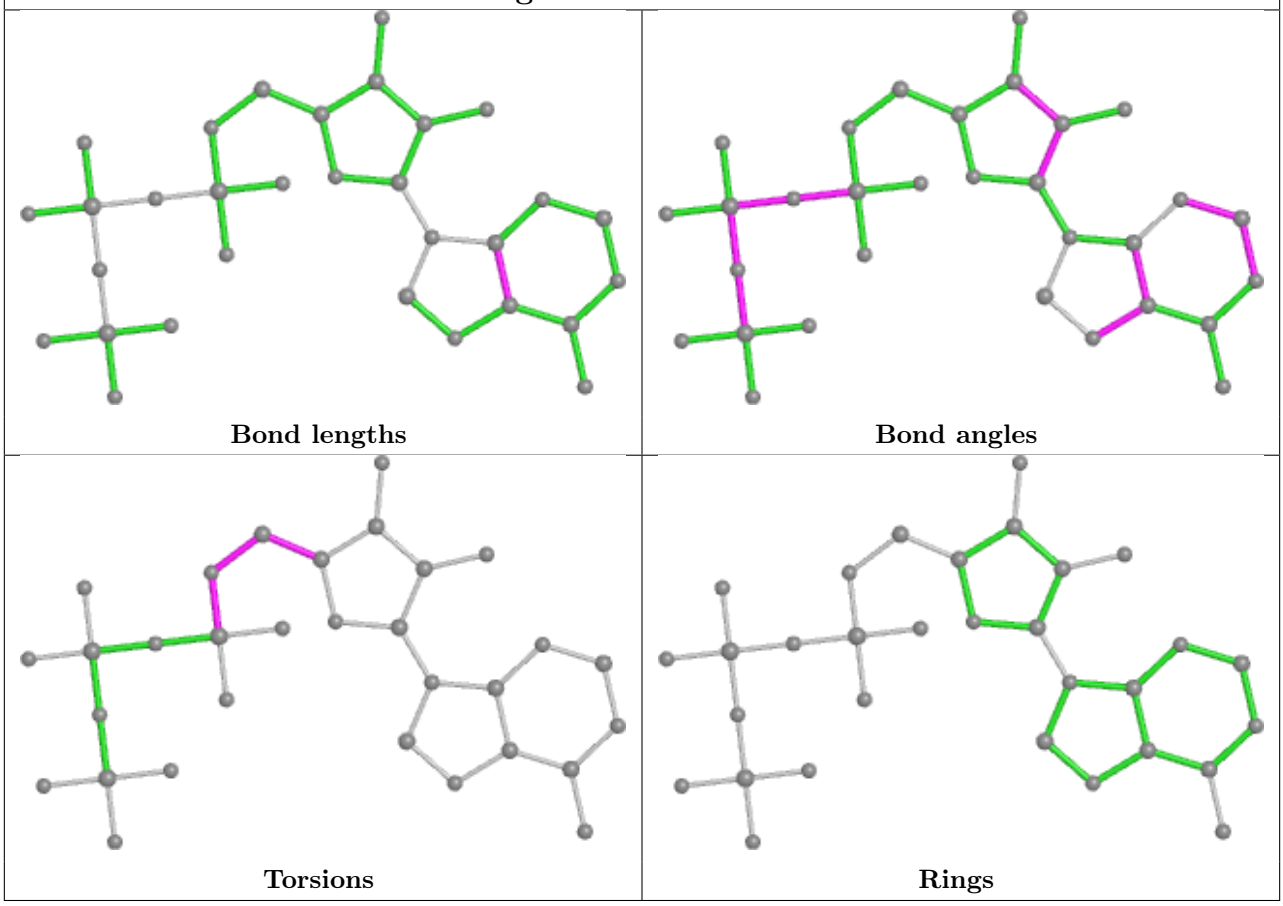


Torsions



Rings

Ligand ATP G 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.

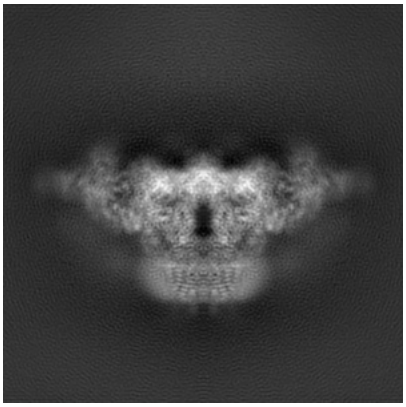
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9837. These allow visual inspection of the internal detail of the map and identification of artifacts.

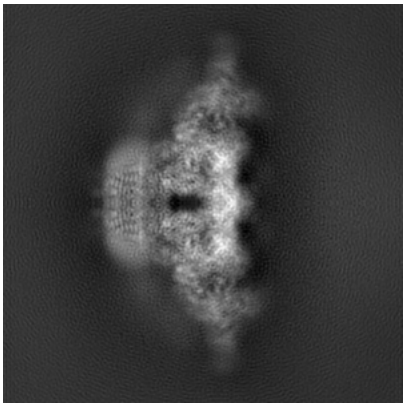
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

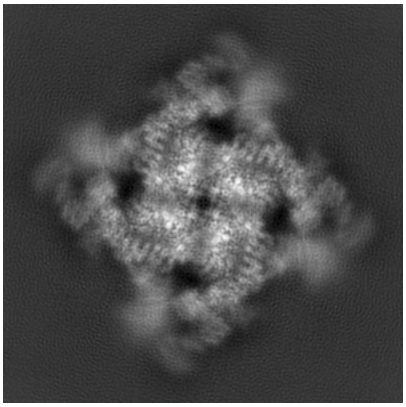
6.1.1 Primary map



X



Y

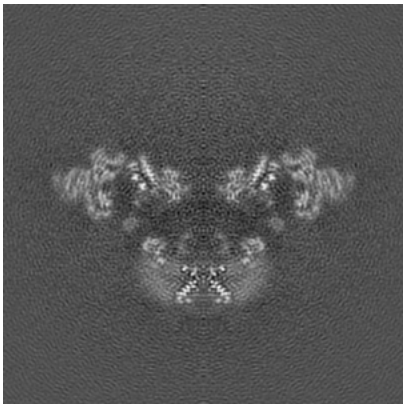


Z

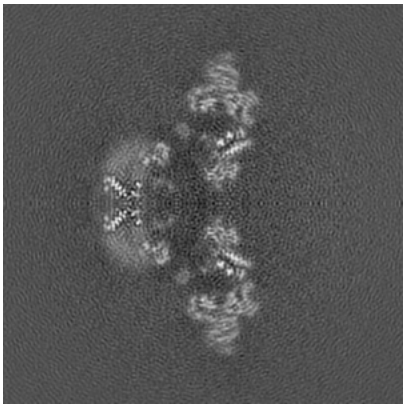
The images above show the map projected in three orthogonal directions.

6.2 Central slices

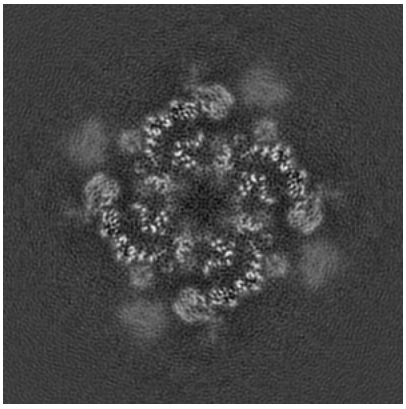
6.2.1 Primary map



X Index: 200



Y Index: 200

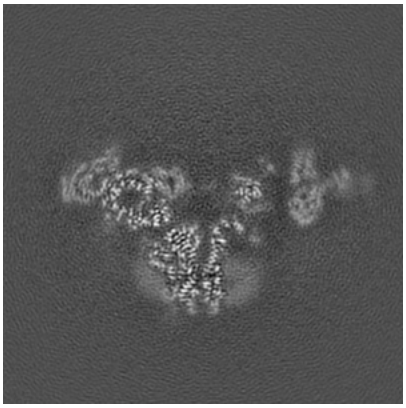


Z Index: 200

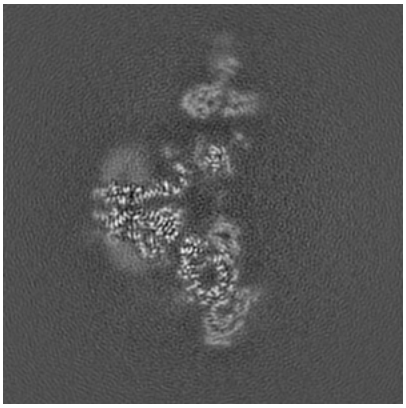
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

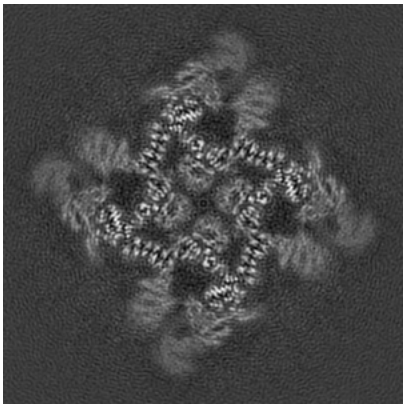
6.3.1 Primary map



X Index: 212



Y Index: 188

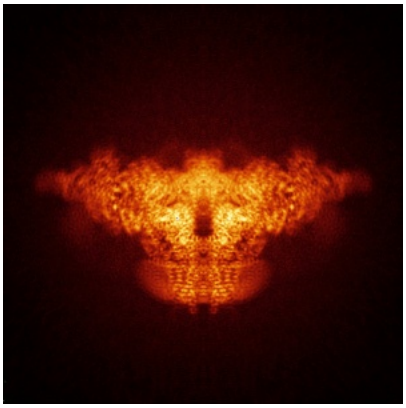


Z Index: 214

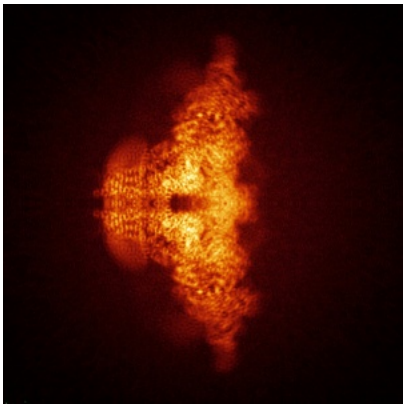
The images above show the largest variance slices of the map in three orthogonal directions.

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

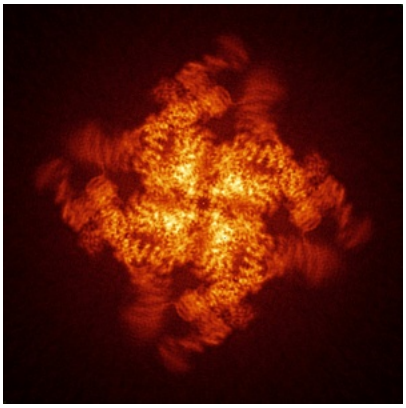
6.4.1 Primary map



X



Y

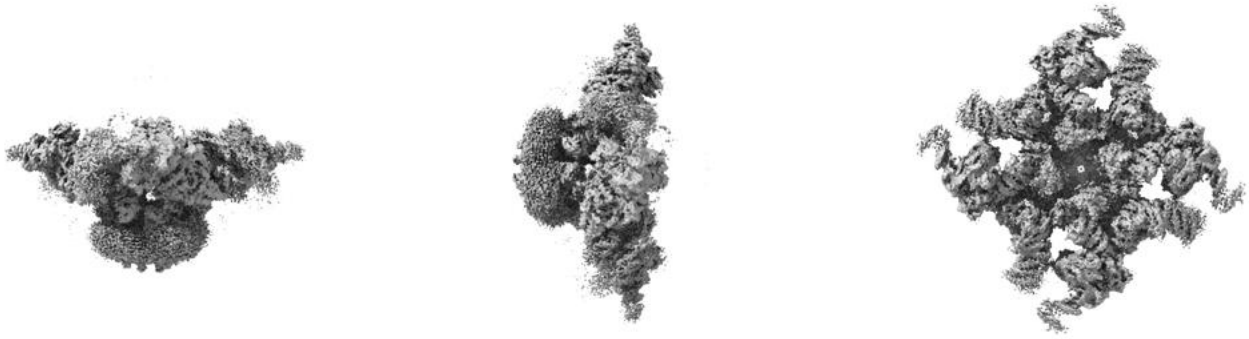


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

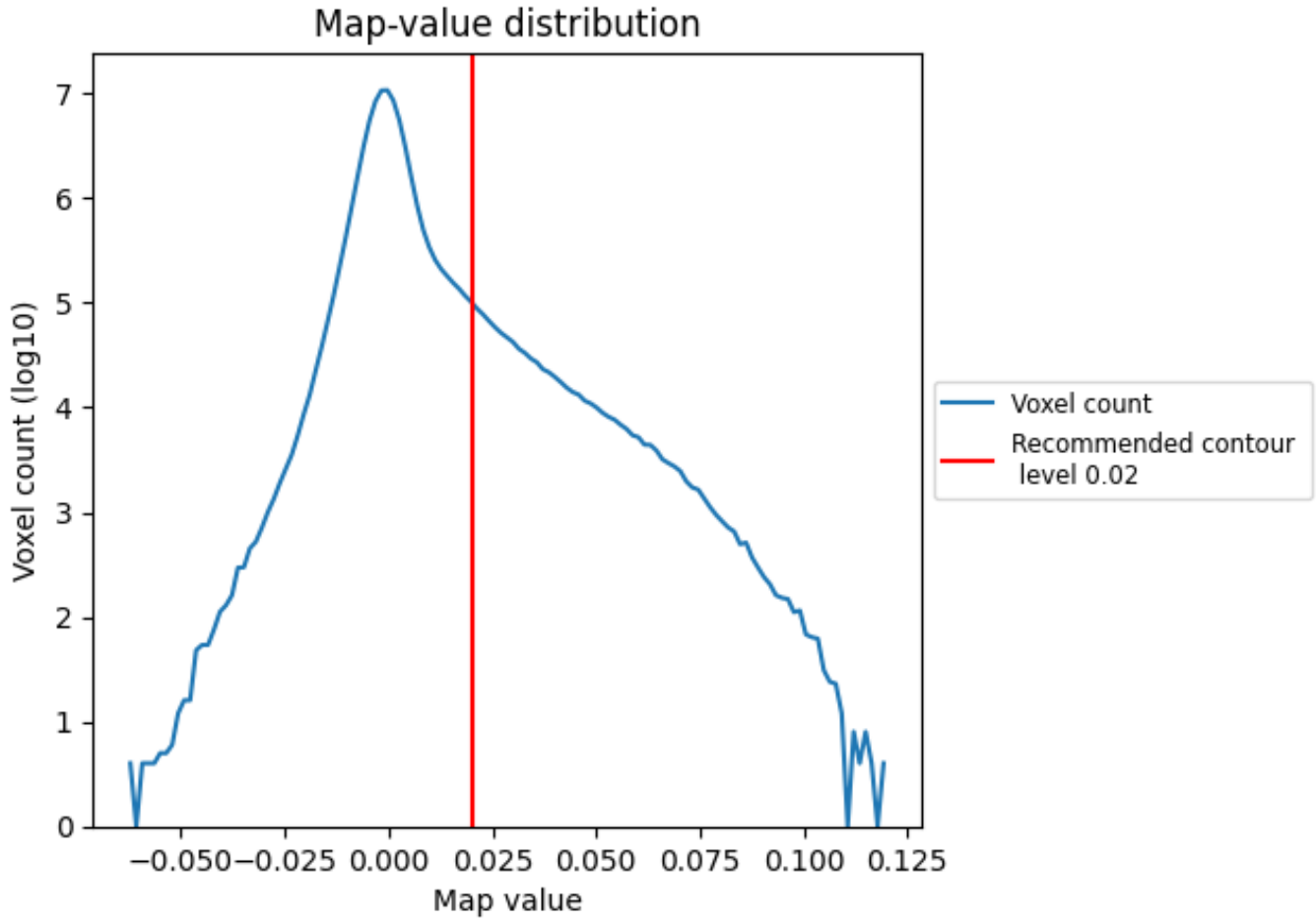
6.6 Mask visualisation (i)

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

7 Map analysis

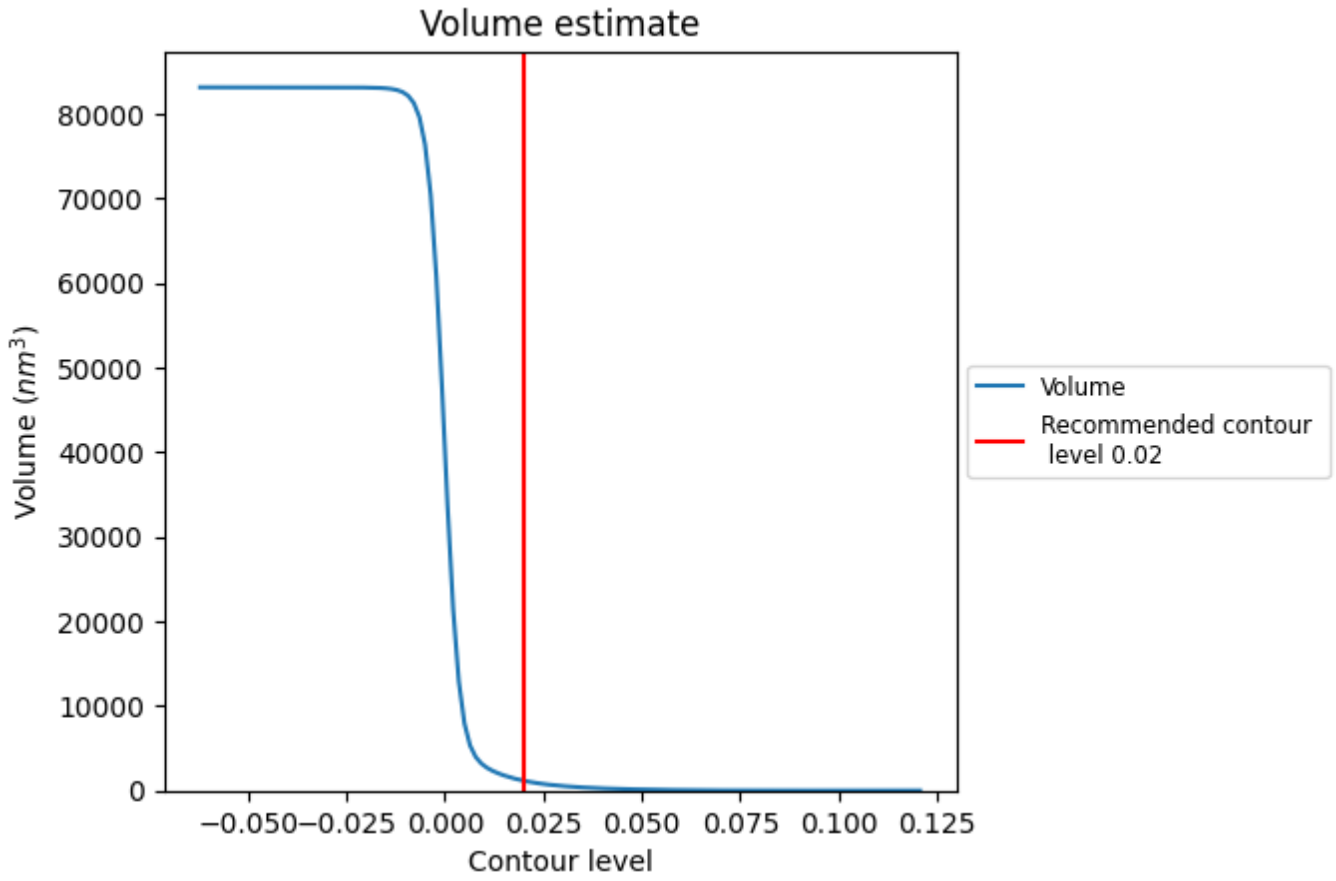
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

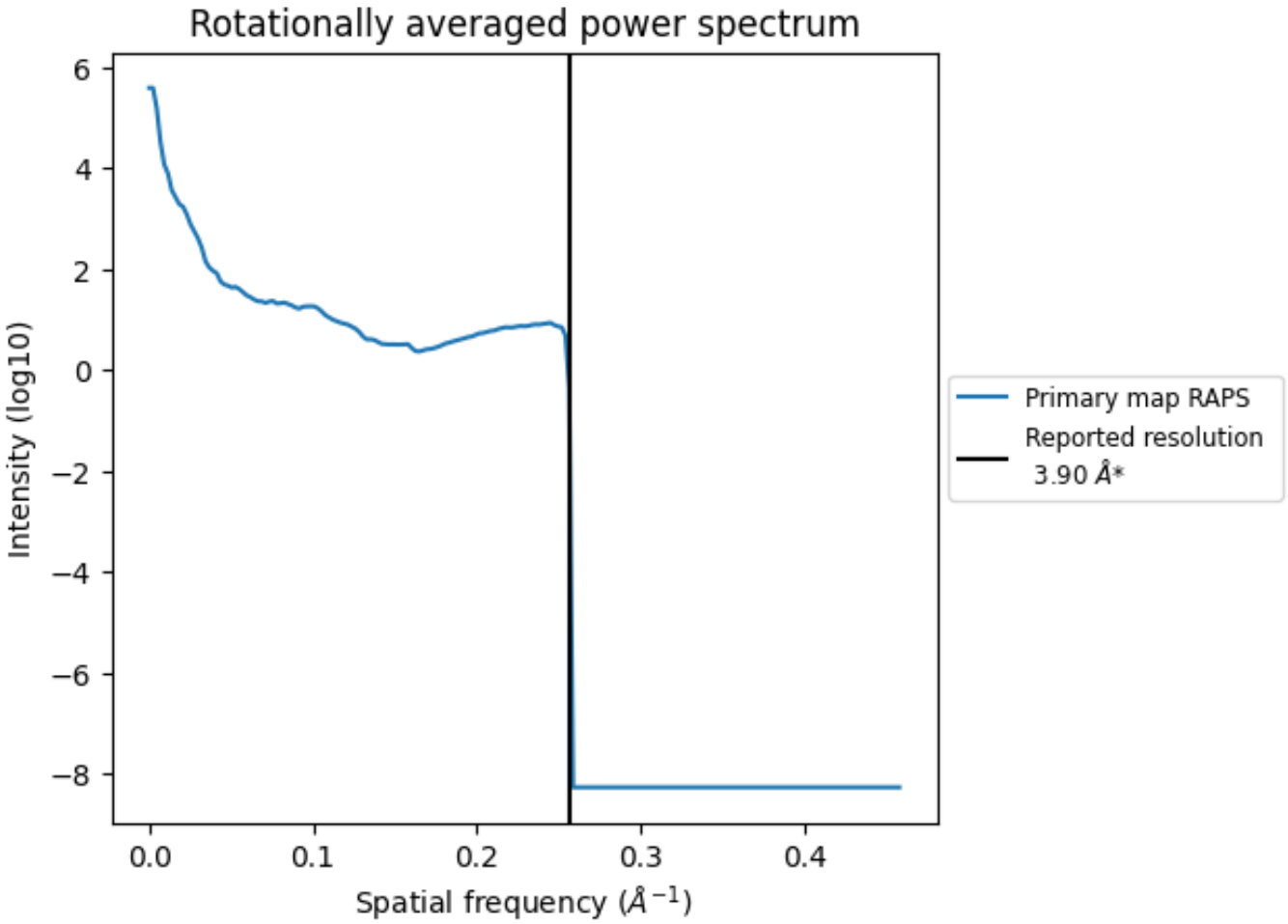
7.2 Volume estimate (i)



The volume at the recommended contour level is 1164 nm^3; this corresponds to an approximate mass of 1051 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)

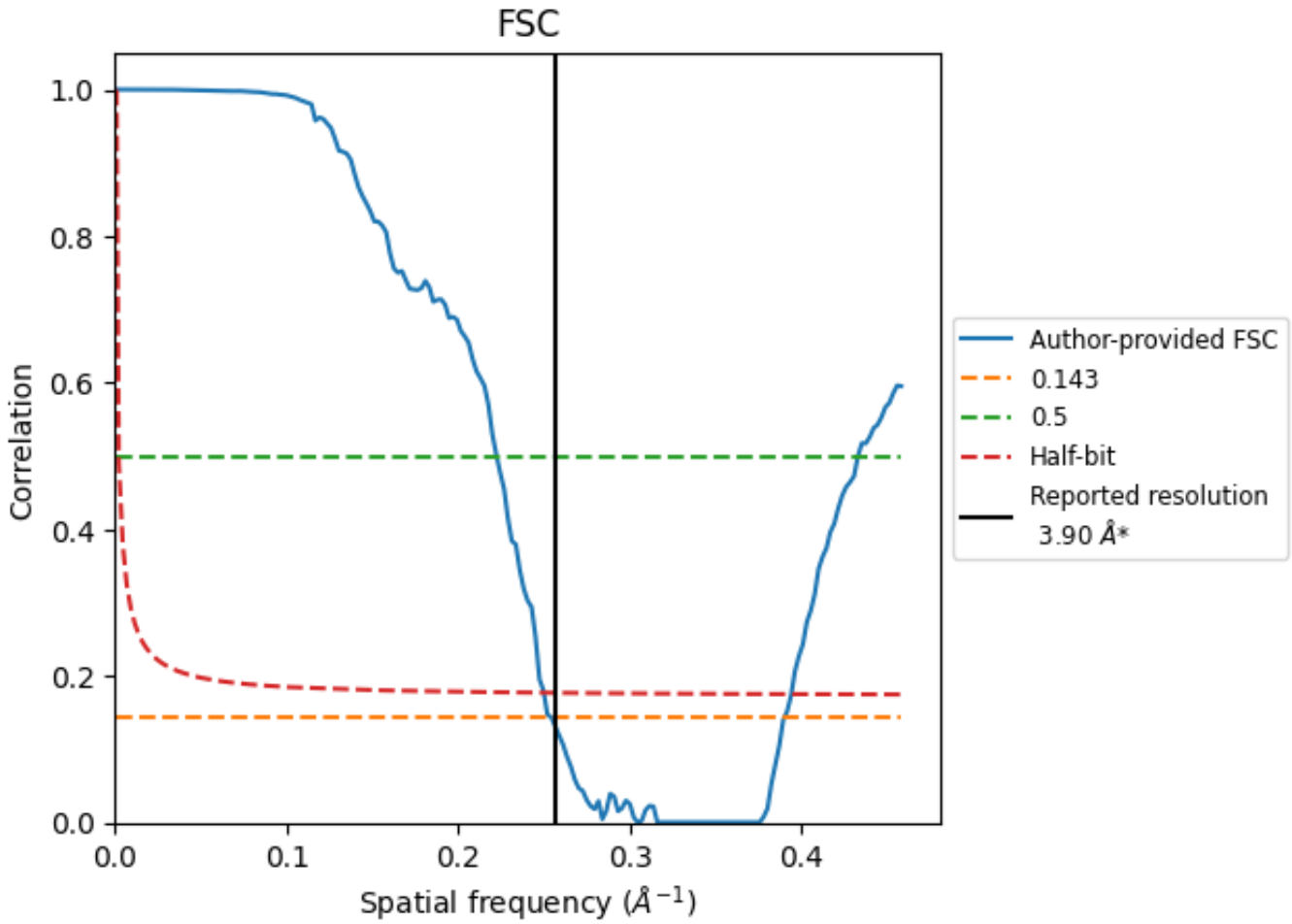


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

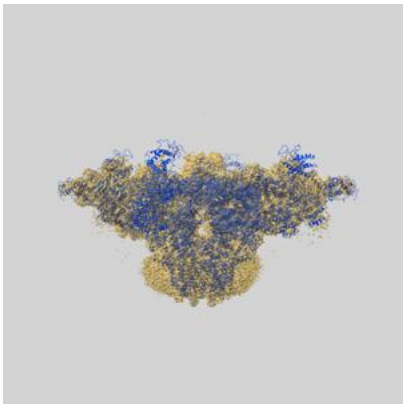
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.49	4.00
Unmasked-calculated*	-	-	-

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

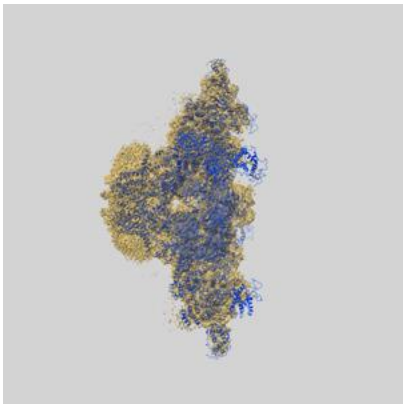
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9837 and PDB model 6JIY. Per-residue inclusion information can be found in section 3 on page 8.

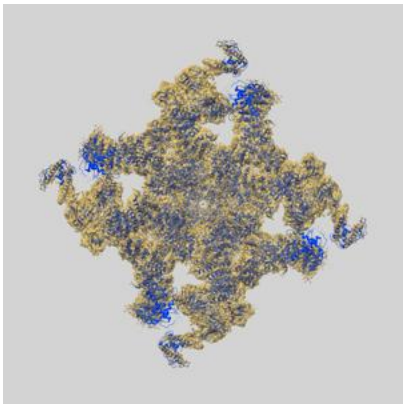
9.1 Map-model overlay



X



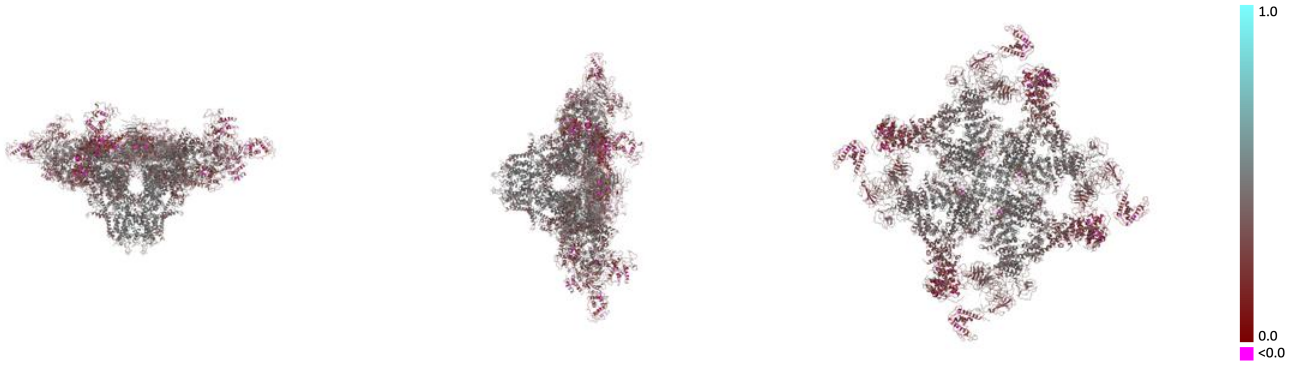
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

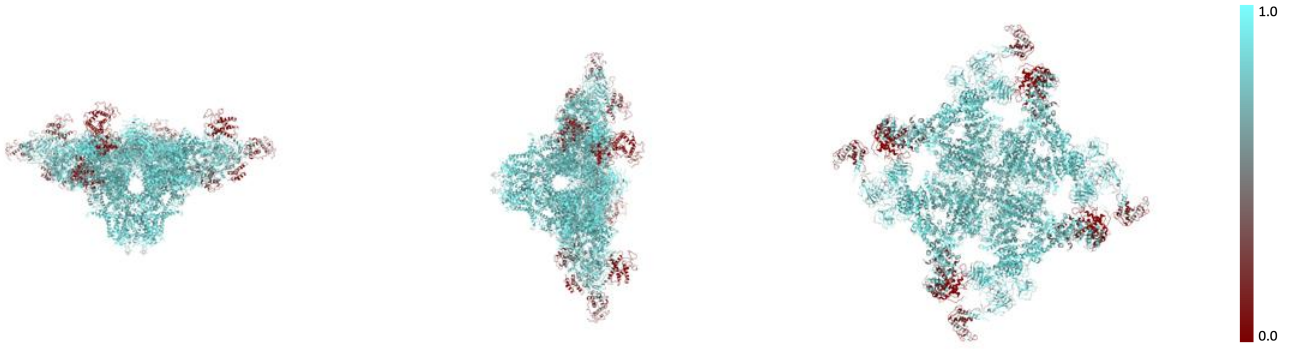
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

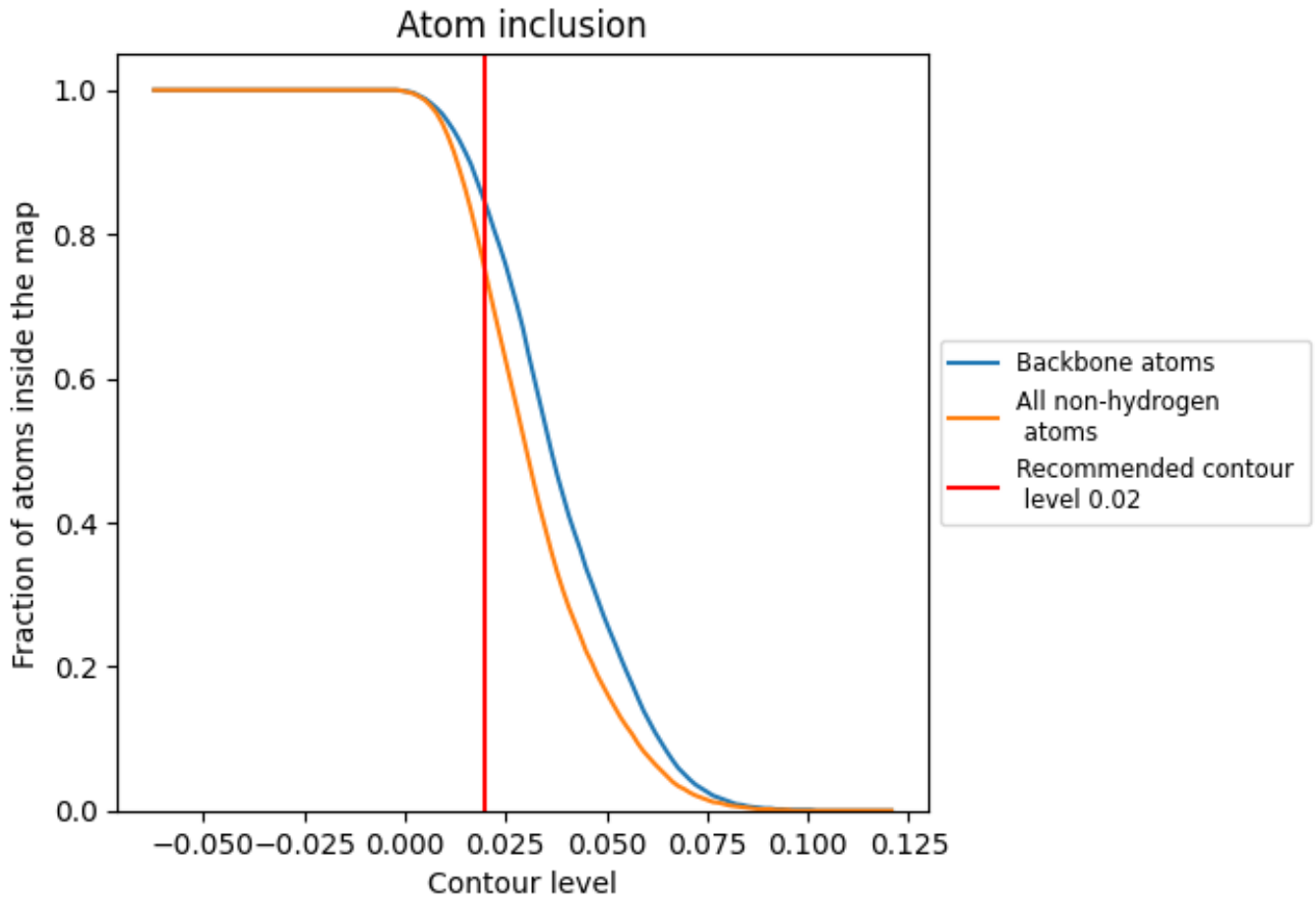
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.3750
A	0.7590	0.3790
B	0.7990	0.3990
C	0.3940	0.2820
D	0.7590	0.3790
E	0.7990	0.3990
F	0.3960	0.2820
G	0.7590	0.3780
H	0.7990	0.3970
I	0.3930	0.2810
J	0.7580	0.3780
K	0.7970	0.3980
L	0.3970	0.2820