wwPDB EM Validation Summary Report

Nov 2, 2022 – 03:37 AM EDT

PDB ID	:	5TAM
EMDB ID	:	EMD-8379
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.30 Å(reported)

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

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

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

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

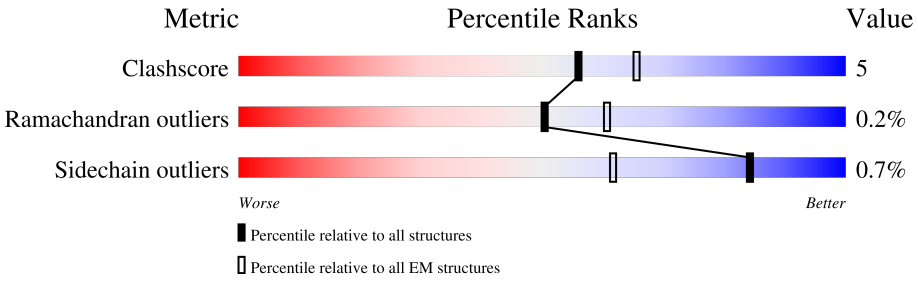
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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	108	56% 79% 20%
1	F	108	56% 81% 19%
1	H	108	57% 81% 19%
1	J	108	56% 81% 19%
2	B	4416	49% 83% 11% 5%
2	E	4416	49% 84% 11% 5%
2	G	4416	50% 83% 11% 5%
2	I	4416	50% 84% 11% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

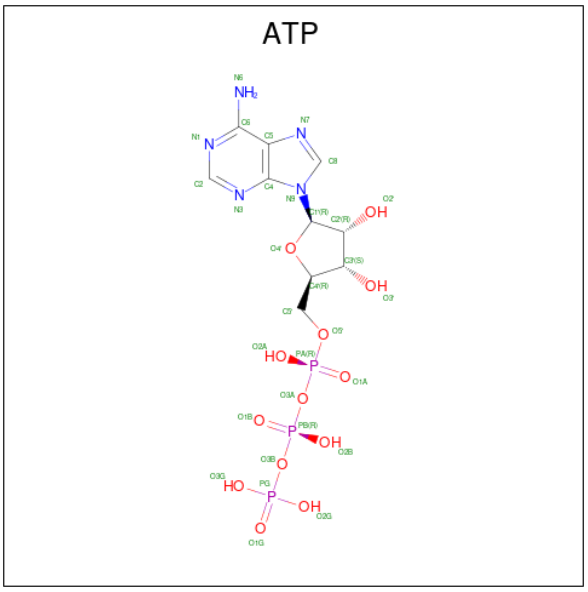
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

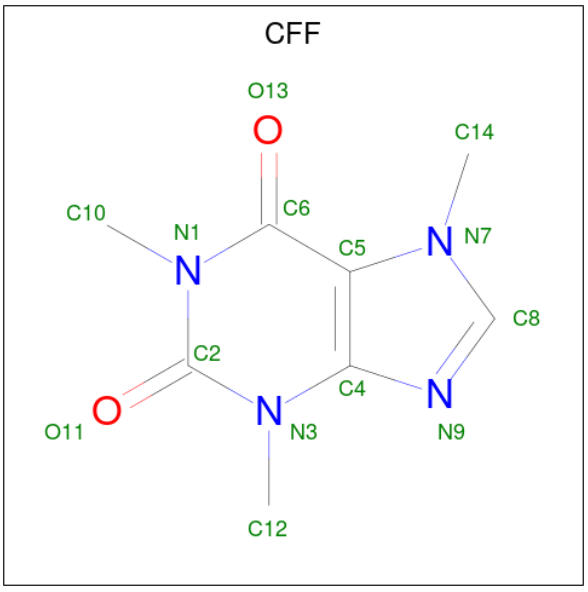
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

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



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

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



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

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

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

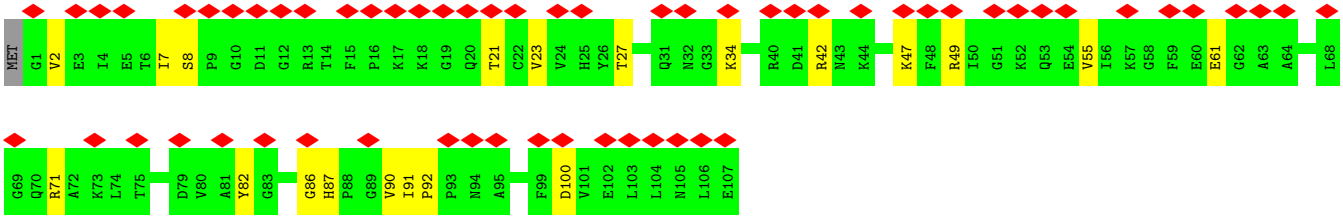
Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total Ca 1 1	0
6	E	1	Total Ca 1 1	0
6	I	1	Total Ca 1 1	0
6	G	1	Total Ca 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

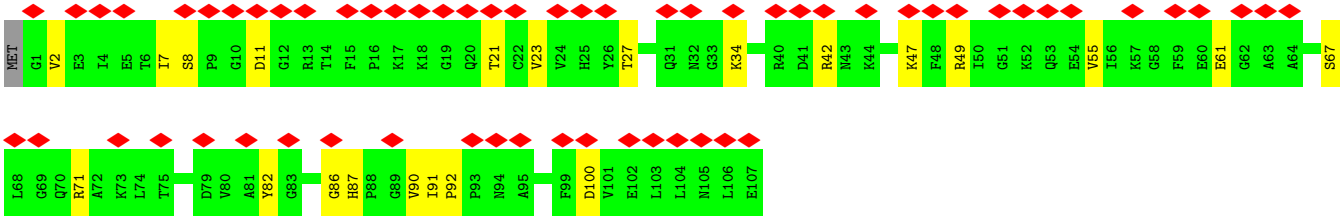
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



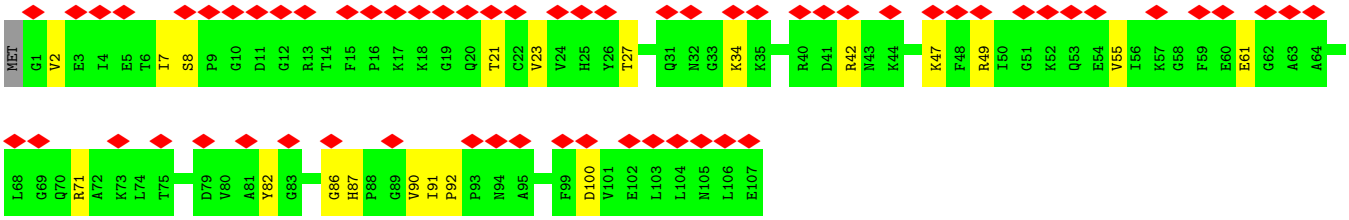
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



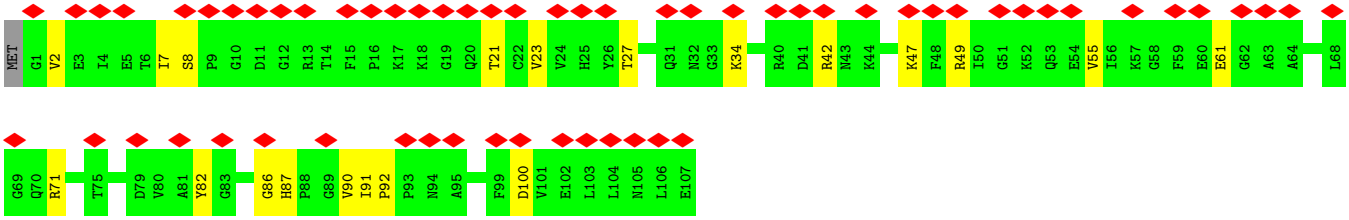
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



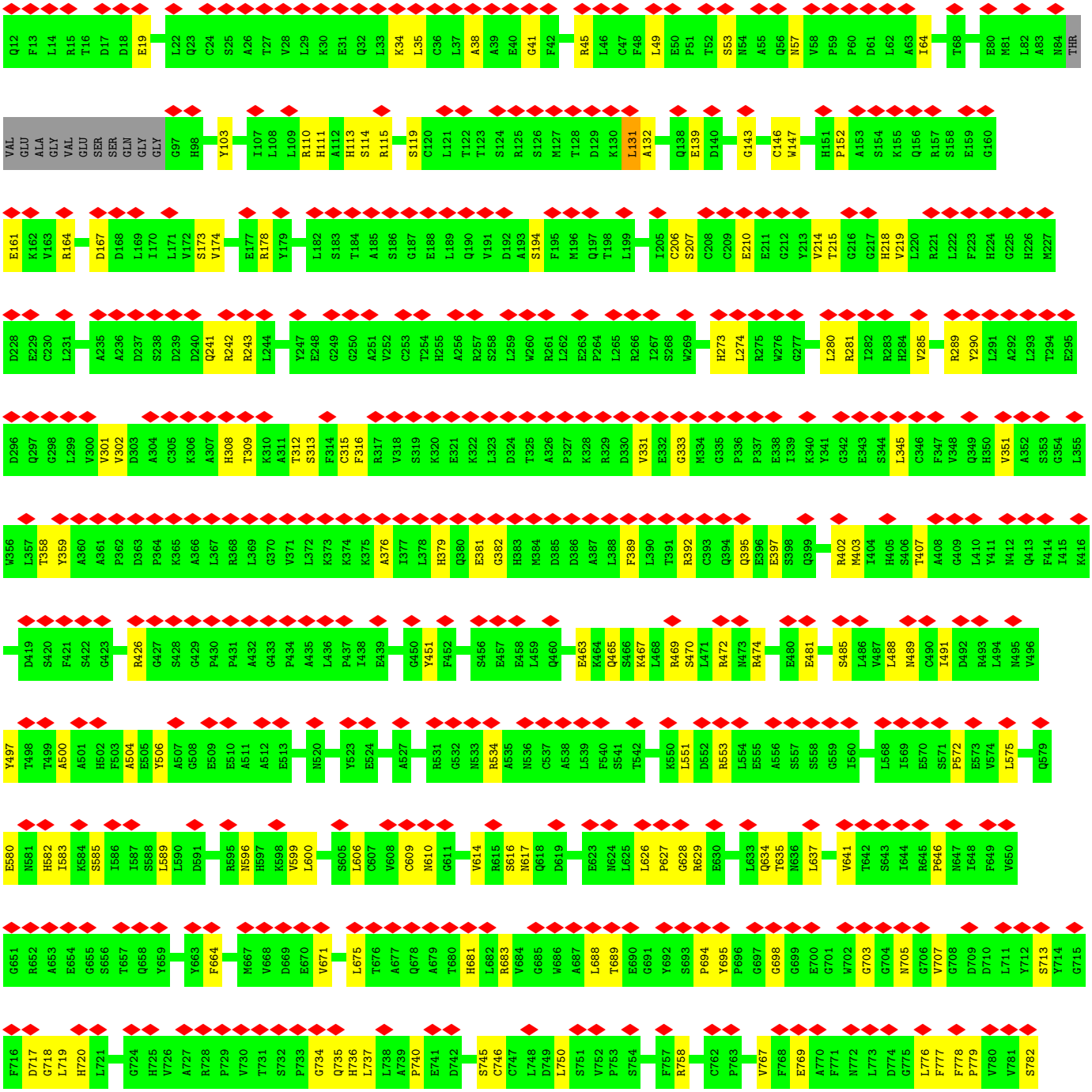
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

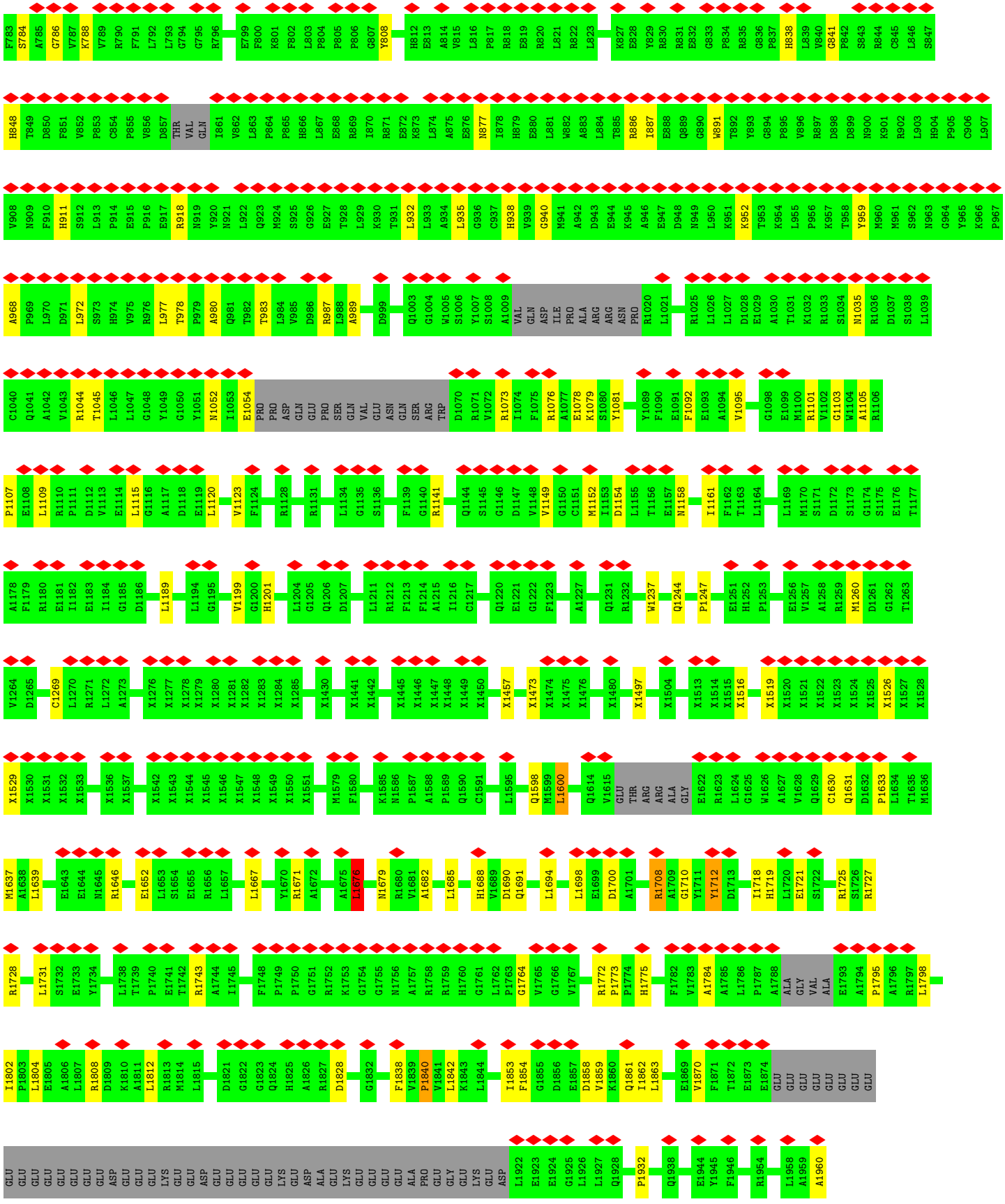
Chain J:



• Molecule 2: Ryanodine receptor 1

Chain B:

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H848 T849 D850 F851 V852 P853 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907
V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967
A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 A989 D999 Q1003 G1004 W1005 S1006 Y1007 S1008 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 R1025 L1026 L1027 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039
C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 I1074 F1075 R1076 A1077 E1078 K1079 S1080 Y1081 Y1089 F1090 E1091 F1092 E1093 A1094 V1095 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106
P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 G1116 A1117 D1118 E1119 L1120 V1123 F1124 R1128 R1131 L1134 G1135 S1136 F1139 G1140 R1141 Q1144 S1145 G1146 D1147 V1148 V1149 G1150 C1151 M1152 I1153 D1154 L1155 T1156 E1157 N1158 I1161 F1162 T1163 L1164 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177
A1178 F1179 R1180 E1181 I1182 E1183 I1184 G1185 D1186 L1189 L1194 G1195 V1199 G1200 H1201 L1204 G1205 Q1206 D1207 L1211 R1212 F1213 F1214 A1215 I1216 C1217 Q1220 E1221 G1222 F1223 A1227 Q1231 R1232 W1237 Q1244 P1247 E1251 H1252 P1253 E1256 V1257 A1258 R1259 M1260 D1261 G1262 T1263
V1264 D1265 C1269 L1270 R1271 L1272 A1273 X1276 X1277 X1278 X1279 X1280 X1281 X1282 X1283 X1284 X1285 X1430 X1441 X1442 X1445 X1446 X1447 X1448 X1449 X1450 X1457 X1473 X1474 X1475 X1476 X1480 X1497 X1504 X1513 X1514 X1515 X1516 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528
X1529 X1530 X1531 X1532 X1533 X1536 X1537 X1542 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 X1551 M1579 F1580 K1585 N1586 P1587 A1588 P1589 Q1590 C1591 L1595 Q1598 M1599 L1600 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624 G1625 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 T1635 M1636
M1637 A1638 L1639 E1643 E1644 N1645 R1646 E1652 L1653 S1654 E1655 R1656 L1657 L1667 Y1670 R1671 A1672 A1675 L1676 N1679 R1680 V1681 A1682 L1685 H1688 V1689 D1690 Q1691 L1694 L1698 E1699 D1700 A1701 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 S1722 R1725 S1726 R1727
R1728 L1731 S1732 E1733 Y1734 L1738 T1739 P1740 E1741 T1742 R1743 A1744 I1745 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1761 L1762 P1763 G1764 V1765 G1766 V1767 R1772 P1773 P1774 H1775 F1782 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798
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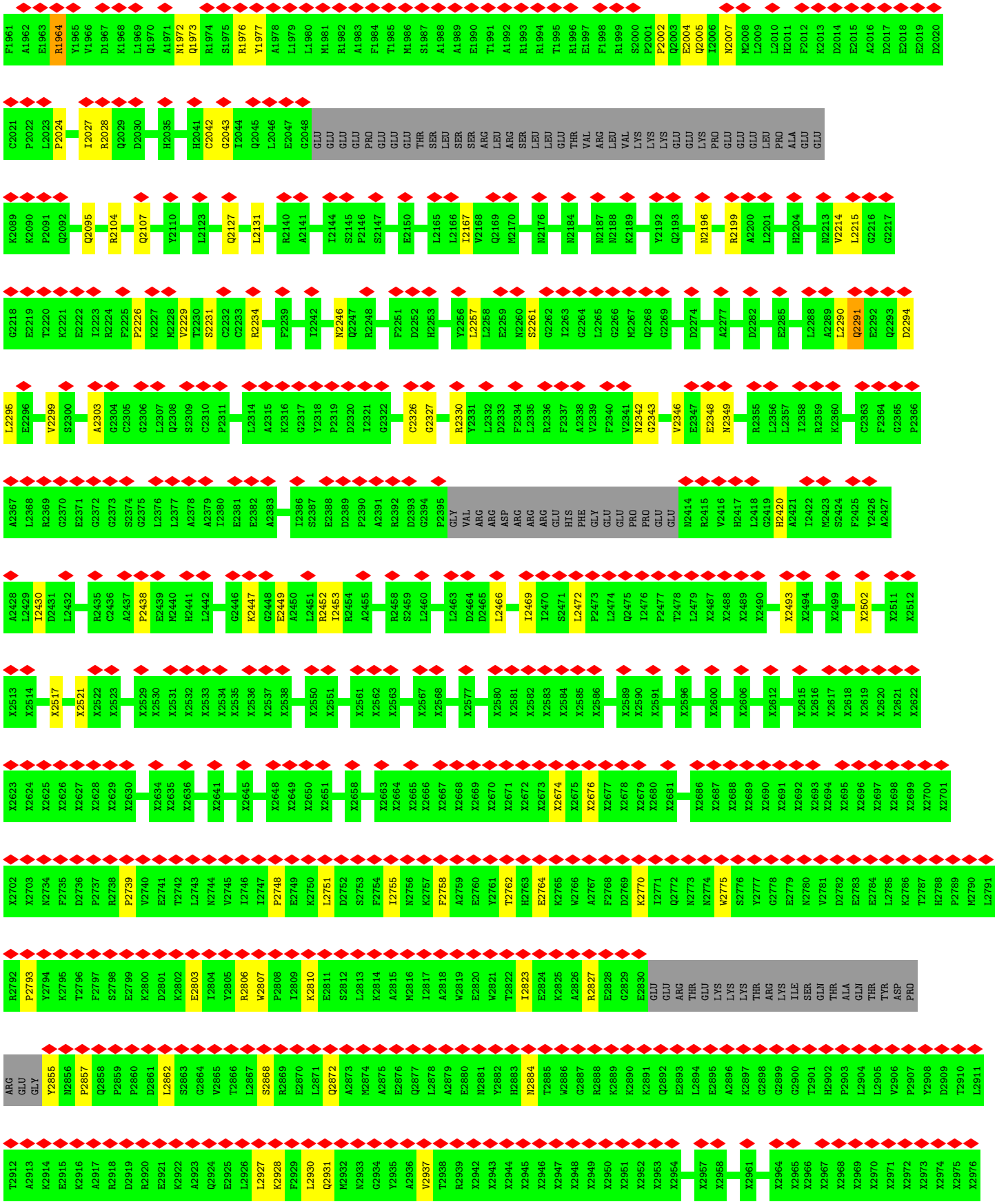
GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 P1932 Q1938 E1944 Y1945 F1946 R1964 L1968 A1959 A1960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C2021 P2022 L2023 P2024 I2027 R2028 Q2029 D2030 H2035 H2041 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU
K2089 K2090 P2091 Q2092 Q2095 R2104 Q2107 Y2110 L2123 Q2127 L2131 R2140 A2141 I2144 S2145 P2146 S2147 E2150 L2165 L2166 I2167 V2168 Q2169 M2170 N2176 N2184 N2187 N2188 K2189 Y2192 Q2193 N2196 R2199 A2200 L2201 H2204 N2213 V2214 L2215 G2216 G2217
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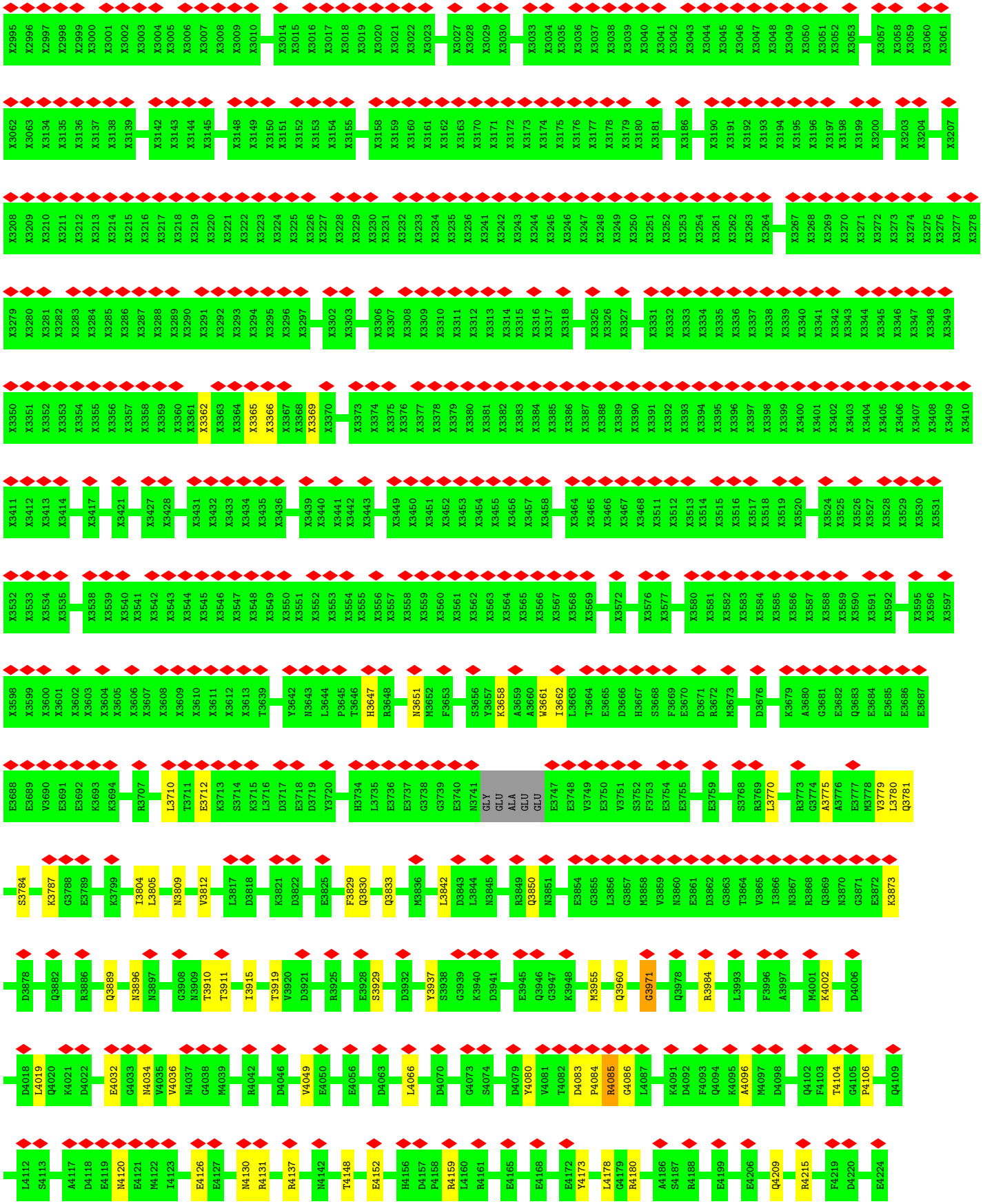
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X3302 X3303
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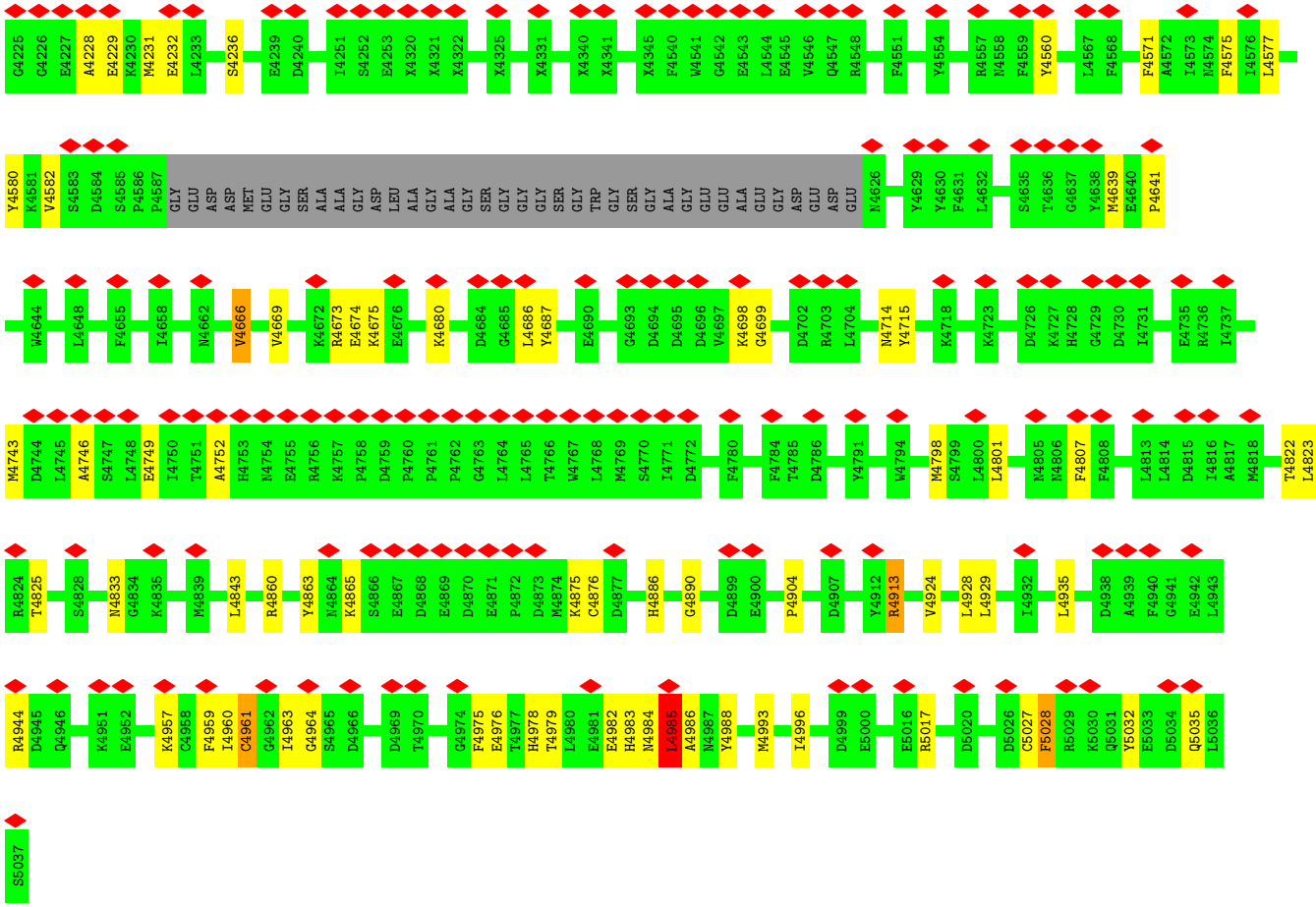

• Molecule 2: Ryanodine receptor 1

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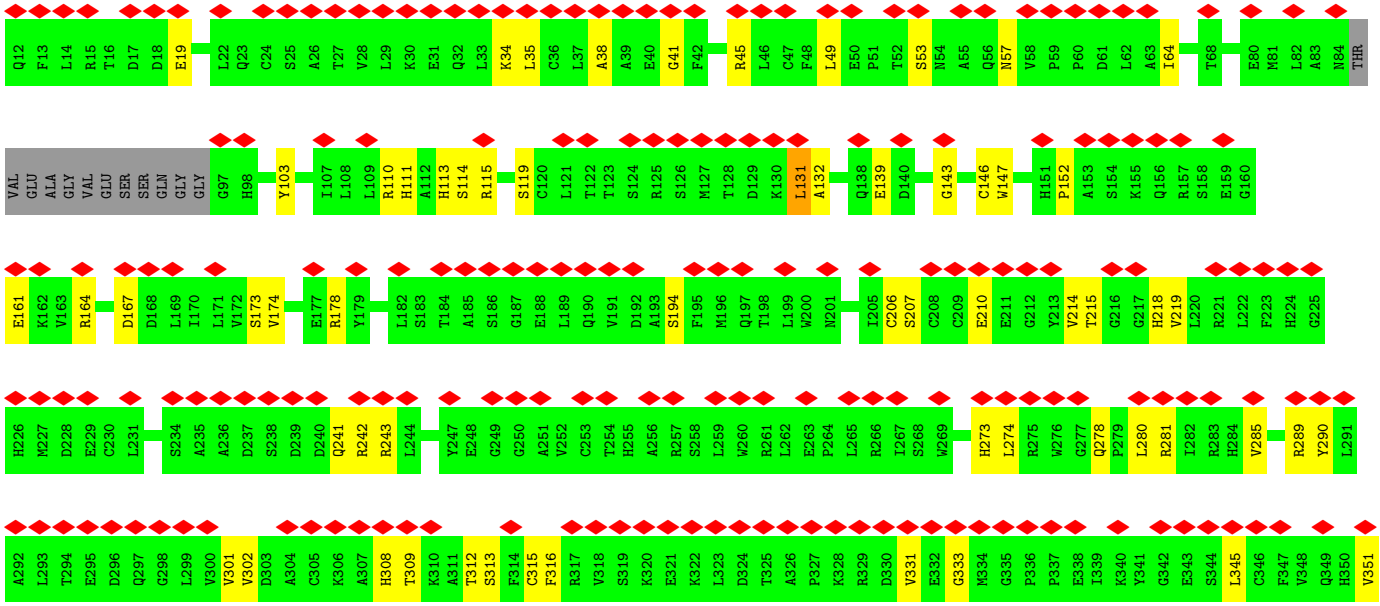

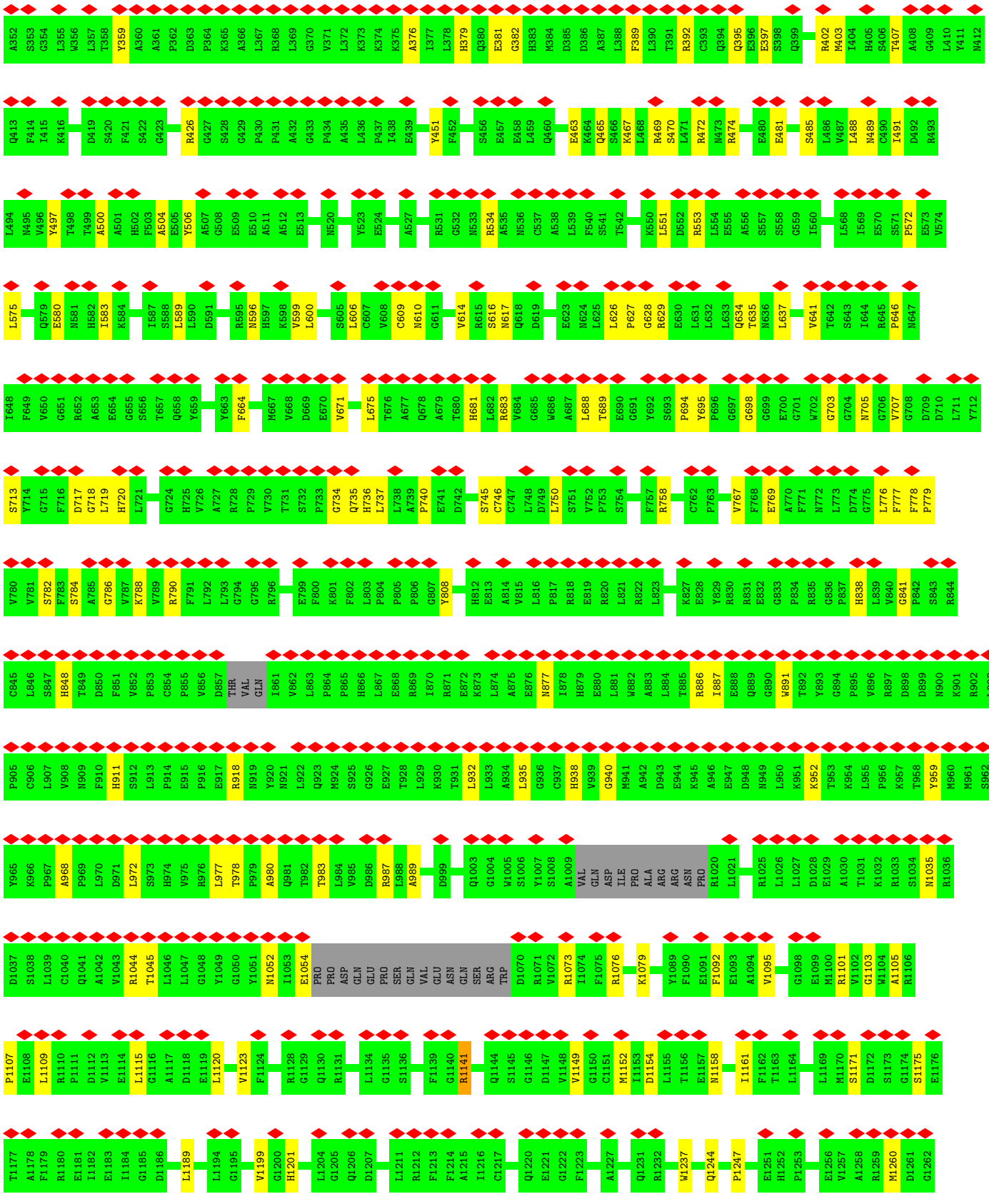
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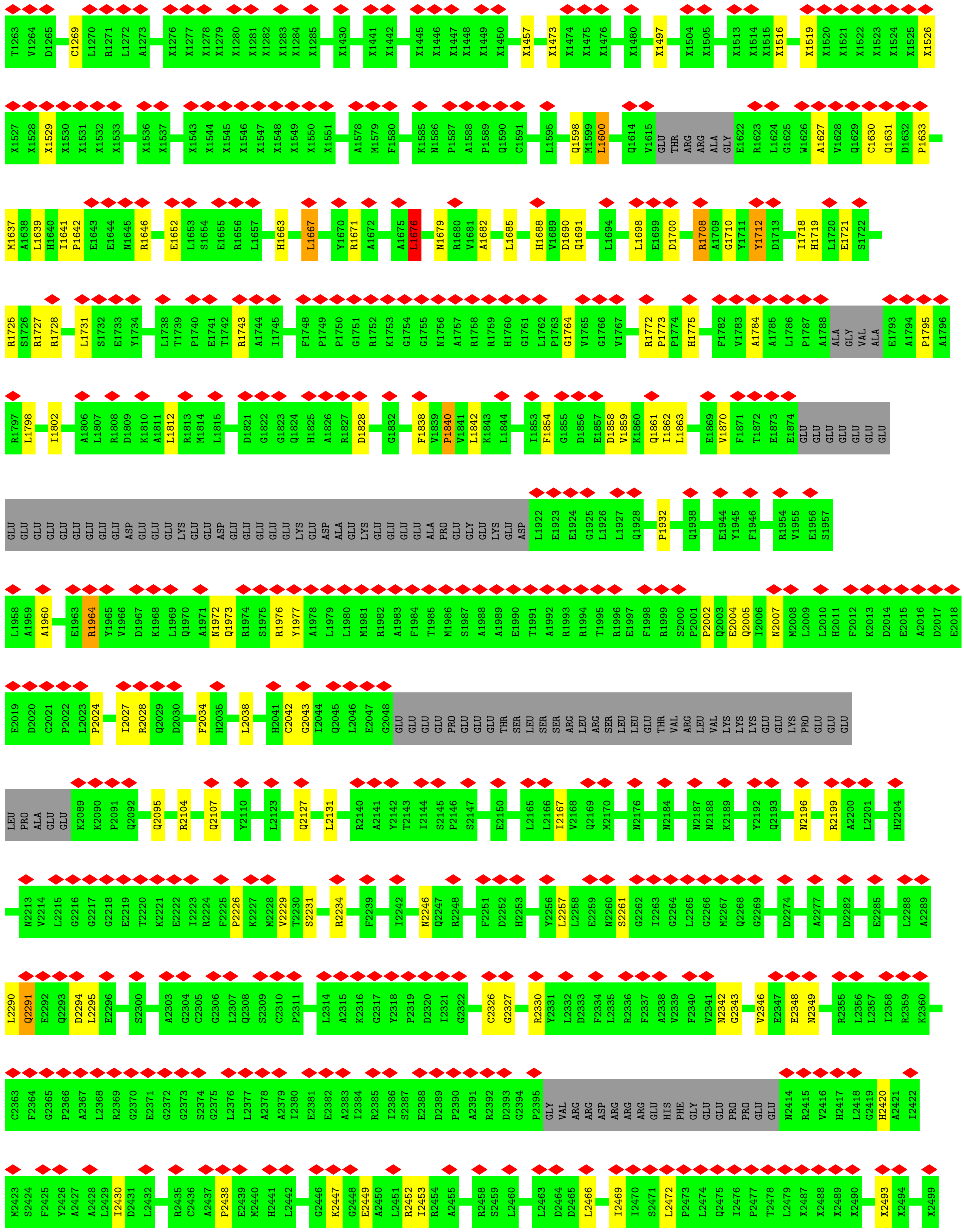
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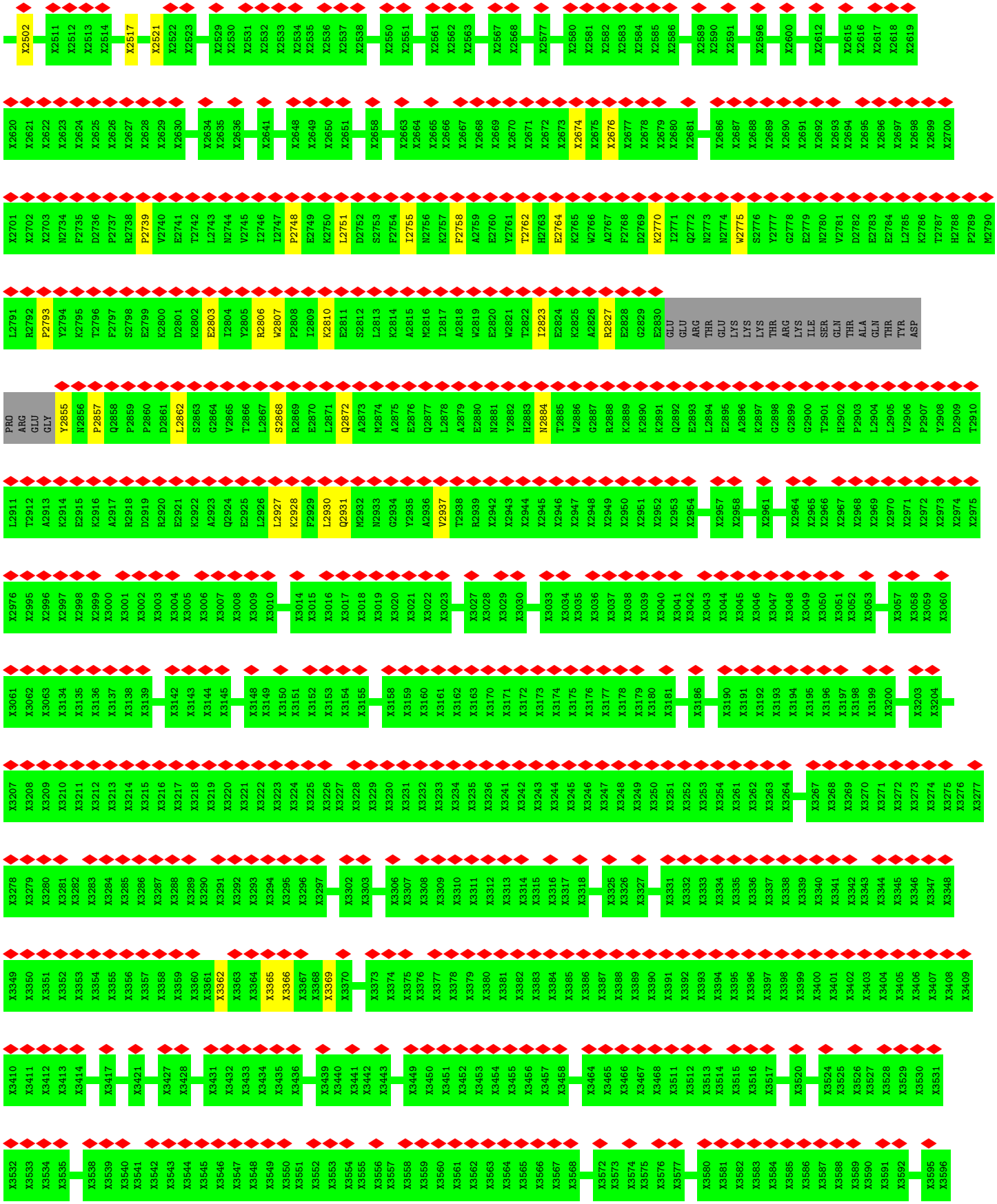
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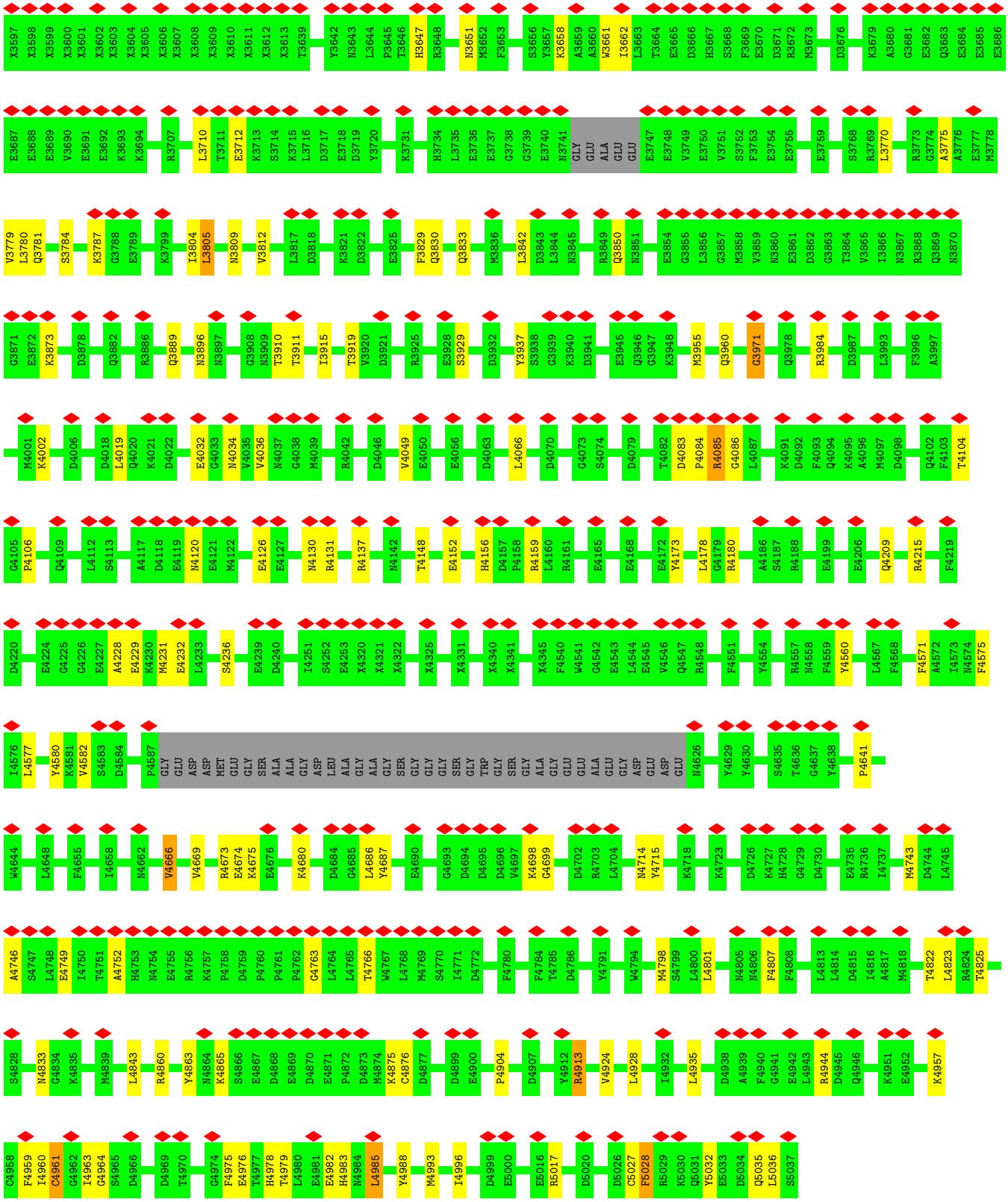

• Molecule 2: Ryanodine receptor 1

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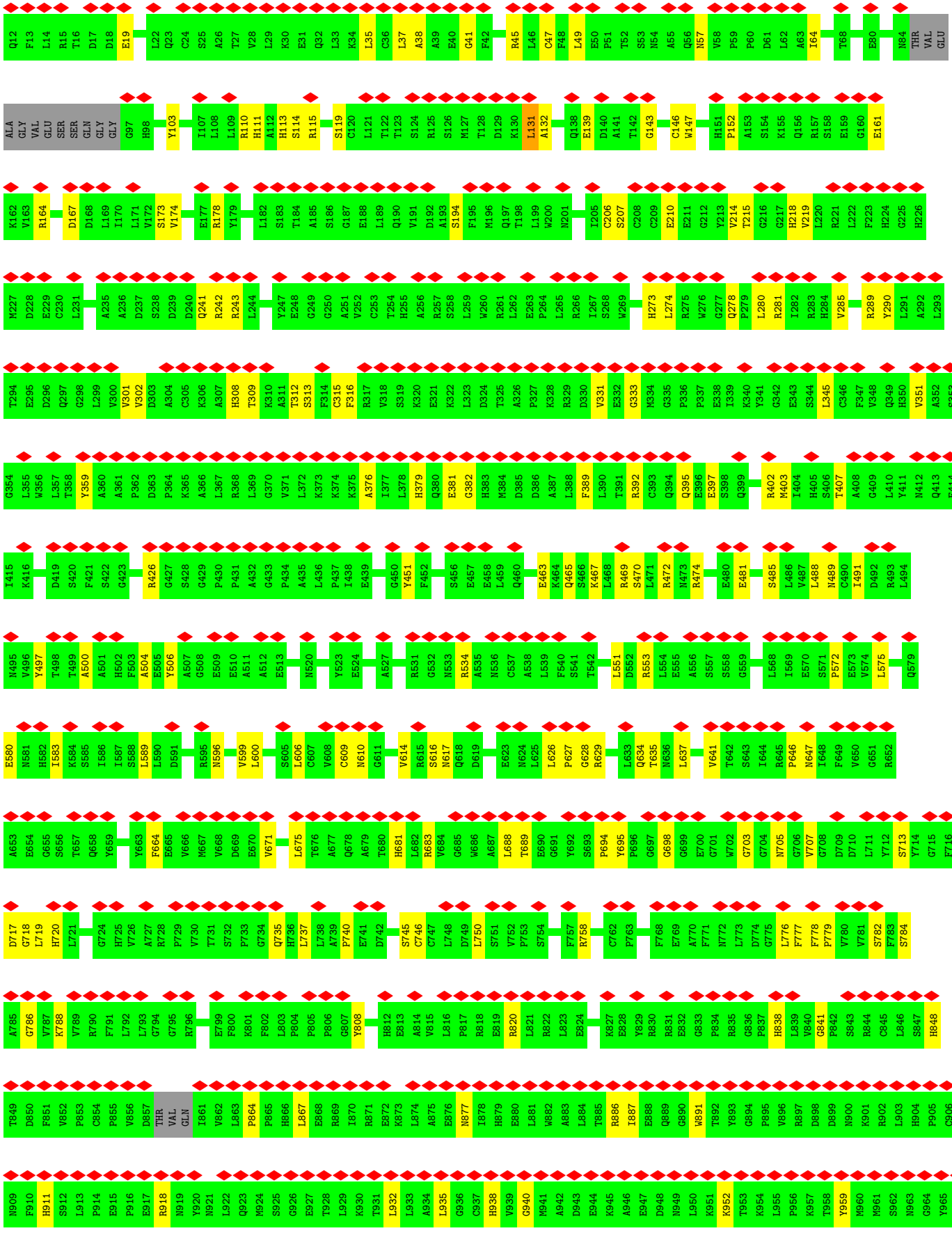
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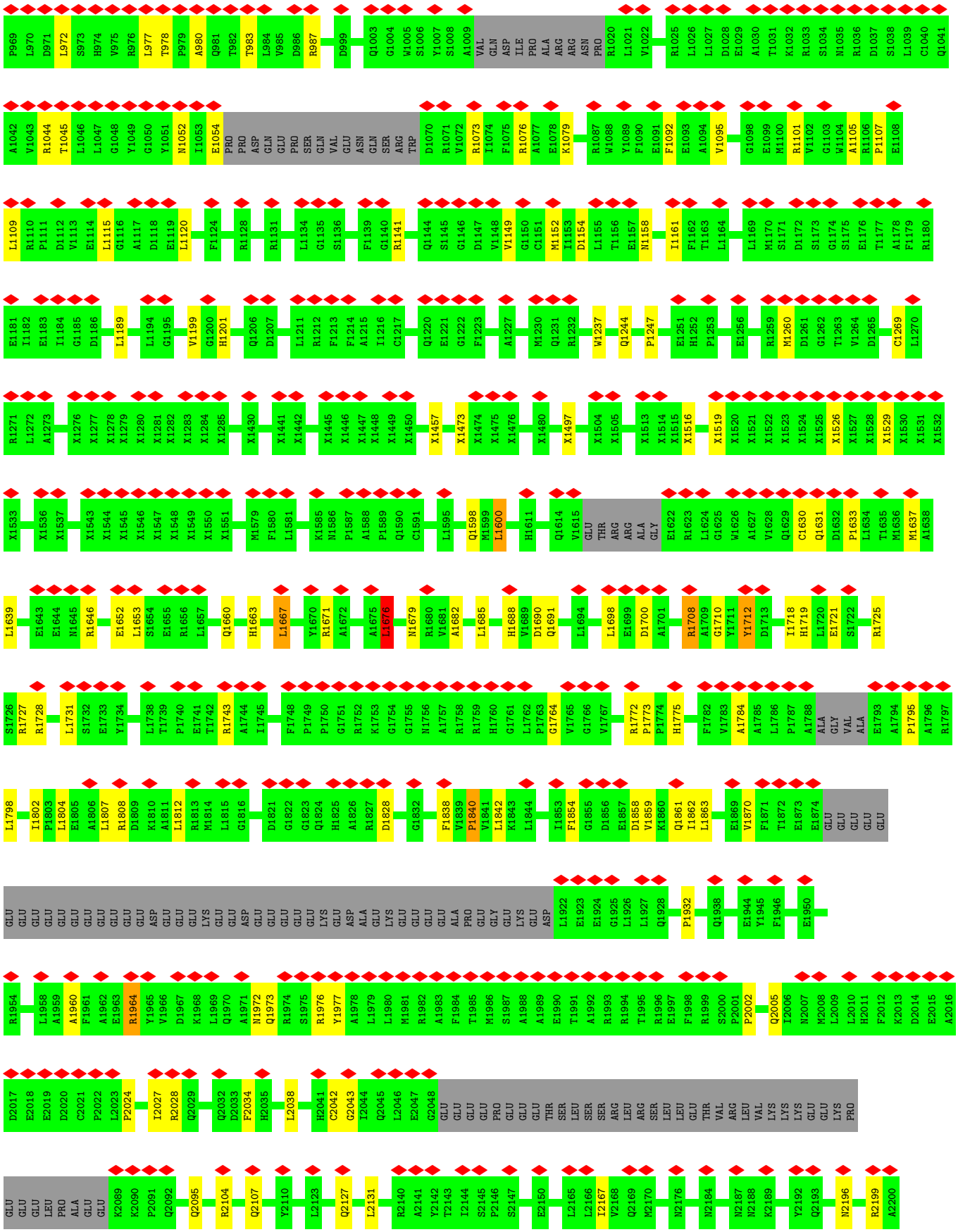
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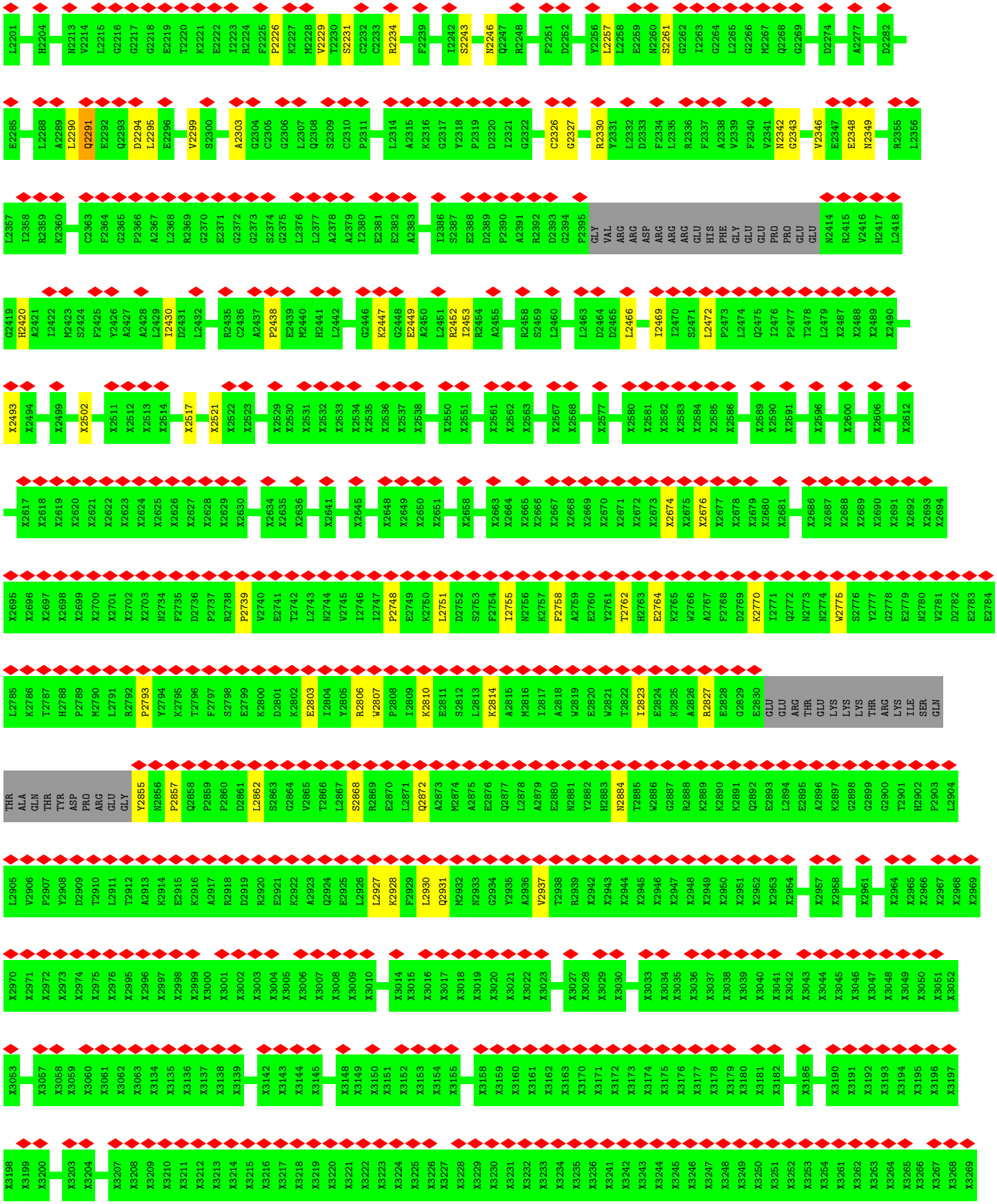
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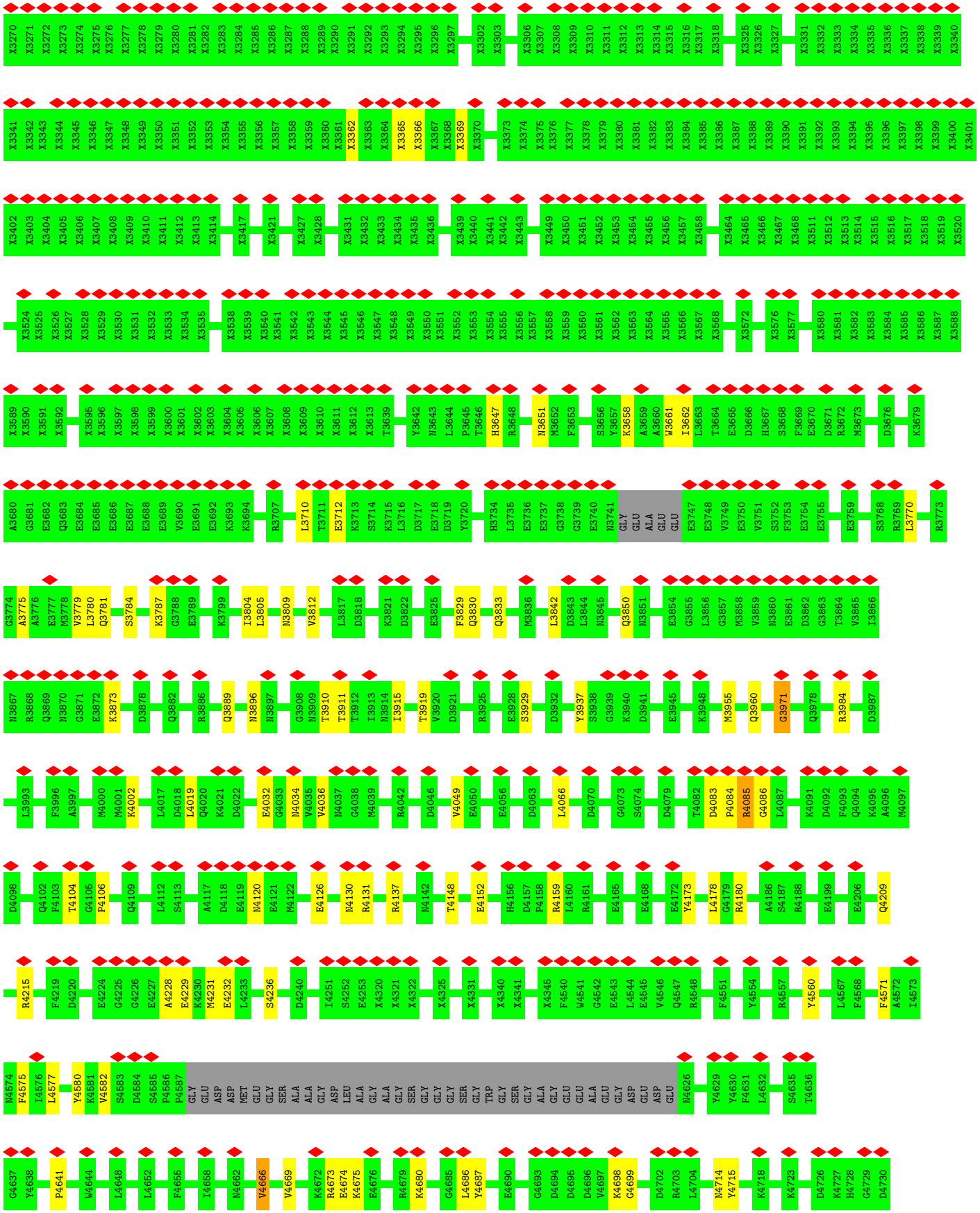
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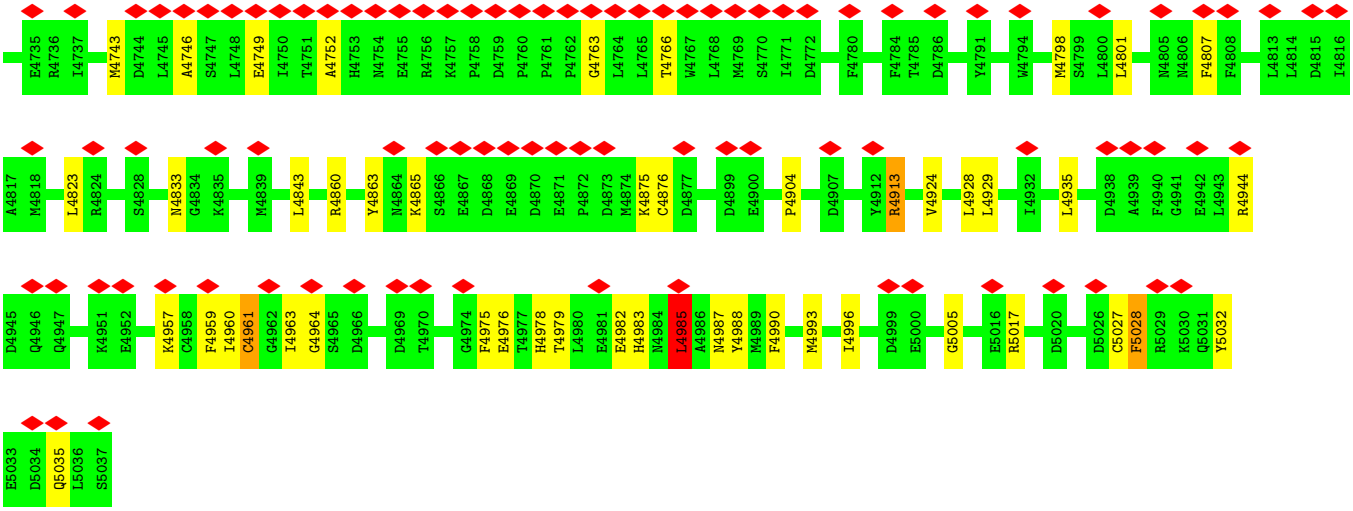
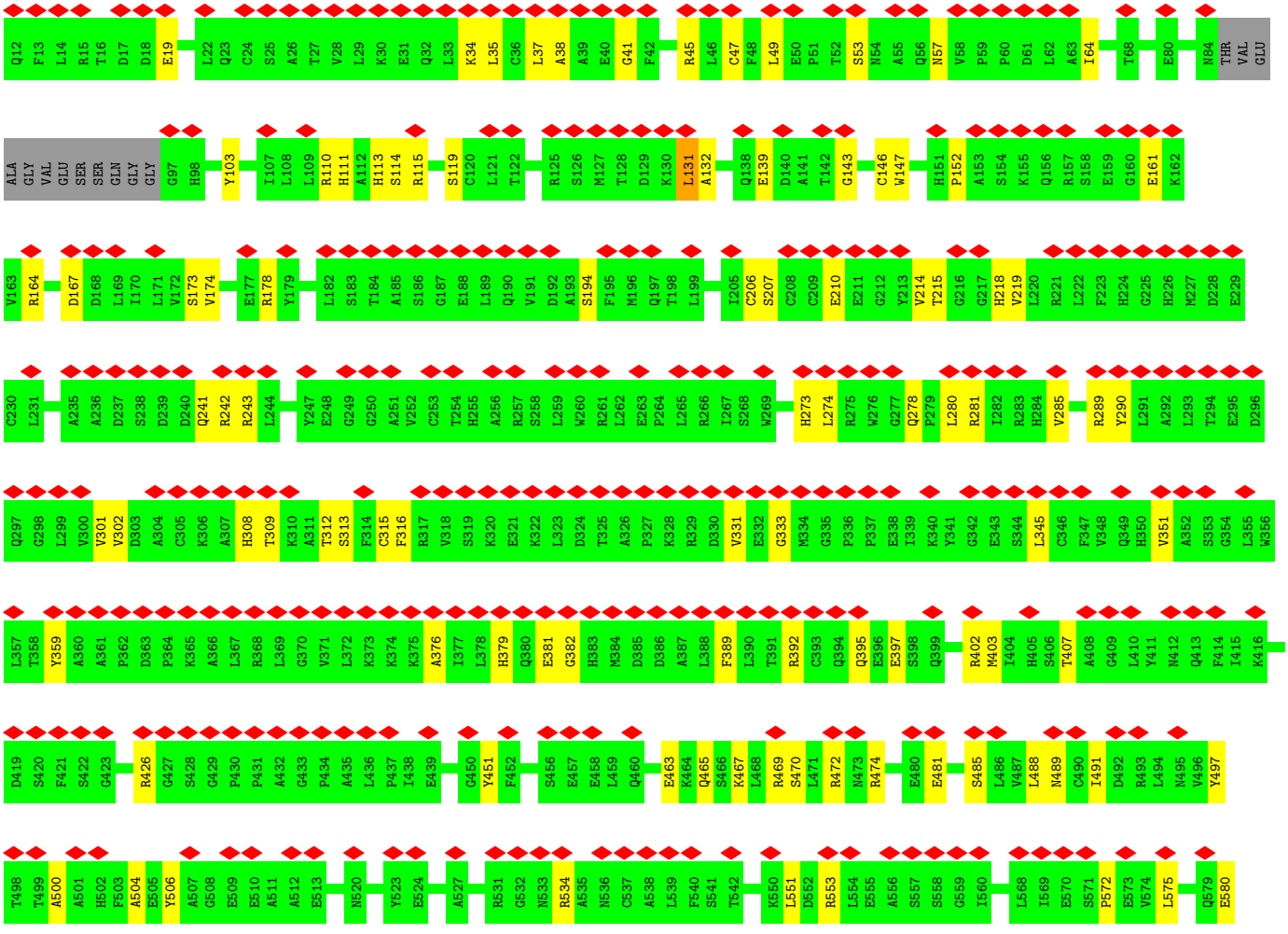
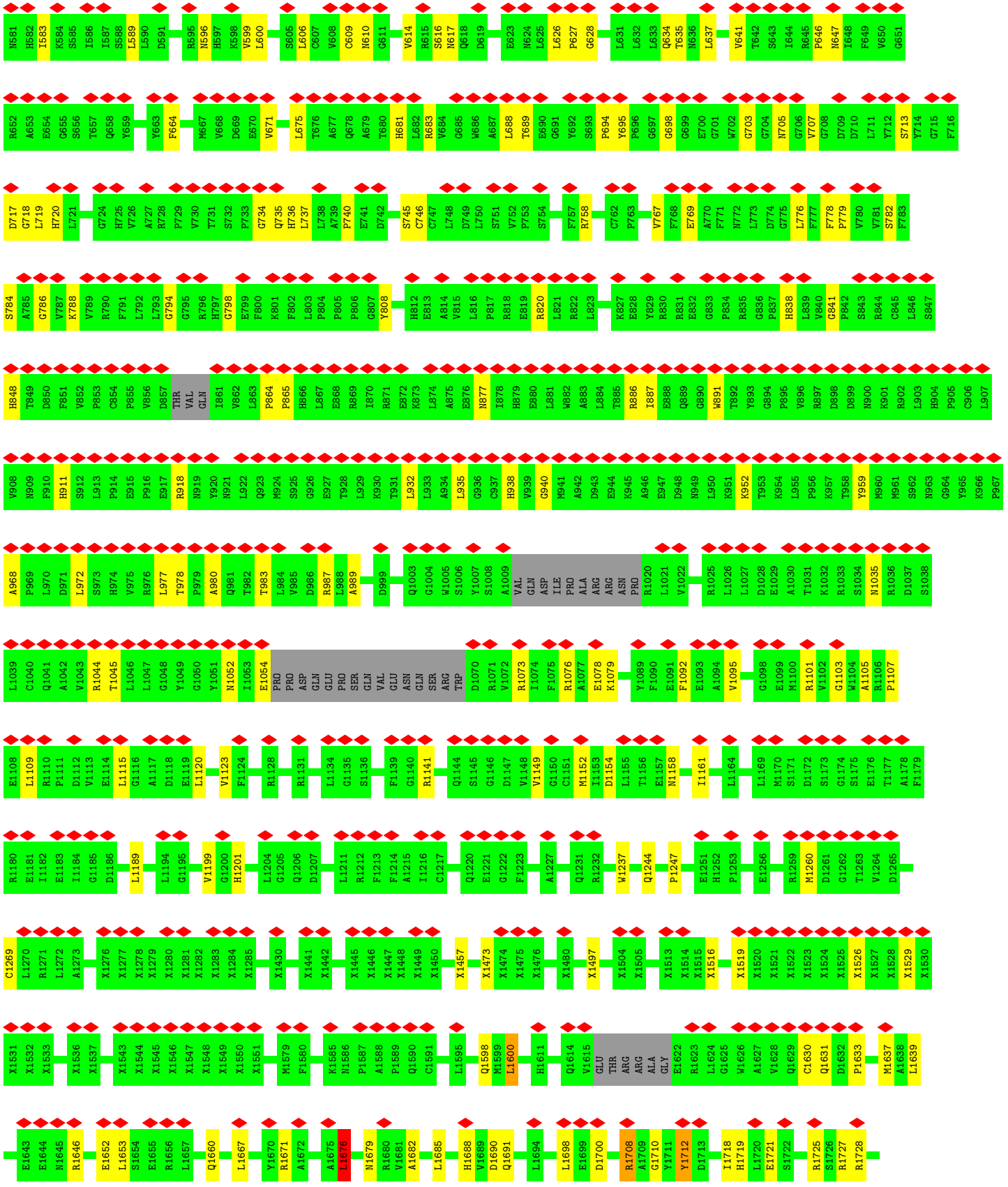


• Molecule 2: Ryanodine receptor 1

Chain G:

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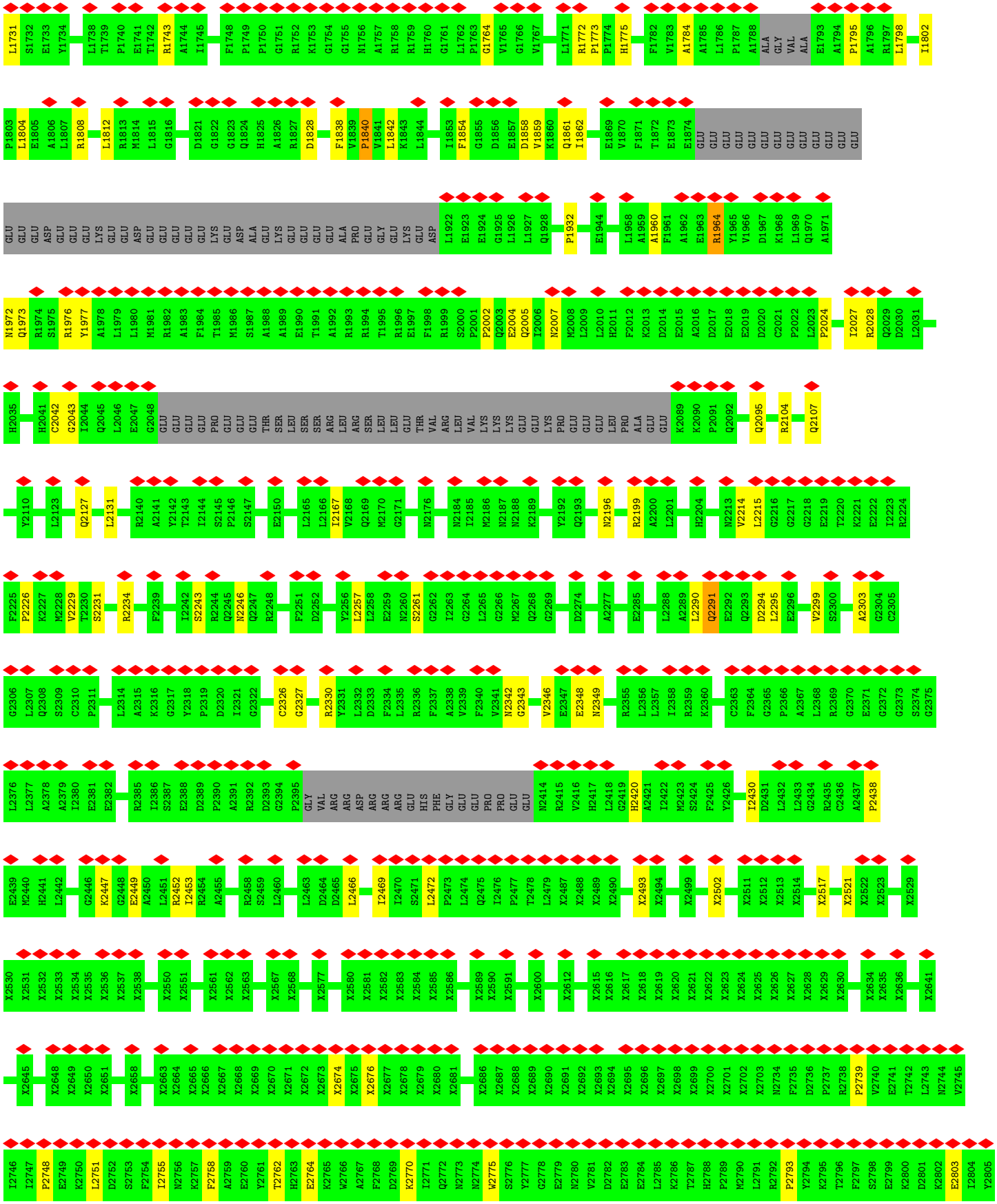
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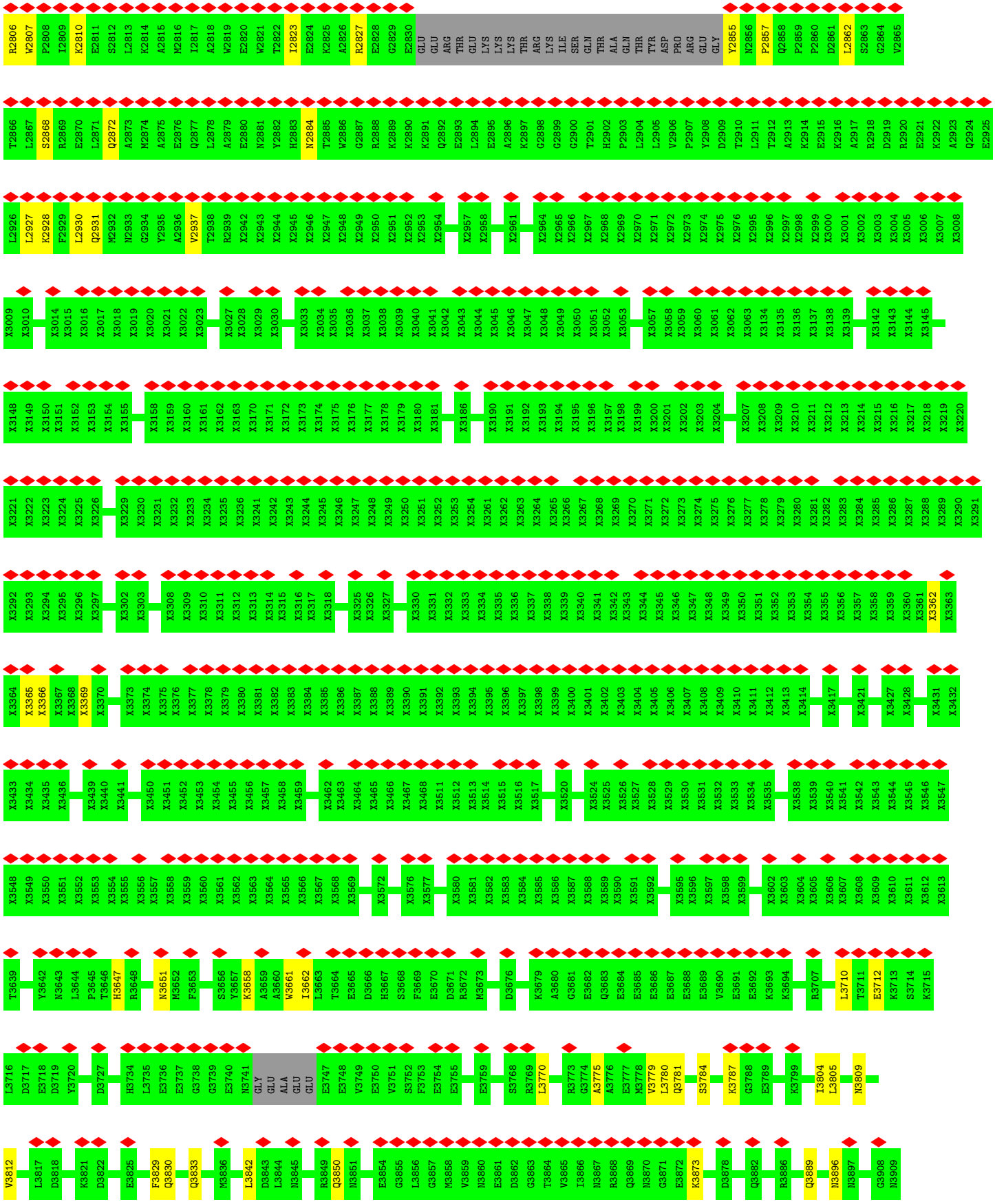
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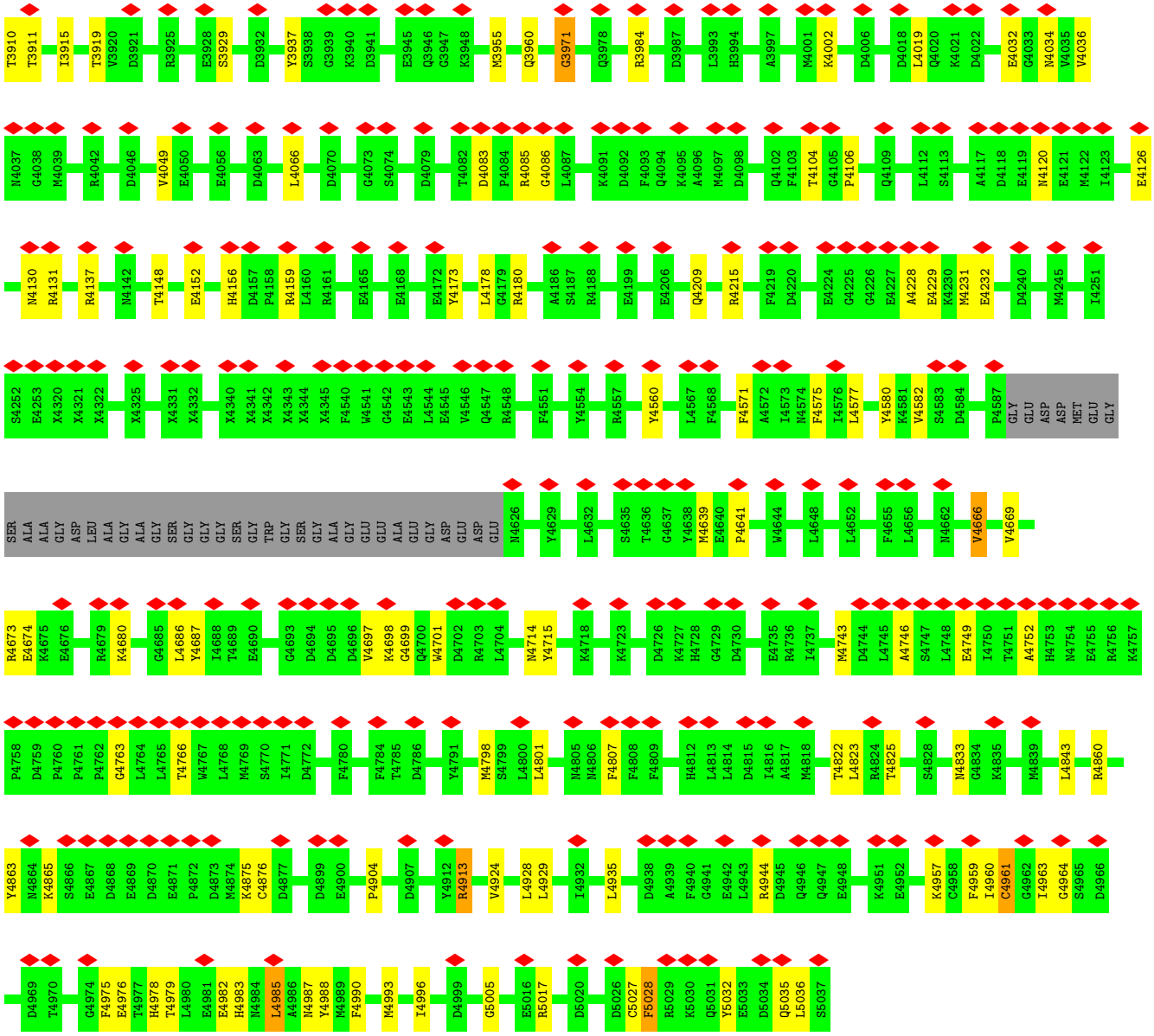
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SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY GLY SER GLY TRP GLY GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 Y4629 L4632 S4635 T4636 G4637 Y4638 M4639 E4640 P4641 W4644 L4648 L4652 F4655 L4656 N4662 V4666 V4669
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	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	0.065	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	9/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	9/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	34/142628 (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	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	8.16	134.07	115.30
2	G	131	LEU	CA-CB-CG	8.16	134.07	115.30
2	B	131	LEU	CA-CB-CG	8.15	134.04	115.30
2	I	131	LEU	CA-CB-CG	8.13	133.99	115.30
2	E	4985	LEU	CA-CB-CG	7.48	132.50	115.30

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
1	F	8	SER	Peptide
1	H	8	SER	Peptide
1	J	8	SER	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	818	0	824	15	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	14	0
2	B	29499	0	24747	289	0
2	E	29499	0	24747	286	0
2	G	29499	0	24747	288	0
2	I	29499	0	24748	285	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102373	1167	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 5.

The worst 5 of 1167 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.85	0.77
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.85	0.76
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.86	0.76
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.86	0.76
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.78	0.71

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	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	F	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	H	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
1	J	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
2	B	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	3235/4416 (73%)	2892 (89%)	338 (10%)	5 (0%)	47	81
2	G	3235/4416 (73%)	2890 (89%)	340 (10%)	5 (0%)	47	81
2	I	3235/4416 (73%)	2889 (89%)	340 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	11954 (90%)	1384 (10%)	22 (0%)	50	81

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1932	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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2475 (99%)	18 (1%)	84	90
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	81	89
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	84	90
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	84	90
All	All	10324/12444 (83%)	10251 (99%)	73 (1%)	84	90

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	553	ARG

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Mol	Chain	Res	Type
2	G	4944	ARG
2	G	1141	ARG
2	G	4034	ASN
2	E	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	4209	GLN
2	G	3889	GLN
2	G	57	ASN
2	G	725	HIS
2	G	4054	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CFF	I	5102	-	8,15,15	2.51	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	G	5102	-	8,15,15	2.51	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	E	5102	-	8,15,15	2.51	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	I	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.51	5 (16%)
3	ATP	G	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.51	5 (16%)
4	CFF	B	5102	-	8,15,15	2.51	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	B	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.52	5 (16%)
3	ATP	E	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.51	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
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	E	5101	-	-	6/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	CFF	C5-C4	-4.59	1.33	1.39
4	E	5102	CFF	C5-C4	-4.59	1.33	1.39
4	I	5102	CFF	C5-C4	-4.59	1.33	1.39
4	G	5102	CFF	C5-C4	-4.59	1.33	1.39
4	G	5102	CFF	C6-N1	-4.05	1.32	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	5101	ATP	PB-O3B-PG	-3.40	121.16	132.83
3	I	5101	ATP	PB-O3B-PG	-3.40	121.16	132.83
3	E	5101	ATP	PB-O3B-PG	-3.40	121.17	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5101	ATP	PB-O3B-PG	-3.39	121.18	132.83
3	G	5101	ATP	PA-O3A-PB	-3.28	121.58	132.83

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O2A
3	I	5101	ATP	C5'-O5'-PA-O1A

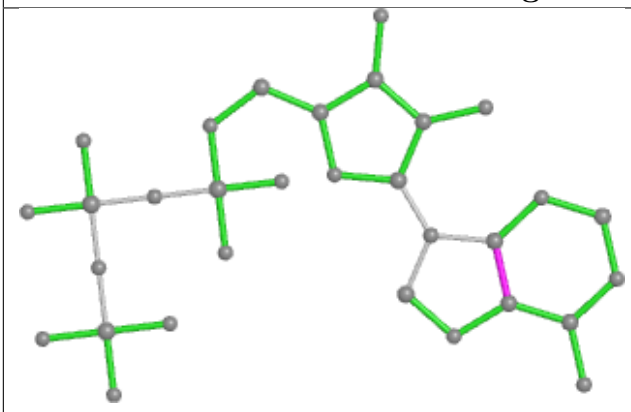
There are no ring outliers.

8 monomers are involved in 12 short contacts:

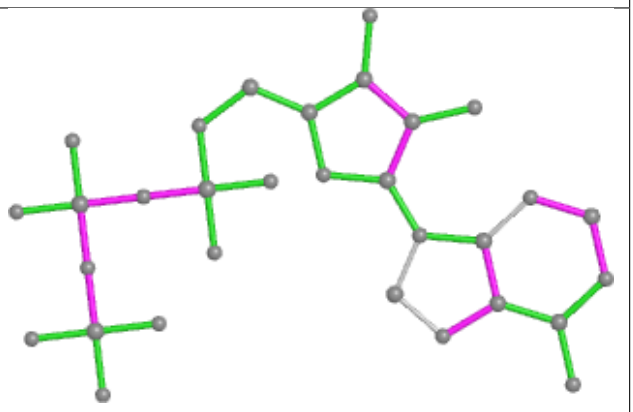
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	5102	CFF	1	0
4	G	5102	CFF	1	0
4	E	5102	CFF	1	0
3	I	5101	ATP	2	0
3	G	5101	ATP	2	0
4	B	5102	CFF	1	0
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0

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

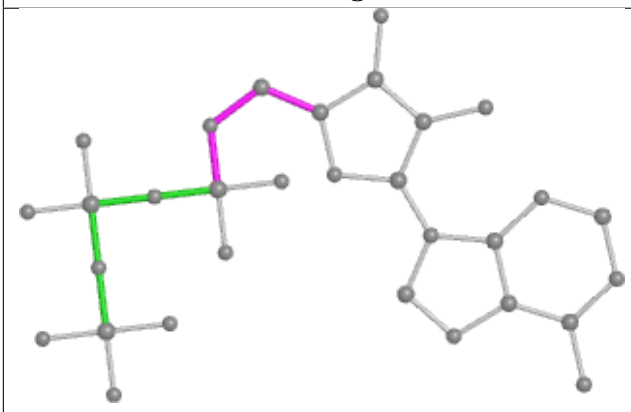
Ligand ATP I 5101



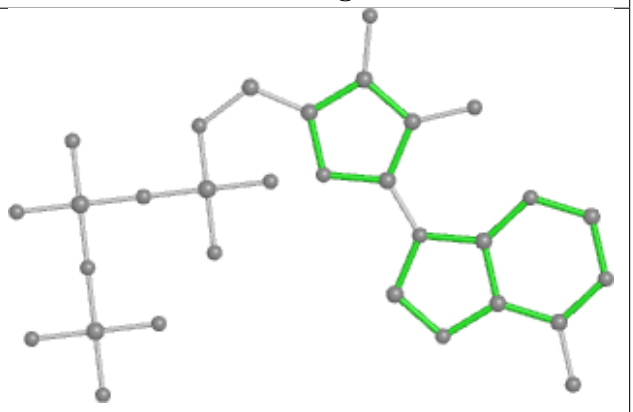
Bond lengths



Bond angles

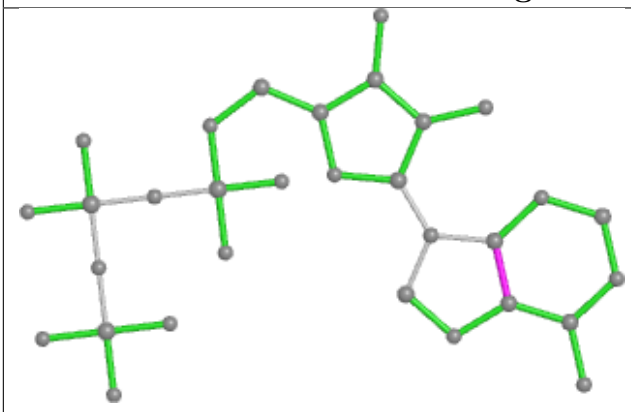


Torsions

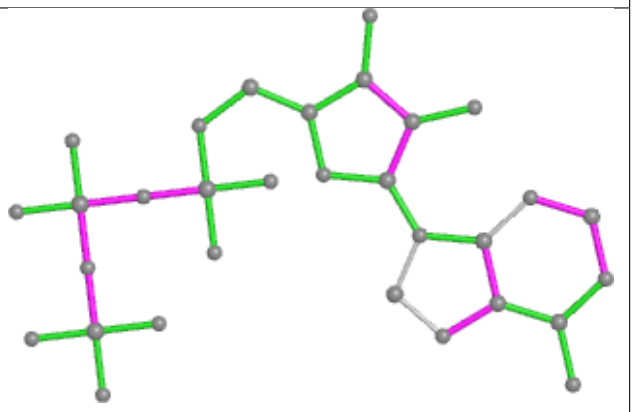


Rings

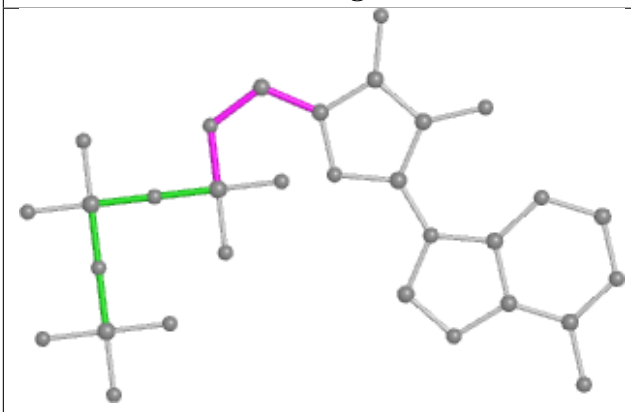
Ligand ATP G 5101



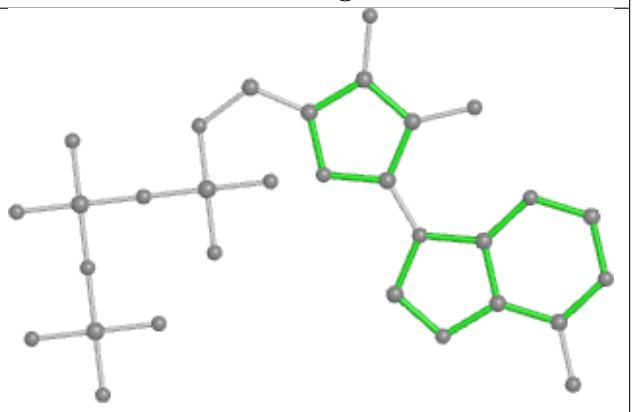
Bond lengths



Bond angles

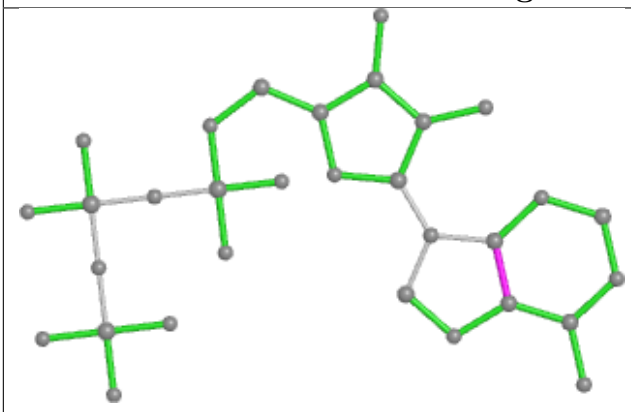


Torsions

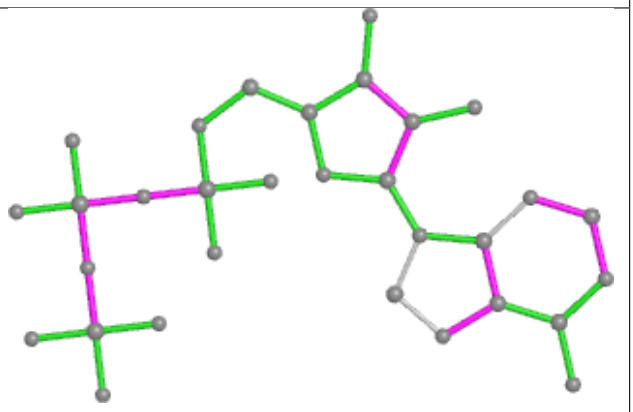


Rings

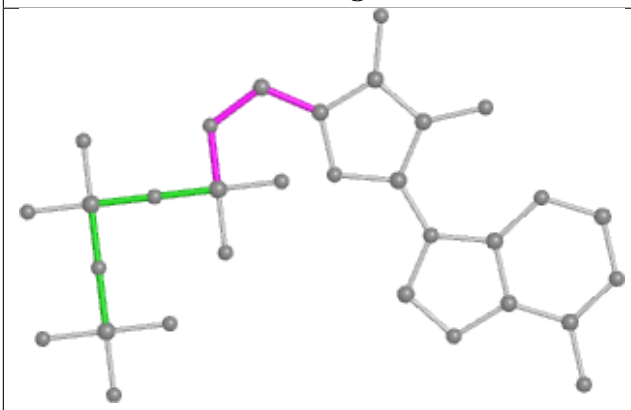
Ligand ATP B 5101



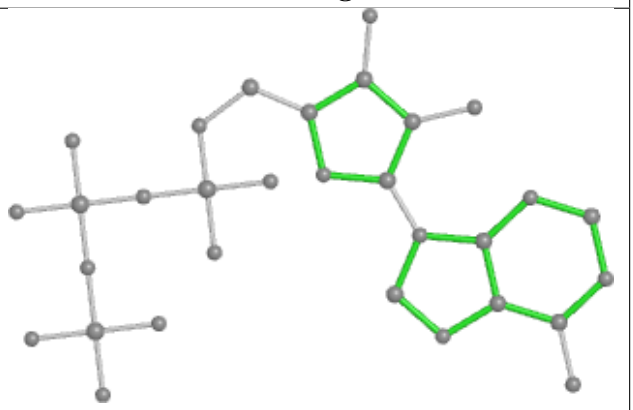
Bond lengths



Bond angles

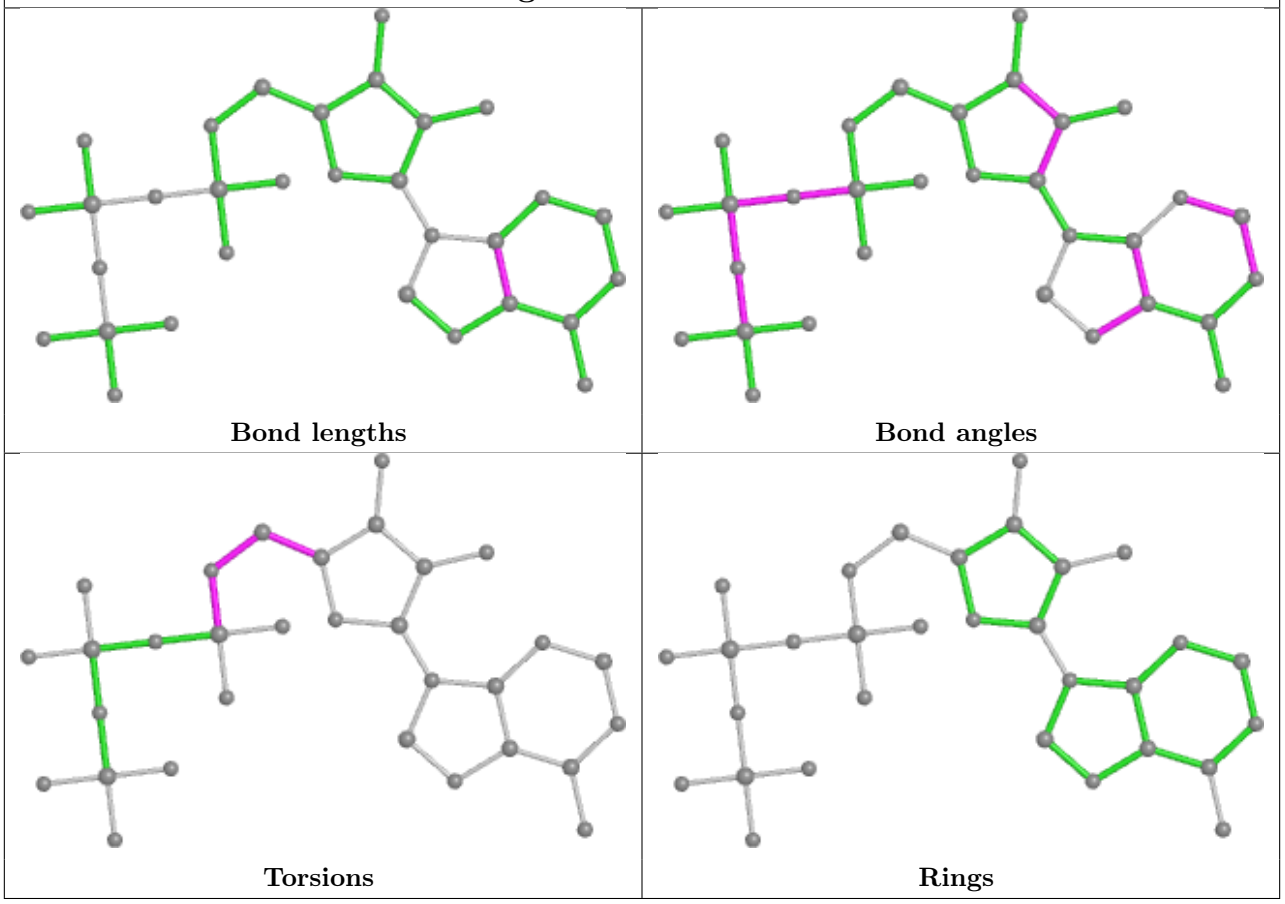


Torsions



Rings

Ligand ATP E 5101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	72.88
1	E	4345:UNK	C	4540:PHE	N	72.88

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.88
1	G	4345:UNK	C	4540:PHE	N	72.88
1	B	3613:UNK	C	3639:THR	N	43.44

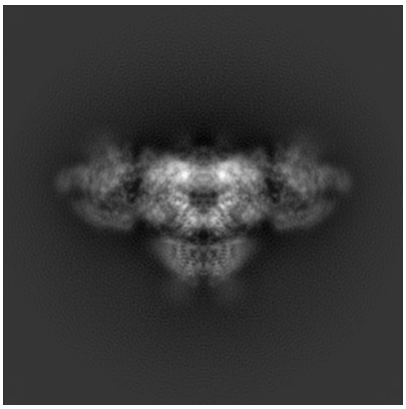
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8379. These allow visual inspection of the internal detail of the map and identification of artifacts.

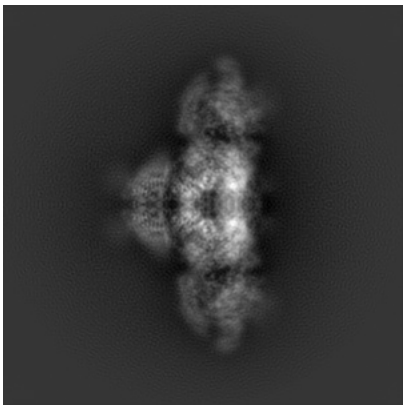
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

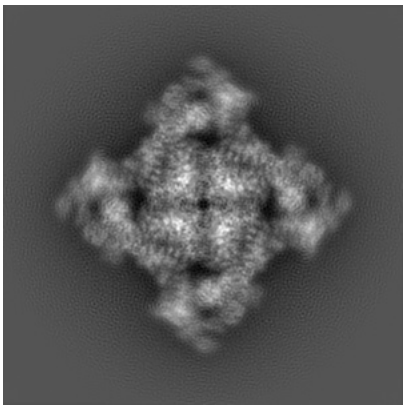
6.1.1 Primary map



X

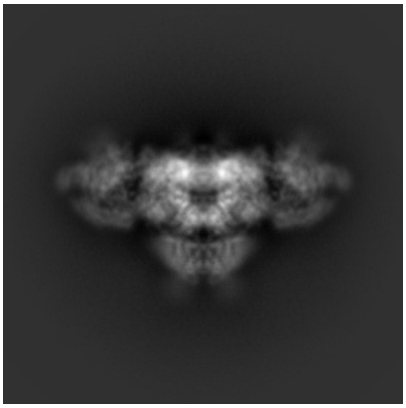


Y

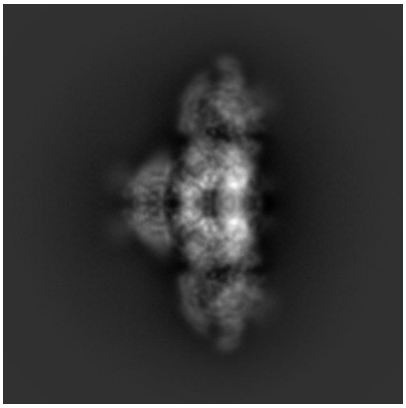


Z

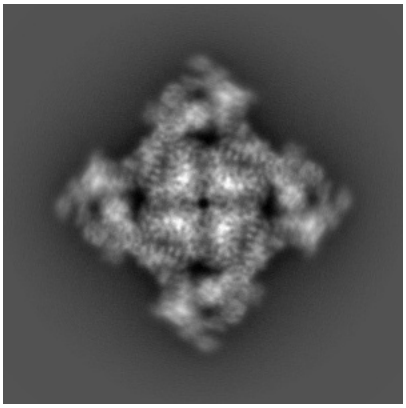
6.1.2 Raw map



X



Y

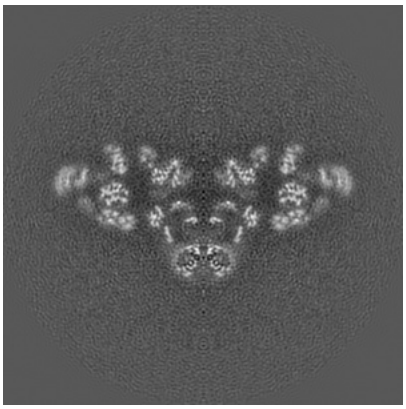


Z

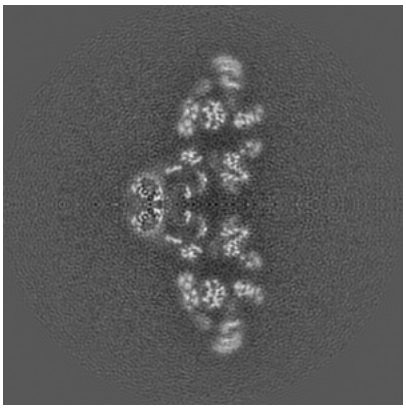
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

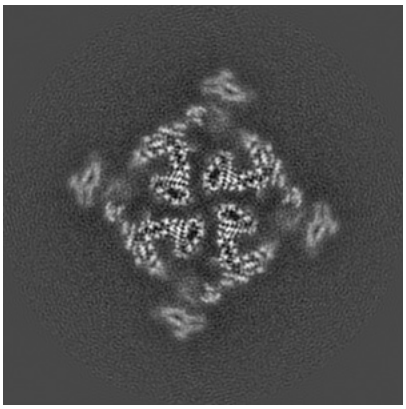
6.2.1 Primary map



X Index: 200

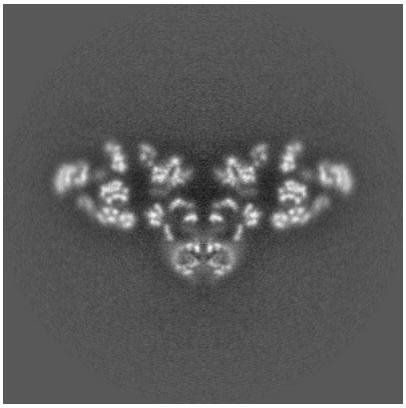


Y Index: 200

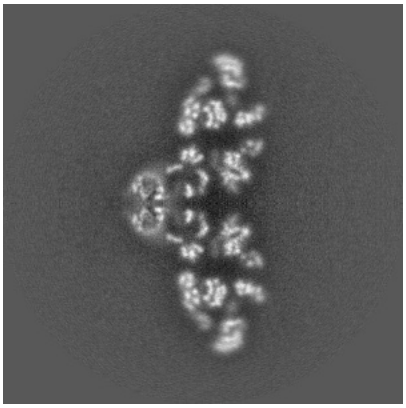


Z Index: 200

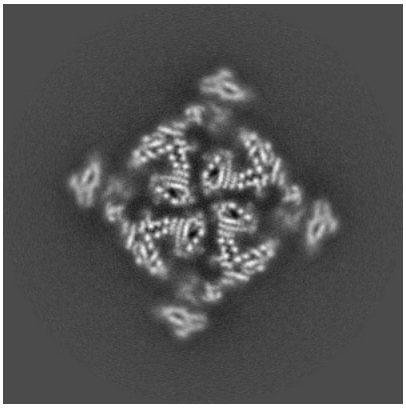
6.2.2 Raw map



X Index: 200



Y Index: 200

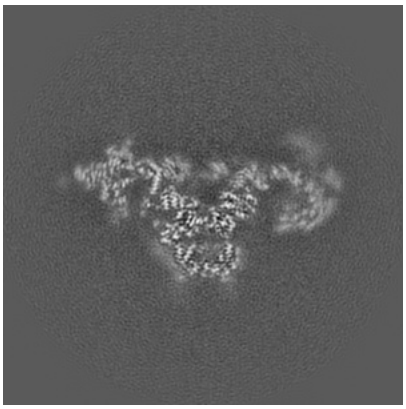


Z Index: 200

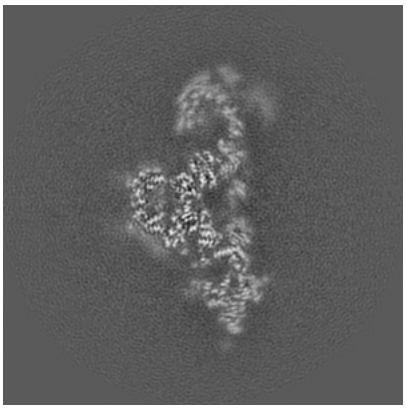
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

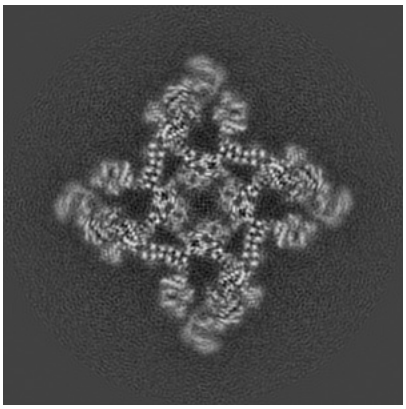
6.3.1 Primary map



X Index: 217

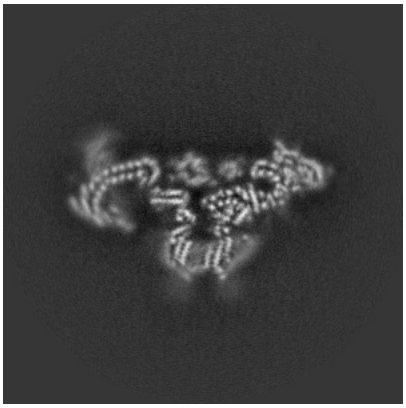


Y Index: 183

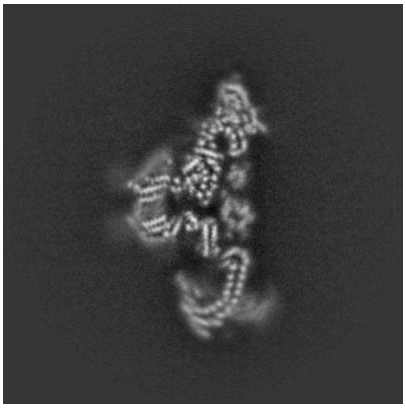


Z Index: 226

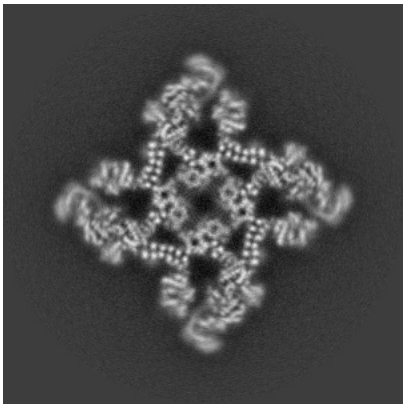
6.3.2 Raw map



X Index: 176



Y Index: 224



Z Index: 227

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

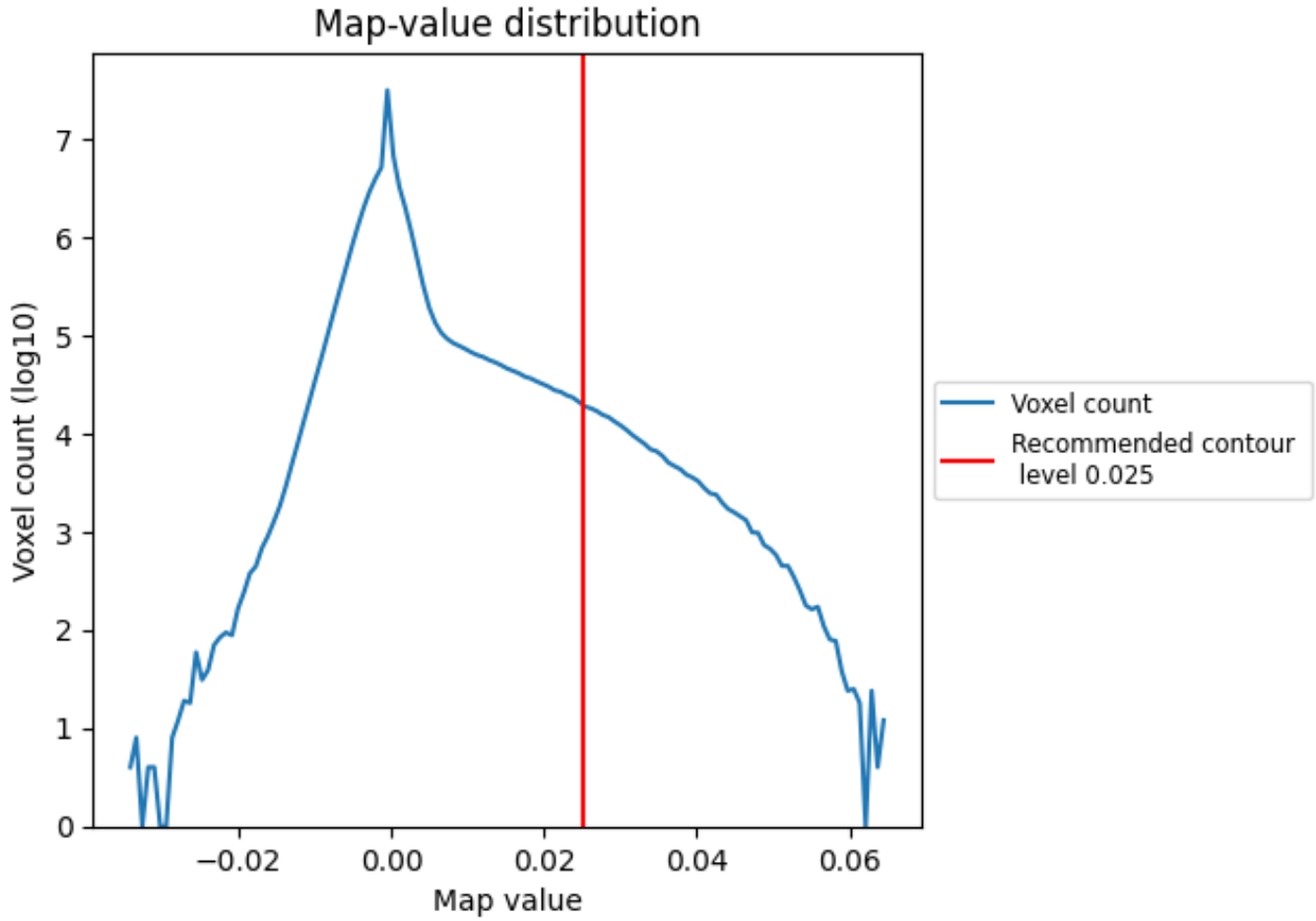
6.5 Mask visualisation (i)

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

7 Map analysis

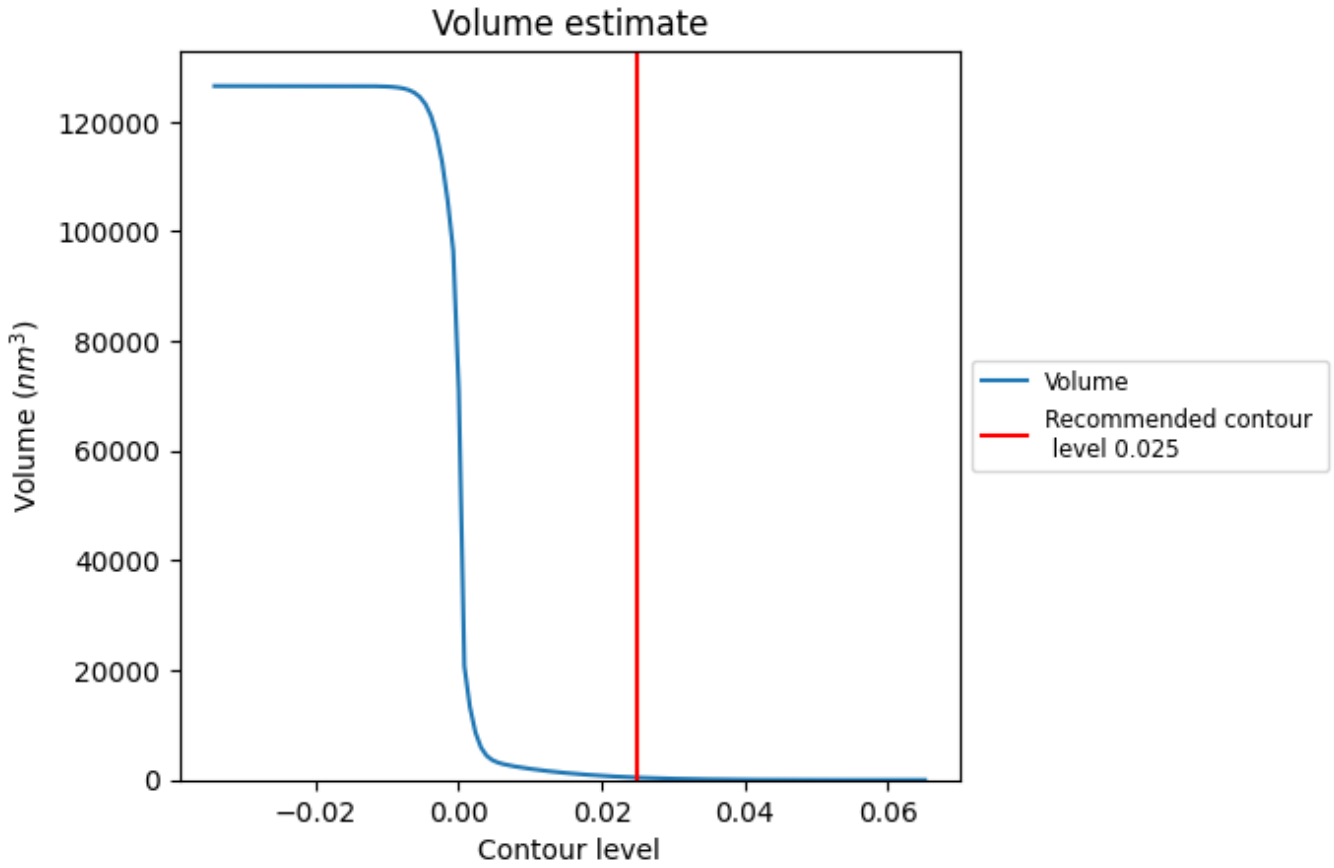
This section contains the results of statistical analysis of the map.

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.

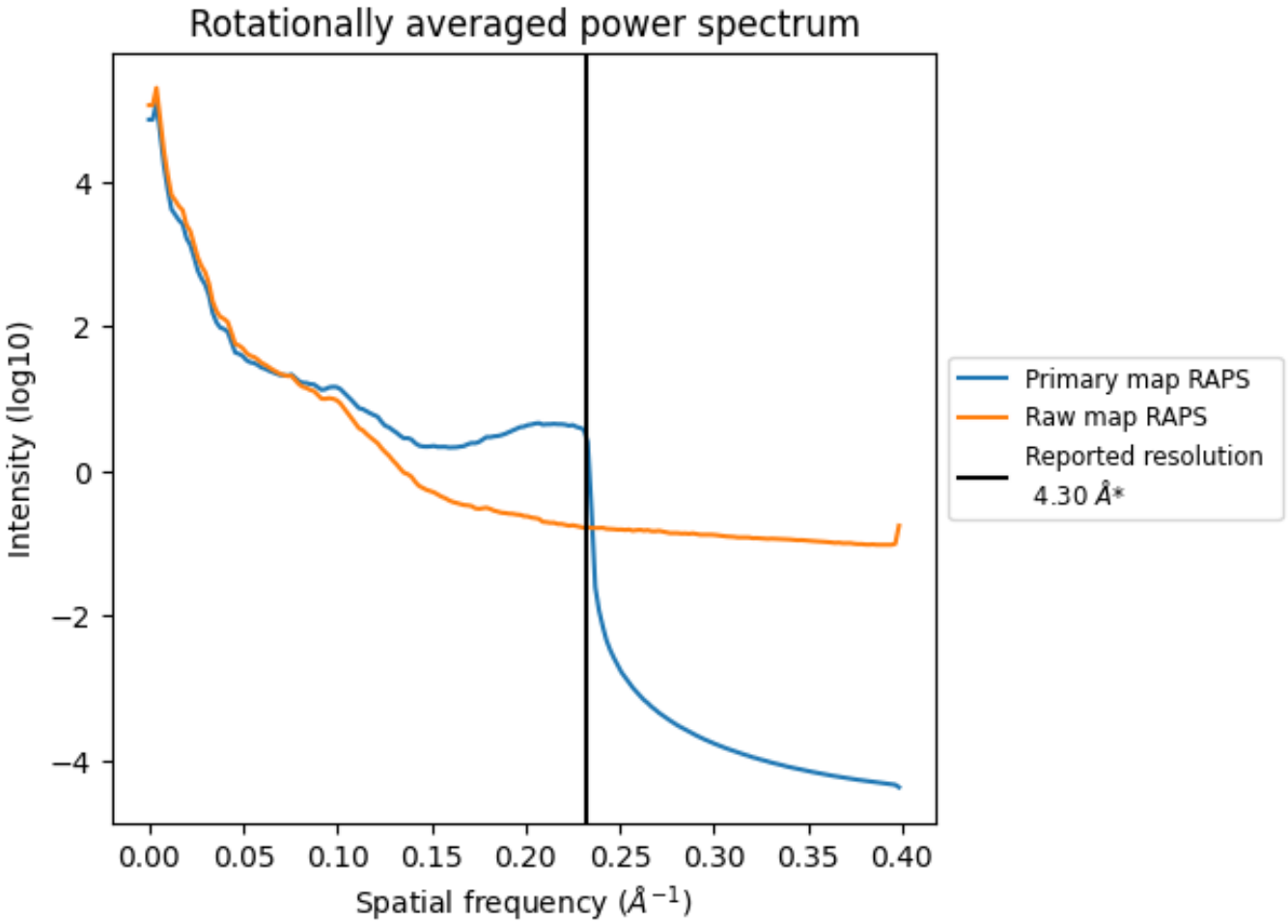
7.2 Volume estimate (i)



The volume at the recommended contour level is 437 nm^3; this corresponds to an approximate mass of 395 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)

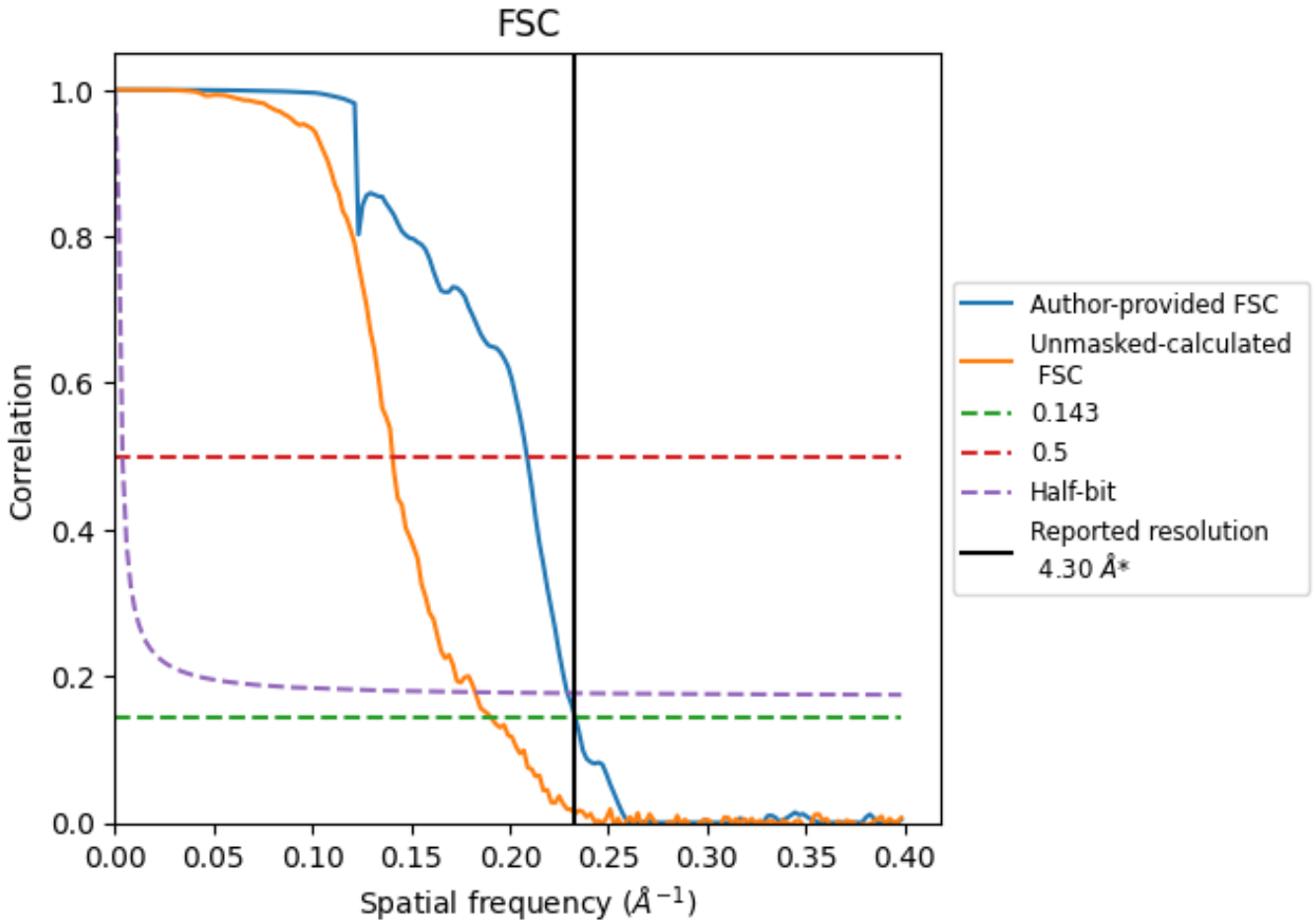


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

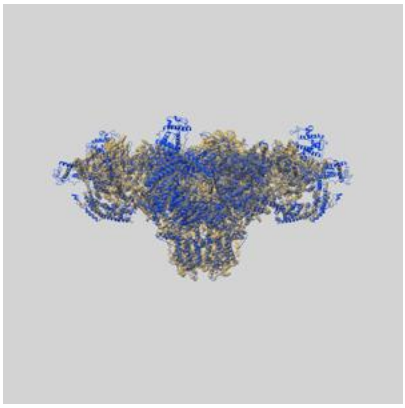
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.29	4.79	4.36
Unmasked-calculated*	5.25	7.11	5.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.25 differs from the reported value 4.3 by more than 10 %

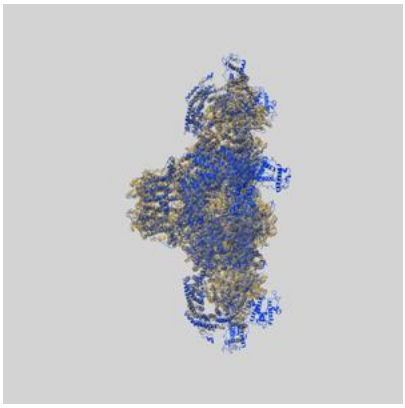
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8379 and PDB model 5TAM. Per-residue inclusion information can be found in section 3 on page 6.

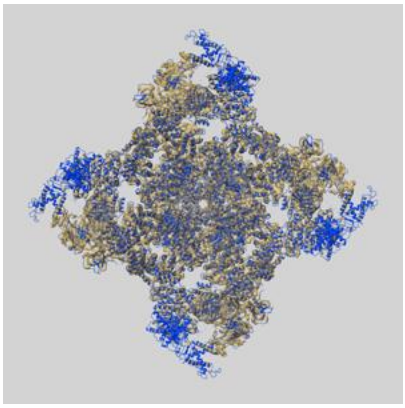
9.1 Map-model overlay



X



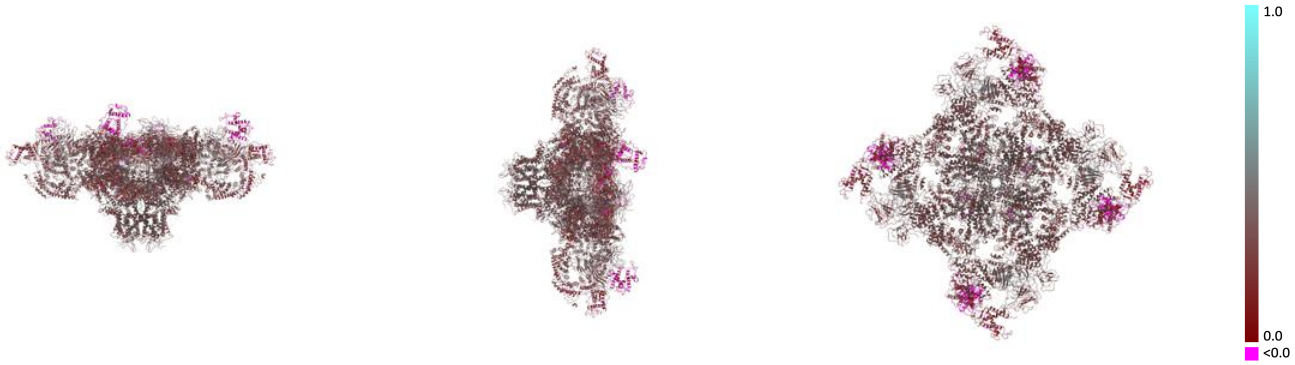
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

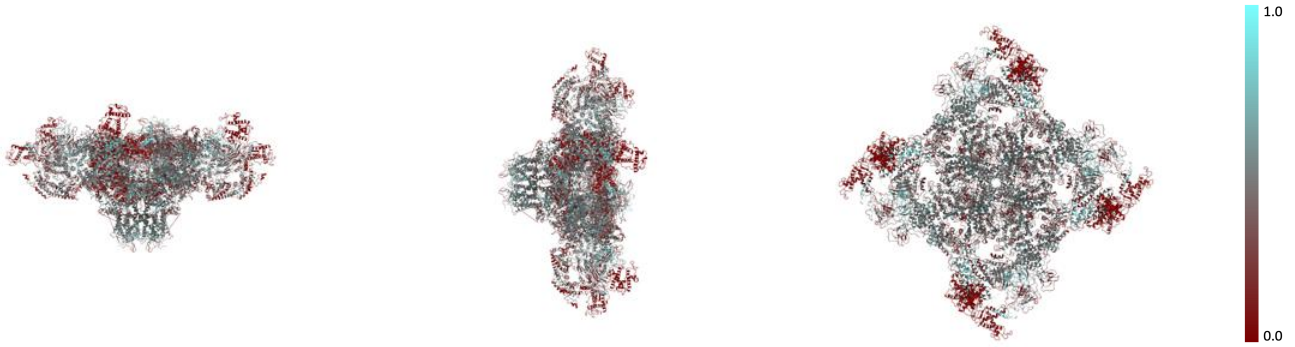
9.2 Q-score mapped to coordinate model



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.

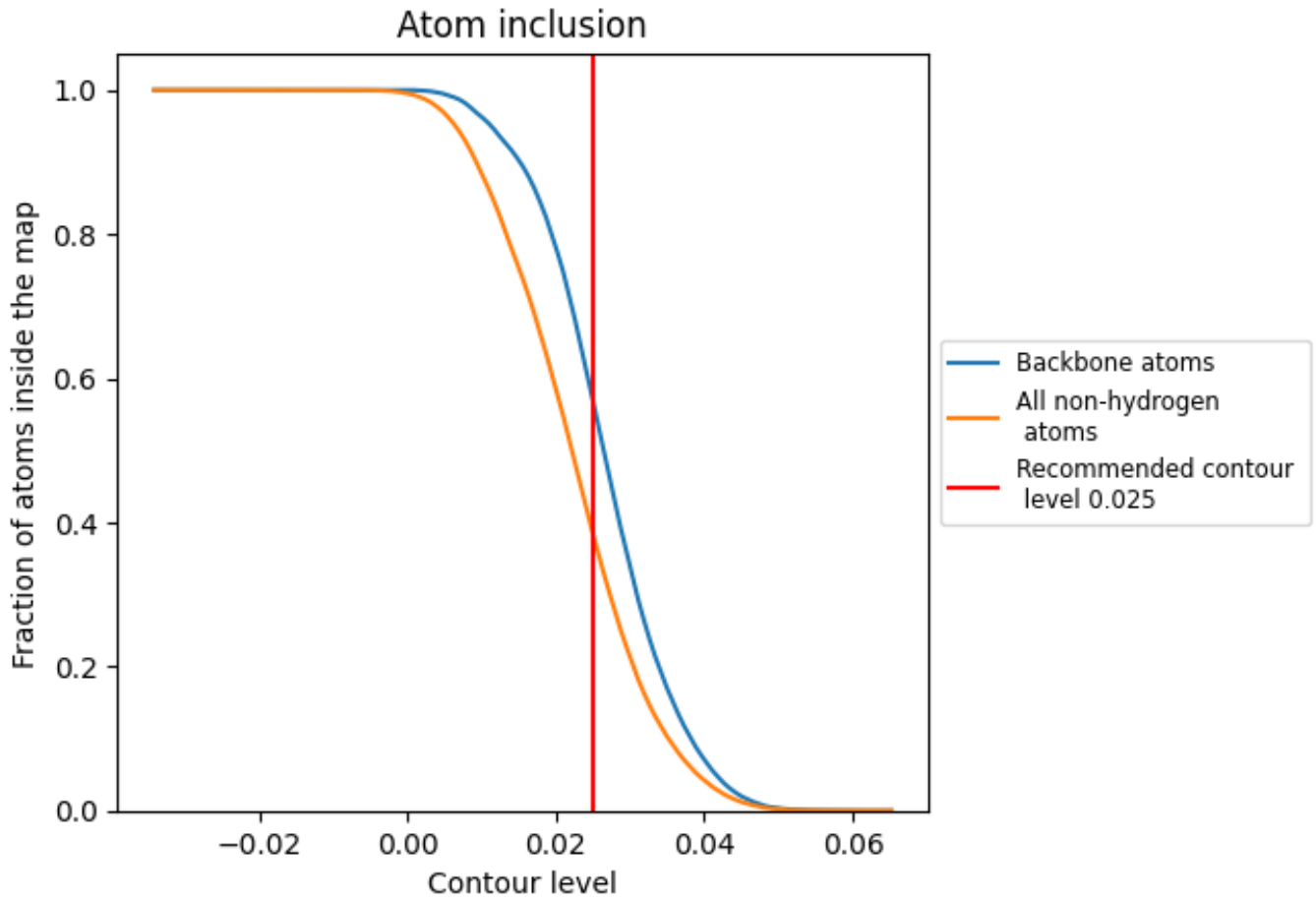
9.3 Atom inclusion mapped to coordinate model



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 57% of all backbone atoms, 38% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3837	0.3030
A	0.3524	0.3310
B	0.3847	0.3020
E	0.3846	0.3020
F	0.3573	0.3360
G	0.3845	0.3020
H	0.3536	0.3360
I	0.3842	0.3020
J	0.3561	0.3340