wwPDB EM Validation Summary Report (i)

Nov 11, 2026 – 03:05 PM EST

PDB ID	:	9Z9P / pdb_00009z9p
EMDB ID	:	EMD-73954
Title	:	Skewed-state T4825I rabbit RyR1 with activating ligands (Ca2+/ATP) and S107
Authors	:	Chen, Y.S.; Van Petegem, F.
Deposited on	:	2025-11-18
Resolution	:	3.02 Å(reported)
Based on initial model	:	7TZC

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:

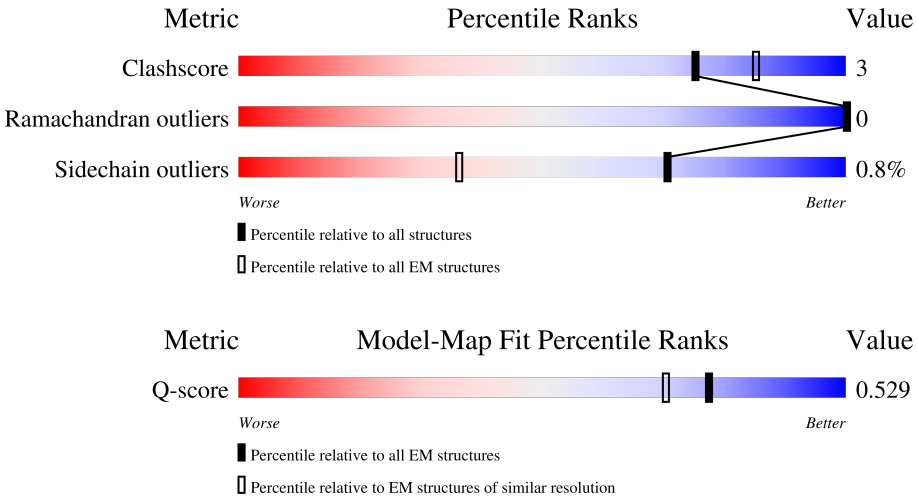
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.02 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.



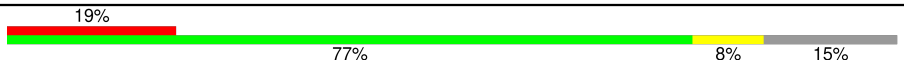
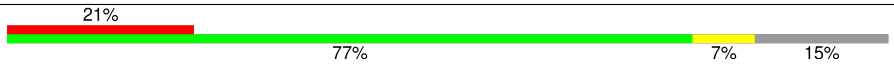
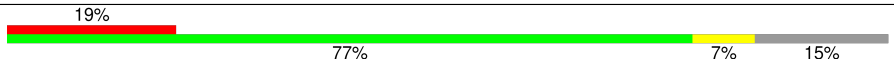
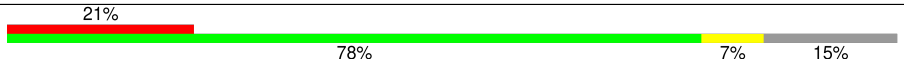
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	110	5% 85% 14%
1	C	110	88% 9%
1	E	110	5% 85% 14%
1	G	110	89% 8%

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Mol	Chain	Length	Quality of chain
2	B	5037	
2	D	5037	
2	F	5037	
2	H	5037	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 135868 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	A	108	Total	C	N	O	S	0	0
			819	517	145	153	4		
1	C	107	Total	C	N	O	S	0	0
			814	513	143	154	4		
1	E	108	Total	C	N	O	S	0	0
			819	517	145	153	4		
1	G	107	Total	C	N	O	S	0	0
			814	513	143	154	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P68106
A	0	ASN	-	expression tag	UNP P68106
A	1	ALA	-	expression tag	UNP P68106
C	-1	SER	-	expression tag	UNP P68106
C	0	ASN	-	expression tag	UNP P68106
C	1	ALA	-	expression tag	UNP P68106
E	-1	SER	-	expression tag	UNP P68106
E	0	ASN	-	expression tag	UNP P68106
E	1	ALA	-	expression tag	UNP P68106
G	-1	SER	-	expression tag	UNP P68106
G	0	ASN	-	expression tag	UNP P68106
G	1	ALA	-	expression tag	UNP P68106

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4274	Total	C	N	O	S	1	0
			33249	21239	5746	6039	225		
2	D	4271	Total	C	N	O	S	0	0
			32972	21075	5702	5975	220		
2	F	4274	Total	C	N	O	S	1	0
			33249	21239	5746	6039	225		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	4271	Total	C	N	O	S	0	0
			32972	21075	5702	5975	220		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	GLY	-	insertion	UNP P11716
B	68	ILE	THR	conflict	UNP P11716
B	208	GLY	CYS	conflict	UNP P11716
B	213	PHE	TYR	conflict	UNP P11716
B	235	PRO	ALA	conflict	UNP P11716
B	236	SER	ALA	conflict	UNP P11716
B	251	PRO	ALA	conflict	UNP P11716
B	4825	ILE	THR	engineered mutation	UNP P11716
D	5	GLY	-	insertion	UNP P11716
D	68	ILE	THR	conflict	UNP P11716
D	208	GLY	CYS	conflict	UNP P11716
D	213	PHE	TYR	conflict	UNP P11716
D	235	PRO	ALA	conflict	UNP P11716
D	236	SER	ALA	conflict	UNP P11716
D	251	PRO	ALA	conflict	UNP P11716
D	4825	ILE	THR	engineered mutation	UNP P11716
F	5	GLY	-	insertion	UNP P11716
F	68	ILE	THR	conflict	UNP P11716
F	208	GLY	CYS	conflict	UNP P11716
F	213	PHE	TYR	conflict	UNP P11716
F	235	PRO	ALA	conflict	UNP P11716
F	236	SER	ALA	conflict	UNP P11716
F	251	PRO	ALA	conflict	UNP P11716
F	4825	ILE	THR	engineered mutation	UNP P11716
H	5	GLY	-	insertion	UNP P11716
H	68	ILE	THR	conflict	UNP P11716
H	208	GLY	CYS	conflict	UNP P11716
H	213	PHE	TYR	conflict	UNP P11716
H	235	PRO	ALA	conflict	UNP P11716
H	236	SER	ALA	conflict	UNP P11716
H	251	PRO	ALA	conflict	UNP P11716
H	4825	ILE	THR	engineered mutation	UNP P11716

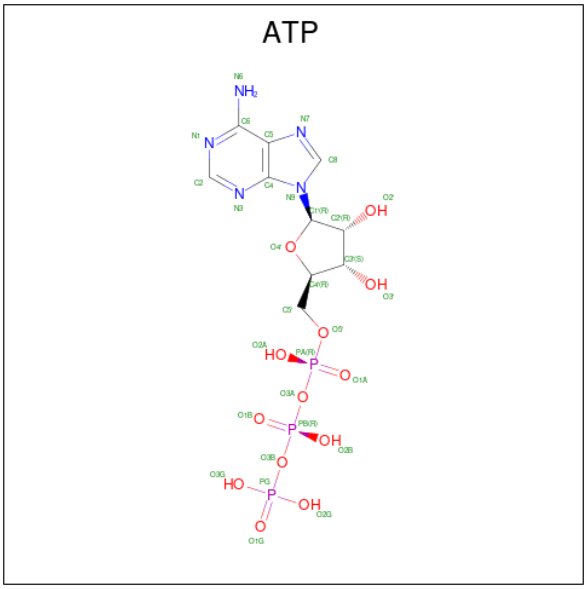
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total Zn 1 1	0
3	D	1	Total Zn 1 1	0
3	F	1	Total Zn 1 1	0
3	H	1	Total Zn 1 1	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	D	1	Total Ca 1 1	0
4	F	1	Total Ca 1 1	0
4	H	1	Total Ca 1 1	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



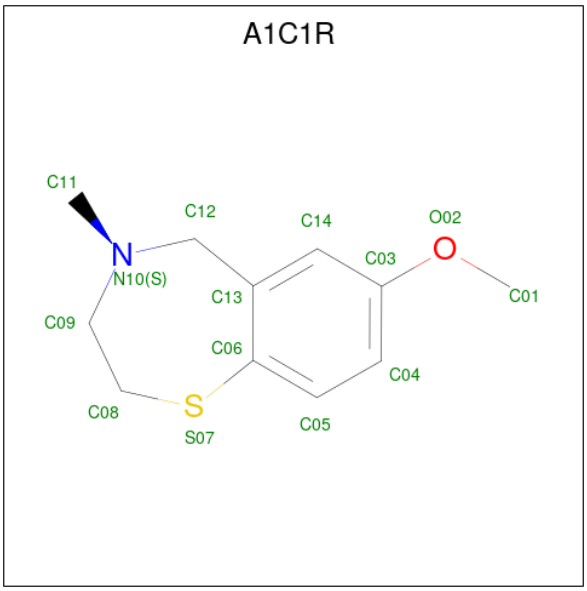
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C N O P 31 10 5 13 3	0
5	D	1	Total C N O P 31 10 5 13 3	0

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Mol	Chain	Residues	Atoms					AltConf
5	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is 7-methoxy-4-methyl-2,3,4,5-tetrahydro-1,4-benzothiazepine (CCD ID: A1C1R) (formula: $C_{11}H_{15}NOS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	S	0
			14	11	1	1	1	
6	D	1	Total	C	N	O	S	0
			14	11	1	1	1	

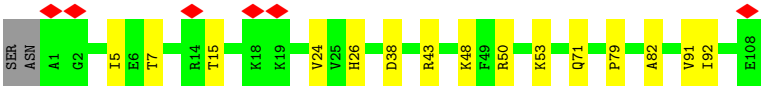
3 Residue-property plots (i)

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 A:

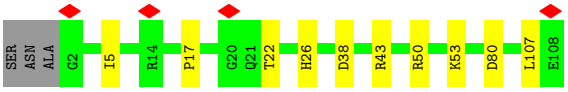




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C:

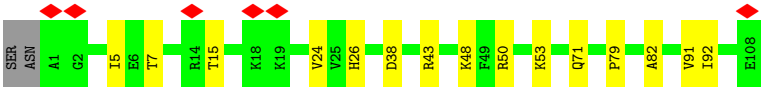




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

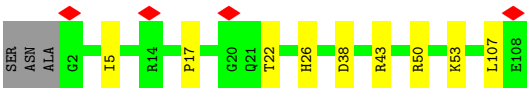




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

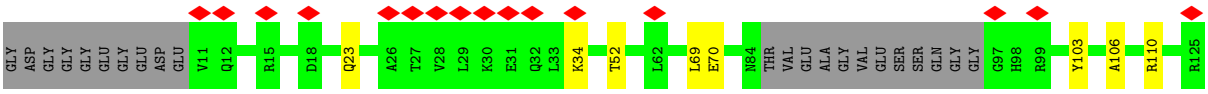


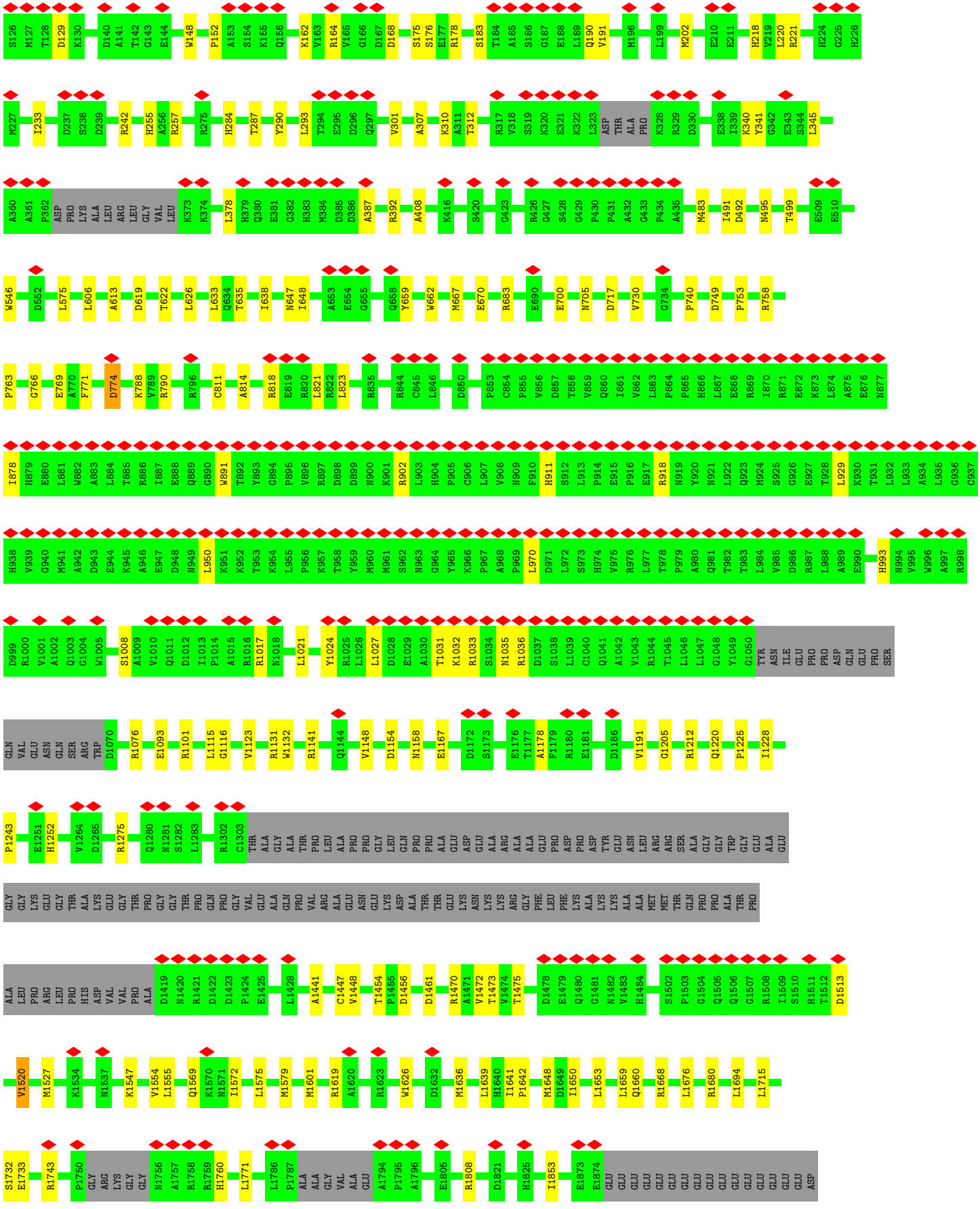


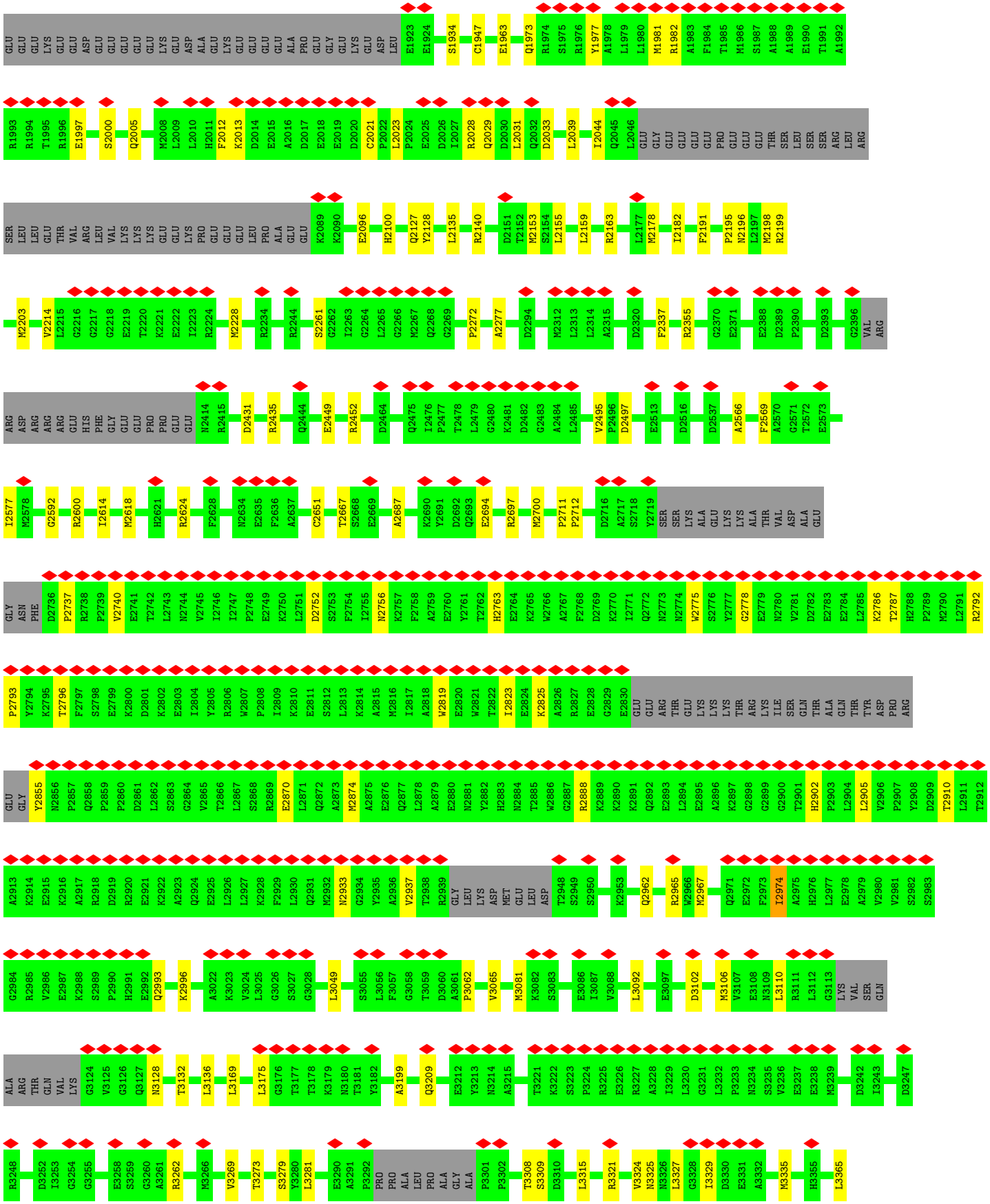
• Molecule 2: Ryanodine receptor 1

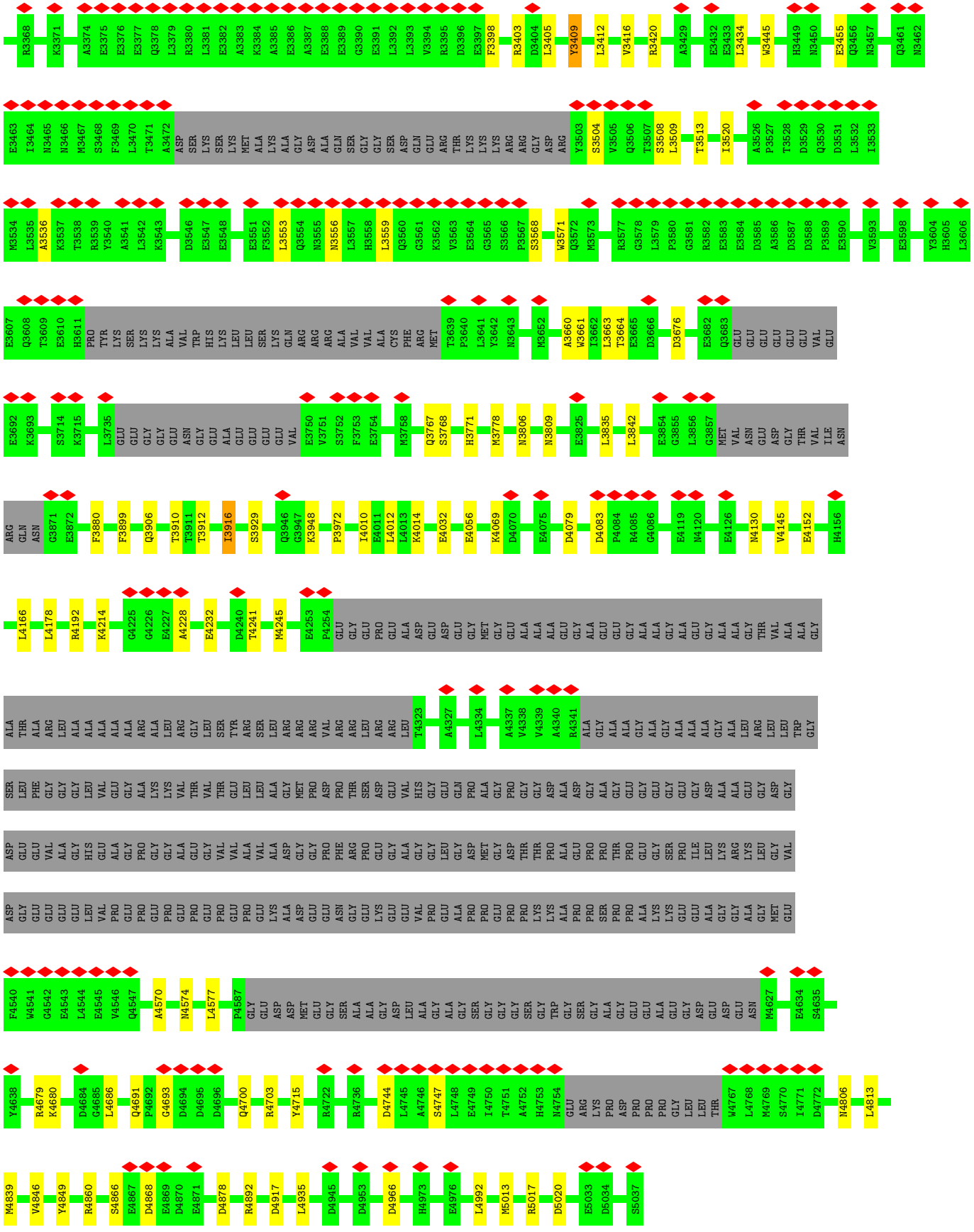
Chain B:





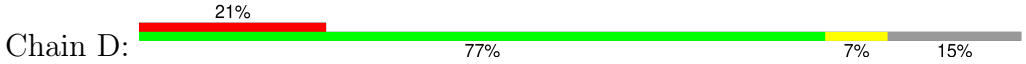

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M227 I233 D237 S238 D239 R242 H255 A256 R257 R275 H284 T287 Y290 L293 T294 E295 D296 Q297 V301 A307 K310 A311 T312 R317 V318 S319 K320 E321 K322 L323 ASP THR ALA PRO K328 R329 D330 E338 I339 K340 Y341 G342 E343 S344 L345
A360 A361 P362 ASP PRO LYS ALA LEU ARG LEU GLY VAL LEU K373 K374 L378 H379 Q380 E381 G382 H383 M384 D385 D386 A387 R392 A408 K416 S420 G423 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 M483 I491 D492 N495 T499 E509 E510
W546 D582 L575 L606 A613 D619 T622 L626 L633 Q634 T635 I638 N647 I648 A653 E654 G655 Q658 Y659 W662 M667 E670 R683 E690 E700 N705 D717 V730 G734 P740 D749 P753 R758
P763 G766 E769 A770 F771 D774 K788 V789 R790 R796 C811 A814 R818 E819 R820 L821 R822 L823 R835 R844 C845 L846 D850 P853 C854 P855 V856 D857 T858 V859 Q860 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 E990 H993 N994 V995 W996 A997 R998
D999 R1000 V1001 A1002 Q1003 G1004 W1005 S1008 A1009 V1010 Q1011 D1012 I1013 P1014 A1015 R1016 R1017 N1018 L1021 Y1024 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 TYR ASN ILE GLU PRO PRO ASP GLN GLU PRO SER
GLN VAL GLU ASN GLN SER ARG TRP D1070 R1076 E1093 R1101 L1115 G1116 V1123 R1131 W1132 R1141 Q1144 V1148 D1154 N1158 E1167 D1172 S1173 E1176 T1177 A1178 F1179 R1180 E1181 D1186 V1191 G1205 R1212 Q1220 P1225 I1228
P1243 E1251 H1252 V1264 D1265 R1275 Q1280 N1281 S1282 L1283 R1302 C1303 THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU
GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO
ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 D1423 P1424 E1425 L1428 A1441 C1447 V1448 T1454 P1455 D1456 D1461 R1470 A1471 V1472 T1473 V1474 T1475 D1478 E1479 Q1480 G1481 N1482 V1483 H1484 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 T1512 D1513
V1520 M1527 K1534 N1537 K1547 V1554 L1555 Q1569 K1570 N1571 I1572 L1575 M1579 M1601 R1619 A1620 R1623 W1626 D1632 M1636 L1639 H1640 I1641 P1642 M1648 D1649 I1650 L1653 L1659 Q1660 R1668 L1676 R1680 L1694 L1715
S1732 E1733 R1743 P1750 GLY ARG LYS GLY GLY N1756 A1757 R1758 R1759 H1760 L1771 L1786 P1787 ALA ALA GLY VAL ALA GLU A1794 P1795 A1796 E1805 R1808 D1821 H1825 I1853 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP

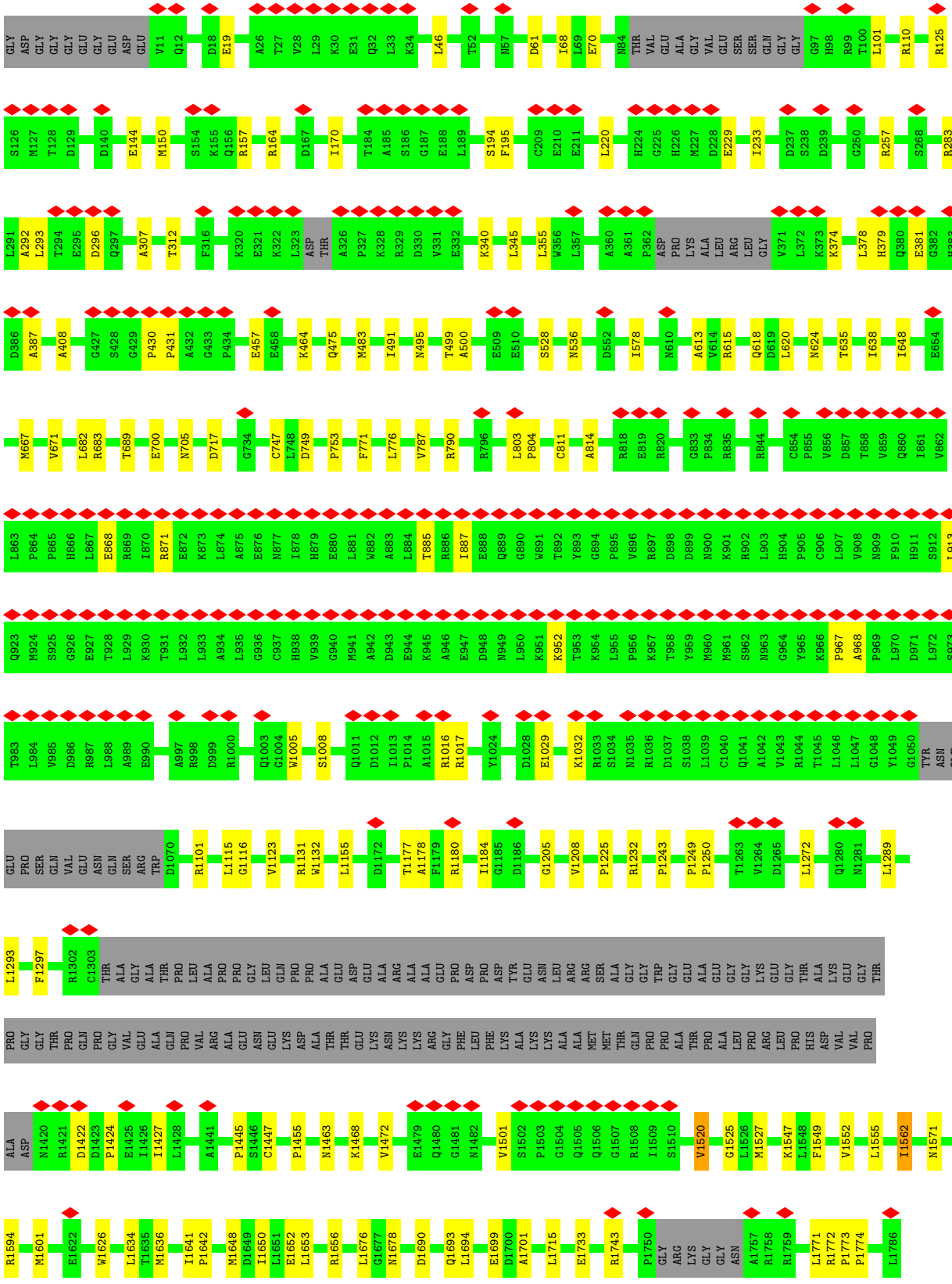

GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU
E1923 E1924 S1934 C1947 E1963 Q1973 R1974 S1975 R1976 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992
R1993 R1994 T1995 R1996 E1997 S2000 Q2005 M2008 L2009 L2010 H2011 F2012 K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 P2022 L2023 P2024 E2025 D2026 I2027 R2028 Q2029 D2030 L2031 Q2032 D2033 L2039 I2044 Q2045 L2046 GLU GLY 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 E2096 H2100 Q2127 Y2128 L2135 R2140 D2151 T2152 M2153 S2154 L2155 L2159 R2163 L2177 M2178 I2182 F2191 P2195 N2196 L2197 M2198 R2199
M2203 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 M2228 R2234 R2244 S2261 G2262 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 P2272 A2277 D2294 M2312 L2313 L2314 A2315 D2320 F2337 R2355 G2370 E2371 E2388 D2389 P2390 D2393 G2396 VAL ARG
ARG ASP ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU GLU
N2414 R2415 D2431 R2435 Q2444 E2449 R2452 D2464 Q2475 I2476 P2477 T2478 L2479 G2480 K2481 D2482 G2483 A2484 L2485 V2495 P2496 D2497 E2513 D2516 D2537 A2566 F2569 A2570 G2571 T2572 E2573
I2577 M2578 G2592 R2600 I2614 M2618 H2621 R2624 F2628 N2634 E2635 F2636 A2637 C2651 T2667 S2668 E2669 A2687 K2690 Y2691 D2692 Q2693 E2694 R2697 M2700 P2711 P2712 D2716 A2717 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU
GLY ASN PHE
D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792
P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG
GLU GLY
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A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP T2948 S2949 S2950 K2953 Q2962 R2965 W2966 M2967 Q2971 E2972 F2973 I2974 A2975 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983
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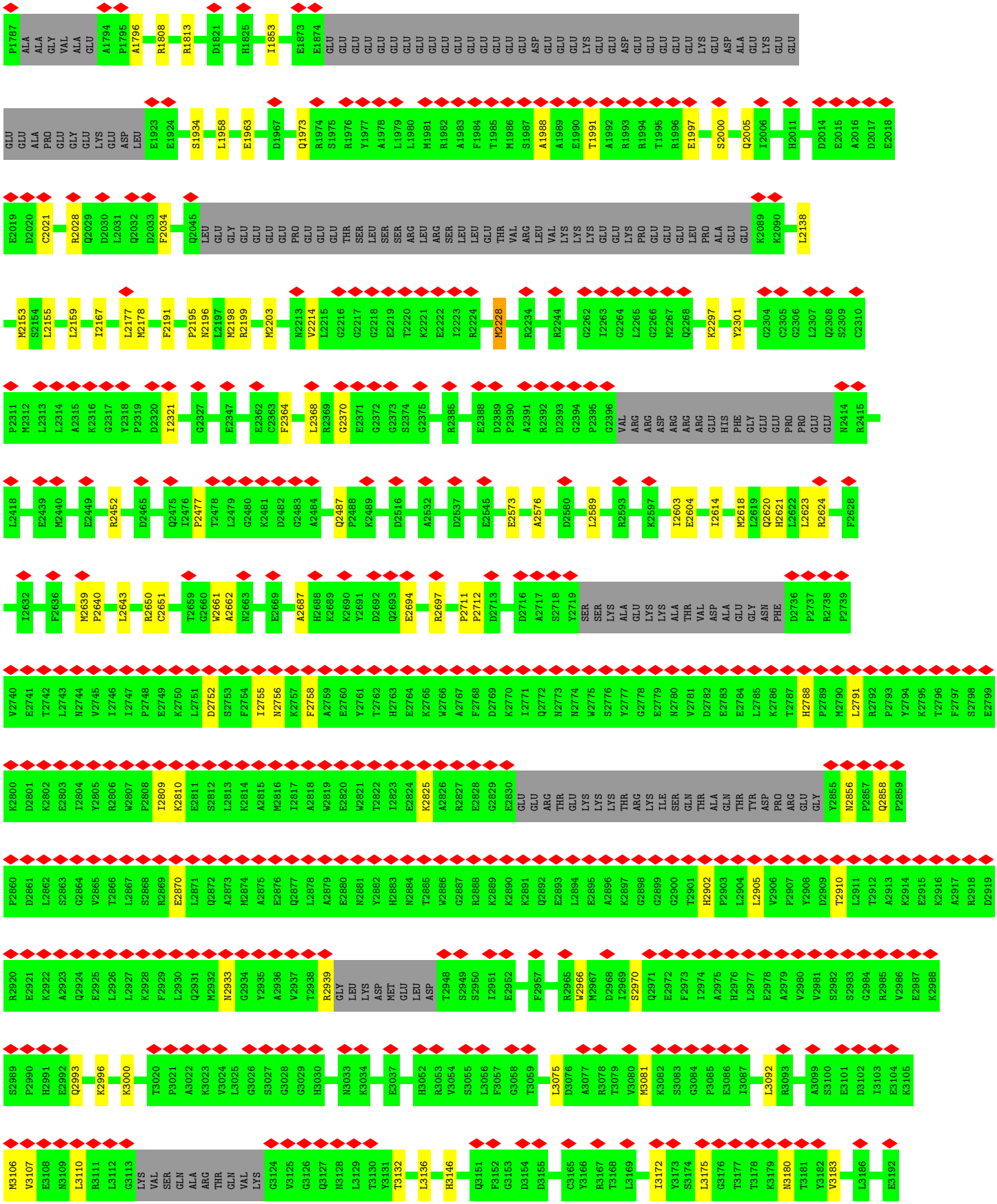


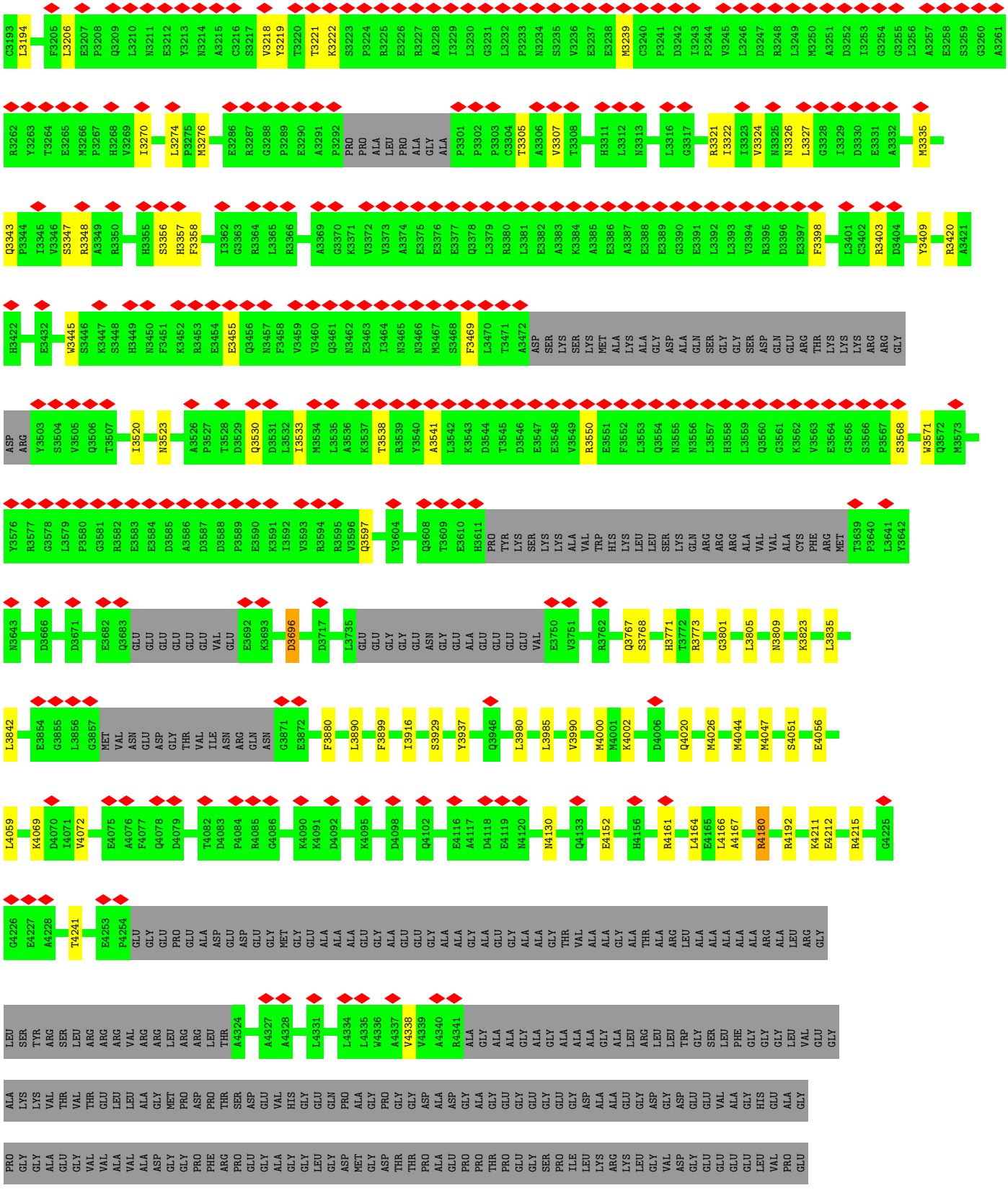
• Molecule 2: Ryanodine receptor 1

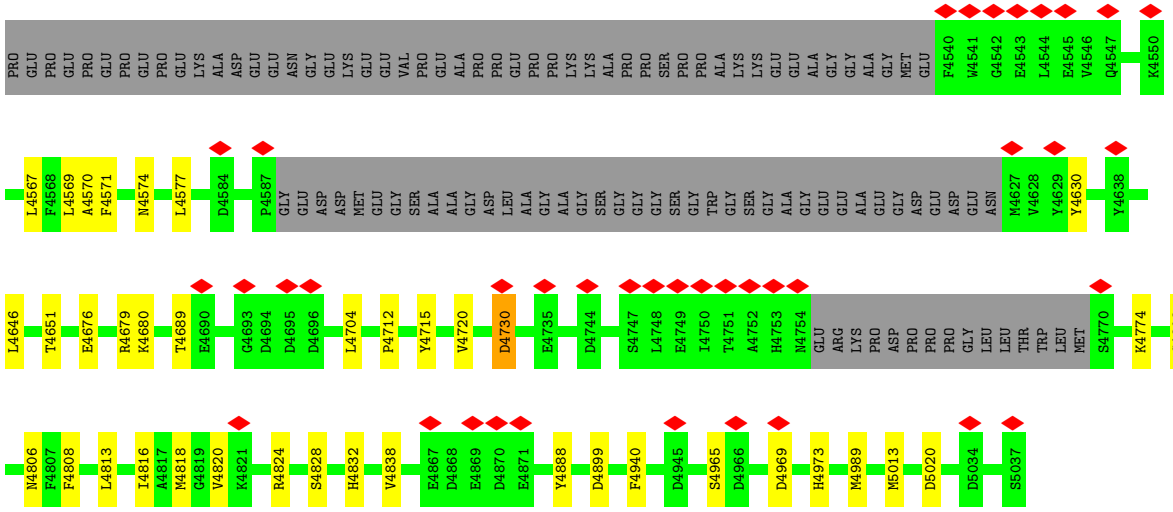
Chain D:







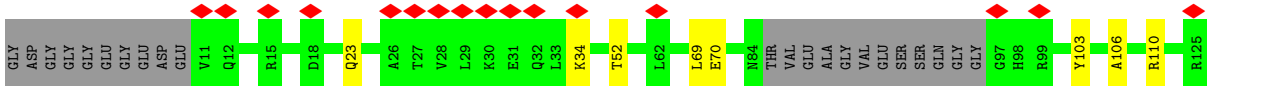

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G4226 E4227 A4228 T4241 E4253 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG ALA LEU ARG GLY
LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG ARG LEU ARG ARG THR A4324 A4327 A4328 L4331 L4334 L4335 W4336 A4337 V4338 V4339 A4340 R4341 ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY
ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY PRO ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA ALA GLU GLY ASP GLY GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY
PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY PRO PHE ARG PRO GLU GLY ALA GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU

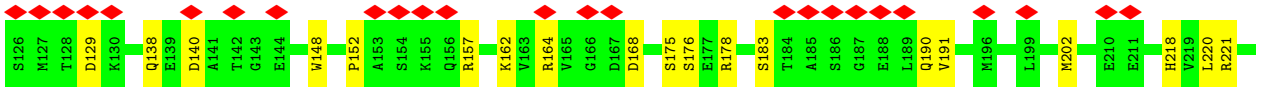


• Molecule 2: Ryanodine receptor 1

Chain F:







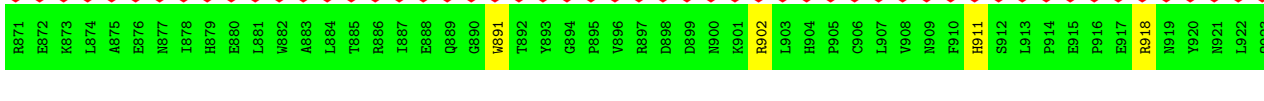


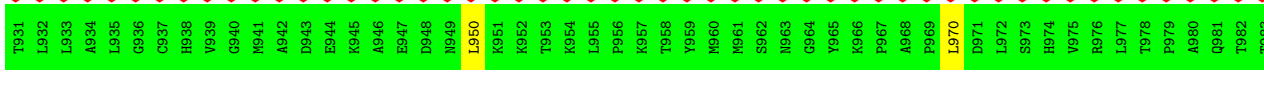


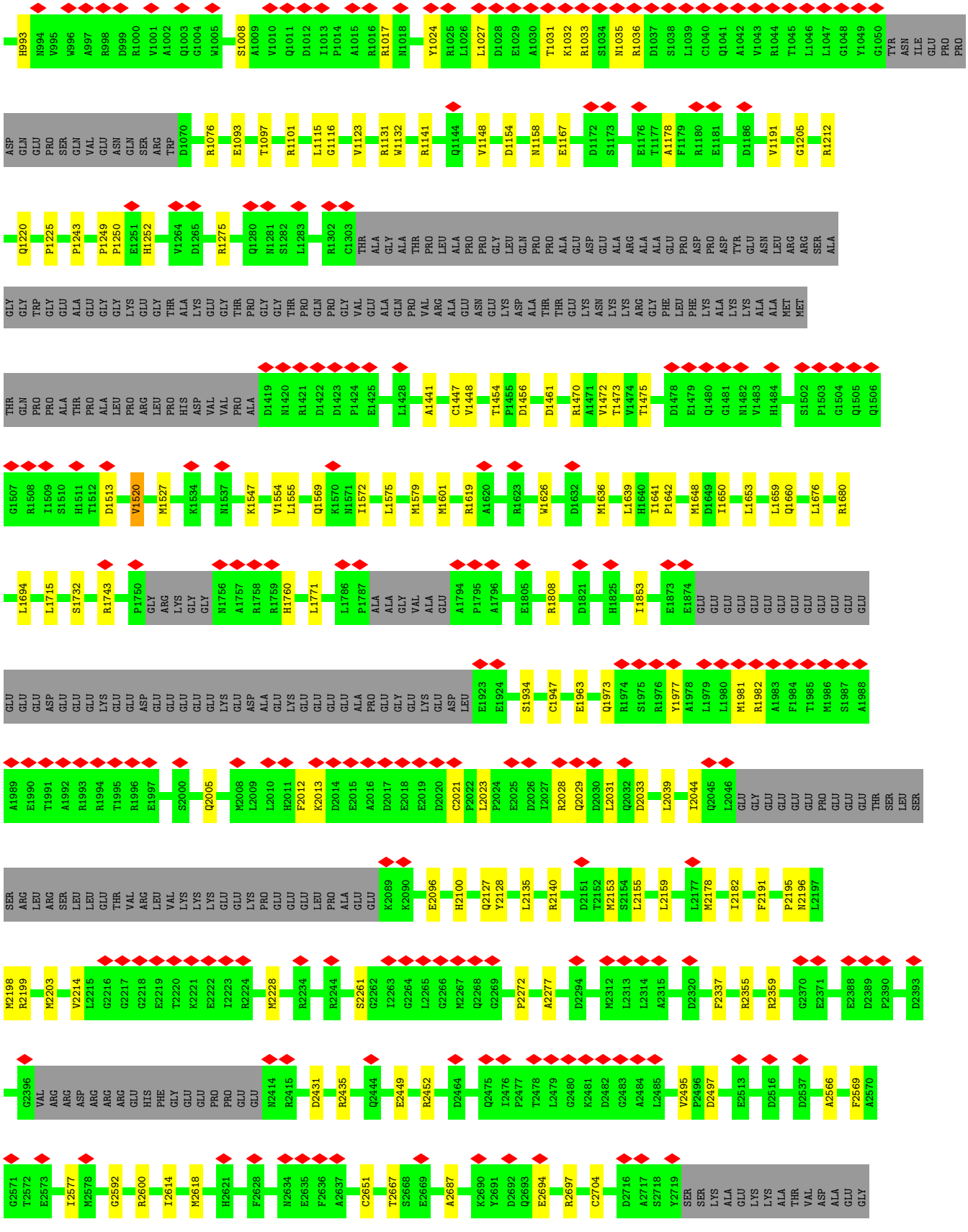


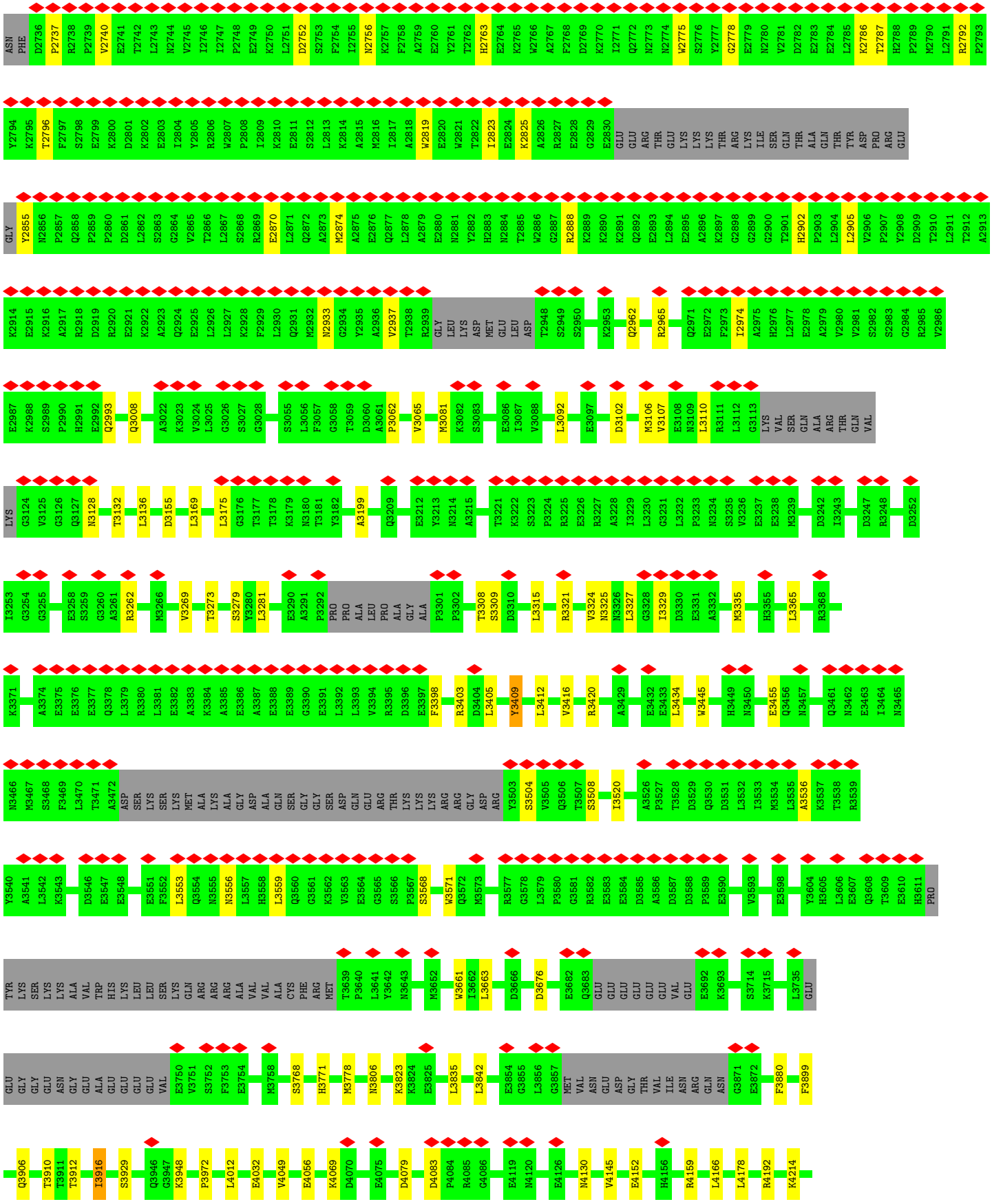


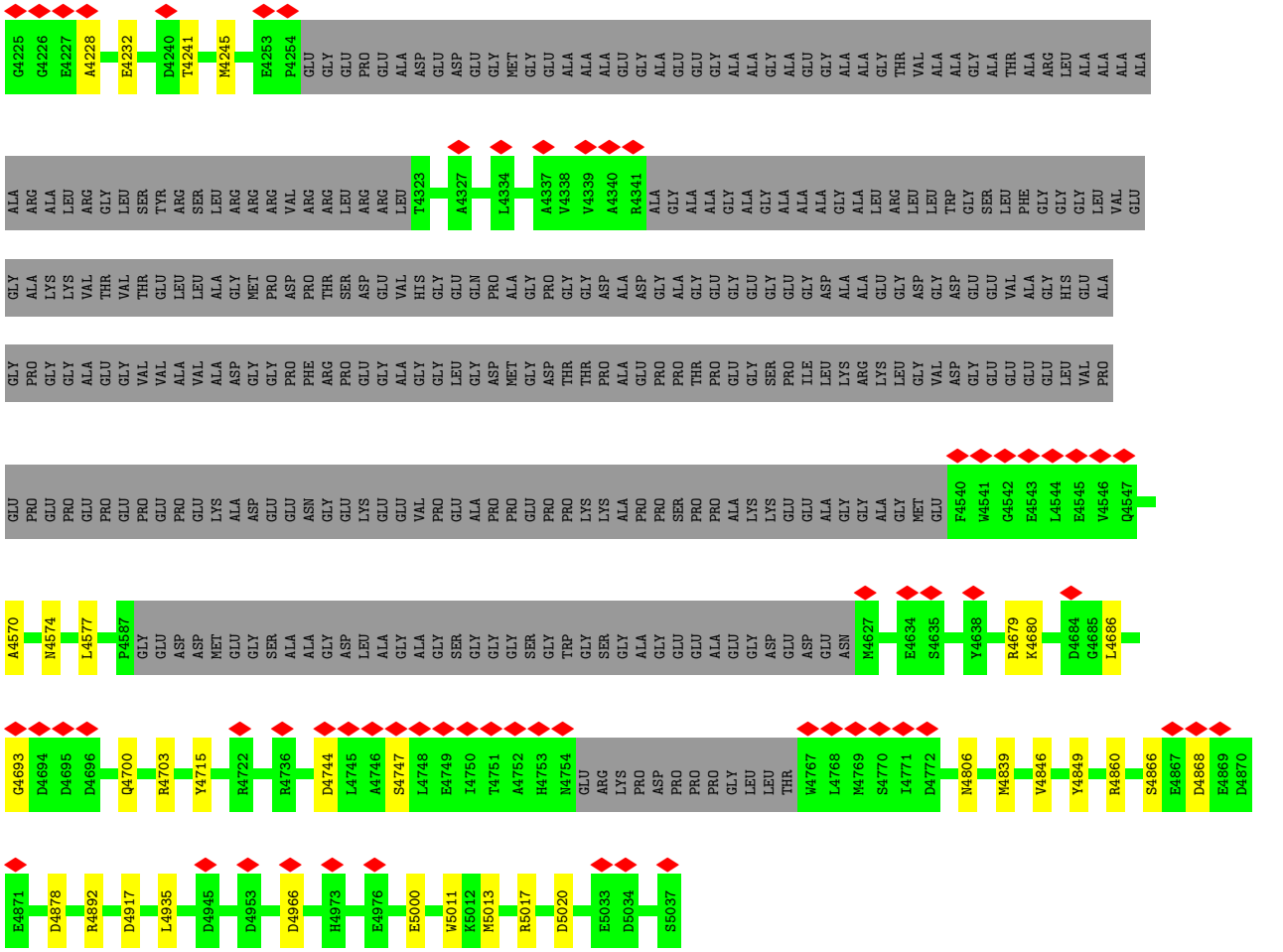







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Q1220 P1225 P1243 P1249 P1250 E1251 H1252 V1264 D1265 R1275 Q1280 N1281 S1282 L1283 R1302 C1303 THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA
GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET
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SER ARG LEU ARG SER LEU LEU GLU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 K2090 E2096 H2100 Q2127 Y2128 L2135 R2140 D2151 T2152 M2153 S2154 L2155 L2159 L2177 M2178 I2182 F2191 P2195 N2196 L2197
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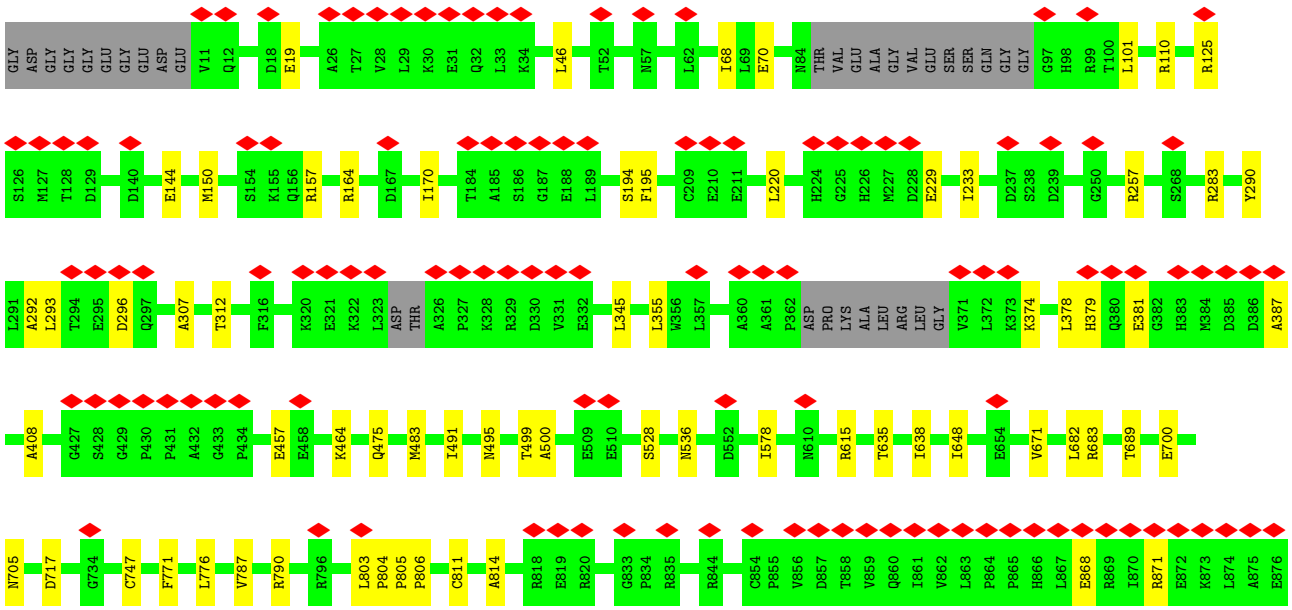

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Q3906 T3910 T3911 T3912 I3916 S3929 Q3946 G3947 K3948 P3972 L4012 E4032 V4049 E4056 K4069 D4070 E4075 D4079 D4083 P4084 R4085 G4086 E4119 N4120 E4126 N4130 V4145 E4152 H4156 R4159 L4166 L4178 R4192 K4214

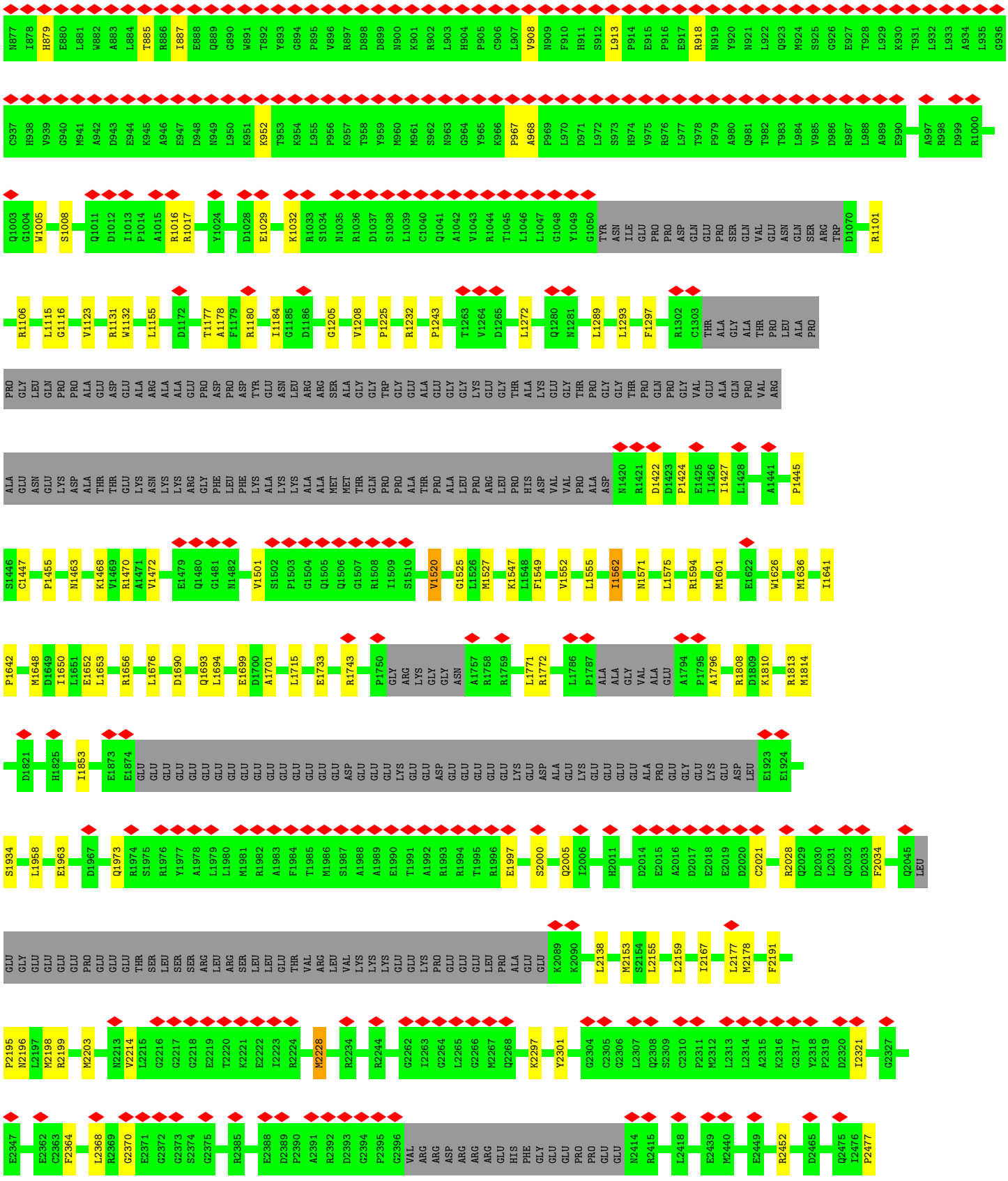


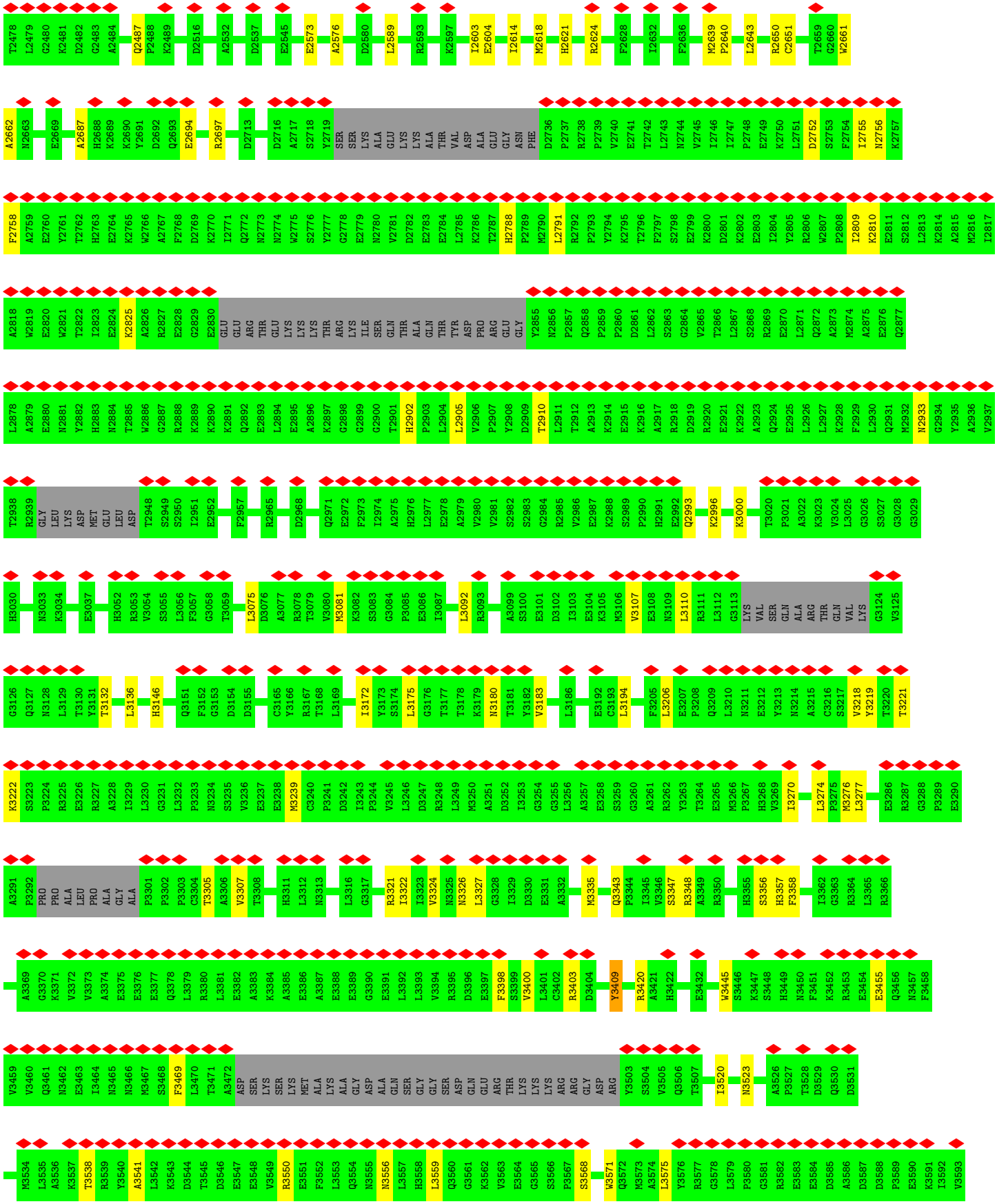
• Molecule 2: Ryanodine receptor 1

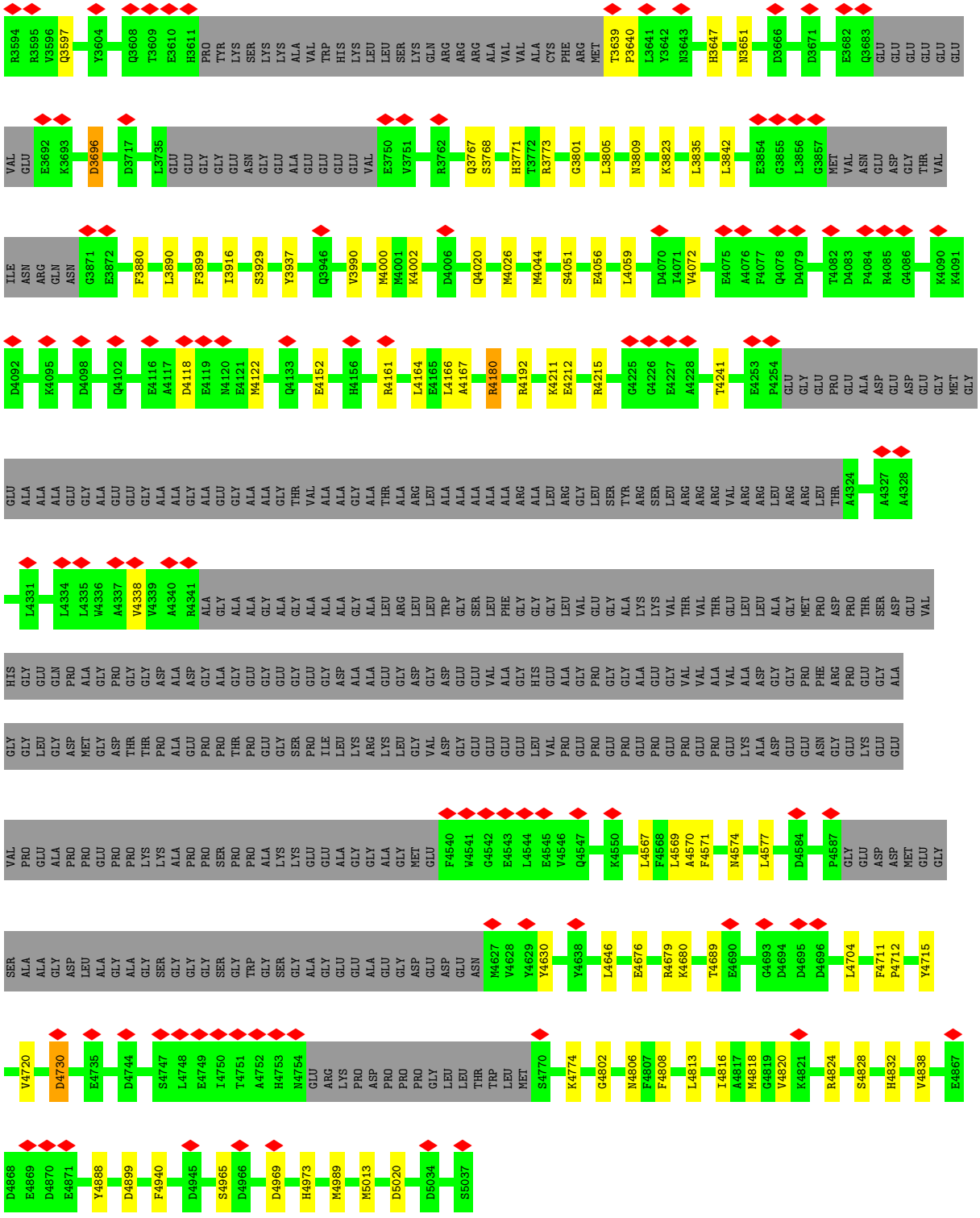
Chain H:






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 E990 A997 R998 D999 R1000
Q1003 G1004 W1005 S1008 Q1011 D1012 I1013 P1014 A1015 R1016 R1017 Y1024 D1028 E1029 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 TYR ASN ILE GLU PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1101
R1106 L1115 G1116 V1123 R1131 W1132 L1155 D1172 T1177 A1178 F1179 R1180 I1184 G1185 D1186 G1205 V1208 P1225 R1232 P1243 T1263 V1264 D1265 L1272 Q1280 N1281 L1289 L1293 F1297 R1302 C1303 THR ALA GLY ALA THR PRO LEU ALA PRO
PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG
ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 D1423 P1424 E1425 I1426 I1427 L1428 A1441 P1445
S1446 C1447 P1455 N1463 K1468 V1469 R1470 A1471 V1472 E1479 Q1480 G1481 N1482 V1501 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 V1520 G1525 L1526 M1527 K1547 L1548 F1549 V1552 L1555 I1562 N1571 L1575 R1594 M1601 E1622 W1626 M1636 I1641
P1642 M1648 D1649 I1650 L1651 E1652 L1653 R1656 L1676 D1690 Q1693 L1694 E1699 D1700 A1701 L1715 E1733 R1743 P1750 GLY ARG LYS GLY GLY ASN A1757 R1758 R1759 L1771 R1772 L1786 P1787 ALA ALA GLY VAL ALA GLU A1794 P1795 A1796 R1808 D1809 K1810 R1813 M1814
D1821 H1825 I1853 E1873 E1874 GLU GLU GLU


T2478 L2479 G2480 K2481 D2482 G2483 A2484 Q2487 P2488 K2489 D2516 A2532 D2537 E2545 E2573 A2576 D2580 L2589 R2593 K2597 I2603 E2604 I2614 M2618 H2621 R2624 F2628 I2632 F2636 M2639 P2640 L2643 R2650 C2651 T2659 G2660 W2661
A2662 N2663 E2669 A2687 H2688 K2689 K2690 Y2691 D2692 Q2693 E2694 R2697 D2713 D2716 A2717 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN PHE D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757
F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817
A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877
L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937
T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP T2948 S2949 S2950 I2951 E2952 F2957 R2965 D2968 Q2971 E2972 F2973 I2974 A2975 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 Q2993 K2996 K3000 T3020 P3021 A3022 K3023 V3024 L3025 G3026 S3027 G3028 G3029
H3030 N3033 K3034 E3037 H3052 R3053 V3054 S3055 L3056 F3057 G3058 T3059 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 S3083 G3084 P3085 E3086 I3087 L3092 R3093 A3099 S3100 E3101 D3102 I3103 E3104 K3105 M3106 V3107 E3108 N3109 L3110 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 V3125
G3126 Q3127 N3128 L3129 T3130 Y3131 T3132 L3136 H3146 Q3151 F3152 G3153 D3154 D3155 C3165 Y3166 R3167 T3168 L3169 I3172 Y3173 S3174 L3175 G3176 T3177 T3178 K3179 N3180 T3181 Y3182 V3183 L3186 E3192 C3193 L3194 F3205 L3206 E3207 P3208 Q3209 L3210 N3211 E3212 Y3213 N3214 A3215 C3216 S3217 V3218 Y3219 T3220 T3221
K3222 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 L3232 P3233 N3234 S3235 V3236 E3237 E3238 M3239 C3240 P3241 D3242 I3243 P3244 V3245 L3246 D3247 R3248 L3249 M3250 A3251 D3252 I3253 G3254 G3255 L3256 A3257 E3258 S3259 G3260 A3261 R3262 Y3263 T3264 E3265 M3266 P3267 H3268 V3269 I3270 L3274 P3275 M3276 L3277 E3286 R3287 G3288 P3289 E3290
A3291 P3292 PRO PRO ALA LEU PRO ALA GLY ALA P3301 P3302 P3303 C3304 T3305 A3306 V3307 T3308 H3311 L3312 N3313 L3316 G3317 R3321 I3322 I3323 V3324 N3325 N3326 L3327 G3328 I3329 D3330 E3331 A3332 M3335 Q3343 P3344 I3345 V3346 S3347 R3348 A3349 R3350 H3355 S3356 H3357 F3358 I3362 G3363 R3364 L3365 R3366
A3369 G3370 K3371 V3372 V3373 A3374 E3375 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 D3396 E3397 F3398 S3399 V3400 L3401 C3402 R3403 D3404 Y3409 R3420 A3421 H3422 E3432 W3445 S3446 K3447 S3448 H3449 N3450 F3451 K3452 R3453 E3454 E3455 Q3456 N3457 F3458
V3459 V3460 Q3461 N3462 E3463 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 A3472 ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG Y3503 S3504 V3505 Q3506 T3507 I3520 N3523 A3526 P3527 T3528 D3529 Q3530 D3531
M3534 L3535 A3536 K3537 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 T3545 D3546 E3547 E3548 V3549 R3550 E3551 F3552 L3553 Q3554 N3555 N3556 L3557 H3558 L3559 Q3560 G3561 K3562 V3563 E3564 G3565 S3566 P3567 S3568 W3571 Q3572 M3573 A3574 L3575 Y3576 R3577 G3578 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 K3591 I3592 V3593


R3594 R3595 V3596 Q3597 Y3604 Q3608 T3609 E3610 H3611 T3639 P3640 L3641 Y3642 N3643 H3647 N3651 D3666 D3671 E3682 Q3683
VAL GLU E3692 K3693 D3696 D3717 L3735 E3750 V3751 R3762 Q3767 S3768 H3771 T3772 R3773 G3801 L3805 N3809 K3823 L3835 L3842 E3854 G3855 L3856 G3857
ILE ASN ARG GLN ASN G3871 E3872 F3880 L3890 F3889 I3916 S3929 Y3937 Q3946 V3990 M4000 M4001 K4002 D4006 Q4020 M4026 M4044 S4051 E4056 L4059 D4070 I4071 V4072 E4075 A4076 F4077 Q4078 D4079 T4082 D4083 P4084 R4085 G4086 K4090 K4091
D4092 K4095 D4098 Q4102 E4116 A4117 D4118 E4119 N4120 E4121 M4122 Q4133 E4152 H4156 R4161 L4164 E4165 L4166 A4167 R4180 R4192 K4211 E4212 R4215 G4225 G4226 E4227 A4228 T4241 E4253 P4254
GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG ARG LEU ARG ARG LEU THR A4324 A4327 A4328
L4331 L4334 L4335 W4336 A4337 V4338 V4339 A4340 R4341
ALA GLY ALA ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL
HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ASP ALA GLU GLY ASP GLU GLU VAL GLU ALA ALA GLY PRO GLY GLY ALA GLU GLY VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA
GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU
VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547 K4550 L4567 F4568 L4569 A4570 F4571 N4574 L4577 D4584 P4587 GLY GLU ASP ASP MET GLU GLY
SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU ASN M4627 V4628 Y4629 Y4630 Y4638 L4646 E4676 R4679 K4680 T4689 E4690 G4693 D4694 D4695 D4696 L4704 F4711 P4712 Y4715
V4720 D4730 E4735 D4744 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 GLU ARG LYS PRO ASP PRO PRO PRO GLY LEU LEU THR TRP LEU MET S4770 K4774 G4802 N4806 F4807 F4808 L4813 I4816 A4817 M4818 G4819 V4820 K4821 R4824 S4828 H4832 V4838 E4867
D4868 E4869 D4870 E4871 Y4888 D4899 F4940 D4945 S4965 D4966 D4969 H4973 M4989 M5013 D5020 D5034 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	169062	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.510	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.078	Depositor
Map size (Å)	477.696, 477.696, 477.696	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.933, 0.933, 0.933	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1C1R, ATP, CA, 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	0.19	0/835	0.37	0/1125
1	C	0.22	0/830	0.37	0/1119
1	E	0.19	0/835	0.37	0/1125
1	G	0.22	0/830	0.37	0/1119
2	B	0.19	0/34005	0.35	0/46137
2	D	0.20	0/33726	0.36	0/45794
2	F	0.19	0/34005	0.35	0/46137
2	H	0.20	0/33726	0.36	0/45794
All	All	0.20	0/138792	0.35	0/188350

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	819	0	825	6	0
1	C	814	0	810	5	0
1	E	819	0	825	6	0
1	G	814	0	810	5	0
2	B	33249	0	32468	223	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	32972	0	32007	213	0
2	F	33249	0	32468	211	0
2	H	32972	0	32007	205	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	B	31	0	12	1	0
5	D	31	0	12	1	0
5	F	31	0	12	1	0
5	H	31	0	12	1	0
6	B	14	0	0	0	0
6	D	14	0	0	0	0
All	All	135868	0	132268	843	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 3.

The worst 5 of 843 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:D:700:GLU:H	2:D:705:ASN:HD21	1.43	0.66
2:D:3523:ASN:HD22	2:F:1220:GLN:NE2	1.94	0.66
2:B:1220:GLN:NE2	2:H:3523:ASN:HD22	1.94	0.65
2:H:101:LEU:HB3	2:H:150:MET:HE1	1.78	0.65
2:D:101:LEU:HB3	2:D:150:MET:HE1	1.78	0.65

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	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	C	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
1	E	106/110 (96%)	104 (98%)	2 (2%)	0	100	100
1	G	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
2	B	4225/5037 (84%)	4170 (99%)	55 (1%)	0	100	100
2	D	4221/5037 (84%)	4156 (98%)	65 (2%)	0	100	100
2	F	4225/5037 (84%)	4170 (99%)	55 (1%)	0	100	100
2	H	4221/5037 (84%)	4156 (98%)	65 (2%)	0	100	100
All	All	17314/20588 (84%)	17064 (99%)	250 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	87/90 (97%)	84 (97%)	3 (3%)	32	64
1	C	87/90 (97%)	85 (98%)	2 (2%)	44	72
1	E	87/90 (97%)	84 (97%)	3 (3%)	32	64
1	G	87/90 (97%)	85 (98%)	2 (2%)	44	72
2	B	3502/4277 (82%)	3476 (99%)	26 (1%)	76	85
2	D	3434/4277 (80%)	3410 (99%)	24 (1%)	76	85
2	F	3502/4277 (82%)	3476 (99%)	26 (1%)	76	85
2	H	3434/4277 (80%)	3410 (99%)	24 (1%)	76	85
All	All	14220/17468 (81%)	14110 (99%)	110 (1%)	70	85

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	26	HIS
2	F	2651	CYS
2	H	4730	ASP
2	H	3398	PHE
2	F	220	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 246 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	4558	ASN
2	H	3149	GLN
2	F	1532	ASN
2	H	3012	ASN
2	H	4043	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	$\#\|Z\|>2$
5	ATP	B	5303	-	32,33,33	0.27	0	48,52,52	0.33	0
6	A1C1R	D	5304	6	14,15,15	3.98	6 (42%)	17,20,20	2.30	2 (11%)
6	A1C1R	B	5304	6	14,15,15	3.98	6 (42%)	17,20,20	2.30	2 (11%)
5	ATP	H	5303	-	32,33,33	0.32	0	48,52,52	0.32	0
5	ATP	F	5303	-	32,33,33	0.27	0	48,52,52	0.33	0
5	ATP	D	5303	-	32,33,33	0.32	0	48,52,52	0.32	0

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
5	ATP	B	5303	-	-	13/22/38/38	0/3/3/3
6	A1C1R	D	5304	6	-	2/2/12/12	0/1/2/2
6	A1C1R	B	5304	6	-	2/2/12/12	0/1/2/2
5	ATP	H	5303	-	-	8/22/38/38	0/3/3/3
5	ATP	F	5303	-	-	13/22/38/38	0/3/3/3
5	ATP	D	5303	-	-	8/22/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5304	A1C1R	C11-N10	-7.34	1.29	1.46
6	D	5304	A1C1R	C11-N10	-7.34	1.29	1.46
6	B	5304	A1C1R	C12-N10	-7.23	1.40	1.47
6	D	5304	A1C1R	C12-N10	-7.23	1.40	1.47
6	B	5304	A1C1R	C06-S07	6.02	1.83	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	5304	A1C1R	C08-S07-C06	8.65	114.97	102.71
6	D	5304	A1C1R	C08-S07-C06	8.65	114.97	102.71
6	B	5304	A1C1R	C11-N10-C12	2.24	114.70	111.04
6	D	5304	A1C1R	C11-N10-C12	2.24	114.70	111.04

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	5303	ATP	C5'-O5'-PA-O1A
5	B	5303	ATP	C5'-O5'-PA-O2A
5	B	5303	ATP	C5'-O5'-PA-O3A
5	B	5303	ATP	C4'-C5'-O5'-PA
5	D	5303	ATP	C5'-O5'-PA-O2A

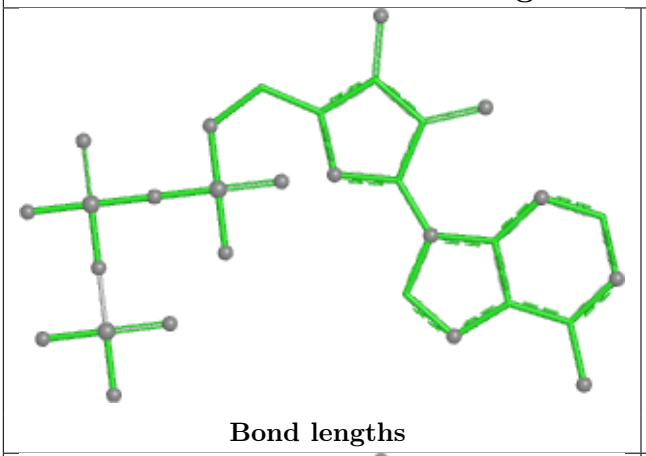
There are no ring outliers.

4 monomers are involved in 4 short contacts:

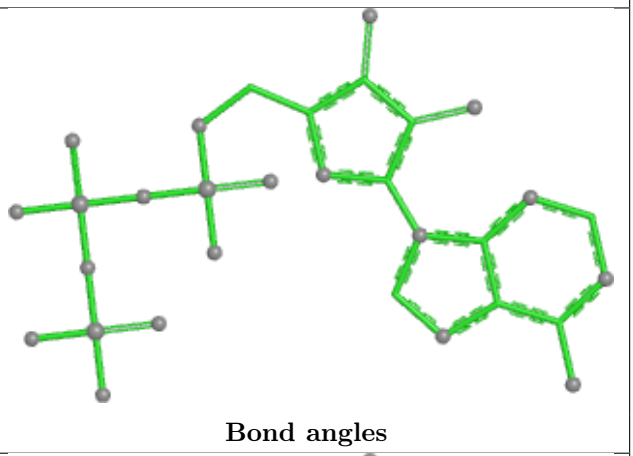
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5303	ATP	1	0
5	H	5303	ATP	1	0
5	F	5303	ATP	1	0
5	D	5303	ATP	1	0

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.

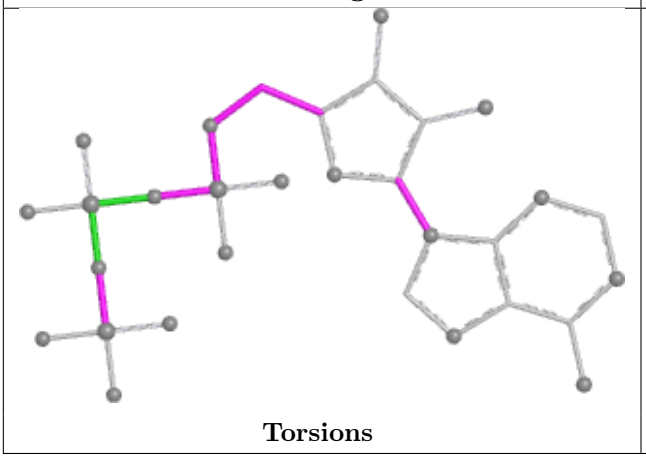
Ligand ATP B 5303



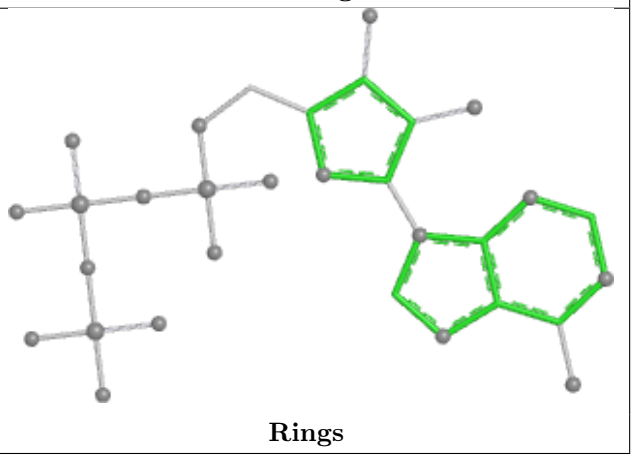
Bond lengths



Bond angles

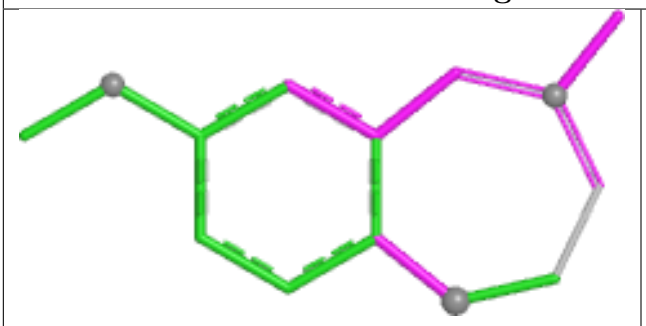


Torsions

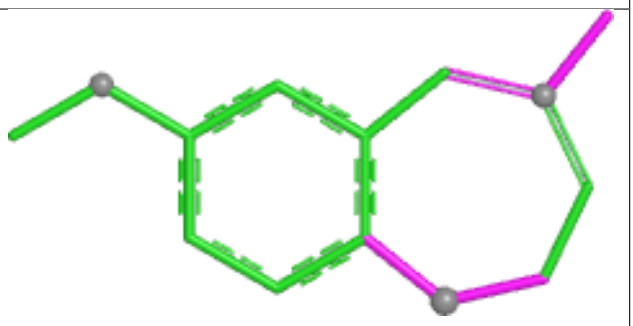


Rings

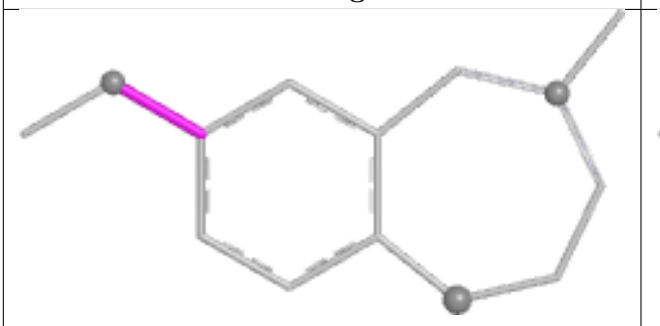
Ligand A1C1R D 5304



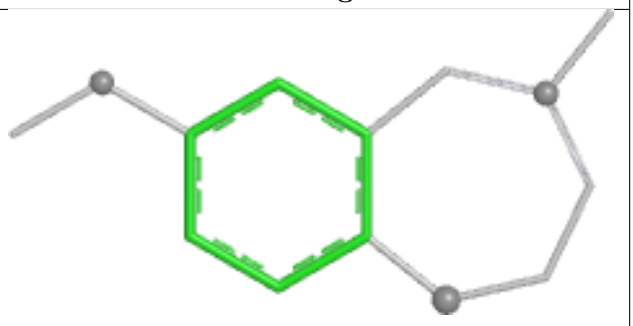
Bond lengths



Bond angles

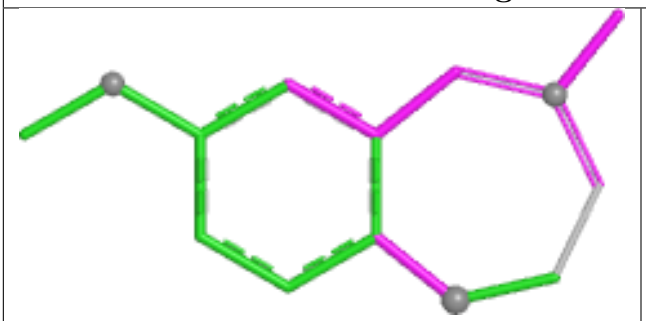


Torsions

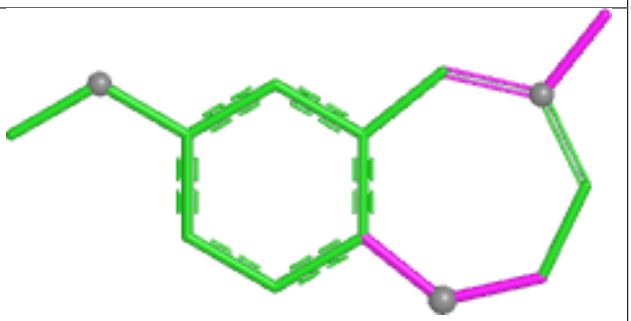


Rings

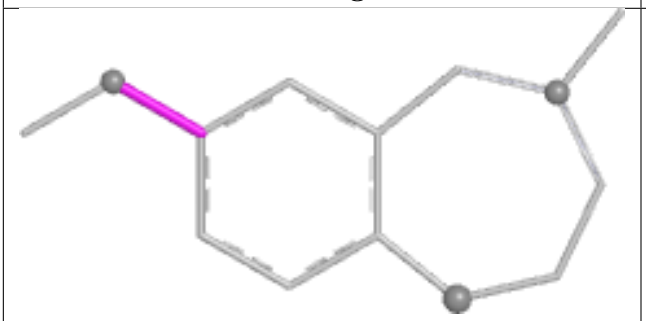
Ligand A1C1R B 5304



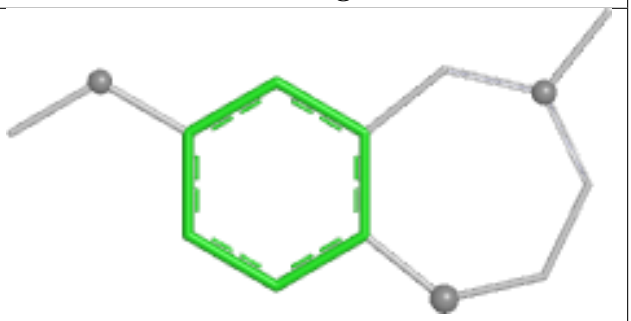
Bond lengths



Bond angles

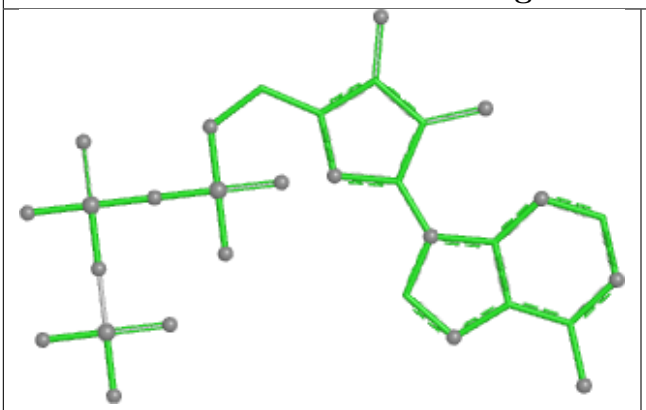


Torsions

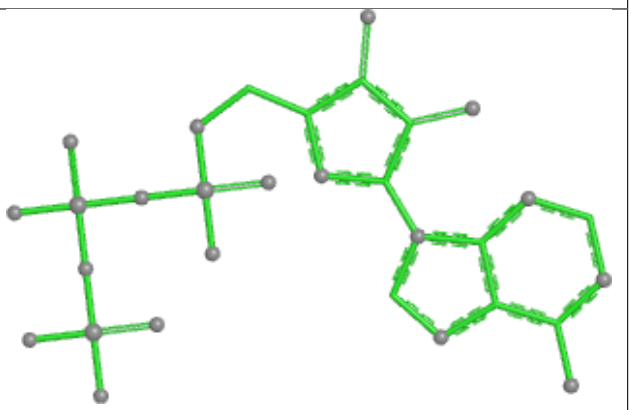


Rings

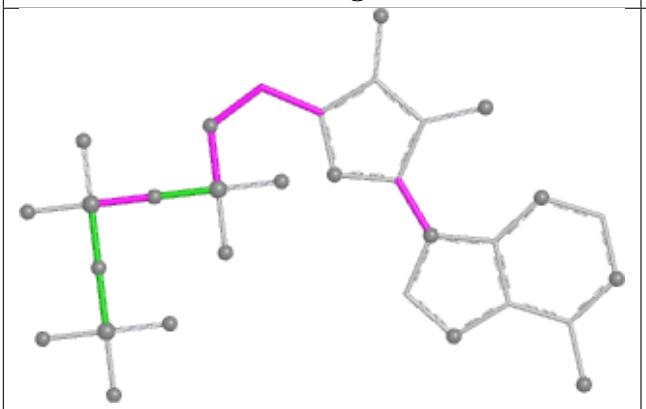
Ligand ATP H 5303



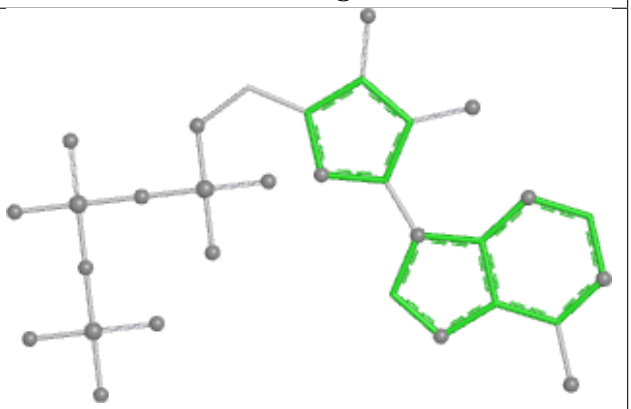
Bond lengths



Bond angles

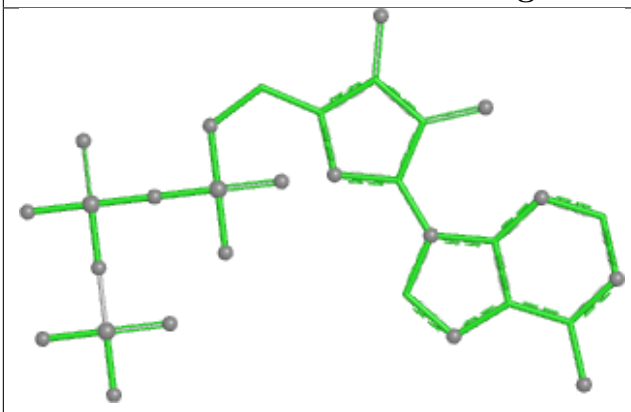


Torsions

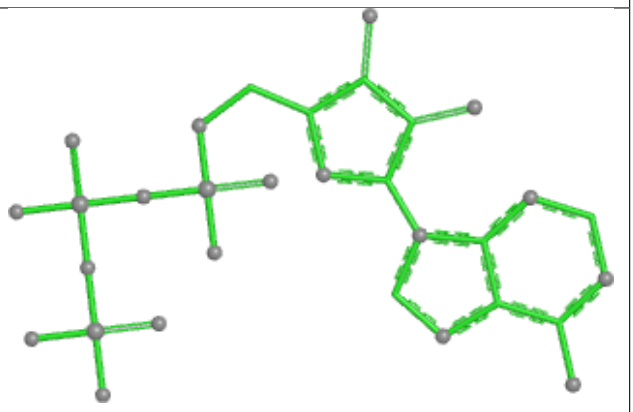


Rings

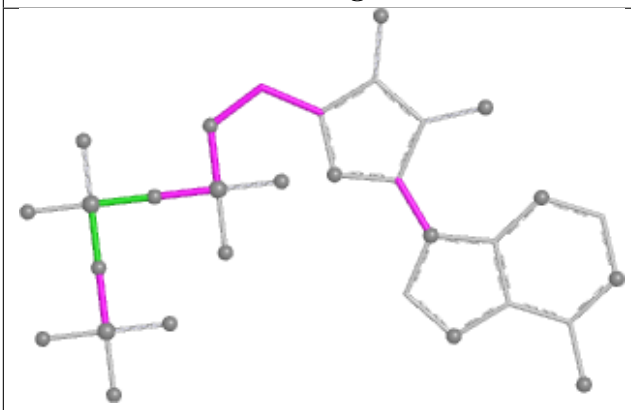
Ligand ATP F 5303



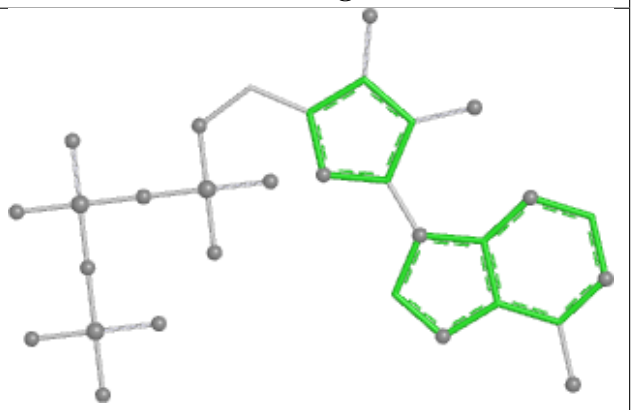
Bond lengths



Bond angles

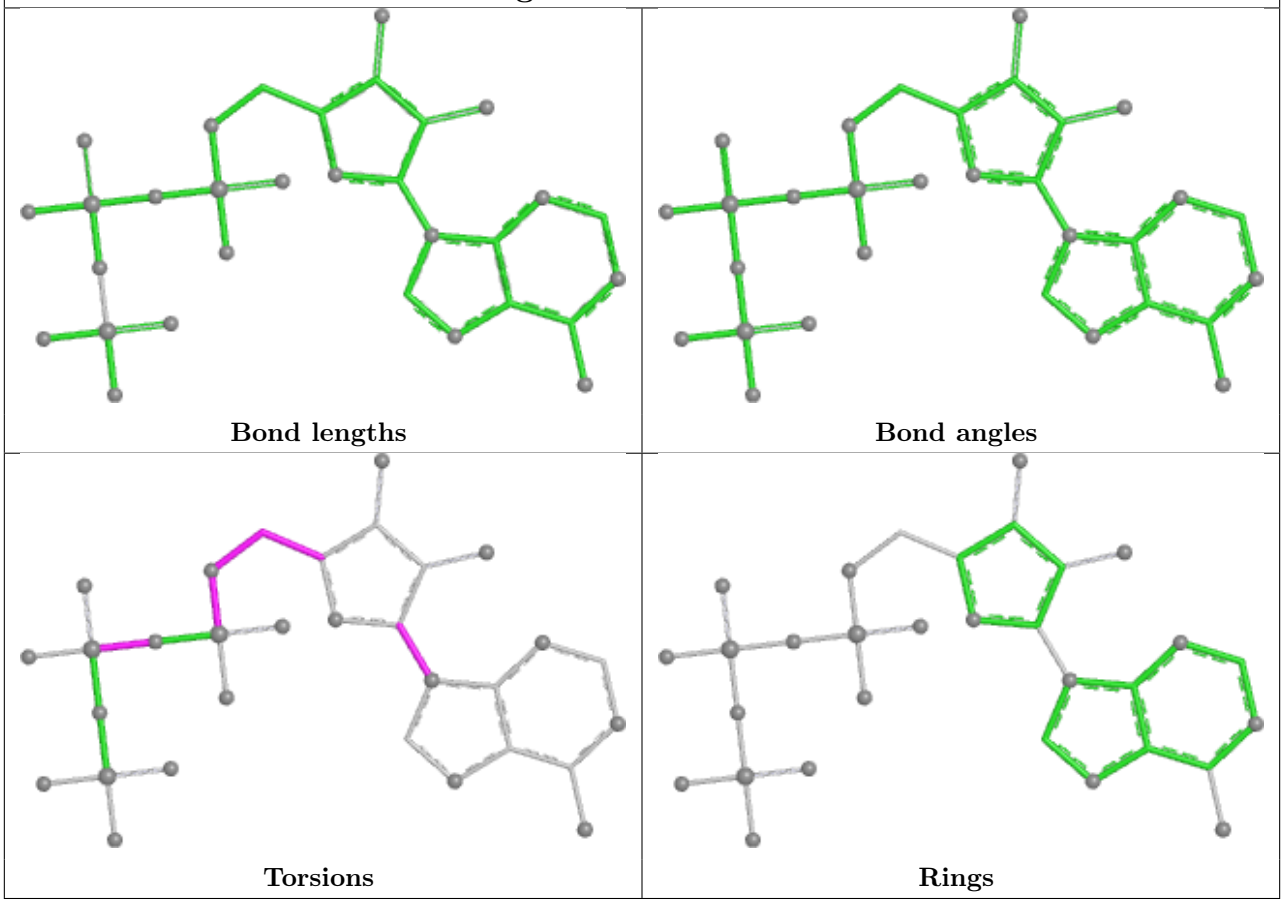


Torsions



Rings

Ligand ATP D 5303



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.

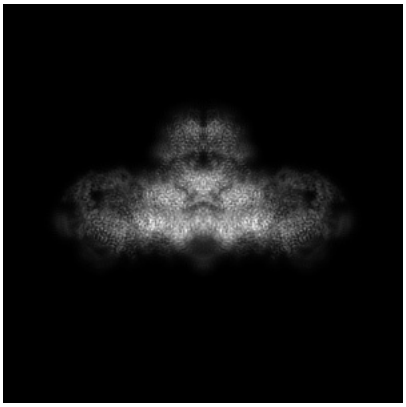
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73954. These allow visual inspection of the internal detail of the map and identification of artifacts.

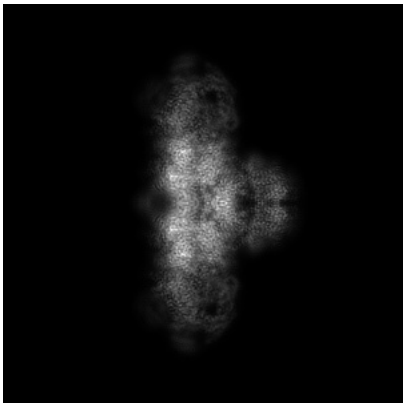
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

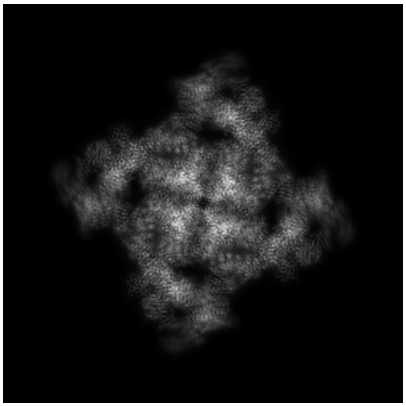
6.1.1 Primary map



X



Y

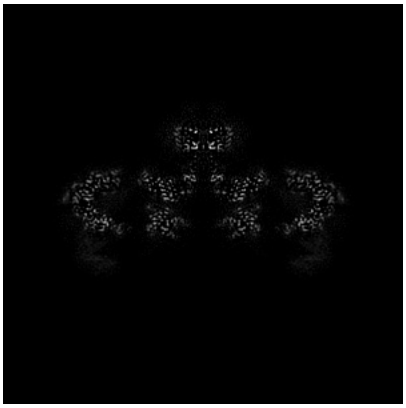


Z

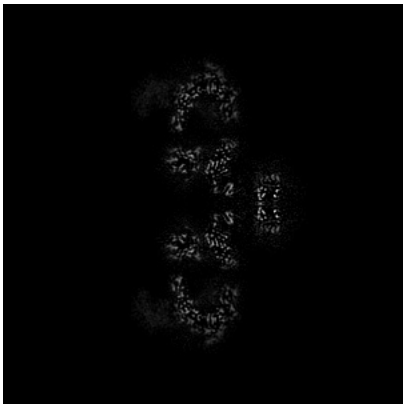
The images above show the map projected in three orthogonal directions.

6.2 Central slices

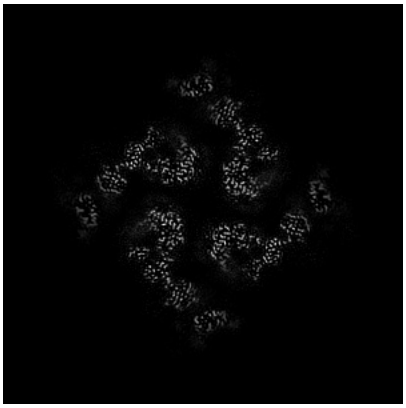
6.2.1 Primary map



X Index: 256



Y Index: 256

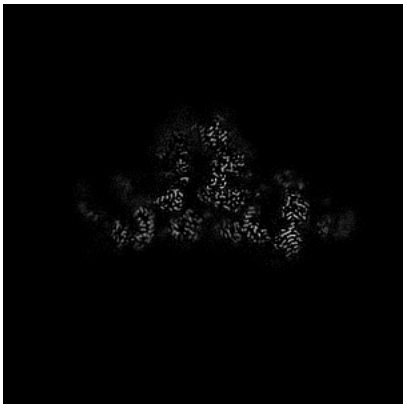


Z Index: 256

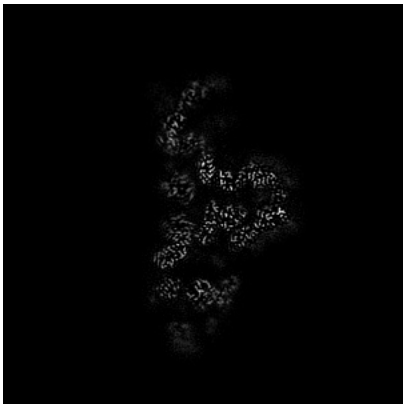
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

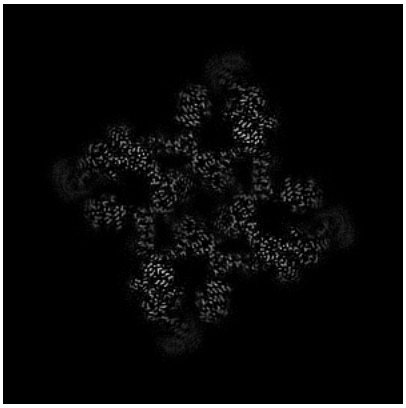
6.3.1 Primary map



X Index: 290



Y Index: 283

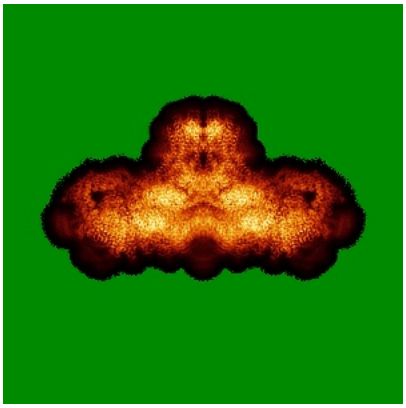


Z Index: 232

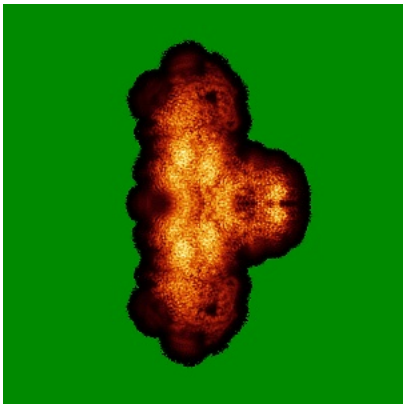
The images above show the largest variance slices of the map in three orthogonal directions.

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

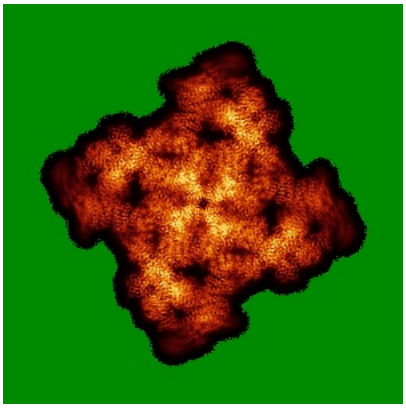
6.4.1 Primary map



X



Y

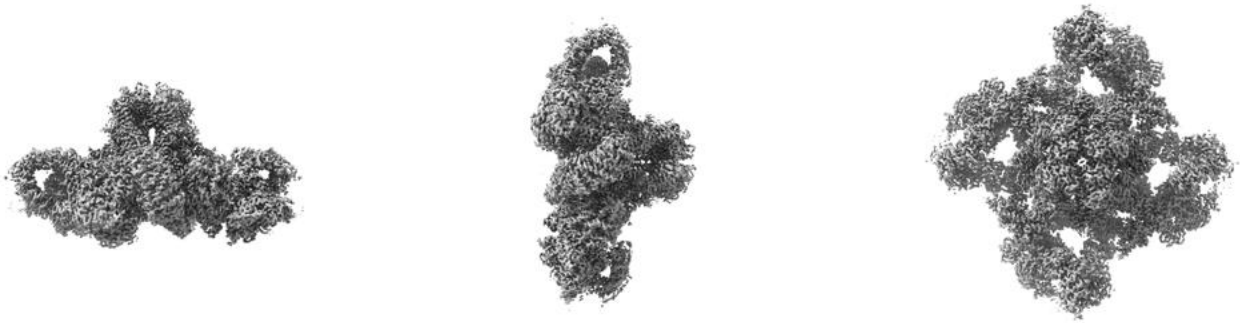


Z

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

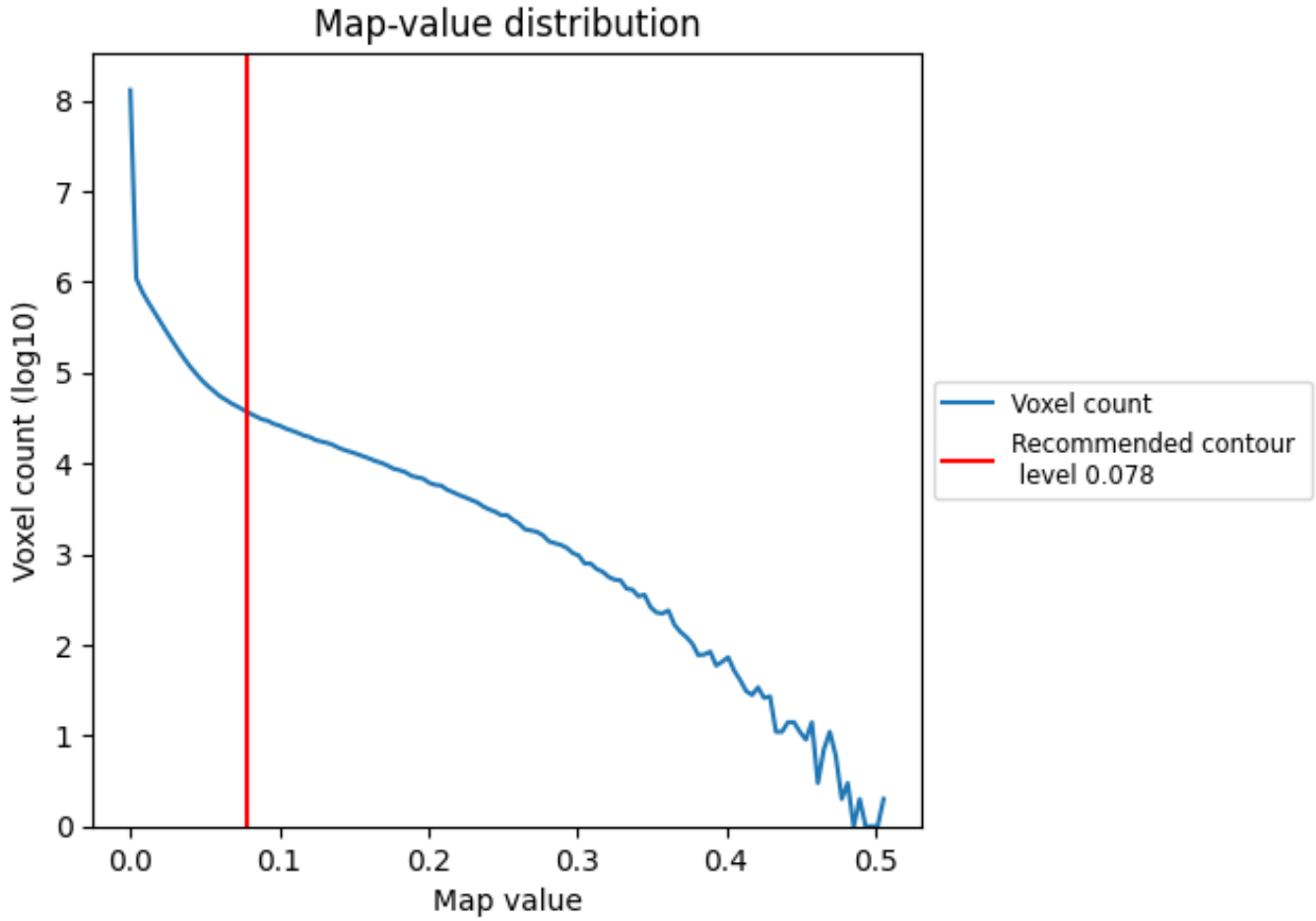
6.6 Mask visualisation (i)

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

7 Map analysis

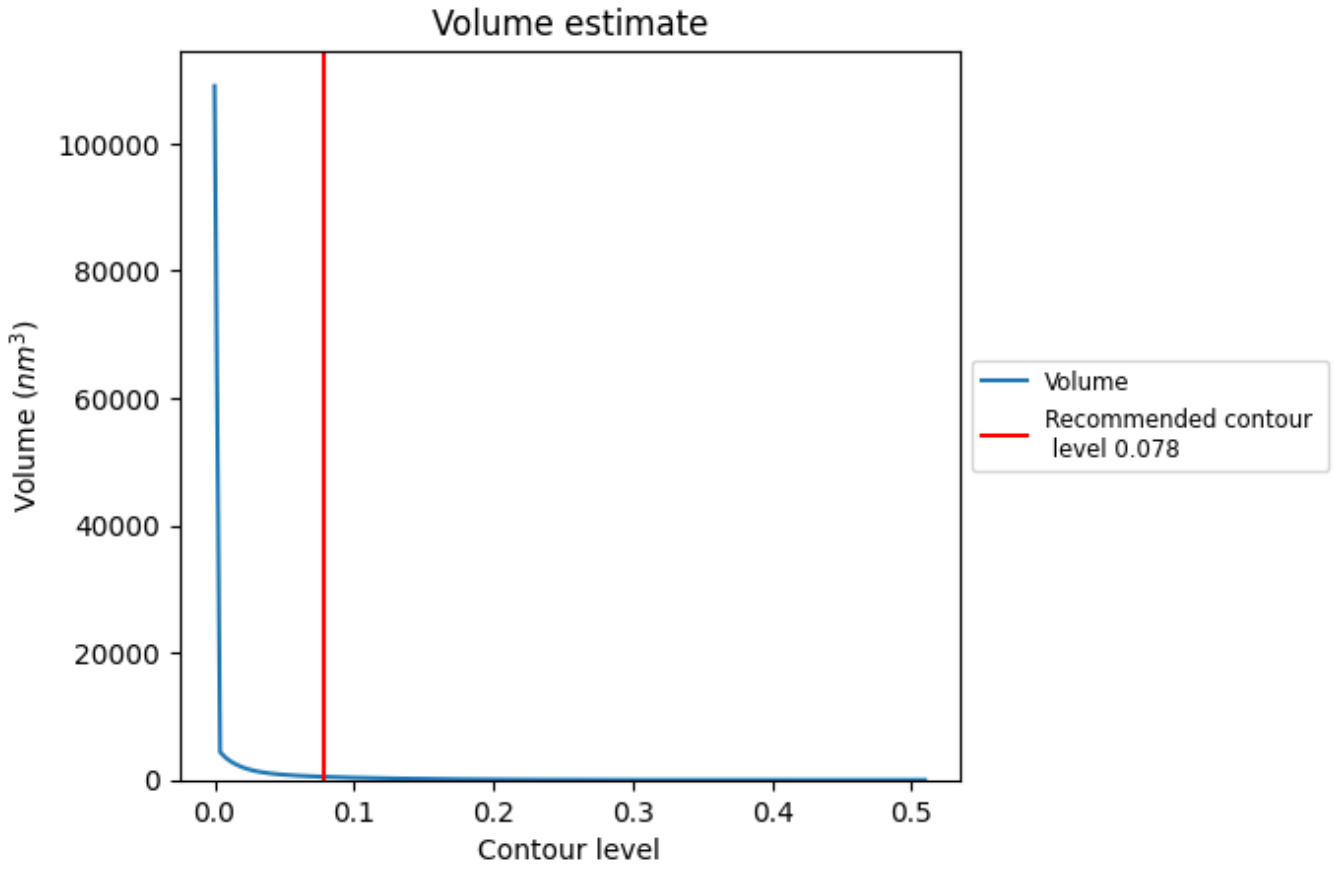
This section contains the results of statistical analysis of the map.

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.

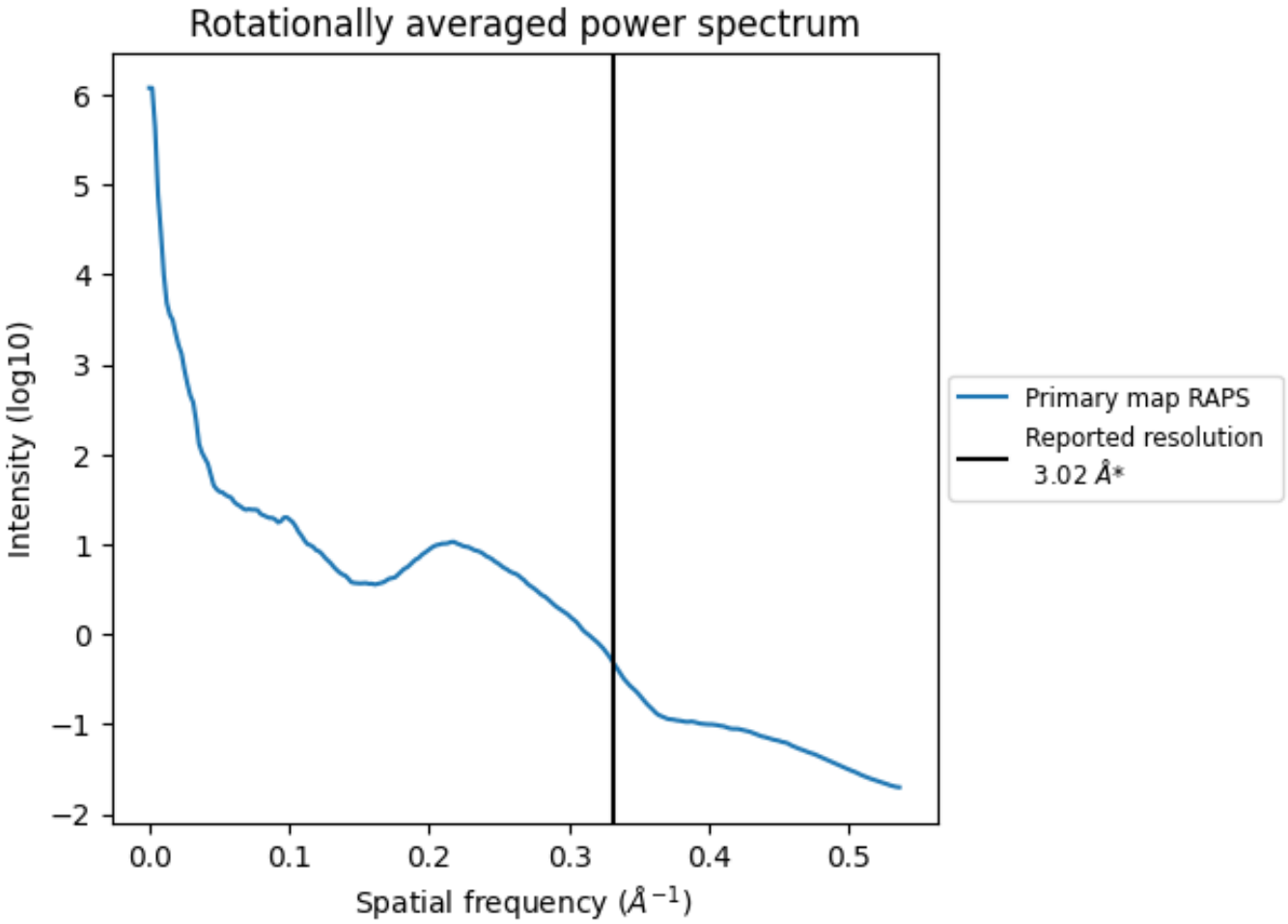
7.2 Volume estimate (i)



The volume at the recommended contour level is 502 nm^3; this corresponds to an approximate mass of 454 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 0.331 Å^{-1}

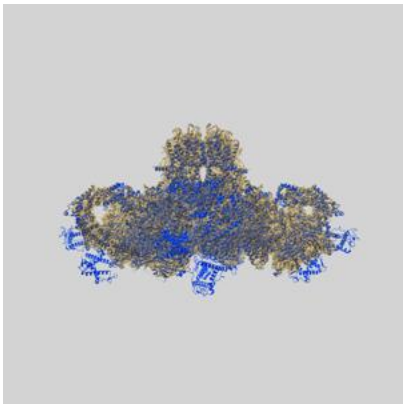
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

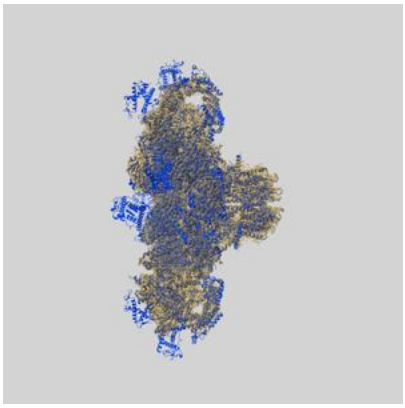
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73954 and PDB model 9Z9P. Per-residue inclusion information can be found in section 3 on page 8.

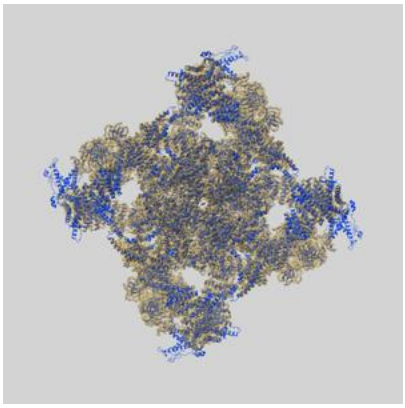
9.1 Map-model overlay



X



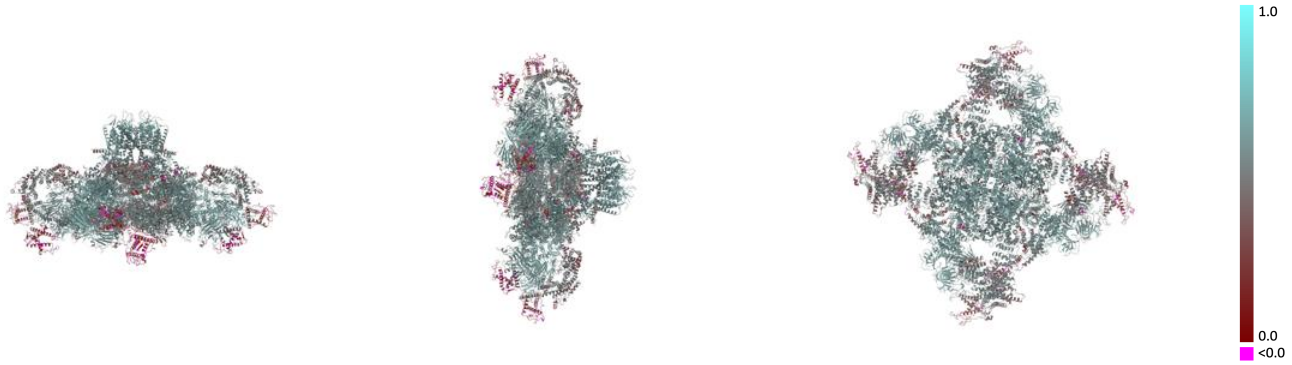
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.078 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

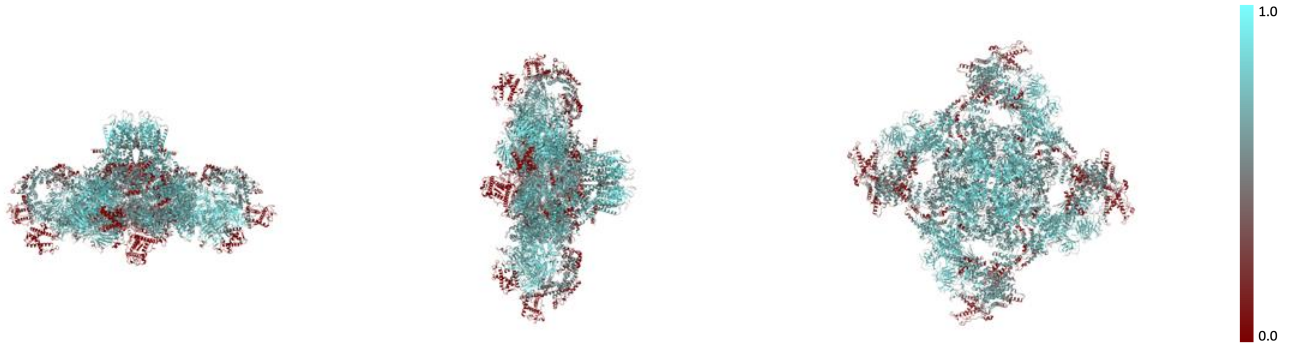
9.2 Q-score mapped to coordinate model (i)



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.

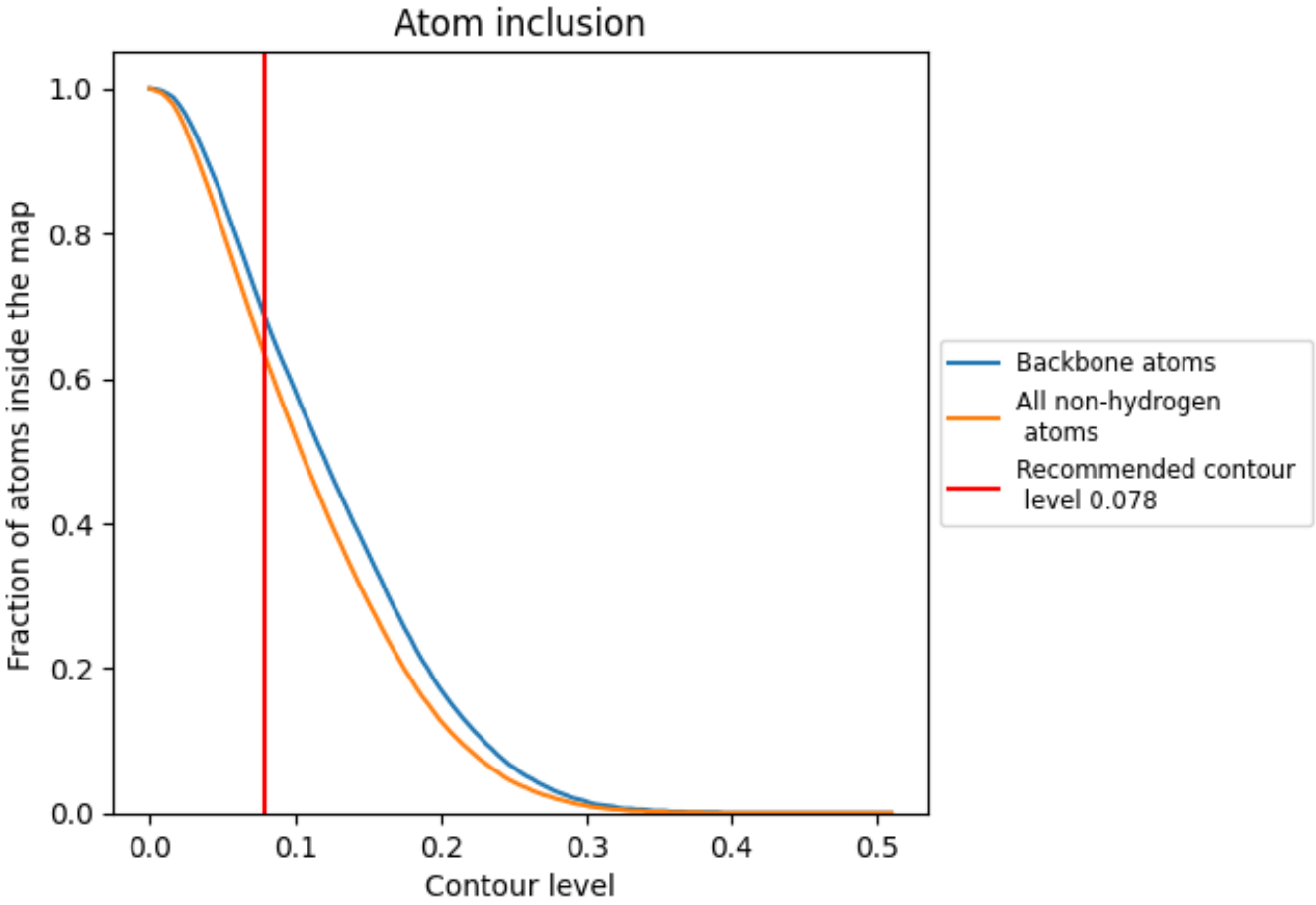
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.078).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 64% 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 (0.078) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.5290
A	0.7350	0.5970
B	0.6390	0.5300
C	0.7770	0.6030
D	0.6280	0.5240
E	0.7340	0.5970
F	0.6390	0.5300
G	0.7740	0.6080
H	0.6270	0.5240

