wwPDB EM Validation Summary Report (i)

Nov 11, 2026 – 03:08 PM EST

PDB ID	:	9Z9R / pdb_00009z9r
EMDB ID	:	EMD-73956
Title	:	Closed-state rabbit RyR1 with activating ligands (Ca2+/ATP)
Authors	:	Chen, Y.S.; Van Petegem, F.
Deposited on	:	2025-11-18
Resolution	:	3.08 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:

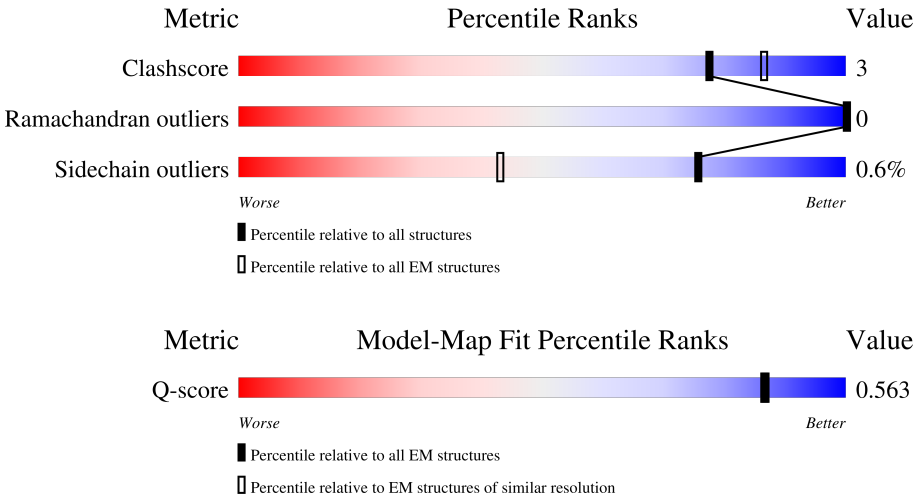
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

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

The reported resolution of this entry is 3.08 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.



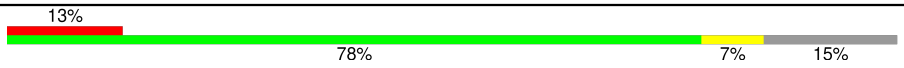
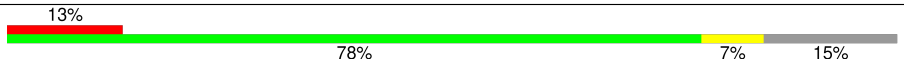
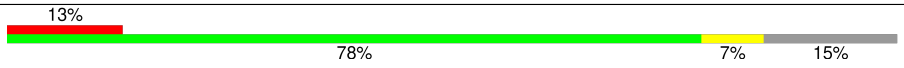
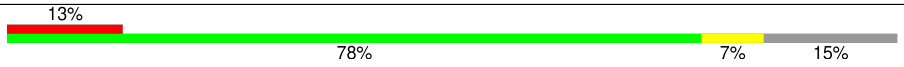
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14000 (2.58 - 3.58)

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	91% 8%
1	C	110	90% 9%
1	E	110	90% 9%
1	G	110	91% 8%

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 137180 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	109	Total	C	N	O	S	0	0
			831	523	147	157	4		
1	C	109	Total	C	N	O	S	0	0
			831	523	147	157	4		
1	E	109	Total	C	N	O	S	0	0
			831	523	147	157	4		
1	G	109	Total	C	N	O	S	0	0
			831	523	147	157	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	4268	Total	C	N	O	S	1	0
			33431	21326	5777	6103	225		
2	D	4268	Total	C	N	O	S	1	0
			33431	21326	5777	6103	225		
2	F	4268	Total	C	N	O	S	1	0
			33431	21326	5777	6103	225		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	4268	Total 33431	C 21326	N 5777	O 6103	S 225	1	0

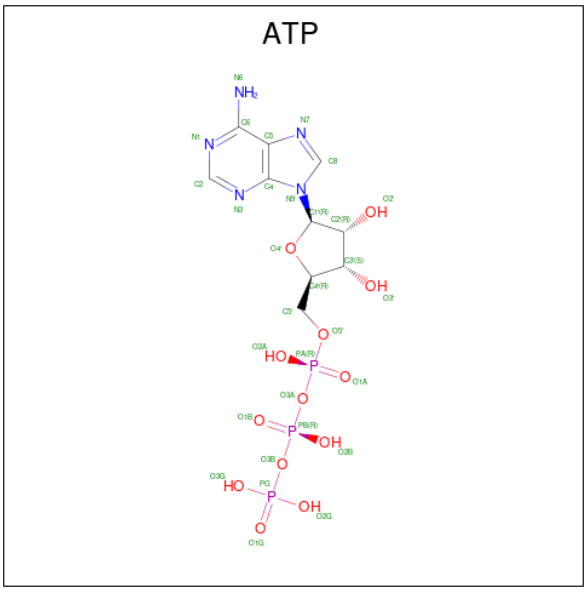
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

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

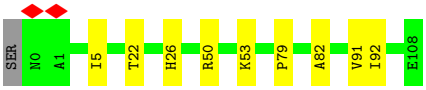
3 Residue-property plots (i)

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:

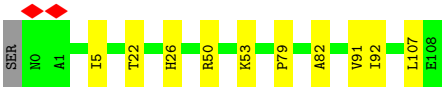




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C:

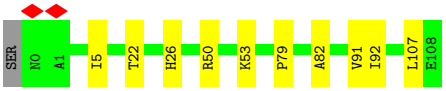




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

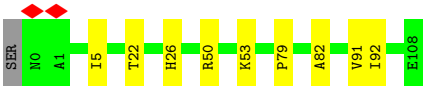




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

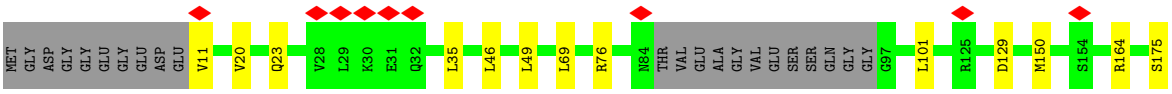


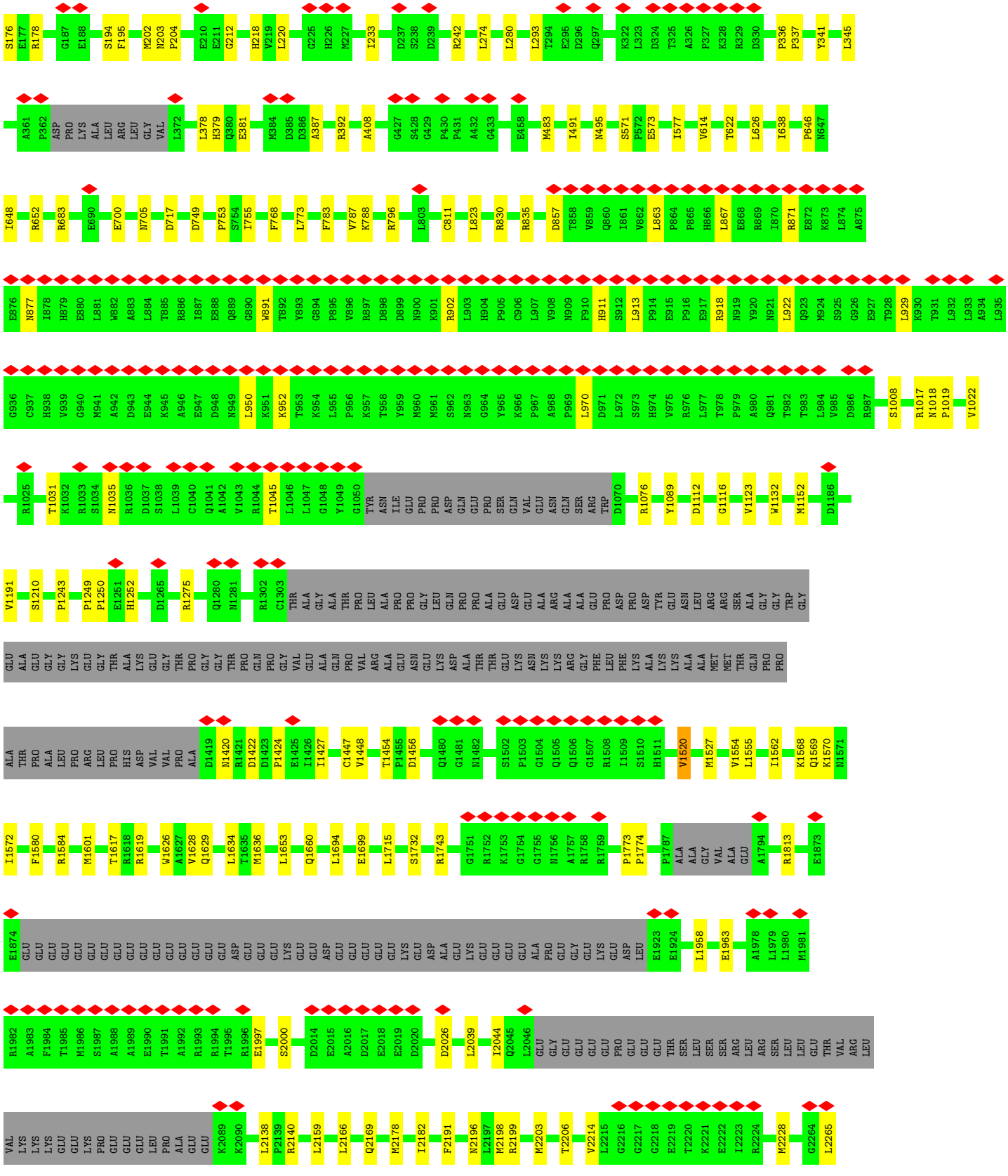


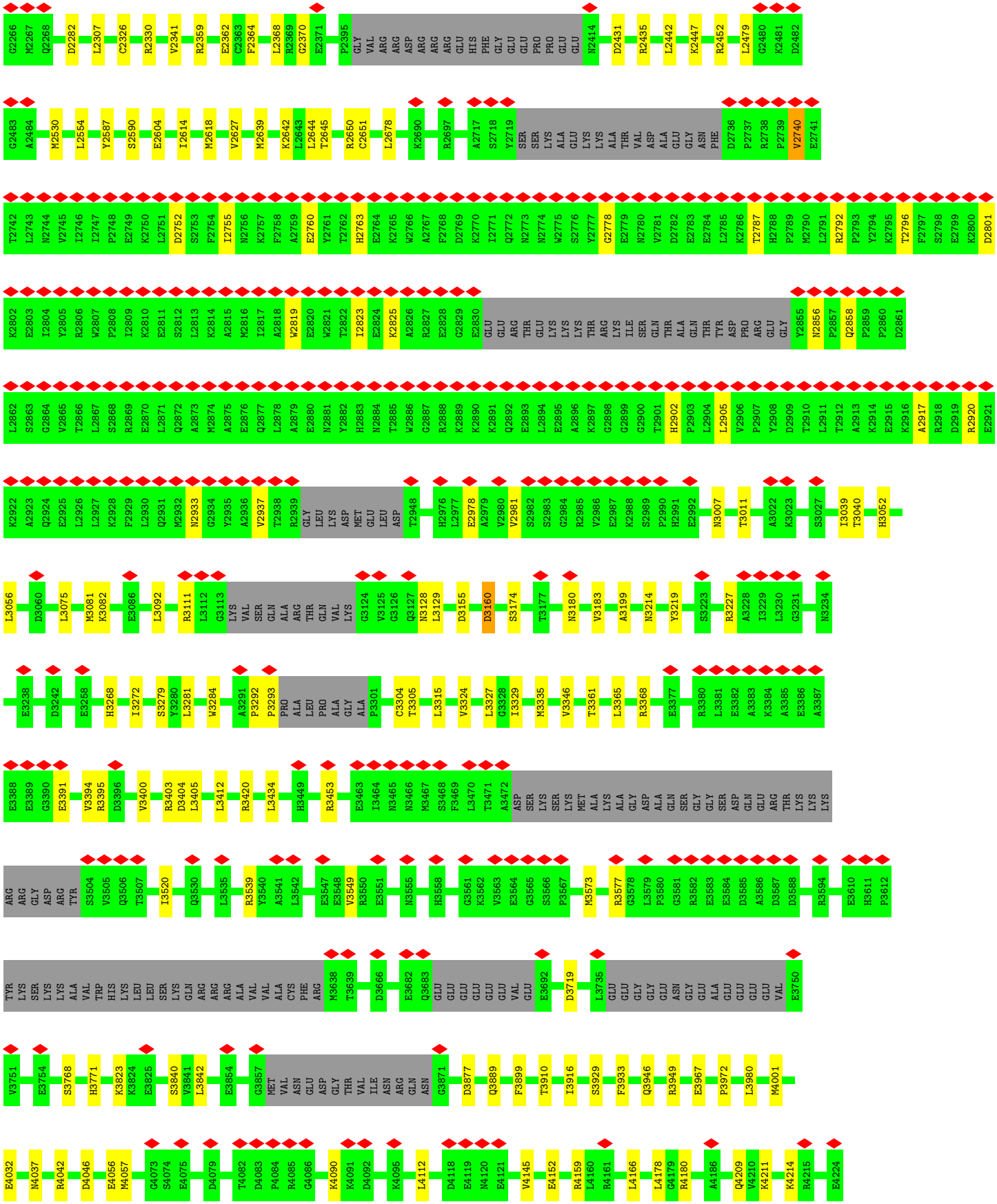
• Molecule 2: Ryanodine receptor 1

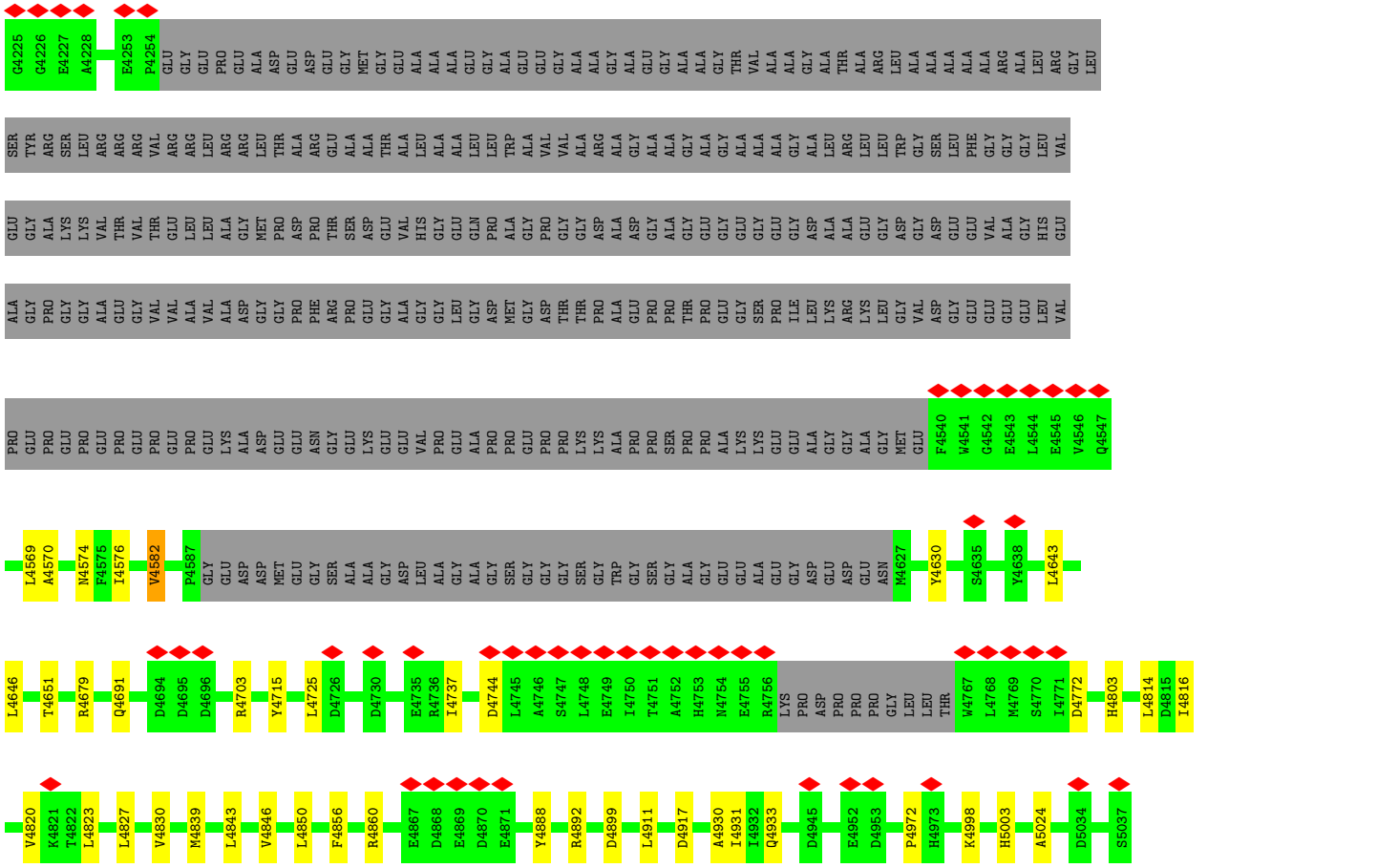
Chain B:






S176 E177 R178 G187 E188 S194 F195 M202 N203 P204 E210 E211 G212 H218 V219 L220 G225 H226 M227 I233 D237 S238 D239 R242 L274 L280 L293 T294 E295 D296 Q297 K322 L323 D324 T325 A326 P327 K328 R329 D330 P336 P337 Y341 L345
A361 P362 ASP PRO LYS ALA LEU ARG LEU GLY VAL L372 L378 H379 Q380 E381 M384 D385 D386 A387 R392 A408 G427 S428 G429 P430 P431 A432 G433 E458 M483 I491 N495 S571 P572 E573 I577 V614 T622 L626 I638 P646 N647
I648 R652 R683 E690 E700 N705 D717 D749 P753 S754 I755 F768 L773 F783 V787 K788 R796 L803 C811 L823 R830 R835 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 D982 T983 L984 V985 D986 R987 S1008 R1017 N1018 P1019 V1022
R1025 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 Y1089 D1112 G1116 V1123 W1132 M1152 D1186
V1191 S1210 P1243 P1249 P1250 E1251 H1252 D1265 R1275 Q1280 N1281 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 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 I1426 I1427 C1447 V1448 T1454 P1455 D1456 Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 V1554 L1555 I1562 K1568 Q1569 K1570 N1571
I1572 F1580 R1584 M1601 T1617 R1618 R1619 W1626 A1627 V1628 Q1629 L1634 T1635 M1636 L1653 Q1660 L1694 E1699 L1715 S1732 R1743 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 P1773 P1774 P1787 ALA ALA GLY VAL ALA GLU A1794 R1813 E1873
E1874 GLU GLU GLU

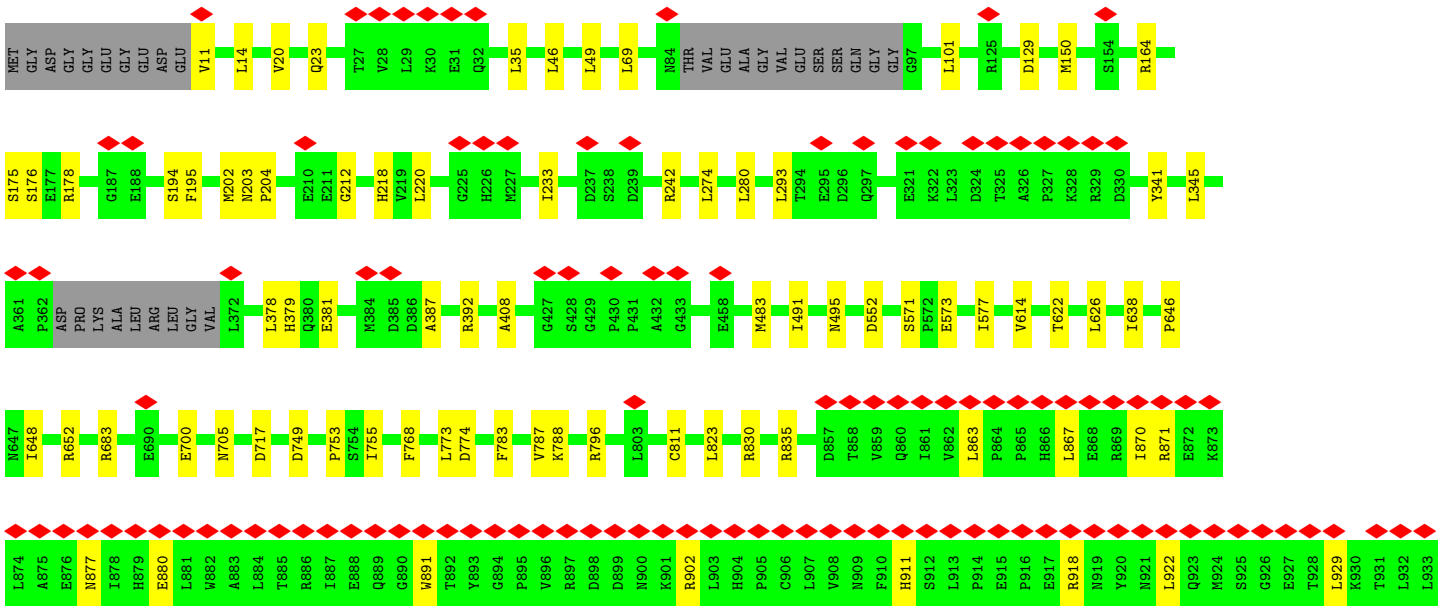

G2266 M2267 Q2268 D2282 L2307 C2326 R2330 V2341 R2359 E2362 C2363 F2364 L2368 R2369 G2370 E2371 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 D2431 R2435 L2442 K2447 R2452 L2479 G2480 K2481 D2482
G2483 A2484 M2530 L2554 Y2587 S2590 E2604 I2614 M2618 V2627 M2639 K2642 L2643 L2644 T2645 R2650 C2651 L2678 K2690 R2697 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 P2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP T2948 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 N3007 T3011 A3022 K3023 S3027 I3039 T3040 H3052
L3056 D3060 L3075 M3081 K3082 E3086 L3092 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 V3125 G3126 Q3127 N3128 L3129 D3155 D3160 S3174 T3177 N3180 V3183 A3199 N3214 Y3219 S3223 R3227 A3228 I3229 L3230 G3231 N3234
E3238 D3242 E3258 H3268 I3272 S3279 Y3280 L3281 W3284 A3291 P3292 P3293 PRO ALA LEU PRO ALA GLY ALA P3301 C3304 T3305 L3315 V3324 L3327 G3328 I3329 M3335 V3346 T3361 L3365 R3368 E3377 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387
E3388 E3389 G3390 E3391 V3394 R3395 D3396 V3400 R3403 D3404 L3405 L3412 R3420 L3434 H3449 R3453 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 GLY SER ASP GLN GLU ARG THR LYS LYS LYS
ARG ARG GLY ASP ARG TYR S3504 V3505 Q3506 T3507 I3520 Q3530 L3535 R3539 Y3540 A3541 L3542 E3547 E3548 V3549 R3550 E3551 N3555 H3558 G3561 K3562 V3563 E3564 G3565 S3566 P3567 M3573 R3577 G3578 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 R3594 E3610 H3611 P3612
TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG M3638 T3639 D3666 E3682 Q3683 GLU GLU GLU GLU GLU VAL GLU E3692 D3719 L3735 GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750
V3751 E3754 S3768 H3771 K3823 K3824 E3825 S3840 V3841 L3842 E3854 G3857 MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN G3871 D3877 Q3889 F3899 T3910 I3916 S3929 F3933 Q3946 R3949 E3967 P3972 L3980 M4001
E4032 N4037 R4042 D4046 E4056 M4057 G4073 S4074 E4075 D4079 T4082 D4083 P4084 R4085 G4086 K4090 K4091 D4092 K4095 L4112 D4118 E4119 M4120 E4121 V4145 E4152 R4159 L4160 R4161 L4166 L4178 G4179 R4180 A4186 Q4209 V4210 K4211 K4214 R4215 E4224

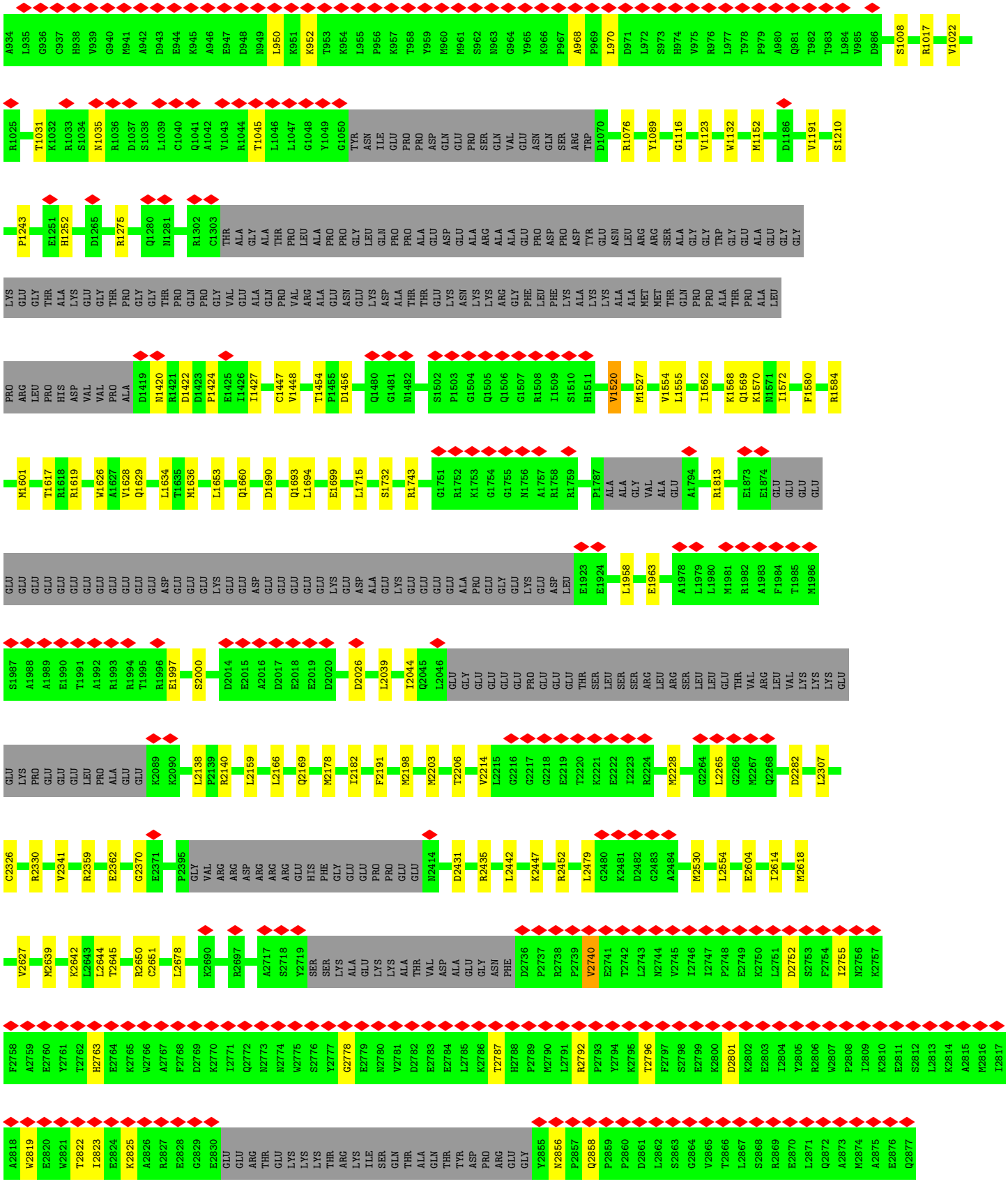


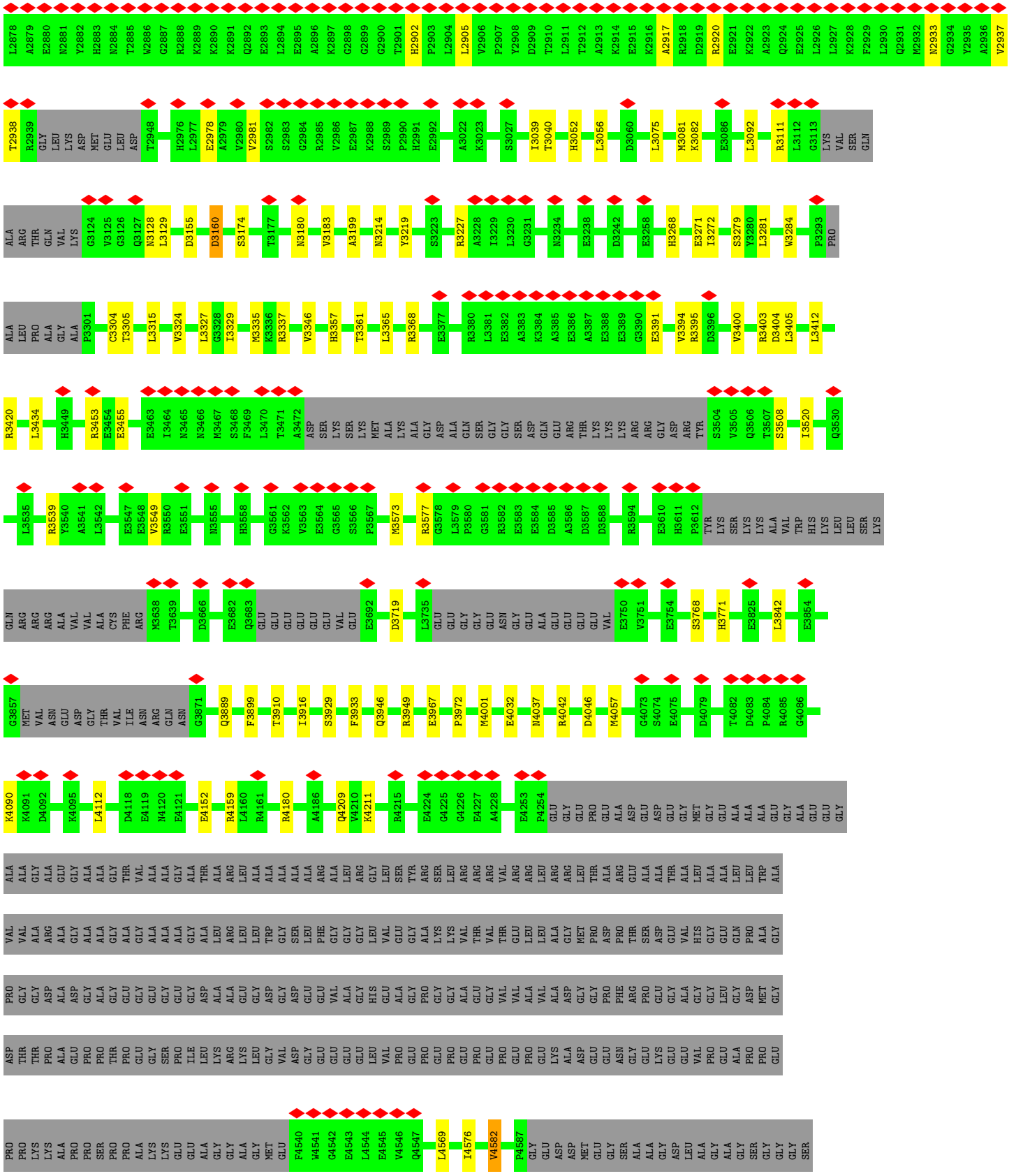
• Molecule 2: Ryanodine receptor 1

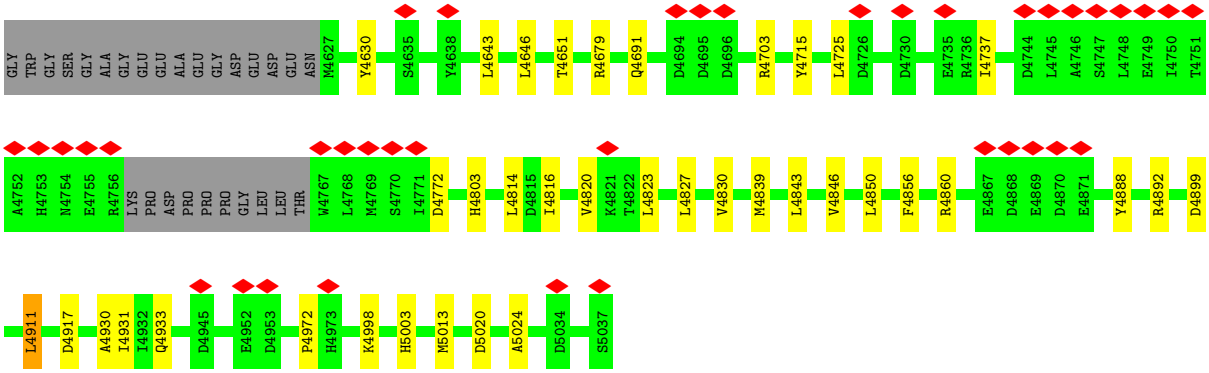
Chain D:






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 S1008 R1017 V1022
R1025 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 Y1089 G1116 V1123 W1132 M1152 D1186 V1191 S1210
P1243 E1251 H1252 D1265 R1275 Q1280 N1281 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 T1426 I1427 C1447 V1448 T1454 P1455 D1456 Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 V1554 L1555 I1562 K1568 Q1569 K1570 N1571 I1572 F1580 R1584
M1601 T1617 R1618 R1619 W1626 A1627 V1628 Q1629 L1634 T1635 M1636 L1653 Q1660 D1690 Q1693 L1694 E1699 L1715 S1732 R1743 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 P1787 ALA ALA GLY VAL ALA GLU A1794 R1813 E1873 E1874 GLU GLU GLU GLU
GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU E1923 E1924 L1958 E1963 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986
S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 S2000 D2014 E2015 A2016 D2017 E2018 E2019 D2020 D2026 L2039 I2044 Q2045 L2046 GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU 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 L2138 P2139 R2140 L2159 L2166 Q2169 M2178 I2182 F2191 M2198 M2203 T2206 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 M2228 G2264 L2265 G2266 M2267 Q2268 D2282 L2307
C2326 R2330 V2341 R2359 E2362 G2370 E2371 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 D2431 R2435 L2442 K2447 R2452 L2479 G2480 K2481 D2482 G2483 A2484 M2530 L2554 E2604 I2614 M2618
V2627 M2639 K2642 L2643 L2644 T2645 R2650 C2651 L2678 K2690 R2697 A2717 S2718 V2719 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 P2768 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

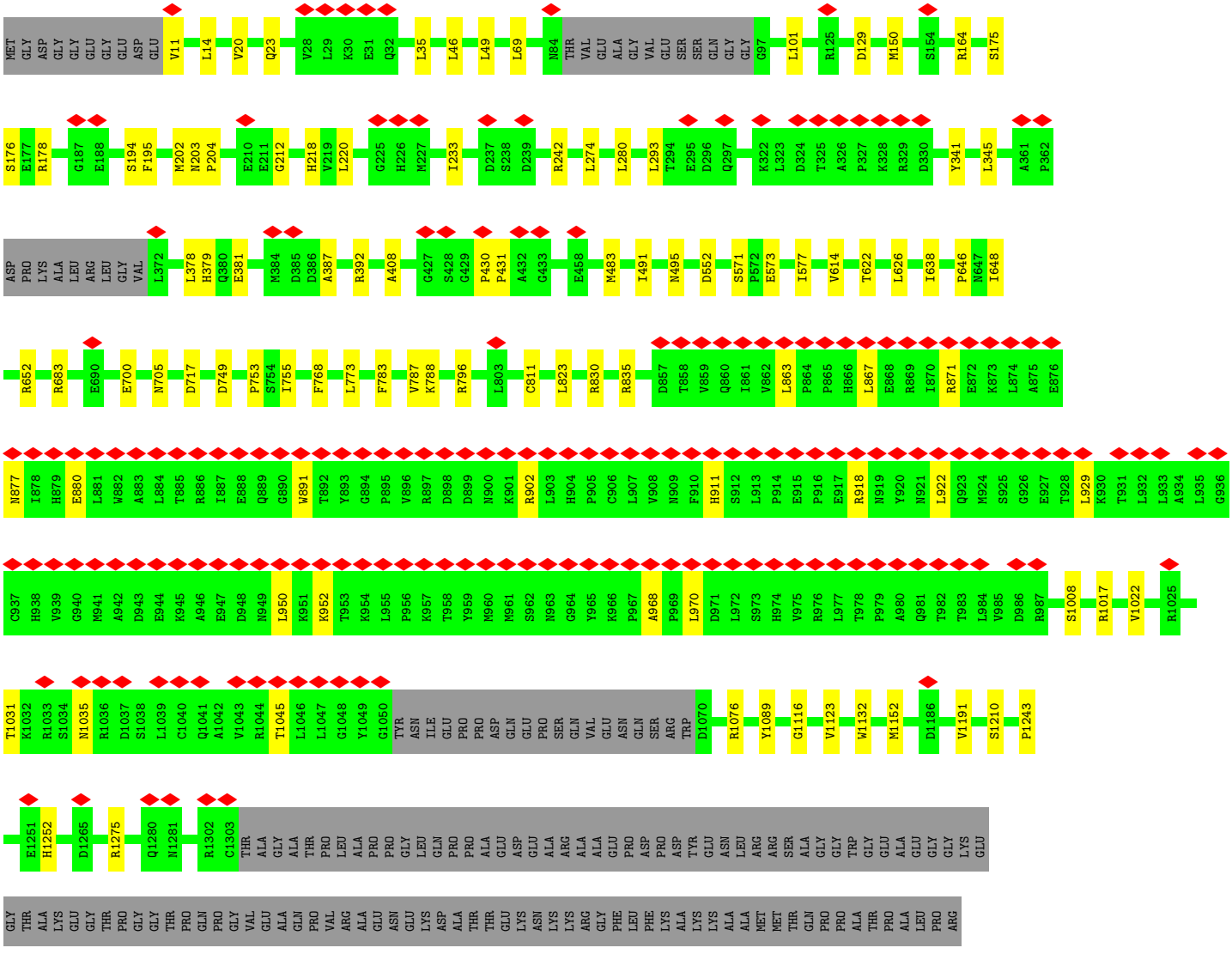

L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937
T2938 R2939 GLY LEU LYS ASP MET GLU LEU ASP T2948 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 A3022 K3023 S3027 I3039 T3040 H3052 L3056 D3060 L3075 M3081 K3082 E3086 L3092 R3111 L3112 G3113 LYS VAL SER GLN
ALA ARG THR GLN VAL LYS G3124 V3125 G3126 Q3127 N3128 L3129 D3155 D3160 S3174 T3177 N3180 V3183 A3199 N3214 Y3219 S3223 R3227 A3228 I3229 L3230 G3231 N3234 E3238 D3242 E3258 H3268 E3271 I3272 S3279 Y3280 L3281 W3284 P3293 PRO
ALA LEU PRO ALA GLY ALA P3301 C3304 T3305 L3315 V3324 L3327 G3328 I3329 M3335 K3336 R3337 V3346 H3357 T3361 L3365 R3368 E3377 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 V3394 R3395 D3396 V3400 R3403 D3404 L3405 L3412
R3420 L3434 H3449 R3453 E3454 E3455 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 TYR S3504 V3505 Q3506 T3507 S3508 I3520 Q3530
L3535 R3539 Y3540 A3541 L3542 E3547 E3548 V3549 R3550 E3551 N3555 H3558 G3561 K3562 V3563 E3564 G3565 S3566 P3567 M3573 R3577 G3578 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 R3594 E3610 H3611 P3612 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS
GLN ARG ARG ARG ALA VAL VAL ALA ALA CYS PHE ARG M3638 T3639 D3666 E3682 Q3683 GLU GLU GLU GLU GLU VAL GLU E3692 D3719 L3735 GLU GLU GLY GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 E3754 S3768 H3771 E3825 L3842 E3854
G3857 MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN G3871 Q3889 F3899 T3910 I3916 S3929 F3933 Q3946 R3949 E3967 P3972 M4001 E4032 N4037 R4042 D4046 M4057 G4073 S4074 E4075 D4079 T4082 D4083 P4084 R4085 G4086
K4090 K4091 D4092 K4095 L4112 D4118 E4119 N4120 E4121 E4152 R4159 L4160 R4161 R4180 A4186 Q4209 V4210 K4211 R4215 E4224 G4225 G4226 E4227 A4228 E4253 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU GLU ALA ALA GLU GLU GLY
ALA ALA GLY ALA GLU GLY GLY THR VAL ALA ALA GLY ALA ALA ALA ARG LEU ALA ALA ALA ARG SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU LEU THR ALA
VAL VAL ALA ARG ALA GLY ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA LEU LEU TRP GLY SER LEU PHE GLY GLY ALA GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU 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 GLU GLY GLU GLY GLY GLY ASP ALA ALA GLY GLU GLY GLU GLY ASP GLY SER GLU GLU VAL ALA ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA ASP GLY PRO GLY PHE ARG PRO GLU GLY ALA GLY LEU GLY LEU GLY ASP MET GLY
ASP THR THR PRO ALA GLU PRO PRO PRO THR PRO GLU GLY GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU ALA GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA 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 L4569 I4576 V4582 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER

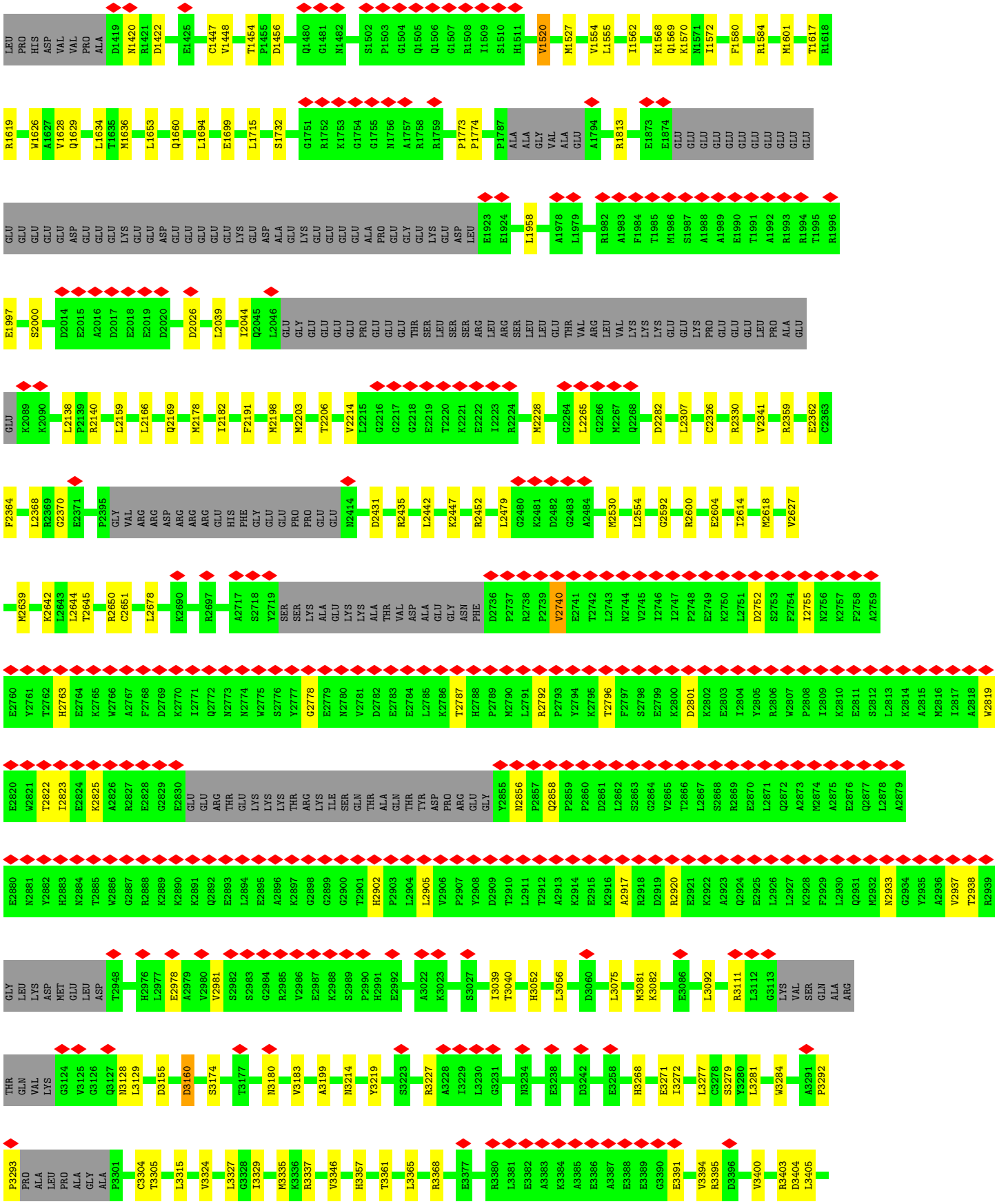


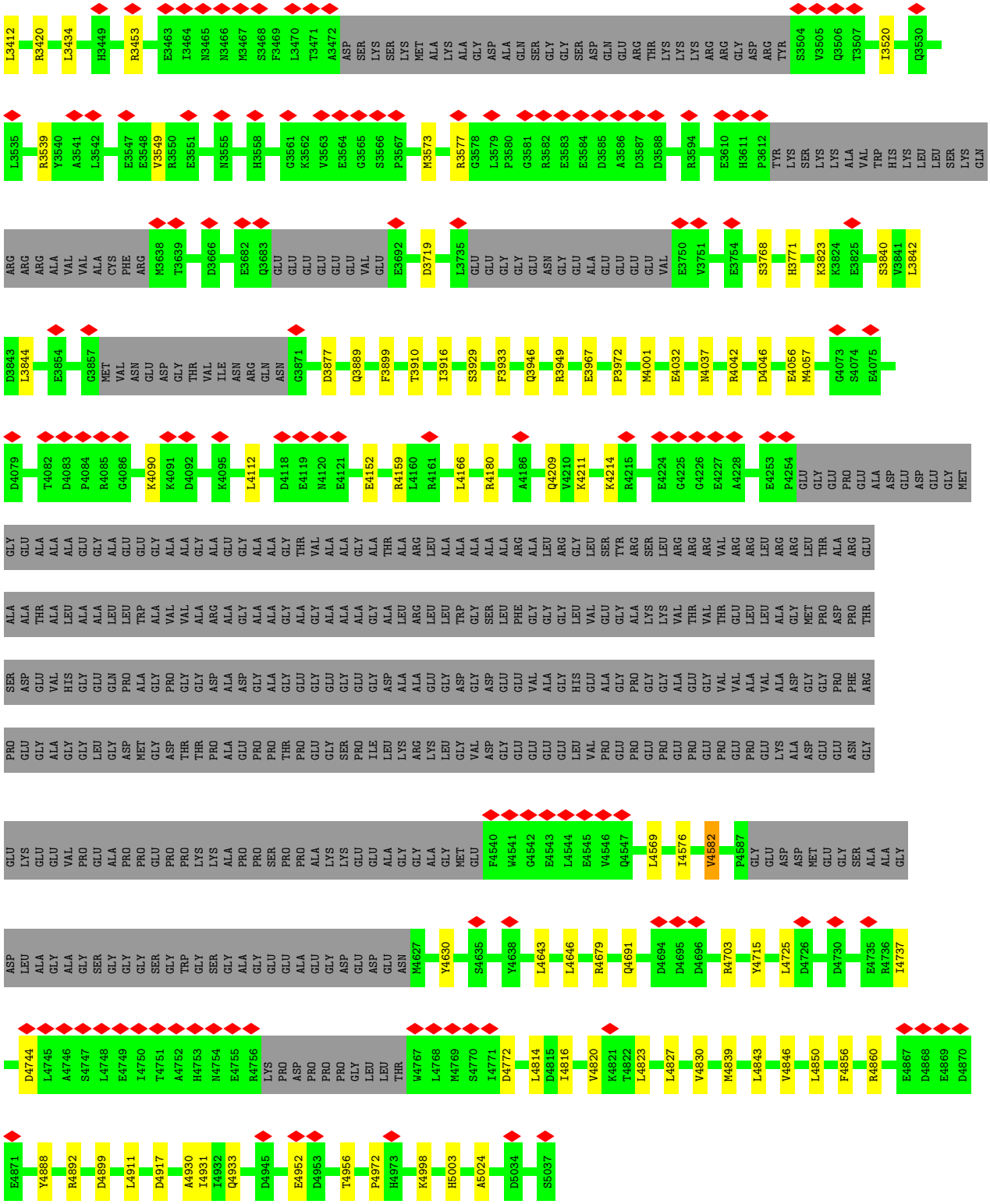
• Molecule 2: Ryanodine receptor 1

Chain F:





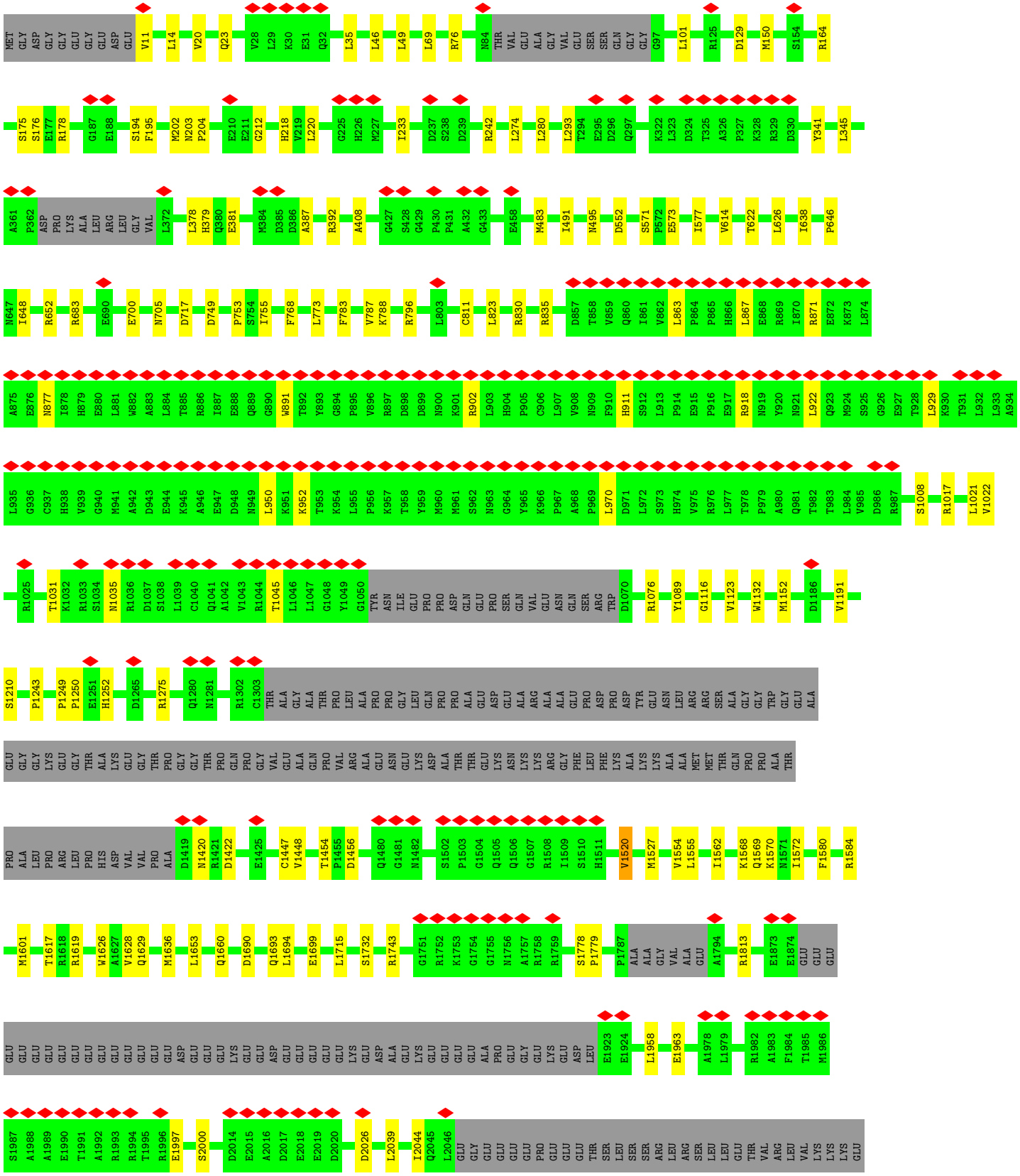

LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 E1425 C1447 V1448 T1454 P1455 D1456 Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 V1554 L1555 I1562 K1568 Q1569 K1570 N1571 I1572 F1580 R1584 M1601 T1617 R1618
R1619 W1626 A1627 V1628 Q1629 L1634 T1635 M1636 L1653 Q1660 L1694 E1699 L1715 S1732 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 P1773 P1774 P1787 ALA ALA GLY VAL ALA GLU A1794 R1813 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU E1923 E1924 L1958 A1978 L1979 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996
E1997 S2000 D2014 E2015 A2016 D2017 E2018 E2019 D2020 D2026 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 VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU
GLU K2089 K2090 L2138 P2139 R2140 L2159 L2166 Q2169 M2178 I2182 F2191 M2198 M2203 T2206 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 M2228 G2264 L2265 G2266 M2267 Q2268 D2282 L2307 C2326 R2330 V2341 R2359 E2362 C2363
F2364 L2368 R2369 G2370 E2371 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 D2431 R2435 L2442 K2447 R2452 L2479 G2480 K2481 D2482 G2483 A2484 M2530 L2554 G2592 R2600 E2604 I2614 M2618 V2627
M2639 K2642 L2643 L2644 T2645 R2650 C2651 L2678 K2690 R2697 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 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 A3022 K3023 S3027 I3039 T3040 H3052 L3056 D3060 L3075 M3081 K3082 E3086 L3092 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG
THR GLN VAL LYS G3124 V3125 G3126 Q3127 N3128 L3129 D3155 D3160 S3174 T3177 N3180 V3183 A3199 N3214 Y3219 S3223 R3227 A3228 I3229 L3230 G3231 N3234 E3238 D3242 E3258 H3268 E3271 I3272 L3277 C3278 S3279 Y3280 L3281 W3284 A3291 P3292
P3293 PRO ALA LEU PRO ALA GLY ALA P3301 C3304 T3305 L3315 V3324 L3327 G3328 I3329 M3335 K3336 R3337 V3346 H3357 T3361 L3365 R3368 E3377 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 V3394 R3395 D3396 V3400 R3403 D3404 L3405

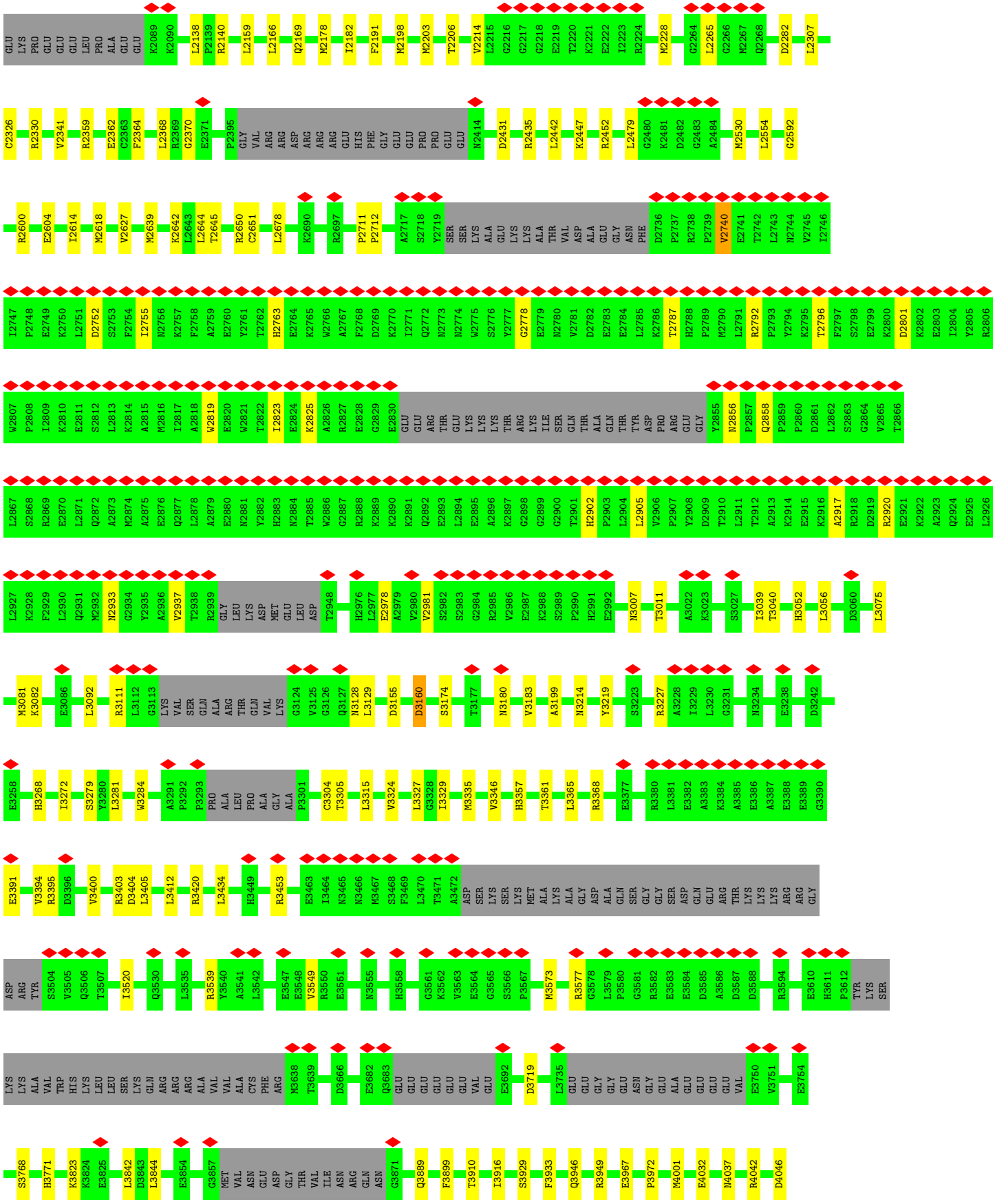


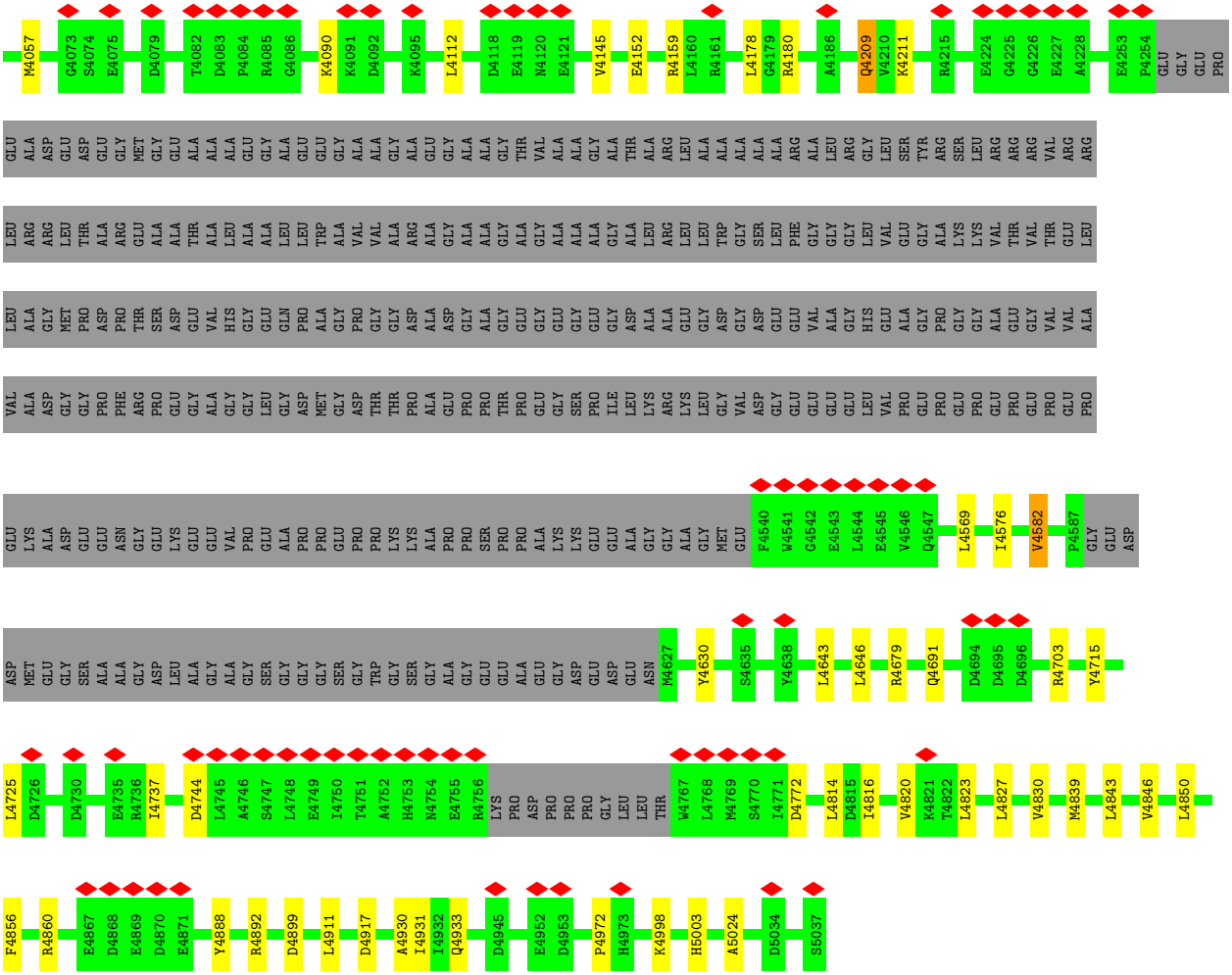
• Molecule 2: Ryanodine receptor 1

Chain H:




MET GLY ASP GLY GLY GLU GLY GLU ASP GLU V11 L14 V20 Q23 V28 L29 K30 E31 Q32 L35 L46 L49 L69 R76 N84 THR VAL GLU ALA GLY VAL GLU SER SER GLN GLY GLY G97 L101 R125 D129 M150 S154 R164
S175 S176 E177 R178 G187 E188 S194 F195 M202 N203 P204 E210 E211 G212 H218 V219 L220 G225 H226 M227 I233 D237 S238 D239 R242 L274 L280 L293 T294 E295 D296 Q297 K322 L323 D324 T325 A326 P327 K328 R329 D330 Y341 L345
A361 P362 ASP PRO LYS ALA LEU ARG LEU GLY VAL L372 L378 H379 Q380 E381 M384 D385 D386 A387 R392 A408 G427 S428 G429 P430 P431 A432 G433 E458 M483 I491 N495 D552 S571 P572 E573 I577 V614 T622 L626 I638 P646
N647 I648 R652 R683 E690 E700 N705 D717 D749 P753 S754 I755 F768 L773 F783 V787 K788 R796 L803 C811 L823 R830 R835 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 S1008 R1017 L1021 V1022
R1025 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 Y1089 G1116 V1123 W1132 M1152 D1186 V1191
S1210 P1243 P1249 P1250 E1251 H1252 D1265 R1275 Q1280 N1281 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 E1425 C1447 V1448 T1454 P1455 D1456 Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 V1554 L1555 I1562 K1568 Q1569 K1570 N1571 I1572 F1580 R1584
M1601 T1617 R1618 R1619 W1626 A1627 V1628 Q1629 M1636 L1653 Q1660 D1690 Q1693 L1694 E1699 L1715 S1732 R1743 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 S1778 P1779 P1787 ALA ALA GLY VAL ALA GLU A1794 R1813 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 GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP LEU E1923 E1924 L1958 E1963 A1978 L1979 R1982 A1983 F1984 T1985 M1986
S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 S2000 D2014 E2015 A2016 D2017 E2018 E2019 D2020 D2026 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 LEU PRO ALA GLU GLU K2089 K2090 L2138 P2139 R2140 L2159 L2166 Q2169 M2178 I2182 F2191 M2198 M2203 T2206 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 M2228 G2264 L2265 G2266 M2267 Q2268 D2282 L2307
C2326 R2330 V2341 R2359 E2362 C2363 F2364 L2368 R2369 G2370 E2371 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 D2431 R2435 L2442 K2447 R2452 L2479 G2480 K2481 D2482 G2483 A2484 M2530 L2554 G2592
R2600 E2604 I2614 M2618 V2627 M2639 K2642 L2643 L2644 T2645 R2650 C2651 L2678 K2690 R2697 P2711 P2712 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 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 P2990 H2991 E2992 N3007 T3011 A3022 K3023 S3027 I3039 T3040 H3052 L3056 D3060 L3075
M3081 K3082 E3086 L3092 R3111 L3112 G3113 LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 V3125 G3126 Q3127 N3128 L3129 D3155 D3160 S3174 T3177 N3180 V3183 A3199 N3214 Y3219 S3223 R3227 A3228 I3229 L3230 G3231 M3234 E3238 D3242
E3258 H3268 T3272 S3279 Y3280 L3281 W3284 A3291 P3292 P3293 PRO ALA LEU PRO ALA GLY ALA P3301 C3304 T3305 L3315 V3324 L3327 G3328 I3329 M3335 V3346 H3357 T3361 L3365 R3368 E3377 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390
E3391 V3394 R3395 D3396 V3400 R3403 D3404 L3405 L3412 R3420 L3434 H3449 R3453 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 TYR S3504 V3505 Q3506 T3507 I3520 Q3530 L3535 R3539 Y3540 A3541 L3542 E3547 E3548 V3549 R3550 E3551 N3555 H3558 G3561 K3562 V3563 E3564 G3565 S3566 P3567 M3573 R3577 G3578 L3579 P3580 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 R3594 E3610 H3611 P3612 TYR LYS SER
LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG M3638 T3639 D3666 E3682 Q3683 GLU GLU GLU GLU GLU VAL GLU E3692 D3719 L3735 GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 E3754
S3768 H3771 K3823 K3824 E3825 L3842 D3843 L3844 E3854 G3857 MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN G3871 Q3889 F3899 T3910 I3916 S3929 F3933 Q3946 R3949 E3967 P3972 M4001 E4032 N4037 R4042 D4046


M4057 G4073 S4074 E4075 D4079 T4082 D4083 P4084 R4085 G4086 K4090 K4091 D4092 K4095 L4112 D4118 E4119 N4120 E4121 V4145 E4152 R4159 L4160 R4161 L4178 G4179 R4180 A4186 Q4209 V4210 K4211 R4215 E4224 G4225 G4226 E4227 A4228 E4253 P4254 GLU GLY GLU PRO
GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ALA ARG LEU ALA ALA ALA ALA ALA ALA ARG ALA ARG LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG
LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA ALA GLY GLU GLY 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 GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP PRO GLY ASP ALA ASP GLU GLY GLU GLY GLU GLY SER GLU ASP ALA ALA GLU GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY GLY ALA GLU GLY GLY VAL ALA ALA
VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY GLY SER PRO ILE LEU 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 PRO GLU PRO
GLU LYS ALA ASP GLU GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO 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 L4569 I4576 V4582 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 Y4630 S4635 Y4638 L4643 L4646 R4679 Q4691 D4694 D4695 D4696 R4703 Y4715
L4725 D4726 D4730 E4735 R4736 I4737 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 LYS PRO ASP PRO PRO PRO GLY LEU LEU THR W4767 L4768 M4769 S4770 I4771 D4772 L4814 D4815 I4816 V4820 K4821 T4822 L4823 L4827 V4830 M4839 L4843 V4846 L4850
F4856 R4860 E4867 D4868 E4869 D4870 E4871 Y4888 R4892 D4899 L4911 D4917 A4930 I4931 I4932 Q4933 D4945 E4952 D4953 P4972 H4973 K4998 H5003 A5024 D5034 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	40197	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	0.583	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	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: CA, ZN, 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	0.15	0/847	0.34	0/1141
1	C	0.15	0/847	0.34	0/1141
1	E	0.15	0/847	0.34	0/1141
1	G	0.15	0/847	0.34	0/1141
2	B	0.15	0/34193	0.31	0/46369
2	D	0.15	0/34193	0.31	0/46369
2	F	0.15	0/34193	0.31	0/46369
2	H	0.15	0/34193	0.31	0/46369
All	All	0.15	0/140160	0.31	0/190040

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	831	0	835	4	0
1	C	831	0	835	5	0
1	E	831	0	835	5	0
1	G	831	0	835	4	0
2	B	33431	0	32724	220	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	33431	0	32724	209	0
2	F	33431	0	32724	213	0
2	H	33431	0	32724	211	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	2	0
5	D	31	0	12	1	0
5	F	31	0	12	2	0
5	H	31	0	12	1	0
All	All	137180	0	134284	775	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 775 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:F:4823:LEU:HG	2:H:4839:MET:CE	2.08	0.83
2:B:4823:LEU:HG	2:D:4839:MET:CE	2.08	0.83
2:B:4839:MET:CE	2:H:4823:LEU:HG	2.08	0.83
2:D:4823:LEU:HG	2:F:4839:MET:CE	2.08	0.83
2:B:4823:LEU:HG	2:D:4839:MET:HE3	1.72	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	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
1	C	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
1	E	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
1	G	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
2	B	4225/5037 (84%)	4159 (98%)	66 (2%)	0	100	100
2	D	4225/5037 (84%)	4159 (98%)	66 (2%)	0	100	100
2	F	4225/5037 (84%)	4159 (98%)	66 (2%)	0	100	100
2	H	4225/5037 (84%)	4159 (98%)	66 (2%)	0	100	100
All	All	17328/20588 (84%)	17056 (98%)	272 (2%)	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	89/90 (99%)	87 (98%)	2 (2%)	45	68
1	C	89/90 (99%)	87 (98%)	2 (2%)	45	68
1	E	89/90 (99%)	87 (98%)	2 (2%)	45	68
1	G	89/90 (99%)	87 (98%)	2 (2%)	45	68
2	B	3553/4276 (83%)	3532 (99%)	21 (1%)	78	81
2	D	3553/4276 (83%)	3532 (99%)	21 (1%)	78	81
2	F	3553/4276 (83%)	3532 (99%)	21 (1%)	78	81
2	H	3553/4276 (83%)	3532 (99%)	21 (1%)	78	81
All	All	14568/17464 (83%)	14476 (99%)	92 (1%)	76	81

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	2326	CYS
2	H	46	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	2740	VAL
2	F	3933	PHE
2	H	577	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 249 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	4078	GLN
2	H	3052	HIS
2	F	1938	GLN
2	H	2991	HIS
2	H	3927	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	0.26	0	48,52,52	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ATP	H	5303	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	F	5303	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	D	5303	-	32,33,33	0.26	0	48,52,52	0.29	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	-	-	7/22/38/38	0/3/3/3
5	ATP	H	5303	-	-	7/22/38/38	0/3/3/3
5	ATP	F	5303	-	-	7/22/38/38	0/3/3/3
5	ATP	D	5303	-	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

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

There are no ring outliers.

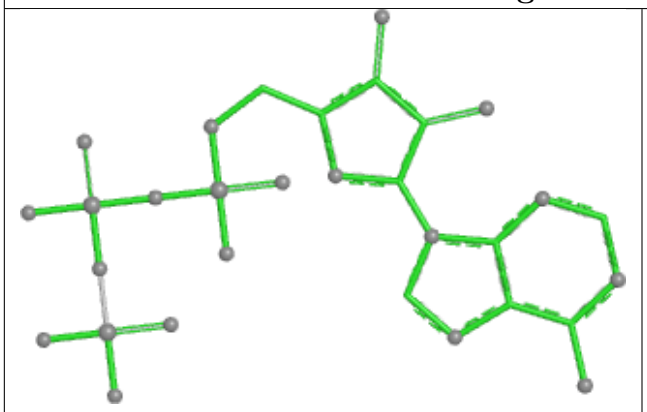
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5303	ATP	2	0
5	H	5303	ATP	1	0
5	F	5303	ATP	2	0
5	D	5303	ATP	1	0

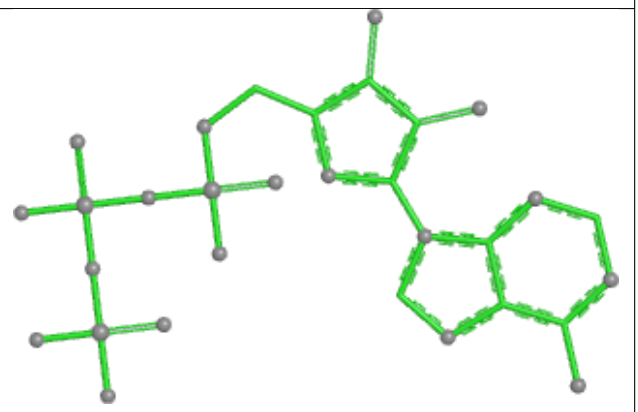
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

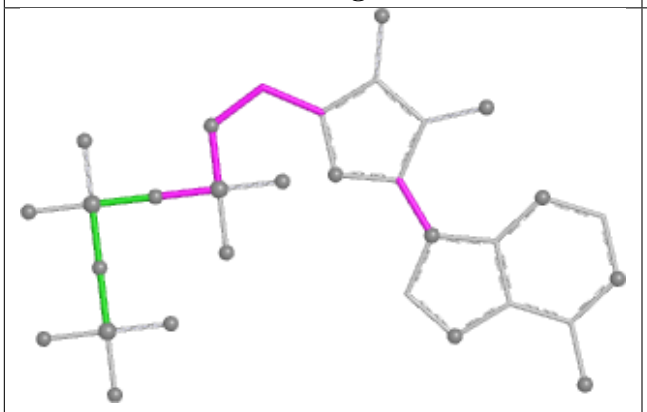
Ligand ATP B 5303



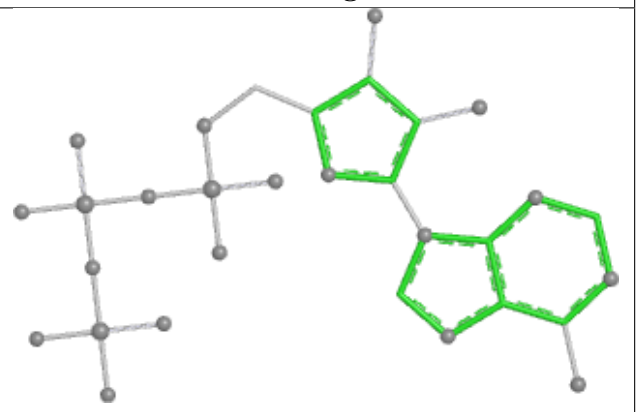
Bond lengths



Bond angles

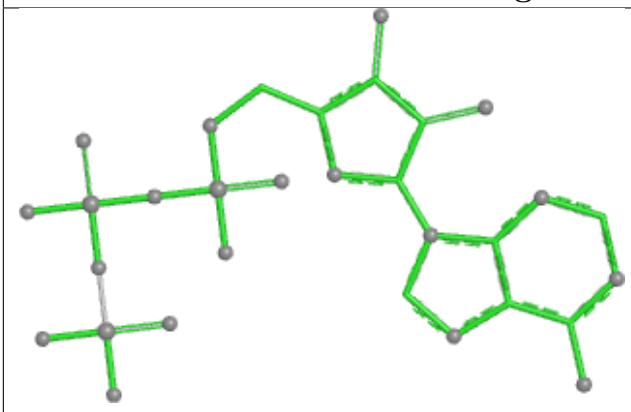


Torsions

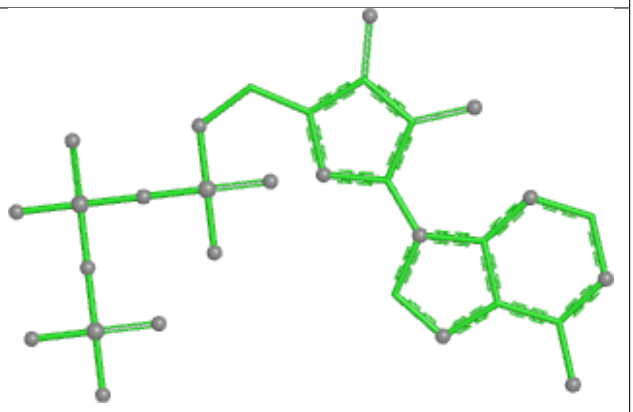


Rings

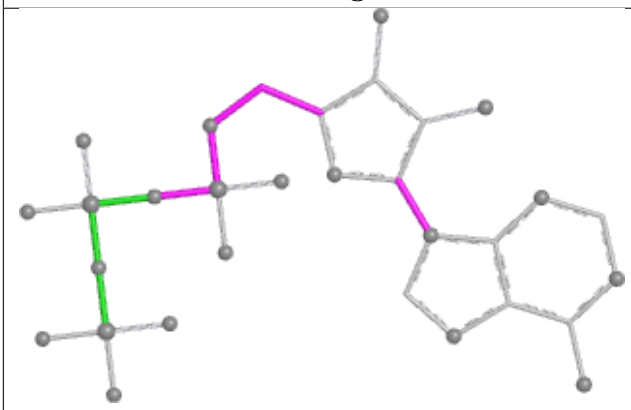
Ligand ATP H 5303



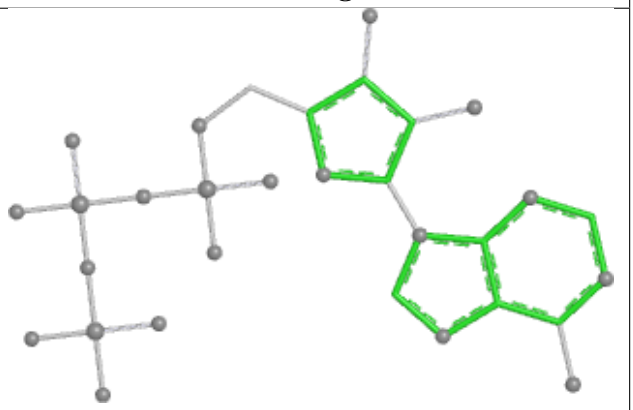
Bond lengths



Bond angles

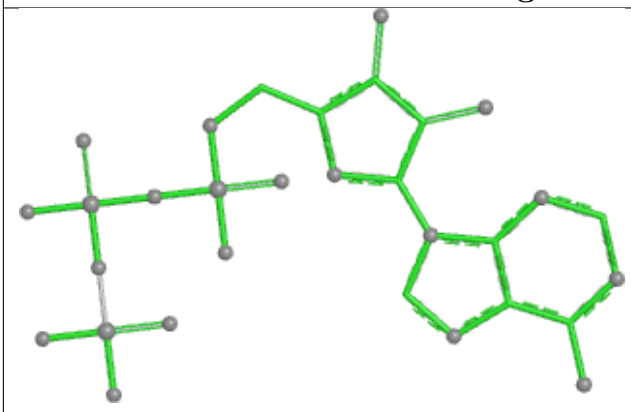


Torsions

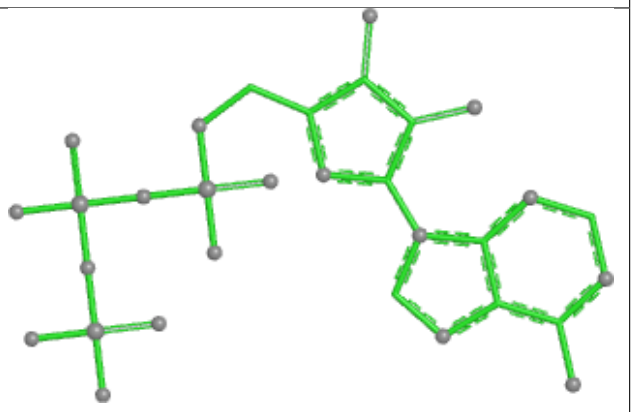


Rings

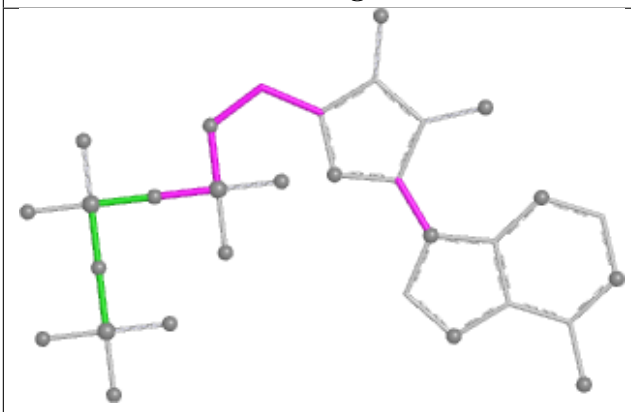
Ligand ATP F 5303



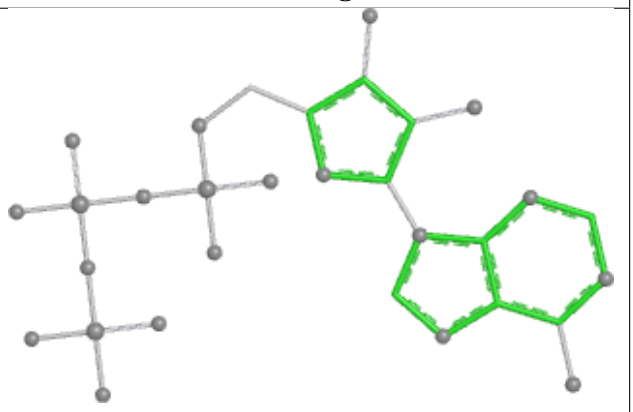
Bond lengths



Bond angles

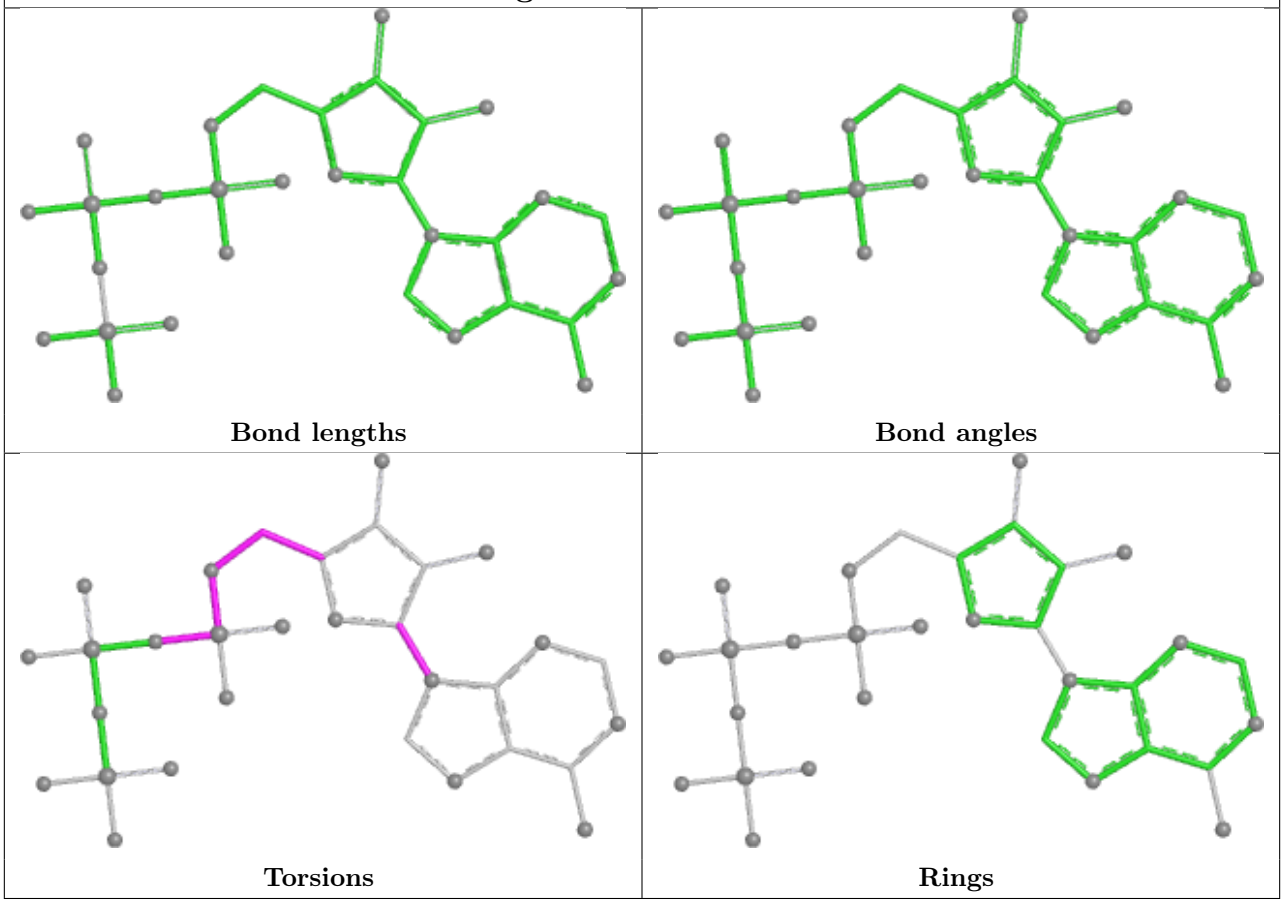


Torsions



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.

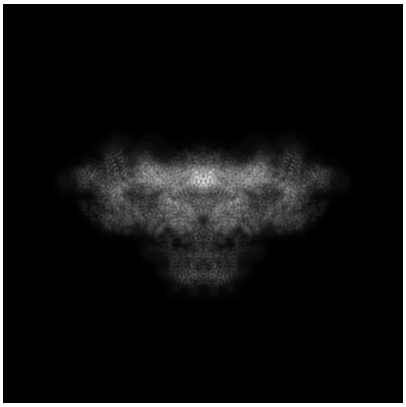
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73956. These allow visual inspection of the internal detail of the map and identification of artifacts.

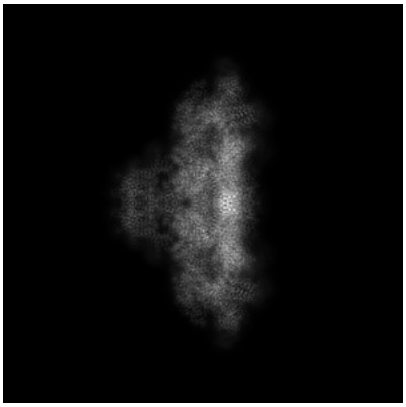
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

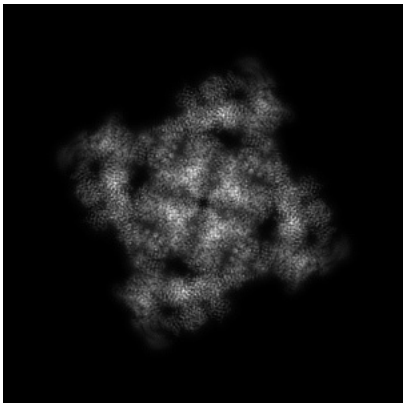
6.1.1 Primary map



X



Y



Z

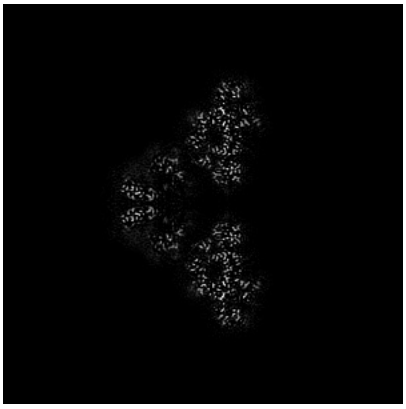
The images above show the map projected in three orthogonal directions.

6.2 Central slices

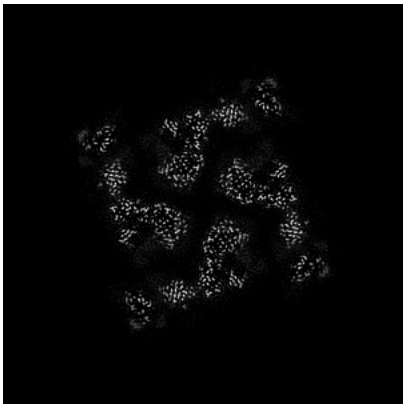
6.2.1 Primary map



X Index: 256



Y Index: 256

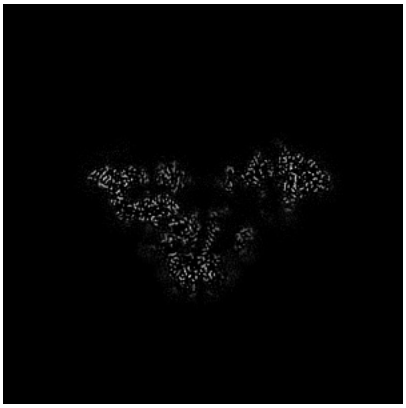


Z Index: 256

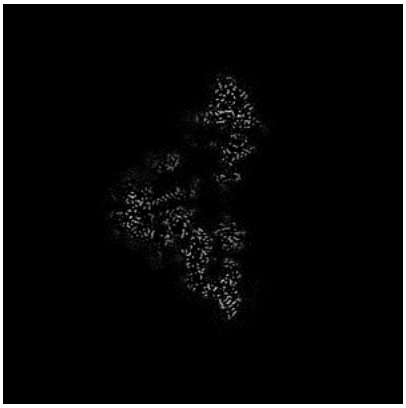
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

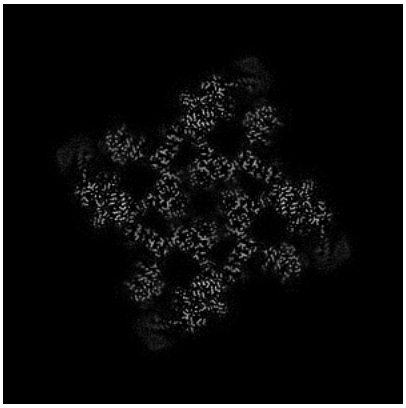
6.3.1 Primary map



X Index: 266



Y Index: 246

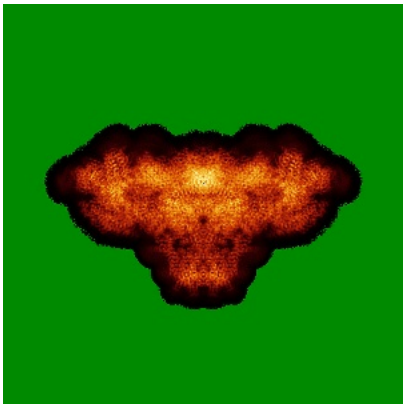


Z Index: 282

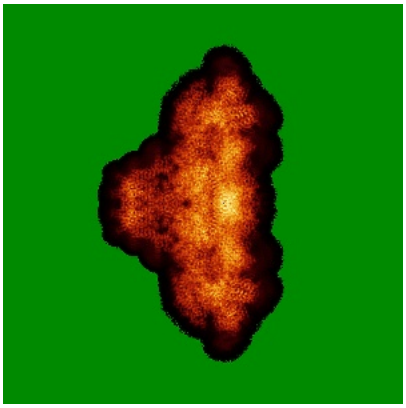
The images above show the largest variance slices of the map in three orthogonal directions.

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

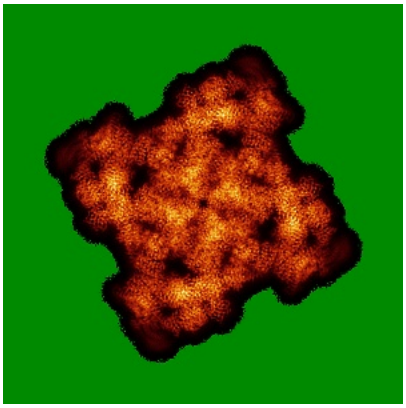
6.4.1 Primary map



X



Y

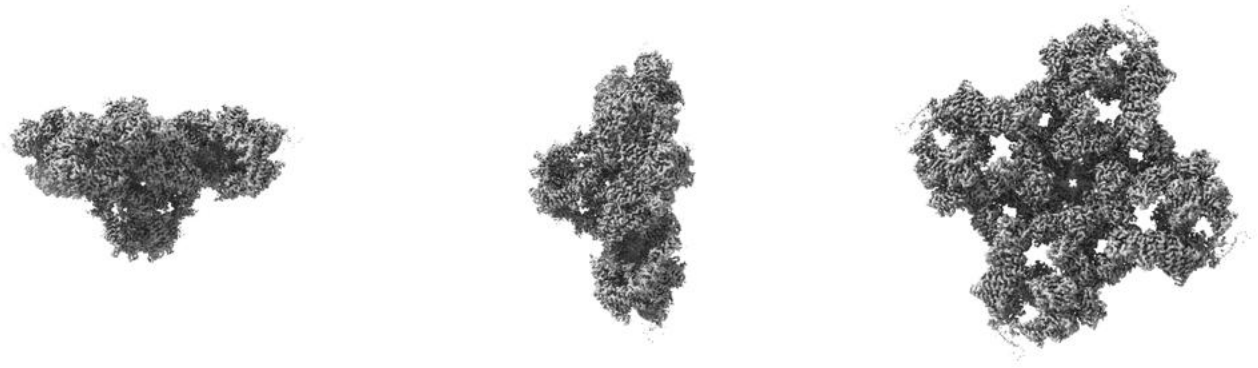


Z

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.

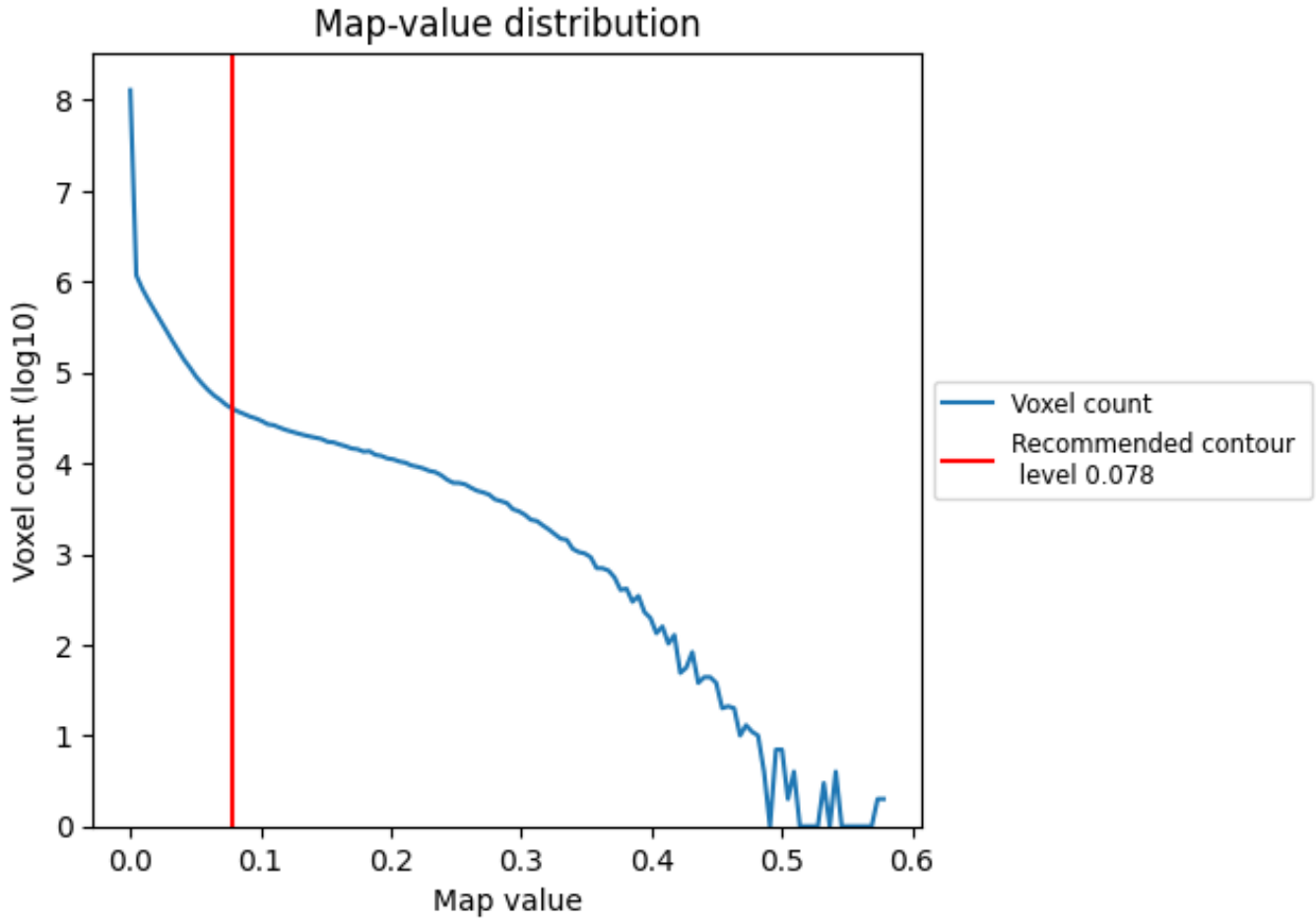
6.6 Mask visualisation (i)

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

7 Map analysis

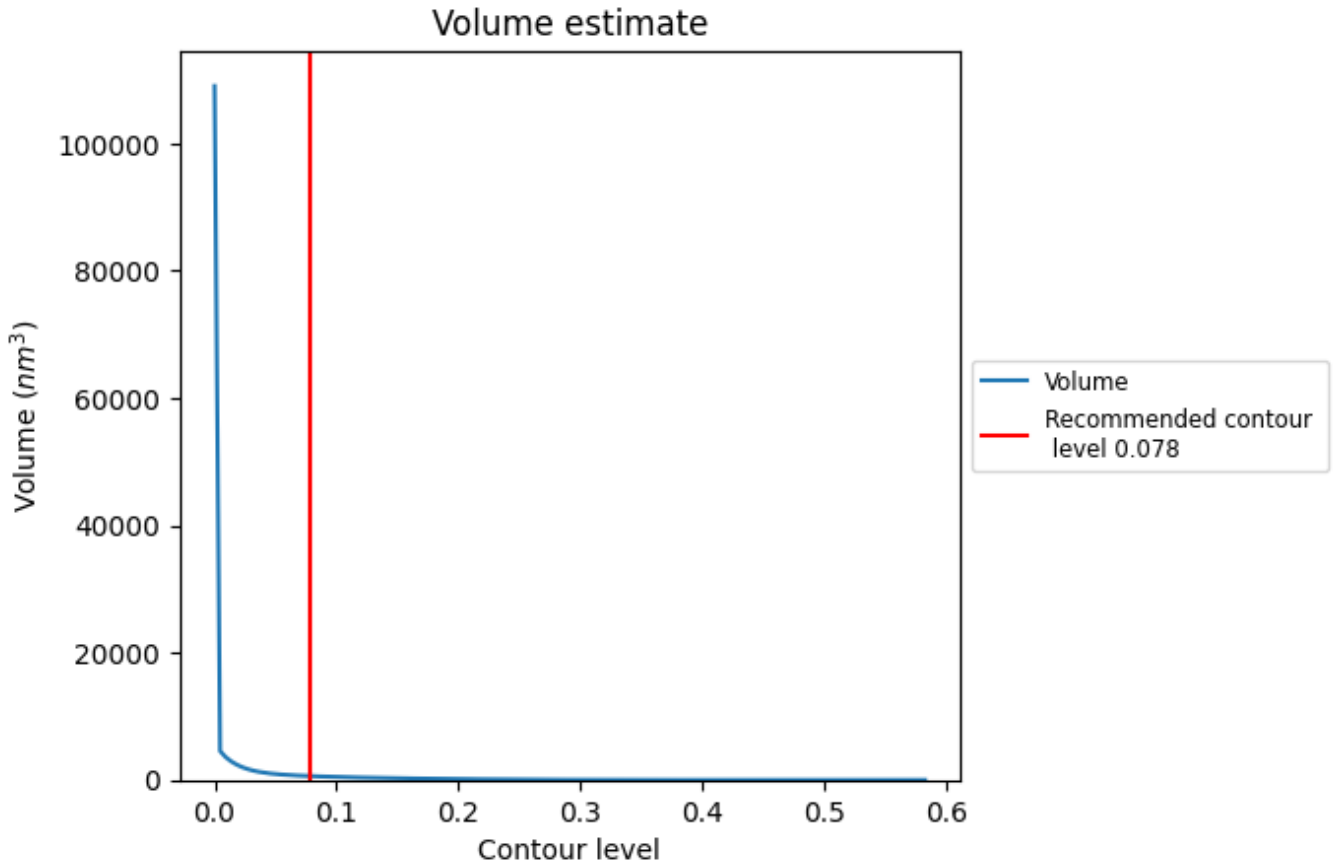
This section contains the results of statistical analysis of the map.

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.

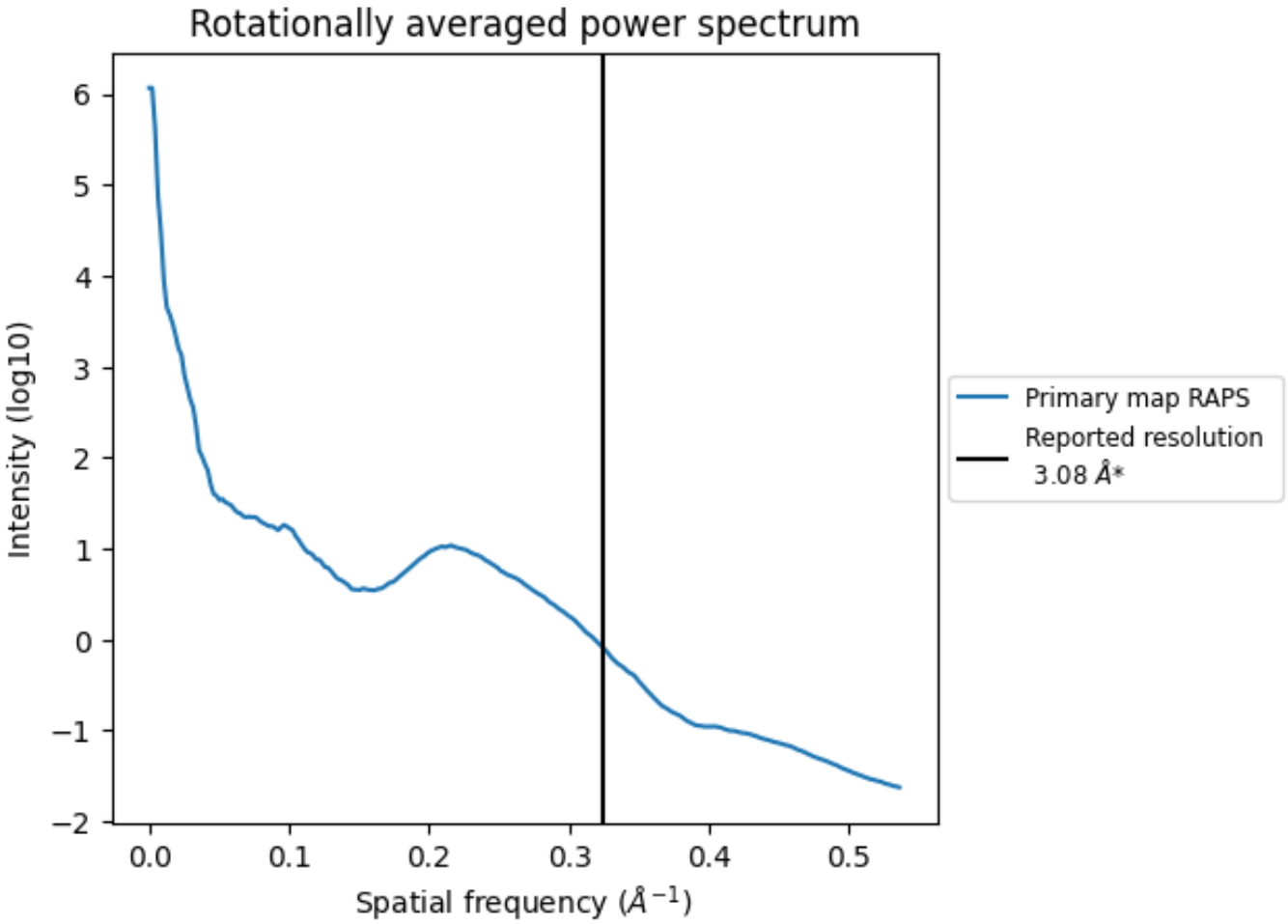
7.2 Volume estimate (i)



The volume at the recommended contour level is 613 nm^3; this corresponds to an approximate mass of 554 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 0.325 Å^{-1}

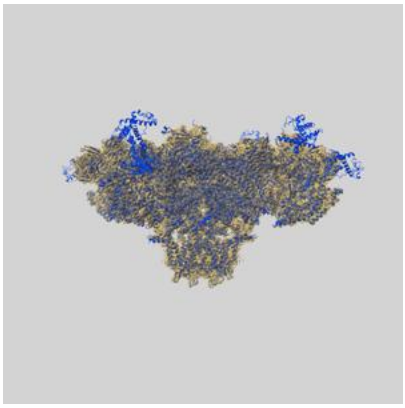
8 Fourier-Shell correlation

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

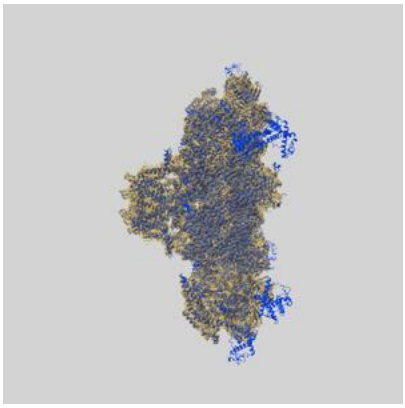
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73956 and PDB model 9Z9R. Per-residue inclusion information can be found in section 3 on page 7.

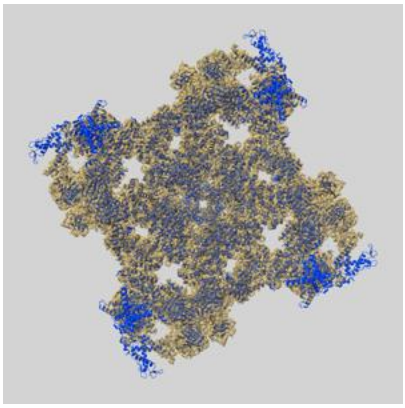
9.1 Map-model overlay



X



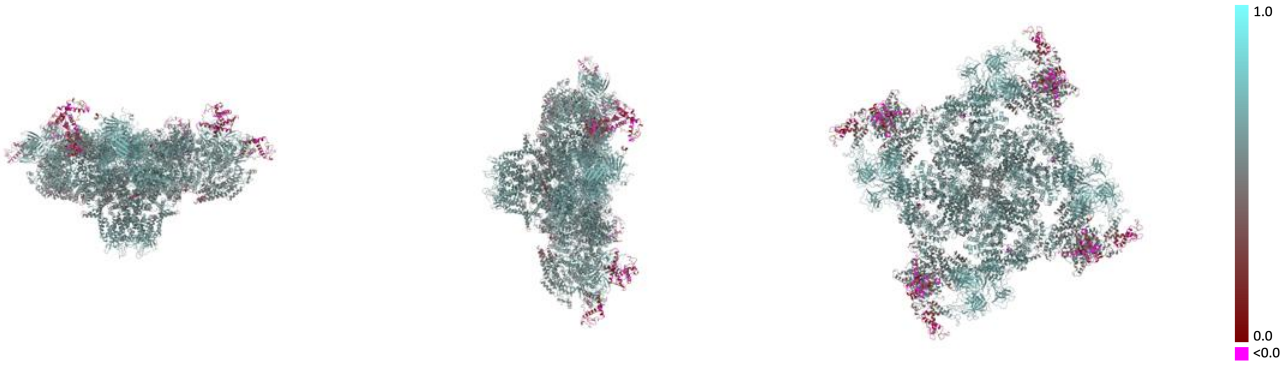
Y



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.

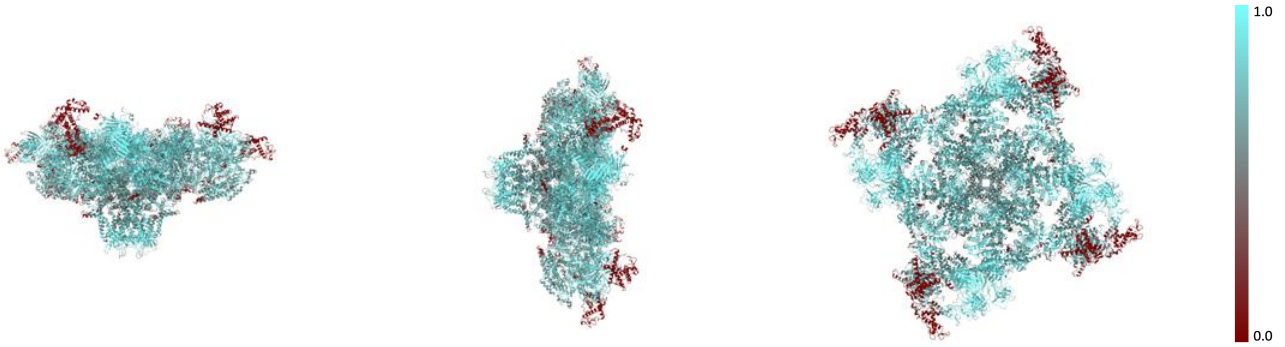
9.2 Q-score mapped to coordinate model (i)



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.

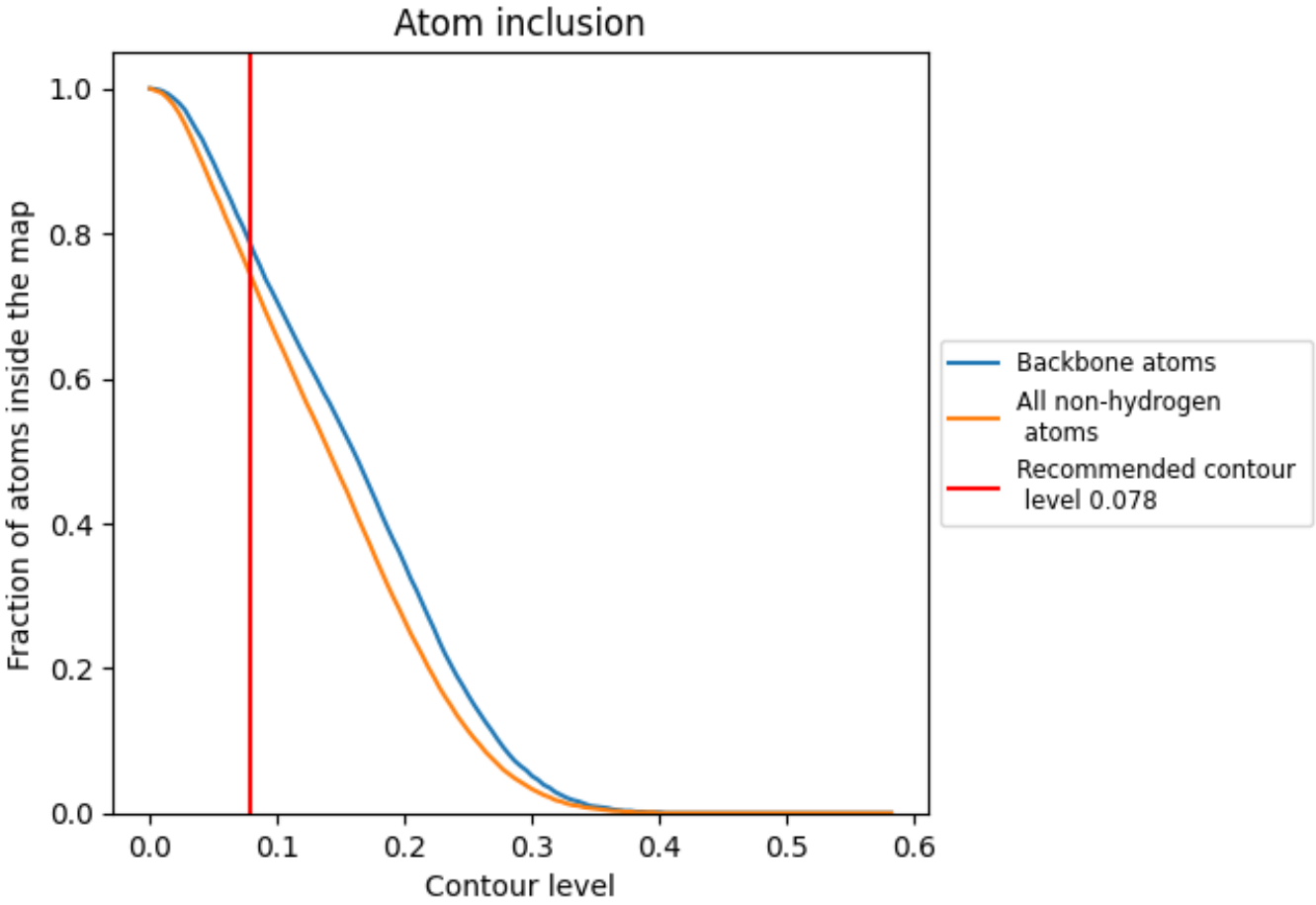
9.3 Atom inclusion mapped to coordinate model (i)



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, 79% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.078) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7460	0.5630
A	0.8660	0.6240
B	0.7430	0.5620
C	0.8690	0.6240
D	0.7440	0.5620
E	0.8660	0.6230
F	0.7430	0.5610
G	0.8660	0.6250
H	0.7430	0.5610

