wwPDB EM Validation Summary Report

Nov 11, 2026 – 03:09 PM EST

PDB ID	:	9Z9O / pdb_00009z9o
EMDB ID	:	EMD-73953
Title	:	Open-state T4825I mouse/rabbit RyR1 with activating ligands (Ca2+/ATP) and dantrolene
Authors	:	Chen, Y.S.; Van Petegem, F.
Deposited on	:	2025-11-18
Resolution	:	2.80 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 (1)) were used in the production of this report:

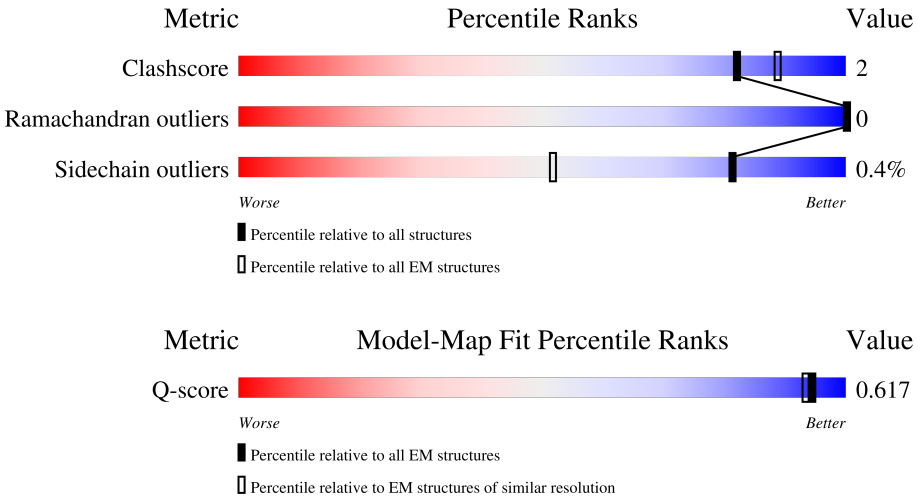
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 2.80 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.



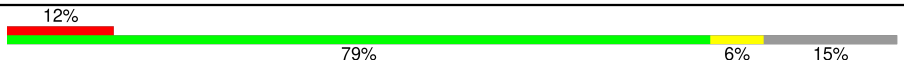
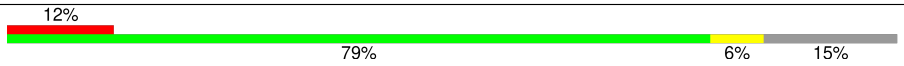
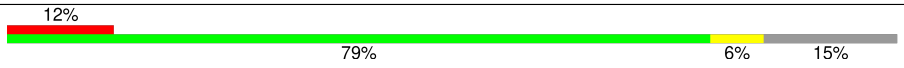
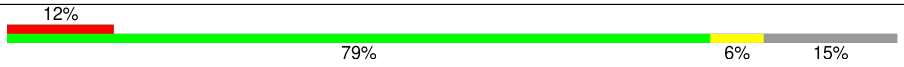
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	87% 9% • •
1	C	110	87% 9% • •
1	E	110	89% 7% • •
1	G	110	89% 7% • •

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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 137024 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	107	Total	C	N	O	S	0	0
			814	513	143	154	4		
1	C	107	Total	C	N	O	S	0	0
			814	513	143	154	4		
1	E	107	Total	C	N	O	S	0	0
			814	513	143	154	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	4268	Total	C	N	O	S	4	0
			33355	21308	5757	6068	222		
2	D	4268	Total	C	N	O	S	4	0
			33355	21308	5757	6068	222		
2	F	4268	Total	C	N	O	S	4	0
			33355	21308	5757	6068	222		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	4268	Total	C	N	O	S	4	0
			33355	21308	5757	6068	222		

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

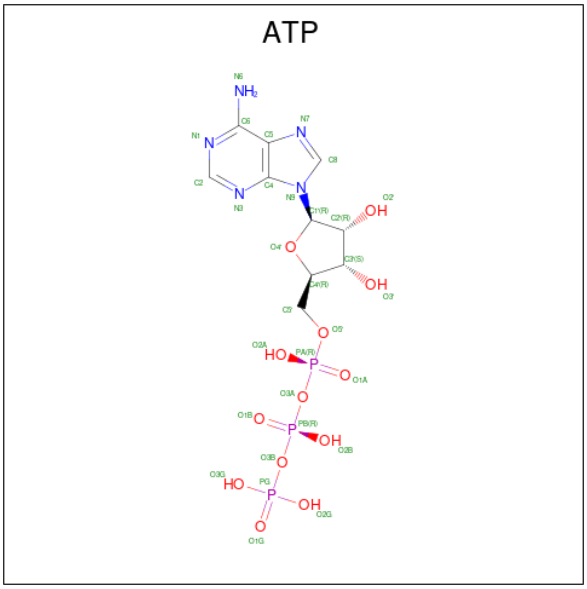
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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: $C_{10}H_{16}N_5O_{13}P_3$).



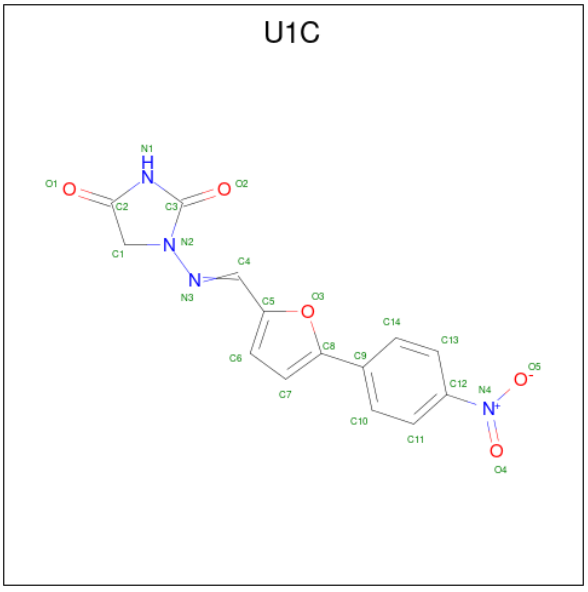
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total C N O P 31 10 5 13 3	0
5	B	1	Total C N O P 31 10 5 13 3	0

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

- Molecule 6 is Dantrolene (CCD ID: U1C) (formula: $C_{14}H_{10}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



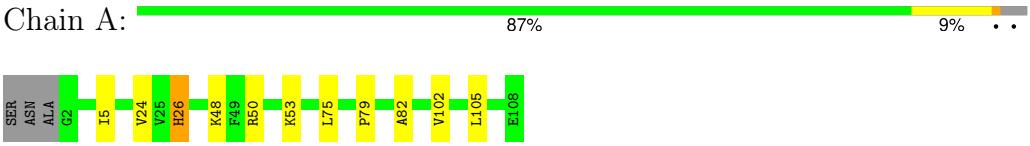
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			23	14	4	5	
6	D	1	Total	C	N	O	0
			23	14	4	5	
6	F	1	Total	C	N	O	0
			23	14	4	5	
6	H	1	Total	C	N	O	0
			23	14	4	5	

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.

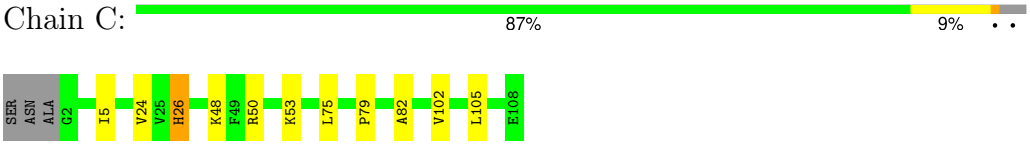
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



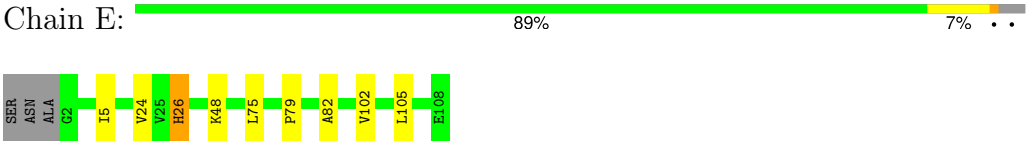
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain C:



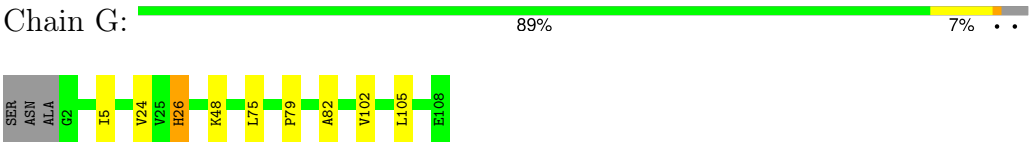
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



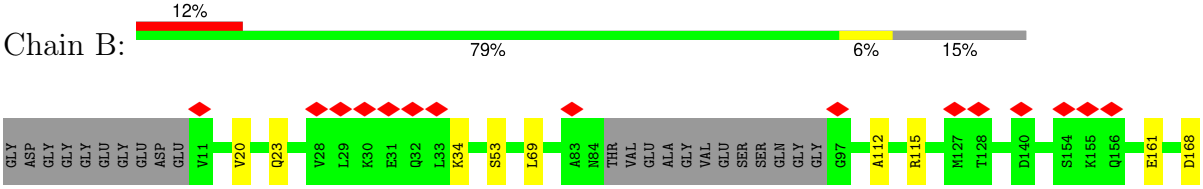
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

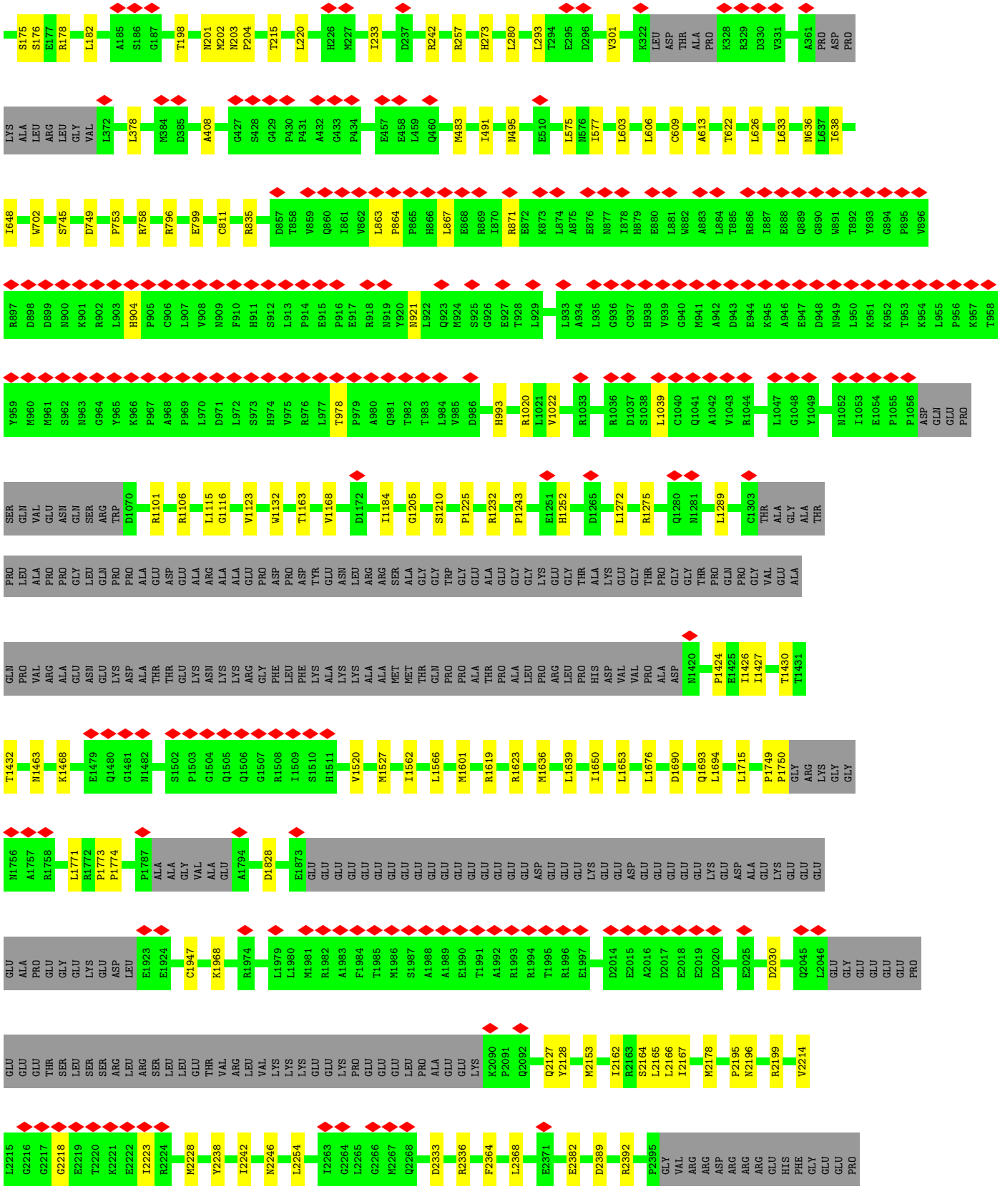
Chain G:

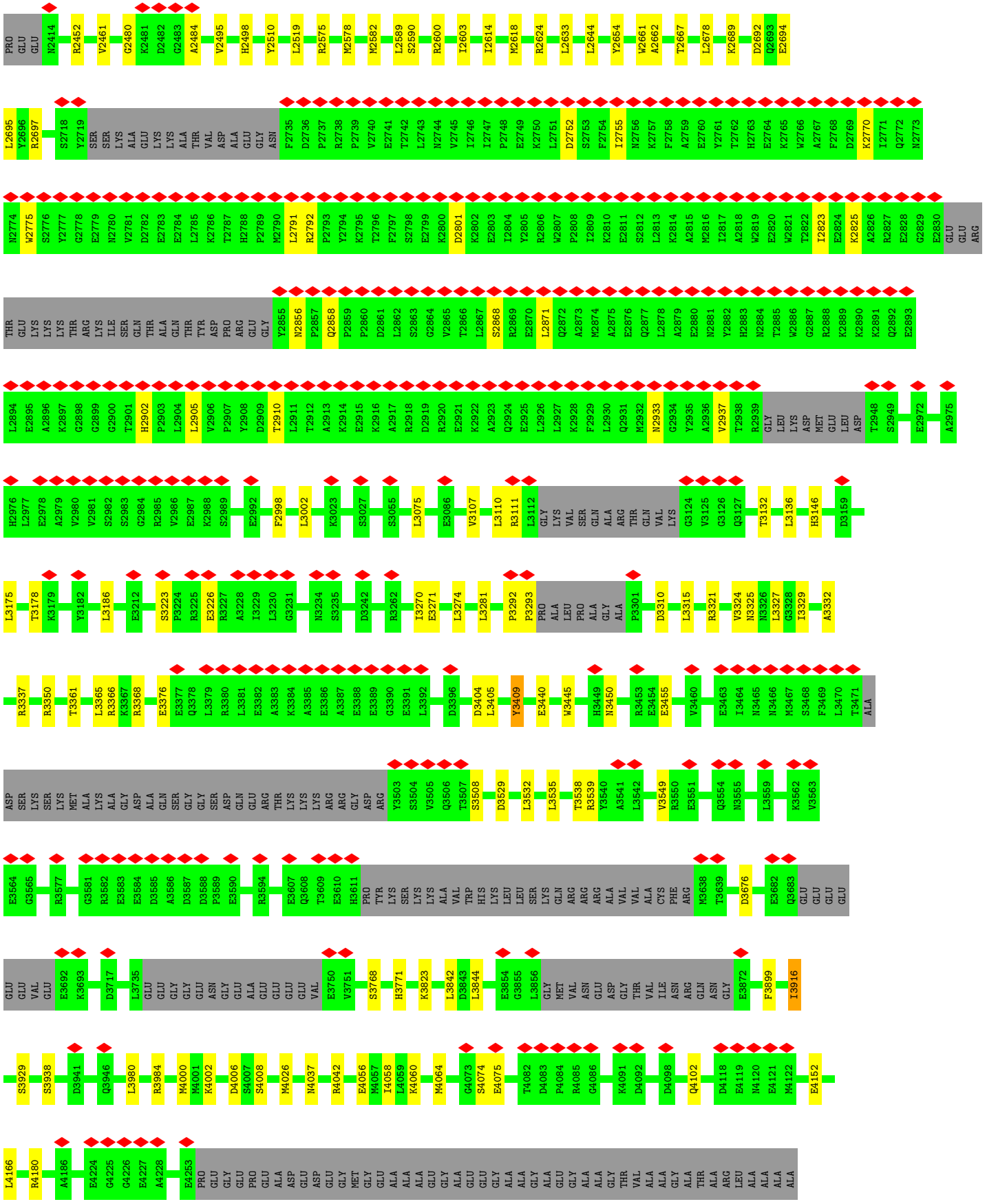


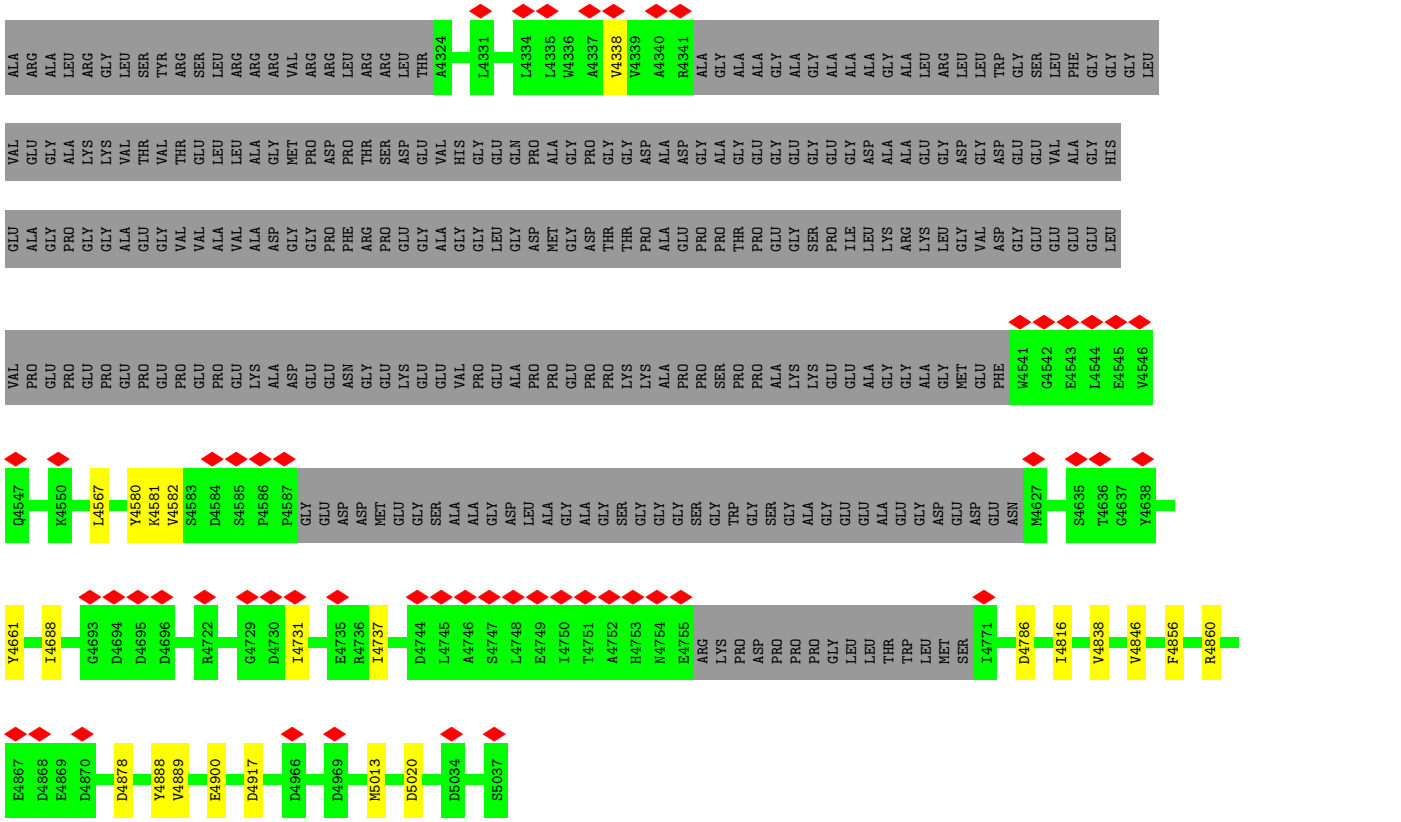
• Molecule 2: Ryanodine receptor 1

Chain B:




S175 S176 E177 R178 L182 A185 S186 G187 T198 N201 M202 N203 P204 T215 L220 H226 M227 I233 D237 R242 R257 H273 L280 L293 T294 E295 D296 V301 K322 LEU ASP THR ALA PRO K328 R329 D330 V331 A361 PRO ASP PRO
LYS ALA LEU ARG LEU GLY VAL L372 L378 M384 D385 A408 G427 S428 G429 P430 P431 A432 G433 P434 E457 E458 L459 Q460 M483 I491 N495 E510 L575 N576 T577 L603 L606 C609 A613 T622 L626 L633 N636 L637 I638
I648 W702 S745 D749 P753 R758 R796 E799 C811 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 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 V908 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 H993 R1020 L1021 V1022 R1033 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 L1047 G1048 Y1049 N1052 I1053 E1054 P1055 P1056 ASP GLN GLU PRO
SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1101 R1106 L1115 G1116 V1123 W1132 T1163 V1168 D1172 I1184 G1205 S1210 P1225 R1232 P1243 E1251 H1252 D1265 L1272 R1275 Q1280 N1281 L1289 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 GLY 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 P1424 E1425 I1426 I1427 T1430 T1431
T1432 N1463 K1468 E1479 Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 I1562 L1566 M1601 R1619 R1623 M1636 L1639 I1650 L1653 L1676 D1690 Q1693 L1694 L1715 P1749 P1750 GLY ARG LYS GLY GLY
N1756 A1757 R1758 L1771 R1772 P1773 P1774 P1787 ALA ALA GLY VAL ALA GLU A1794 D1828 E1873 GLU GLU GLU

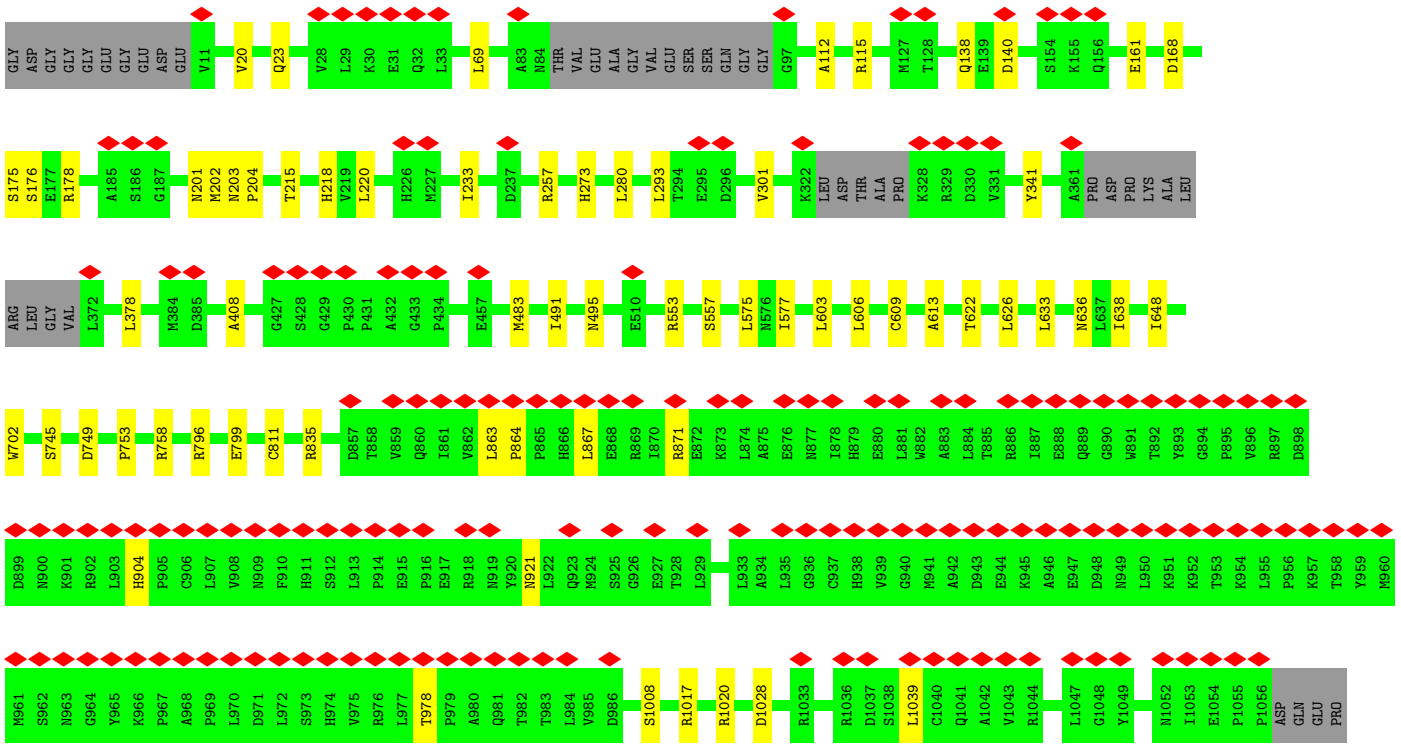

PRO GLU GLU N2414 R2452 V2461 G2480 K2481 D2482 G2483 A2484 V2495 H2498 Y2510 L2519 R2575 M2578 M2582 L2589 S2590 R2600 I2603 I2614 M2618 R2624 L2633 L2644 Y2654 W2661 A2662 T2667 L2678 K2689 D2692 Q2693 E2694
L2695 Y2696 R2697 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN F2735 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 E2972 A2975
H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 E2992 F2998 L3002 K3023 S3027 S3055 L3075 E3086 V3107 L3110 R3111 L3112 GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 V3125 G3126 Q3127 T3132 L3136 H3146 D3159
L3175 T3178 K3179 Y3182 L3186 E3212 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 N3234 S3235 D3242 R3262 I3270 E3271 L3274 L3281 P3292 P3293 PRO ALA LEU PRO ALA GLY ALA P3301 D3310 L3315 R3321 V3324 N3325 N3326 L3327 G3328 I3329 A3332
R3337 R3350 T3361 L3365 R3366 K3367 R3368 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 D3396 D3404 L3405 Y3409 E3440 W3445 H3449 N3450 R3453 E3454 E3455 V3460 E3463 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 ALA
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 S3508 D3529 L3532 L3535 T3538 R3539 Y3540 A3541 L3542 V3549 R3550 E3551 Q3554 N3555 L3559 K3562 V3563
E3564 G3565 R3577 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 R3594 E3607 Q3608 T3609 E3610 H3611 PRO 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 D3676 E3682 Q3683 GLU GLU GLU GLU
GLU GLU VAL GLU E3692 K3693 D3717 L3735 GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 S3768 H3771 K3823 L3842 D3843 L3844 E3854 G3855 L3856 GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY E3872 F3899 I3916
S3929 S3938 D3941 Q3946 L3980 R3984 M4000 M4001 K4002 D4006 S4007 S4008 M4026 N4037 R4042 E4056 M4067 I4058 L4059 K4060 M4064 G4073 S4074 E4075 T4082 D4083 P4084 R4085 G4086 K4091 D4092 D4098 Q4102 D4118 E4119 N4120 E4121 M4122 E4152
L4166 R4180 A4186 E4224 G4225 G4226 E4227 A4228 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA 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

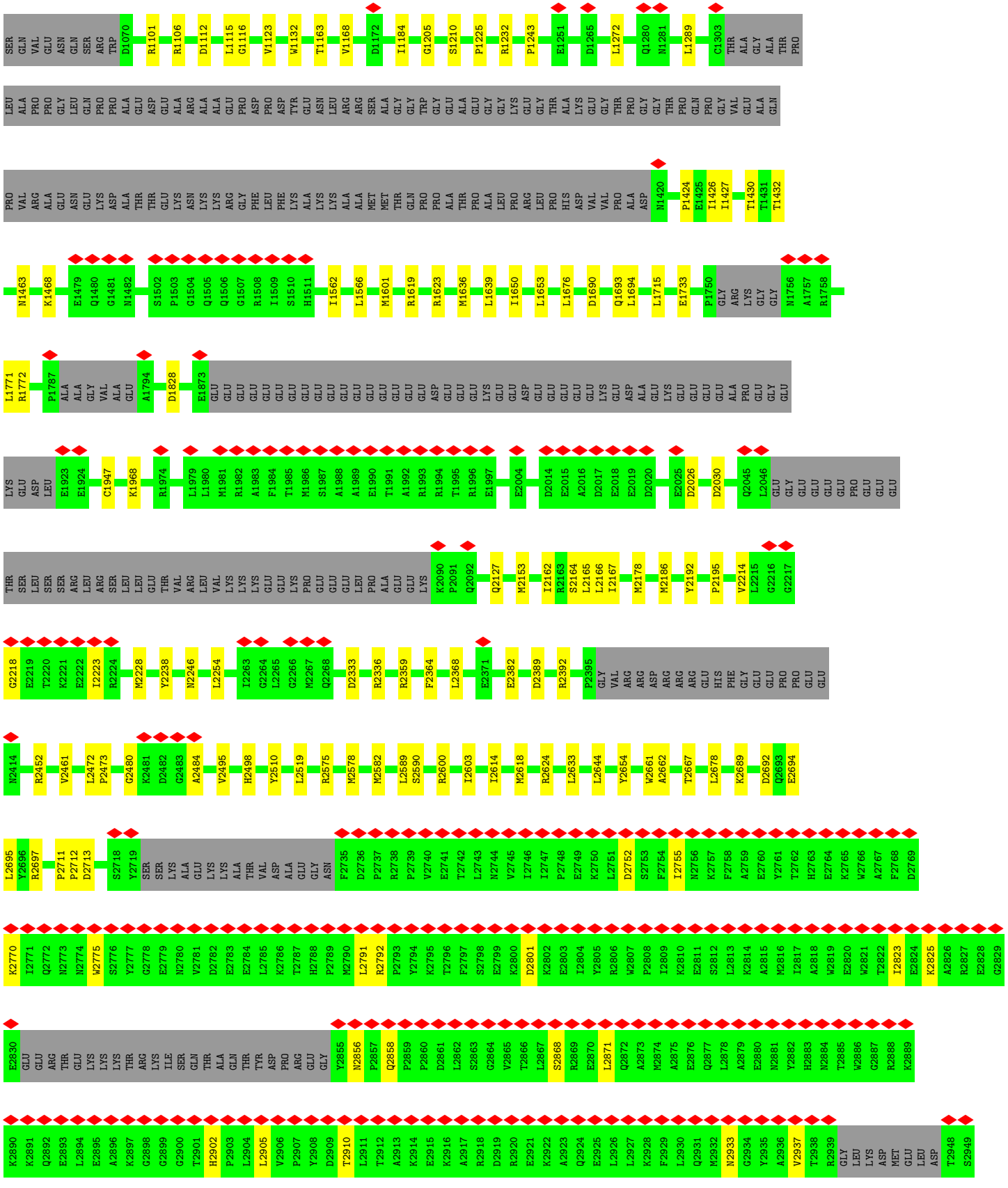


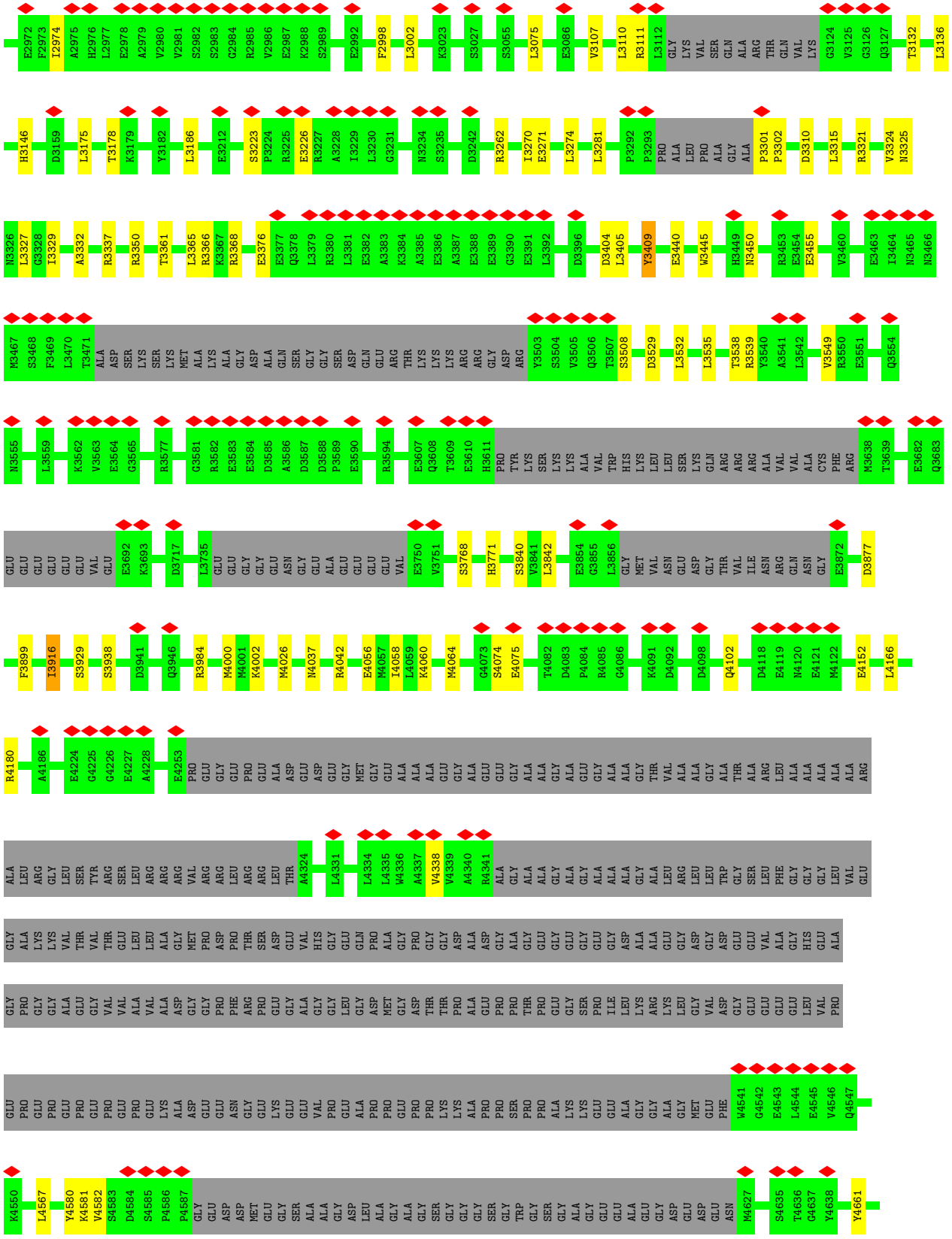
• Molecule 2: Ryanodine receptor 1

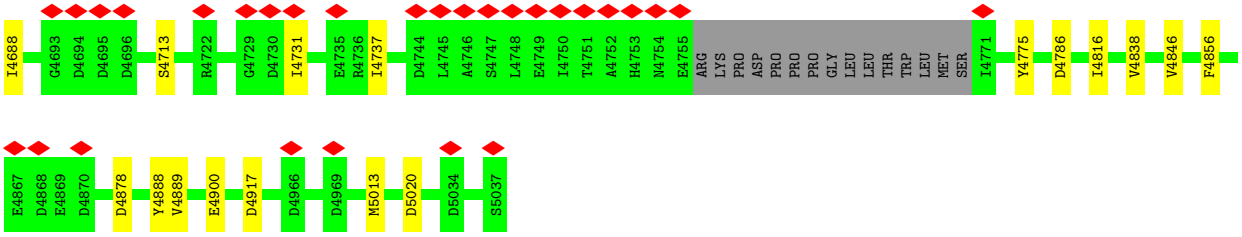
Chain D:






SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1101 R1106 D1112 L1115 G1116 V1123 W1132 T1163 V1168 D1172 I1184 G1205 S1210 P1225 R1232 P1243 E1251 D1265 L1272 Q1280 N1281 L1289 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 P1424 E1425 I1426 I1427 T1430 T1431 T1432
N1463 K1468 E1479 Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 I1562 L1566 M1601 R1619 R1623 M1636 L1639 I1650 L1653 L1676 D1690 Q1693 L1694 L1715 E1733 P1750 GLY ARG LYS GLY GLY N1756 A1757 R1758
L1771 R1772 P1787 ALA ALA GLY VAL ALA GLU A1794 D1828 E1873 GLU GLU GLU

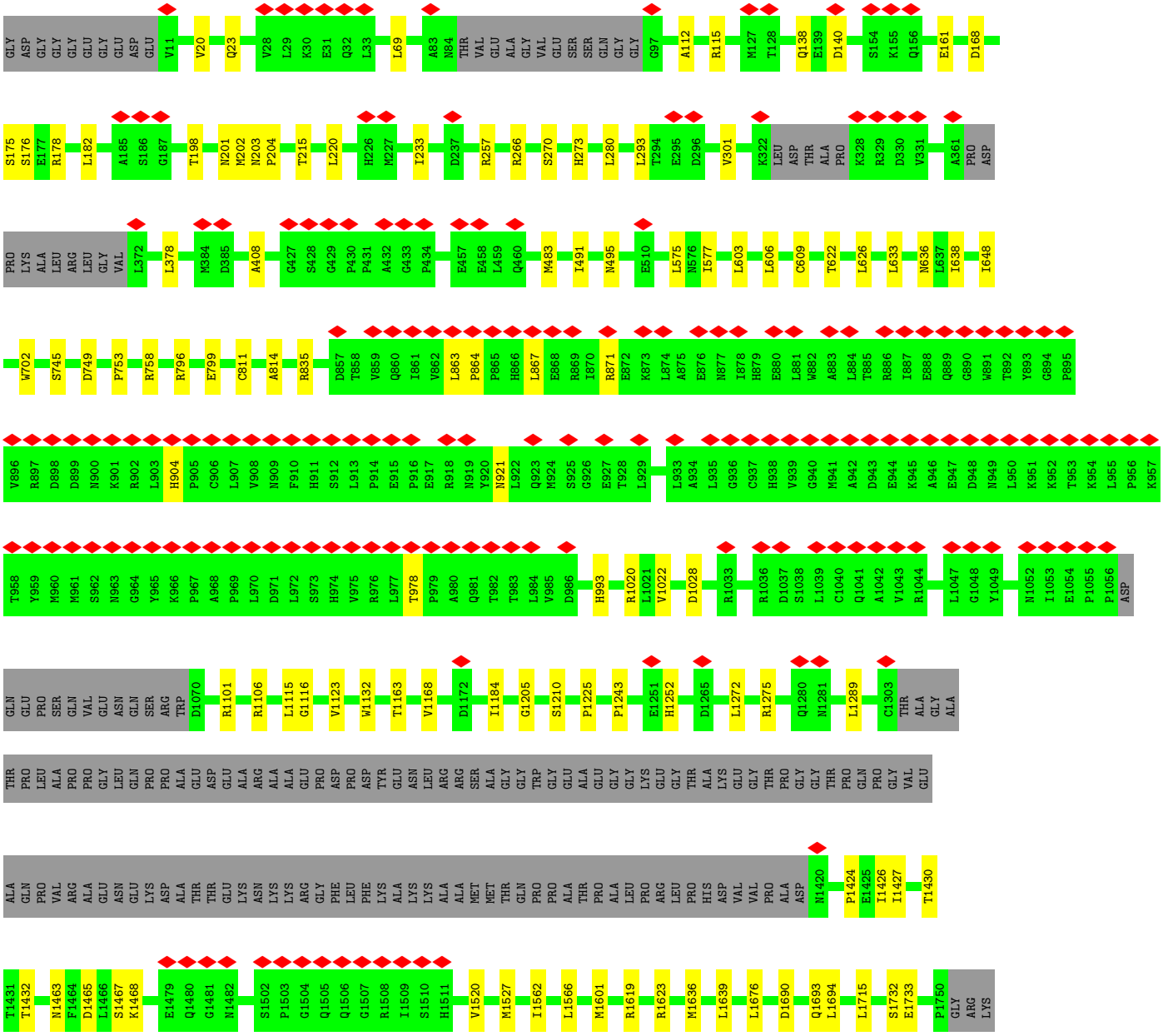

E2972 F2973 I2974 A2975 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 E2992 F2998 L3002 K3023 S3027 S3055 L3075 E3086 V3107 L3110 R3111 L3112 GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS G3124 V3125 G3126 Q3127 T3132 L3136
H3146 D3159 L3175 T3178 K3179 Y3182 L3186 E3212 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 N3234 S3235 D3242 R3262 I3270 E3271 L3274 L3281 P3292 P3293 PRO ALA LEU PRO ALA GLY ALA P3301 P3302 D3310 L3315 R3321 V3324 N3325
N3326 L3327 G3328 I3329 A3332 R3337 R3350 T3361 L3365 R3366 K3367 R3368 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 D3396 D3404 L3405 Y3409 E3440 W3445 H3449 N3450 R3453 E3454 E3455 V3460 E3463 I3464 N3465 N3466
M3467 S3468 F3469 L3470 T3471 ALA 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 S3508 D3529 L3532 L3535 T3538 R3539 Y3540 A3541 L3542 V3549 R3550 E3551 Q3554
N3555 L3559 K3562 V3563 E3564 G3565 R3577 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 R3594 E3607 Q3608 T3609 E3610 H3611 PRO 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 E3682 Q3683
GLU GLU GLU GLU GLU VAL GLU E3692 K3693 D3717 L3735 GLU GLU GLY GLY GLU GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 S3768 H3771 S3840 V3841 L3842 E3854 G3855 L3856 GLY MET VAL ASN GLU ASP GLY THR VAL ILE ASN ARG GLN ASN GLY E3872 D3877
F3899 I3916 S3929 S3938 D3941 Q3946 R3984 M4000 M4001 K4002 M4026 M4037 R4042 E4056 M4057 I4058 L4059 K4060 M4064 G4073 S4074 E4075 T4082 D4083 P4084 R4085 G4086 K4091 D4092 D4098 Q4102 D4118 E4119 N4120 E4121 M4122 E4152 L4166
R4180 A4186 E4224 G4225 G4226 E4227 A4228 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ARG
ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR A4324 L4331 L4334 L4335 W4336 A4337 V4338 V4339 A4340 R4341 ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA ALA LEU ARG LEU 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 GLY PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY GLU ASP ALA ALA GLU GLY GLU VAL GLU ALA GLY
GLY PRO GLY GLY ALA GLU GLY VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ASP MET GLY ASP THR THR PRO ALA 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 PRO GLU 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 GLU GLU ALA GLY GLY ALA GLY MET GLU PHE W4541 G4542 E4543 L4544 E4545 V4546 Q4547
K4550 L4567 Y4580 K4581 V4582 S4583 D4584 S4585 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU ASN M4627 S4635 T4636 G4637 Y4638 Y4661

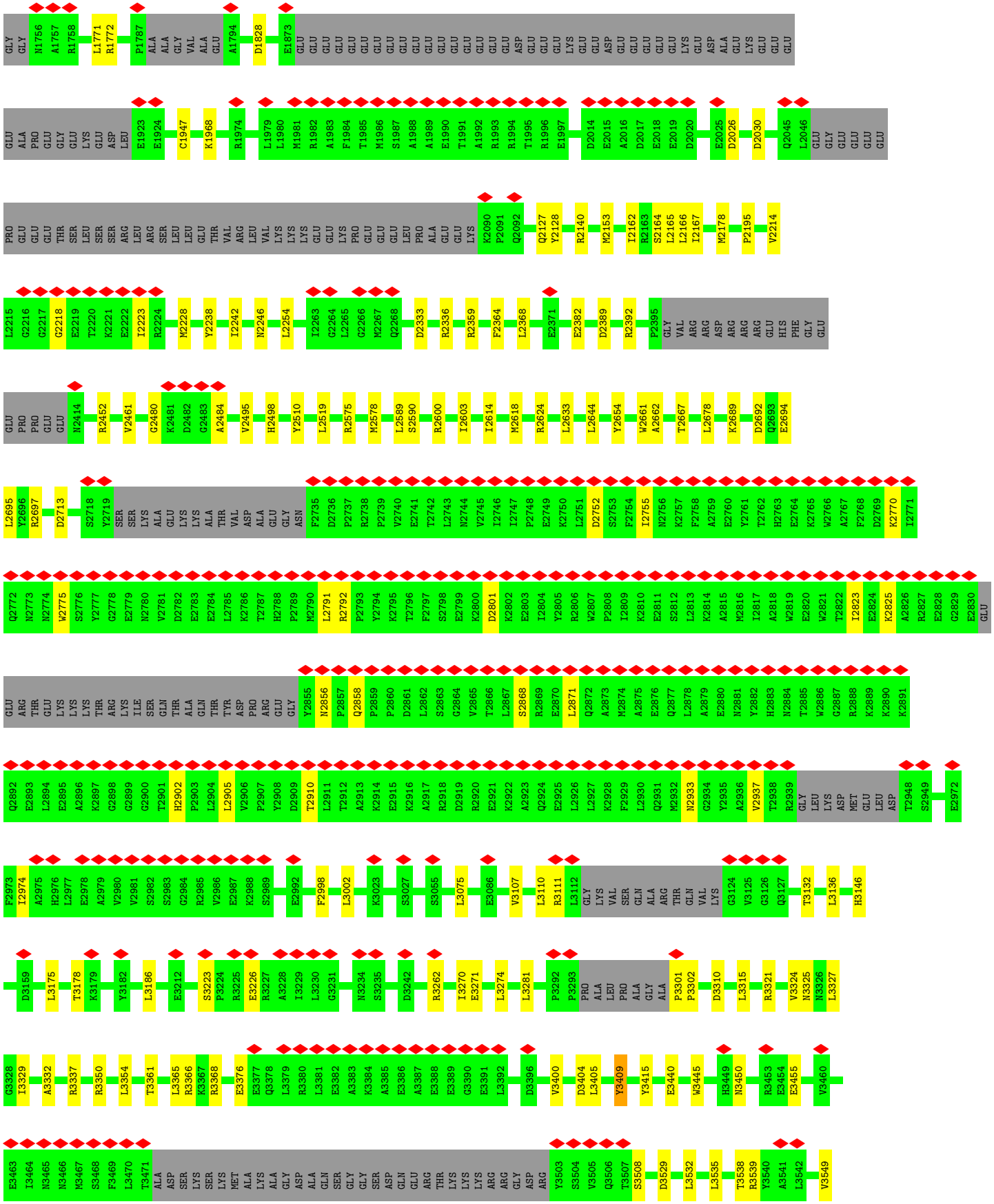


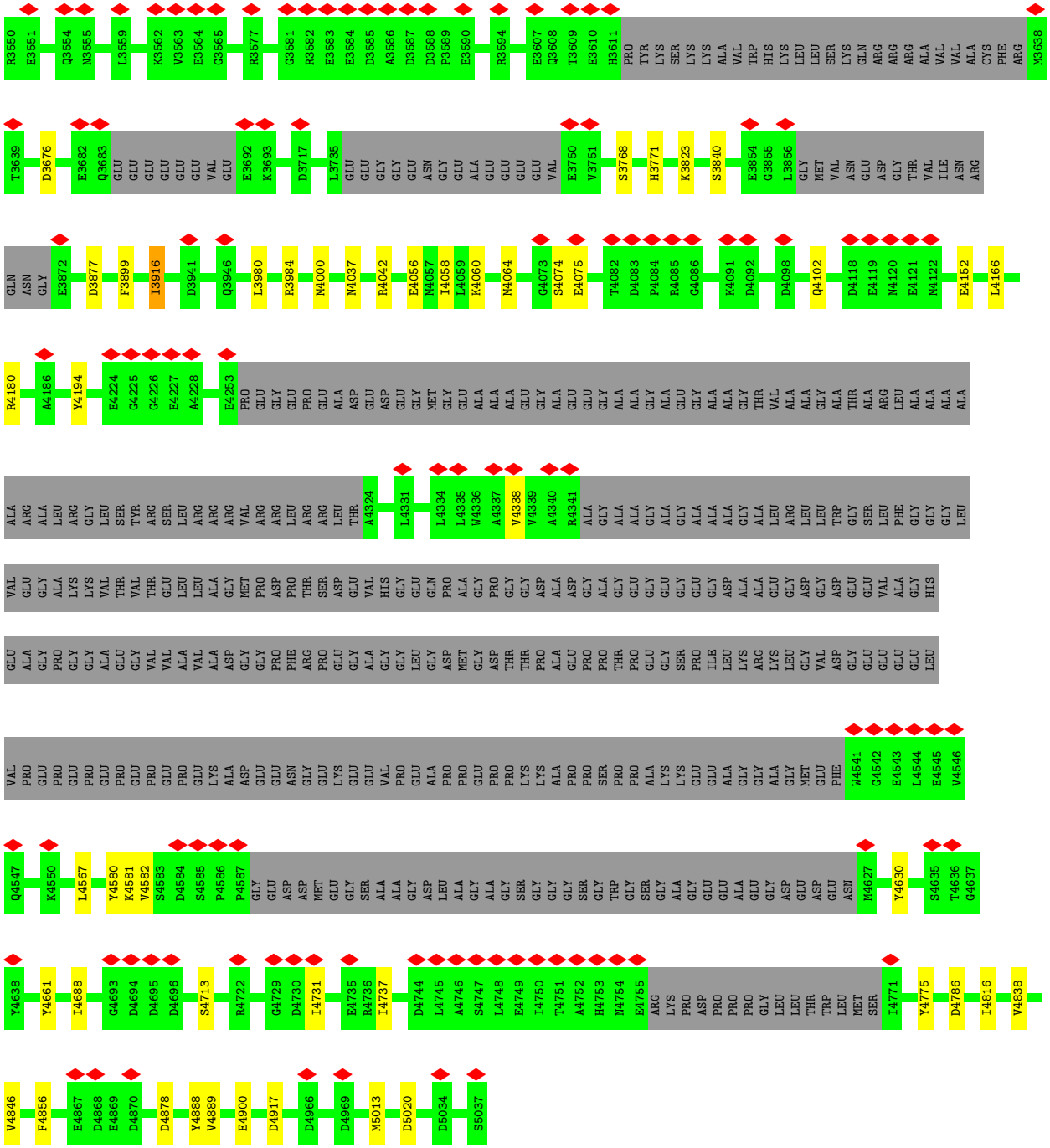
• Molecule 2: Ryanodine receptor 1

Chain F:





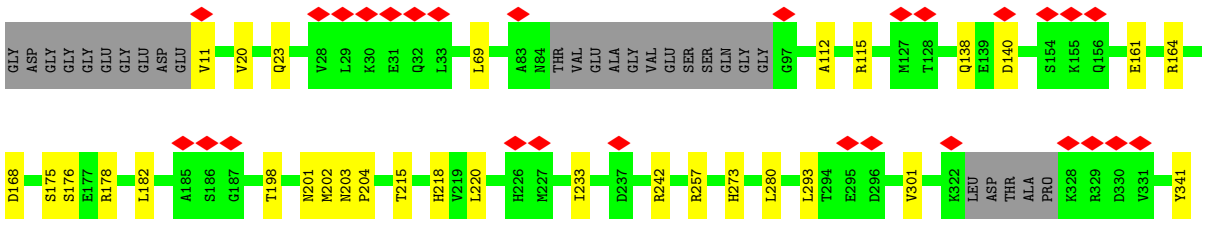

GLY GLY N1756 A1757 R1758 L1771 R1772 P1787 ALA ALA GLY VAL ALA GLU A1794 D1828 E1873 GLU GLU GLU

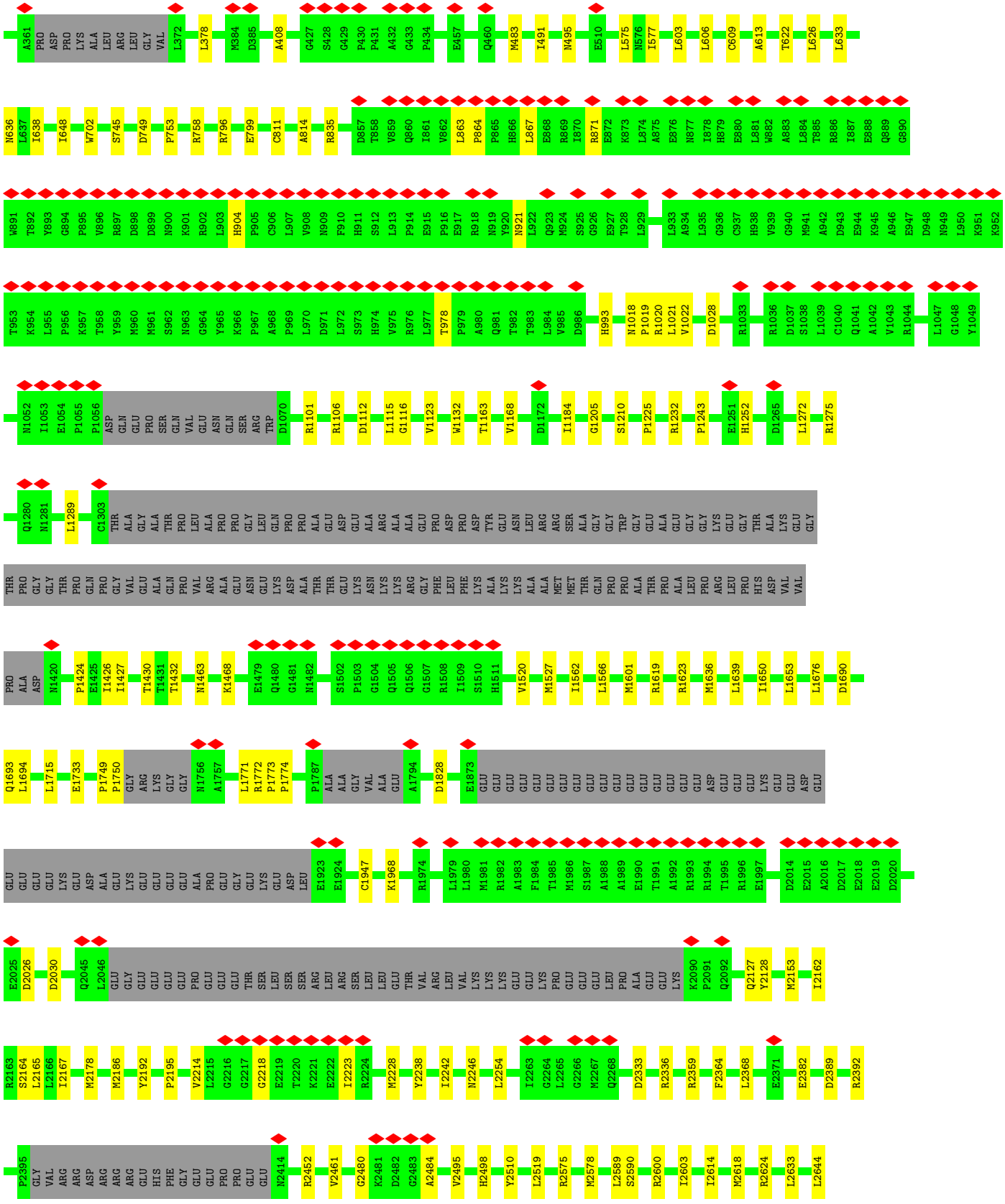


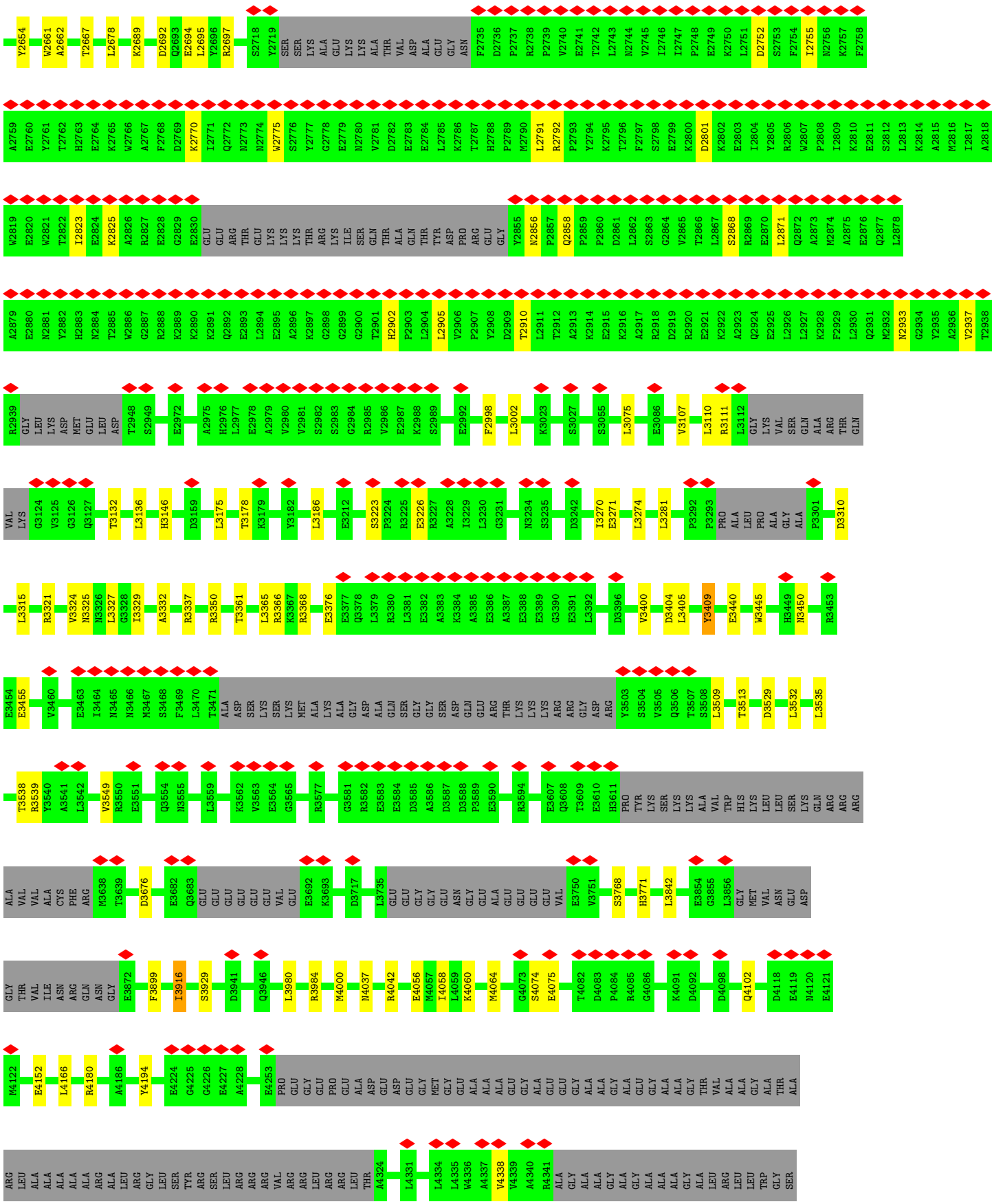
• Molecule 2: Ryanodine receptor 1

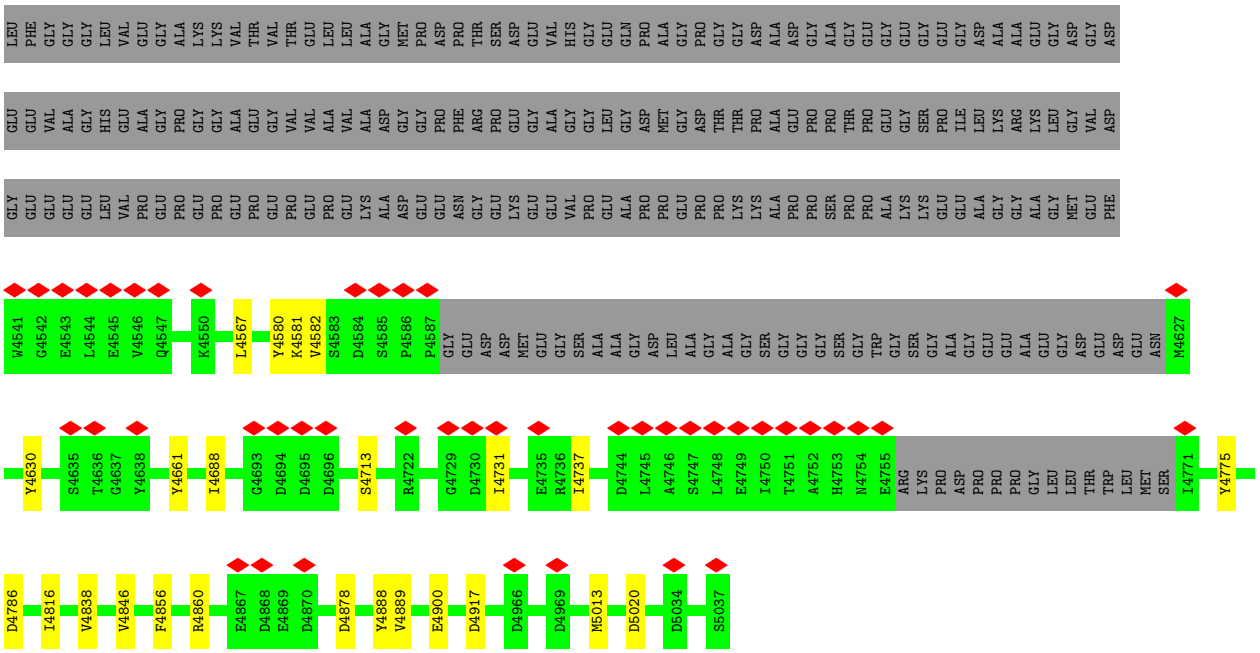
Chain H:






A361 PRO ASP PRO LYS ALA LEU ARG LEU GLY VAL L372 L378 M384 D385 A408 G427 S428 G429 P430 P431 A432 G433 P434 E457 Q460 M483 I491 N495 E510 L575 N576 I577 L603 L606 C609 A613 T622 L626 L633
N636 L637 I638 I648 W702 S745 D749 P753 R758 R796 E799 C811 A814 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 P910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 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 H993 N1018 P1019 R1020 L1021 V1022 D1028 R1033 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 L1047 G1048 Y1049
N1052 I1053 E1054 P1055 P1056 ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1101 R1106 D1112 L1115 G1116 V1123 W1132 T1163 V1168 D1172 I1184 G1205 S1210 P1225 R1232 P1243 E1251 H1252 D1265 L1272 R1275
Q1280 N1281 L1289 C1303 THR ALA GLY 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 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 P1424 E1425 I1426 I1427 T1430 T1431 T1432 N1463 K1468 E1479 Q1480 G1481 N1482 S1502 P1503 G1504 Q1505 Q1506 G1507 R1508 I1509 S1510 H1511 V1520 M1527 I1562 L1566 M1601 R1619 R1623 M1636 L1639 I1650 L1653 L1676 D1690
Q1693 L1694 L1715 E1733 P1749 P1750 GLY ARG LYS GLY GLY N1756 A1757 L1771 R1772 P1773 P1774 P1787 ALA ALA GLY VAL ALA GLU A1794 D1828 E1873 GLU GLU GLU


Y2654 W2661 A2662 T2667 L2678 K2689 D2692 Q2693 E2694 L2695 Y2696 R2697 S2718 Y2719 SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY ASN F2735 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 E2972 A2975 H2976 L2977 E2978 A2979 V2980 V2981 S2982 S2983 G2984 R2985 V2986 E2987 K2988 S2989 E2992 F2998 L3002 K3023 S3027 S3055 L3075 E3086 V3107 L3110 R3111 L3112 GLY LYS VAL SER GLN ALA ARG THR GLN
VAL LYS G3124 V3125 G3126 Q3127 T3132 L3136 H3146 D3159 L3175 T3178 K3179 Y3182 L3186 E3212 S3223 P3224 R3225 E3226 R3227 A3228 I3229 L3230 G3231 N3234 S3235 D3242 I3270 E3271 L3274 L3281 P3292 P3293 PRO ALA LEU PRO ALA GLY ALA P3301 D3310
L3315 R3321 V3324 N3325 N3326 L3327 G3328 I3329 A3332 R3337 R3350 T3361 L3365 R3366 K3367 R3368 E3376 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 D3396 V3400 D3404 L3405 Y3409 E3440 W3445 H3449 N3450 R3453
E3454 E3455 V3460 E3463 I3464 N3465 N3466 M3467 S3468 F3469 L3470 T3471 ALA 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 S3508 L3509 T3513 D3529 L3532 L3535
T3538 R3539 Y3540 A3541 L3542 V3549 R3550 E3551 Q3554 N3555 L3559 K3562 V3563 E3564 G3565 R3577 G3581 R3582 E3583 E3584 D3585 A3586 D3587 D3588 P3589 E3590 R3594 E3607 Q3608 T3609 E3610 H3611 PRO 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 D3676 E3682 Q3683 GLU GLU GLU GLU GLU VAL GLU E3692 K3693 D3717 L3735 GLU GLU GLY GLY GLU ASN GLY GLU ALA GLU GLU GLU GLU VAL E3750 V3751 S3768 H3771 L3842 E3854 G3855 L3856 GLY MET VAL ASN GLU ASP
GLY THR VAL ILE ASN ARG GLN ASN GLY E3872 F3899 I3916 S3929 D3941 Q3946 L3980 R3984 M4000 N4037 R4042 E4056 M4057 I4058 L4059 K4060 M4064 G4073 S4074 E4075 T4082 D4083 P4084 R4085 G4086 K4091 D4092 D4098 Q4102 D4118 E4119 N4120 E4121
M4122 E4152 L4166 R4180 A4186 Y4194 E4224 G4225 G4226 E4227 A4228 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA ALA ALA GLY THR VAL ALA 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 LEU ARG ARG ARG LEU THR A4324 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 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 ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY
GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY GLY ALA GLU PRO GLY VAL 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 THR PRO GLU GLY SER PRO ILE LEU ALA 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 PRO GLU LYS ALA ASP GLY GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU PHE
W4541 G4542 E4543 L4544 E4545 V4546 Q4547 K4550 L4567 Y4580 K4581 V4582 S4583 D4584 S4585 P4586 P4587 GLY GLU 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 T4636 G4637 Y4638 Y4661 I4688 G4693 D4694 D4695 D4696 S4713 R4722 G4729 D4730 I4731 E4735 R4736 I4737 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 ARG LYS PRO ASP PRO PRO PRO GLY LEU LEU THR TRP LEU MET SER I4771 Y4775
D4786 I4816 V4838 V4846 F4856 R4860 E4867 D4868 E4869 D4870 D4878 Y4888 V4889 E4900 D4917 D4966 D4969 M5013 D5020 D5034 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	593532	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	0.755	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.086	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: ZN, U1C, CA, 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	0.17	0/830	0.37	0/1119
1	C	0.17	0/830	0.37	0/1119
1	E	0.17	0/830	0.37	0/1119
1	G	0.17	0/830	0.37	0/1119
2	B	0.16	0/34123	0.33	0/46303
2	D	0.16	0/34123	0.33	0/46303
2	F	0.16	0/34123	0.33	0/46303
2	H	0.16	0/34123	0.33	0/46303
All	All	0.16	0/139812	0.33	0/189688

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	814	0	810	5	0
1	C	814	0	810	5	0
1	E	814	0	810	4	0
1	G	814	0	810	4	0
2	B	33355	0	32544	172	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	33355	0	32544	174	0
2	F	33355	0	32544	174	0
2	H	33355	0	32544	177	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	62	0	24	2	0
5	D	62	0	24	2	0
5	F	62	0	24	2	0
5	H	62	0	24	2	0
6	B	23	0	0	1	0
6	D	23	0	0	1	0
6	F	23	0	0	1	0
6	H	23	0	0	1	0
All	All	137024	0	133512	665	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 2.

The worst 5 of 665 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4581:LYS:HG3	2:D:4878:ASP:HB3	1.47	0.97
2:D:4581:LYS:HG3	2:F:4878:ASP:HB3	1.47	0.95
2:B:4878:ASP:HB3	2:H:4581:LYS:HG3	1.47	0.94
2:F:4581:LYS:HG3	2:H:4878:ASP:HB3	1.47	0.94
2:H:1430:THR:HG22	2:H:1432:THR:H	1.55	0.72

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
1	C	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
1	E	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
1	G	105/110 (96%)	103 (98%)	2 (2%)	0	100	100
2	B	4222/5037 (84%)	4173 (99%)	49 (1%)	0	100	100
2	D	4222/5037 (84%)	4173 (99%)	49 (1%)	0	100	100
2	F	4222/5037 (84%)	4173 (99%)	49 (1%)	0	100	100
2	H	4222/5037 (84%)	4173 (99%)	49 (1%)	0	100	100
All	All	17308/20588 (84%)	17104 (99%)	204 (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%)	85 (98%)	2 (2%)	44	78
1	C	87/90 (97%)	85 (98%)	2 (2%)	44	78
1	E	87/90 (97%)	85 (98%)	2 (2%)	44	78
1	G	87/90 (97%)	85 (98%)	2 (2%)	44	78
2	B	3521/4277 (82%)	3508 (100%)	13 (0%)	84	94
2	D	3521/4277 (82%)	3508 (100%)	13 (0%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	3521/4277 (82%)	3508 (100%)	13 (0%)	84 94
2	H	3521/4277 (82%)	3508 (100%)	13 (0%)	84 94
All	All	14432/17468 (83%)	14372 (100%)	60 (0%)	81 94

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	3916	ILE
2	H	2254	LEU
2	F	577	ILE
2	H	2238	TYR
2	H	4580	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 254 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	4133	GLN
2	H	2599	GLN
2	F	1532	ASN
2	H	2441	HIS
2	H	3560	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	5305	-	32,33,33	0.28	0	48,52,52	0.28	0
6	U1C	D	5304	-	25,25,25	0.60	0	33,35,35	0.50	0
6	U1C	F	5304	-	25,25,25	0.60	0	33,35,35	0.50	0
6	U1C	H	5304	-	25,25,25	0.60	0	33,35,35	0.50	0
5	ATP	H	5305	-	32,33,33	0.28	0	48,52,52	0.28	0
5	ATP	B	5303	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	D	5305	-	32,33,33	0.28	0	48,52,52	0.28	0
5	ATP	D	5303	-	32,33,33	0.26	0	48,52,52	0.30	0
5	ATP	F	5303	-	32,33,33	0.26	0	48,52,52	0.30	0
6	U1C	B	5304	-	25,25,25	0.60	0	33,35,35	0.50	0
5	ATP	F	5305	-	32,33,33	0.28	0	48,52,52	0.28	0
5	ATP	H	5303	-	32,33,33	0.26	0	48,52,52	0.30	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	5305	-	-	4/22/38/38	0/3/3/3
6	U1C	D	5304	-	-	0/11/25/25	0/3/3/3
6	U1C	F	5304	-	-	0/11/25/25	0/3/3/3
6	U1C	H	5304	-	-	0/11/25/25	0/3/3/3
5	ATP	H	5305	-	-	4/22/38/38	0/3/3/3
5	ATP	B	5303	-	-	8/22/38/38	0/3/3/3
5	ATP	D	5305	-	-	4/22/38/38	0/3/3/3
5	ATP	D	5303	-	-	8/22/38/38	0/3/3/3
5	ATP	F	5303	-	-	8/22/38/38	0/3/3/3
6	U1C	B	5304	-	-	0/11/25/25	0/3/3/3
5	ATP	F	5305	-	-	4/22/38/38	0/3/3/3
5	ATP	H	5303	-	-	8/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 48 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	5305	ATP	C5'-O5'-PA-O1A
5	B	5305	ATP	C5'-O5'-PA-O2A

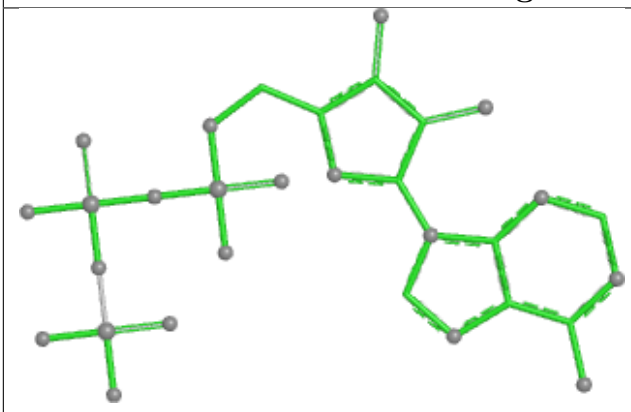
There are no ring outliers.

8 monomers are involved in 12 short contacts:

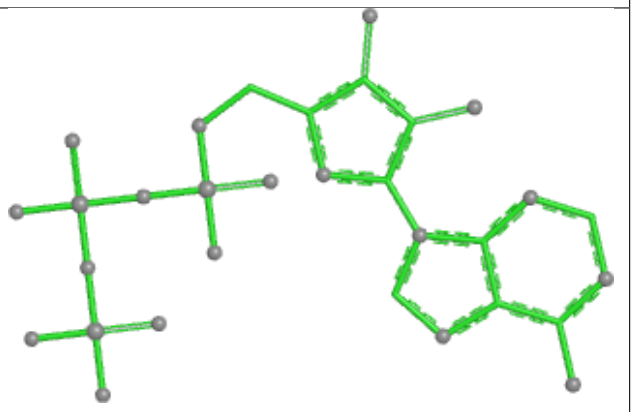
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5305	ATP	2	0
6	D	5304	U1C	1	0
6	F	5304	U1C	1	0
6	H	5304	U1C	1	0
5	H	5305	ATP	2	0
5	D	5305	ATP	2	0
6	B	5304	U1C	1	0
5	F	5305	ATP	2	0

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

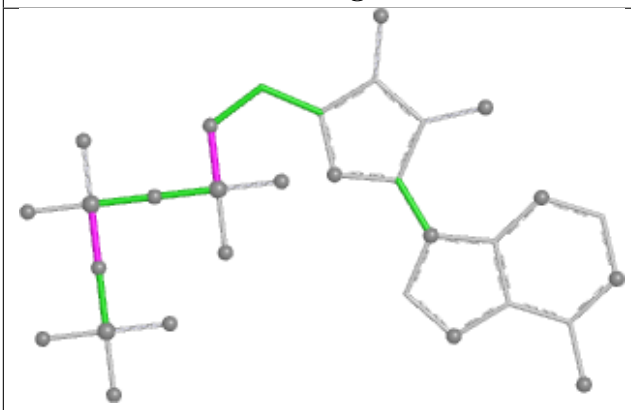
Ligand ATP B 5305



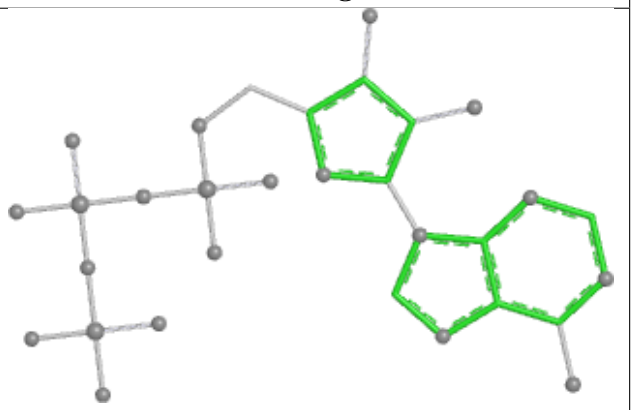
Bond lengths



Bond angles

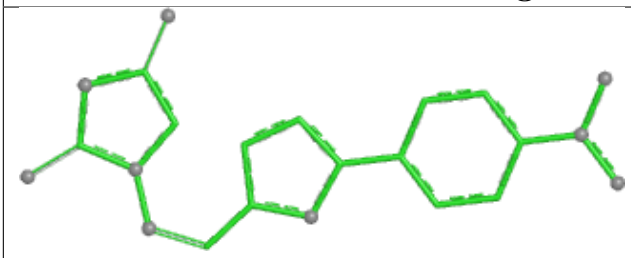


Torsions

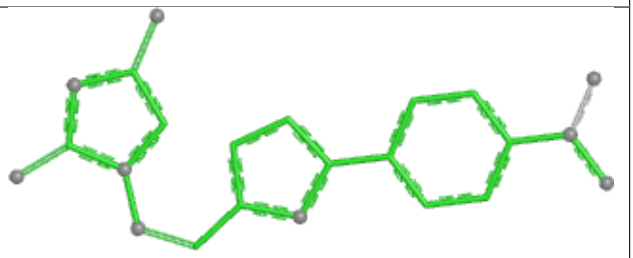


Rings

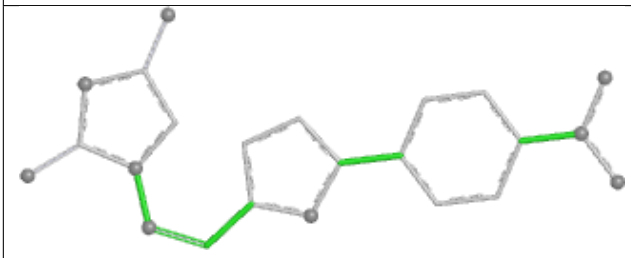
Ligand U1C D 5304



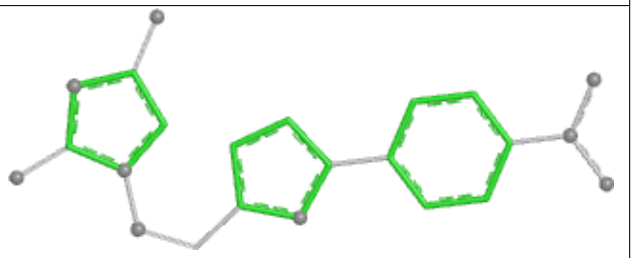
Bond lengths



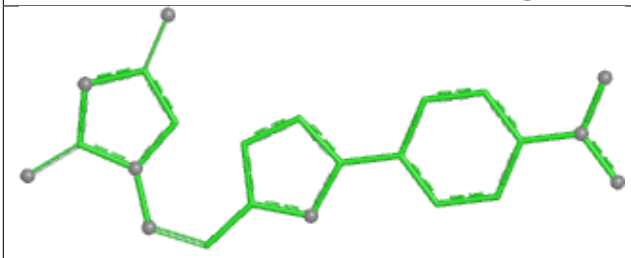
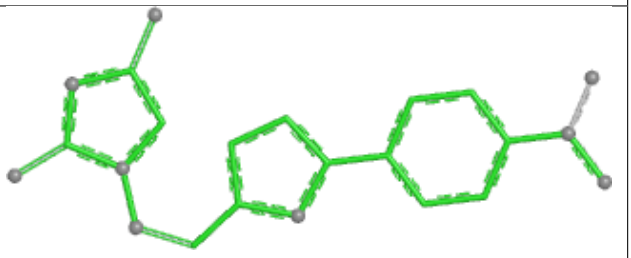
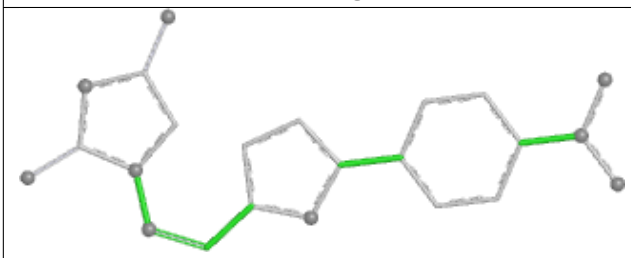
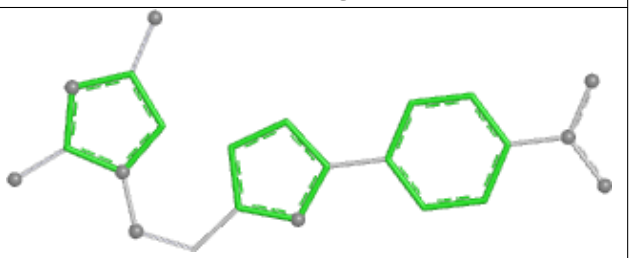
Bond angles

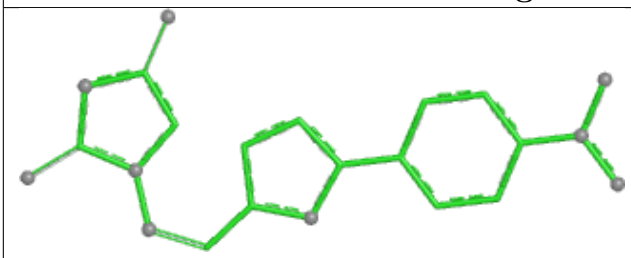
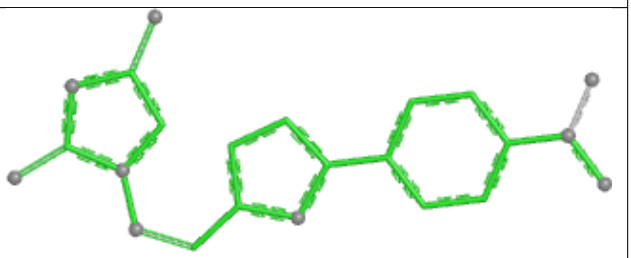
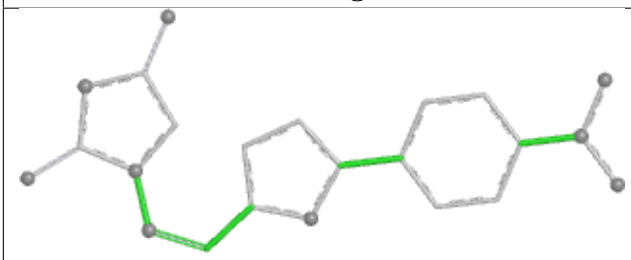
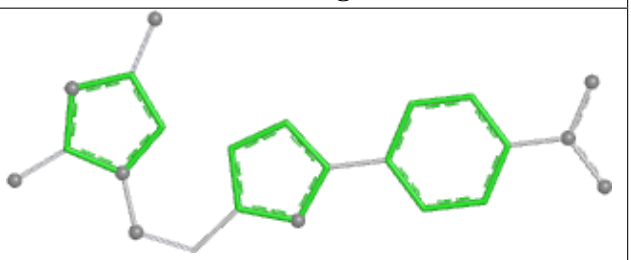


Torsions

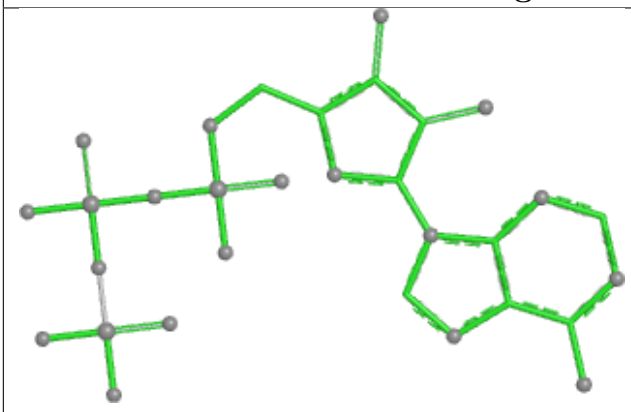


Rings

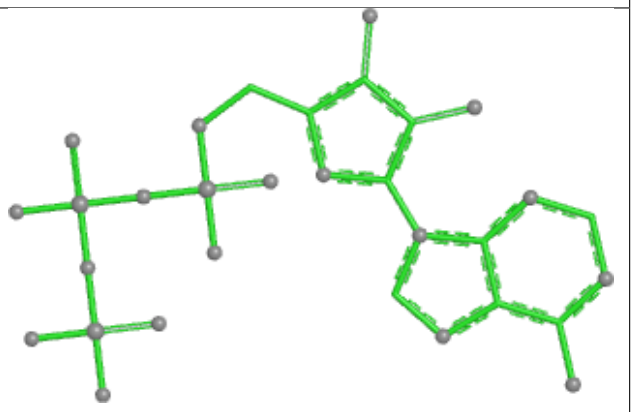
Ligand U1C F 5304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand U1C H 5304	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

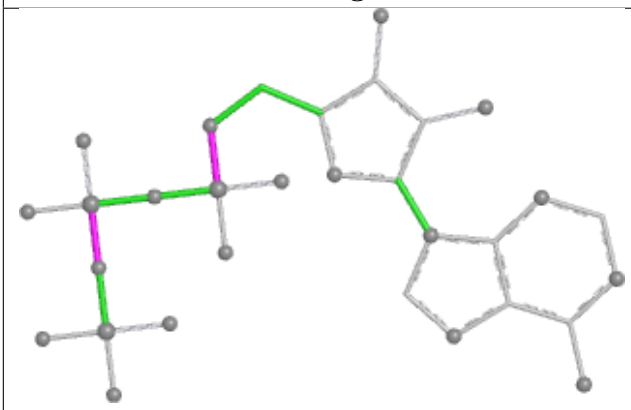
Ligand ATP H 5305



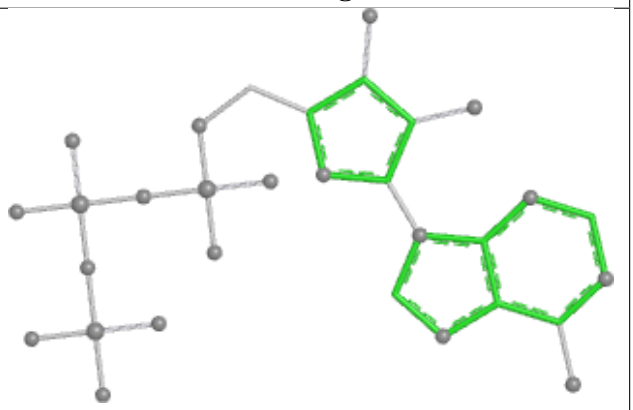
Bond lengths



Bond angles

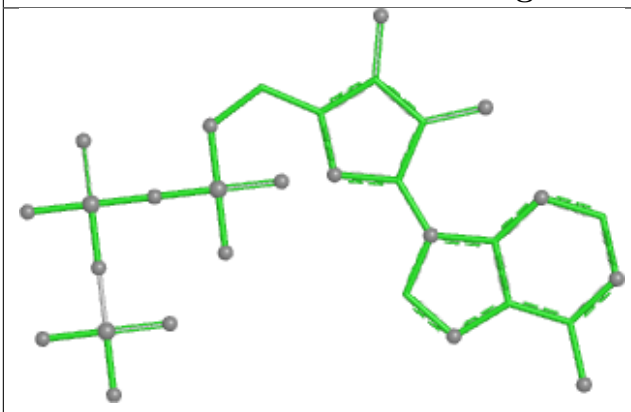


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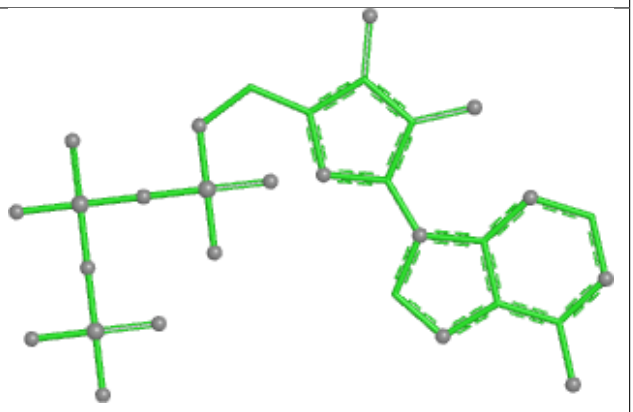


Rings

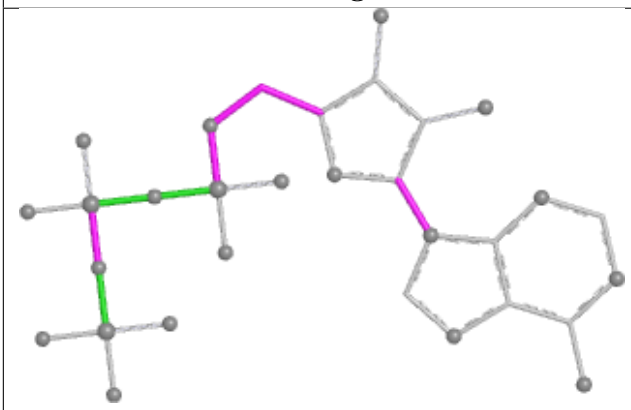
Ligand ATP B 5303



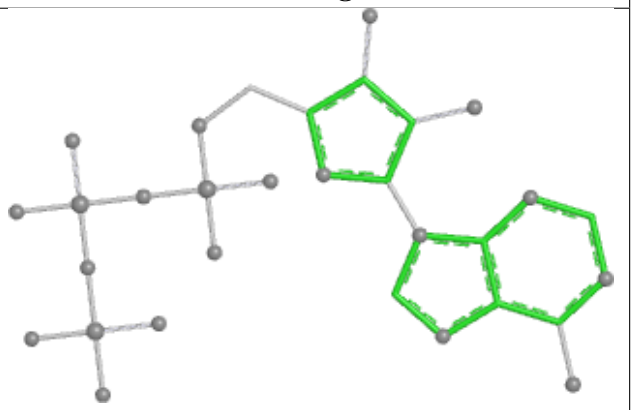
Bond lengths



Bond angles

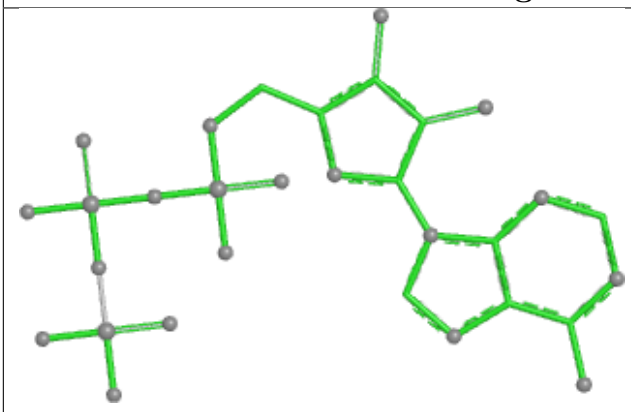


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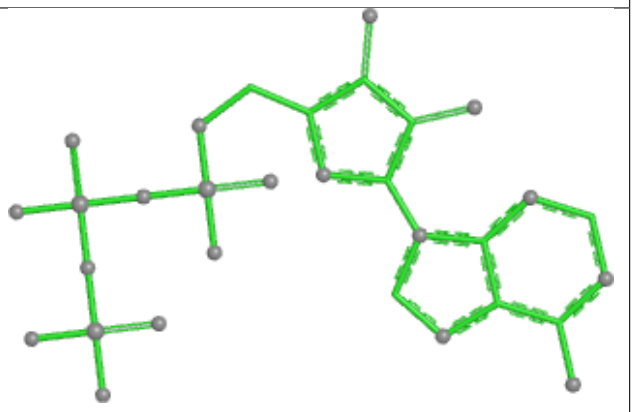


Rings

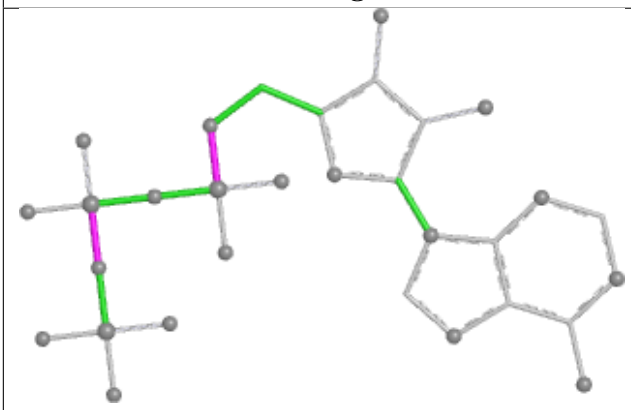
Ligand ATP D 5305



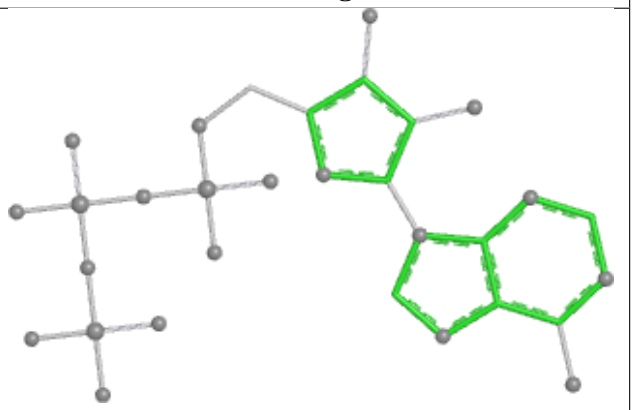
Bond lengths



Bond angles

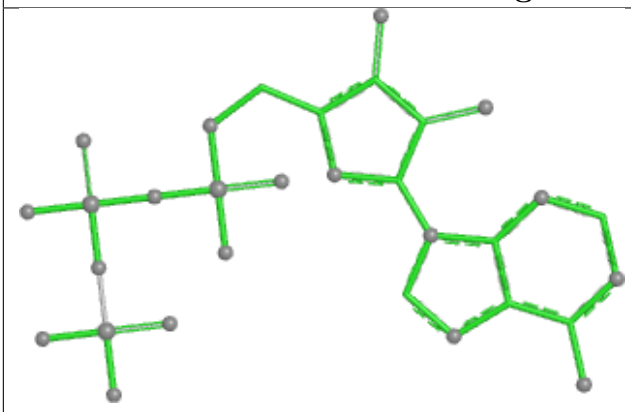


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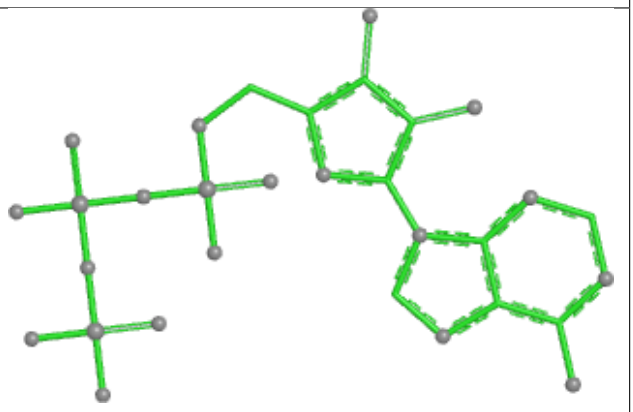


Rings

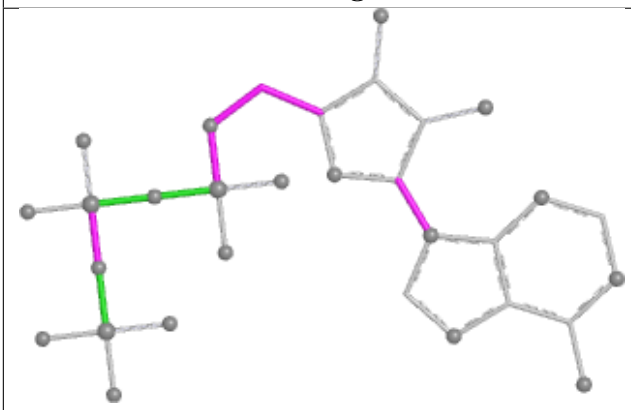
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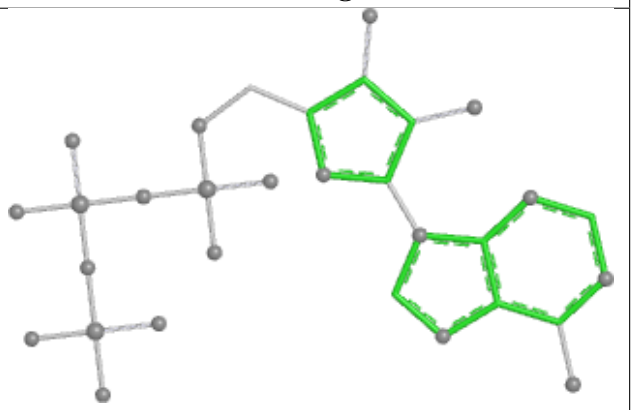
Bond lengths



Bond angles

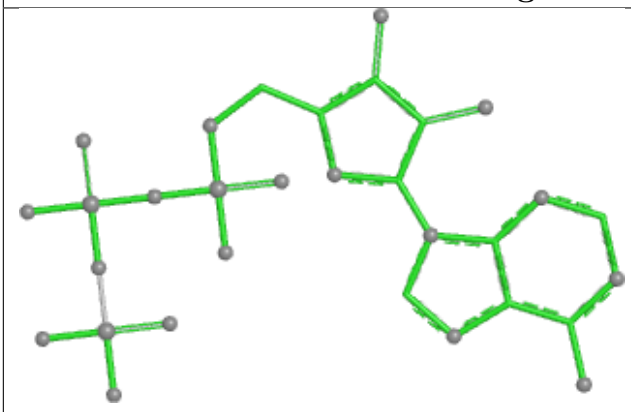


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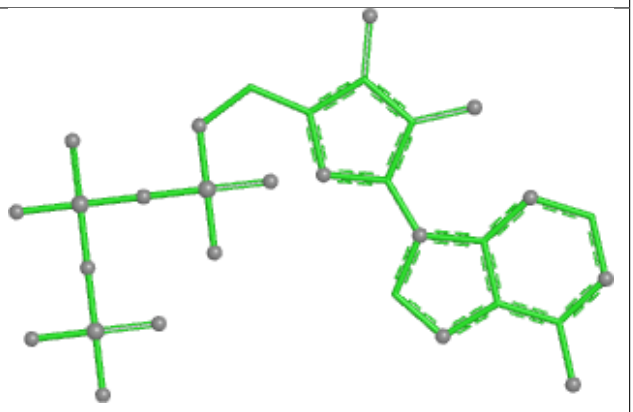


Rings

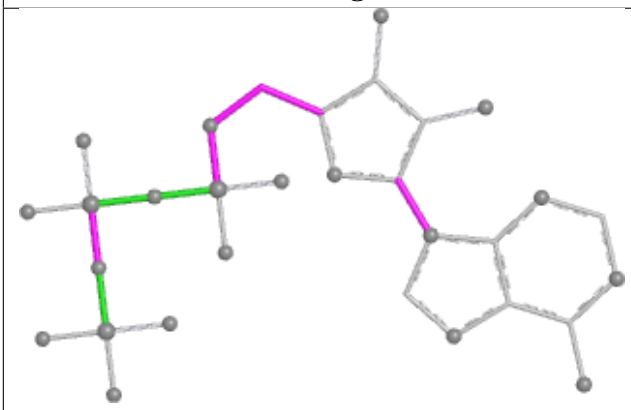
Ligand ATP F 5303



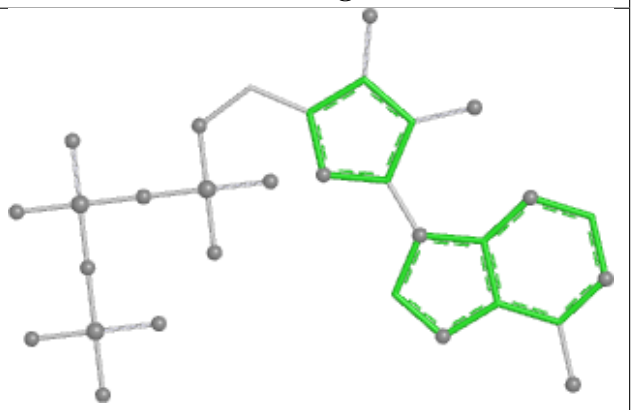
Bond lengths



Bond angles

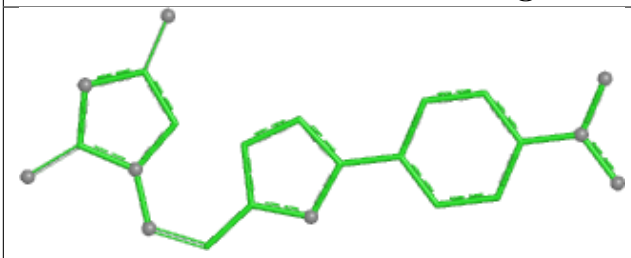


Torsions

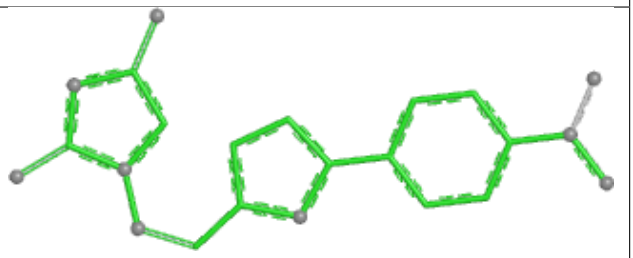


Rings

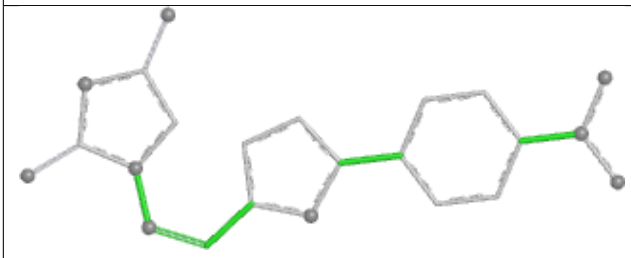
Ligand U1C B 5304



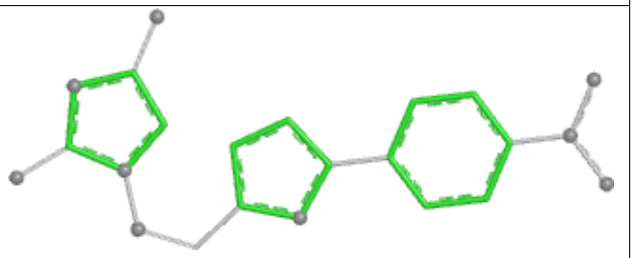
Bond lengths



Bond angles

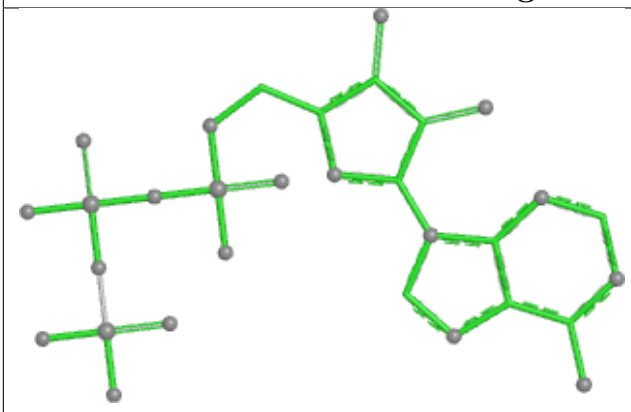


Torsions

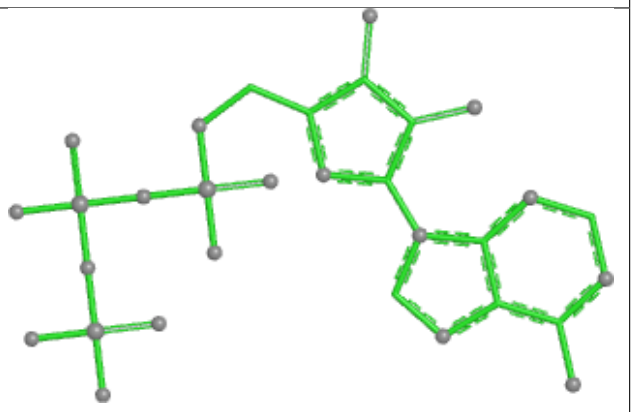


Rings

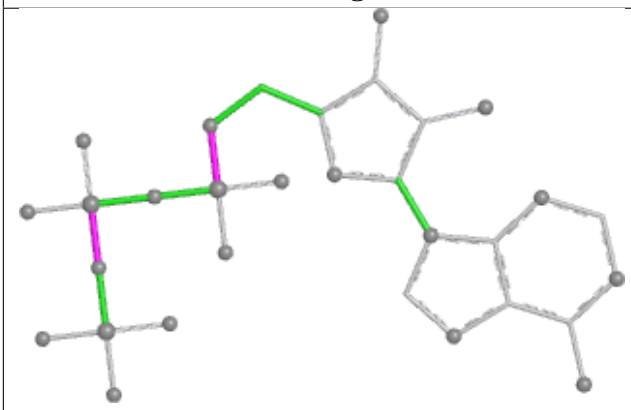
Ligand ATP F 5305



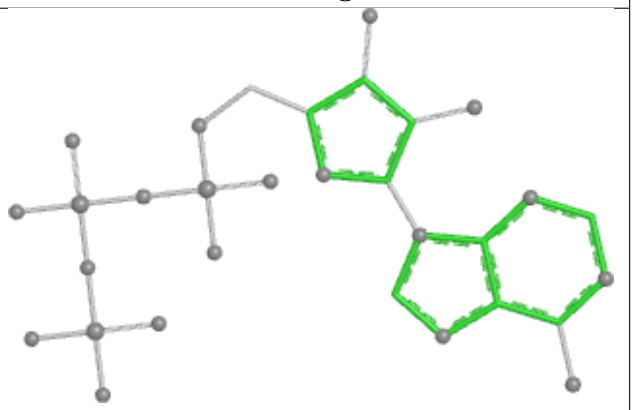
Bond lengths



Bond angles

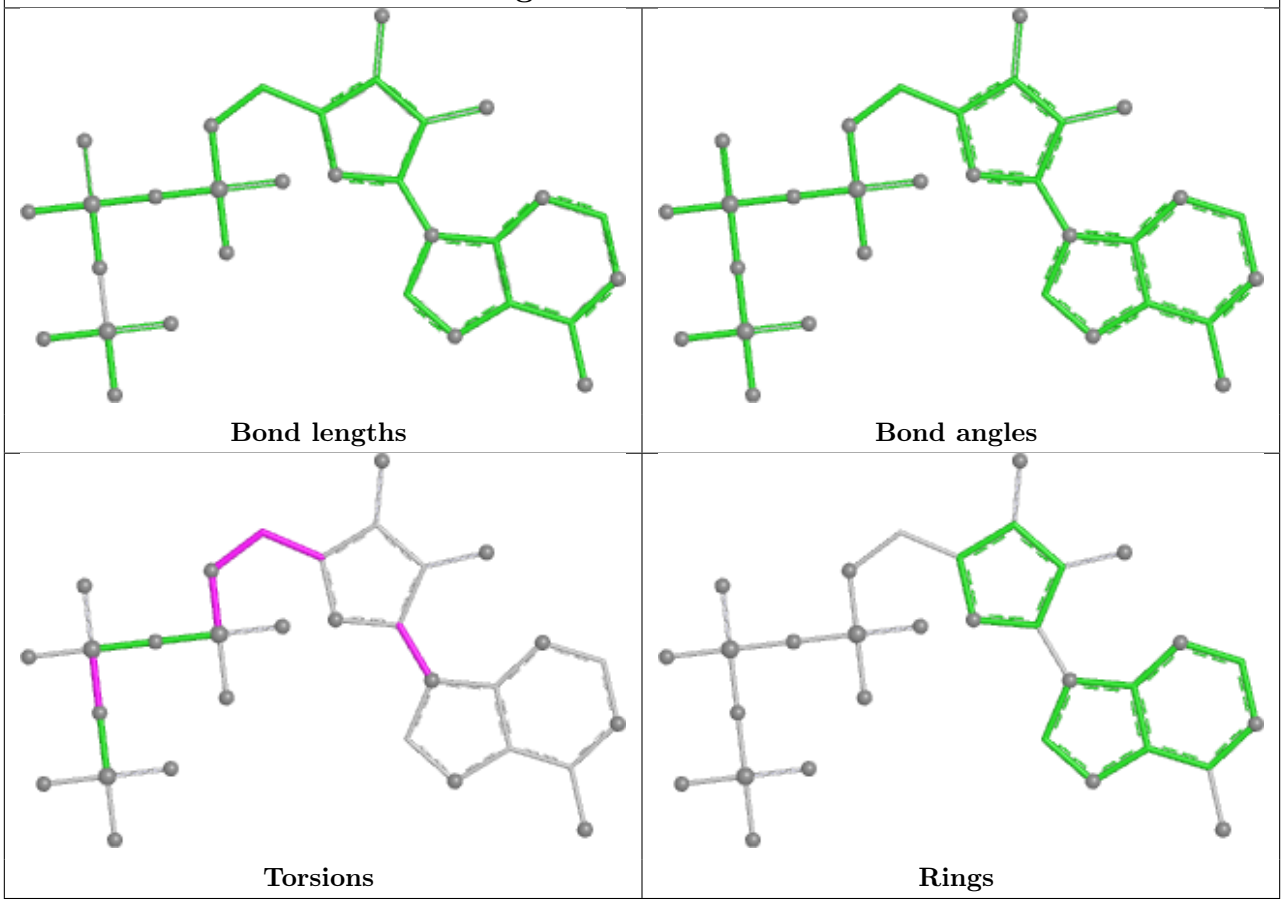


Torsions



Rings

Ligand ATP H 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.

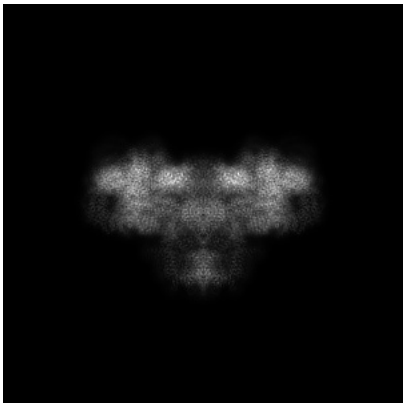
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73953. These allow visual inspection of the internal detail of the map and identification of artifacts.

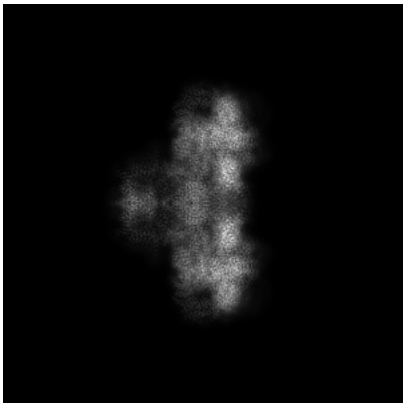
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

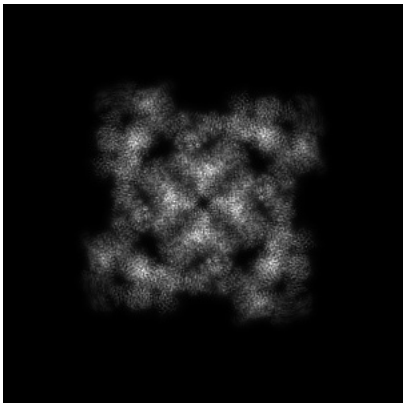
6.1.1 Primary map



X



Y



Z

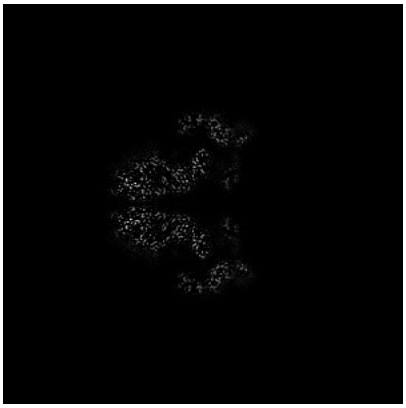
The images above show the map projected in three orthogonal directions.

6.2 Central slices

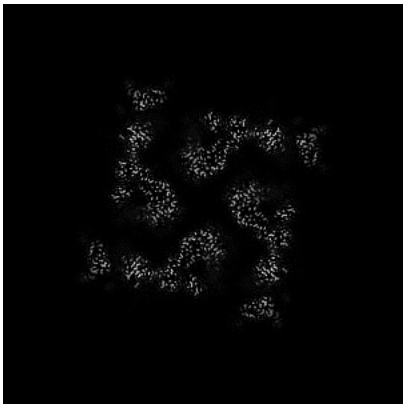
6.2.1 Primary map



X Index: 256



Y Index: 256

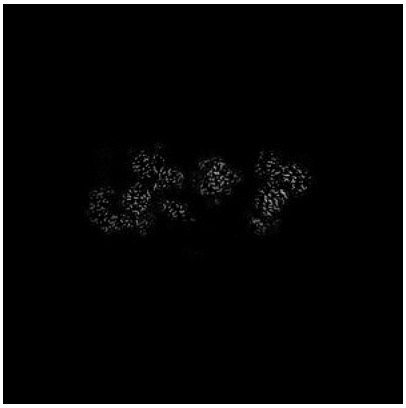


Z Index: 256

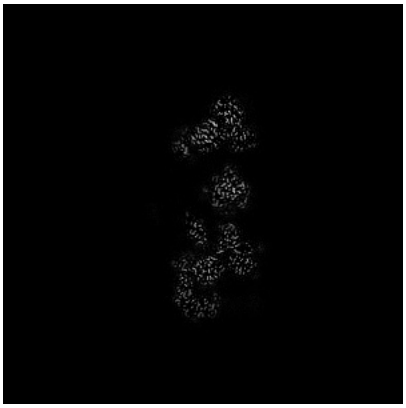
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

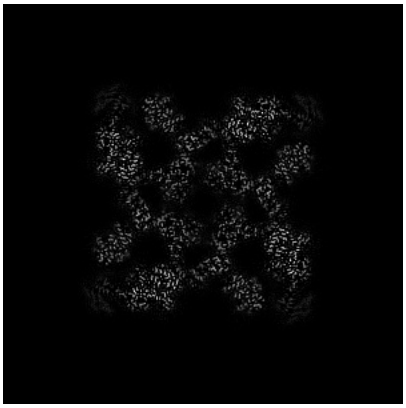
6.3.1 Primary map



X Index: 339



Y Index: 173

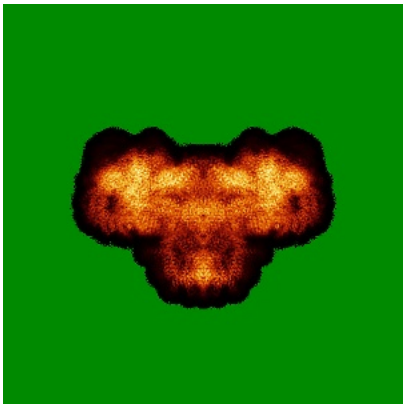


Z Index: 281

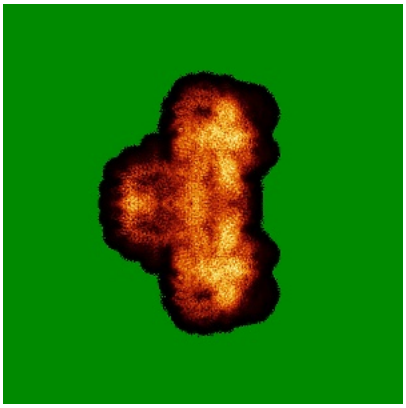
The images above show the largest variance slices of the map in three orthogonal directions.

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

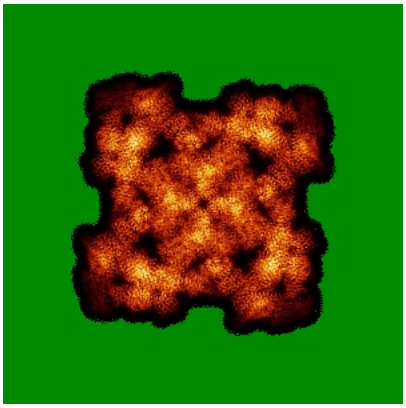
6.4.1 Primary map



X



Y

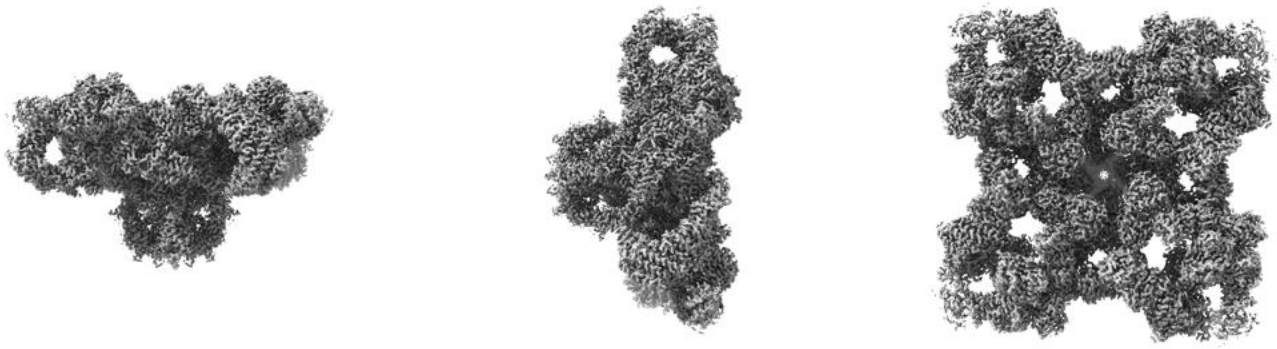


Z

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

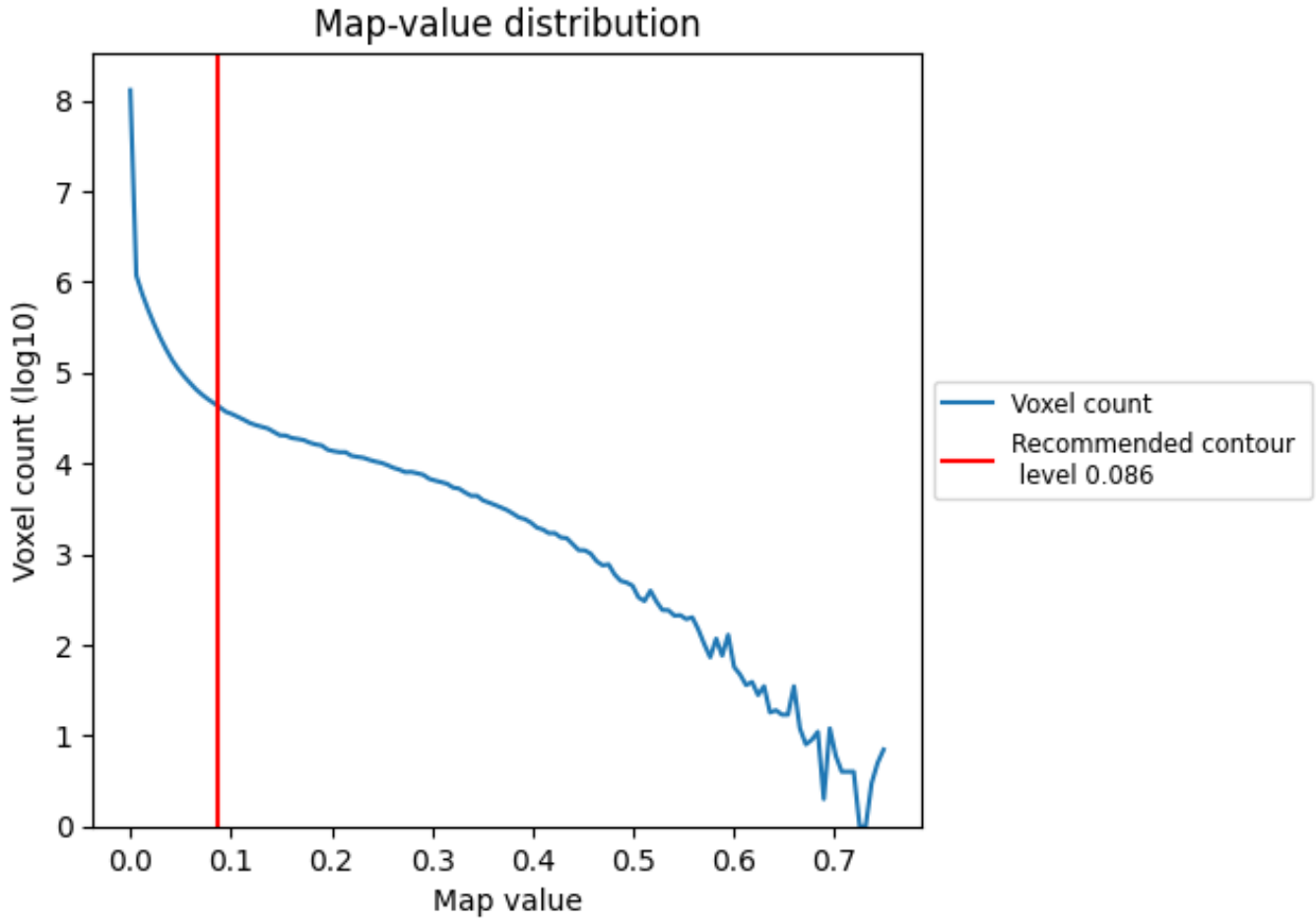
6.6 Mask visualisation (i)

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

7 Map analysis

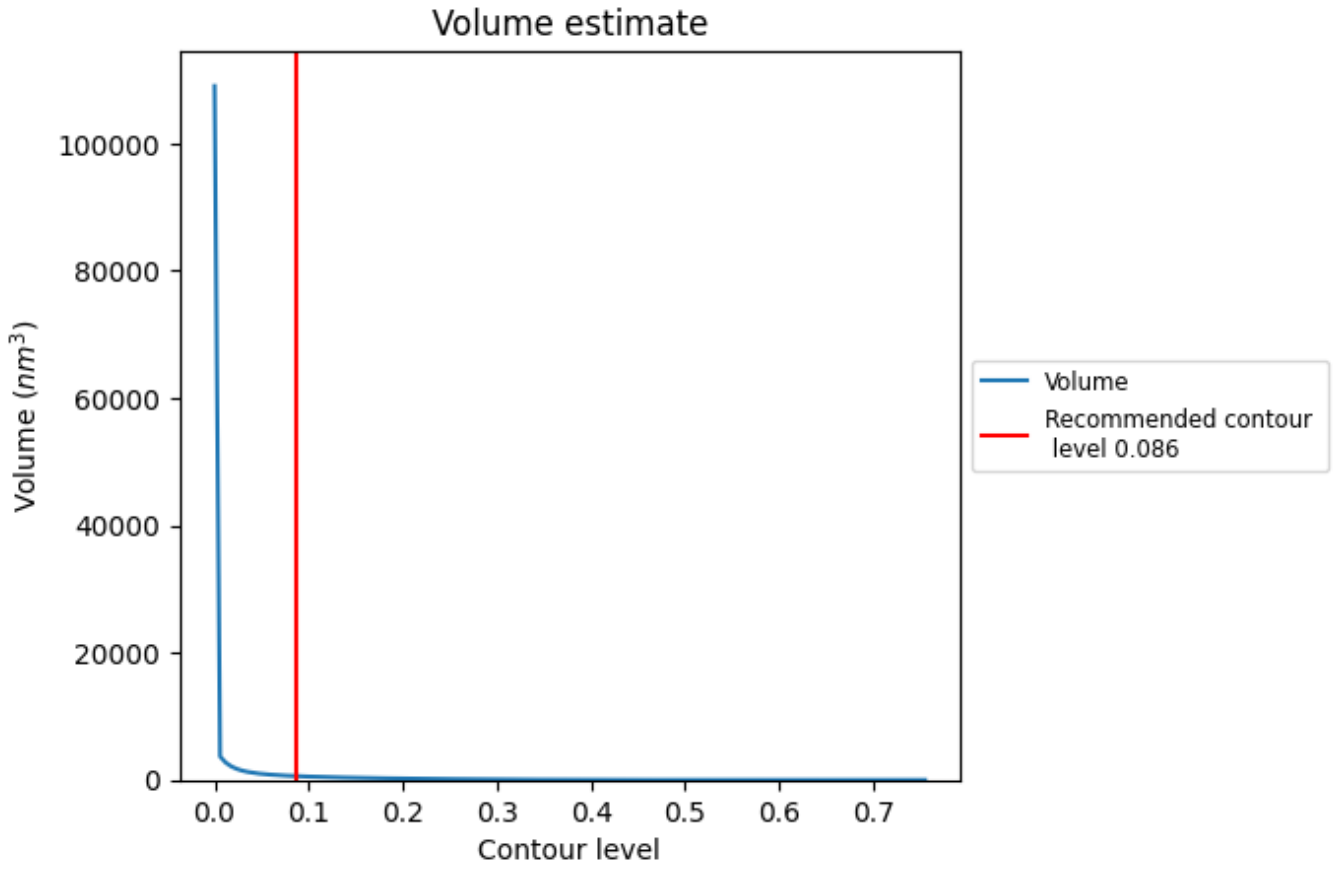
This section contains the results of statistical analysis of the map.

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.

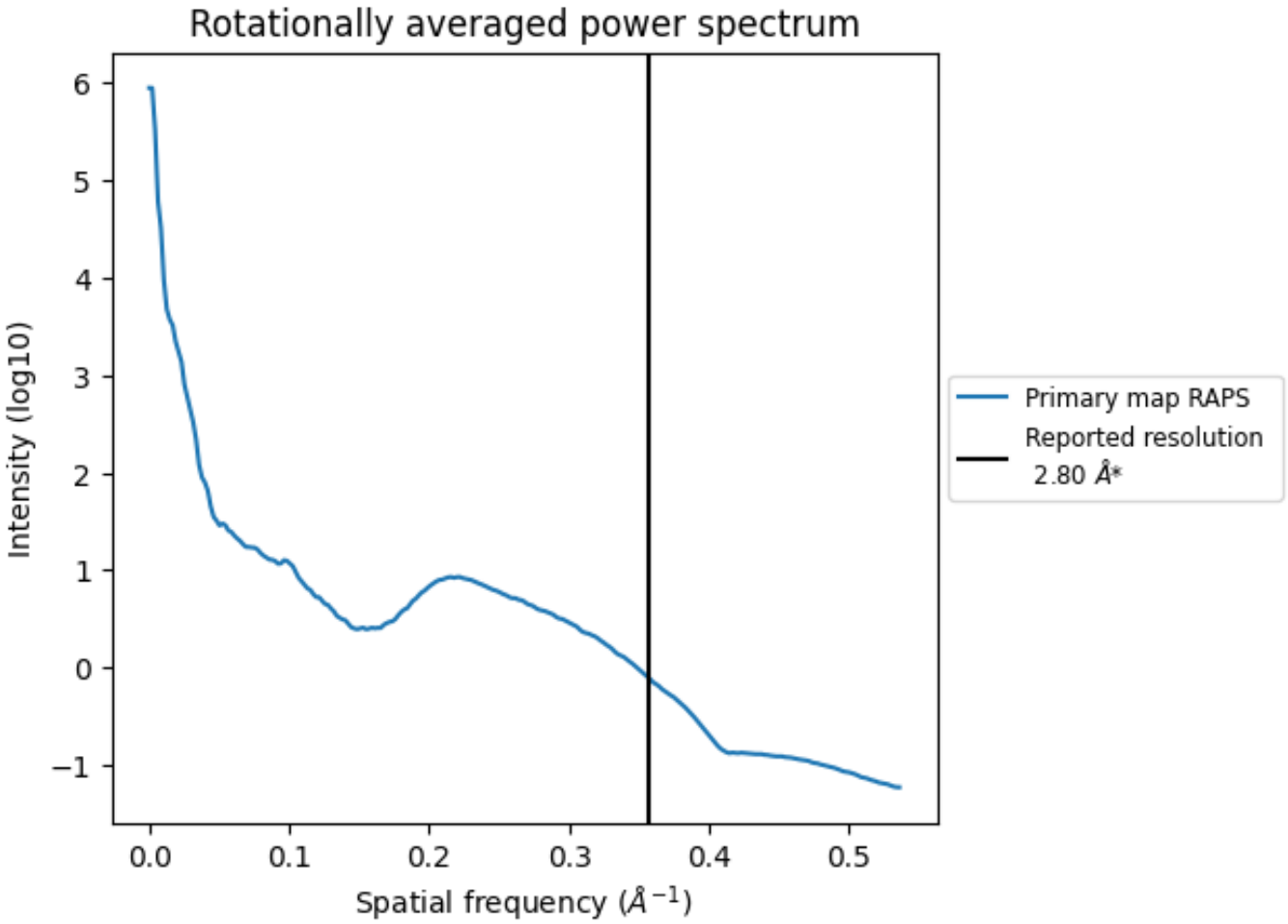
7.2 Volume estimate



The volume at the recommended contour level is 610 nm^3; this corresponds to an approximate mass of 551 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 0.357 Å^{-1}

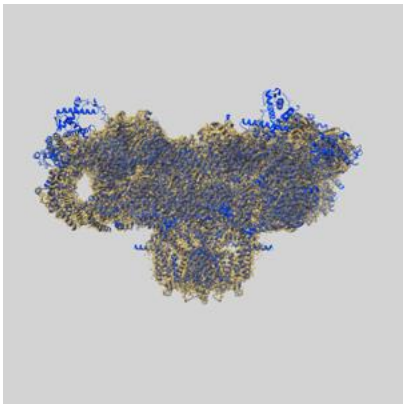
8 Fourier-Shell correlation

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

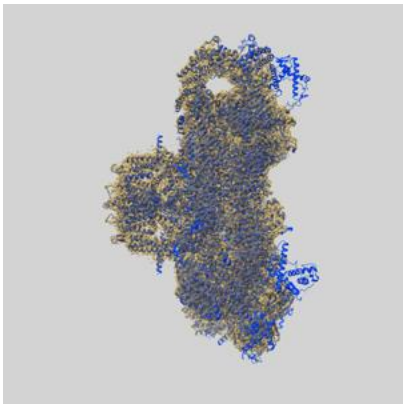
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73953 and PDB model 9Z9O. Per-residue inclusion information can be found in section 3 on page 8.

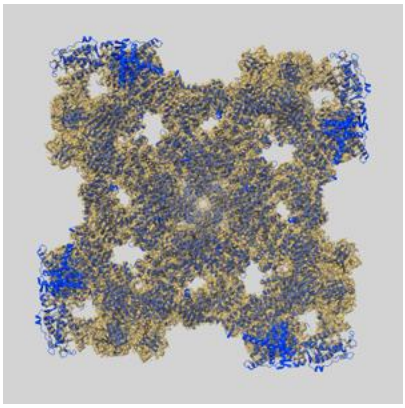
9.1 Map-model overlay



X



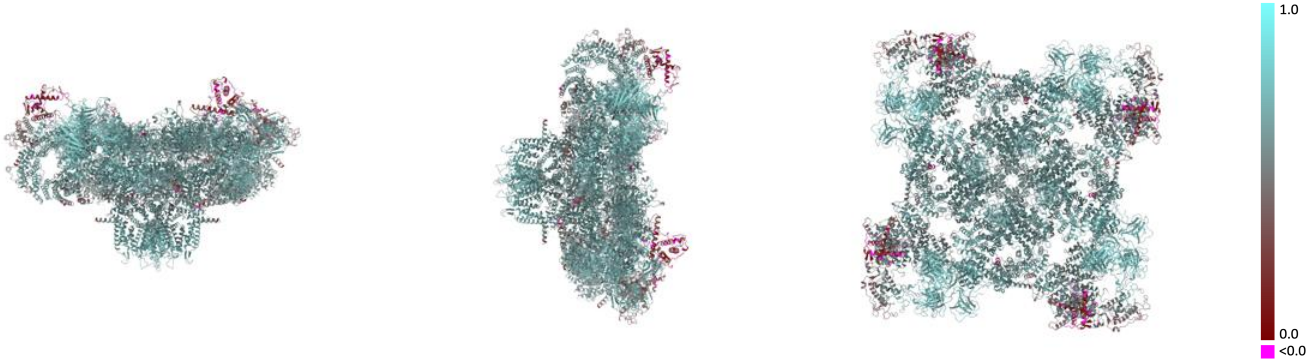
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.086 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

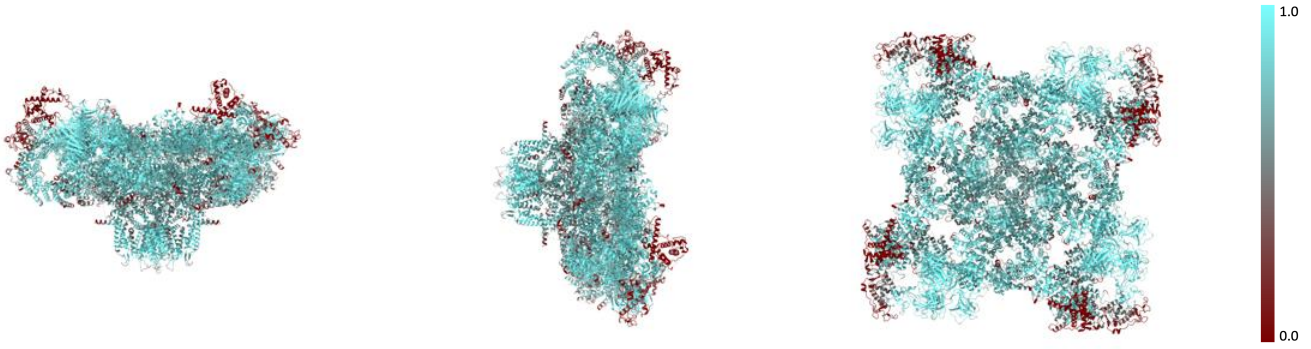
9.2 Q-score mapped to coordinate model



X Y Z

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

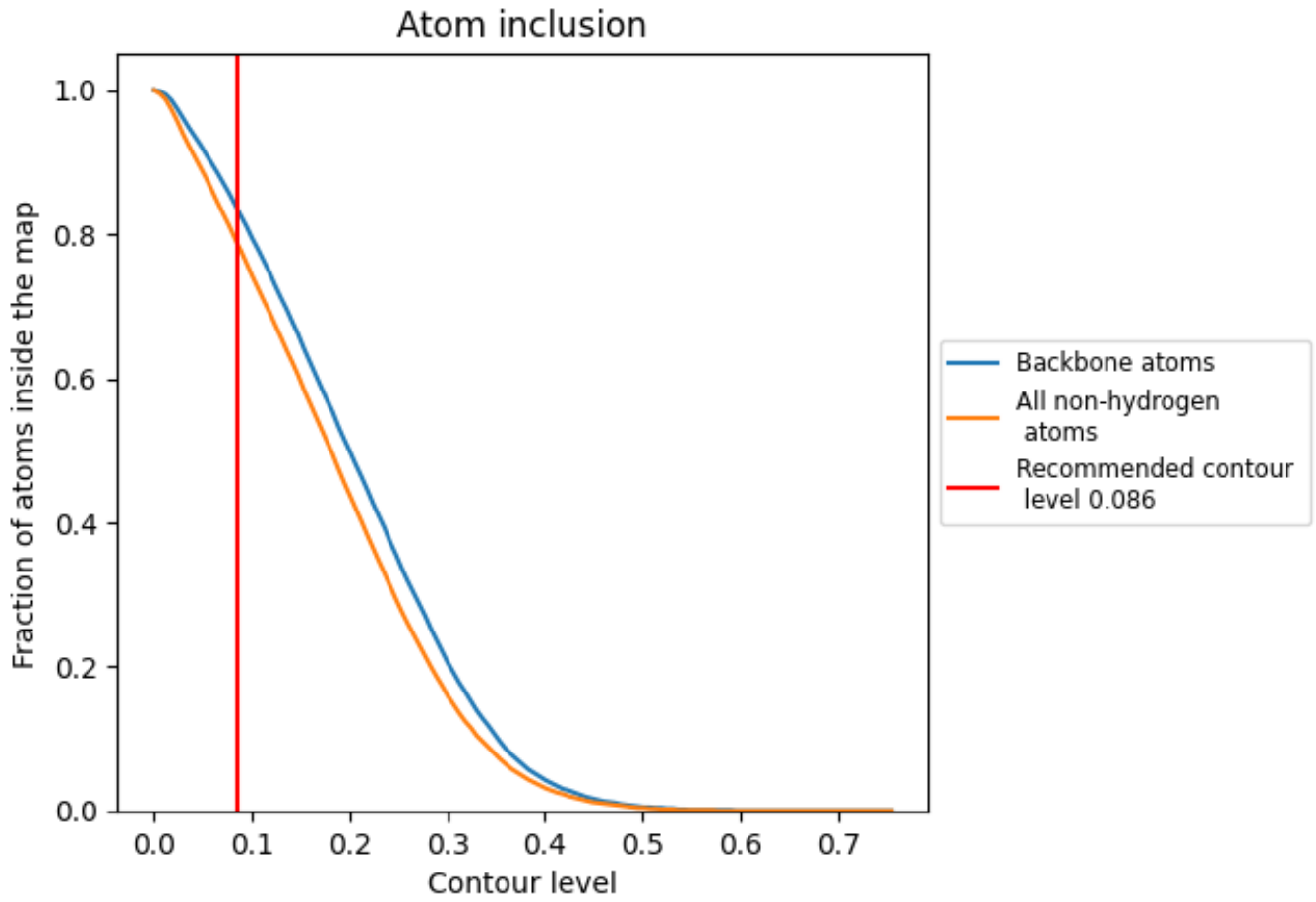
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.086).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.086) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7840	0.6170
A	0.9140	0.6850
B	0.7810	0.6160
C	0.9140	0.6870
D	0.7810	0.6160
E	0.9140	0.6860
F	0.7810	0.6150
G	0.9140	0.6860
H	0.7810	0.6150

