wwPDB EM Validation Summary Report (i)

Oct 28, 2024 – 01:49 AM EDT

PDB ID	:	7UA3
EMDB ID	:	EMD-26413
Title	:	Structure of PKA phosphorylated human RyR2-R2474S in the closed state in the presence of Calmodulin
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2022-03-11
Resolution	:	2.97 Å(reported)
Based on initial model	:	7U9X

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:

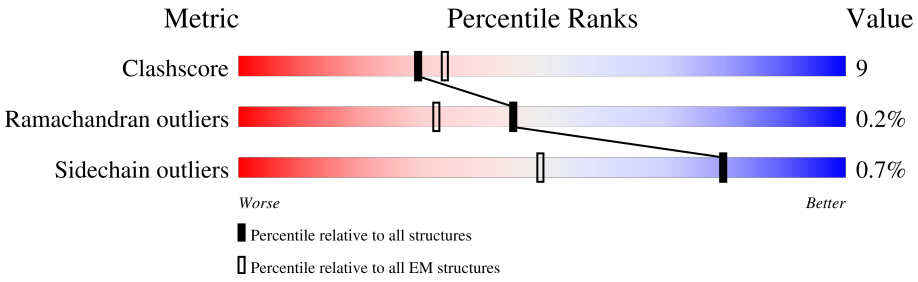
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4967	11% 70% 19% 11%
1	B	4967	11% 70% 19% 11%
1	C	4967	11% 70% 19% 11%
1	D	4967	11% 70% 19% 11%
2	E	108	73% 25% ••
2	F	108	70% 28% ••
2	G	108	73% 25% ••
2	H	108	73% 25% ••

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Mol	Chain	Length	Quality of chain
3	I	149	64% 56% 34% 5% 5%
3	J	149	64% 56% 34% 5% 5%
3	K	149	63% 55% 35% 5% 5%
3	L	149	66% 56% 34% 5% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 150252 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4443	Total 35570	C 22656	N 6059	O 6618	S 237	2	0
1	B	4443	Total 35570	C 22656	N 6059	O 6618	S 237	2	0
1	C	4443	Total 35570	C 22656	N 6059	O 6618	S 237	2	0
1	D	4443	Total 35570	C 22656	N 6059	O 6618	S 237	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2474	SER	ARG	variant	UNP Q92736
B	2474	SER	ARG	variant	UNP Q92736
C	2474	SER	ARG	variant	UNP Q92736
D	2474	SER	ARG	variant	UNP Q92736

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	F	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	G	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	H	107	Total 818	C 516	N 144	O 154	S 4	0	0

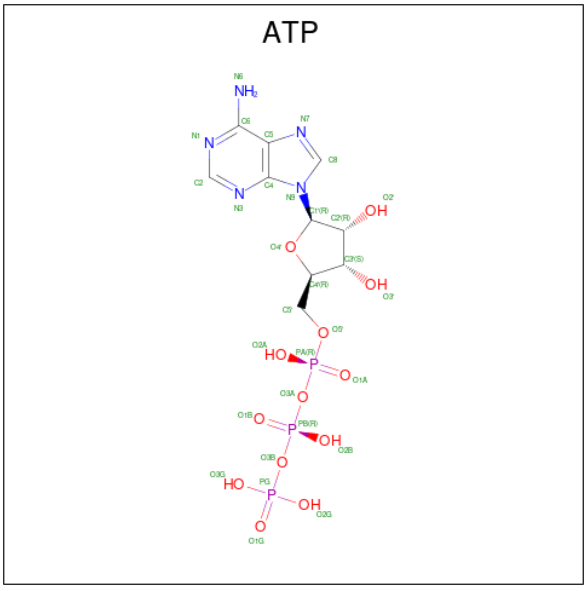
- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
3	J	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
3	K	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
3	L	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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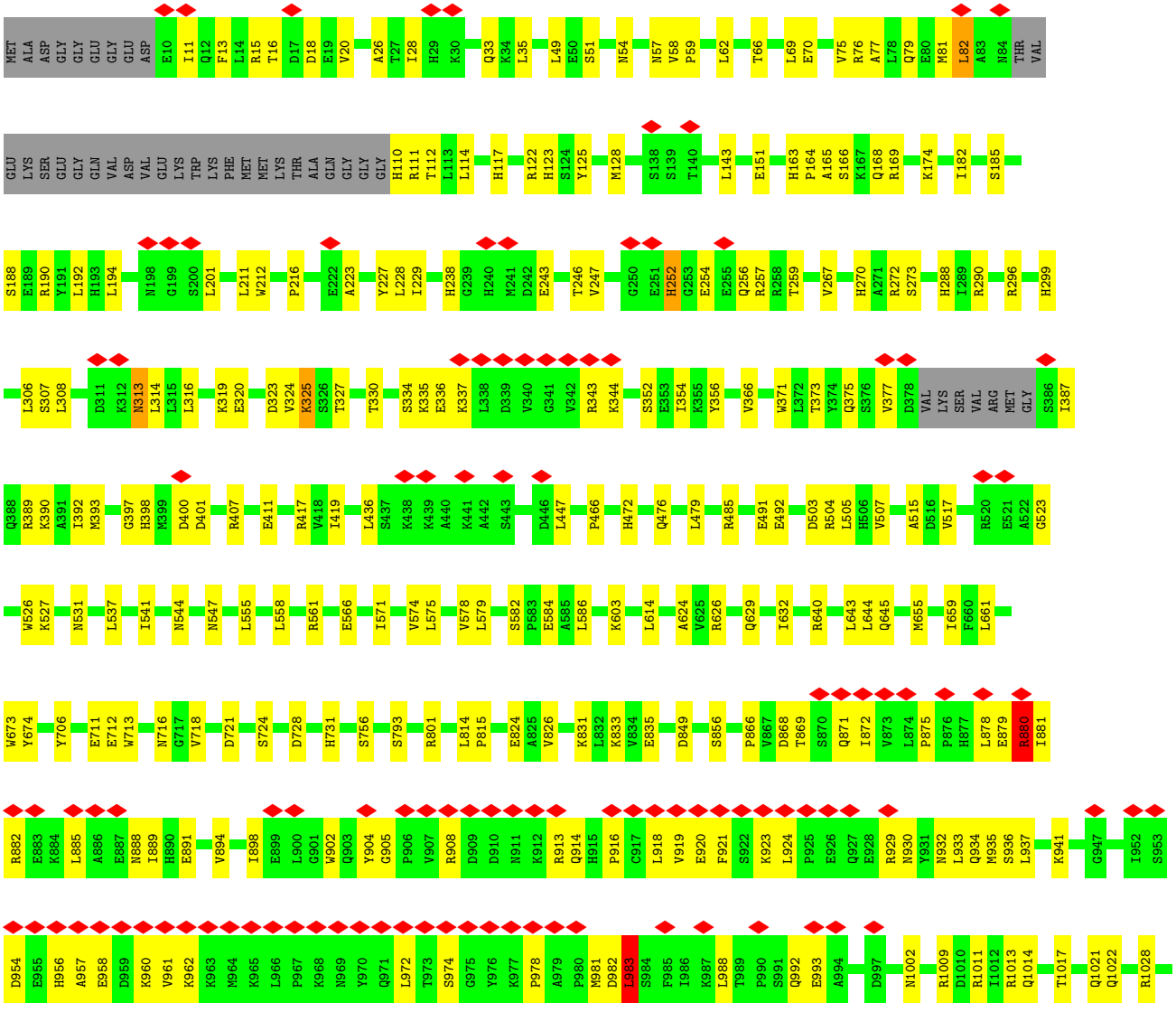
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	D	1	Total	C	N	O	P	0
			31	10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

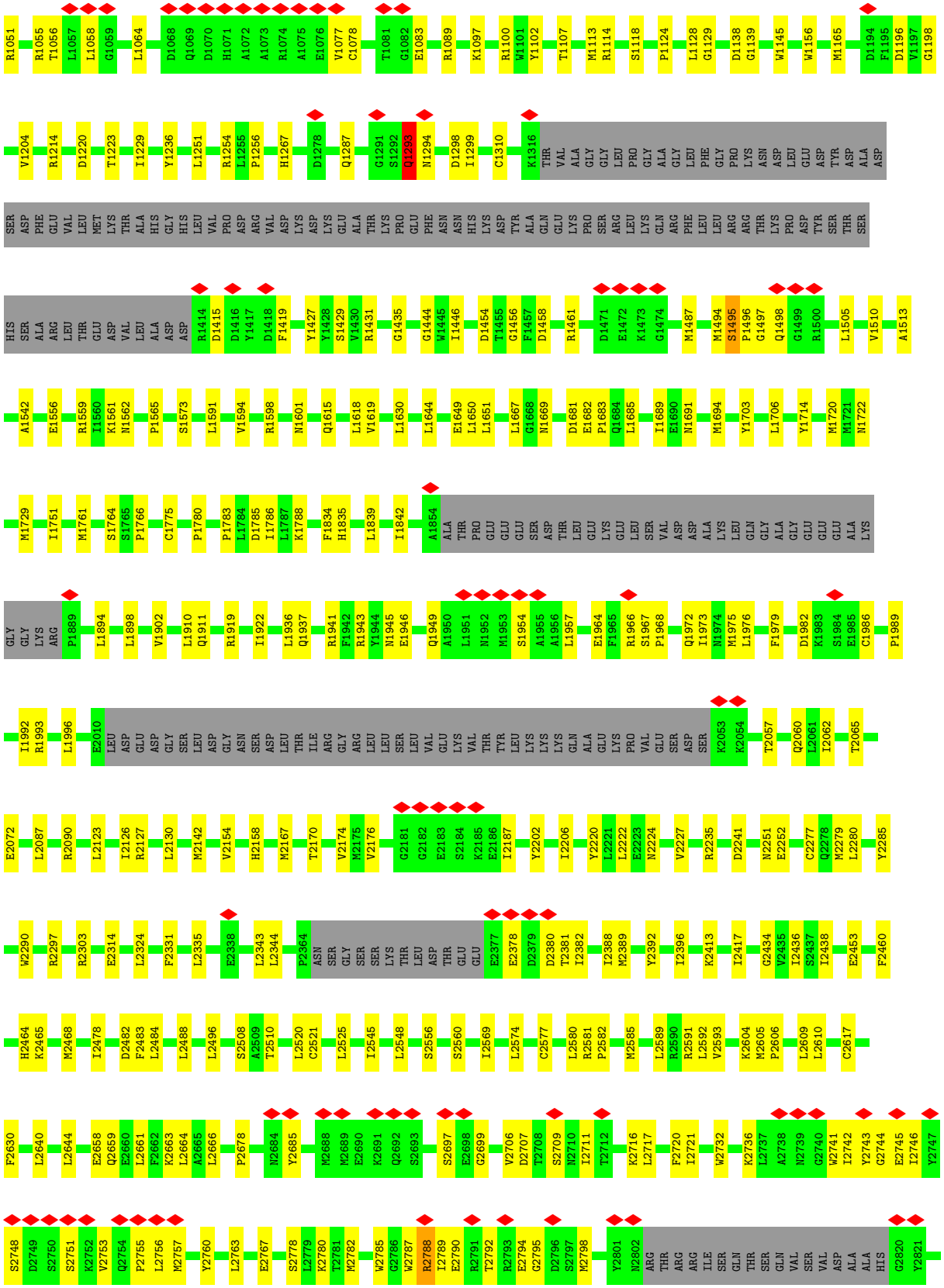
3 Residue-property plots (i)

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: Ryanodine receptor 2

Chain A:

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V1204 R1214 D1220 T1223 I1229 Y1236 L1251 R1254 L1255 P1256 H1267 D1278 Q1287 G1291 S1292 Q1293 N1294 D1298 I1299 C1310 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP
SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER
HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 F1419 Y1427 Y1428 S1429 V1430 R1431 G1435 G1444 W1445 I1446 D1454 T1455 G1456 F1457 D1458 R1461 D1471 E1472 K1473 G1474 M1487 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 L1505 V1510 A1513
A1542 E1556 R1559 I1560 K1561 N1562 P1565 S1573 L1591 V1594 R1598 N1601 Q1615 L1618 V1619 L1630 L1644 E1649 L1650 L1651 L1667 G1668 N1669 D1681 E1682 P1683 Q1684 L1685 I1689 E1690 N1691 M1694 Y1703 L1706 Y1714 M1720 M1721 N1722
M1729 I1751 M1761 S1764 S1765 P1766 C1775 P1780 P1783 L1784 D1785 I1786 L1787 K1788 F1834 H1835 L1839 I1842 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS
GLY GLY LYS ARG P1889 L1894 L1898 V1902 L1910 Q1911 R1919 I1922 L1936 Q1937 R1941 F1942 R1943 Y1944 N1945 E1946 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 E1964 F1965 R1966 S1967 P1968 Q1972 I1973 N1974 M1975 L1976 F1979 D1982 K1983 S1984 E1985 C1986 P1989
I1992 R1993 L1996 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 T2057 Q2060 L2061 I2062 T2065
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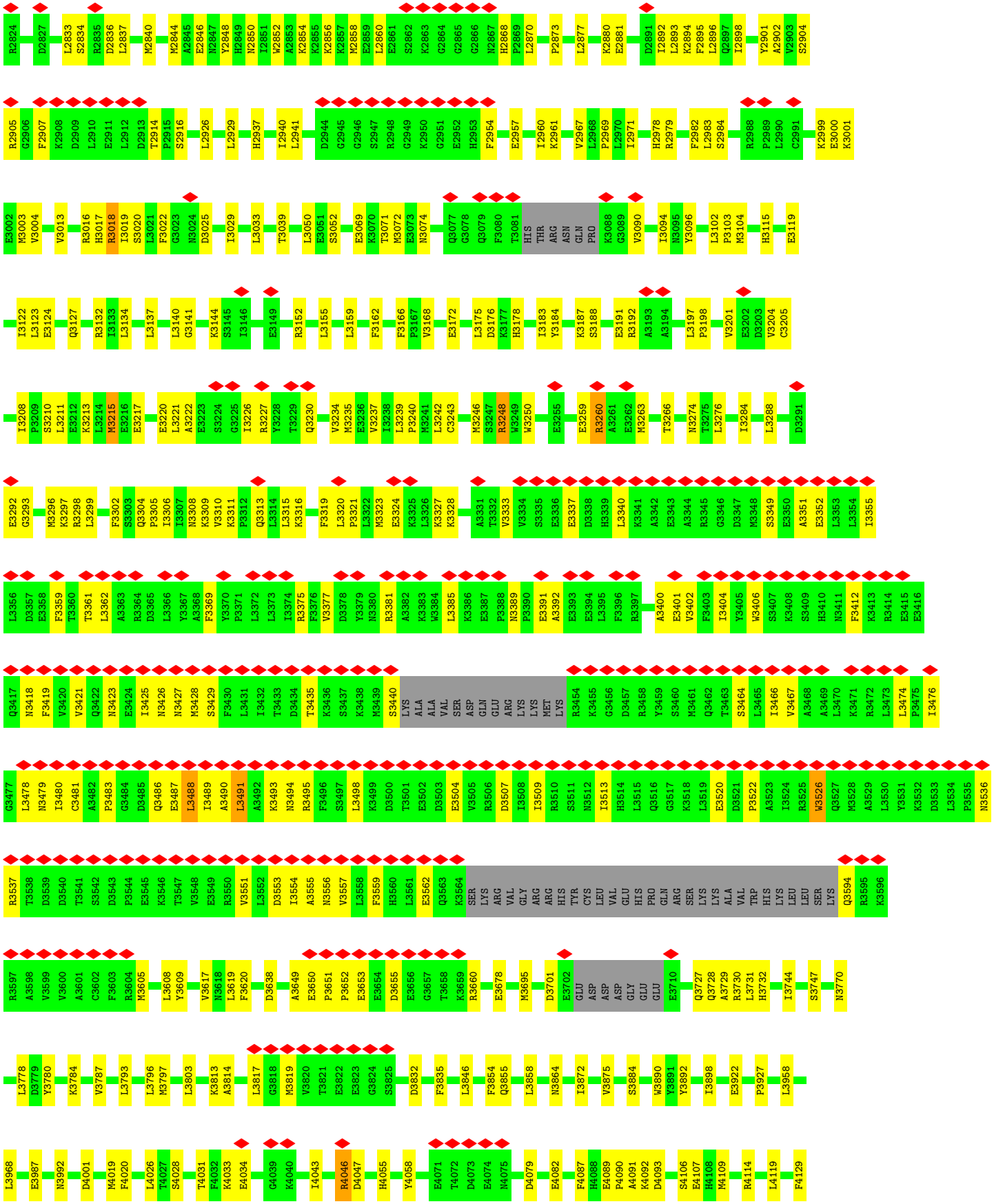
H2464 K2465 M2468 I2478 D2482 F2483 L2484 L2488 L2496 S2508 A2509 T2510 L2520 C2521 L2525 I2545 L2548 S2556 S2560 I2569 L2574 C2577 L2580 R2581 P2582 M2585 L2589 R2590 R2591 L2592 V2593 K2604 M2605 P2606 L2609 L2610 C2617
F2630 L2640 L2644 E2658 Q2659 E2660 L2661 F2662 K2663 L2664 A2665 L2666 P2678 N2684 Y2685 M2688 M2689 E2690 K2691 Q2692 S2693 S2697 E2698 G2699 V2706 D2707 T2708 S2709 W2710 I2711 T2712 K2716 L2717 F2720 I2721 W2732 K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745 I2746 Y2747
S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 Y2760 L2763 E2767 S2778 L2779 K2780 T2781 M2782 W2785 G2786 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796 S2797 M2798 Y2801 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821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R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 S2916 L2926 L2929 H2937 I2940 L2941 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 E2957 I2960 K2961 V2967 L2968 P2969 L2970 I2971 H2978 R2979 F2982 L2983 S2984 R2988 P2989 L2990 C2991 K2999 E3000 K3001
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I3122 L3123 E3124 Q3127 R3132 I3133 L3134 L3137 L3140 G3141 K3144 S3145 I3146 E3149 R3152 L3155 L3159 F3162 F3166 P3167 V3168 E3172 L3175 D3176 K3177 H3178 I3183 Y3184 K3187 S3188 E3191 R3192 A3193 A3194 L3197 P3198 V3201 E3202 D3203 V3204 C3205
I3208 P3209 S3210 L3211 E3212 K3213 L3214 M3215 E3216 E3217 E3220 L3221 A3222 E3223 S3224 G3225 I3226 R3227 Y3228 T3229 Q3230 V3234 M3235 E3236 V3237 I3238 L3239 P3240 M3241 L3242 C3243 M3246 S3247 R3248 W3249 W3250 E3255 E3259 R3260 A3261 E3262 M3263 T3266 N3274 T3275 L3276 I3284 L3288 D3291
E3292 G3293 M3296 K3297 R3298 L3299 F3302 S3303 Q3304 P3305 I3306 I3307 N3308 K3309 V3310 K3311 P3312 Q3313 L3314 L3315 K3316 F3319 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 K3328 A3331 T3332 V3333 V3334 S3335 E3336 E3337 D3338 H3339 L3340 K3341 A3342 E3343 A3344 R3345 G3346 D3347 M3348 S3349 E3350 A3351 E3352 L3353 L3354 I3355
L3356 D3357 E3358 F3359 T3360 T3361 L3362 A3363 R3364 D3365 L3366 Y3367 A3368 F3369 Y3370 P3371 L3372 L3373 I3374 R3375 F3376 V3377 D3378 Y3379 N3380 R3381 A3382 K3383 W3384 L3385 K3386 E3387 P3388 N3389 P3390 E3391 A3392 E3393 E3394 L3395 F3396 R3397 A3400 E3401 V3402 F3403 I3404 Y3405 W3406 S3407 K3408 S3409 H3410 N3411 F3412 K3413 R3414 E3415 E3416
Q3417 N3418 F3419 V3420 V3421 Q3422 N3423 E3424 I3425 N3426 N3427 M3428 S3429 F3430 L3431 I3432 T3433 D3434 T3435 K3436 S3437 K3438 M3439 S3440 LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS R3454 K3455 G3456 D3457 R3458 Y3459 S3460 M3461 Q3462 T3463 S3464 L3465 I3466 V3467 A3468 A3469 L3470 K3471 R3472 L3473 L3474 P3475 I3476
G3477 L3478 N3479 I3480 C3481 A3482 P3483 G3484 D3485 Q3486 E3487 L3488 I3489 A3490 L3491 A3492 K3493 N3494 R3495 F3496 S3497 L3498 K3499 D3500 T3501 E3502 D3503 E3504 V3505 R3506 D3507 I3508 I3509 R3510 S3511 N3512 I3513 H3514 L3515 Q3516 G3517 K3518 L3519 E3520 D3521 P3522 A3523 I3524 R3525 W3526 Q3527 M3528 A3529 L3530 Y3531 K3532 D3533 L3534 P3535 N3536
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R3597 A3598 V3599 V3600 A3601 C3602 F3603 R3604 M3605 L3608 Y3609 V3617 N3618 L3619 F3620 D3638 A3649 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 E3678 M3695 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 Q3727 Q3728 A3729 R3730 L3731 H3732 I3744 S3747 N3770
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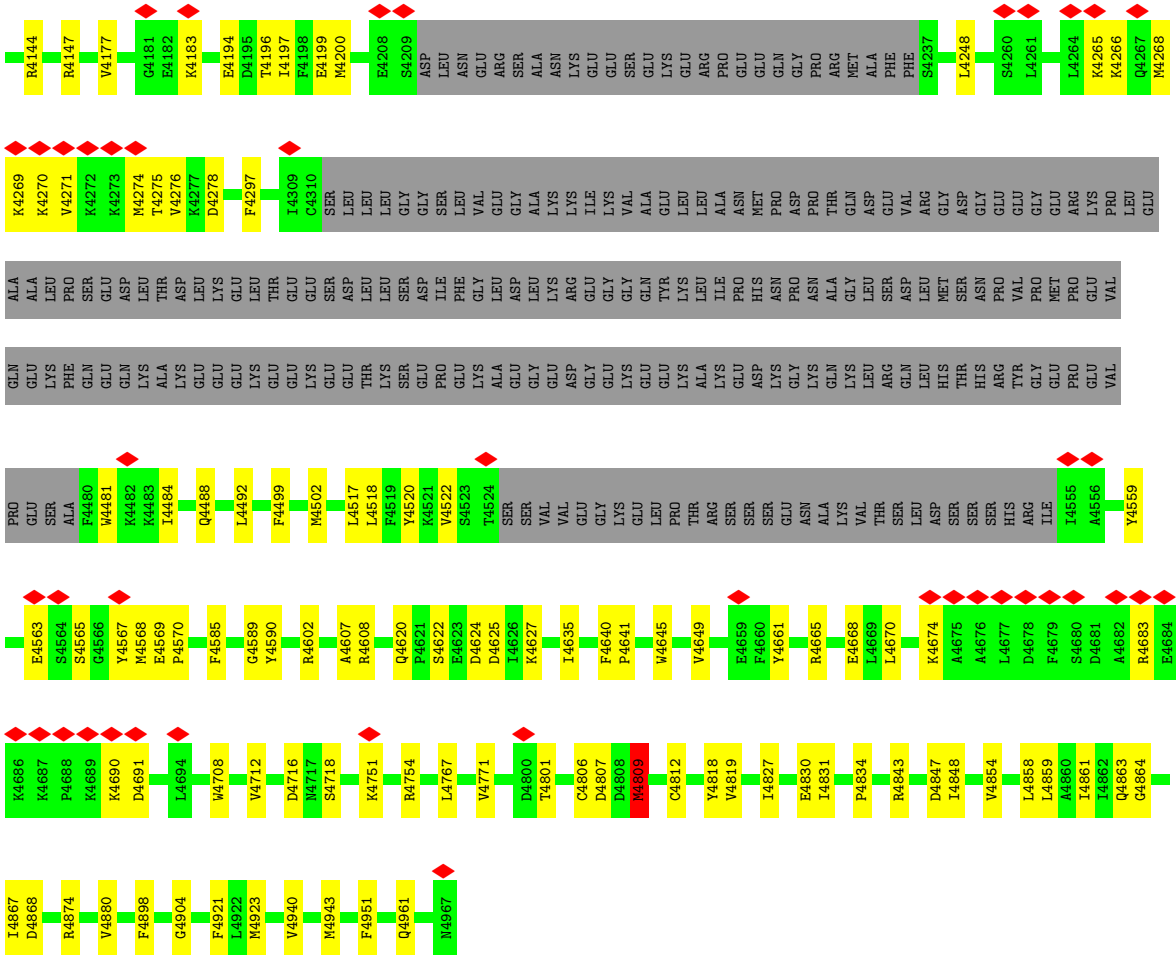
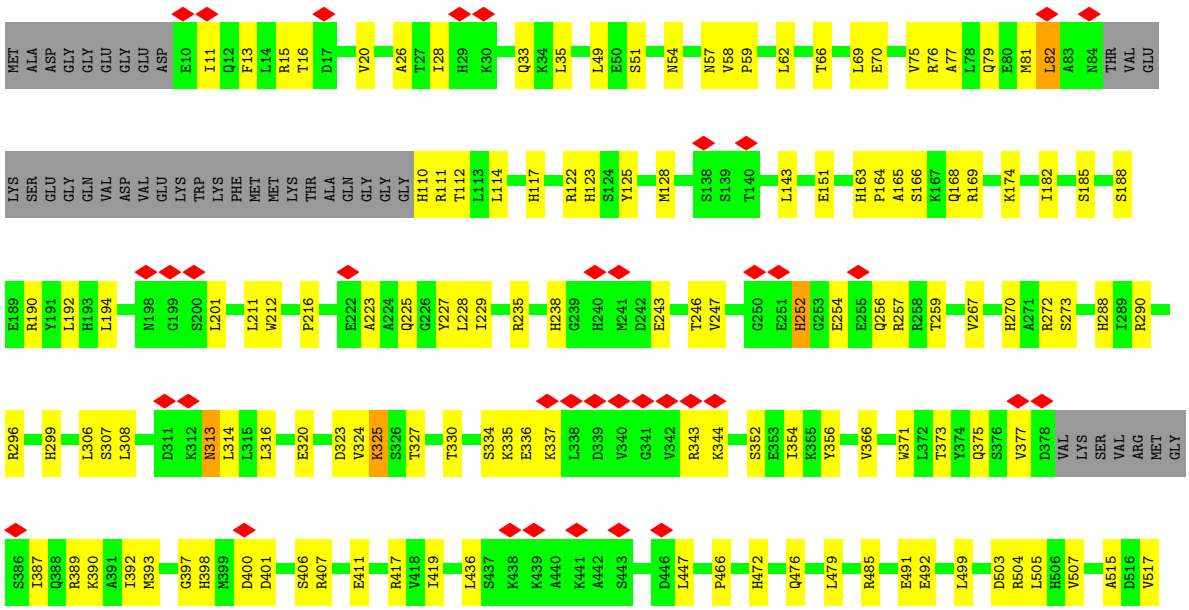
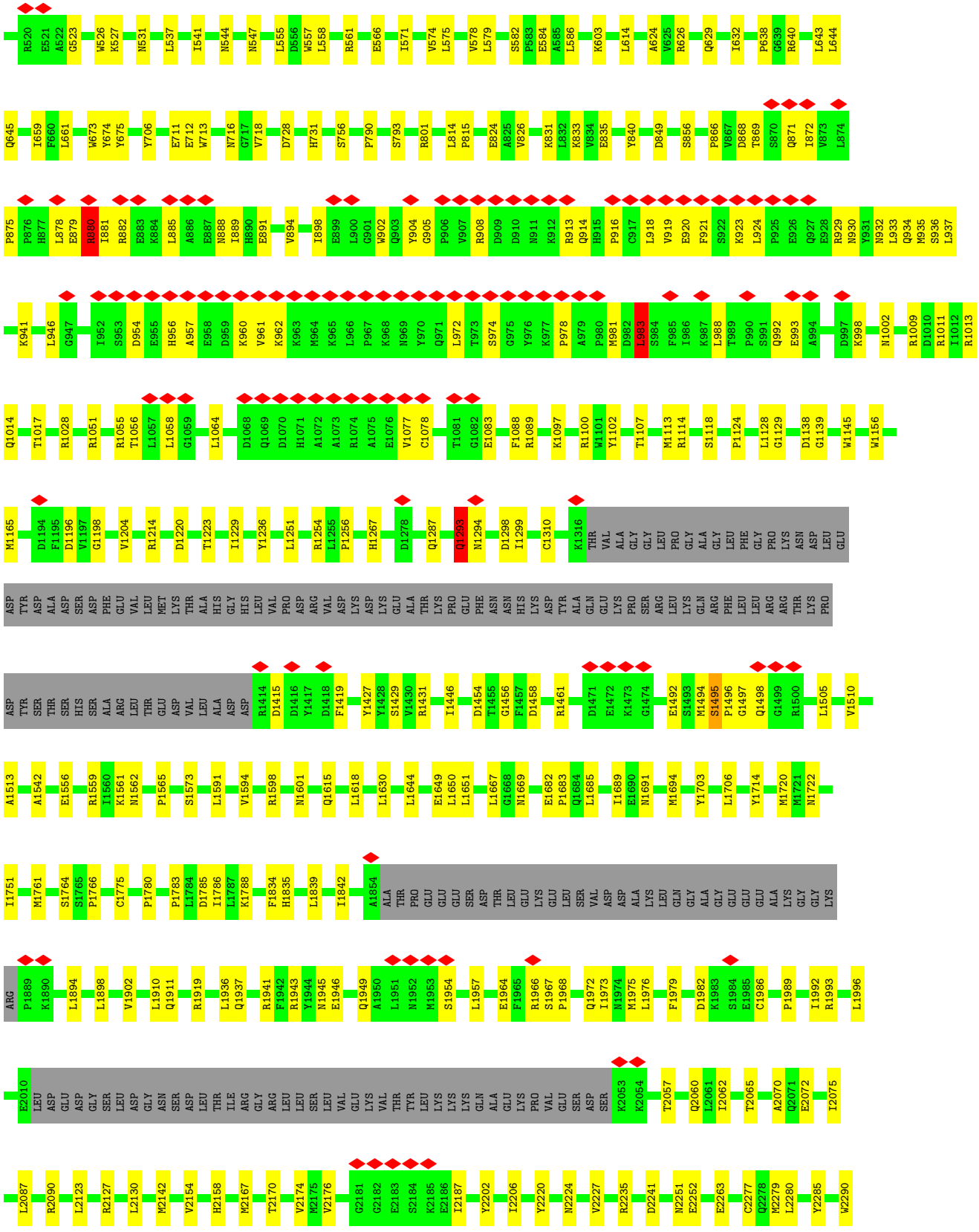


• Molecule 1: Ryanodine receptor 2

Chain B:

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Q1014 T1017 R1028 R1051 R1055 T1056 L1057 L1058 G1059 L1064 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 T1081 G1082 E1083 F1088 R1089 K1097 R1100 W1101 Y1102 T1107 M1113 R1114 S1118 P1124 L1128 G1129 D1138 G1139 W1145 W1156
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ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO
ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 F1419 Y1427 Y1428 S1429 V1430 R1431 I1446 D1454 T1455 G1456 F1457 D1458 R1461 D1471 E1472 K1473 G1474 E1492 S1493 M1494 S1495 P1496 G1497 Q1498 G1499 R1500 L1505 V1510
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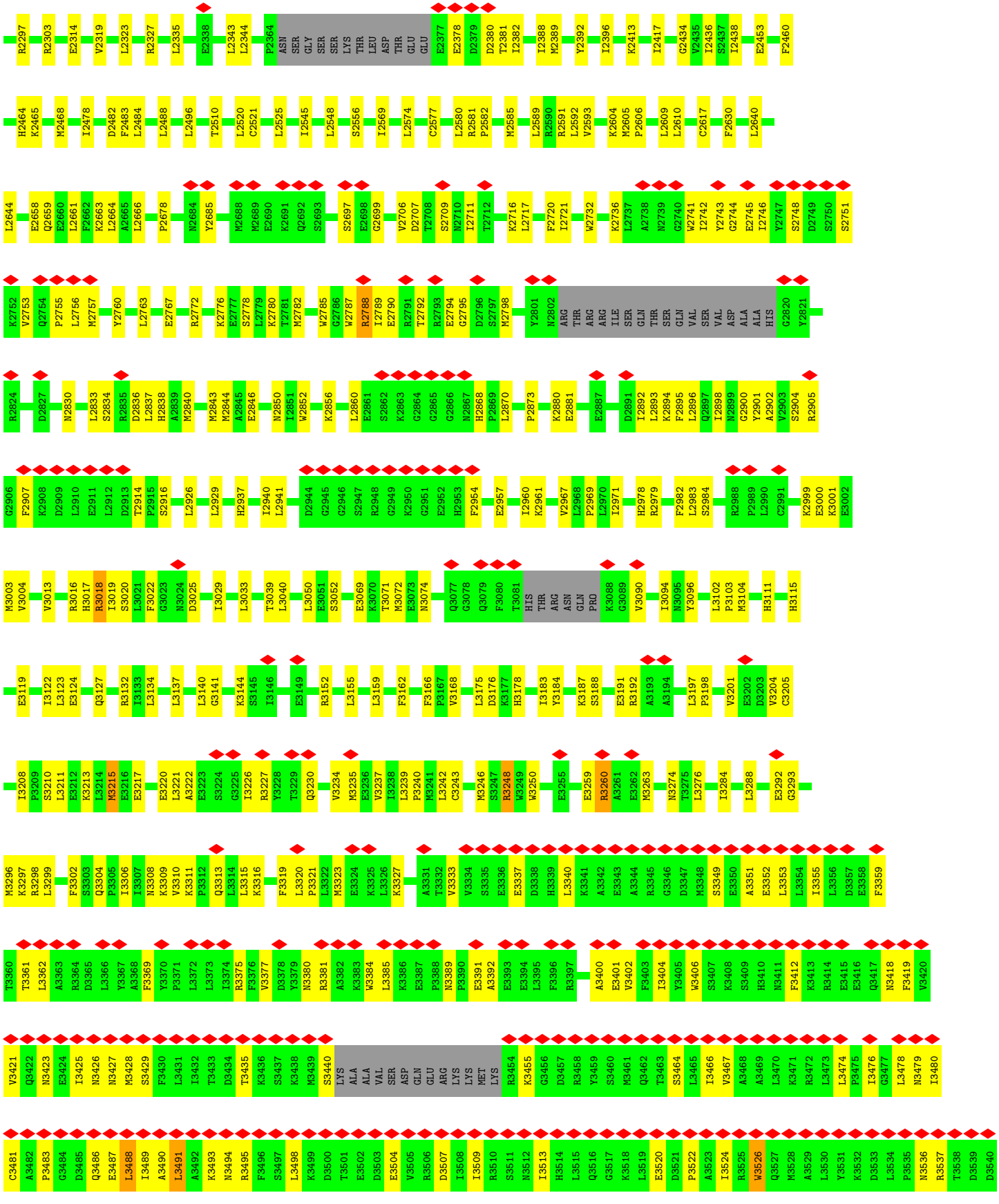
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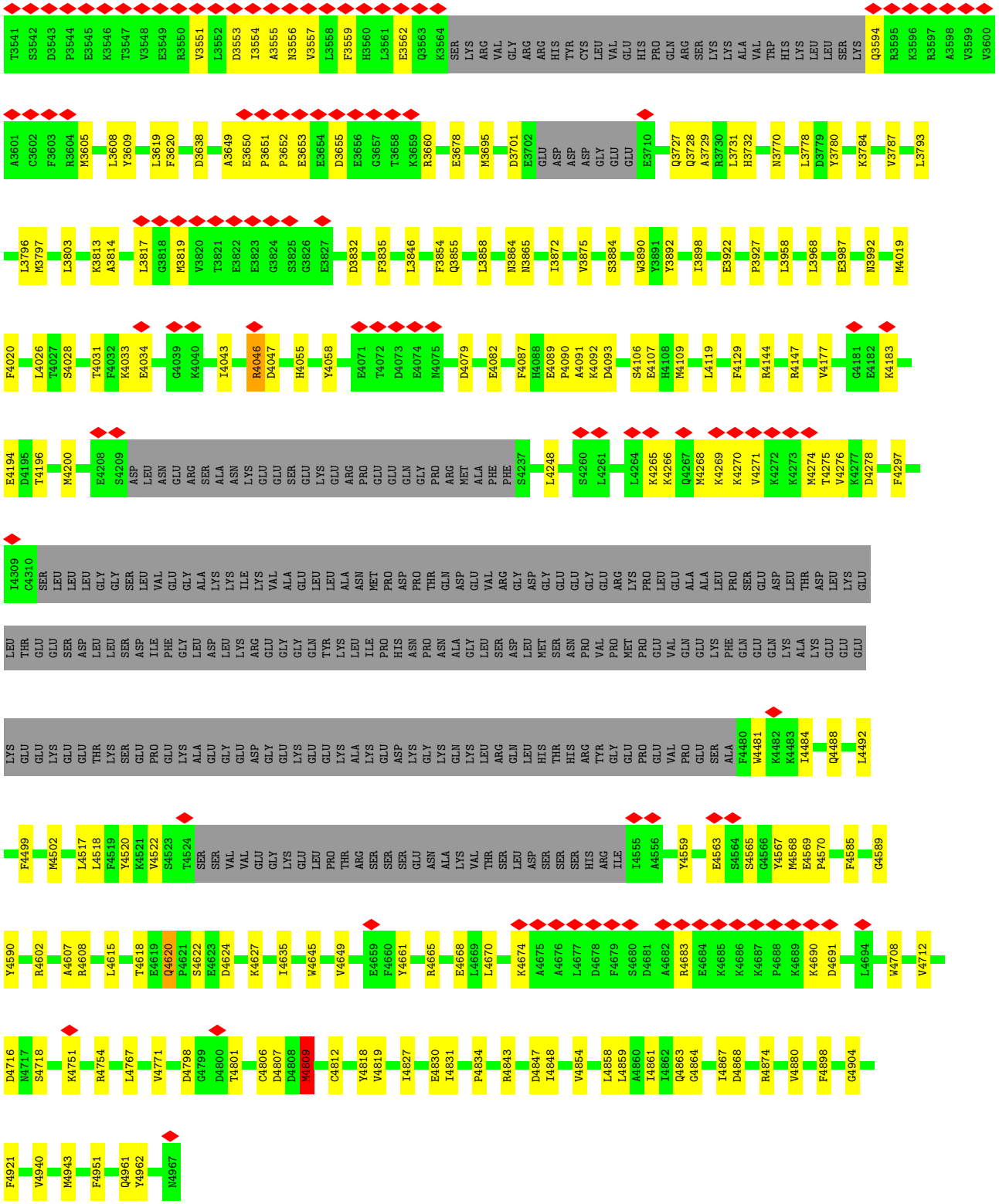
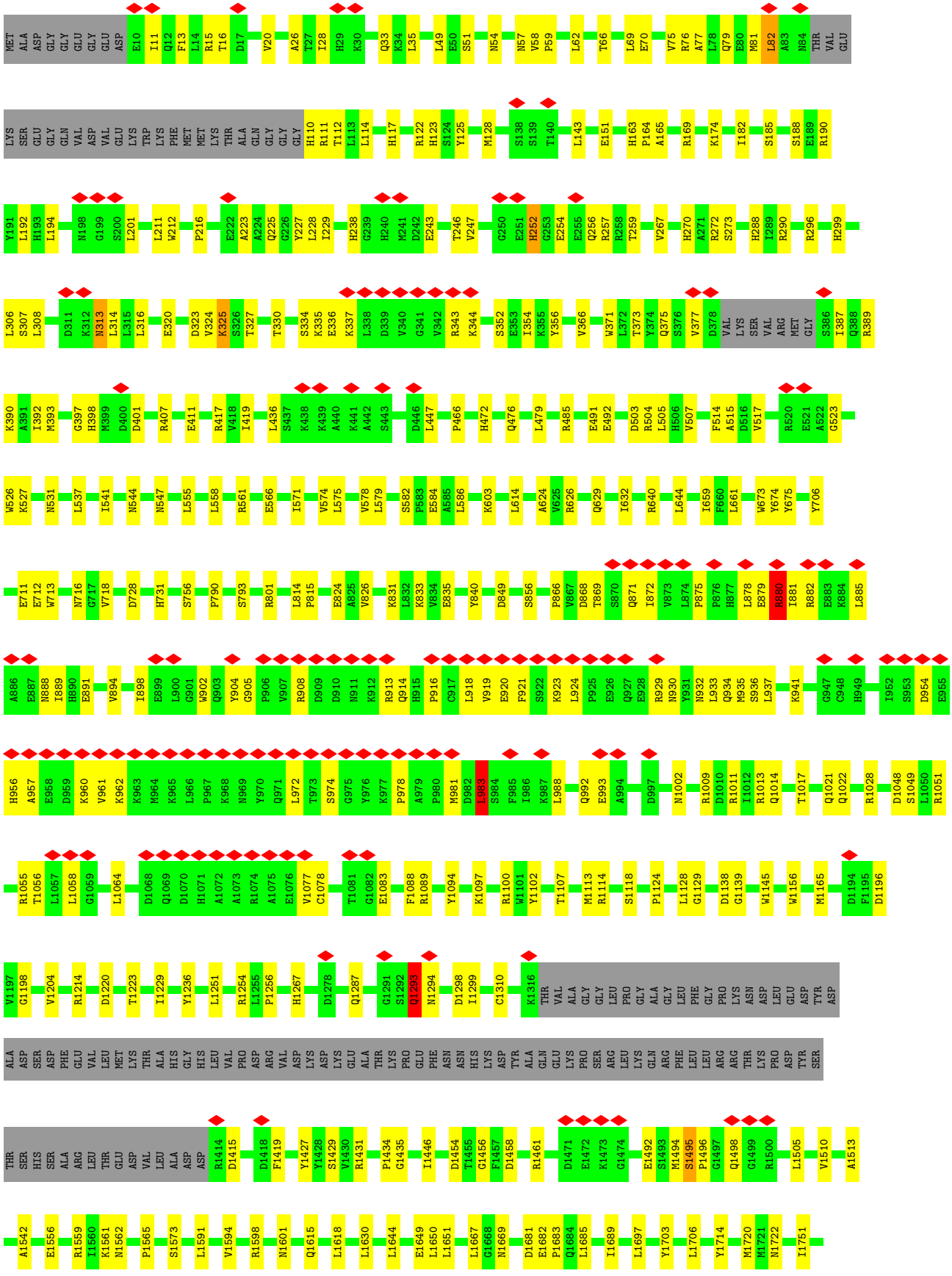


• Molecule 1: Ryanodine receptor 2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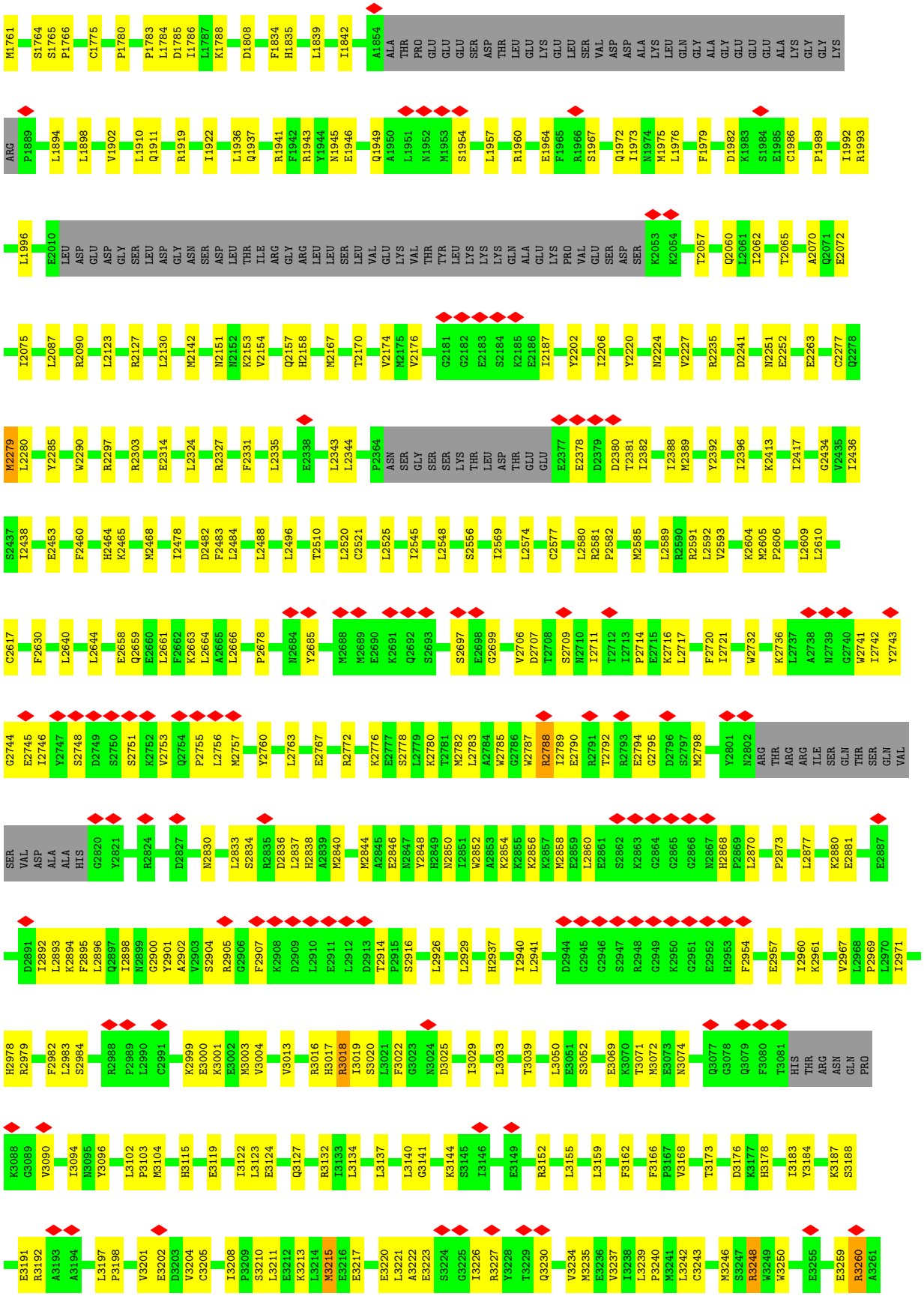
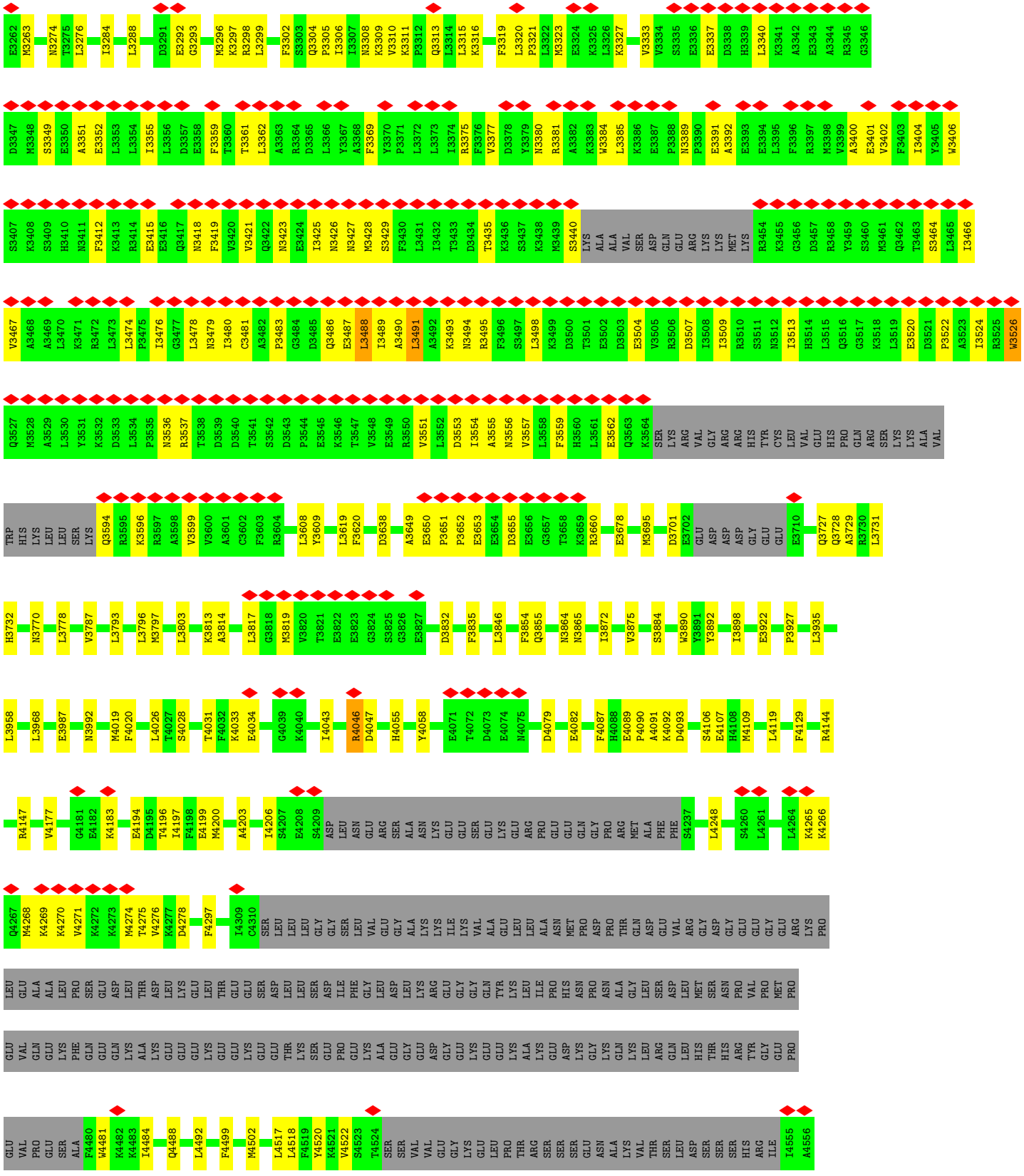
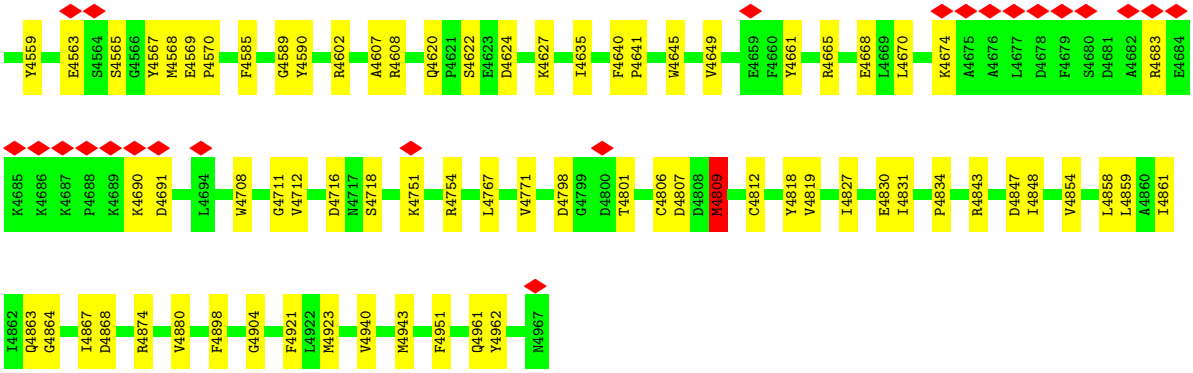
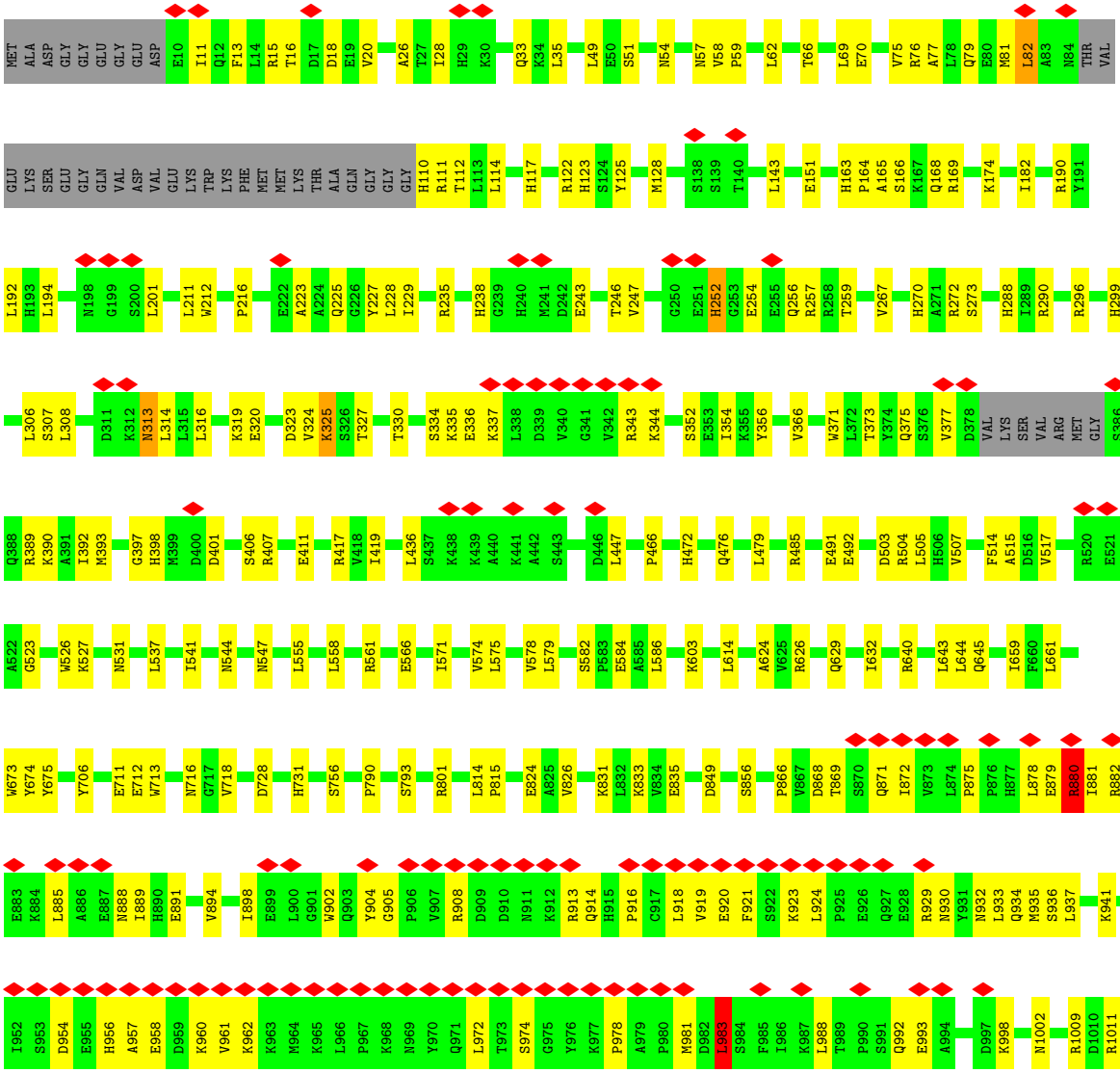


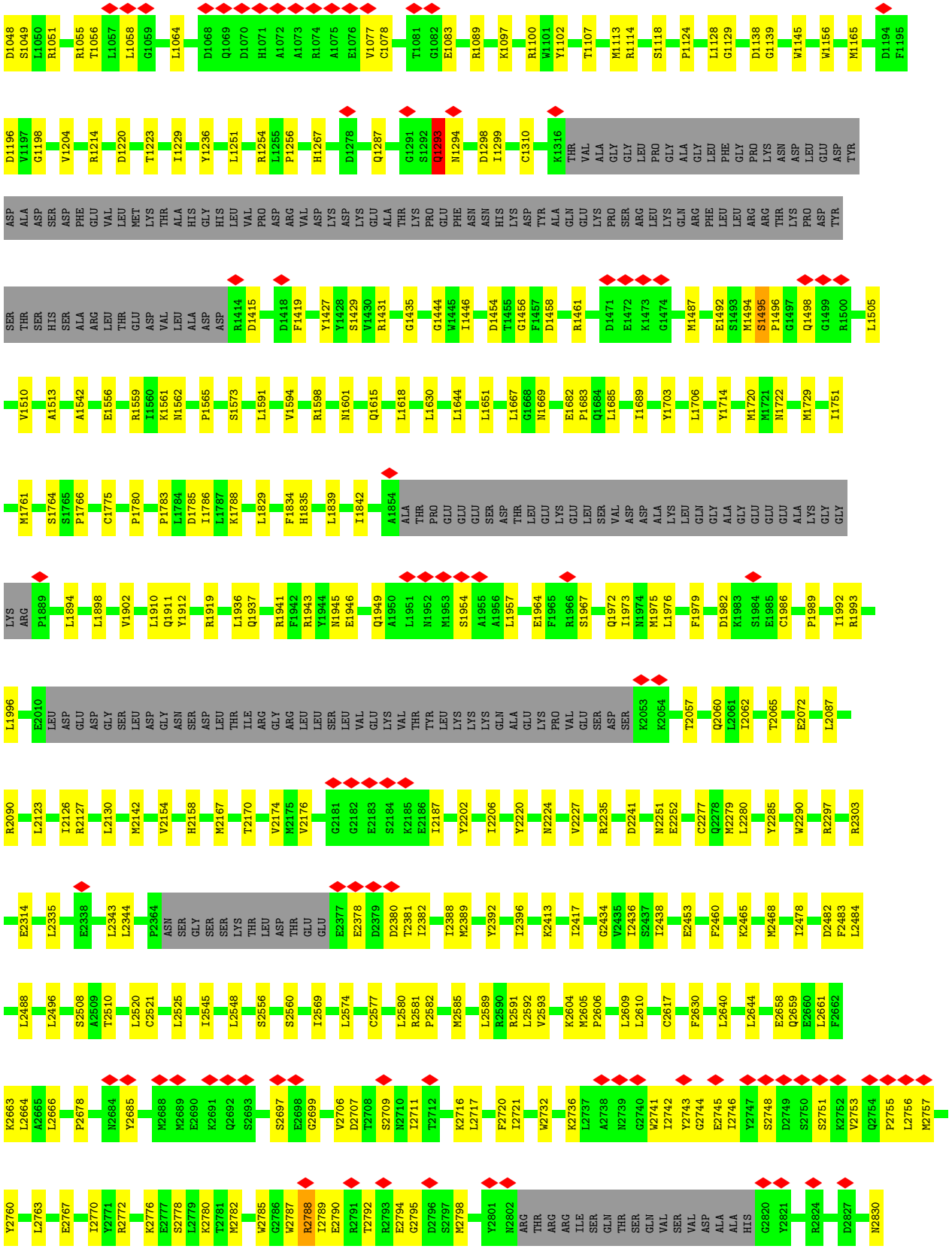




• Molecule 1: Ryanodine receptor 2

Chain D:

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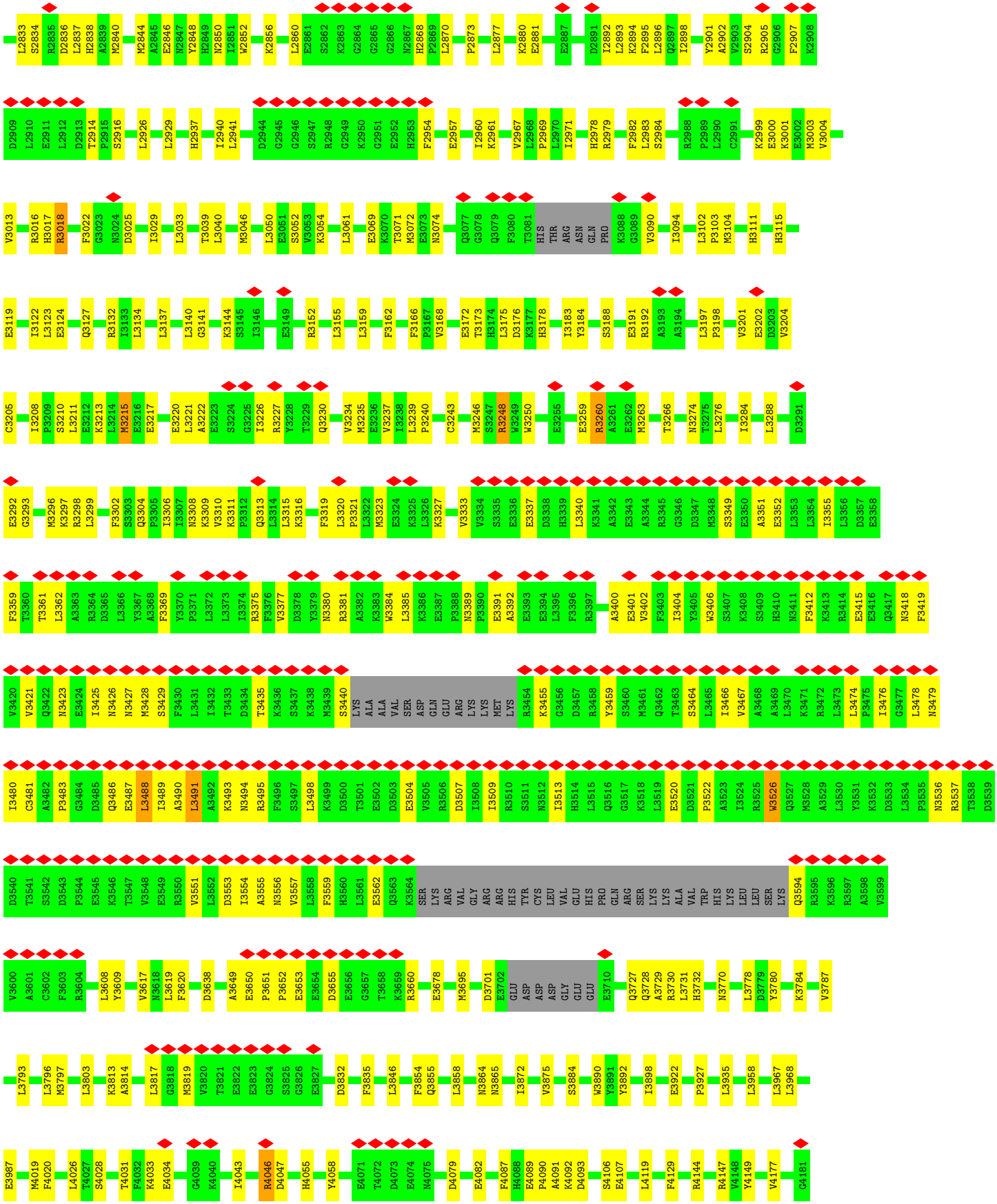
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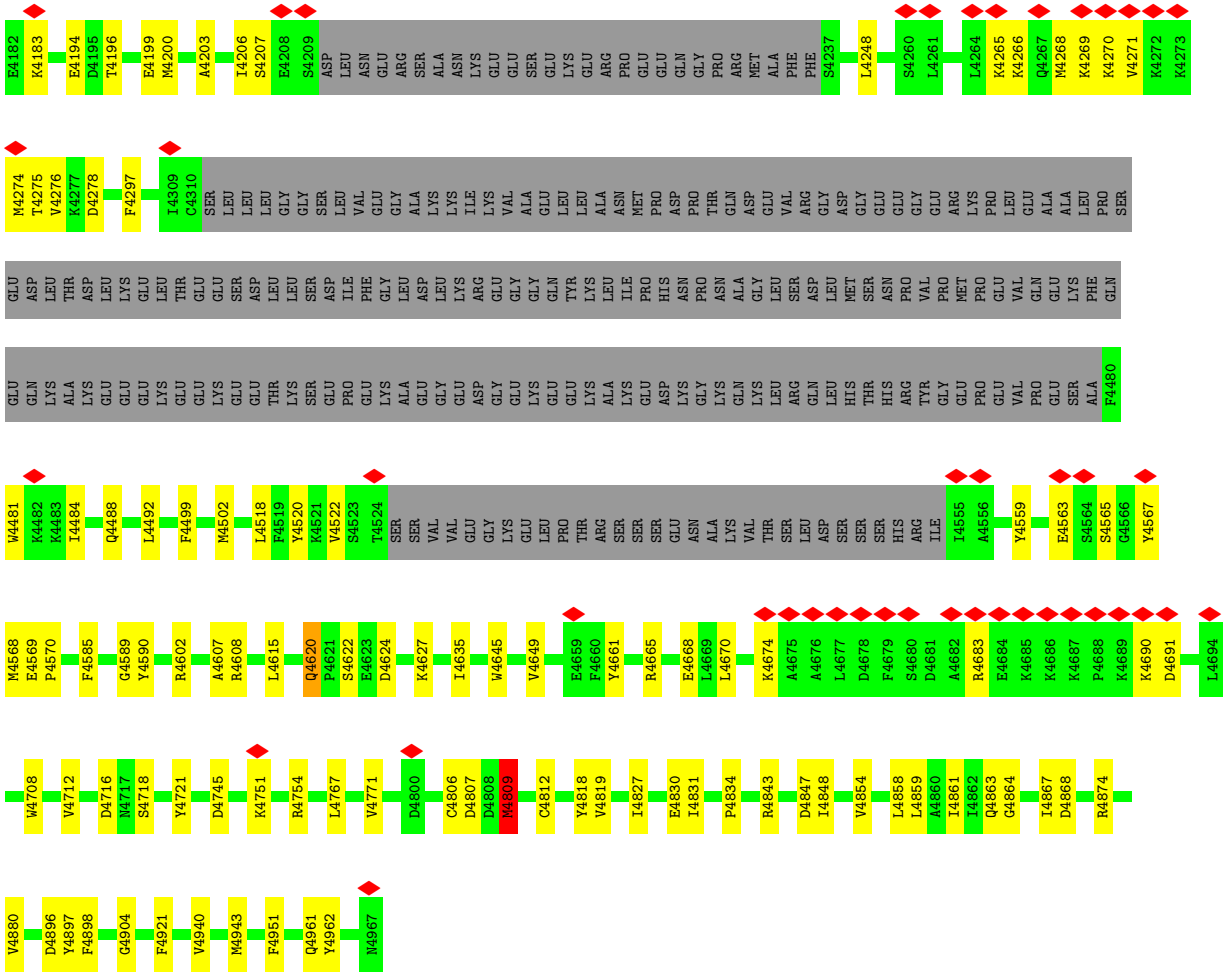
D3540 T3541 S3542 D3543 P3544 E3545 K3546 T3547 V3548 E3549 R3550 V3551 L3552 D3553 I3554 A3555 N3556 V3557 L3558 F3559 H3560 L3561 E3562 Q3563 K3564 SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU LEU SER LYS Q3594 R3595 K3596 R3597 A3598 V3599
V3600 A3601 C3602 F3603 R3604 L3608 Y3609 V3617 N3618 L3619 F3620 D3638 A3649 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 E3678 M3695 D3701 E3702 GLU ASP ASP GLY GLU GLU E3710 Q3727 Q3728 A3729 R3730 L3731 H3732 N3770 L3778 D3779 Y3780 K3784 V3787
L3793 L3796 M3797 L3803 K3813 A3814 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 G3826 E3827 D3832 F3835 L3846 F3854 Q3855 L3858 N3864 N3865 I3872 V3875 S3884 W3890 Y3891 Y3892 I3898 E3922 P3927 L3935 L3968 L3967 L3968
E3987 M4019 F4020 L4026 T4027 S4028 T4031 F4032 K4033 E4034 G4039 K4040 I4043 R4046 D4047 H4055 Y4058 E4071 T4072 D4073 E4074 N4075 D4079 E4082 F4087 H4088 E4089 P4090 A4091 K4092 D4093 S4106 E4107 L4119 F4129 R4144 R4147 V4148 Y4149 V4177 G4181

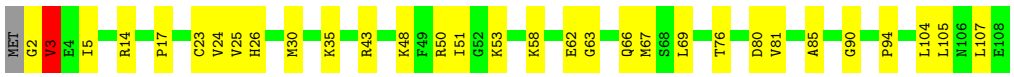


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

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

Chain F:

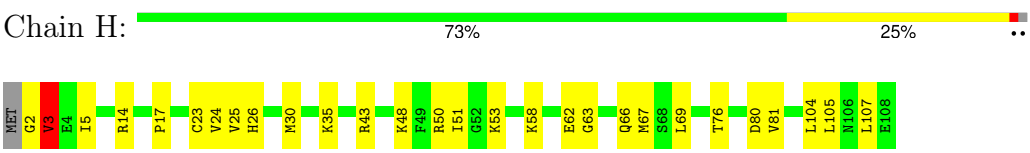


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

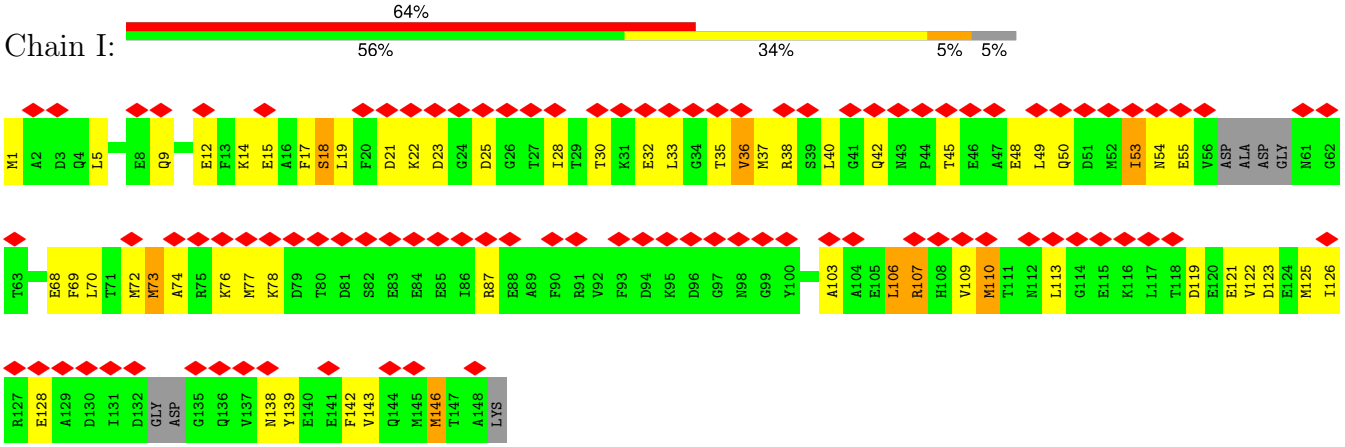
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



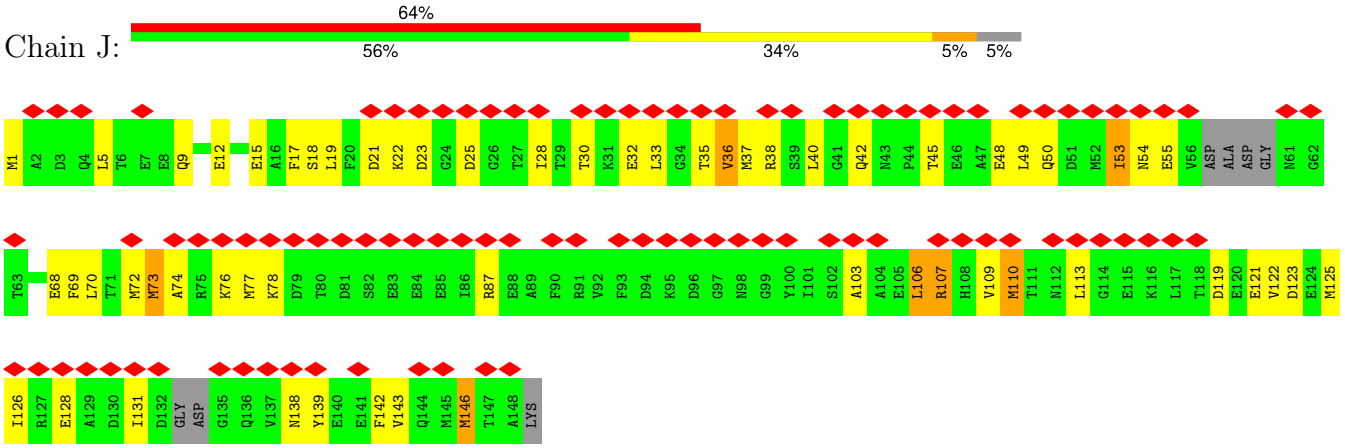
• Molecule 3: Calmodulin-1

Chain I:



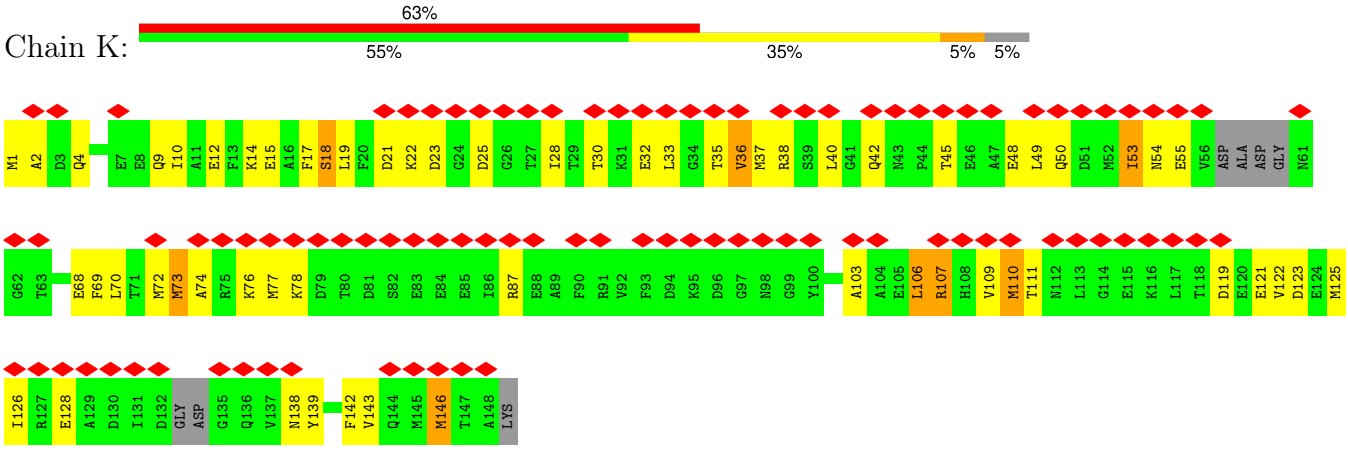
• Molecule 3: Calmodulin-1

Chain J:



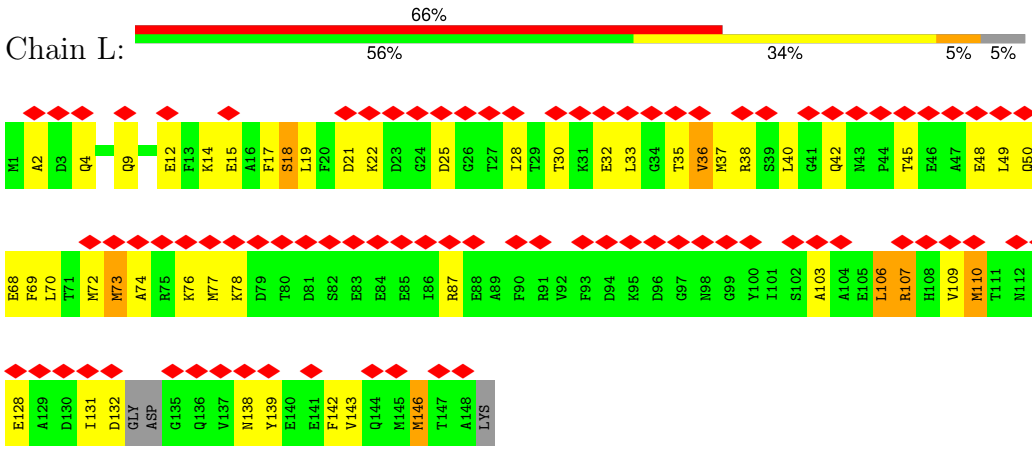
• Molecule 3: Calmodulin-1

Chain K:



• Molecule 3: Calmodulin-1

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73052	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.746	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/36343	0.50	10/49085 (0.0%)
1	B	0.26	0/36343	0.50	10/49085 (0.0%)
1	C	0.26	0/36343	0.50	10/49085 (0.0%)
1	D	0.26	0/36343	0.50	10/49085 (0.0%)
2	E	0.29	0/834	0.55	0/1123
2	F	0.29	0/834	0.55	0/1123
2	G	0.29	0/834	0.55	0/1123
2	H	0.29	0/834	0.55	0/1123
3	I	0.33	0/1122	0.82	5/1504 (0.3%)
3	J	0.33	0/1122	0.82	5/1504 (0.3%)
3	K	0.33	0/1122	0.82	5/1504 (0.3%)
3	L	0.33	0/1122	0.82	5/1504 (0.3%)
All	All	0.26	0/153196	0.51	60/206848 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
3	I	0	1
3	J	0	1
3	K	0	1
3	L	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	1293	GLN	CA-CB-CG	7.56	130.02	113.40
1	A	1293	GLN	CA-CB-CG	7.54	129.98	113.40
1	B	1293	GLN	CA-CB-CG	7.53	129.96	113.40
1	C	1293	GLN	CA-CB-CG	7.52	129.94	113.40
1	B	983	LEU	CA-CB-CG	7.18	131.81	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3520	GLU	Peptide
3	I	107	ARG	Sidechain
3	J	107	ARG	Sidechain
3	K	107	ARG	Sidechain
3	L	107	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	35570	0	35258	638	0
1	B	35570	0	35258	632	0
1	C	35570	0	35258	647	0
1	D	35570	0	35258	639	0
2	E	818	0	821	19	0
2	F	818	0	821	21	0
2	G	818	0	821	19	0
2	H	818	0	821	19	0
3	I	1112	0	1053	31	0
3	J	1112	0	1053	32	0
3	K	1112	0	1053	39	0
3	L	1112	0	1053	31	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	62	0	24	0	0
5	B	62	0	24	0	0
5	C	62	0	24	0	0
5	D	62	0	24	0	0
All	All	150252	0	148624	2702	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 9.

The worst 5 of 2702 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2905:ARG:NH1	1:C:2907:PHE:O	1.97	0.98
1:D:2905:ARG:NH1	1:D:2907:PHE:O	1.97	0.97
1:B:2905:ARG:NH1	1:B:2907:PHE:O	1.97	0.97
1:A:2905:ARG:NH1	1:A:2907:PHE:O	1.97	0.97
3:I:138:ASN:O	3:I:142:PHE:HB2	1.64	0.96

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	4415/4967 (89%)	4241 (96%)	168 (4%)	6 (0%)	48	79
1	B	4415/4967 (89%)	4240 (96%)	169 (4%)	6 (0%)	48	79
1	C	4415/4967 (89%)	4241 (96%)	168 (4%)	6 (0%)	48	79
1	D	4415/4967 (89%)	4241 (96%)	168 (4%)	6 (0%)	48	79
2	E	105/108 (97%)	101 (96%)	3 (3%)	1 (1%)	13	43
2	F	105/108 (97%)	100 (95%)	4 (4%)	1 (1%)	13	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	G	105/108 (97%)	99 (94%)	5 (5%)	1 (1%)	13 43
2	H	105/108 (97%)	100 (95%)	4 (4%)	1 (1%)	13 43
3	I	136/149 (91%)	126 (93%)	10 (7%)	0	100 100
3	J	136/149 (91%)	126 (93%)	10 (7%)	0	100 100
3	K	136/149 (91%)	126 (93%)	10 (7%)	0	100 100
3	L	136/149 (91%)	126 (93%)	10 (7%)	0	100 100
All	All	18624/20896 (89%)	17867 (96%)	729 (4%)	28 (0%)	45 74

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	VAL
1	A	1495	SER
2	E	3	VAL
2	F	3	VAL
2	G	3	VAL

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	3905/4358 (90%)	3889 (100%)	16 (0%)	89 95
1	B	3905/4358 (90%)	3887 (100%)	18 (0%)	86 94
1	C	3905/4358 (90%)	3887 (100%)	18 (0%)	86 94
1	D	3905/4358 (90%)	3887 (100%)	18 (0%)	86 94
2	E	88/89 (99%)	85 (97%)	3 (3%)	32 64
2	F	88/89 (99%)	85 (97%)	3 (3%)	32 64
2	G	88/89 (99%)	85 (97%)	3 (3%)	32 64
2	H	88/89 (99%)	85 (97%)	3 (3%)	32 64
3	I	119/127 (94%)	109 (92%)	10 (8%)	9 31
3	J	119/127 (94%)	109 (92%)	10 (8%)	9 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	K	119/127 (94%)	109 (92%)	10 (8%)	9 31
3	L	119/127 (94%)	109 (92%)	10 (8%)	9 31
All	All	16448/18296 (90%)	16326 (99%)	122 (1%)	80 91

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	146	MET
1	D	2279	MET
1	B	983	LEU
1	D	1293	GLN
1	D	3260	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2868	HIS
1	D	3178	HIS
1	B	2868	HIS
1	B	1691	ASN
1	D	3274	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ATP	C	5002	-	28,33,33	0.62	0	34,52,52	0.60	1 (2%)
5	ATP	A	5003	-	28,33,33	0.65	0	34,52,52	0.58	1 (2%)
5	ATP	A	5002	-	28,33,33	0.62	0	34,52,52	0.60	1 (2%)
5	ATP	C	5003	-	28,33,33	0.63	0	34,52,52	0.58	1 (2%)
5	ATP	B	5003	-	28,33,33	0.64	0	34,52,52	0.59	1 (2%)
5	ATP	B	5002	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
5	ATP	D	5002	-	28,33,33	0.62	0	34,52,52	0.60	1 (2%)
5	ATP	D	5003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)

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	C	5002	-	-	7/18/38/38	0/3/3/3
5	ATP	A	5003	-	-	5/18/38/38	0/3/3/3
5	ATP	A	5002	-	-	7/18/38/38	0/3/3/3
5	ATP	C	5003	-	-	5/18/38/38	0/3/3/3
5	ATP	B	5003	-	-	5/18/38/38	0/3/3/3
5	ATP	B	5002	-	-	7/18/38/38	0/3/3/3
5	ATP	D	5002	-	-	7/18/38/38	0/3/3/3
5	ATP	D	5003	-	-	5/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	5003	ATP	C5-C6-N6	2.35	123.89	120.31
5	D	5003	ATP	C5-C6-N6	2.34	123.88	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	5003	ATP	C5-C6-N6	2.32	123.84	120.31
5	D	5002	ATP	C5-C6-N6	2.32	123.84	120.31
5	C	5002	ATP	C5-C6-N6	2.30	123.81	120.31

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

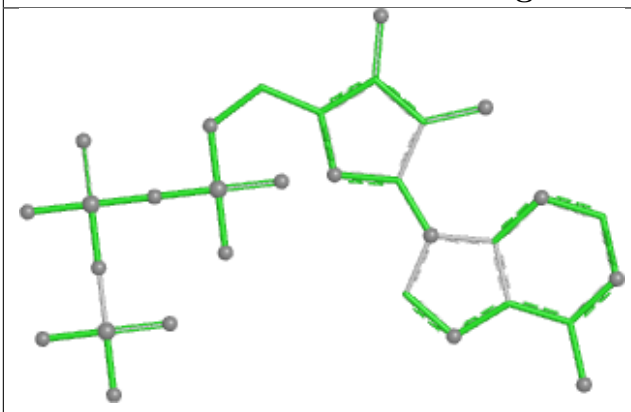
Mol	Chain	Res	Type	Atoms
5	A	5002	ATP	C5'-O5'-PA-O1A
5	A	5002	ATP	C5'-O5'-PA-O2A
5	A	5002	ATP	C5'-O5'-PA-O3A
5	A	5003	ATP	C5'-O5'-PA-O1A
5	A	5003	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

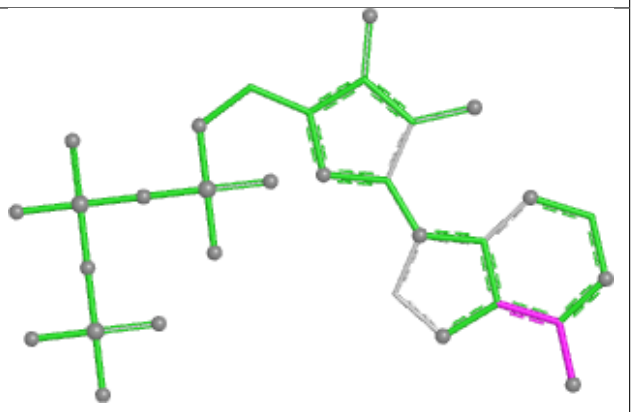
No monomer is involved in short contacts.

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.

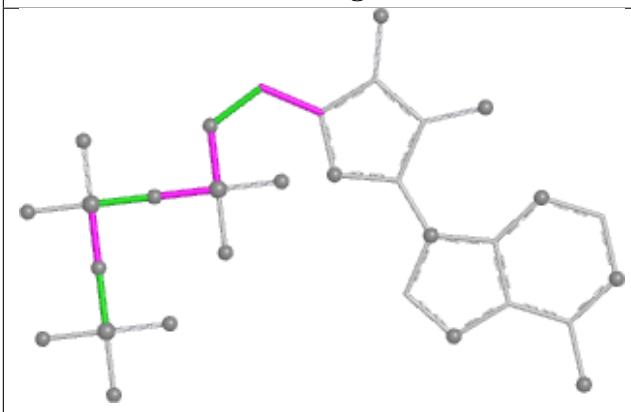
Ligand ATP C 5002



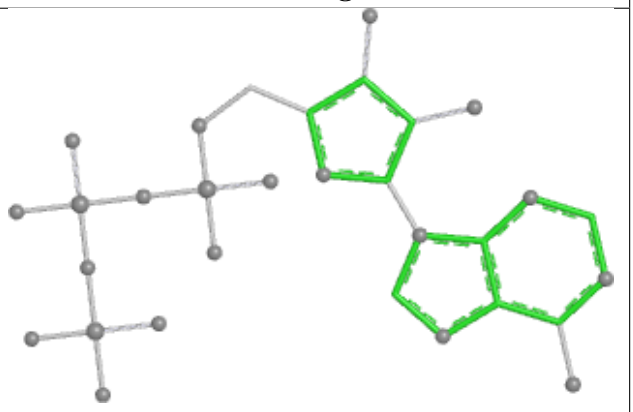
Bond lengths



Bond angles

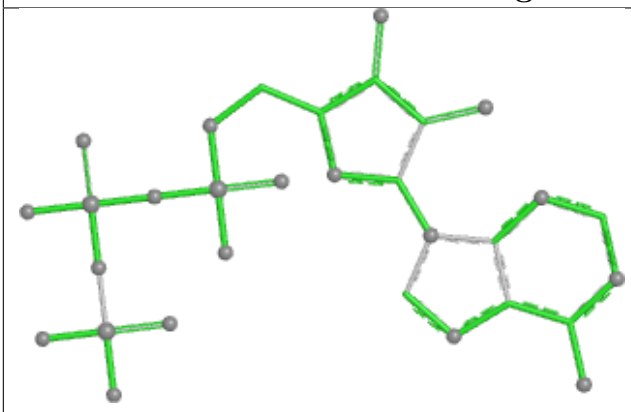


Torsions

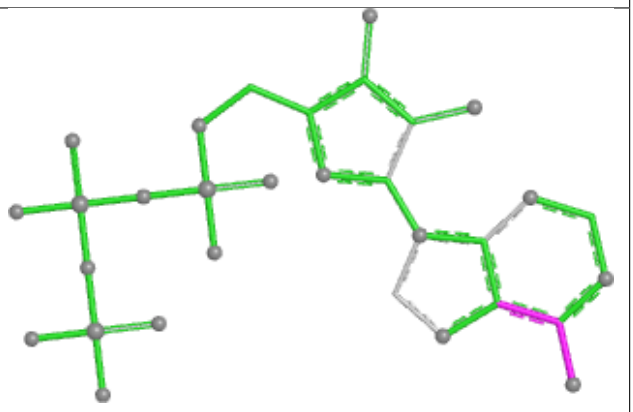


Rings

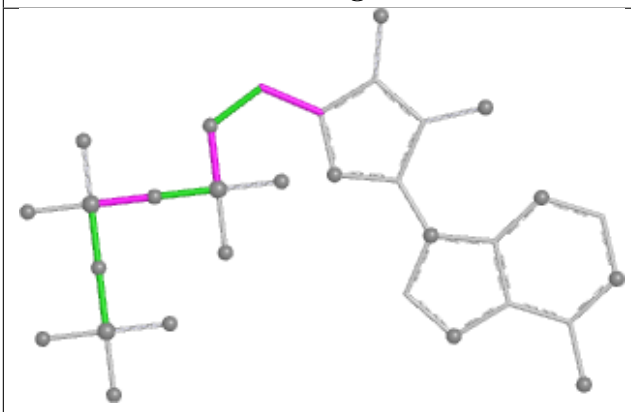
Ligand ATP A 5003



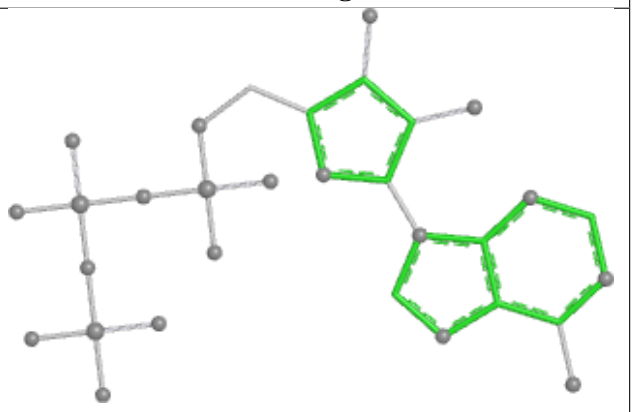
Bond lengths



Bond angles

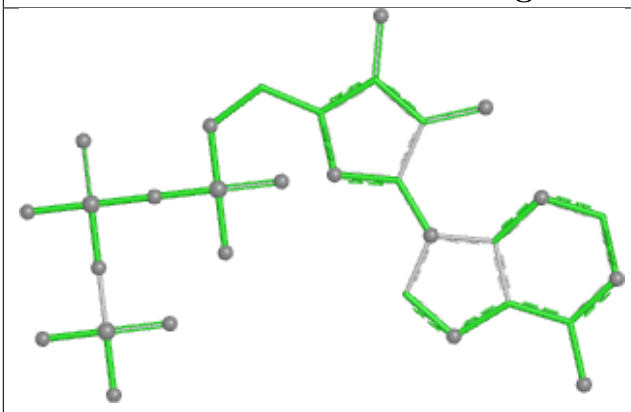


Torsions

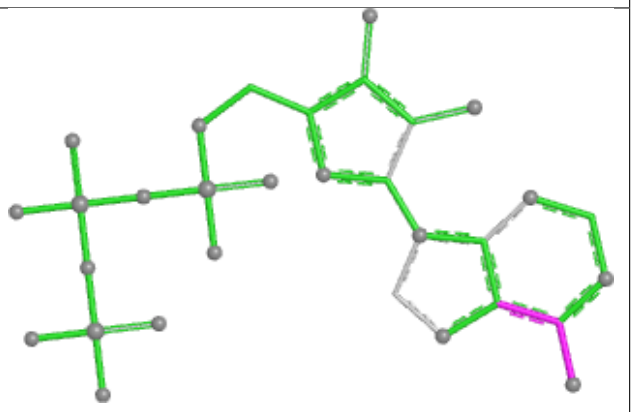


Rings

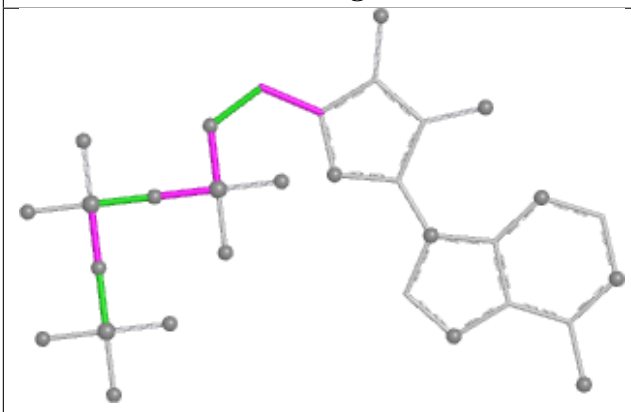
Ligand ATP A 5002



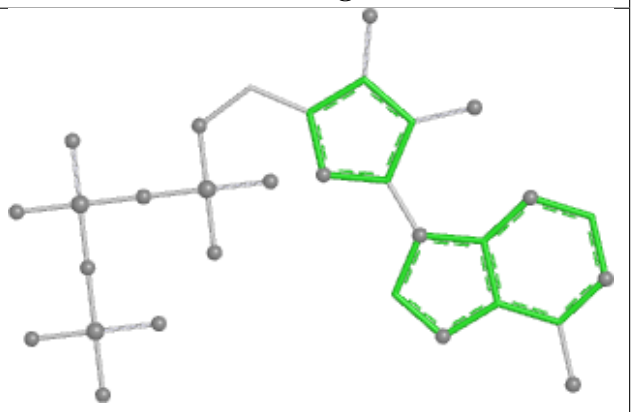
Bond lengths



Bond angles

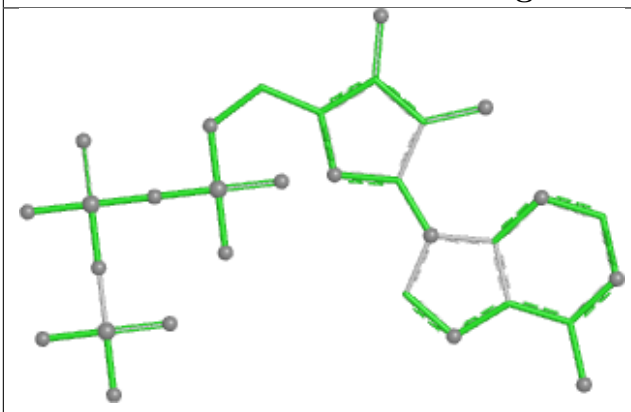


Torsions

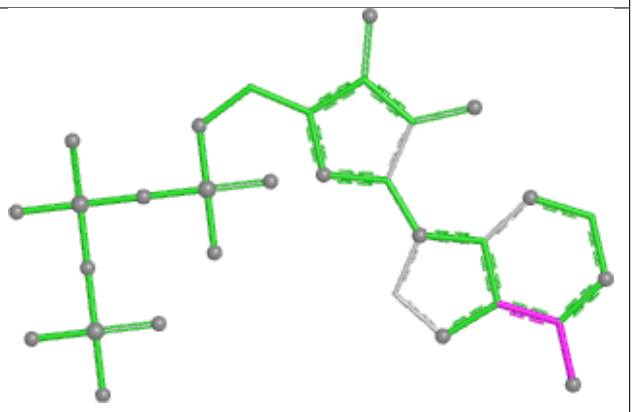


Rings

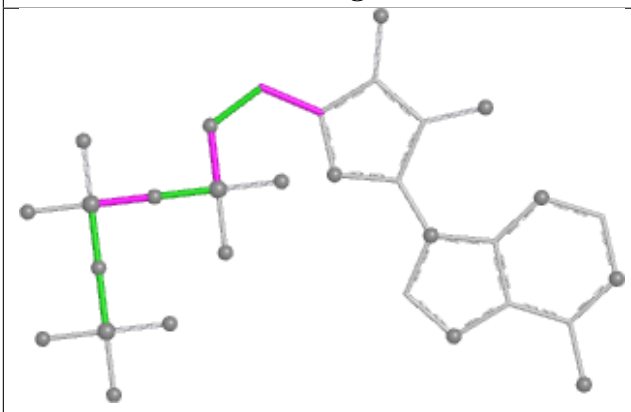
Ligand ATP C 5003



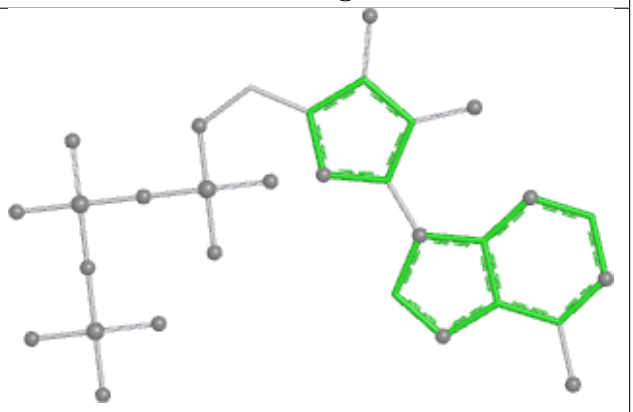
Bond lengths



Bond angles

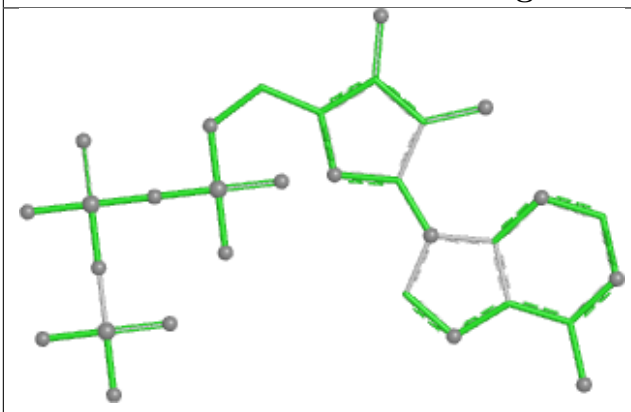


Torsions

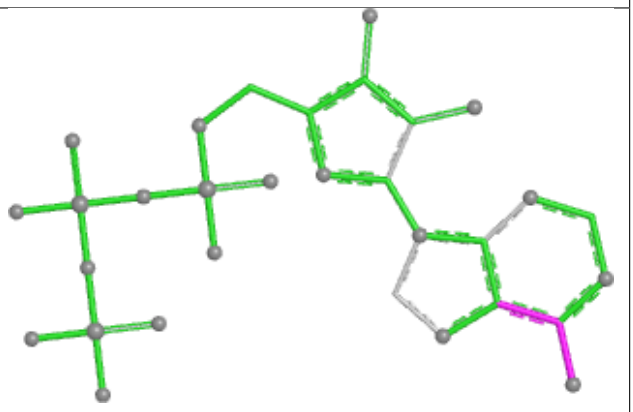


Rings

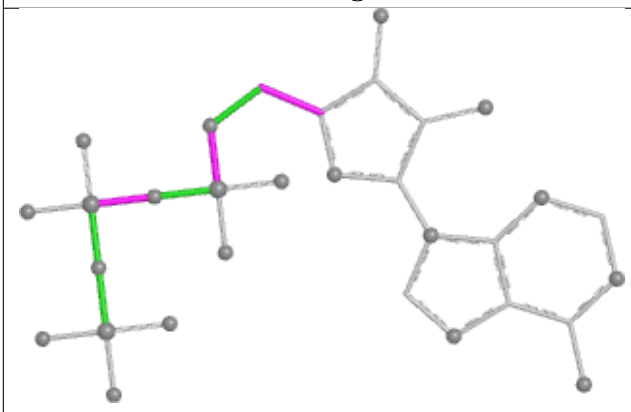
Ligand ATP B 5003



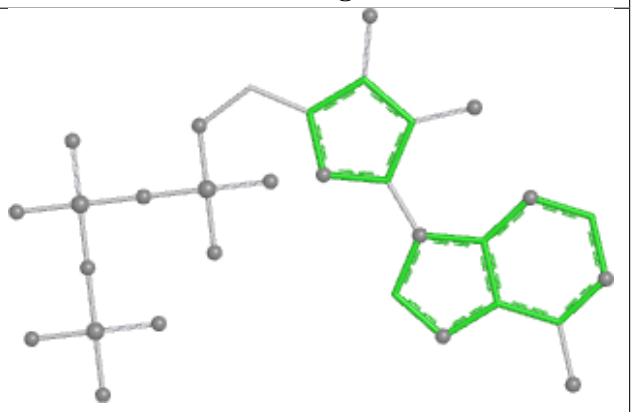
Bond lengths



Bond angles

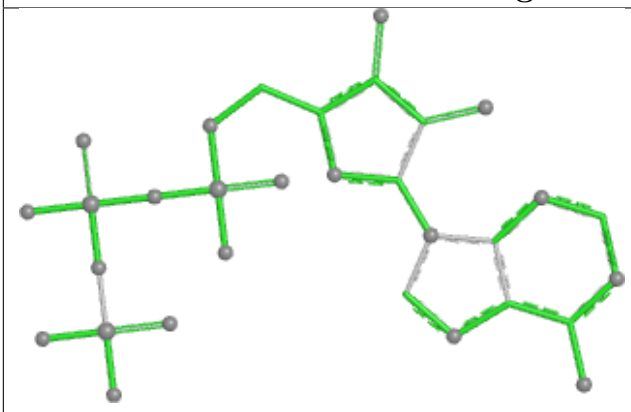


Torsions

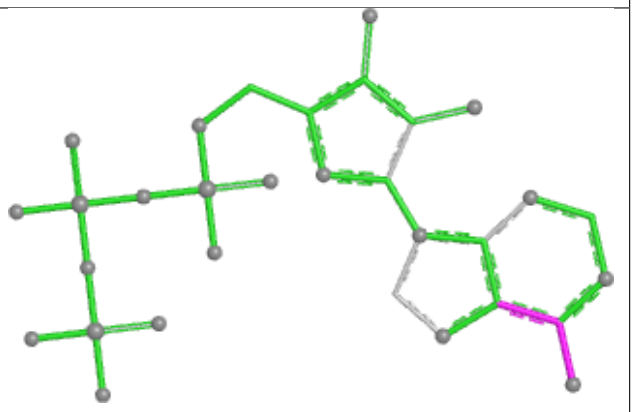


Rings

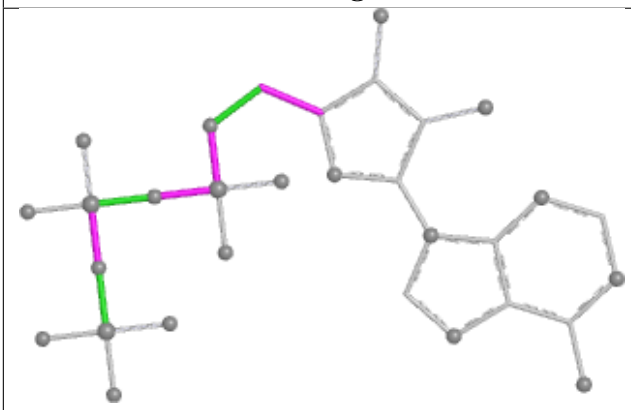
Ligand ATP B 5002



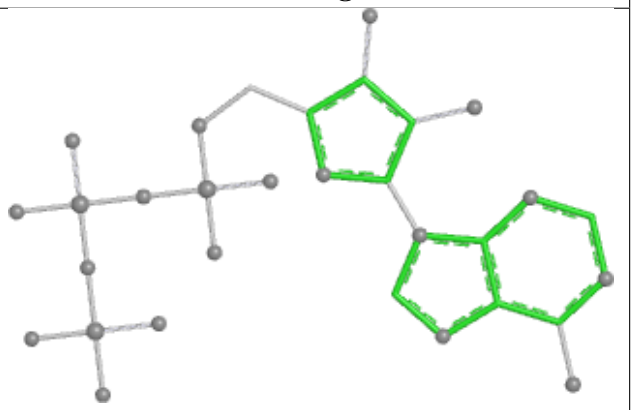
Bond lengths



Bond angles

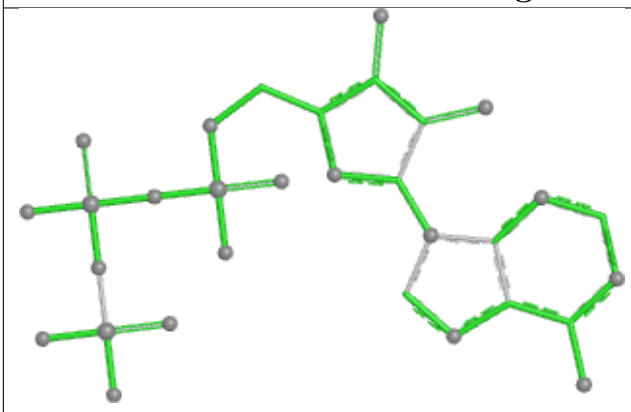


Torsions

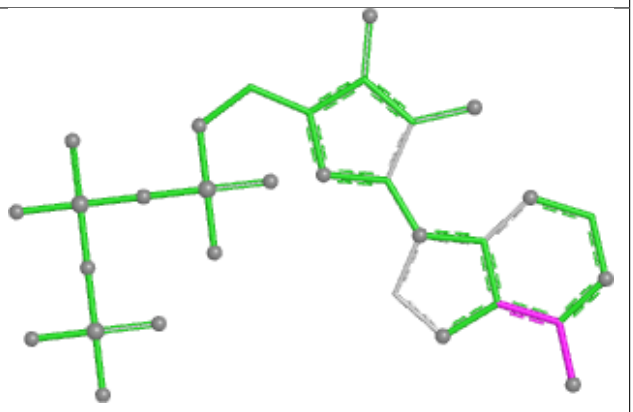


Rings

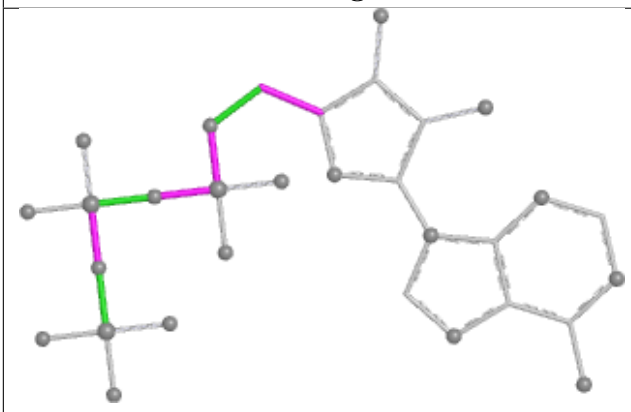
Ligand ATP D 5002



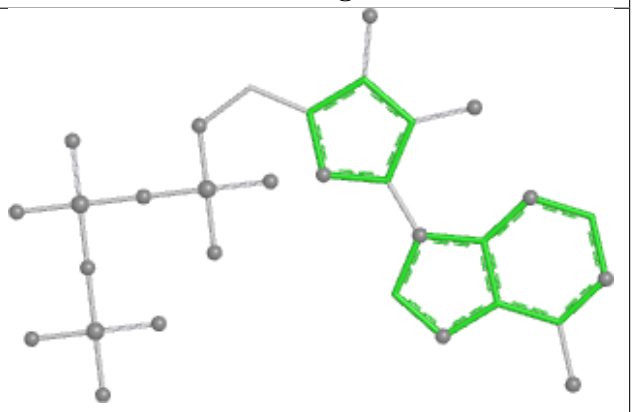
Bond lengths



Bond angles

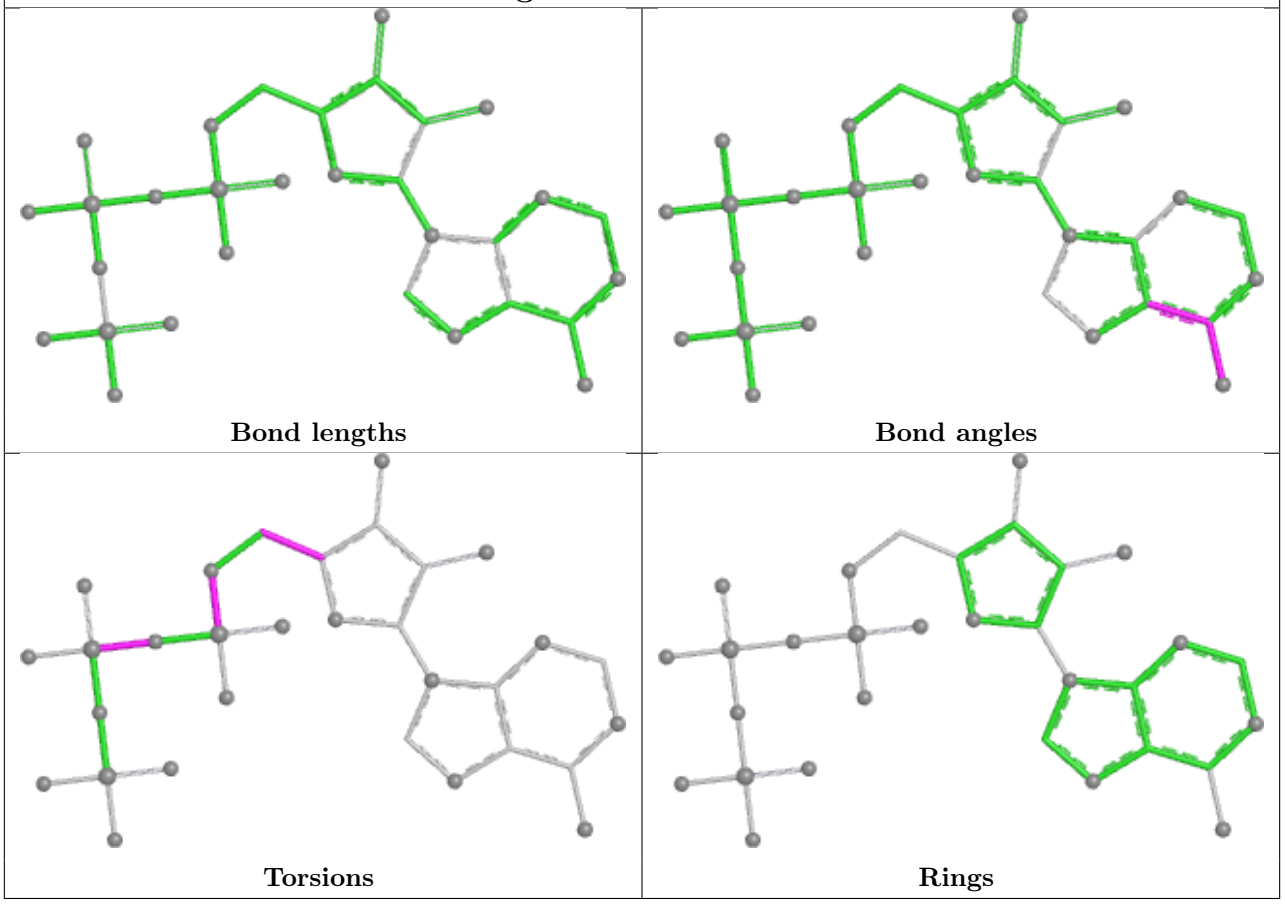


Torsions



Rings

Ligand ATP D 5003



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.

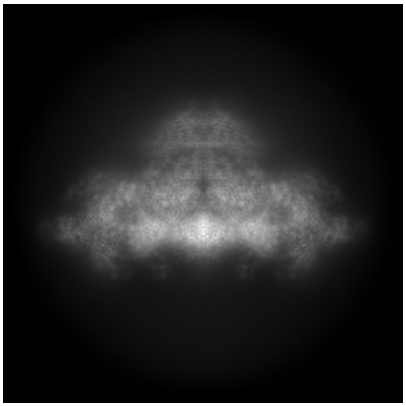
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26413. These allow visual inspection of the internal detail of the map and identification of artifacts.

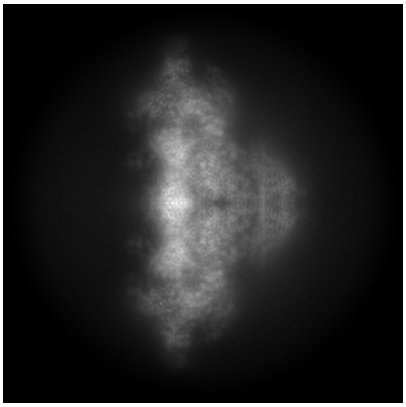
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

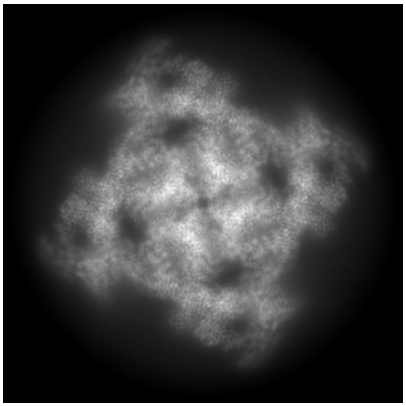
6.1.1 Primary map



X



Y

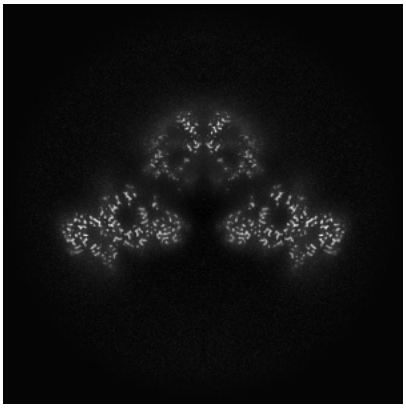


Z

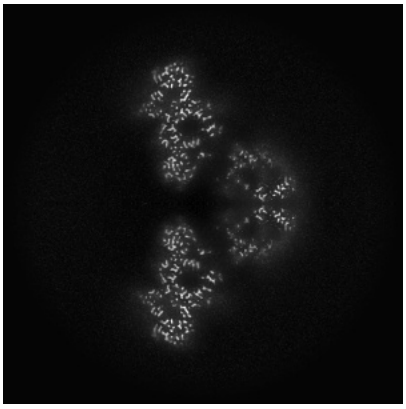
The images above show the map projected in three orthogonal directions.

6.2 Central slices

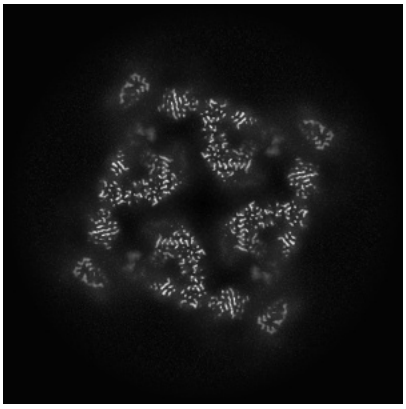
6.2.1 Primary map



X Index: 256



Y Index: 256

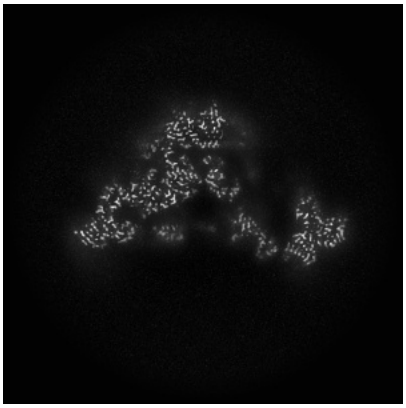


Z Index: 256

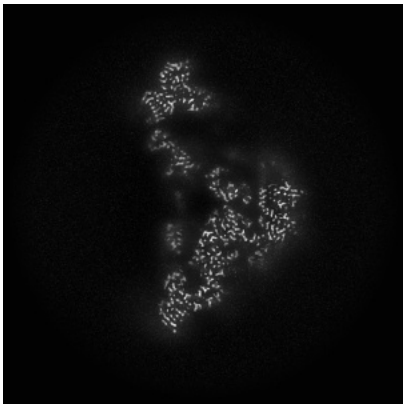
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

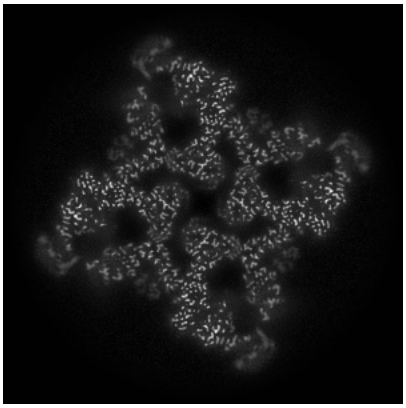
6.3.1 Primary map



X Index: 237



Y Index: 275

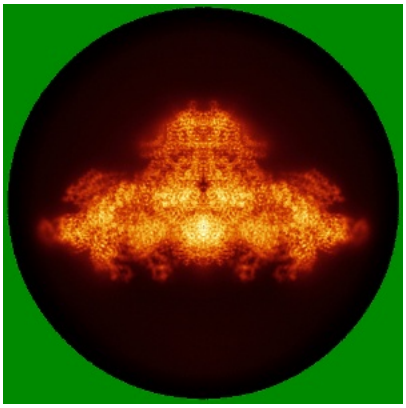


Z Index: 223

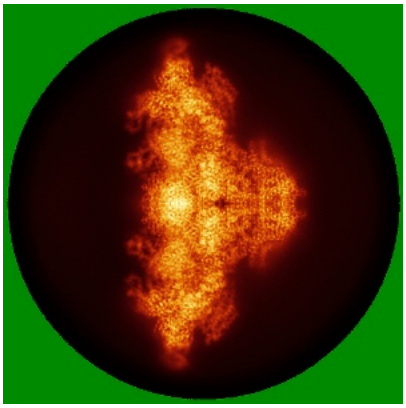
The images above show the largest variance slices of the map in three orthogonal directions.

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

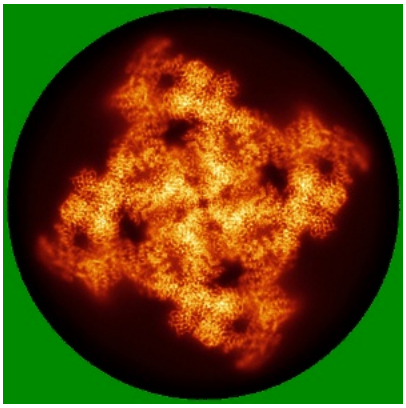
6.4.1 Primary map



X



Y

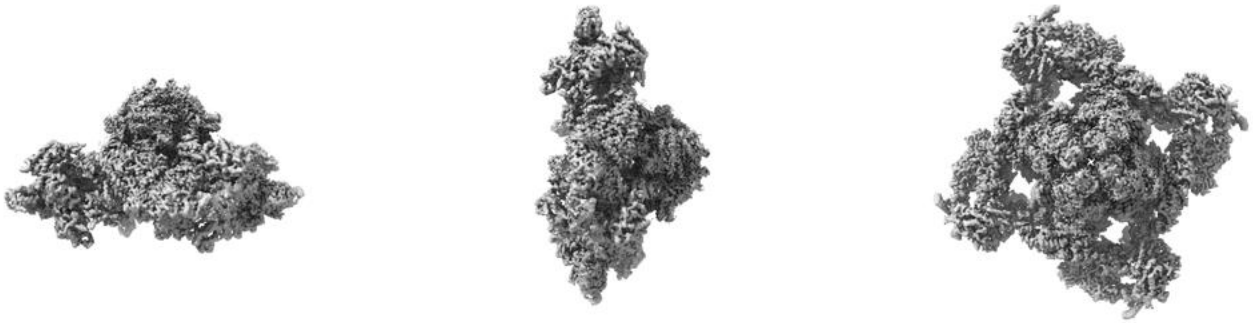


Z

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

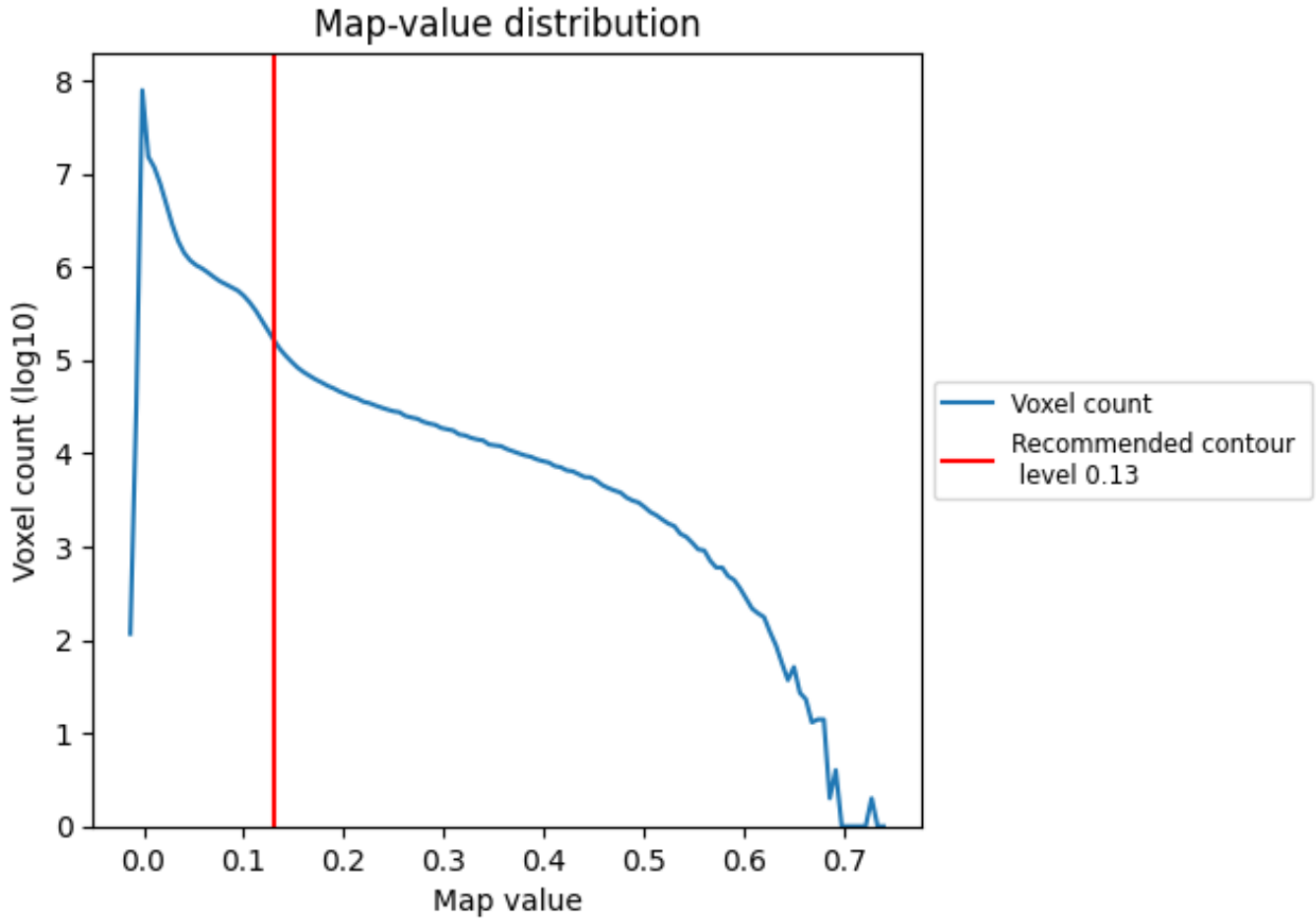
6.6 Mask visualisation (i)

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

7 Map analysis

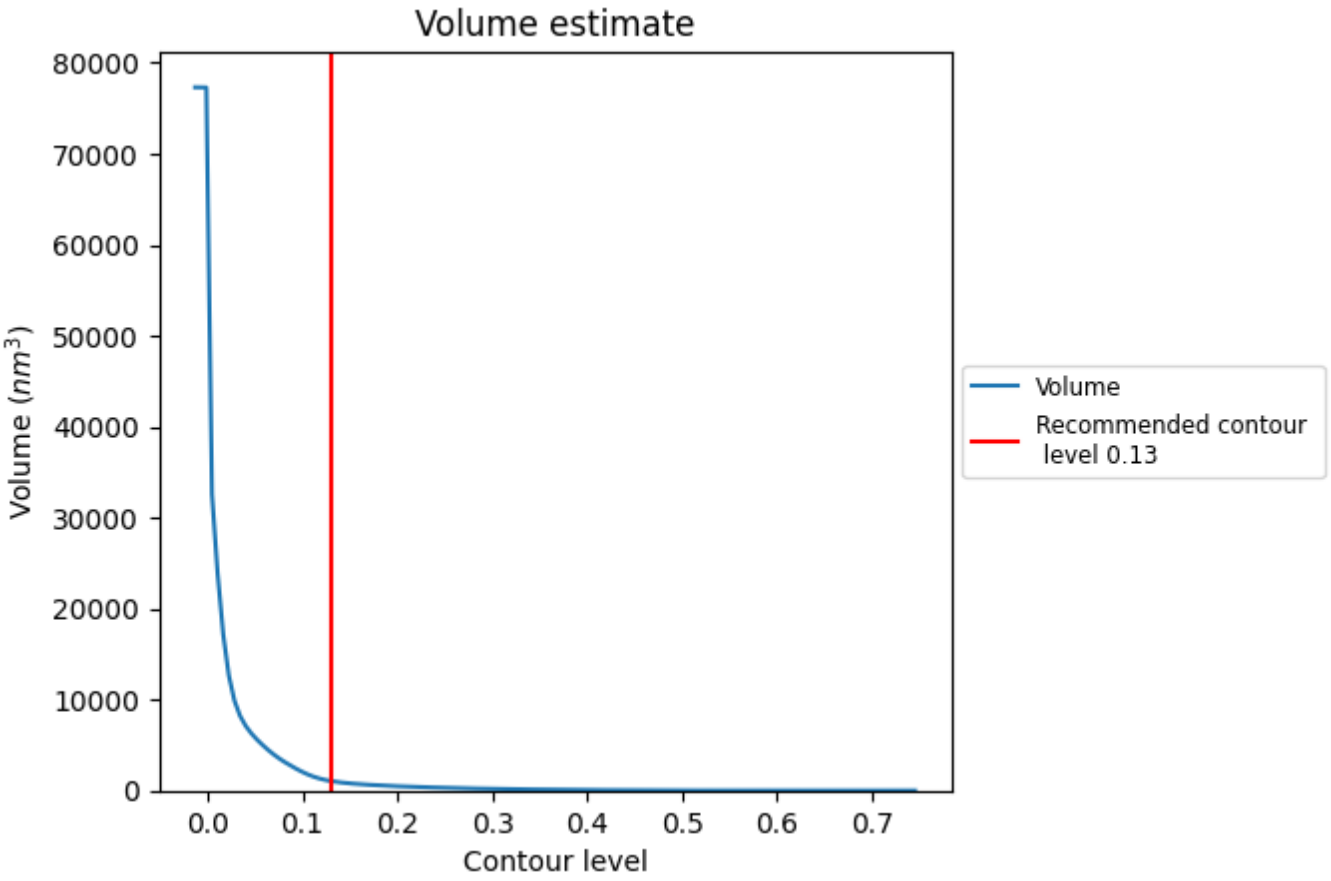
This section contains the results of statistical analysis of the map.

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.

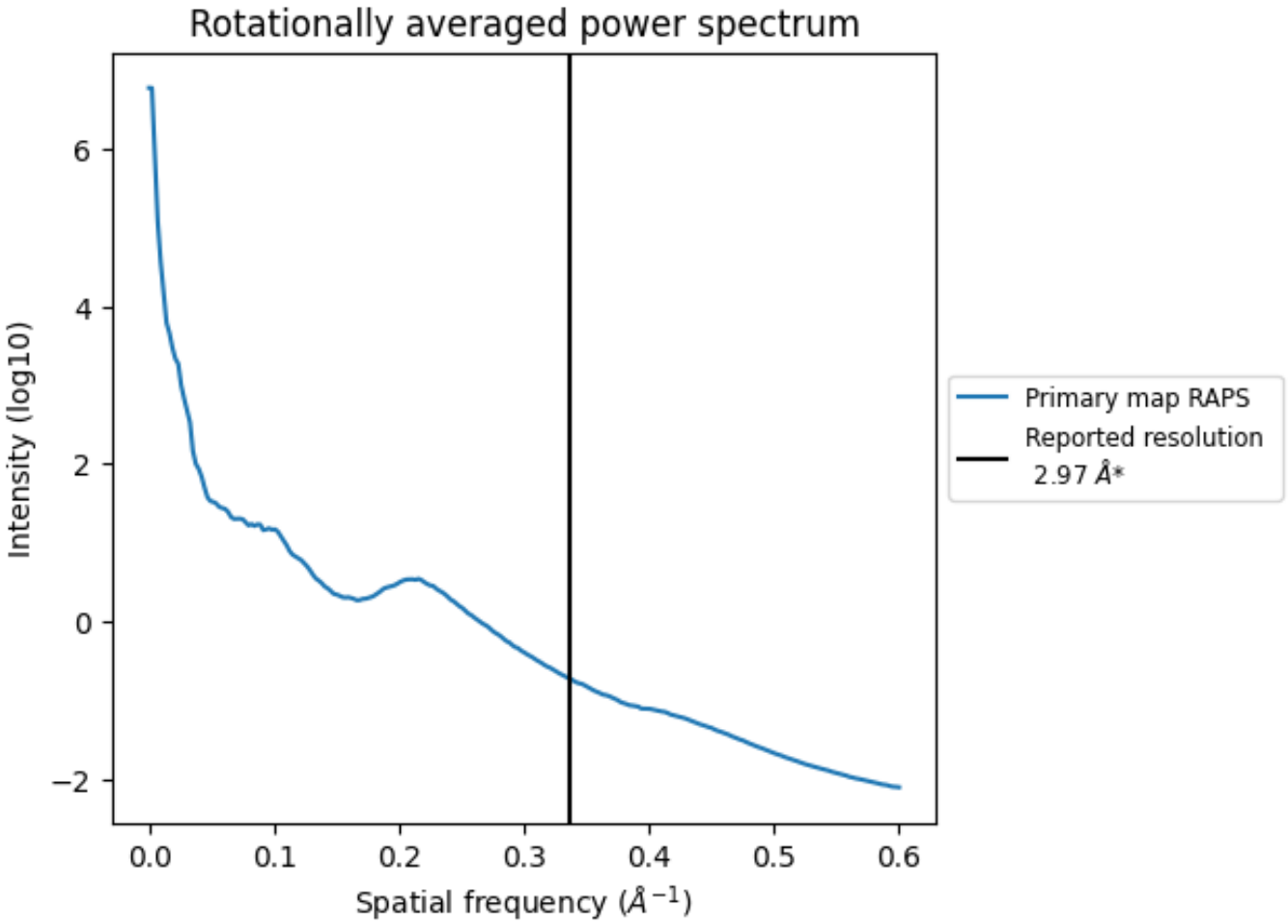
7.2 Volume estimate (i)



The volume at the recommended contour level is 1047 nm^3; this corresponds to an approximate mass of 946 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 0.337 Å^{-1}

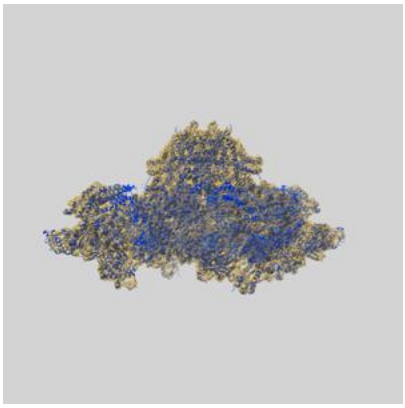
8 Fourier-Shell correlation

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

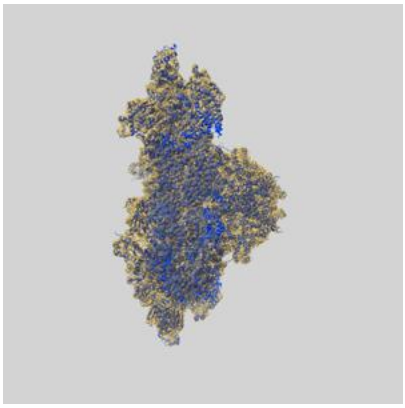
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26413 and PDB model 7UA3. Per-residue inclusion information can be found in section 3 on page 7.

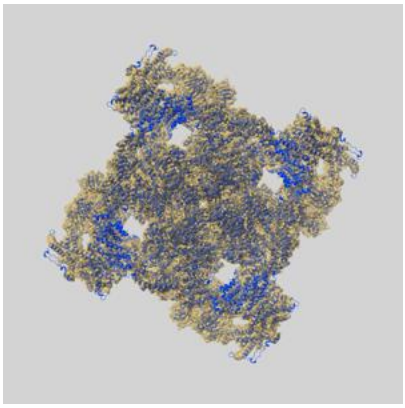
9.1 Map-model overlay



X



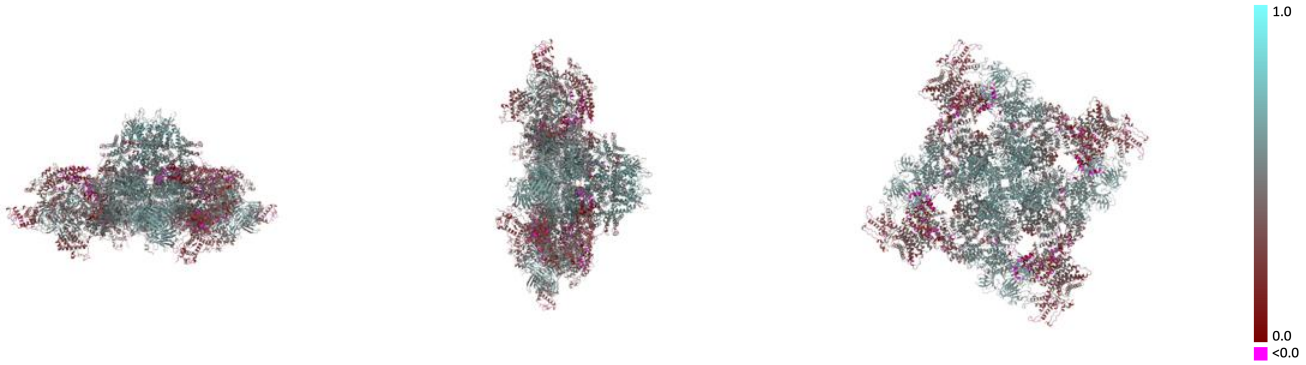
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

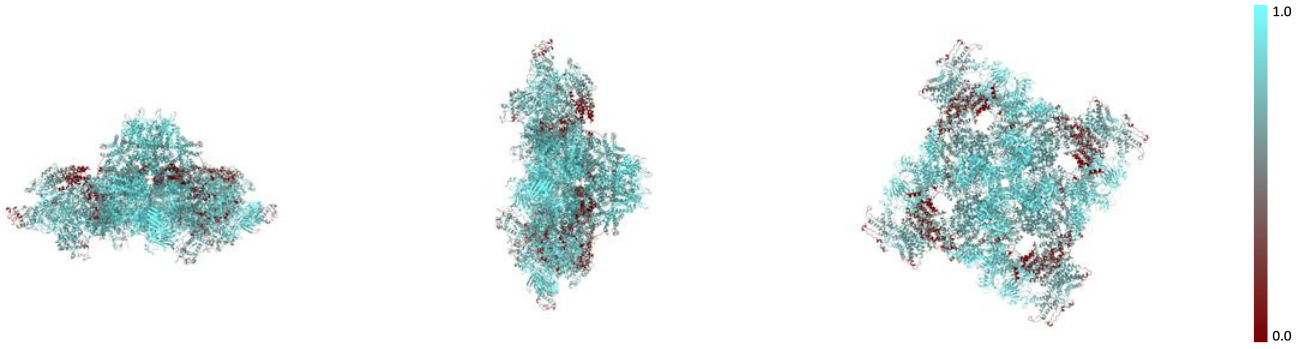
9.2 Q-score mapped to coordinate model (i)



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.

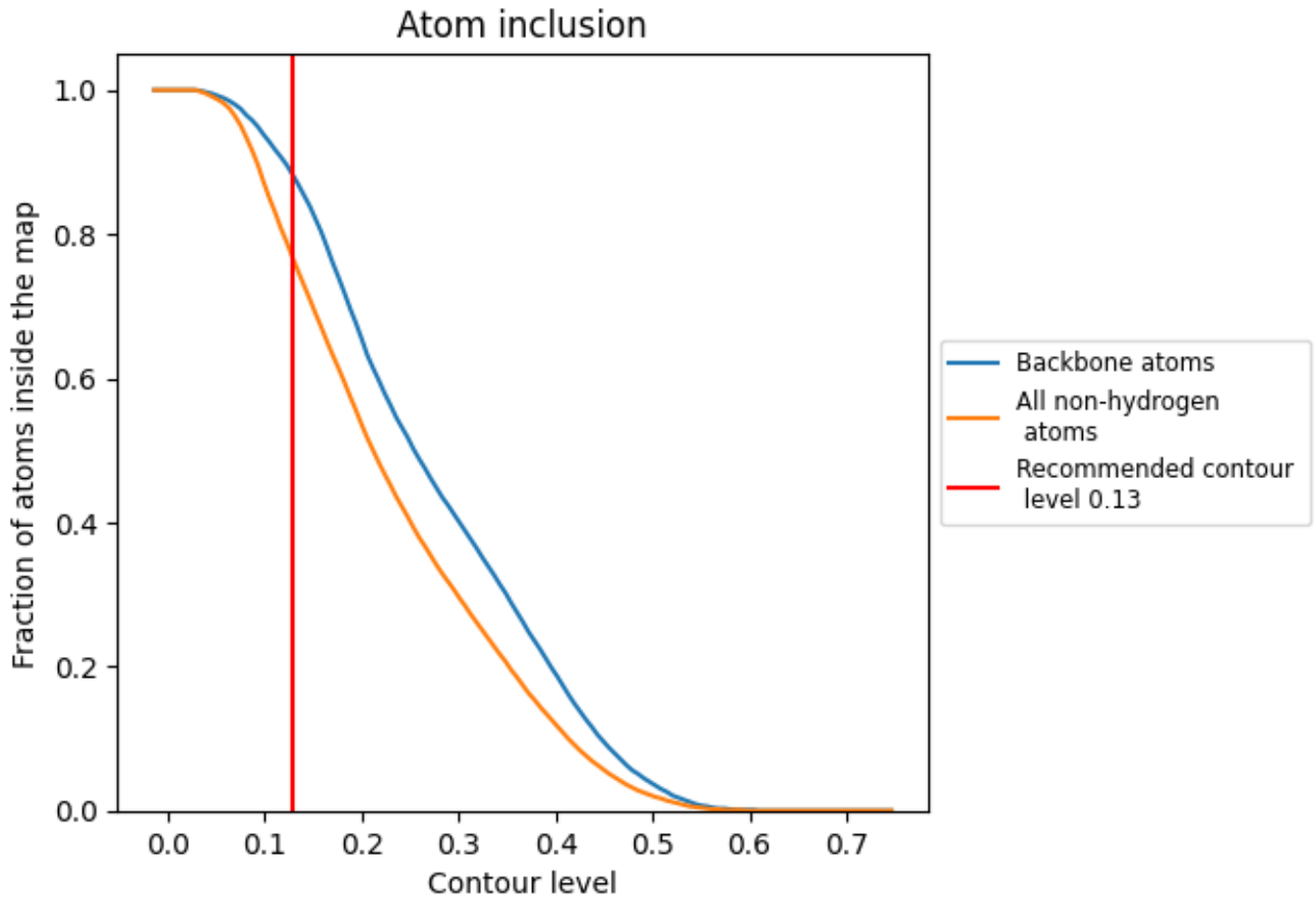
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7650	0.4470
A	0.7770	0.4530
B	0.7760	0.4520
C	0.7760	0.4520
D	0.7760	0.4520
E	0.9270	0.5680
F	0.9290	0.5710
G	0.9330	0.5700
H	0.9300	0.5710
I	0.2810	0.1610
J	0.2820	0.1670
K	0.2950	0.1660
L	0.2820	0.1640