wwPDB EM Validation Summary Report

Nov 10, 2024 – 02:59 pm GMT

PDB ID	:	8RRX
EMDB ID	:	EMD-19468
Title	:	Structure of RyR1 reconstituted into lipid nanodisc in primed state in complex with Ca2+, ATP, caffeine and Nb9657
Authors	:	Li, C.; Efremov, R.G.
Deposited on	:	2024-01-23
Resolution	:	3.10 Å(reported)

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

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

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

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

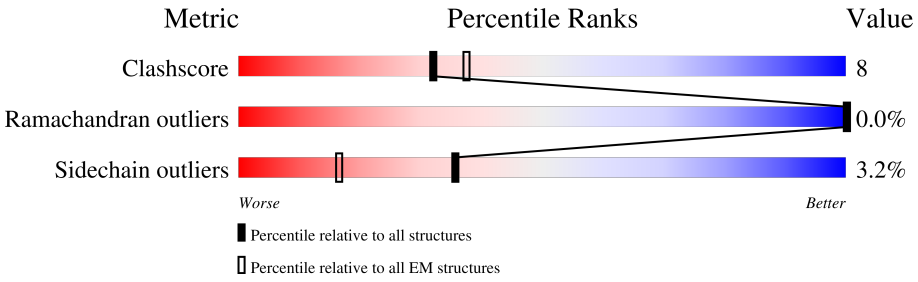
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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.



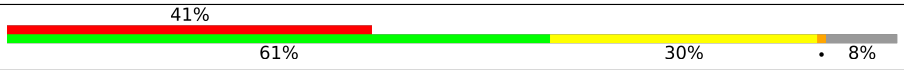
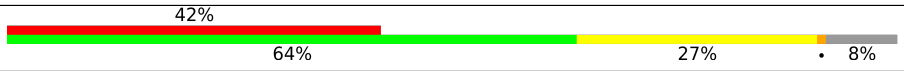
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	F	107	82% 16%
1	H	107	82% 16%
1	J	107	85% 14%
1	L	107	83% 15%
2	A	5027	5% 67% 18% 14%
2	D	5027	5% 67% 18% 14%
2	G	5027	5% 67% 18% 14%
2	I	5027	5% 67% 18% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	137	
3	E	137	
3	K	137	
3	M	137	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 144144 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	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	L	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	100	ASP	GLY	conflict	UNP Q8HYX6
L	100	ASP	GLY	conflict	UNP Q8HYX6
J	100	ASP	GLY	conflict	UNP Q8HYX6
F	100	ASP	GLY	conflict	UNP Q8HYX6

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	4319	Total	C	N	O	S	1	0
			34151	21750	5888	6285	228		
2	A	4319	Total	C	N	O	S	1	0
			34153	21752	5888	6285	228		
2	D	4319	Total	C	N	O	S	1	0
			34153	21752	5888	6285	228		
2	G	4319	Total	C	N	O	S	1	0
			34151	21750	5888	6285	228		

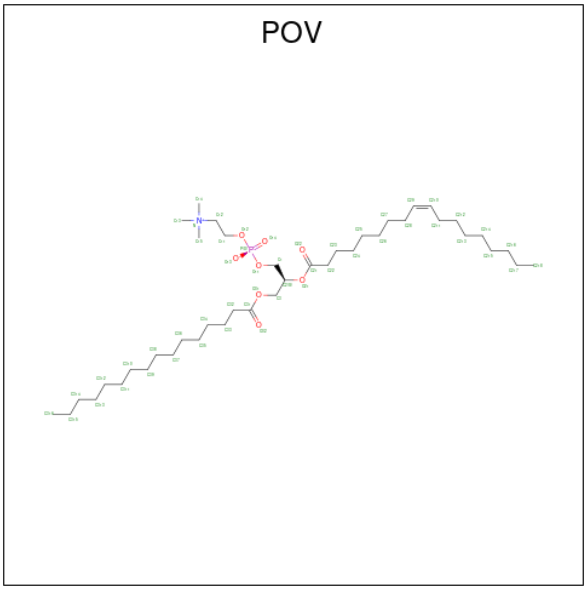
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	C	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	E	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	M	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	I	1	Total	Zn	0
			1	1	
4	A	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).



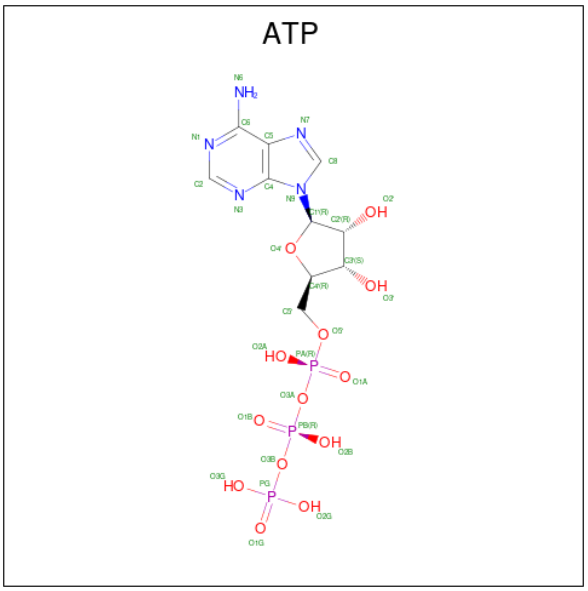
Mol	Chain	Residues	Atoms					AltConf
5	I	1	Total	C	N	O	P	0
			52	42	1	8	1	

Continued on next page...

Continued from previous page...

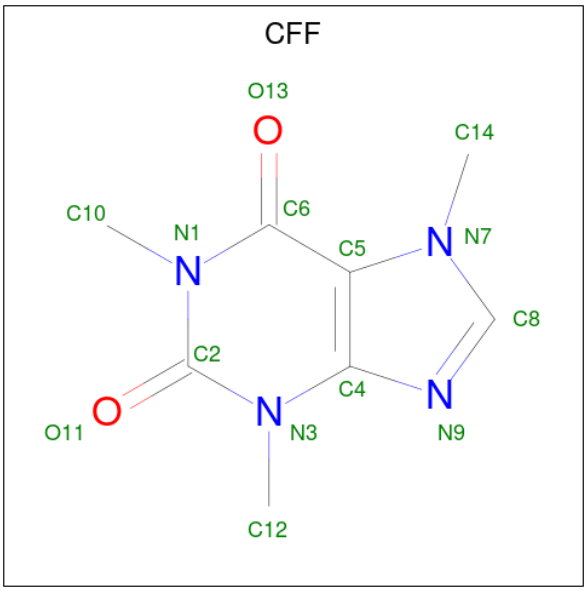
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	D	1	Total	C	N	O	P	0
			52	42	1	8	1	
5	G	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 6 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
6	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	I	1	Total C N O 14 8 4 2	0
7	A	1	Total C N O 14 8 4 2	0
7	D	1	Total C N O 14 8 4 2	0
7	G	1	Total C N O 14 8 4 2	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

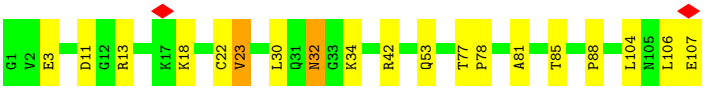
Mol	Chain	Residues	Atoms	AltConf
8	I	1	Total Ca 1 1	0
8	A	1	Total Ca 1 1	0
8	D	1	Total Ca 1 1	0
8	G	1	Total Ca 1 1	0

3 Residue-property plots (i)

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

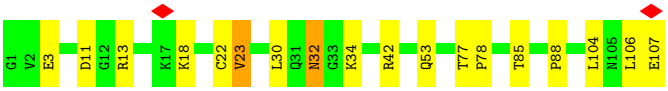
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



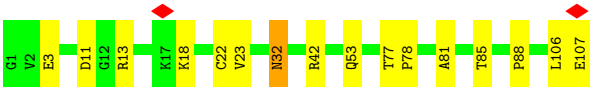
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain L:



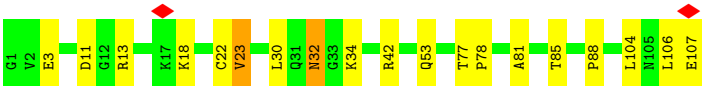
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:



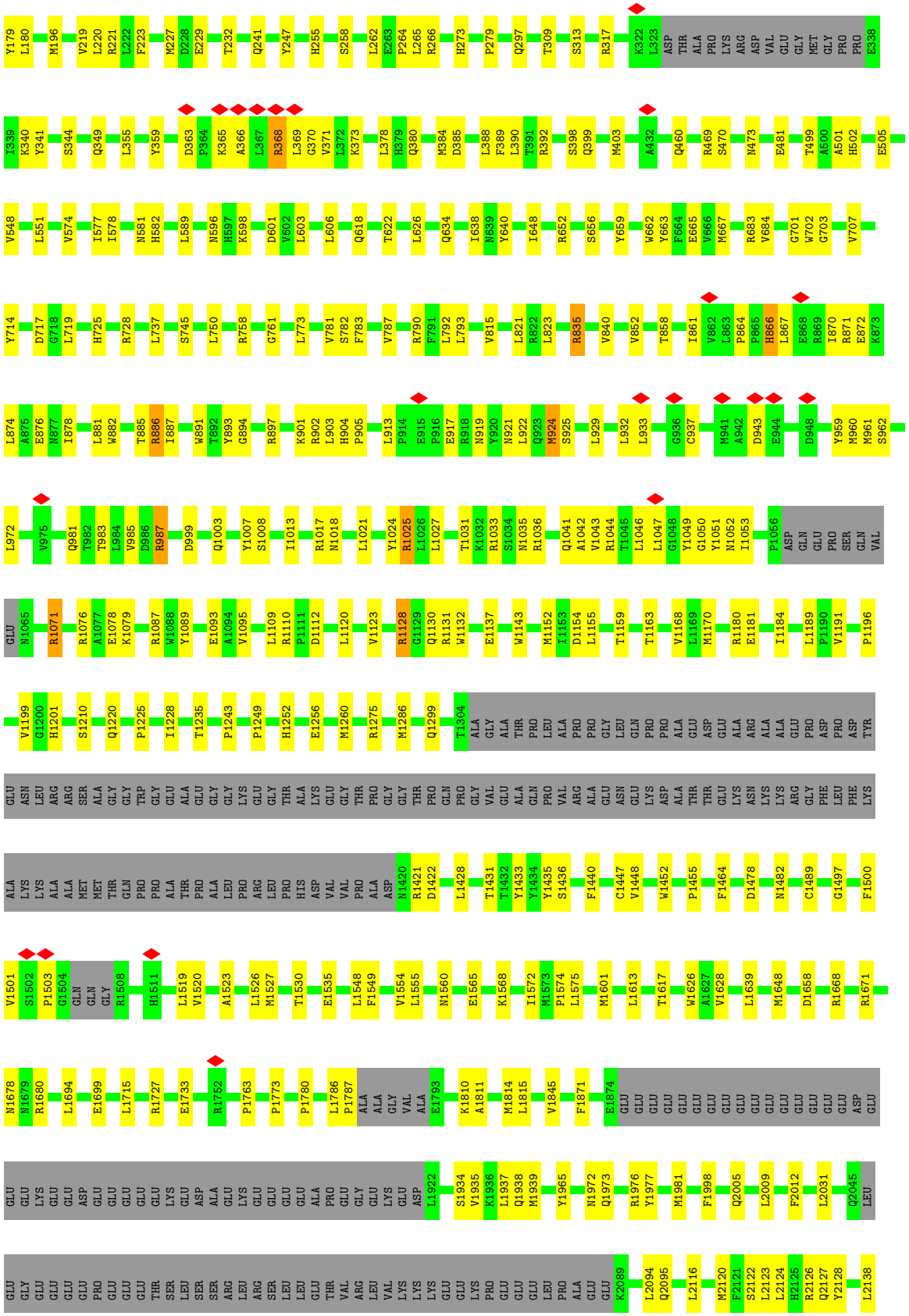
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

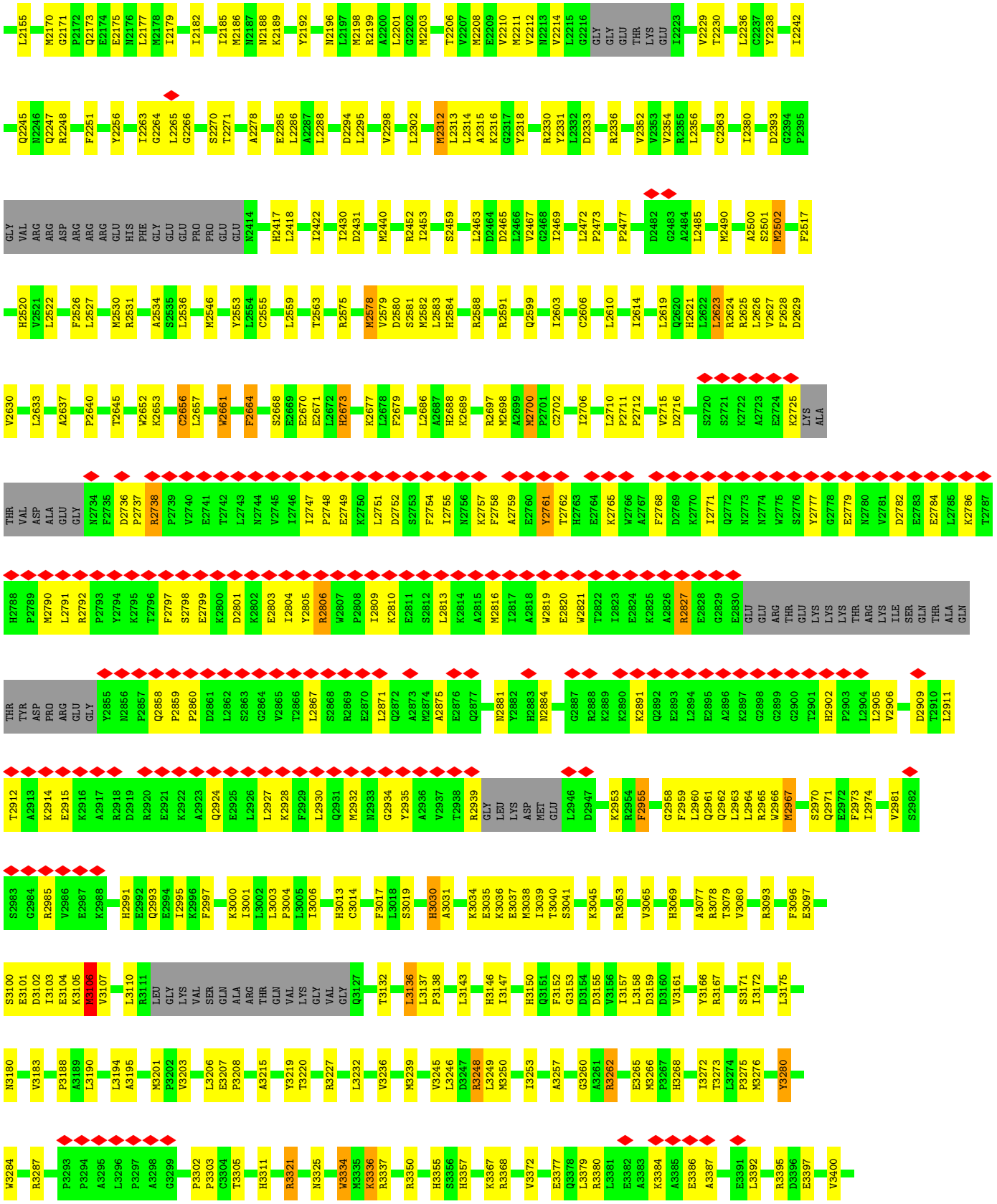
Chain F:

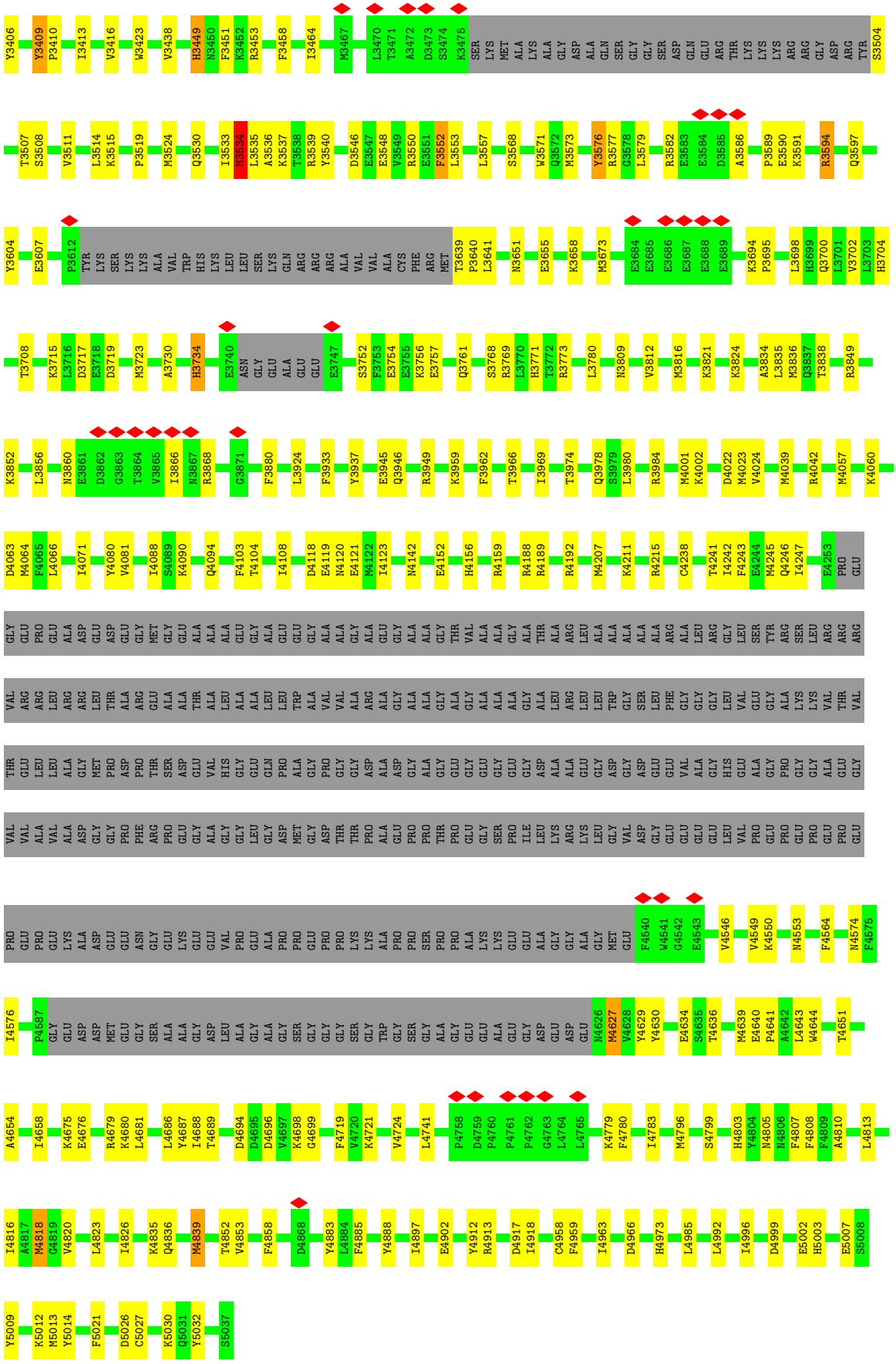


• Molecule 2: Ryanodine receptor 1

Chain I:

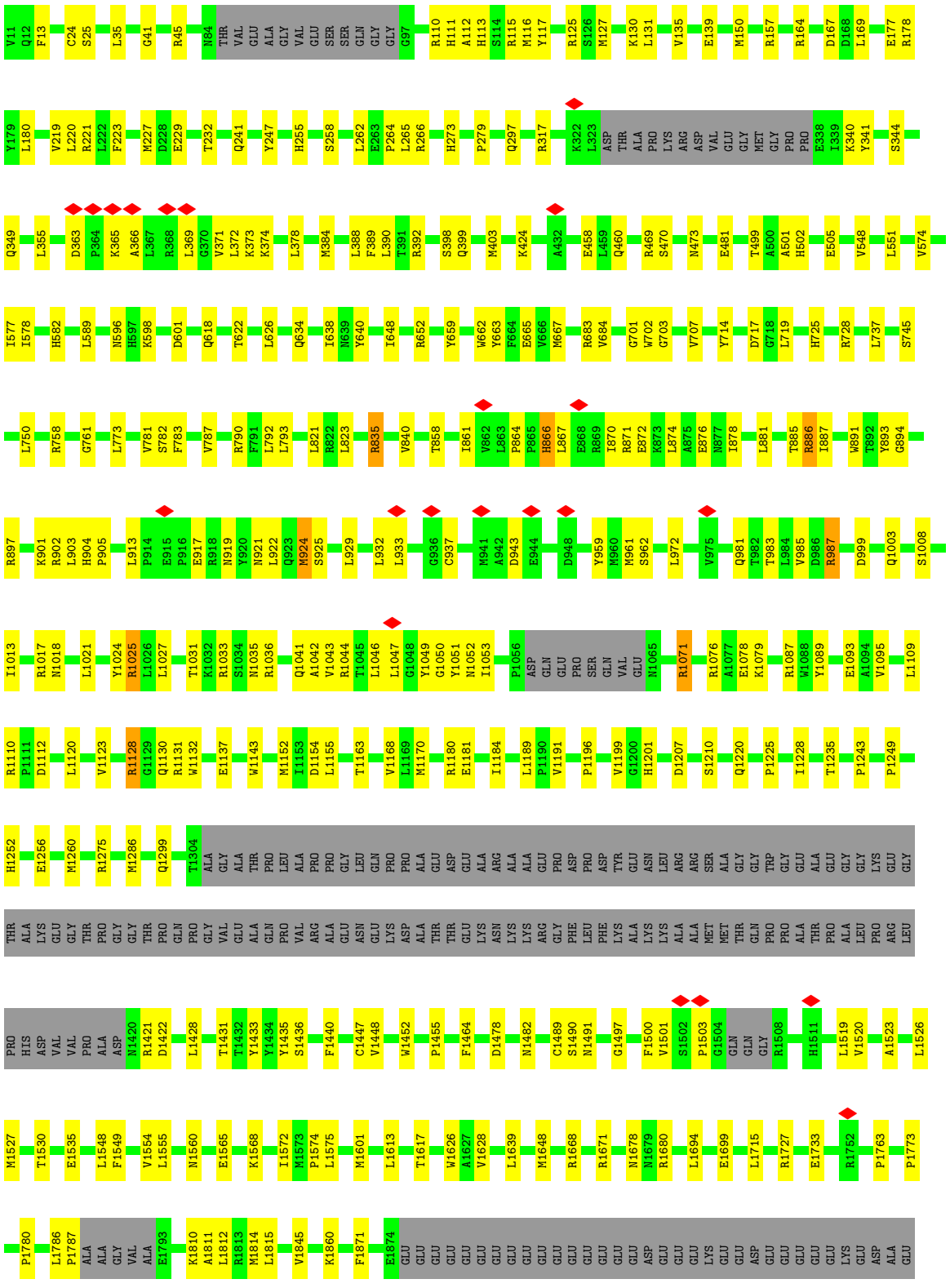

Y179 L180 M196 V219 L220 R221 L222 F223 M227 D228 E229 T232 Q241 Y247 H255 S258 L262 E263 P264 L265 R266 H273 P279 Q297 T309 S313 R317 K322 L323 ASP THR ALA PRO LYS ARG ASP VAL GLU GLY MET GLY PRO PRO E338
I339 K340 Y341 S344 Q349 L355 Y359 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 K373 L378 H379 Q380 M384 D385 L388 F389 L390 T391 R392 S398 Q399 M403 A432 Q460 R469 S470 N473 E481 T499 A500 A501 H502 E505
V548 L551 V574 I577 I578 N581 H582 L589 N596 H597 K598 D601 V602 L603 L606 Q618 T622 L626 Q634 I638 W639 Y640 I648 R652 S656 Y659 W662 Y663 F664 E665 V666 M667 R683 V684 G701 W702 G703 V707
Y714 D717 G718 L719 H725 R728 L737 S745 L750 R758 G761 L773 V781 S782 F783 V787 R790 F791 L792 L793 V815 L821 R822 L823 R835 V840 V852 T858 I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873
L874 A875 E876 N877 I878 L881 W882 T885 R886 I887 W891 T892 Y893 G894 R897 K901 R902 L903 H904 P905 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924 S925 L929 V932 L933 G936 C937 M941 A942 D943 E944 D948 Y959 M960 M961 S962
L972 V975 Q981 T982 T983 L984 V985 D986 R987 D999 Q1003 Y1007 S1008 I1013 R1017 N1018 L1021 Y1024 R1025 L1026 L1027 T1031 K1032 R1033 S1034 N1035 R1036 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 P1056 ASP GLN GLU PRO SER GLN VAL
GLU N1065 R1071 R1076 A1077 E1078 K1079 R1087 W1088 Y1089 E1093 A1094 V1095 L1109 R1110 P1111 D1112 L1120 V1123 R1128 G1129 Q1130 R1131 W1132 E1137 W1143 M1152 I1153 D1154 L1155 T1159 T1163 V1168 L1169 M1170 R1180 E1181 I1184 L1189 P1190 V1191 P1196
V1199 G1200 H1201 S1210 Q1220 P1225 I1228 T1235 P1243 P1249 H1252 E1256 M1260 R1275 M1286 Q1299 T1304 ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR
GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS
ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 L1428 T1431 T1432 Y1433 Y1434 Y1435 S1436 F1440 C1447 V1448 W1452 P1455 F1464 D1478 N1482 C1489 G1497 F1500
V1501 S1502 P1503 G1504 GLN GLN GLY R1508 H1511 L1519 V1520 A1523 L1526 M1527 T1530 E1535 L1548 F1549 V1554 L1555 N1560 E1565 K1568 I1572 M1573 P1574 L1575 M1601 L1613 T1617 W1626 A1627 V1628 L1639 M1648 D1658 R1668 R1671
N1678 N1679 R1680 L1694 E1699 L1715 R1727 E1733 R1752 P1763 P1773 P1780 L1786 P1787 ALA ALA GLY VAL ALA E1793 K1810 A1811 M1814 L1815 V1845 F1871 E1874 GLU GLU GLU

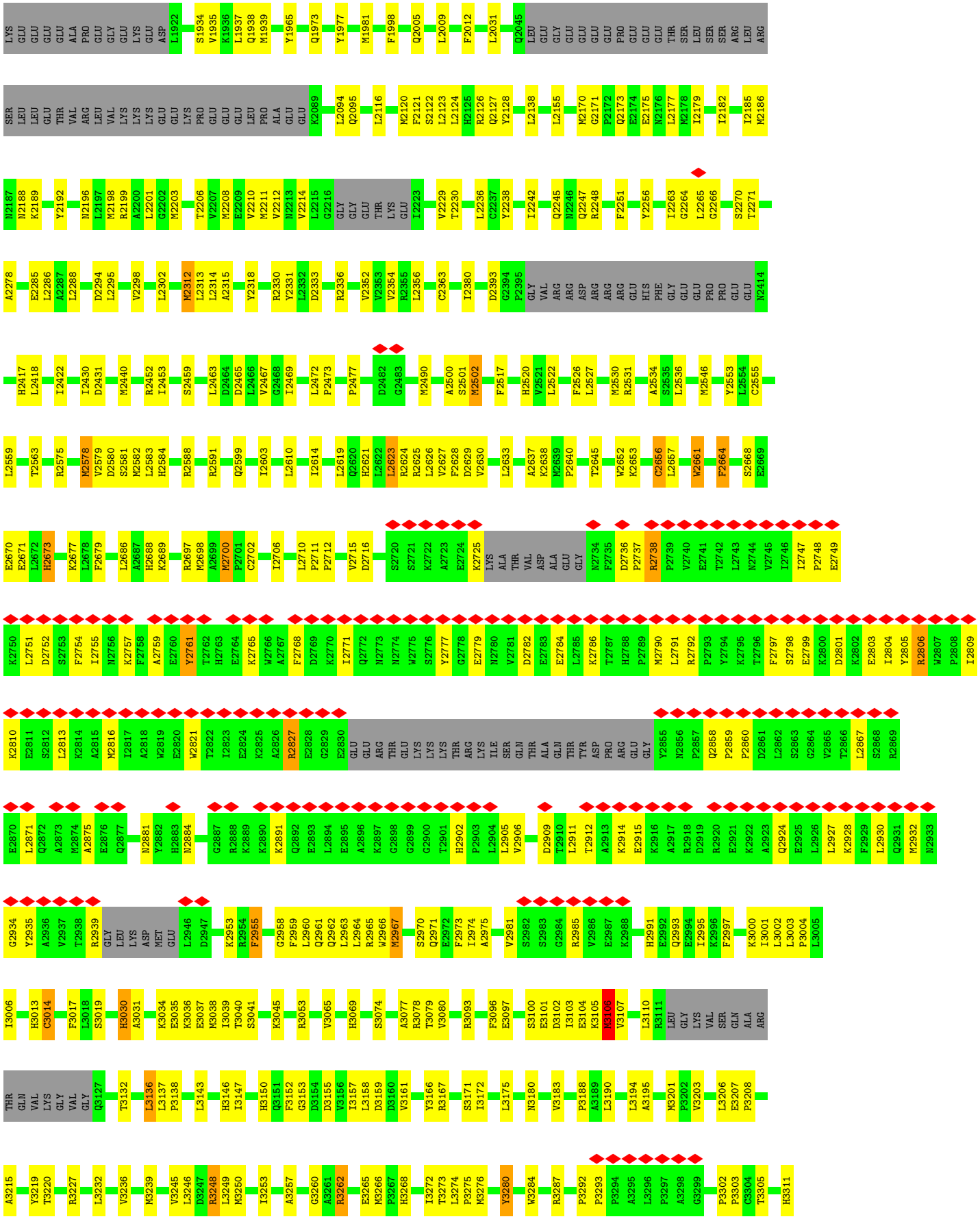

L2155 M2170 G2171 P2172 Q2173 E2174 E2175 N2176 L2177 M2178 I2179 I2182 I2185 M2186 N2187 N2188 K2189 Y2192 N2196 L2197 M2198 R2199 A2200 L2201 G2202 M2203 T2206 V2207 M2208 E2209 V2210 M2211 V2212 N2213 V2214 L2215 G2216 GLY GLY GLU THR LYS GLU I2223 V2229 T2230 L2236 C2237 Y2238 I2242
Q2245 W2246 Q2247 R2248 F2251 Y2256 I2263 G2264 L2265 G2266 S2270 T2271 A2278 E2285 L2286 A2287 L2288 D2294 L2295 V2298 L2302 M2312 L2313 L2314 A2315 K2316 G2317 Y2318 R2330 Y2331 L2332 D2333 R2336 V2352 V2353 V2354 R2355 L2356 C2363 I2380 D2393 G2394 P2395
GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2417 L2418 I2422 I2430 D2431 M2440 R2452 I2453 S2459 L2463 D2464 D2465 L2466 V2467 G2468 I2469 L2472 P2473 P2477 D2482 G2483 A2484 L2485 M2490 A2500 S2501 M2502 F2517
H2520 V2521 L2522 F2526 L2527 M2530 R2531 A2534 S2535 L2536 M2546 Y2553 L2554 C2555 L2559 T2563 R2575 M2578 V2579 D2580 S2581 M2582 L2583 H2584 R2588 R2591 Q2599 I2603 C2606 L2610 I2614 L2619 Q2620 H2621 L2622 L2623 R2624 R2625 L2626 V2627 F2628 D2629
V2630 L2633 A2637 P2640 T2645 W2652 K2653 C2656 L2657 W2661 F2664 S2668 E2669 E2670 E2671 L2672 H2673 K2677 L2678 F2679 L2686 A2687 H2688 K2689 R2697 M2698 A2699 M2700 P2701 C2702 I2706 L2710 P2711 P2712 V2715 D2716 S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA
THR VAL ASP ALA GLU GLY N2734 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 N2881 Y2882 H2883 N2884 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 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 L2946 D2947 K2953 R2954 F2955 G2958 F2959 L2960 Q2961 Q2962 L2963 L2964 R2965 W2966 M2967 S2970 Q2971 E2972 F2973 I2974 V2981 S2982
S2983 G2984 R2985 V2986 E2987 K2988 H2991 E2992 Q2993 E2994 I2995 K2996 F2997 K3000 I3001 L3002 L3003 P3004 L3005 I3006 H3013 C3014 F3017 L3018 S3019 H3030 A3031 K3034 E3035 K3036 E3037 M3038 I3039 T3040 S3041 K3045 R3053 V3065 H3069 A3077 R3078 T3079 V3080 R3093 F3096 E3097
S3100 E3101 D3102 I3103 E3104 K3105 M3106 V3107 L3110 R3111 LEU GLY LYS VAL SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 T3132 L3136 L3137 P3138 L3143 H3146 I3147 H3150 Q3151 F3152 G3153 D3154 D3155 V3156 I3157 L3158 D3159 D3160 V3161 Y3166 R3167 S3171 I3172 L3175
N3180 V3183 P3188 A3189 L3190 L3194 A3195 M3201 P3202 V3203 L3206 E3207 P3208 A3215 Y3219 T3220 R3227 L3232 V3236 M3239 V3245 L3246 D3247 R3248 L3249 M3250 I3253 A3257 G3260 A3261 R3262 E3265 M3266 P3267 H3268 I3272 T3273 L3274 P3275 M3276 Y3280
W3284 R3287 P3293 P3294 A3296 L3296 P3297 A3298 G3299 P3302 P3303 C3304 T3305 H3311 R3321 N3326 W3334 M3335 K3336 R3337 R3350 H3355 S3356 H3357 K3367 R3368 V3372 E3377 Q3378 L3379 R3380 L3381 E3382 A3383 K3384 A3385 E3386 A3387 E3391 L3392 R3395 D3396 E3397 V3400

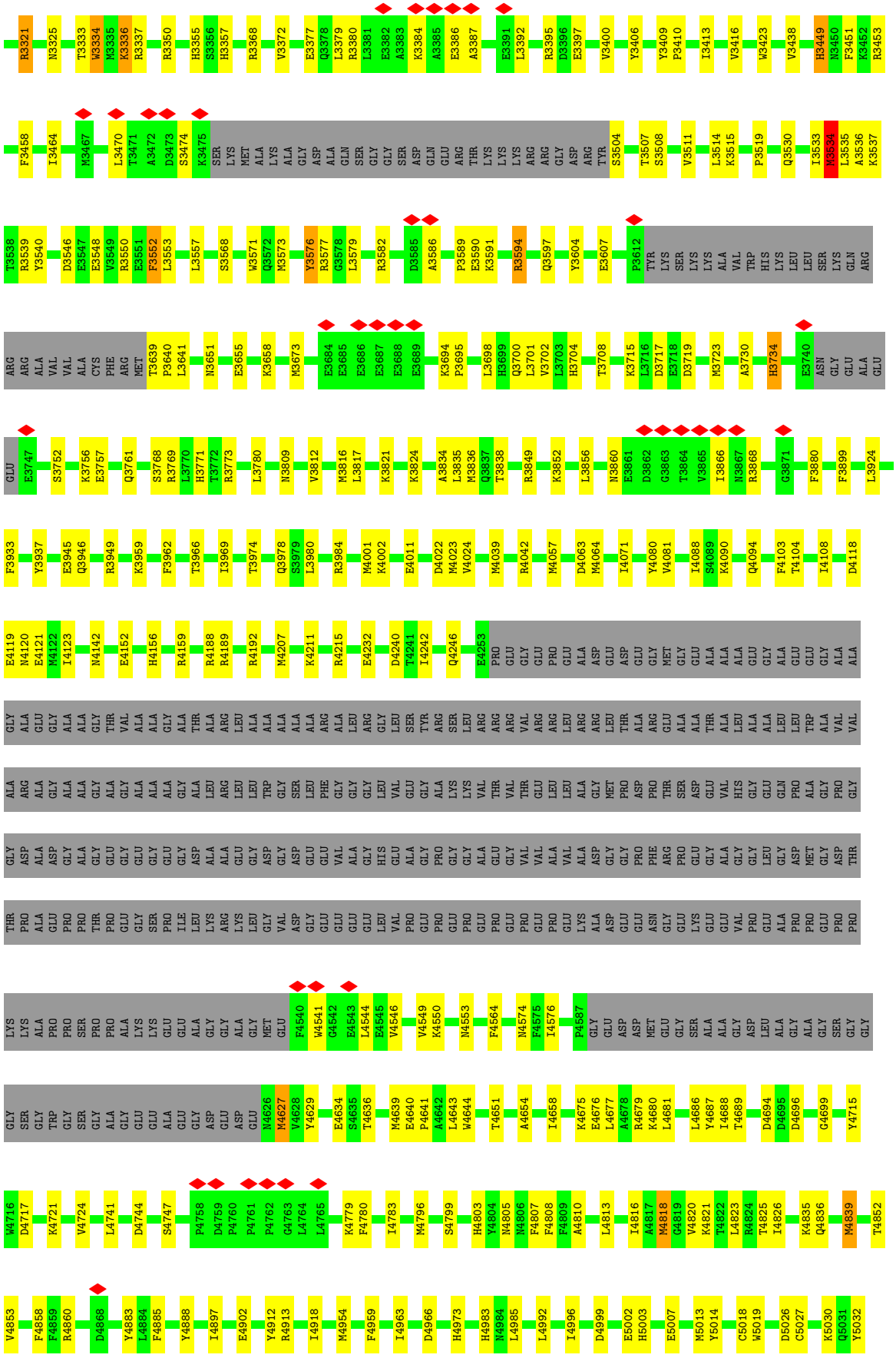


• Molecule 2: Ryanodine receptor 1

Chain A:

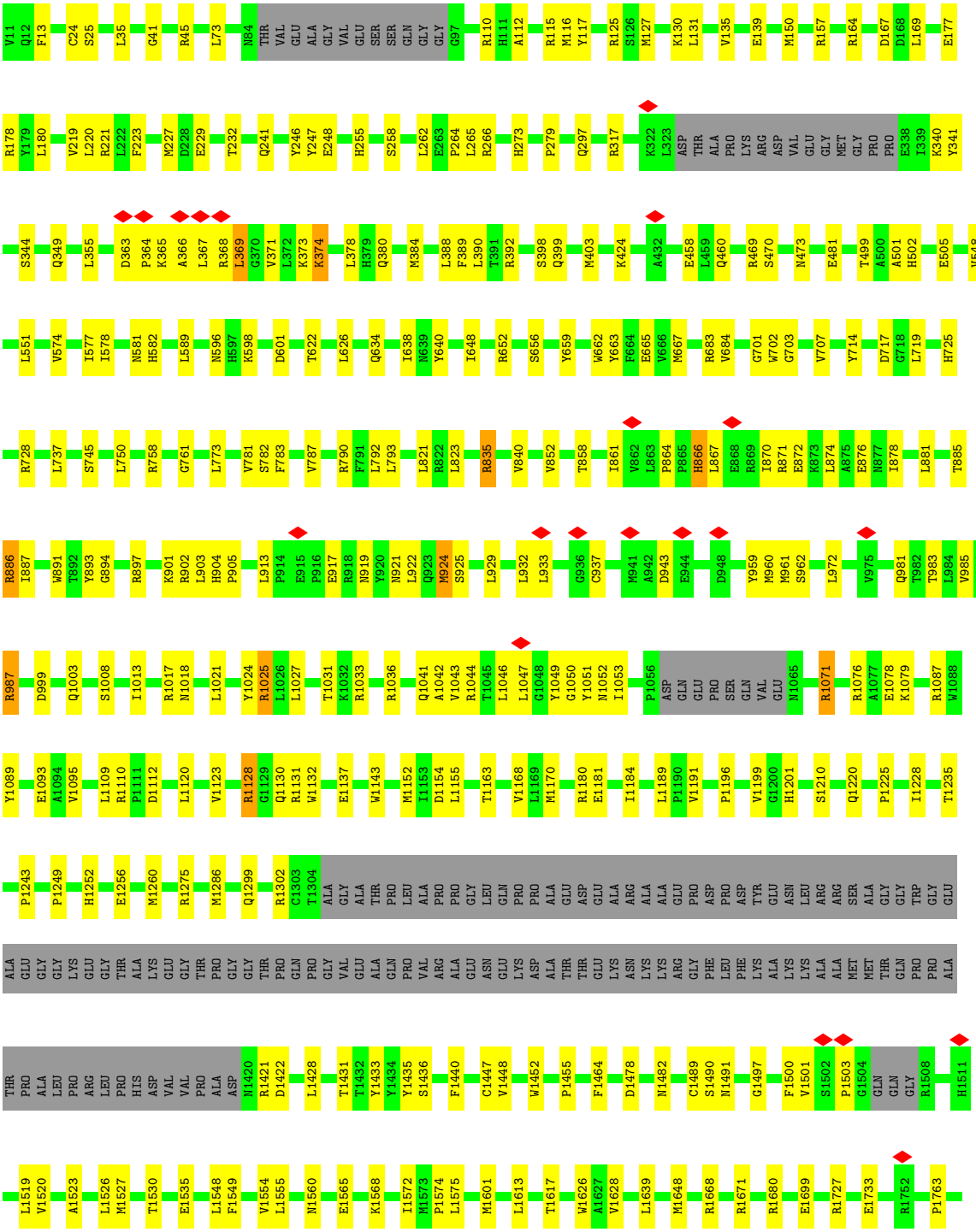


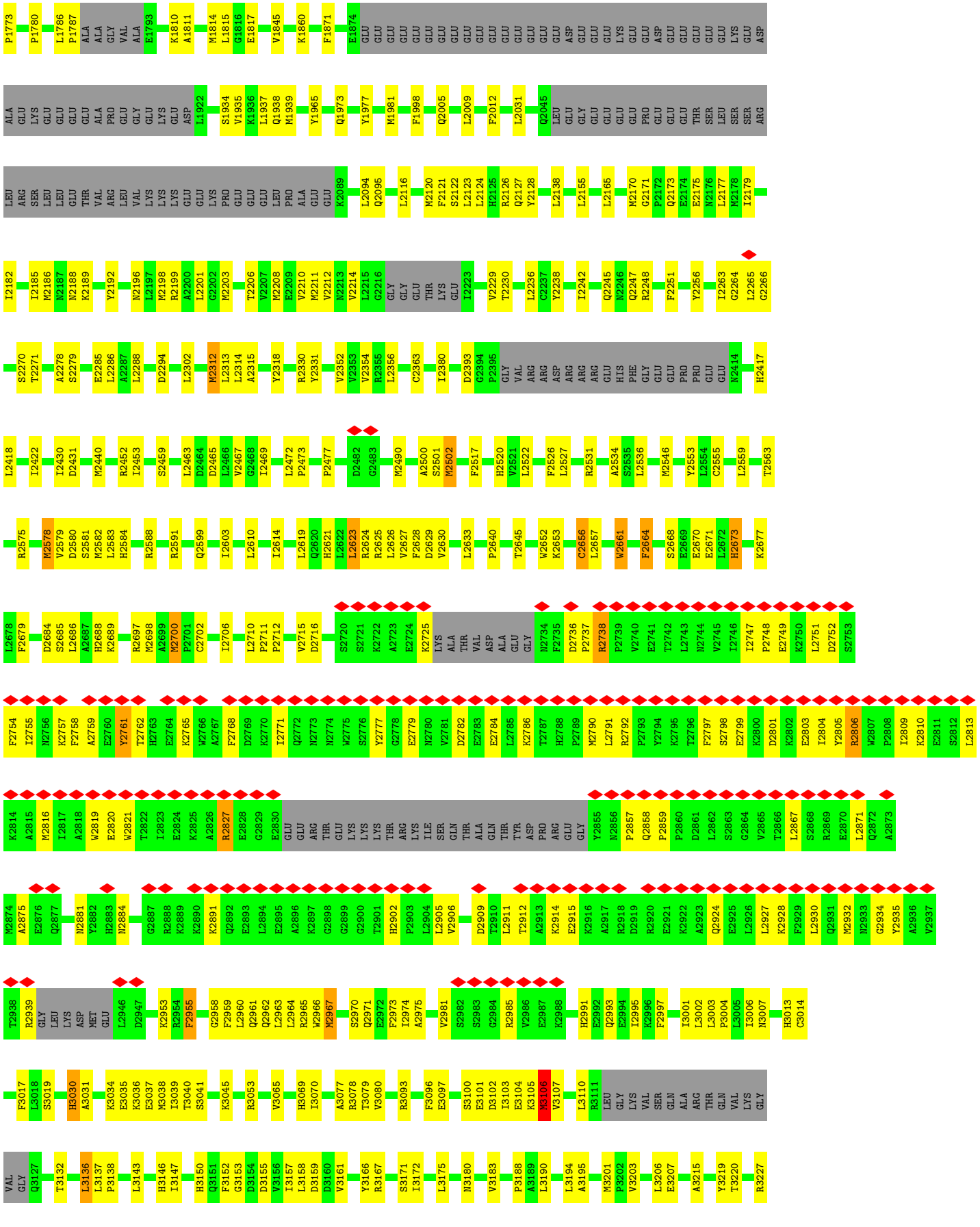


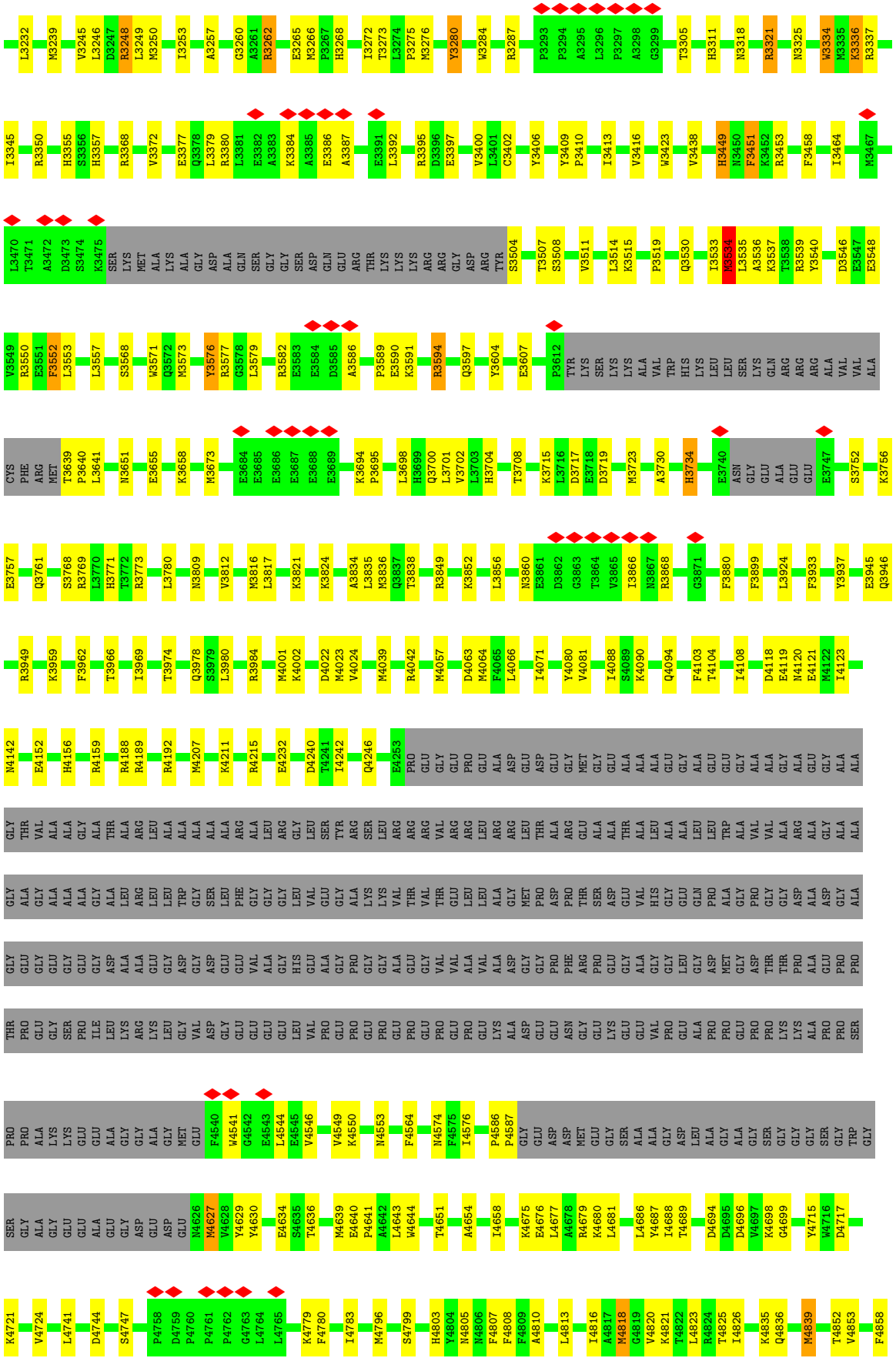


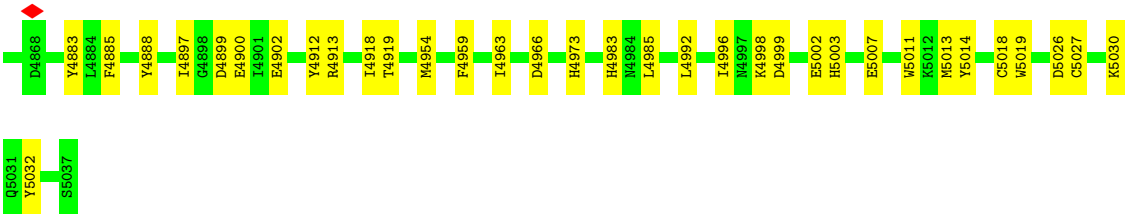
• Molecule 2: Ryanodine receptor 1

Chain D:



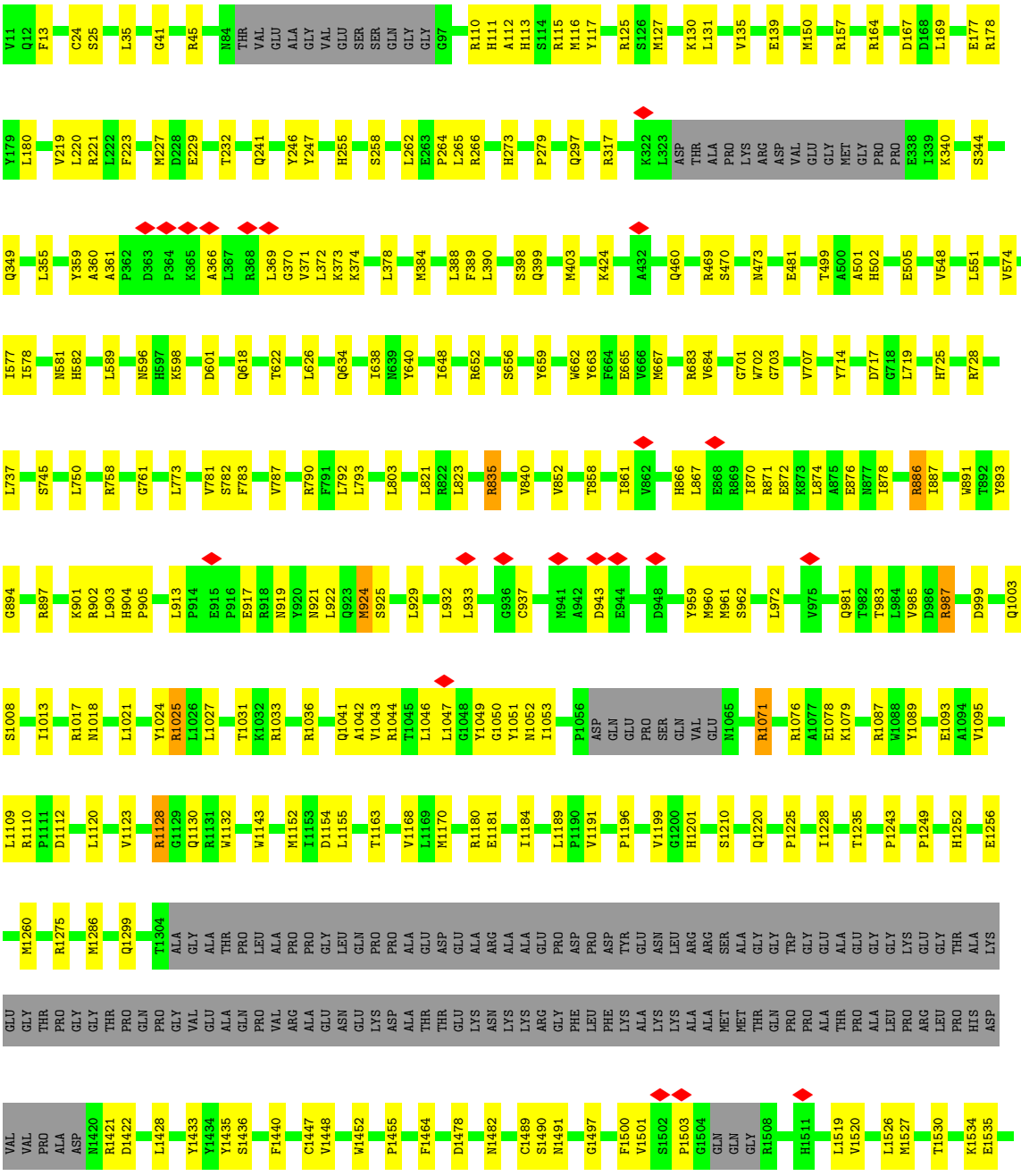


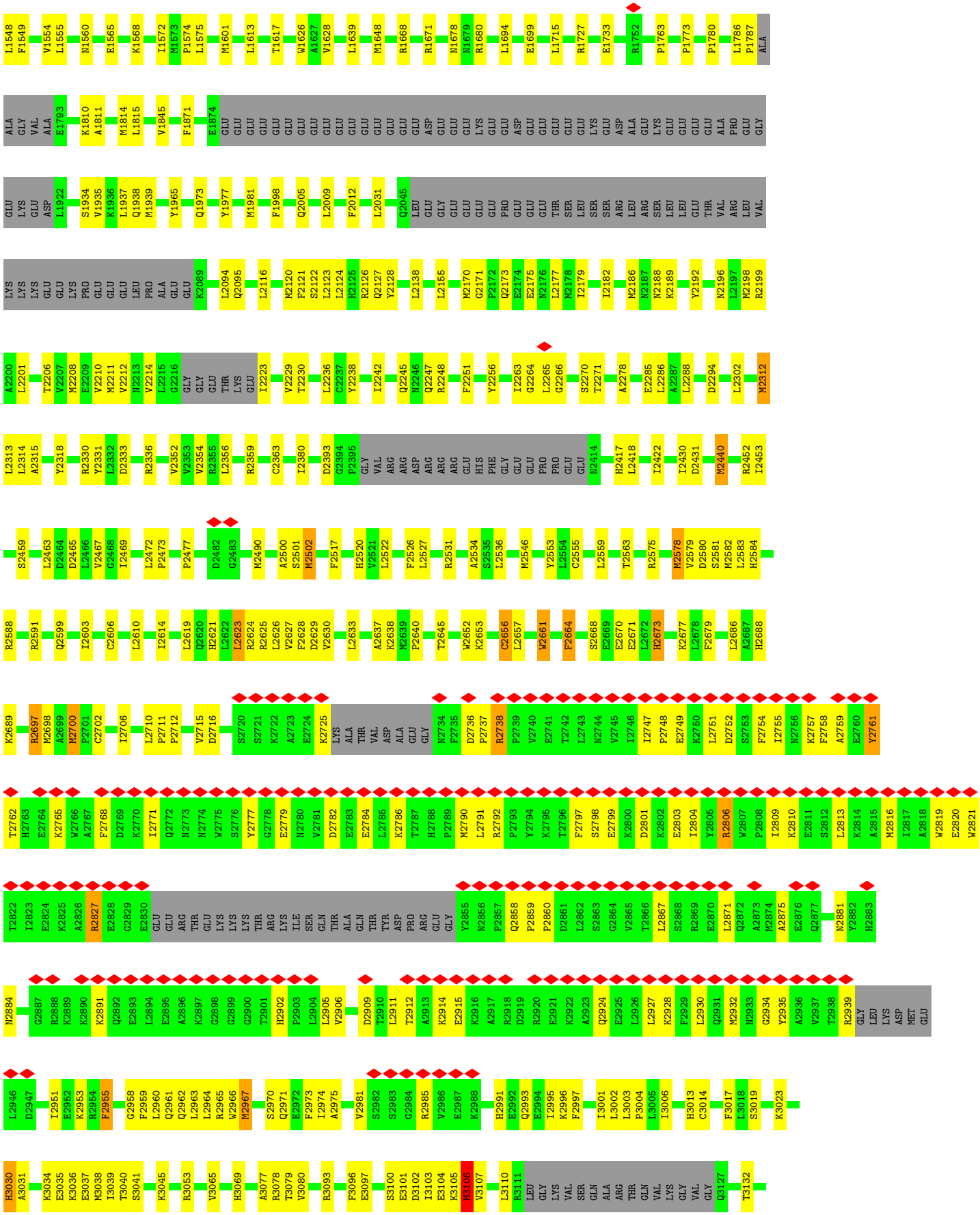


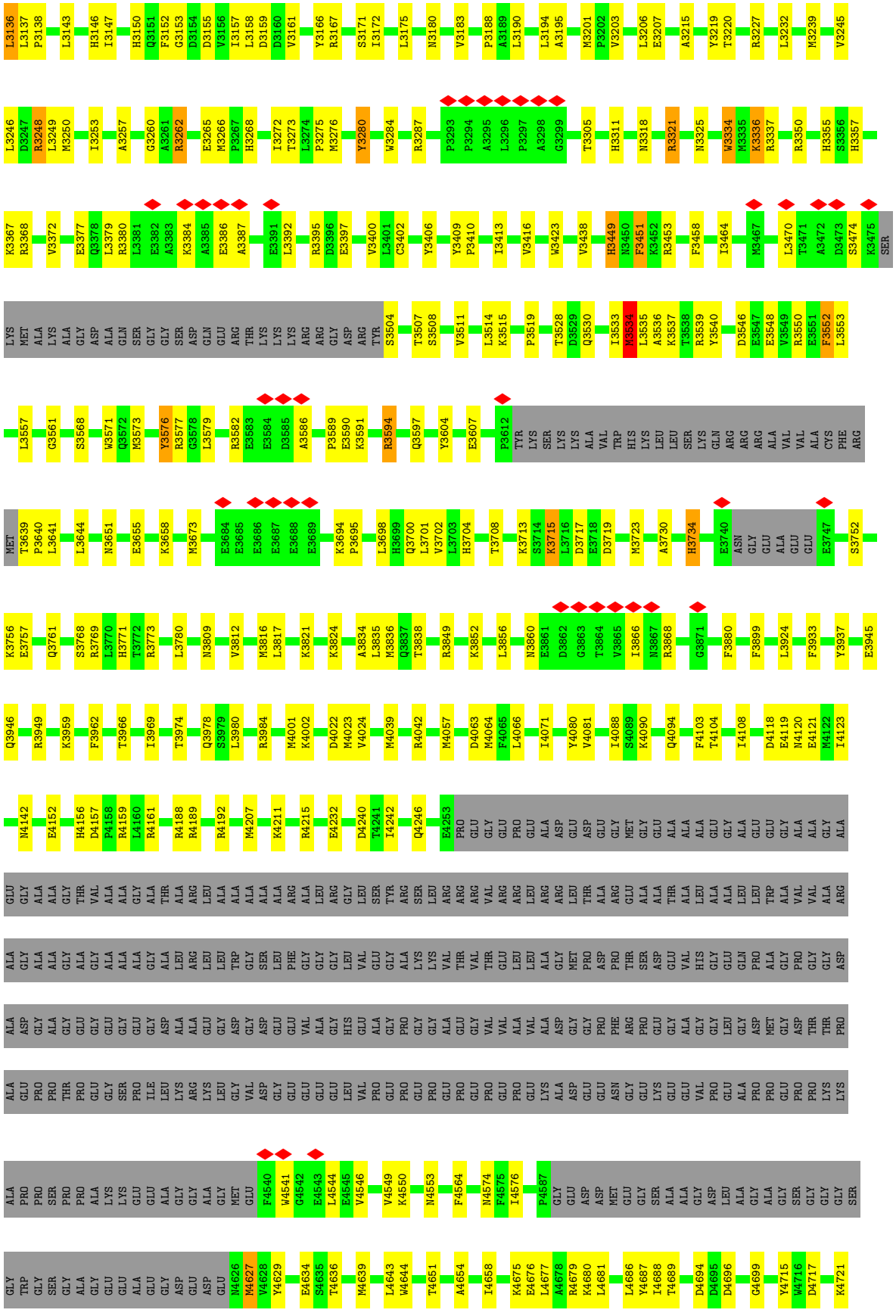


• Molecule 2: Ryanodine receptor 1

Chain G:

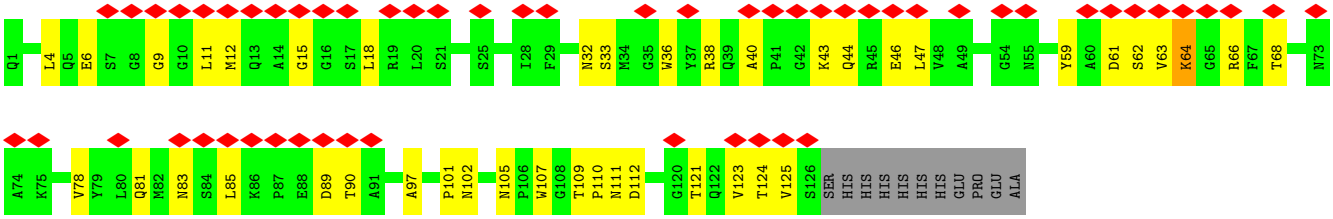






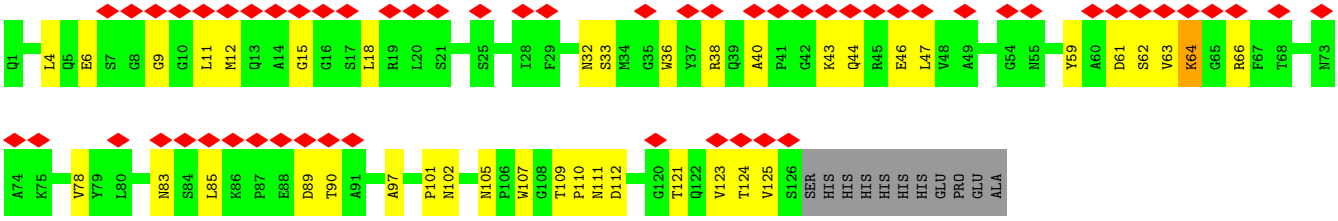
• Molecule 3: Nanobody 9657

Chain K:



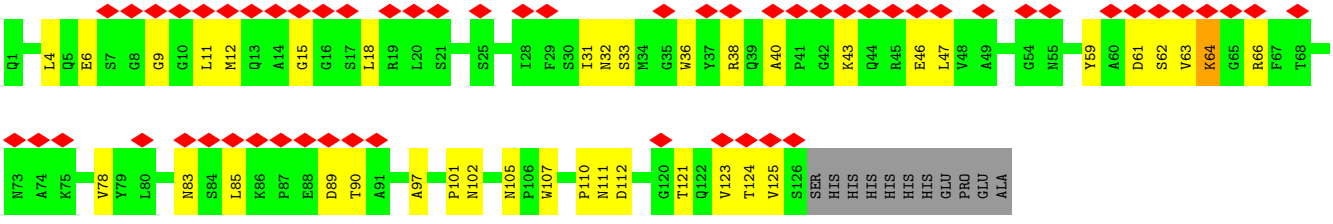
• Molecule 3: Nanobody 9657

Chain C:



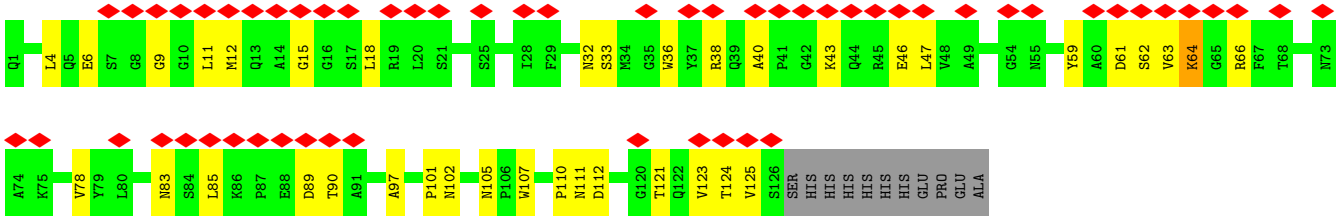
• Molecule 3: Nanobody 9657

Chain E:



• Molecule 3: Nanobody 9657

Chain M:


Q1 L4 Q5 E6 S7 G8 G9 G10 L11 M12 Q13 A14 G15 G16 S17 L18 R19 L20 S21 S25 I28 F29 N32 S33 M34 G35 W36 Y37 R38 Q39 A40 P41 G42 K43 Q44 R45 E46 L47 V48 A49 G54 N55 Y59 A60 D61 S62 V63 K64 G65 R66 F67 T68 N73
A74 K75 V78 Y79 L80 N83 S84 L85 K86 P87 E88 D89 T90 A91 A97 P101 N102 N105 P106 W107 P110 N111 D112 G120 T121 Q122 V123 T124 V125 S126 SER HIS HIS HIS HIS HIS HIS GLU PRO GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	175535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.601	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	511.65, 511.65, 511.65	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.137, 1.137, 1.137	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, CFF, POV, CA

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	F	0.27	0/834	0.56	0/1123
1	H	0.27	0/834	0.56	0/1123
1	J	0.27	0/834	0.56	0/1123
1	L	0.27	0/834	0.56	0/1123
2	A	0.25	0/34923	0.49	4/47330 (0.0%)
2	D	0.25	0/34923	0.49	4/47330 (0.0%)
2	G	0.25	0/34920	0.49	4/47325 (0.0%)
2	I	0.25	0/34920	0.49	4/47325 (0.0%)
3	C	0.25	0/987	0.52	0/1340
3	E	0.25	0/987	0.52	0/1340
3	K	0.25	0/987	0.52	0/1340
3	M	0.25	0/987	0.52	0/1340
All	All	0.25	0/146970	0.49	16/199162 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1503	PRO	N-CA-CB	5.72	110.16	103.30
2	I	1503	PRO	N-CA-CB	5.71	110.16	103.30
2	D	1503	PRO	N-CA-CB	5.71	110.16	103.30
2	A	1503	PRO	N-CA-CB	5.68	110.12	103.30
2	D	3136	LEU	CA-CB-CG	5.66	128.32	115.30

There are no chirality outliers.

There are no planarity outliers.

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	F	818	0	824	14	0
1	H	818	0	824	13	0
1	J	818	0	824	11	0
1	L	818	0	824	12	0
2	A	34153	0	33544	573	0
2	D	34153	0	33544	576	0
2	G	34151	0	33538	575	0
2	I	34151	0	33538	580	0
3	C	967	0	916	25	0
3	E	967	0	916	25	0
3	K	967	0	916	28	0
3	M	967	0	916	23	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
5	A	52	0	82	1	0
5	D	52	0	82	3	0
5	G	52	0	82	3	0
5	I	52	0	82	1	0
6	A	31	0	12	3	0
6	D	31	0	12	3	0
6	G	31	0	12	3	0
6	I	31	0	12	2	0
7	A	14	0	10	1	0
7	D	14	0	10	2	0
7	G	14	0	10	2	0
7	I	14	0	10	1	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	I	1	0	0	0	0
All	All	144144	0	141540	2394	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 8.

The worst 5 of 2394 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:A:3132:THR:HA	2:A:3136:LEU:HB3	1.61	0.83
2:G:3132:THR:HA	2:G:3136:LEU:HB3	1.61	0.82
2:I:3132:THR:HA	2:I:3136:LEU:HB3	1.61	0.82
2:I:4823:LEU:HD13	2:G:4839:MET:HE2	1.61	0.81
2:I:4839:MET:HE2	2:A:4823:LEU:HD13	1.62	0.81

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	F	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	H	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	J	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	L	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	A	4280/5027 (85%)	4203 (98%)	77 (2%)	0	100	100
2	D	4280/5027 (85%)	4201 (98%)	78 (2%)	1 (0%)	100	100
2	G	4280/5027 (85%)	4201 (98%)	79 (2%)	0	100	100
2	I	4280/5027 (85%)	4203 (98%)	77 (2%)	0	100	100
3	C	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	E	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	K	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
3	M	124/137 (90%)	118 (95%)	6 (5%)	0	100	100
All	All	18036/21084 (86%)	17684 (98%)	351 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	374	LYS

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	F	88/88 (100%)	85 (97%)	3 (3%)	32	62
1	H	88/88 (100%)	85 (97%)	3 (3%)	32	62
1	J	88/88 (100%)	85 (97%)	3 (3%)	32	62
1	L	88/88 (100%)	85 (97%)	3 (3%)	32	62
2	A	3674/4270 (86%)	3555 (97%)	119 (3%)	34	63
2	D	3674/4270 (86%)	3553 (97%)	121 (3%)	33	62
2	G	3673/4270 (86%)	3552 (97%)	121 (3%)	33	62
2	I	3673/4270 (86%)	3552 (97%)	121 (3%)	33	62
3	C	104/114 (91%)	102 (98%)	2 (2%)	52	75
3	E	104/114 (91%)	102 (98%)	2 (2%)	52	75
3	K	104/114 (91%)	102 (98%)	2 (2%)	52	75
3	M	104/114 (91%)	102 (98%)	2 (2%)	52	75
All	All	15462/17888 (86%)	14960 (97%)	502 (3%)	36	63

5 of 502 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4156	HIS
2	G	3014	CYS
2	D	2294	ASP
2	G	2914	LYS
2	G	3836	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	981	GLN
2	G	1299	GLN
2	G	4246	GLN
2	A	3146	HIS
2	A	981	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	POV	I	5102	-	51,51,51	0.49	0	57,59,59	0.45	0
7	CFF	A	5104	-	8,15,15	2.40	3 (37%)	8,23,23	1.20	1 (12%)
5	POV	D	5102	-	51,51,51	0.49	0	57,59,59	0.45	0
6	ATP	A	5103	-	26,33,33	0.59	0	31,52,52	0.85	3 (9%)
6	ATP	I	5103	-	26,33,33	0.91	1 (3%)	31,52,52	1.59	5 (16%)
7	CFF	I	5104	-	8,15,15	2.40	3 (37%)	8,23,23	1.20	1 (12%)
7	CFF	G	5104	-	8,15,15	2.38	3 (37%)	8,23,23	1.18	1 (12%)
6	ATP	G	5103	-	26,33,33	0.58	0	31,52,52	0.84	3 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	POV	G	5102	-	51,51,51	0.49	0	57,59,59	0.45	0
7	CFF	D	5104	-	8,15,15	2.41	3 (37%)	8,23,23	1.19	1 (12%)
6	ATP	D	5103	-	26,33,33	0.59	0	31,52,52	0.85	3 (9%)
5	POV	A	5101	-	51,51,51	0.49	0	57,59,59	0.45	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	POV	I	5102	-	-	17/55/55/55	-
7	CFF	A	5104	-	-	-	0/2/2/2
5	POV	D	5102	-	-	17/55/55/55	-
6	ATP	A	5103	-	-	5/18/38/38	0/3/3/3
6	ATP	I	5103	-	-	3/18/38/38	0/3/3/3
7	CFF	I	5104	-	-	-	0/2/2/2
7	CFF	G	5104	-	-	-	0/2/2/2
6	ATP	G	5103	-	-	5/18/38/38	0/3/3/3
5	POV	G	5102	-	-	17/55/55/55	-
7	CFF	D	5104	-	-	-	0/2/2/2
6	ATP	D	5103	-	-	5/18/38/38	0/3/3/3
5	POV	A	5101	-	-	17/55/55/55	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5104	CFF	C5-C4	4.54	1.45	1.39
7	I	5104	CFF	C5-C4	4.53	1.45	1.39
7	D	5104	CFF	C5-C4	4.53	1.45	1.39
7	G	5104	CFF	C5-C4	4.52	1.45	1.39
7	D	5104	CFF	C5-C6	4.35	1.48	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	5103	ATP	PA-O3A-PB	-3.89	119.48	132.83
6	I	5103	ATP	PB-O3B-PG	-3.87	119.54	132.83
6	I	5103	ATP	N3-C2-N1	-3.20	123.67	128.68
6	I	5103	ATP	C3'-C2'-C1'	3.07	105.60	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	5103	ATP	C4-C5-N7	-2.42	106.87	109.40

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	5102	POV	C1-O11-P-O14
5	A	5101	POV	C1-O11-P-O14
5	D	5102	POV	C1-O11-P-O14
5	G	5102	POV	C1-O11-P-O14
6	I	5103	ATP	C5'-O5'-PA-O1A

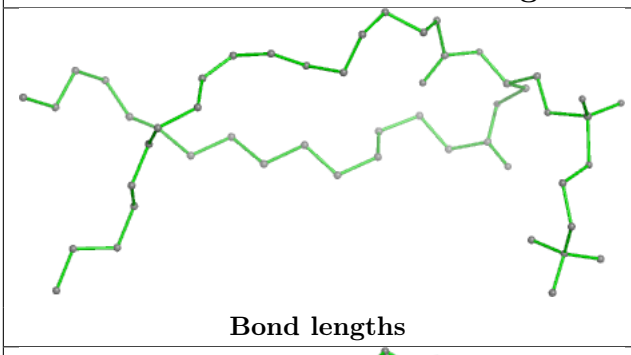
There are no ring outliers.

12 monomers are involved in 25 short contacts:

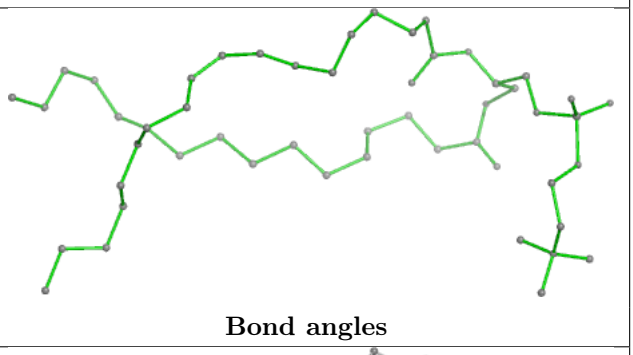
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	5102	POV	1	0
7	A	5104	CFF	1	0
5	D	5102	POV	3	0
6	A	5103	ATP	3	0
6	I	5103	ATP	2	0
7	I	5104	CFF	1	0
7	G	5104	CFF	2	0
6	G	5103	ATP	3	0
5	G	5102	POV	3	0
7	D	5104	CFF	2	0
6	D	5103	ATP	3	0
5	A	5101	POV	1	0

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

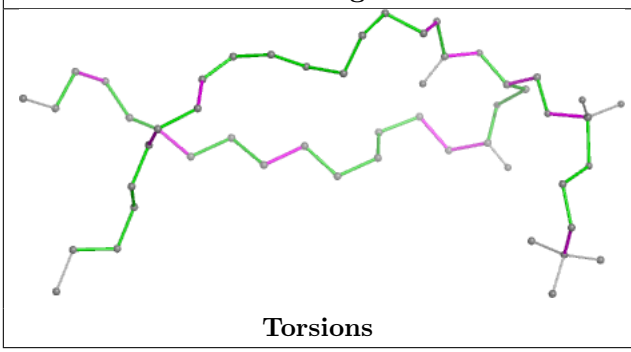
Ligand POV I 5102



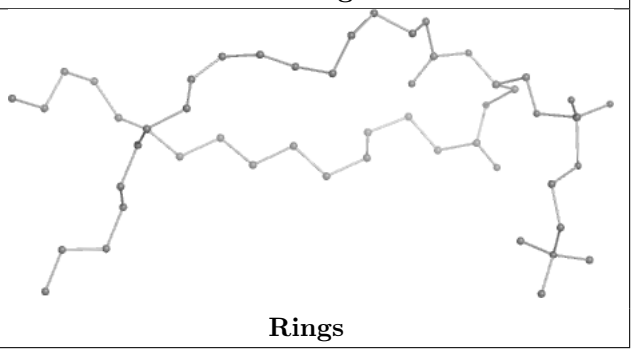
Bond lengths



Bond angles

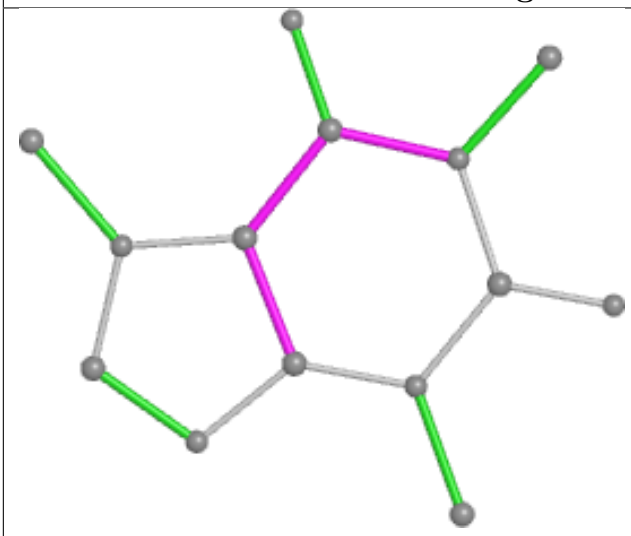


Torsions

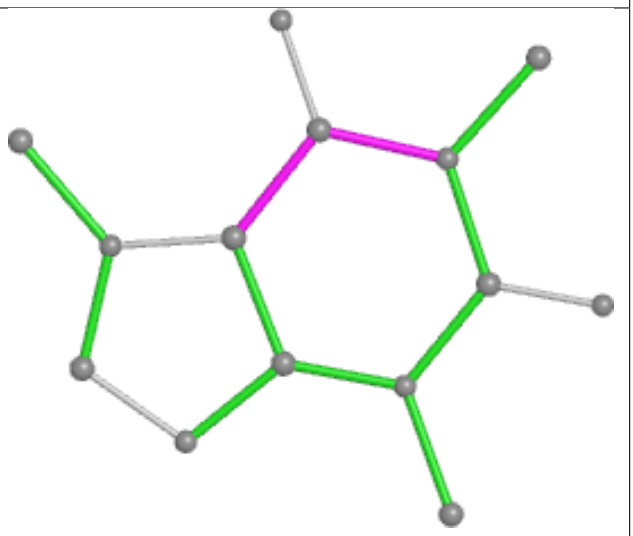


Rings

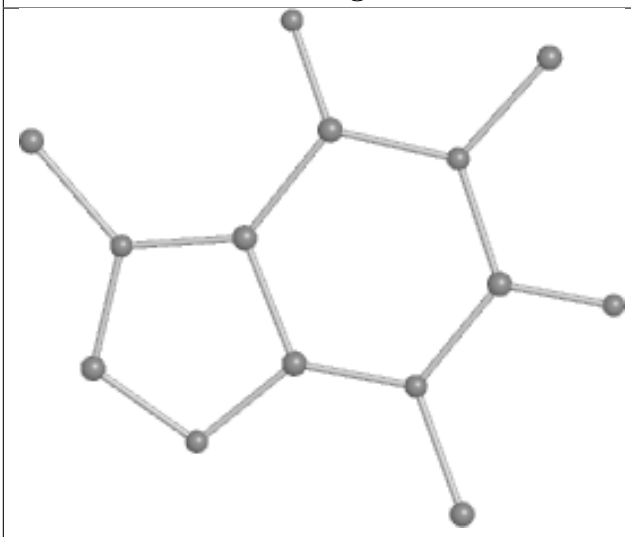
Ligand CFF A 5104



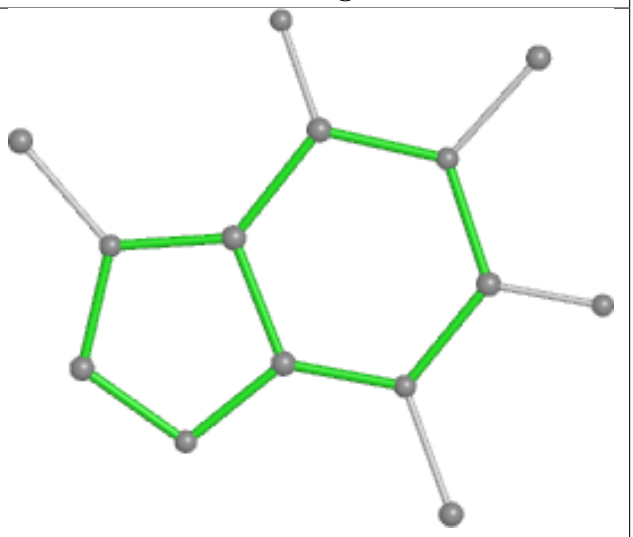
Bond lengths



Bond angles

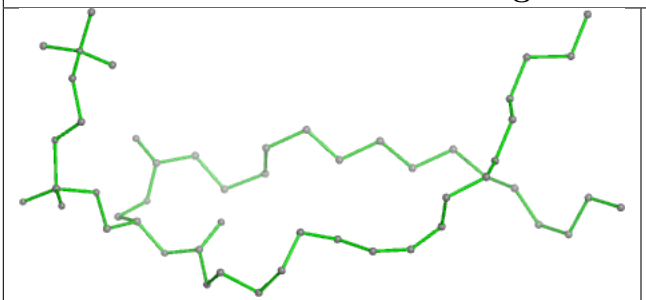


Torsions

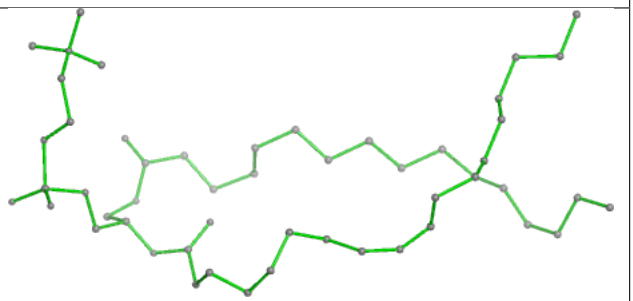


Rings

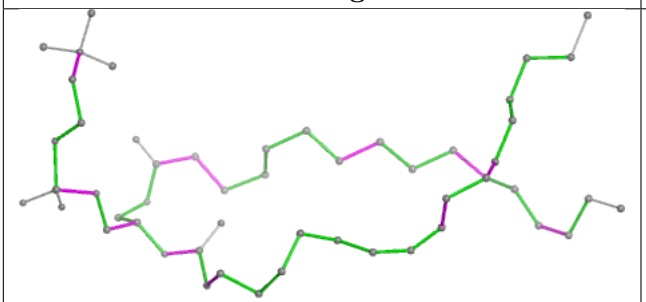
Ligand POV D 5102



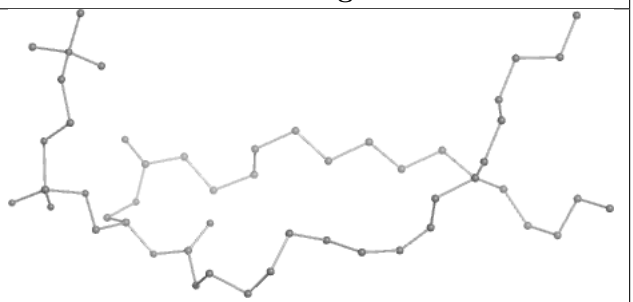
Bond lengths



Bond angles

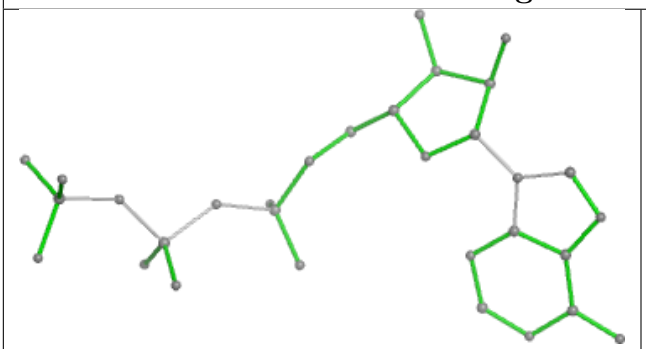


Torsions

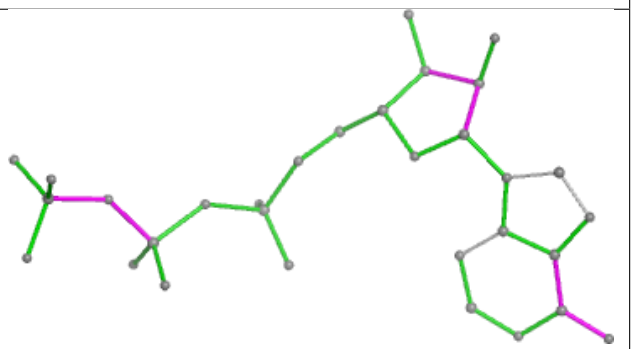


Rings

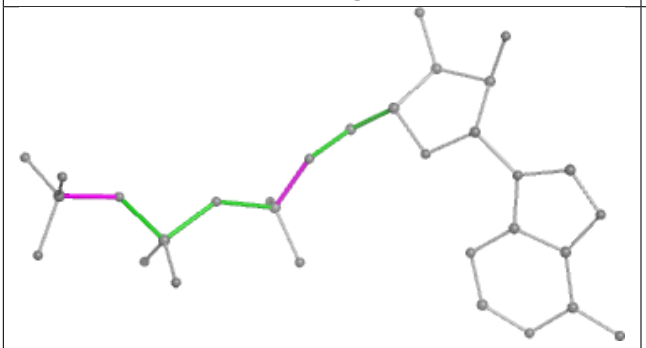
Ligand ATP A 5103



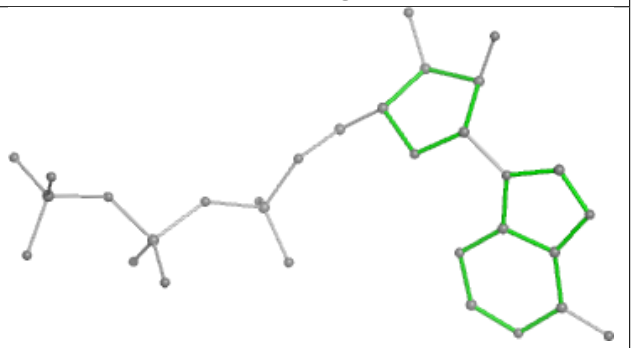
Bond lengths



Bond angles

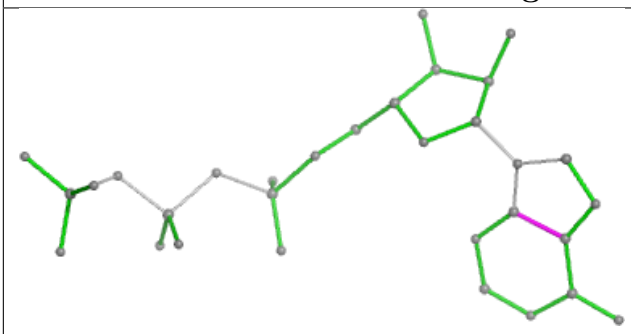


Torsions

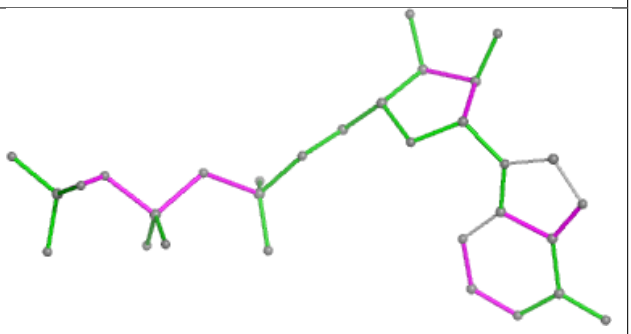


Rings

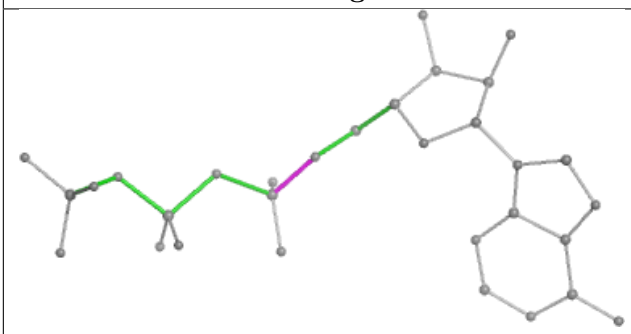
Ligand ATP I 5103



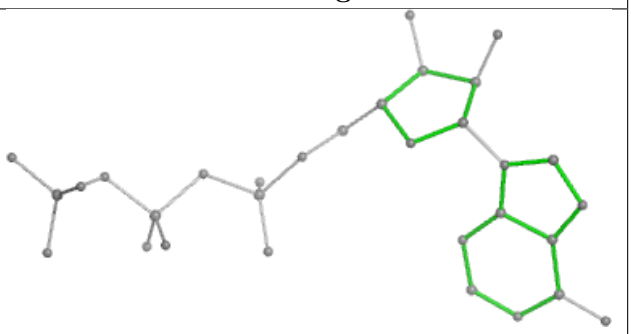
Bond lengths



Bond angles

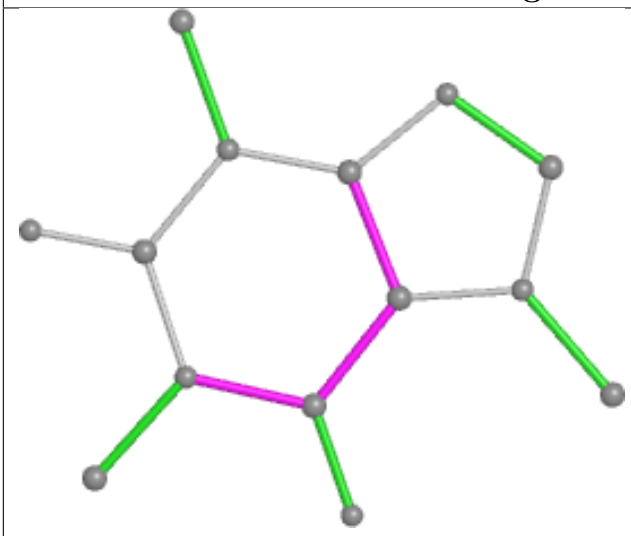


Torsions

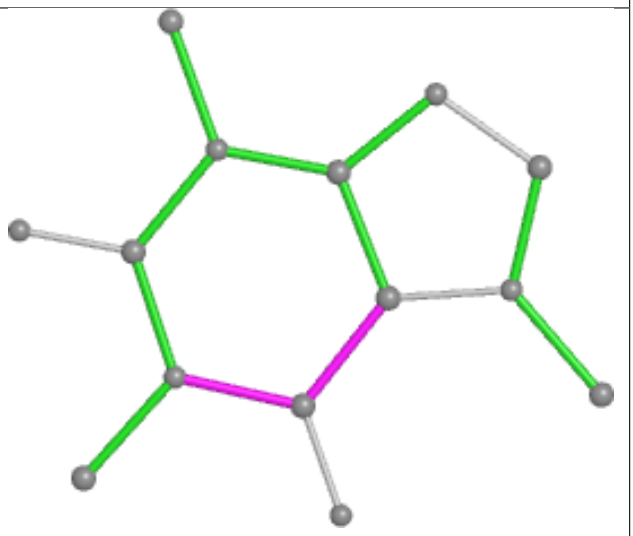


Rings

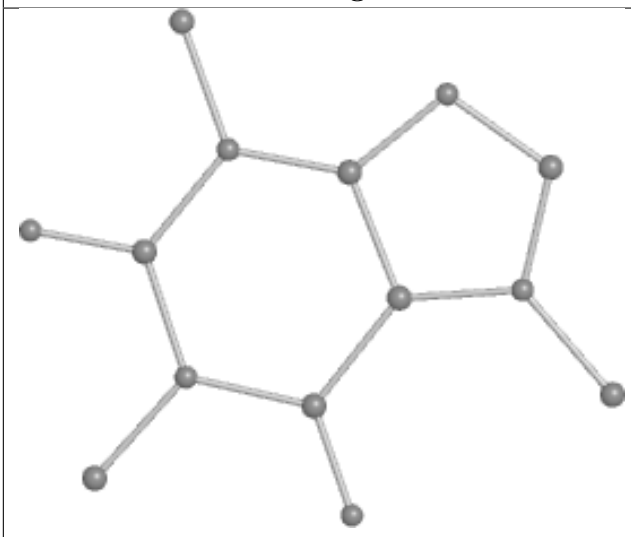
Ligand CFF I 5104



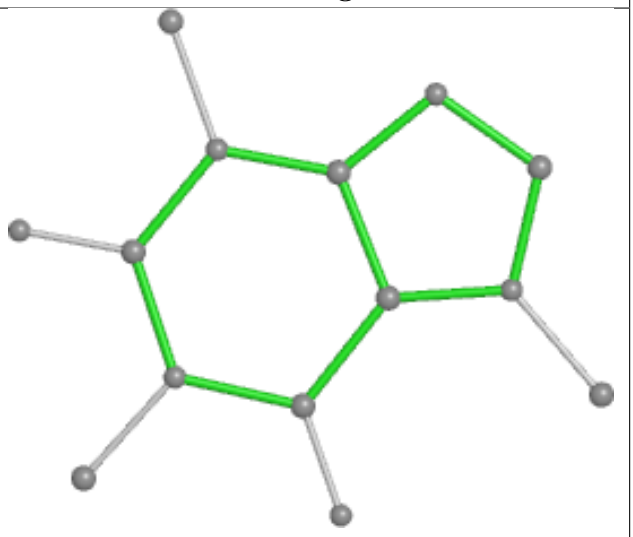
Bond lengths



Bond angles

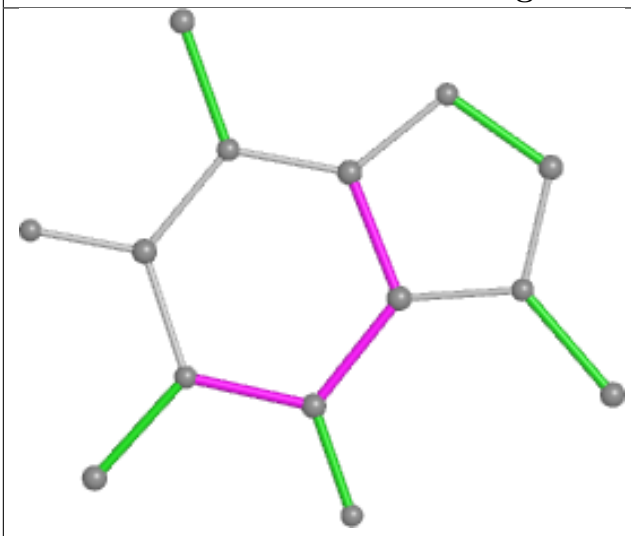


Torsions

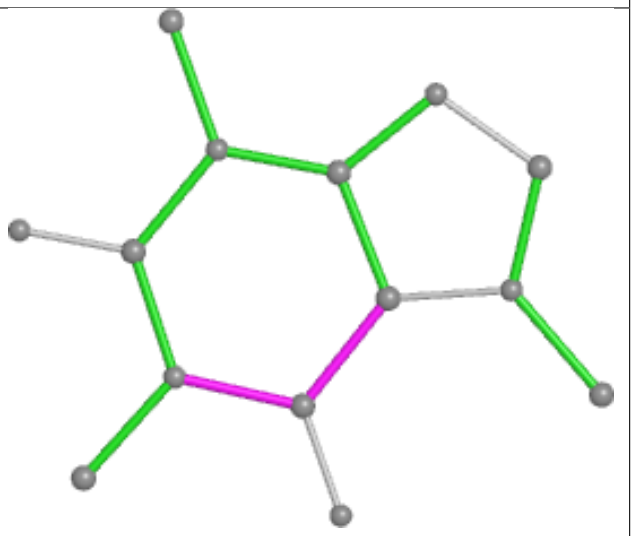


Rings

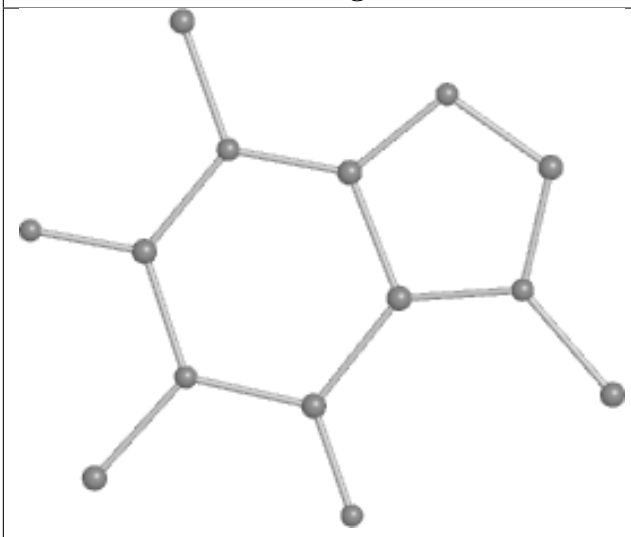
Ligand CFF G 5104



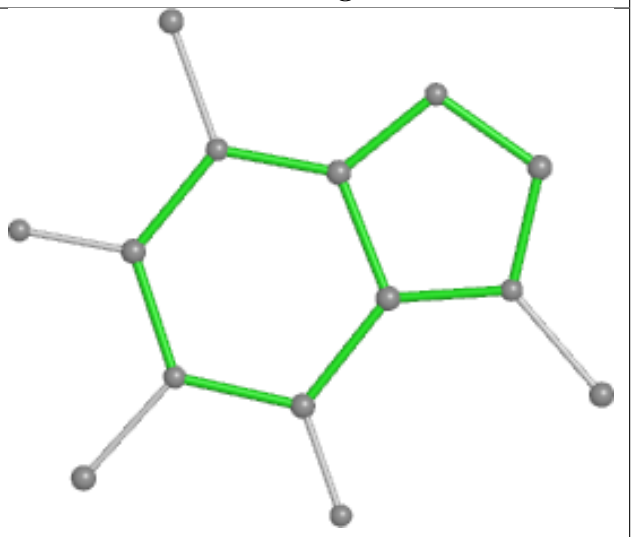
Bond lengths



Bond angles

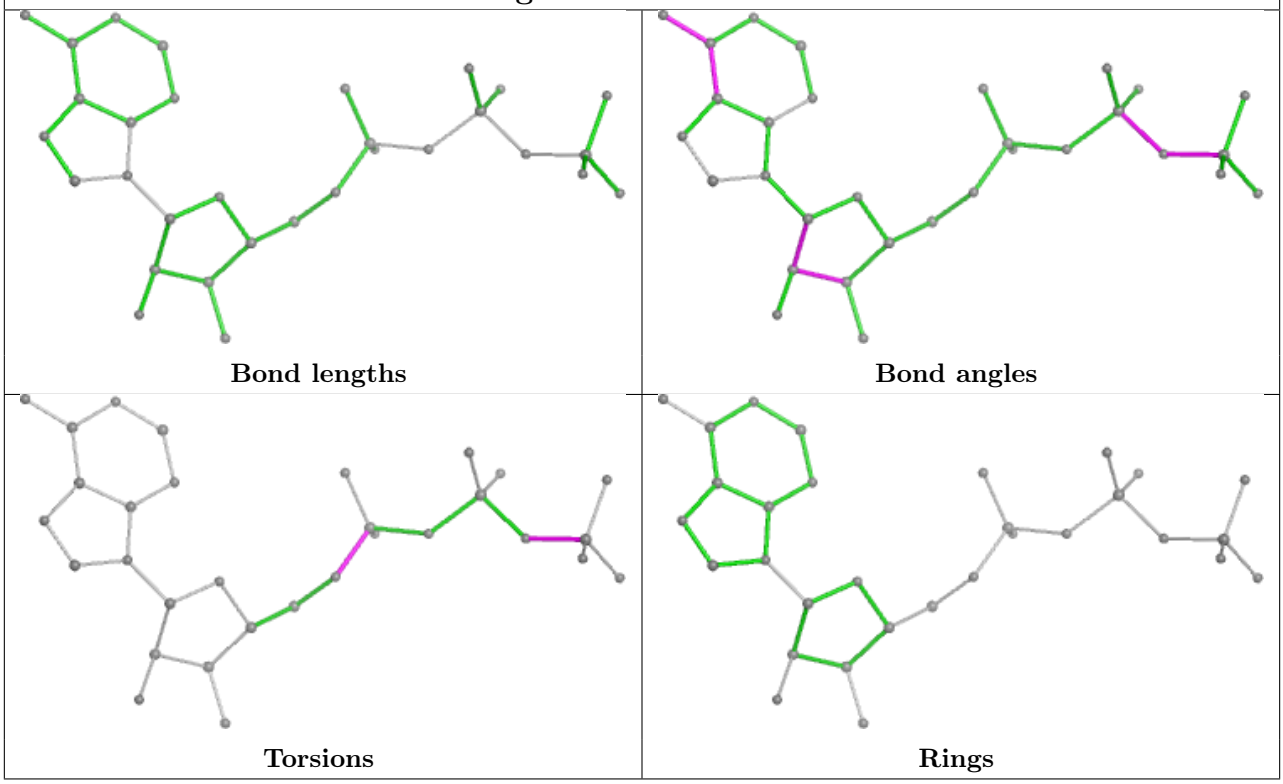


Torsions

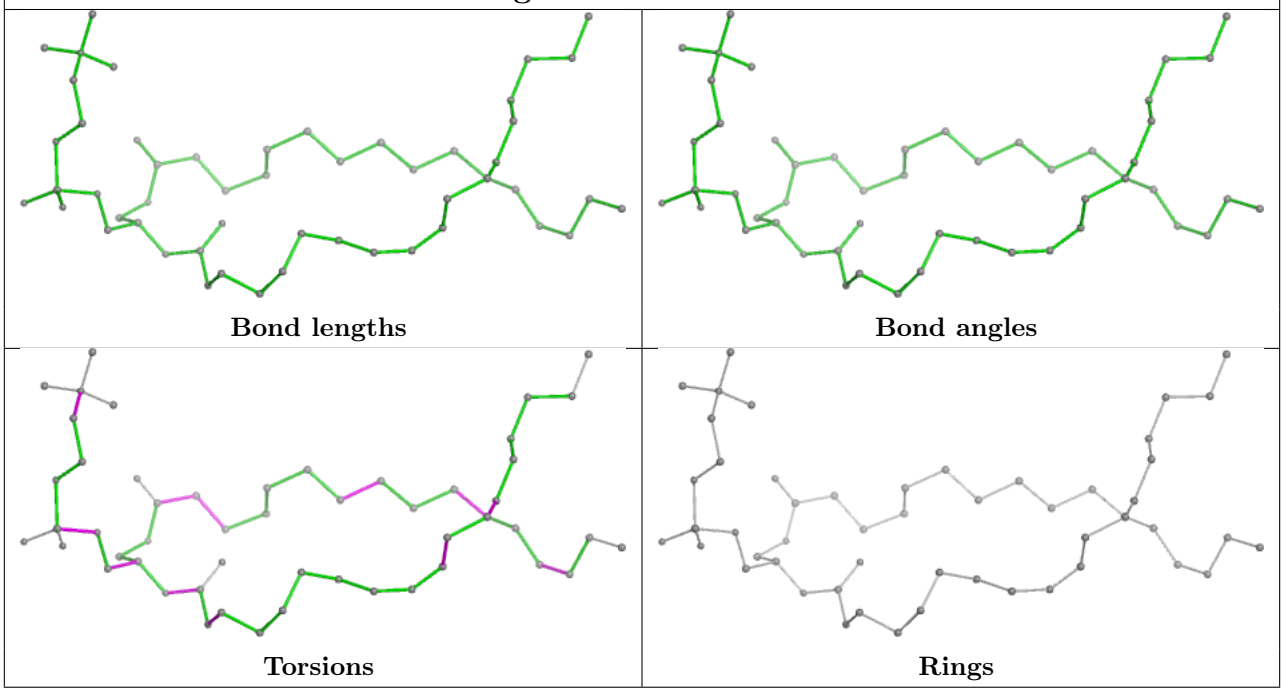


Rings

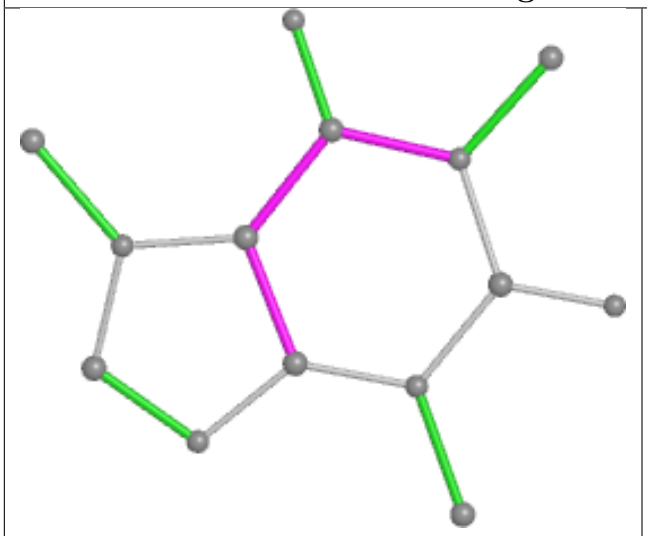
Ligand ATP G 5103



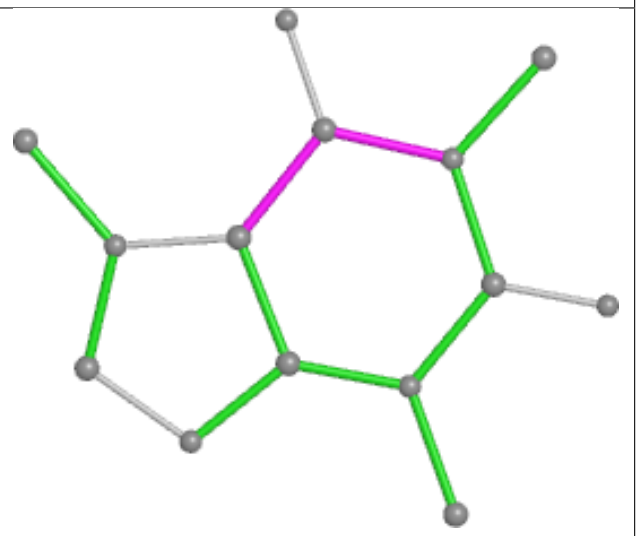
Ligand POV G 5102



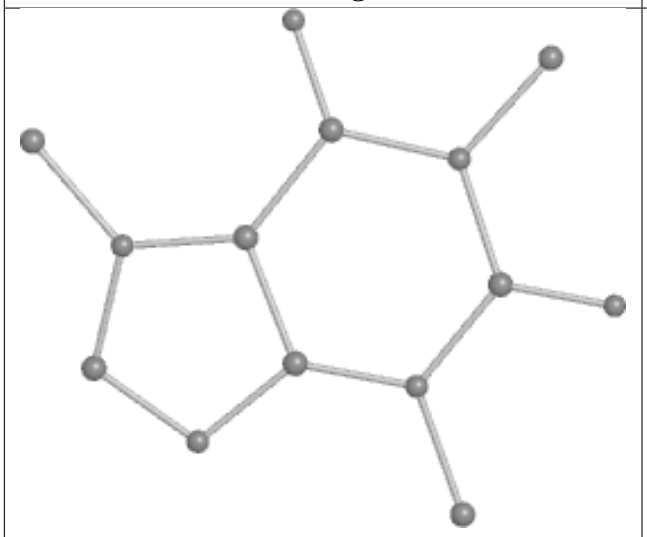
Ligand CFF D 5104



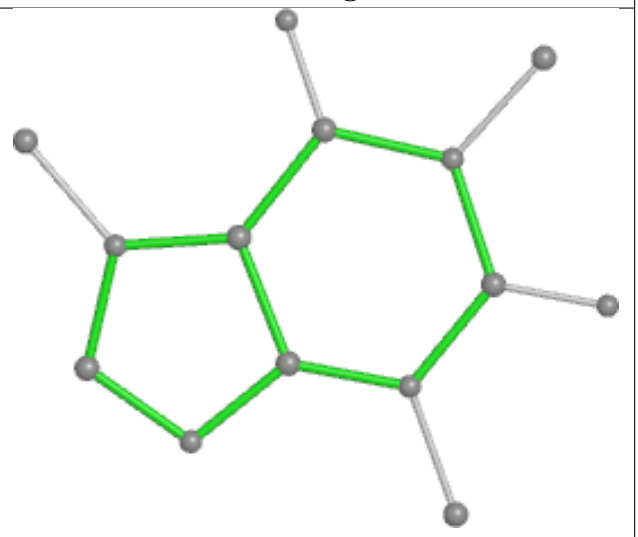
Bond lengths



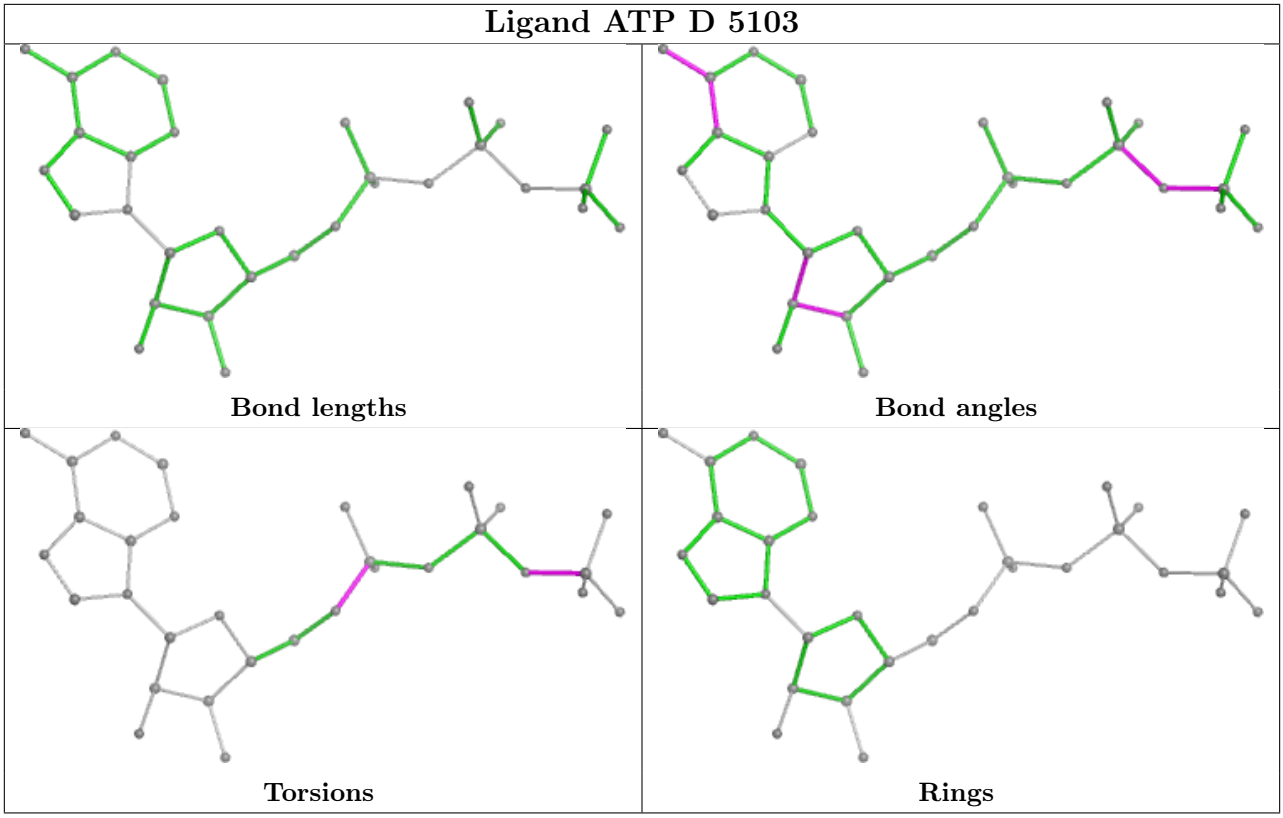
Bond angles

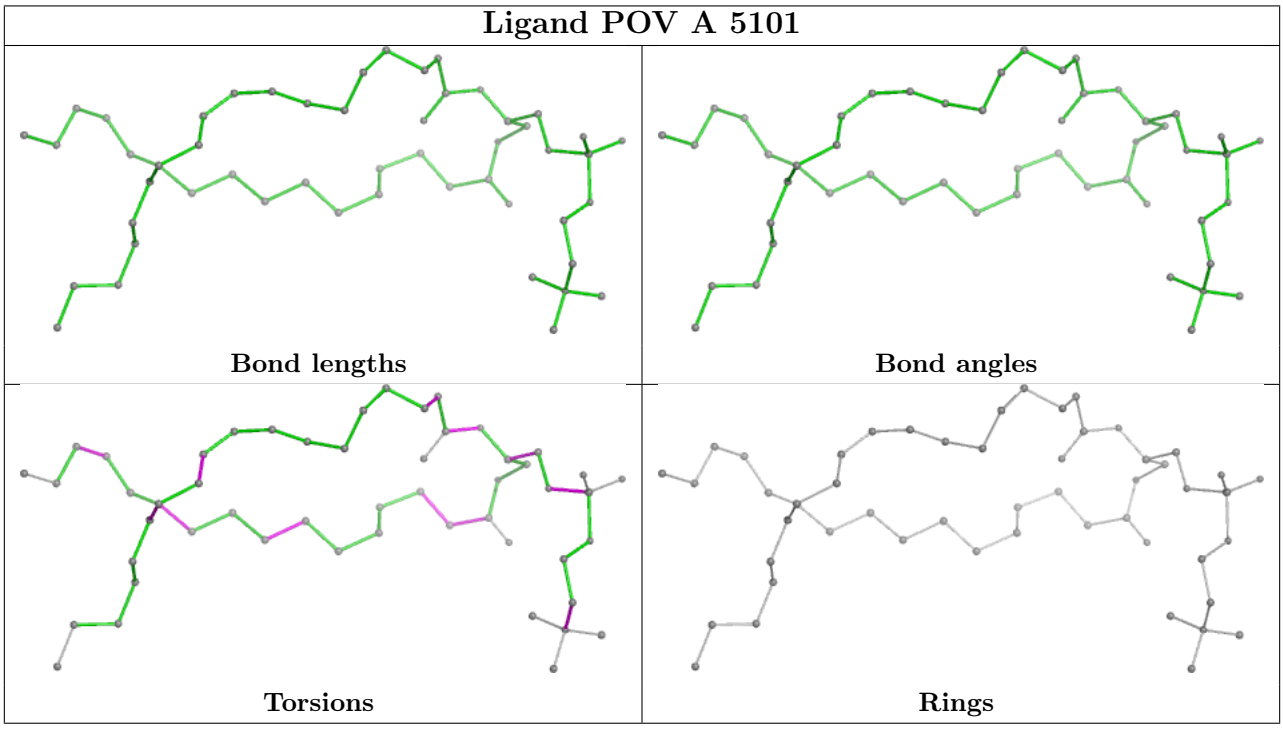


Torsions



Rings





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.

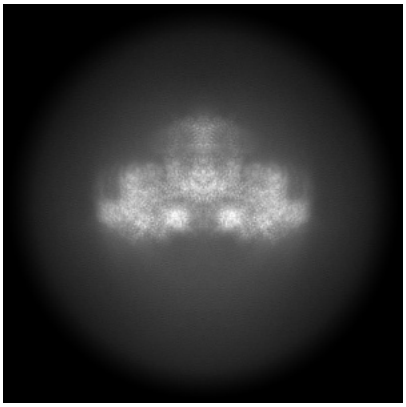
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19468. These allow visual inspection of the internal detail of the map and identification of artifacts.

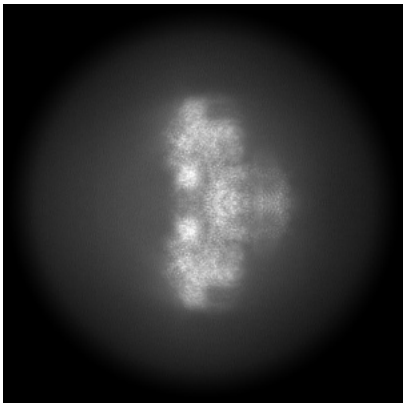
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

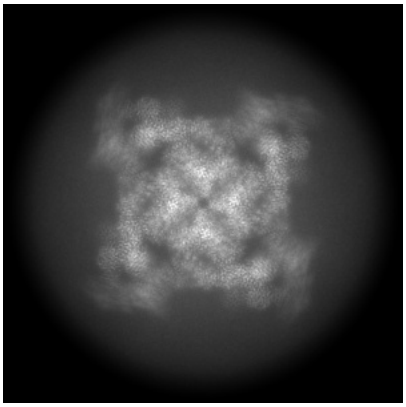
6.1.1 Primary map



X



Y

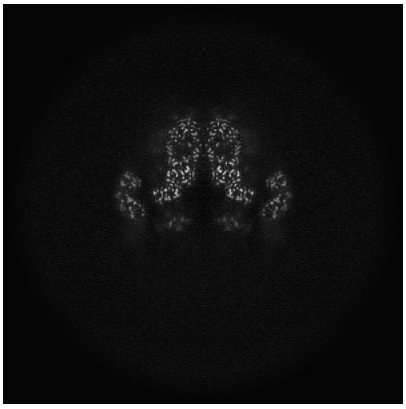


Z

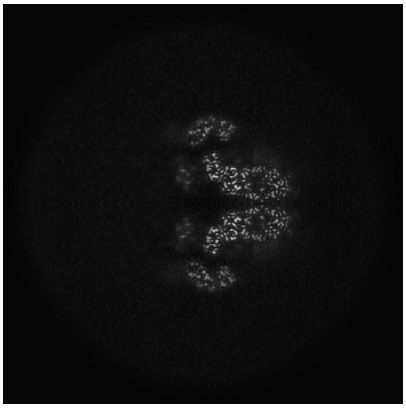
The images above show the map projected in three orthogonal directions.

6.2 Central slices

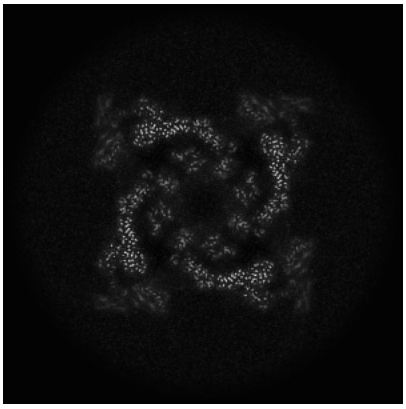
6.2.1 Primary map



X Index: 225



Y Index: 225

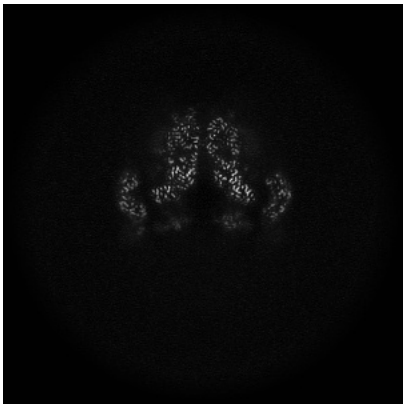


Z Index: 225

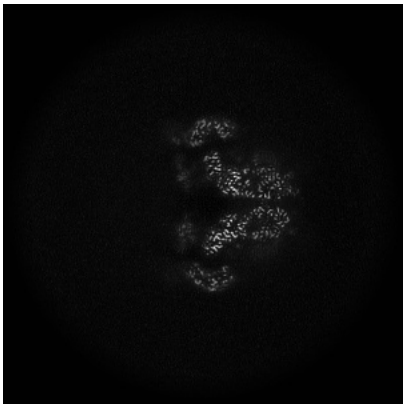
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

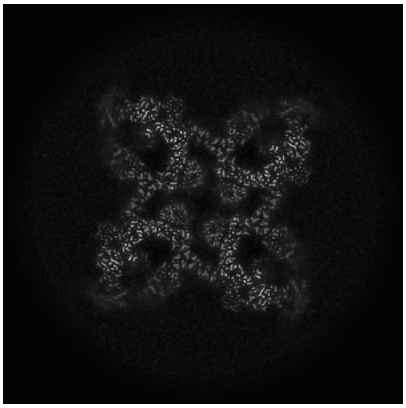
6.3.1 Primary map



X Index: 223



Y Index: 223

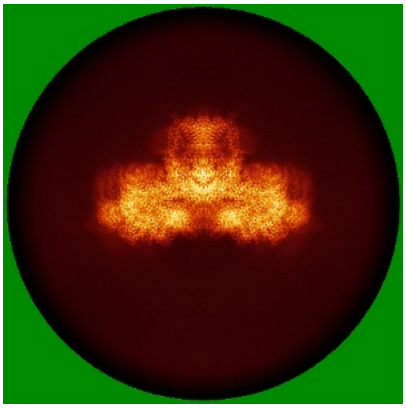


Z Index: 210

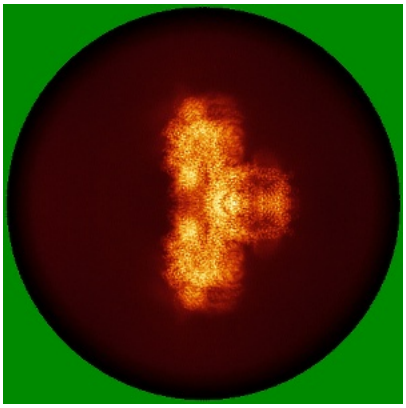
The images above show the largest variance slices of the map in three orthogonal directions.

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

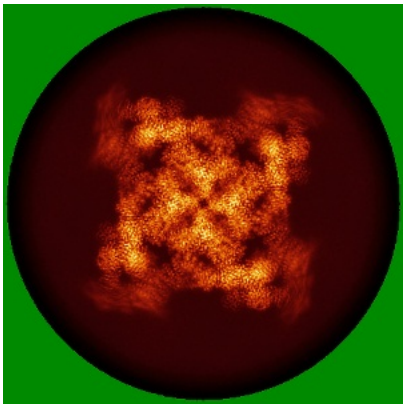
6.4.1 Primary map



X



Y

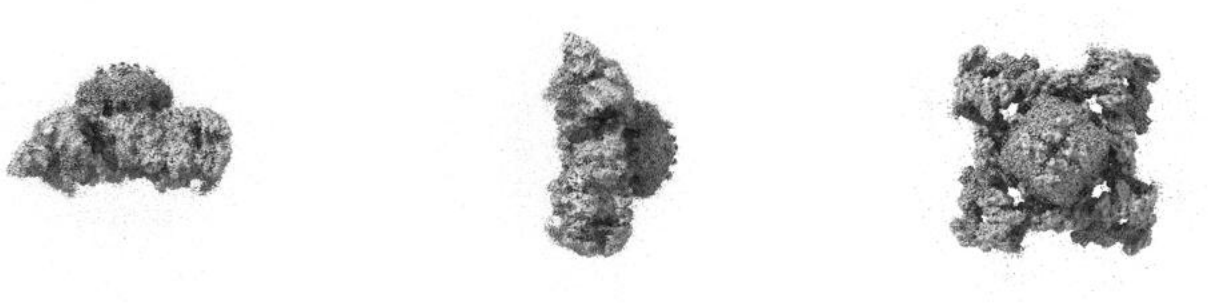


Z

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

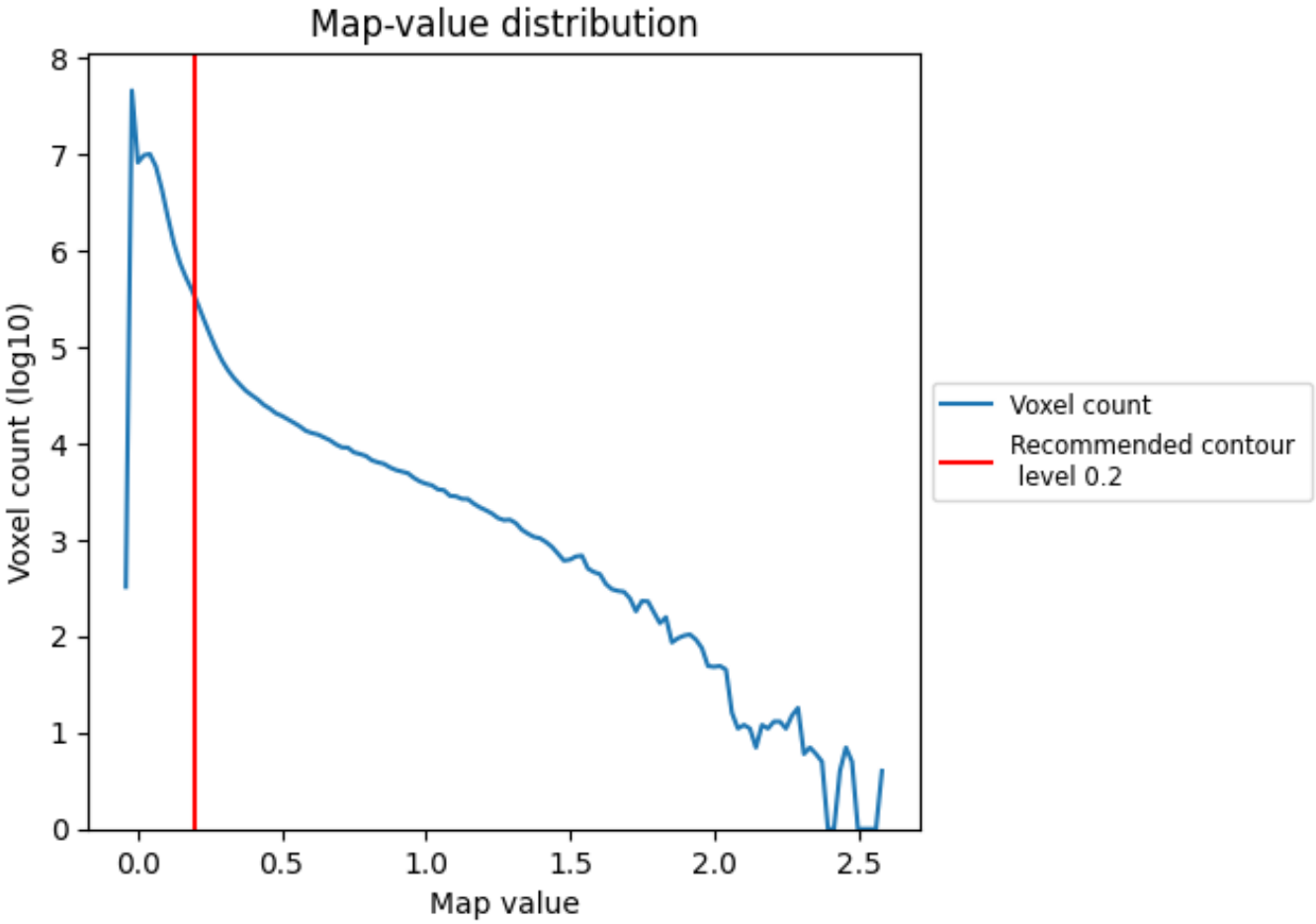
6.6 Mask visualisation (i)

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

7 Map analysis

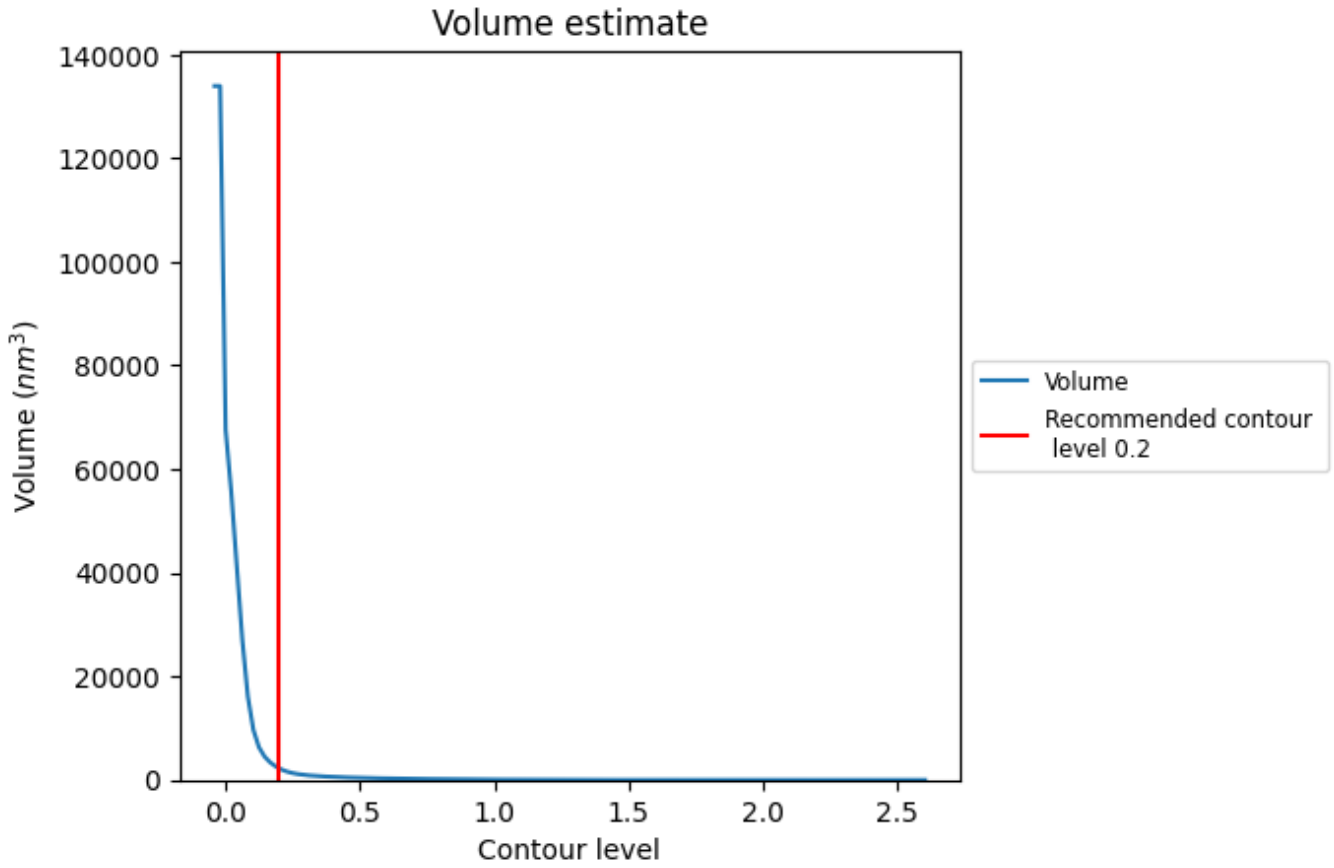
This section contains the results of statistical analysis of the map.

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.

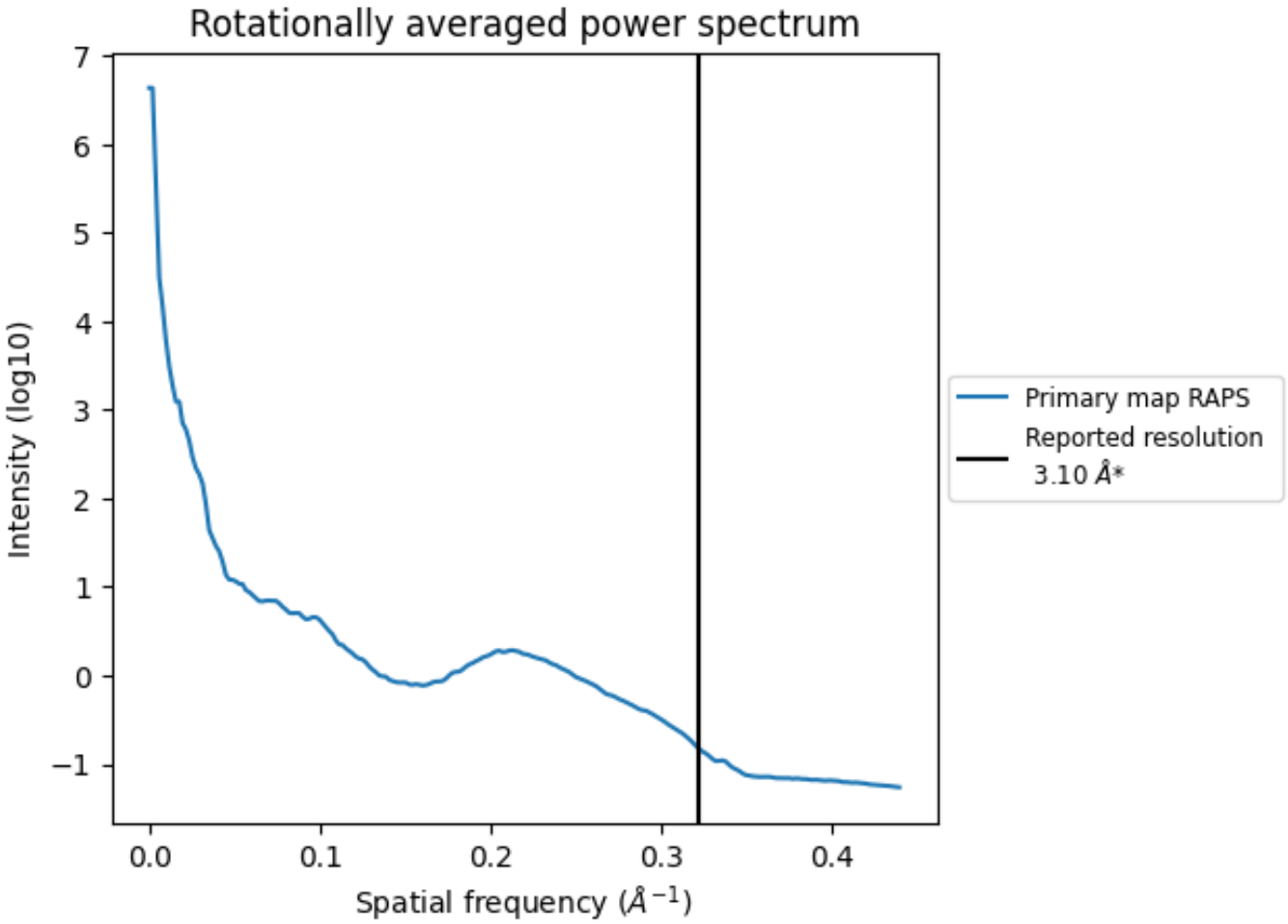
7.2 Volume estimate



The volume at the recommended contour level is 2259 nm^3; this corresponds to an approximate mass of 2041 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)

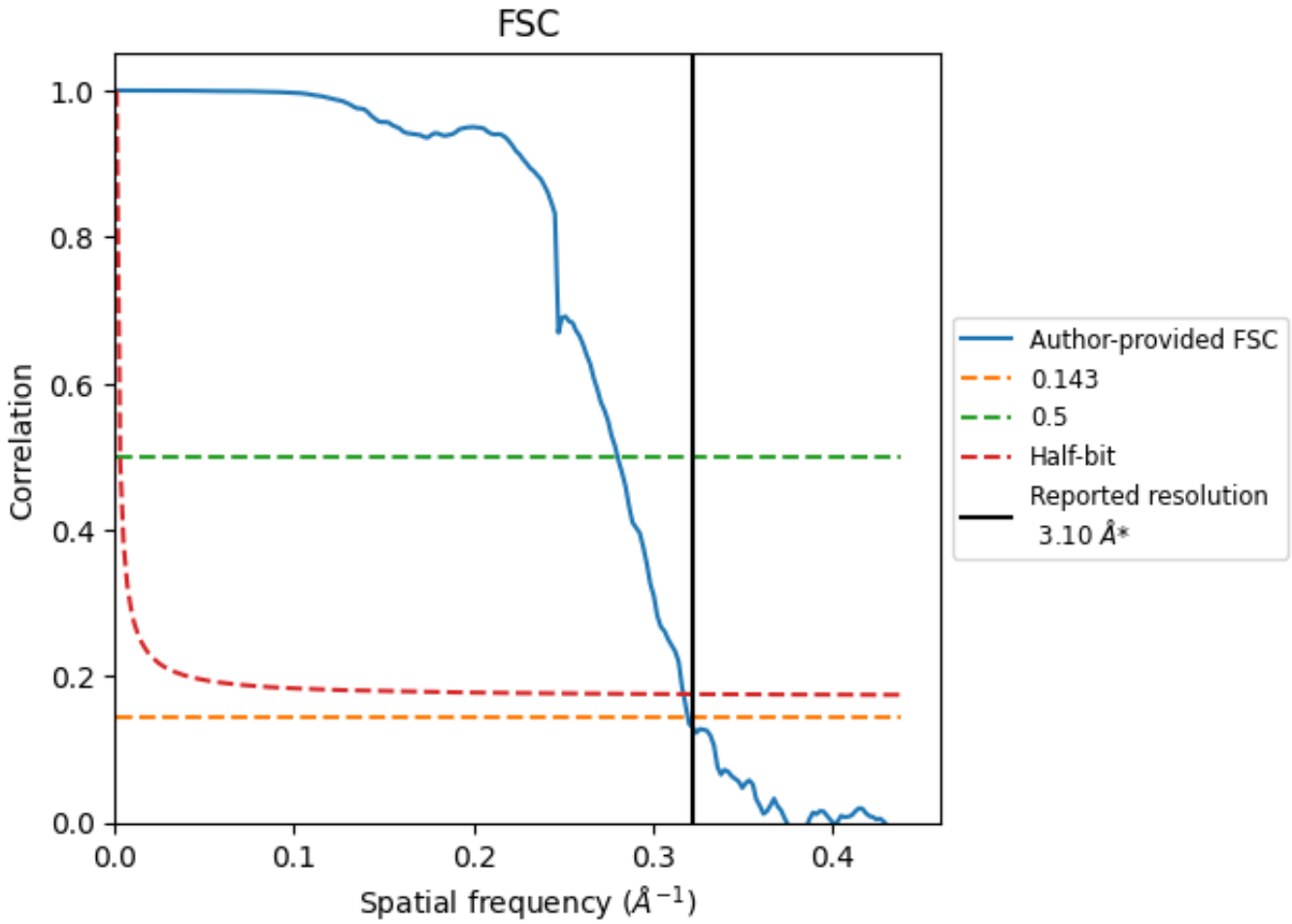


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

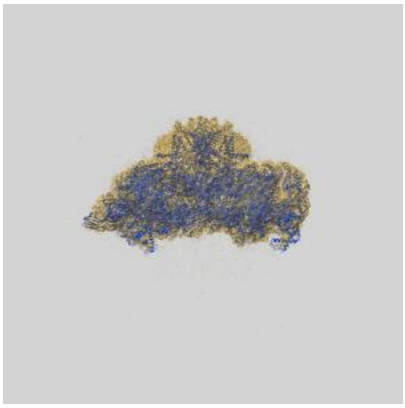
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.13	3.57	3.15
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

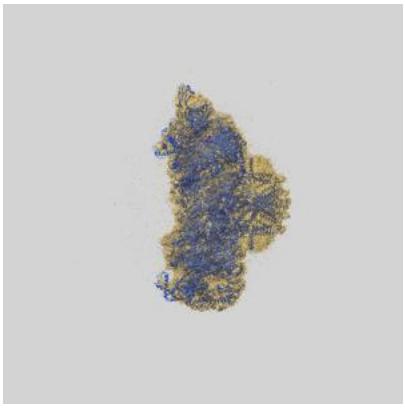
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19468 and PDB model 8RRX. Per-residue inclusion information can be found in section 3 on page 8.

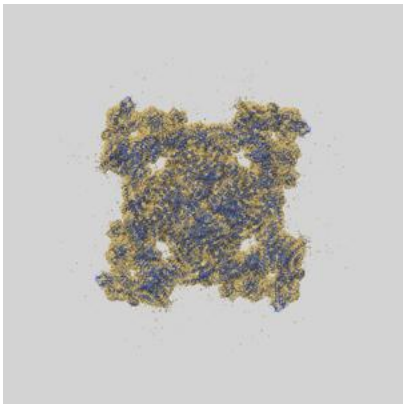
9.1 Map-model overlay



X



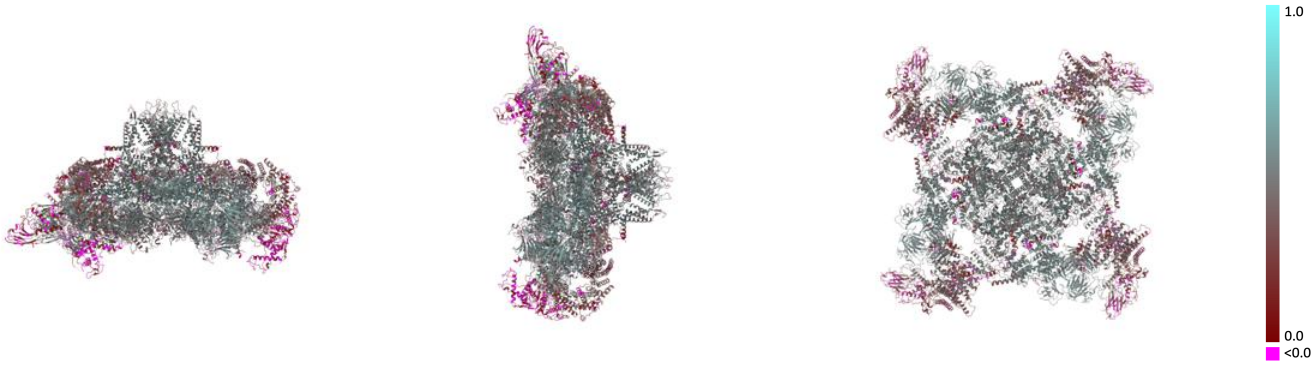
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

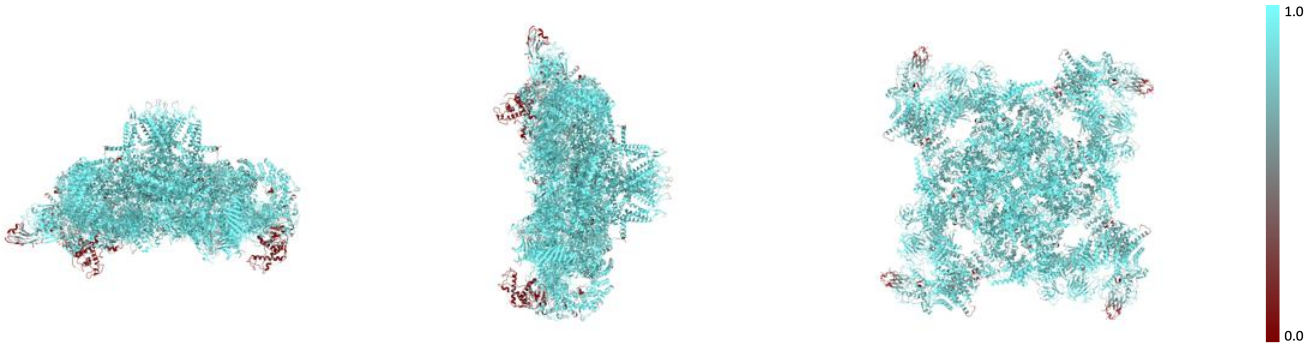
9.2 Q-score mapped to coordinate model (i)



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.

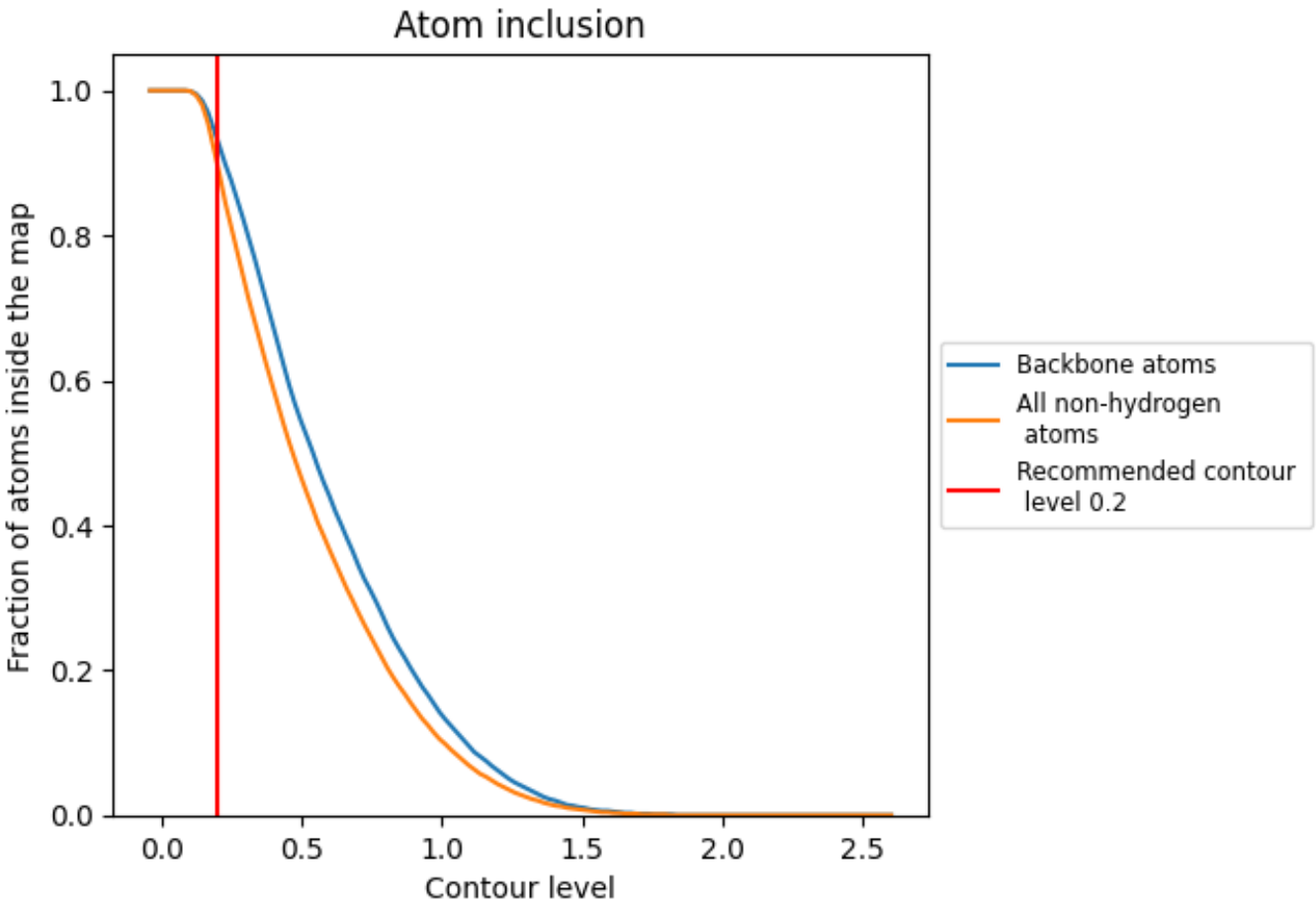
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.4240
A	0.9090	0.4300
C	0.4850	0.1360
D	0.9090	0.4300
E	0.4900	0.1350
F	0.9070	0.5000
G	0.9090	0.4300
H	0.9020	0.5020
I	0.9090	0.4300
J	0.9070	0.5040
K	0.4870	0.1370
L	0.9030	0.5030
M	0.4910	0.1370