wwPDB EM Validation Summary Report

Oct 19, 2024 – 10:59 AM EDT

PDB ID	:	5TAS
EMDB ID	:	EMD-8383
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 1)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	6.20 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:

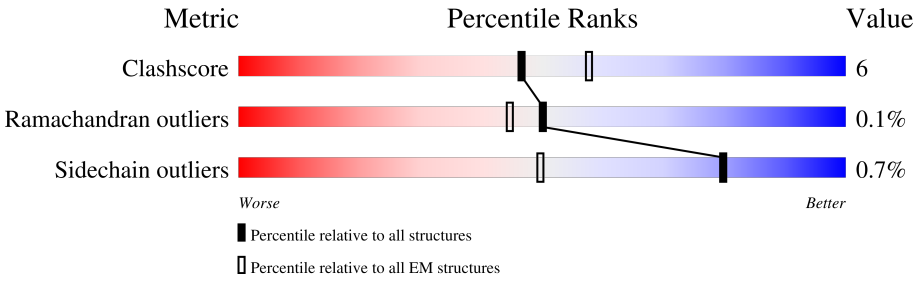
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 6.20 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	108	25% 69% 31%
1	F	108	24% 70% 29%
1	H	108	22% 71% 28%
1	J	108	22% 72% 27%
2	B	4416	33% 82% 12% 5%
2	E	4416	33% 82% 12% 5%
2	G	4416	32% 82% 12% 5%
2	I	4416	33% 83% 12% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

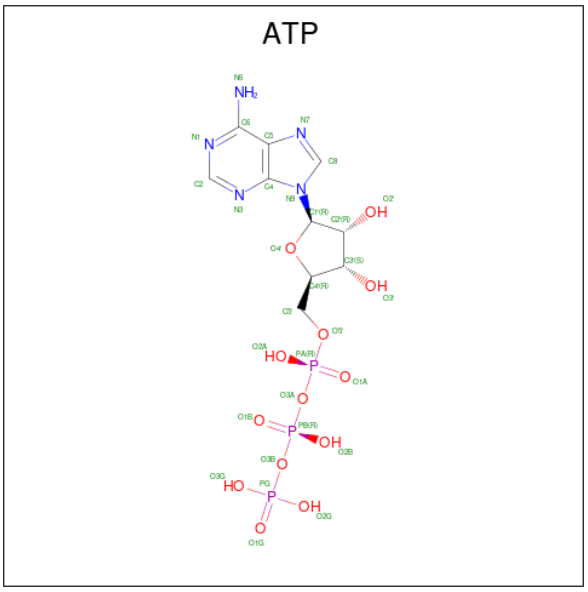
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

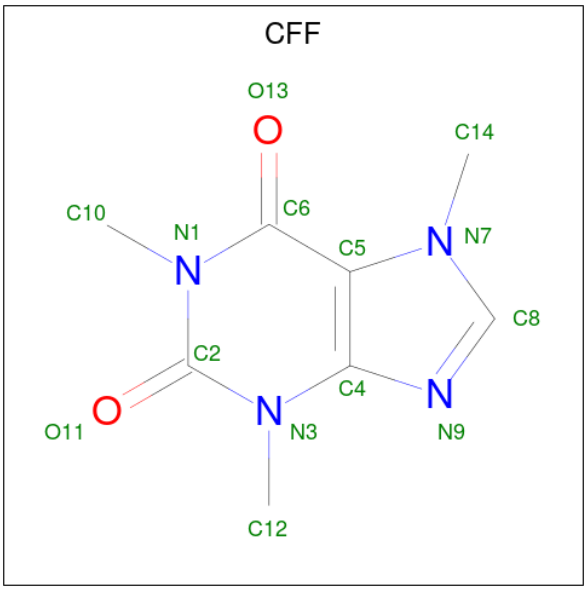
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

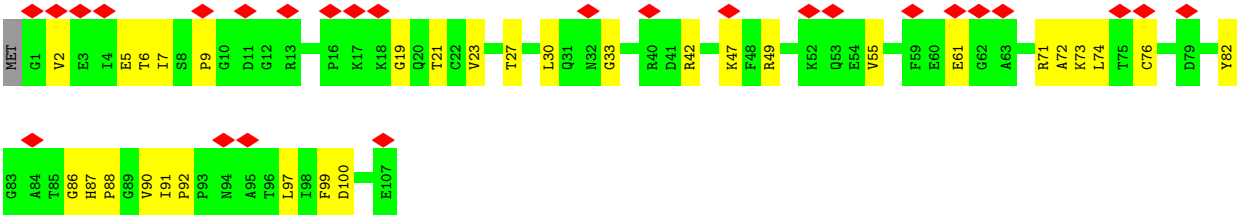
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

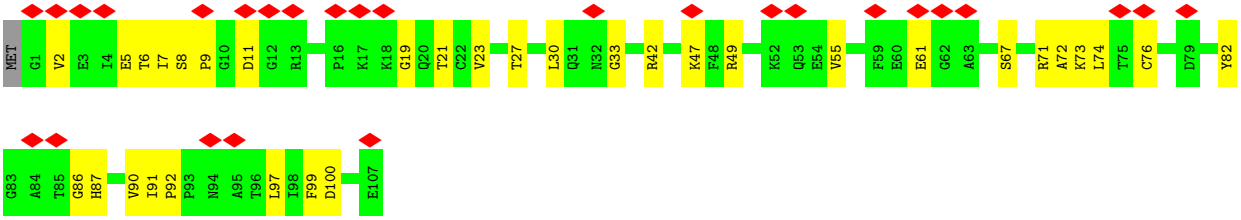
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



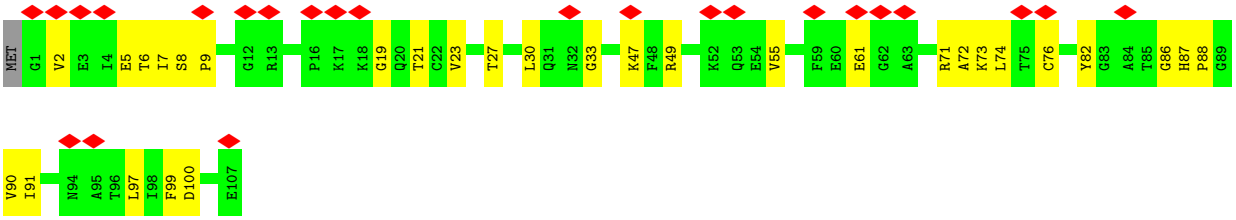
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



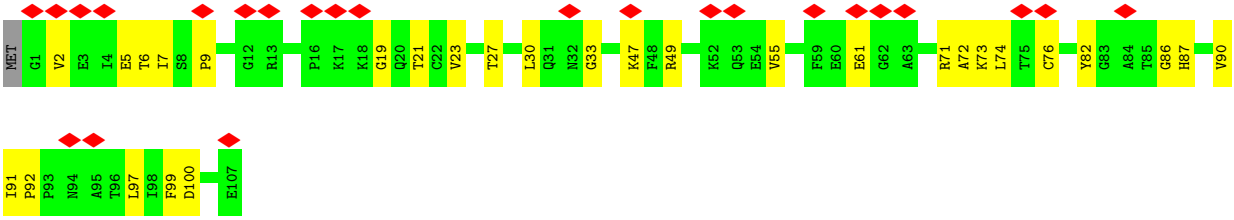
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



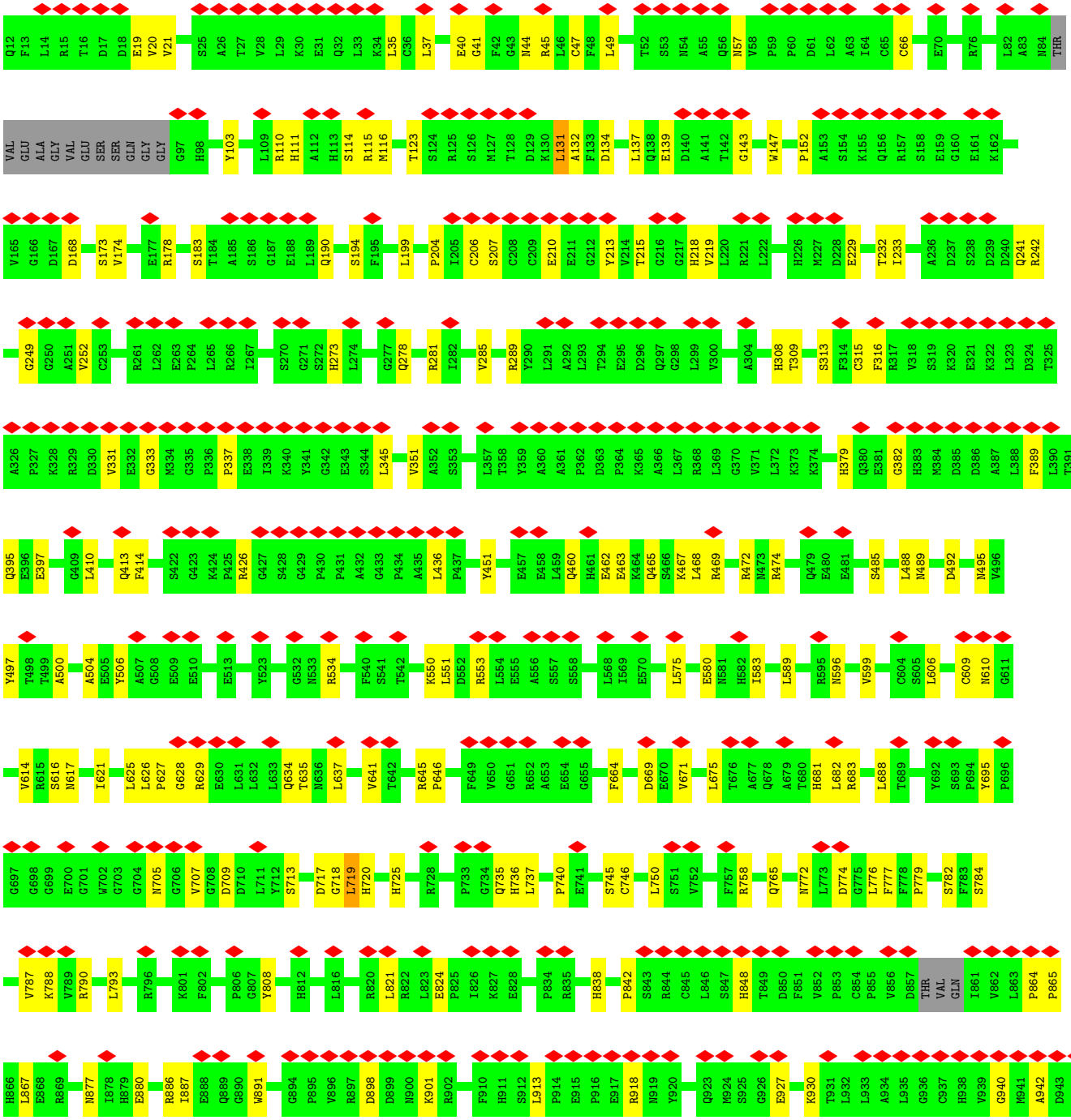
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

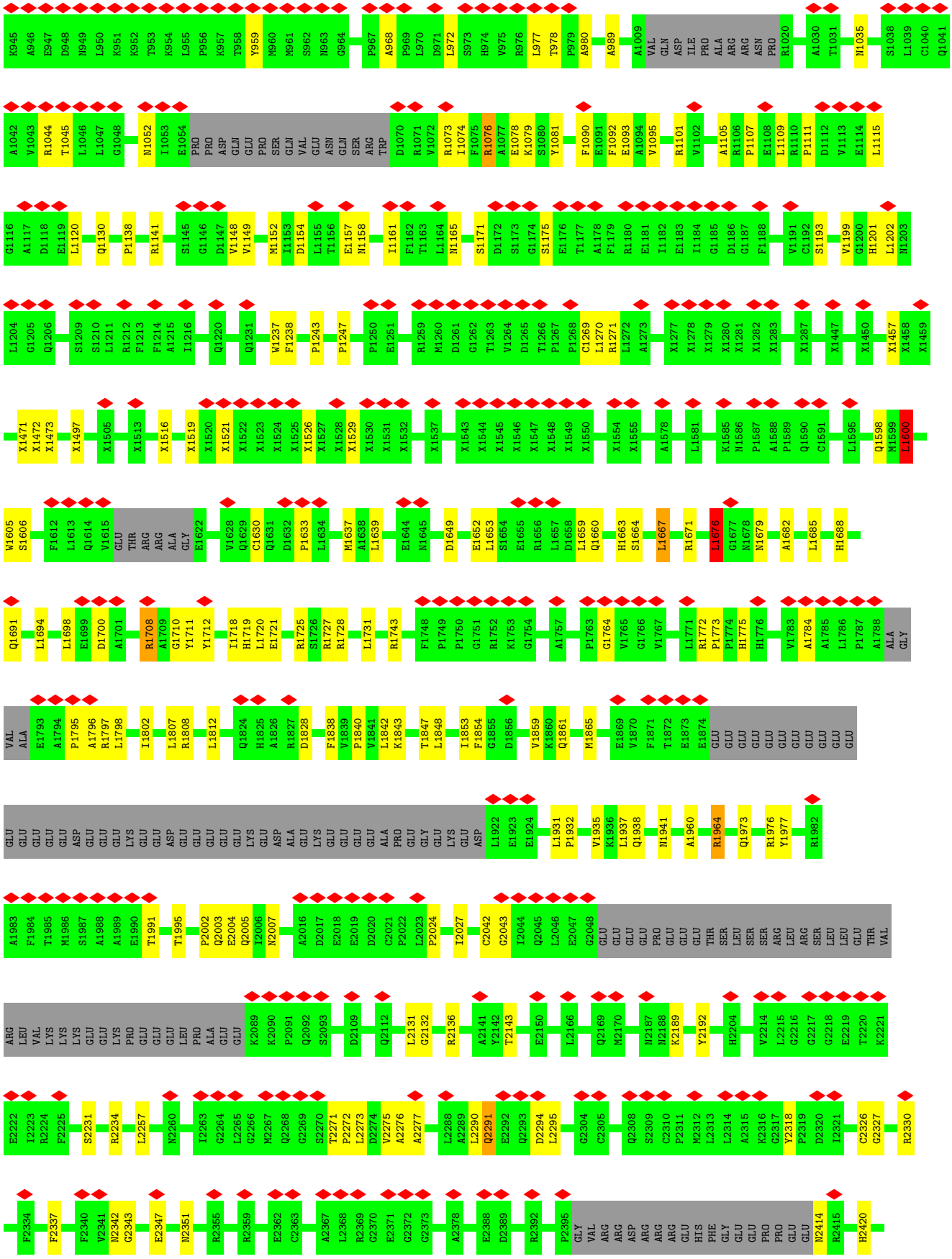
Chain J:



• Molecule 2: Ryanodine receptor 1

Chain B:

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L1204 G1205 Q1206 S1209 S1210 L1211 R1212 F1213 F1214 A1215 I1216 Q1220 Q1231 W1237 F1238 P1243 P1247 P1250 E1251 R1259 M1260 D1261 G1262 T1263 V1264 D1265 T1266 P1267 P1268 C1269 L1270 R1271 L1272 A1273 X1277 X1278 X1279 X1280 X1281 X1282 X1283 X1287 X1447 X1450 X1457 X1458 X1459
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VAL ALA E1793 A1794 P1795 A1796 R1797 L1798 I1802 L1807 R1808 L1812 Q1824 H1825 A1826 R1827 D1828 F1838 V1839 P1840 V1841 L1842 K1843 T1847 L1848 I1853 F1854 G1855 D1856 V1859 K1860 Q1861 M1865 E1869 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 L1931 P1932 V1935 K1936 L1937 Q1938 N1941 A1960 R1964 Q1973 R1976 Y1977 R1982
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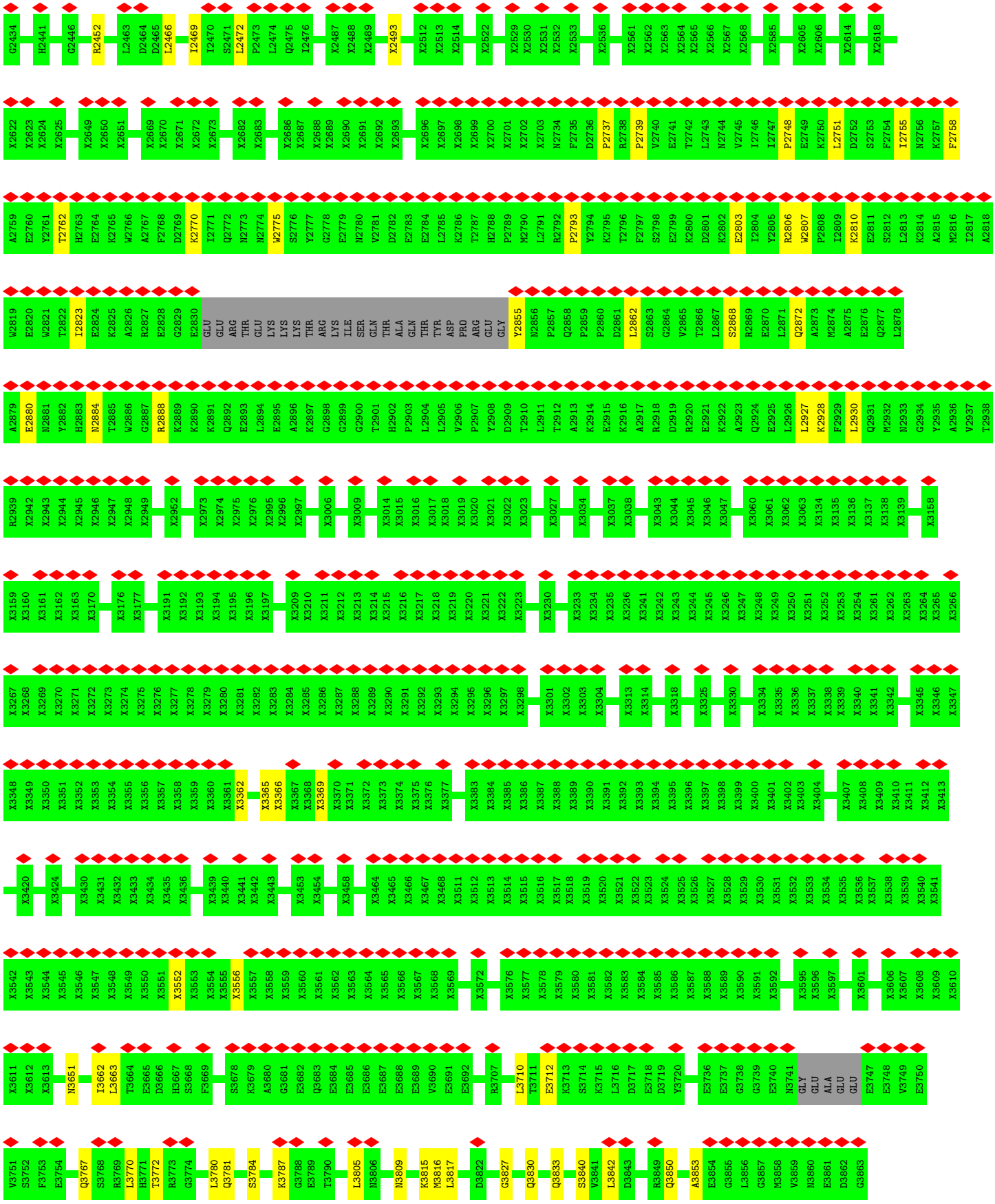
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W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878
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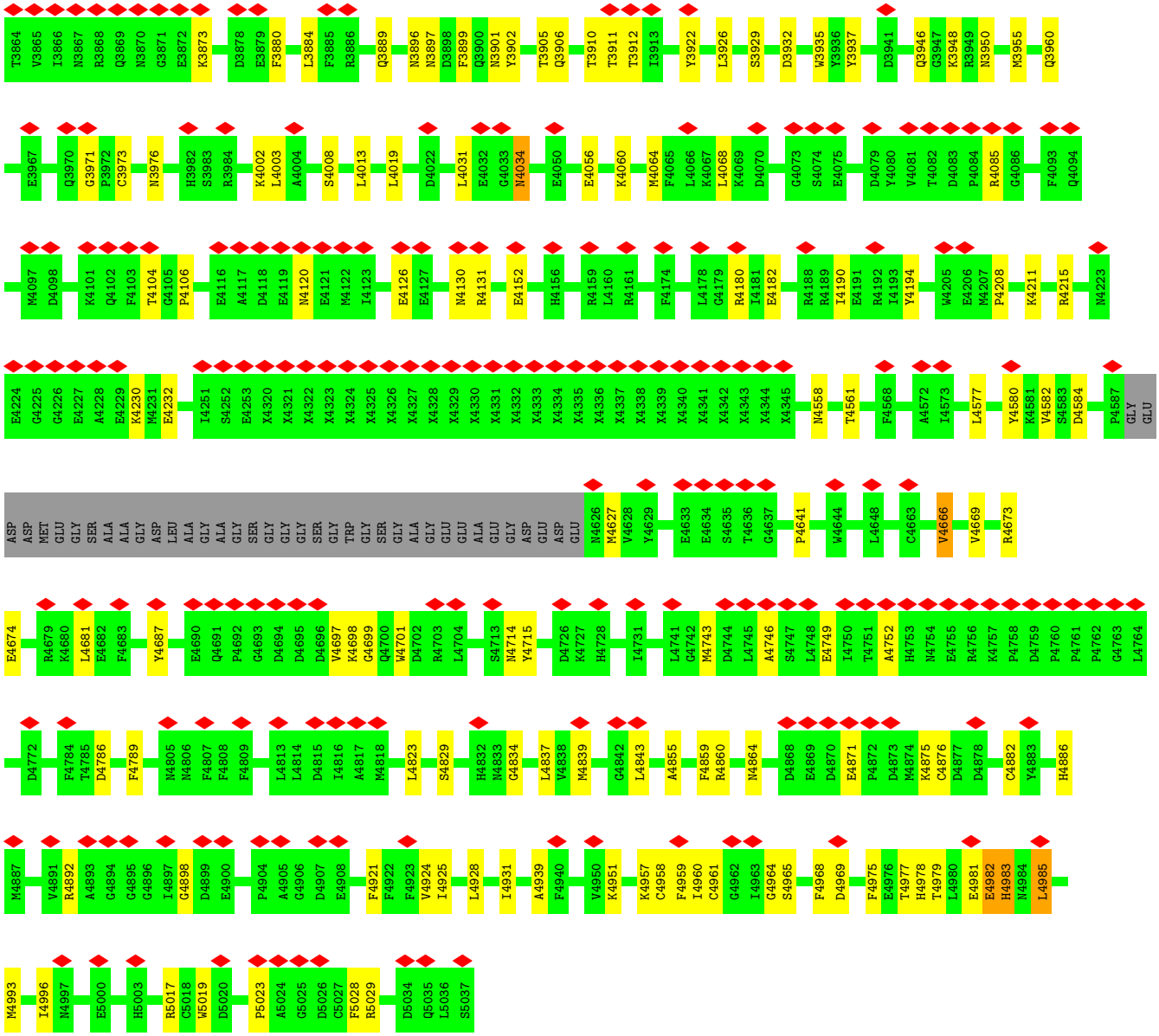
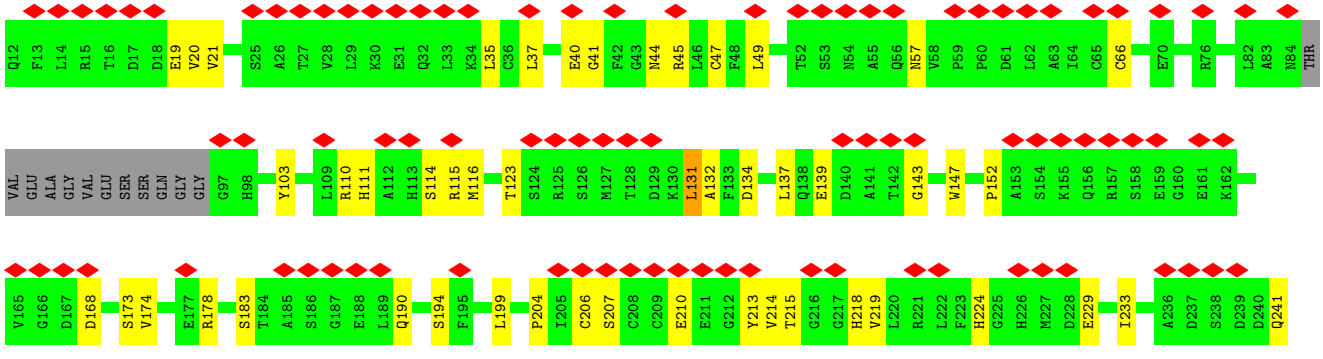
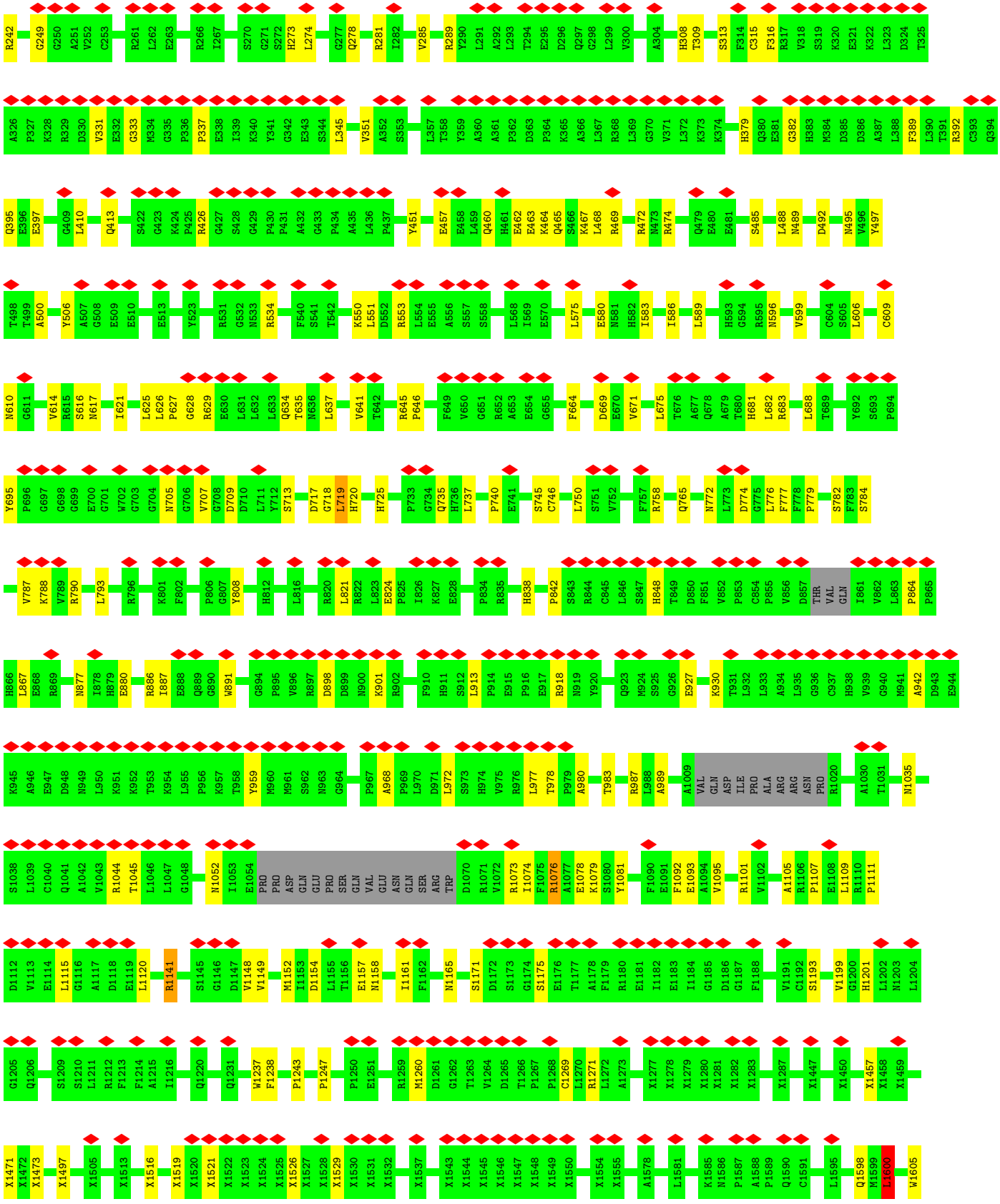
V3751 S3752 F3753 E3754 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 L3780 Q3781 S3784 K3787 G3788 E3789 T3790 L3805 N3806 N3809 K3815 M3816 L3817 D3822 G3827 Q3830 Q3833 S3840 V3841 L3842 D3843 R3849 Q3850 A3853 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863



• Molecule 2: Ryanodine receptor 1

Chain I:

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A326 P327 K328 R329 D330 V331 E332 G333 M334 G335 P336 P337 E338 I339 K340 Y341 G342 E343 S344 L345 V351 A352 S353 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 K373 K374 H379 Q380 E381 G382 H383 M384 D385 D386 A387 L388 F389 L390 T391 R392 C393 Q394
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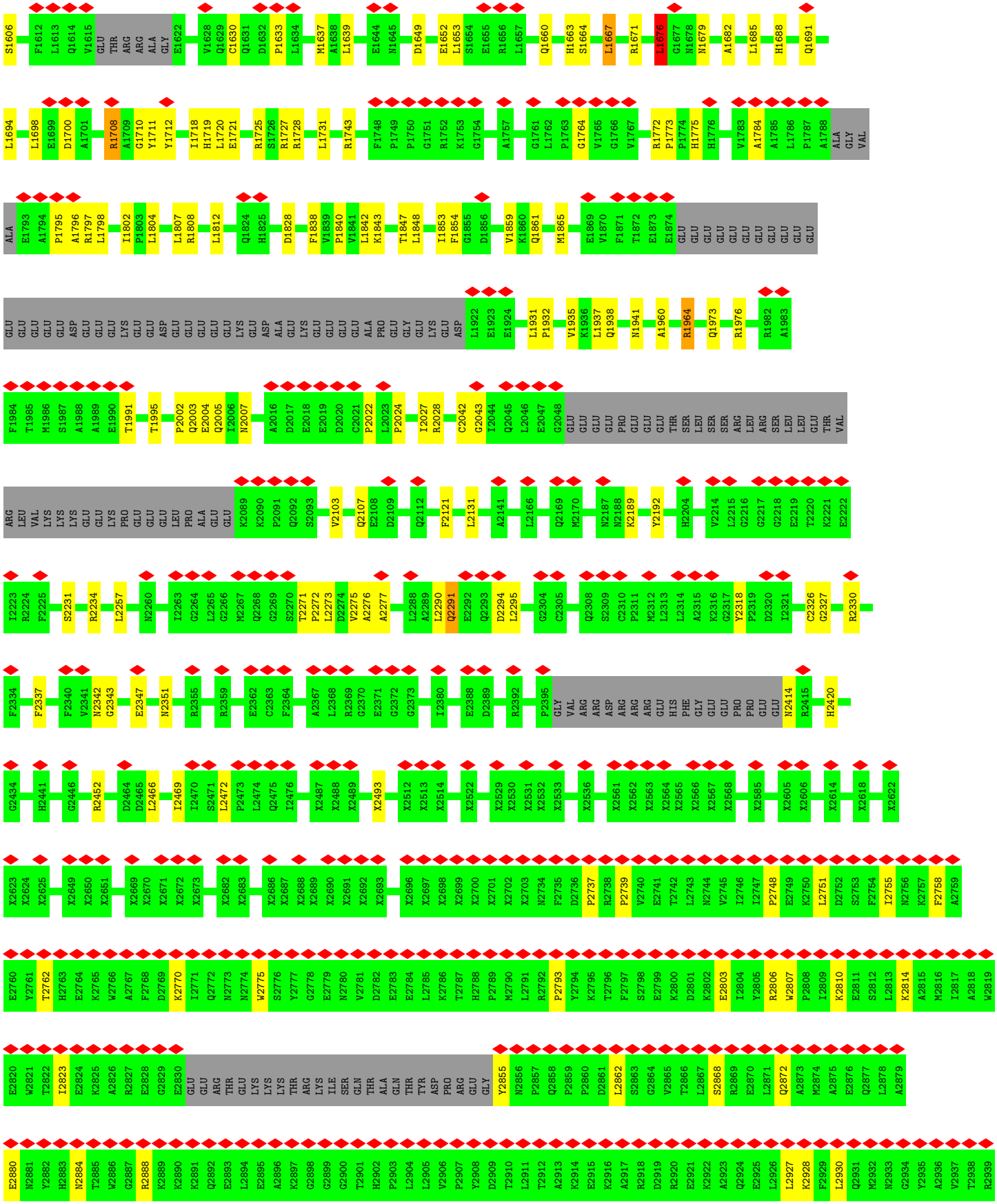
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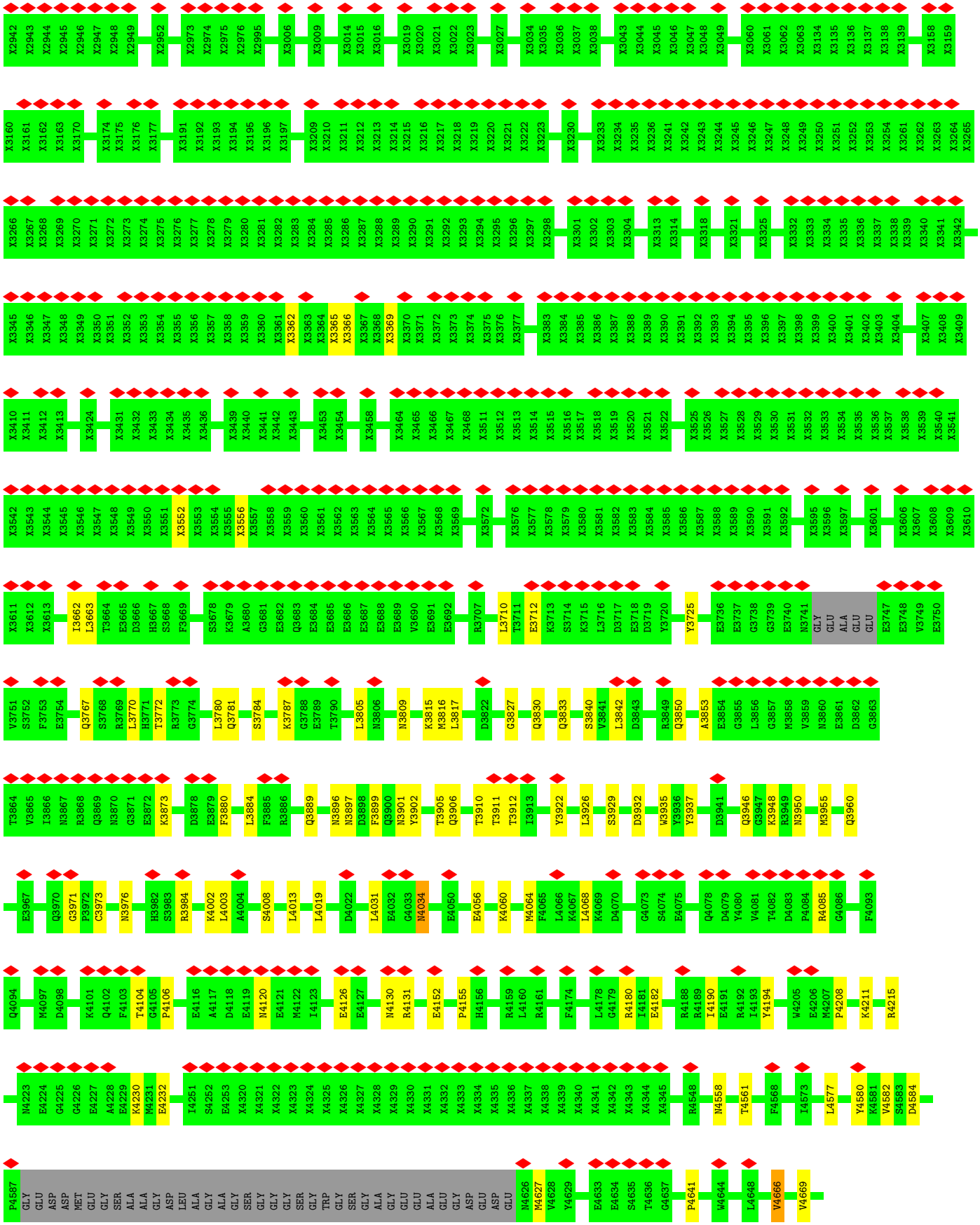
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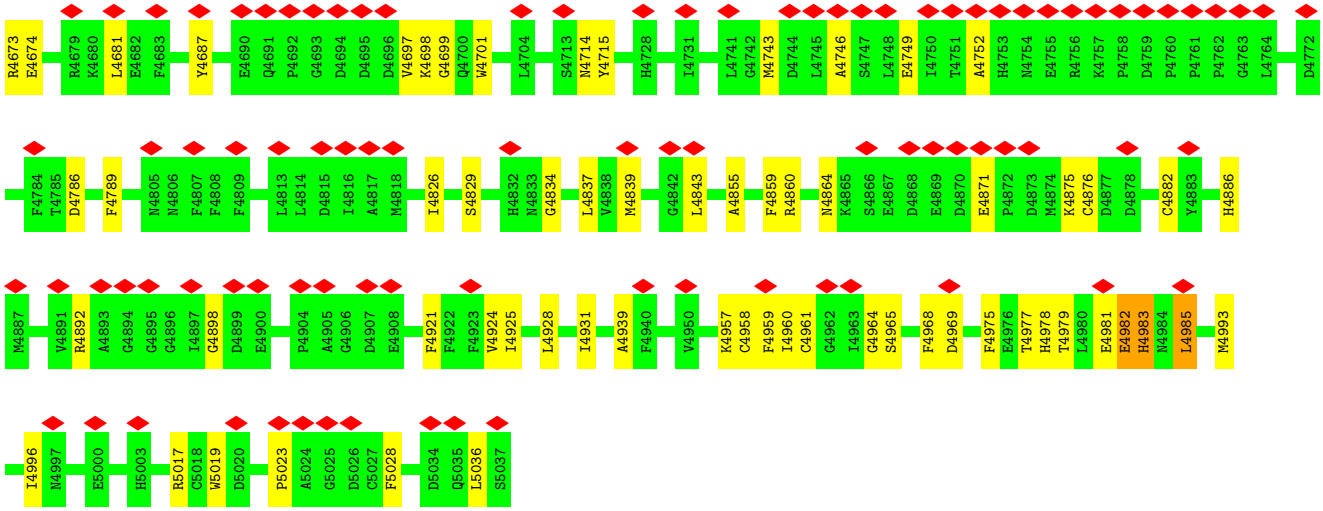
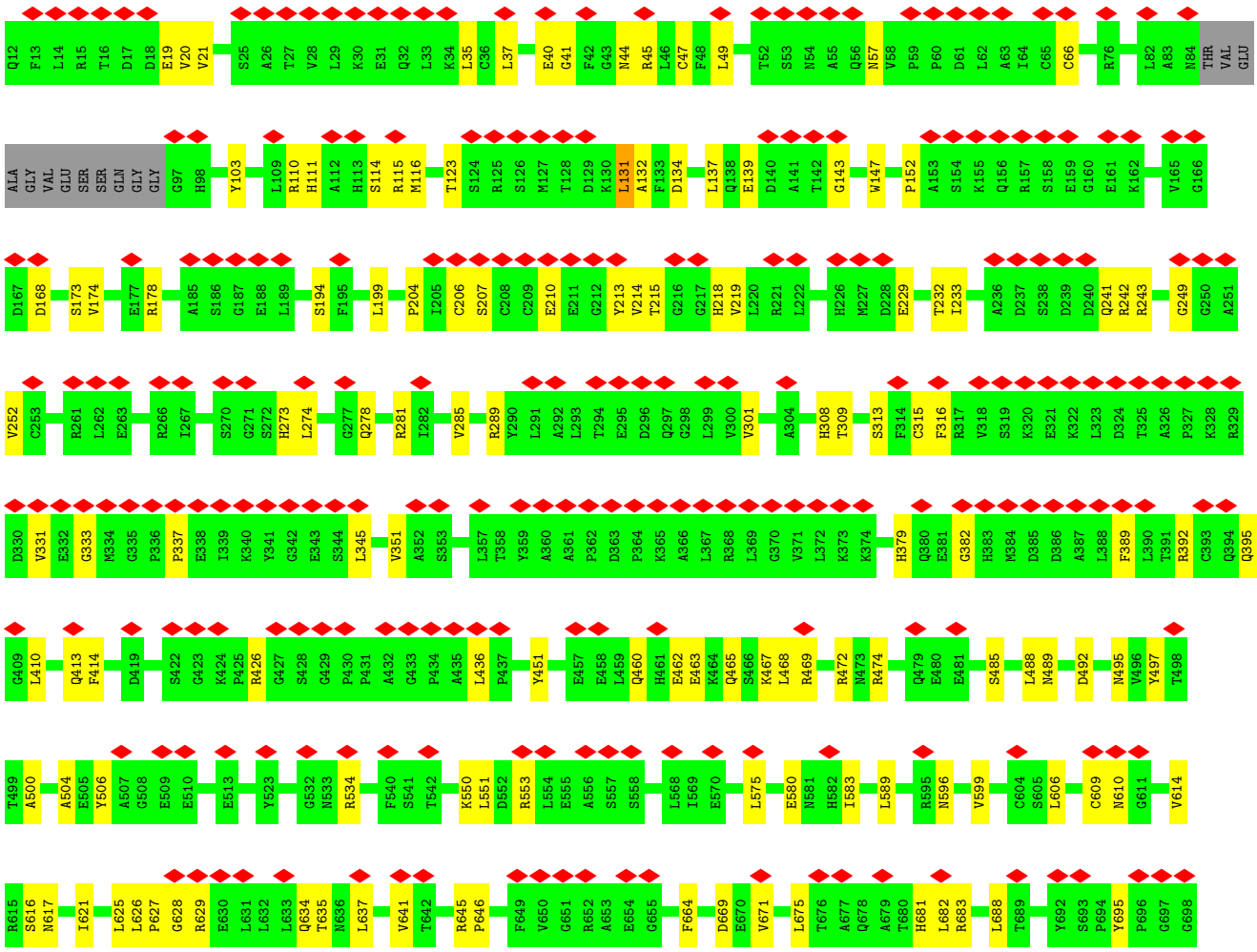
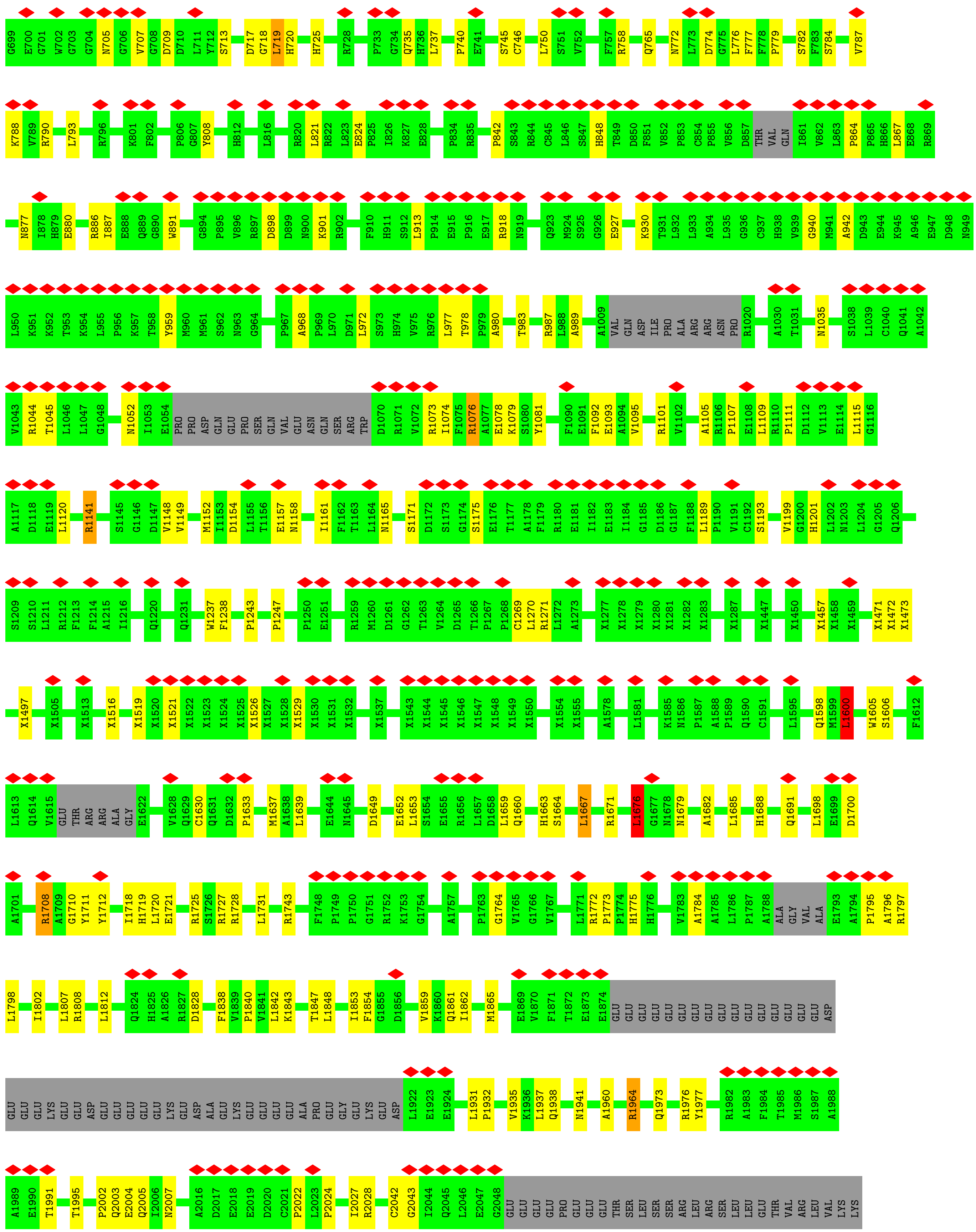


• Molecule 2: Ryanodine receptor 1

Chain E:

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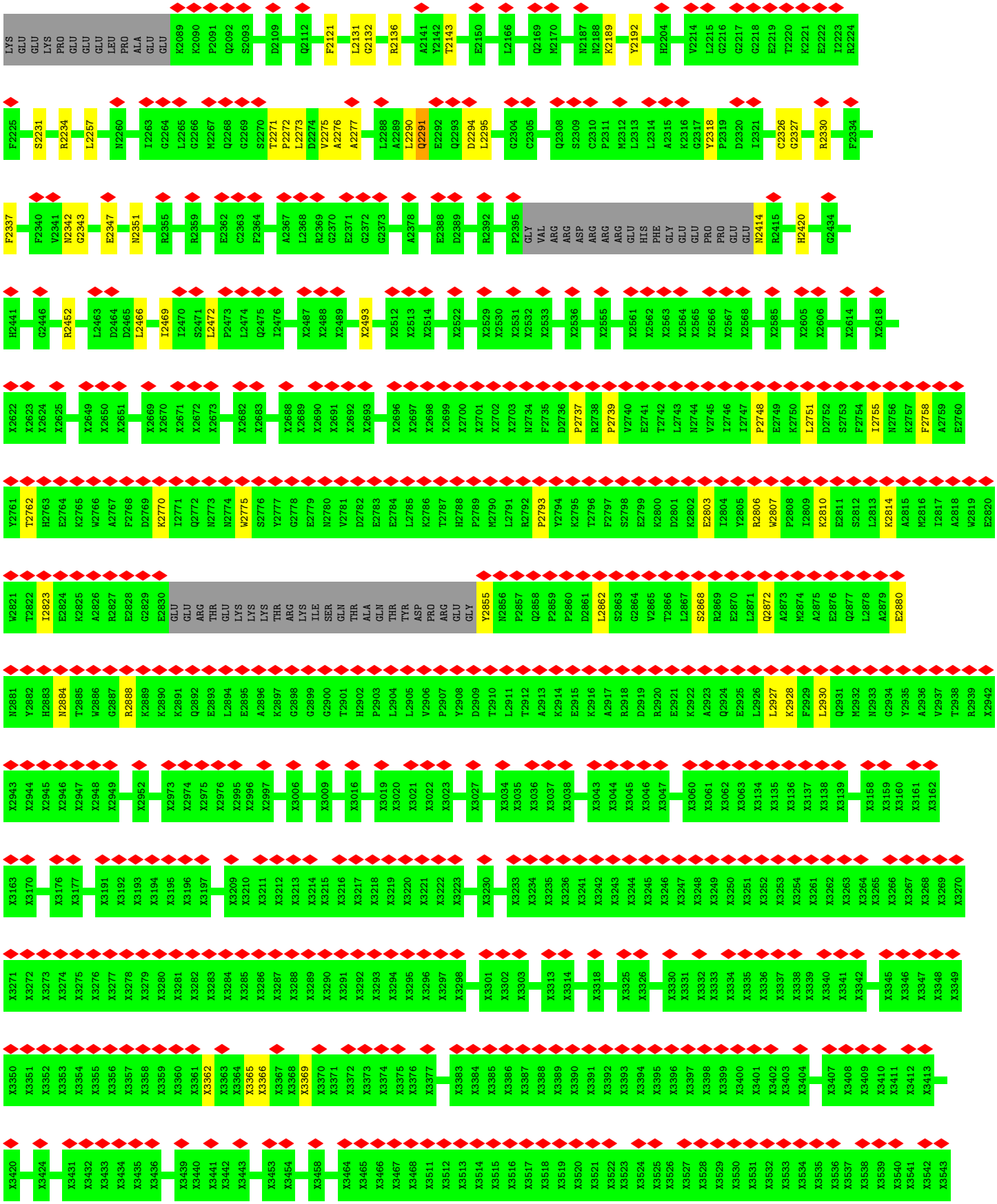
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X2622 X2623 X2624 X2625 X2649 X2650 X2651 X2669 X2670 X2671 X2672 X2673 X2682 X2683 X2688 X2689 X2690 X2691 X2692 X2693 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 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 L2878 A2879 E2880
N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942
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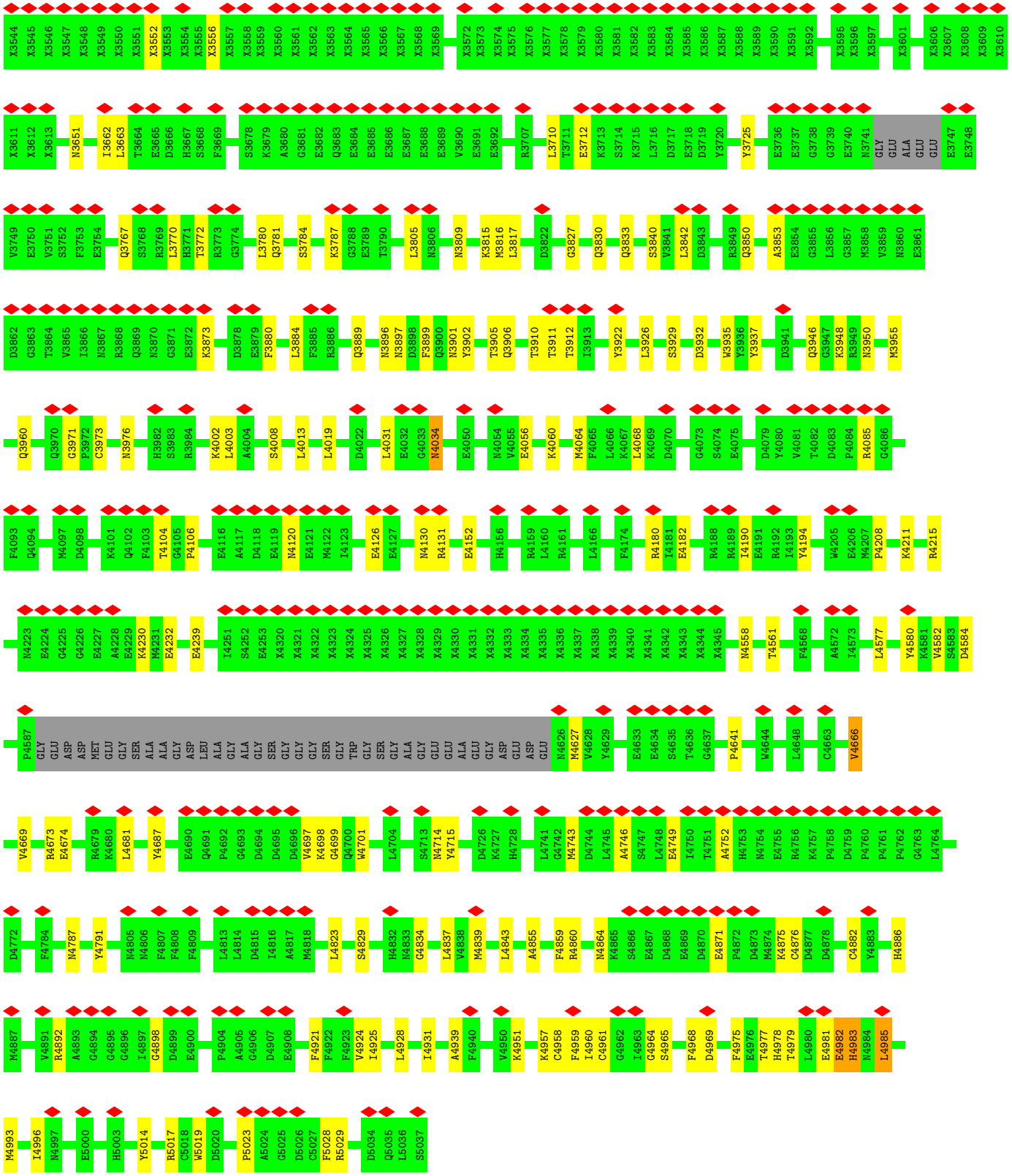
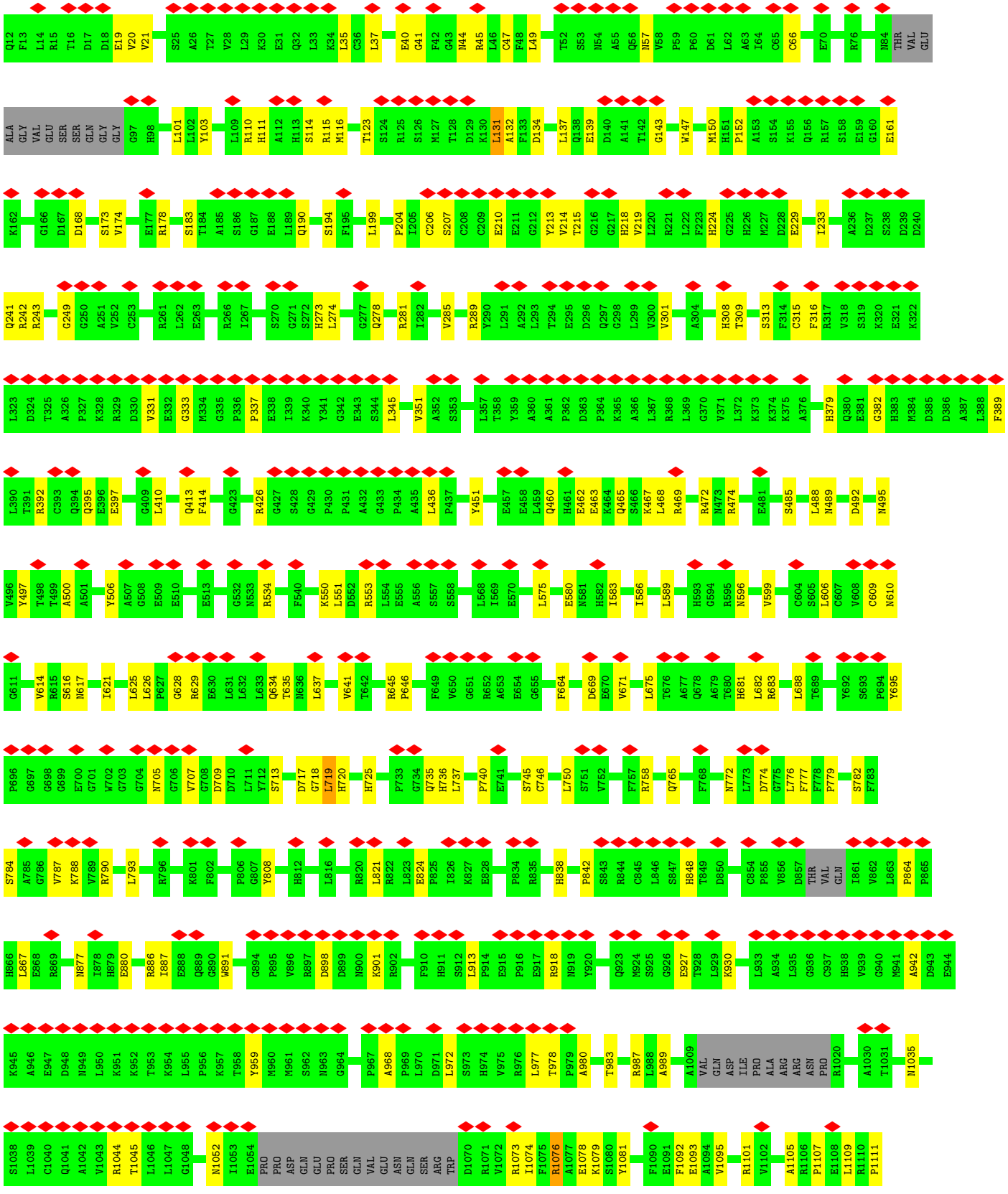


• Molecule 2: Ryanodine receptor 1

Chain G: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ALA GLY VAL GLU SER SER GLN GLY GLY G97 H98 L101 L102 Y103 L109 R110 H111 A112 H113 S114 R115 M116 T123 S124 R125 S126 M127 T128 D129 K130 L131 A132 F133 D134 L137 Q138 E139 D140 A141 T142 G143 W147 M150 H151 P152 A153 S154 K155 Q156 R157 S158 E159 G160 E161
K162 G166 D167 D168 S173 V174 E177 R178 S183 T184 A185 S186 G187 E188 L189 Q190 S194 F195 L199 P204 I205 C206 S207 C208 C209 E210 E211 G212 Y213 V214 T215 G216 G217 H218 V219 L220 R221 L222 F223 H224 G225 H226 M227 D228 E229 I233 A236 D237 S238 D239 D240
Q241 R242 R243 G249 G250 A251 V252 C253 R261 L262 E263 R266 I267 S270 G271 S272 H273 L274 G277 Q278 R281 I282 V285 R289 Y290 L291 A292 L293 T294 E295 D296 Q297 G298 L299 V300 V301 A304 H308 T309 S313 F314 C315 F316 R317 V318 S319 K320 E321 K322
L323 D324 T325 A326 P327 K328 R329 D330 V331 E332 G333 M334 G335 P336 P337 E338 I339 K340 Y341 G342 E343 S344 L345 V351 A352 S353 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 K373 K374 K375 A376 H379 Q380 E381 G382 H383 M384 D385 D386 A387 L388 F389
L390 T391 R392 C393 Q394 Q395 E396 E397 G409 L410 Q413 F414 G423 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 L436 P437 Y451 E457 E458 L459 Q460 H461 E462 E463 K464 Q465 S466 K467 L468 R469 R472 N473 R474 E481 S485 L488 N489 D492 N495
V496 Y497 T498 T499 A500 A501 Y506 A507 G508 E509 E510 E513 G532 N533 R534 F540 K550 L551 D552 R553 L554 E555 A556 S557 S558 L568 I569 E570 L575 E580 N581 H582 I583 I586 L589 H593 G594 R595 N596 V599 C604 S605 L606 C607 V608 C609 N610
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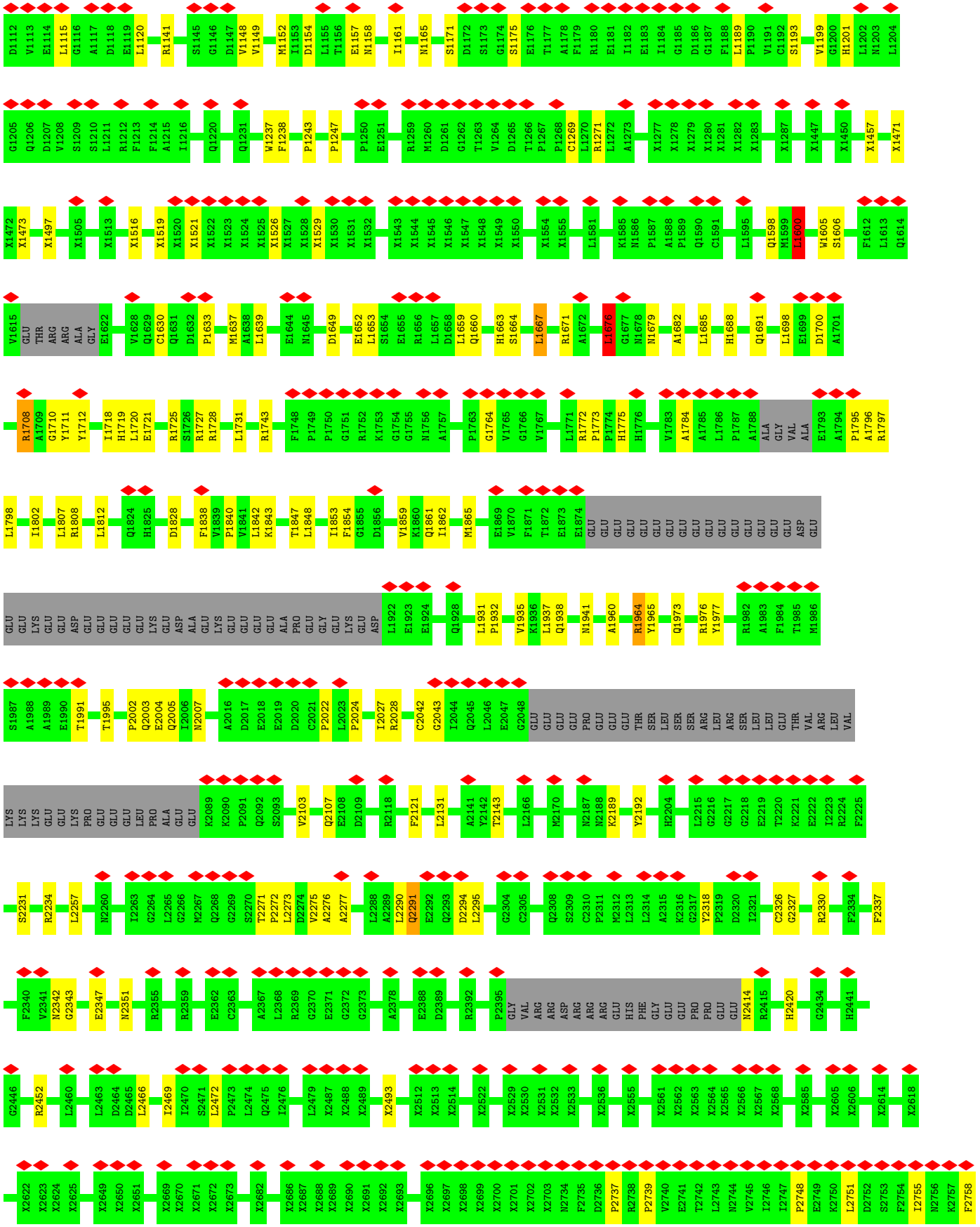
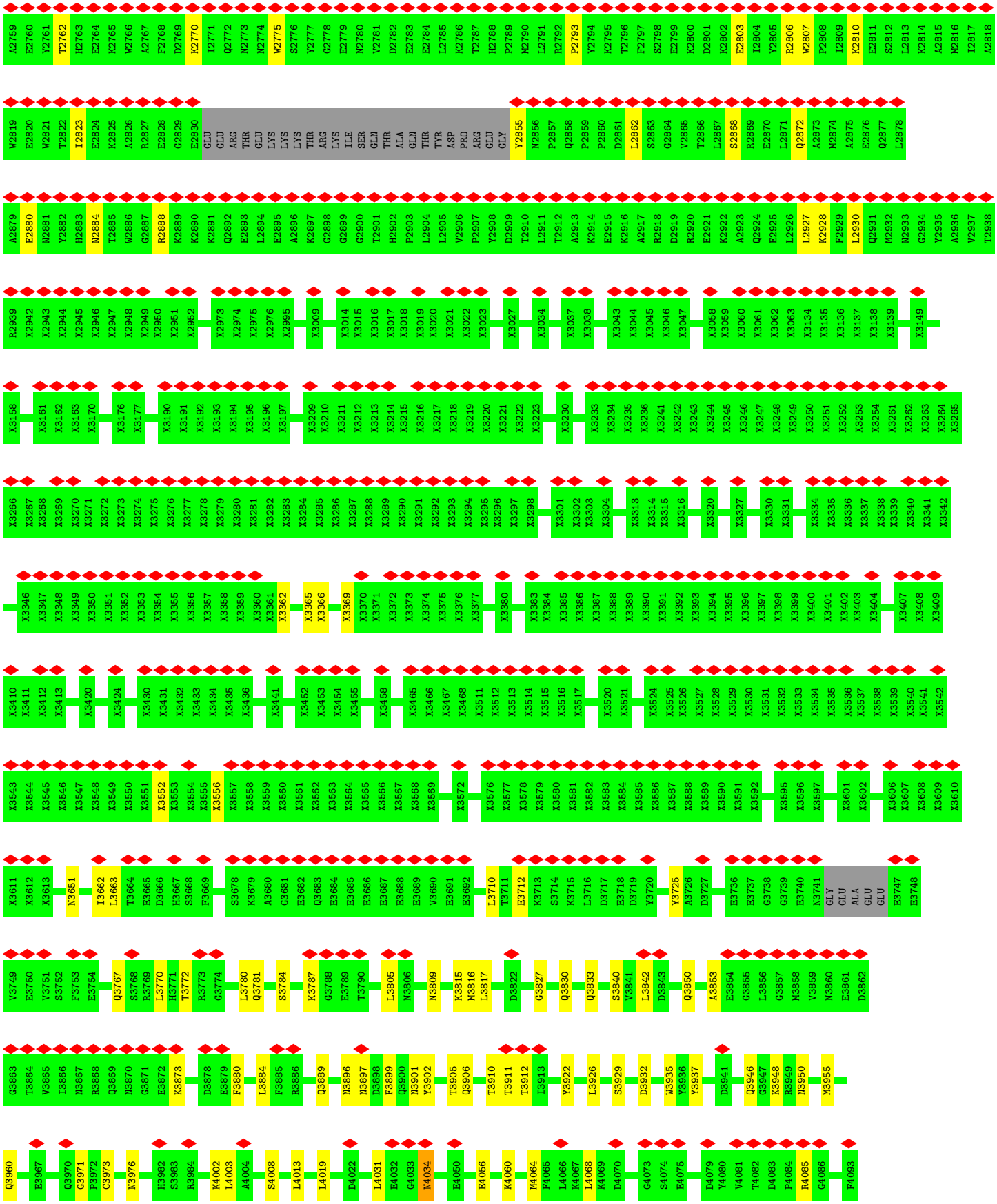
K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 T983 R987 L988 A989 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 A1030 T1031 N1035
S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 N1052 I1053 E1054 PRO PRO ASP GLN GLU GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 I1074 F1075 R1076 A1077 E1078 K1079 S1080 Y1081 F1090 E1091 F1092 E1093 A1094 V1095 R1101 V1102 A1105 R1106 P1107 E1108 L1109 R1110 P1111

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W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878
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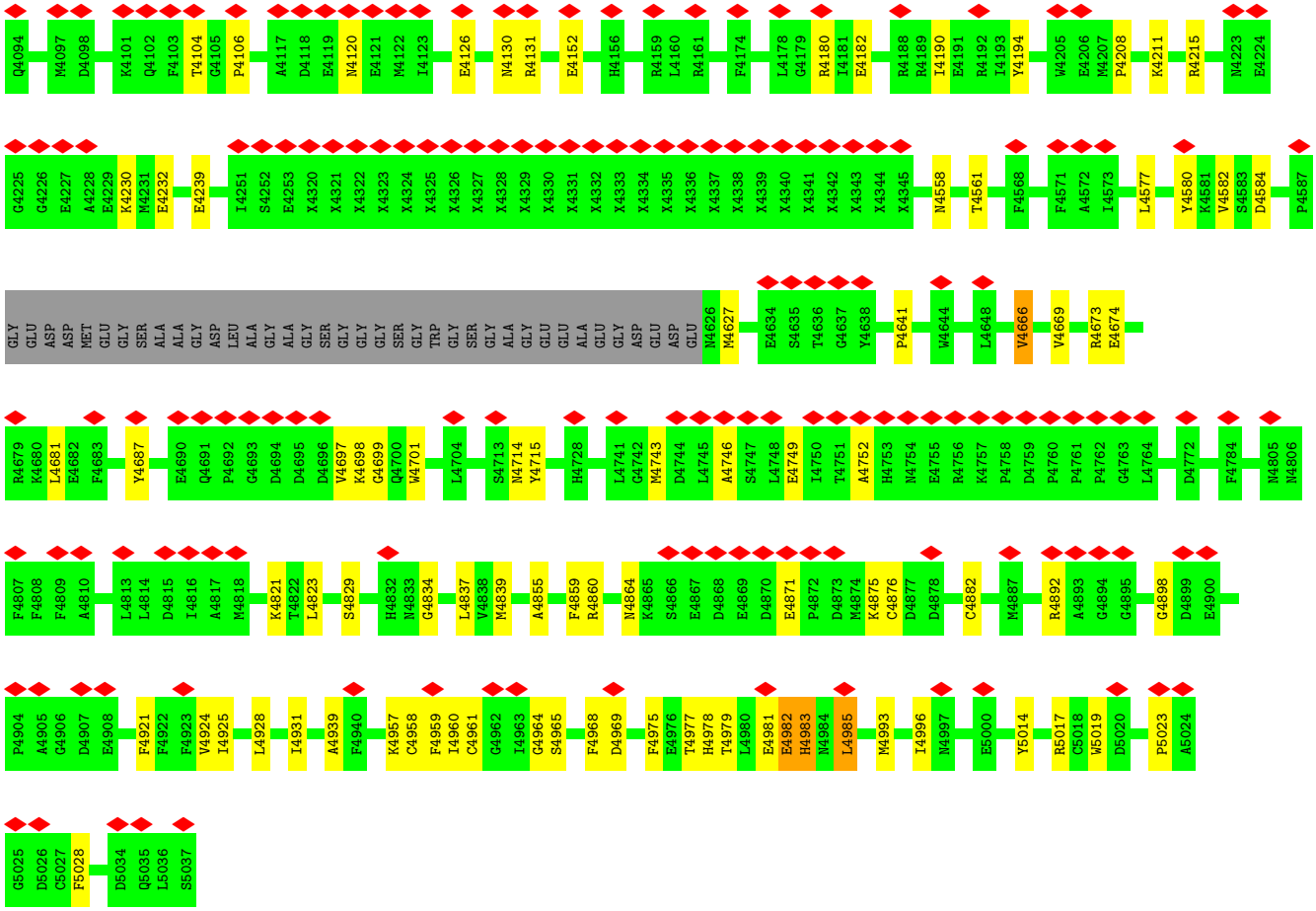
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, 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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.29	0/25428	0.53	9/34534 (0.0%)
2	E	0.29	0/25428	0.53	9/34534 (0.0%)
2	G	0.29	0/25428	0.53	9/34534 (0.0%)
2	I	0.29	0/25428	0.53	9/34534 (0.0%)
All	All	0.29	0/105048	0.53	36/142628 (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
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.04	133.78	115.30
2	B	131	LEU	CA-CB-CG	8.02	133.75	115.30
2	I	131	LEU	CA-CB-CG	8.01	133.73	115.30
2	E	131	LEU	CA-CB-CG	8.00	133.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1600	LEU	CA-CB-CG	7.20	131.87	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	808	TYR	Peptide

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	818	0	824	21	0
1	F	818	0	824	20	0
1	H	818	0	824	18	0
1	J	818	0	824	18	0
2	B	29499	0	24746	316	0
2	E	29499	0	24746	322	0
2	G	29499	0	24746	319	0
2	I	29499	0	24746	317	0
3	B	31	0	12	2	0
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102368	1324	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 6.

The worst 5 of 1324 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:G:4230:LYS:HD2	2:G:4959:PHE:CE2	1.25	1.69
2:E:4230:LYS:HD2	2:E:4959:PHE:CE2	1.25	1.64
2:I:4230:LYS:HD2	2:I:4959:PHE:CE2	1.25	1.60
2:B:4230:LYS:HD2	2:B:4959:PHE:CE2	1.25	1.58
2:B:4230:LYS:HD2	2:B:4959:PHE:CZ	1.55	1.42

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2929 (90%)	302 (9%)	4 (0%)	48	83
2	E	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	48	83
2	G	3235/4416 (73%)	2930 (91%)	301 (9%)	4 (0%)	48	83
2	I	3235/4416 (73%)	2928 (90%)	303 (9%)	4 (0%)	48	83
All	All	13360/18096 (74%)	12101 (91%)	1243 (9%)	16 (0%)	50	83

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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Mol	Chain	Res	Type
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1840	PRO

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	81	87
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	80	87

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1076	ARG
2	G	4983	HIS
2	G	1600	LEU
2	G	4034	ASN
2	I	1676	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 158 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	4034	ASN

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Mol	Chain	Res	Type
2	G	3830	GLN
2	E	4833	ASN
2	G	949	ASN
2	G	3976	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	$\#\|Z\| > 2$
4	CFF	I	5102	-	8,15,15	1.98	3 (37%)	8,23,23	1.36	1 (12%)
3	ATP	B	5101	-	28,33,33	0.94	0	34,52,52	1.16	2 (5%)
3	ATP	E	5101	-	28,33,33	0.93	0	34,52,52	1.15	2 (5%)
3	ATP	G	5101	-	28,33,33	0.94	0	34,52,52	1.16	2 (5%)
4	CFF	B	5102	-	8,15,15	1.99	3 (37%)	8,23,23	1.36	1 (12%)
3	ATP	I	5101	-	28,33,33	0.95	0	34,52,52	1.16	2 (5%)
4	CFF	G	5102	-	8,15,15	1.98	3 (37%)	8,23,23	1.35	1 (12%)
4	CFF	E	5102	-	8,15,15	1.99	3 (37%)	8,23,23	1.36	1 (12%)

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
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	E	5101	-	-	6/18/38/38	0/3/3/3
3	ATP	G	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	6/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	5102	CFF	C6-N1	-3.27	1.32	1.38
4	E	5102	CFF	C6-N1	-3.27	1.32	1.38
4	G	5102	CFF	C6-N1	-3.26	1.32	1.38
4	I	5102	CFF	C6-N1	-3.23	1.32	1.38
4	I	5102	CFF	C5-C4	-3.23	1.33	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	5101	ATP	N3-C2-N1	-3.78	123.54	128.67
3	G	5101	ATP	N3-C2-N1	-3.75	123.58	128.67
3	B	5101	ATP	N3-C2-N1	-3.75	123.58	128.67
3	E	5101	ATP	N3-C2-N1	-3.73	123.61	128.67
4	B	5102	CFF	C14-N7-C8	-2.82	111.86	125.43

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	B	5101	ATP	C5'-O5'-PA-O2A
3	B	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O2A

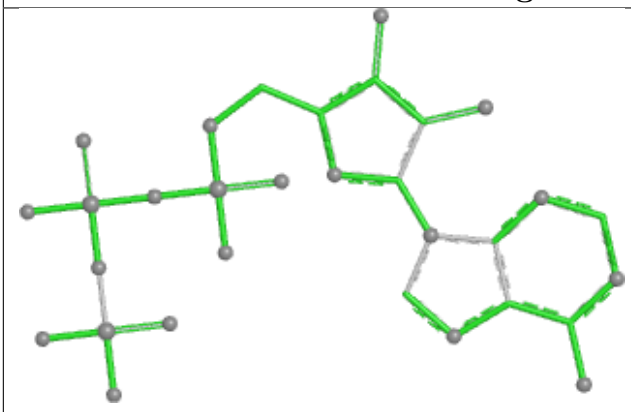
There are no ring outliers.

8 monomers are involved in 12 short contacts:

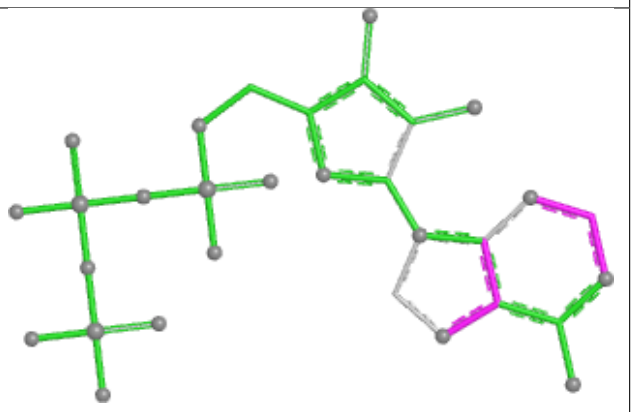
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	5102	CFF	1	0
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0
3	G	5101	ATP	2	0
4	B	5102	CFF	1	0
3	I	5101	ATP	2	0
4	G	5102	CFF	1	0
4	E	5102	CFF	1	0

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

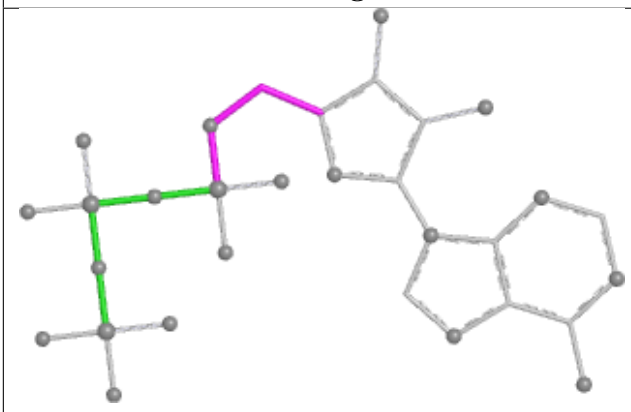
Ligand ATP B 5101



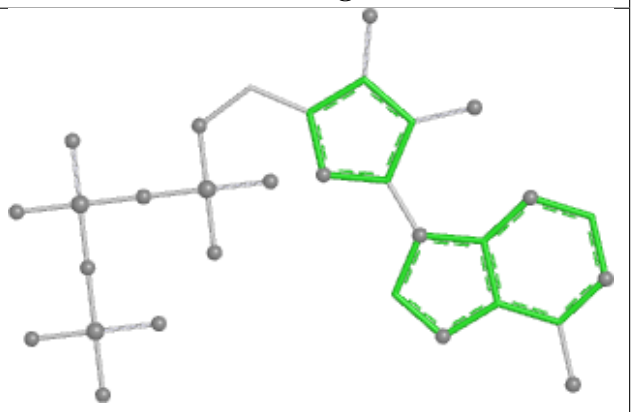
Bond lengths



Bond angles

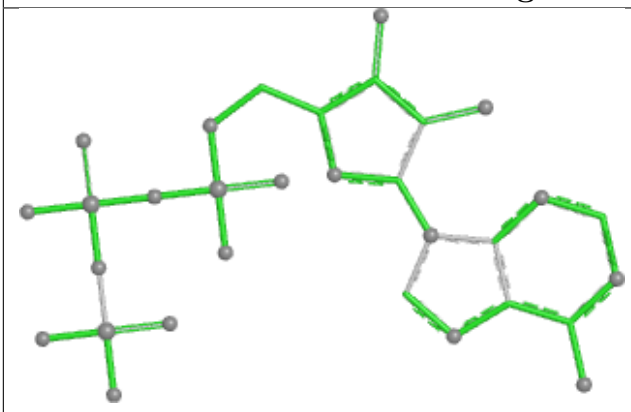


Torsions

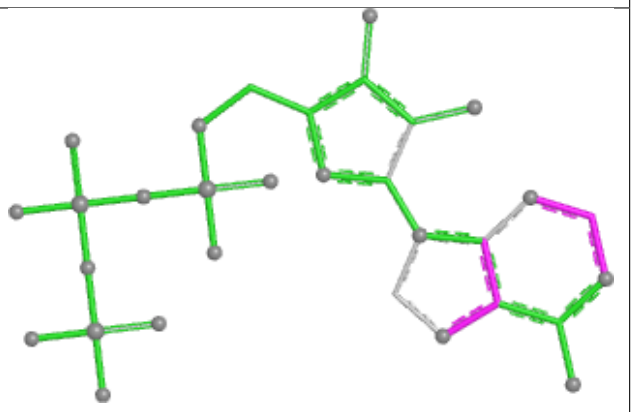


Rings

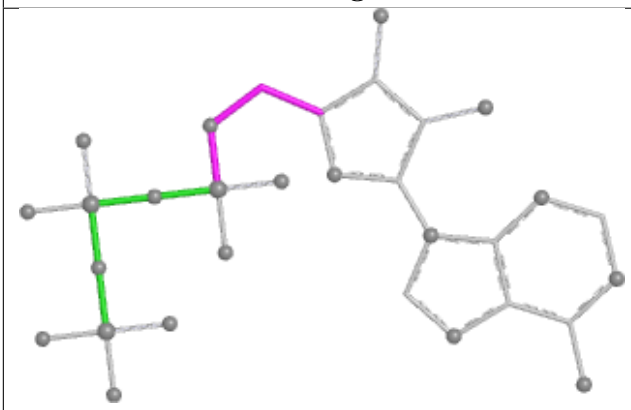
Ligand ATP E 5101



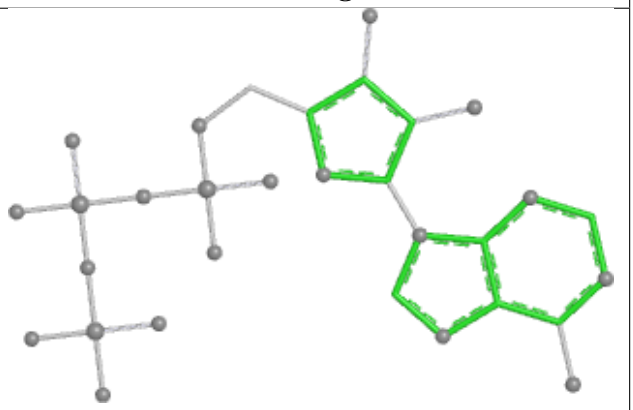
Bond lengths



Bond angles

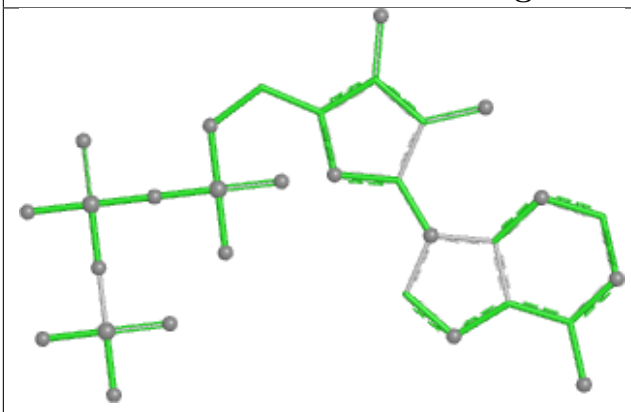


Torsions

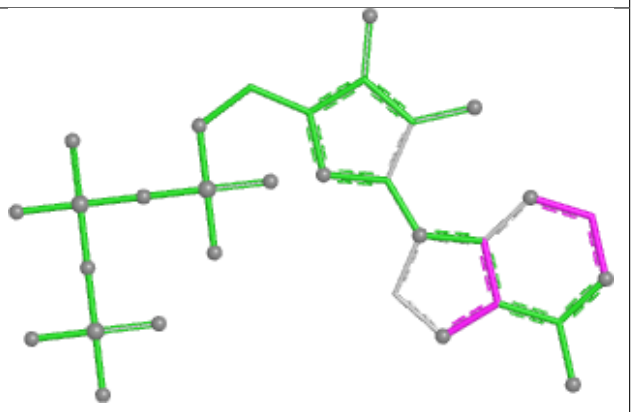


Rings

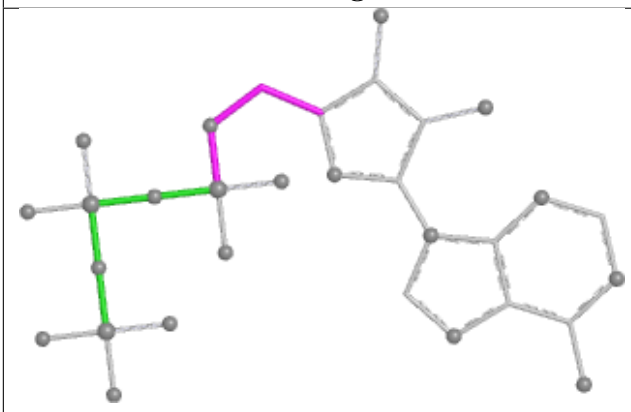
Ligand ATP G 5101



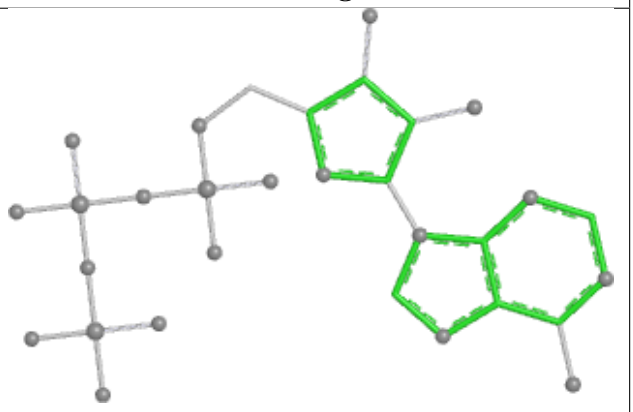
Bond lengths



Bond angles

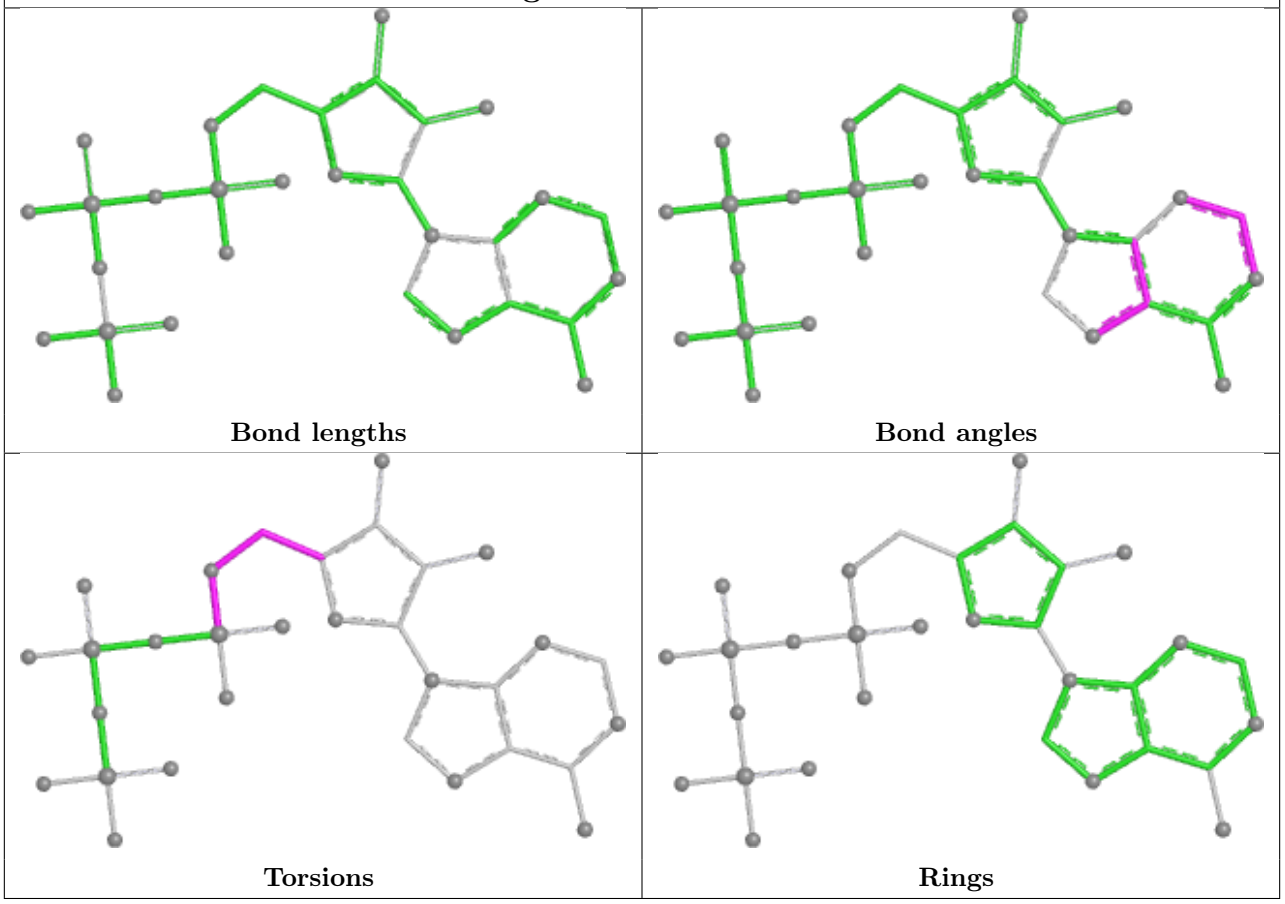


Torsions



Rings

Ligand ATP I 5101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	I	14
2	E	14
2	G	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.19
1	I	4345:UNK	C	4540:PHE	N	73.19

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4345:UNK	C	4540:PHE	N	73.19
1	G	4345:UNK	C	4540:PHE	N	73.19
1	B	3613:UNK	C	3639:THR	N	44.63

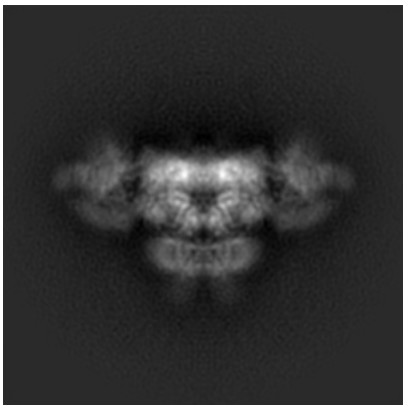
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8383. These allow visual inspection of the internal detail of the map and identification of artifacts.

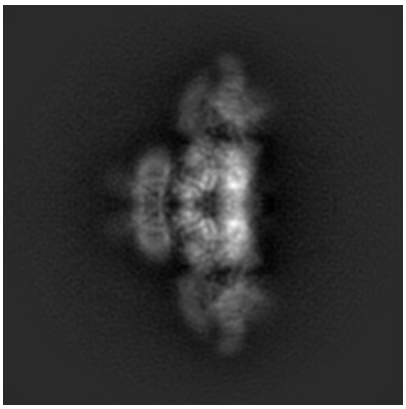
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

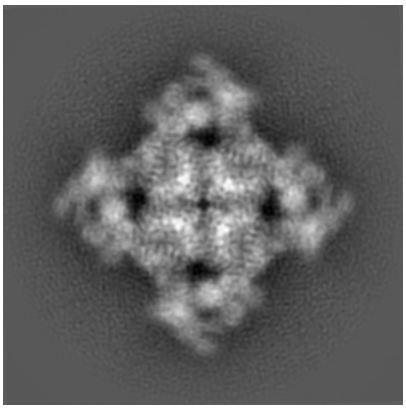
6.1.1 Primary map



X

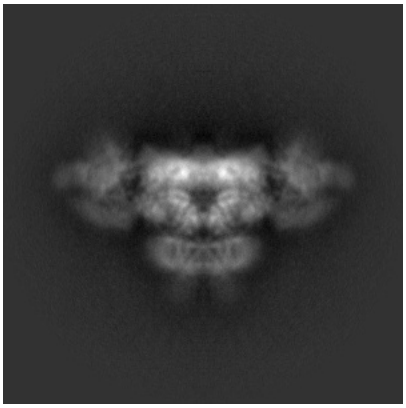


Y

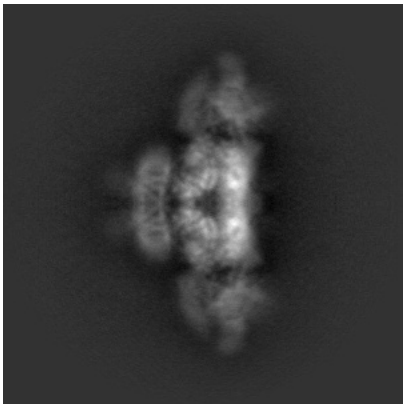


Z

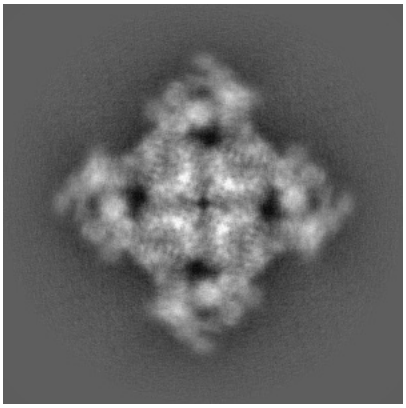
6.1.2 Raw map



X



Y

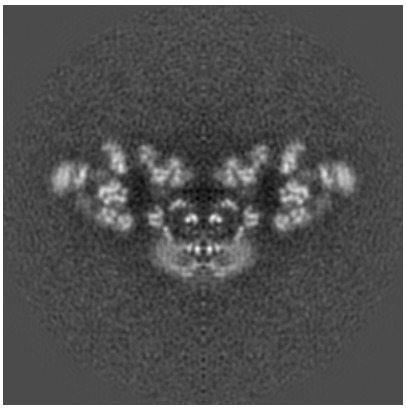


Z

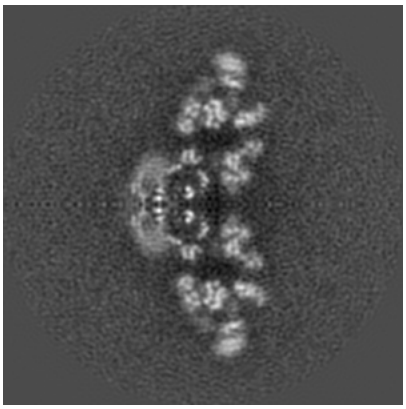
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

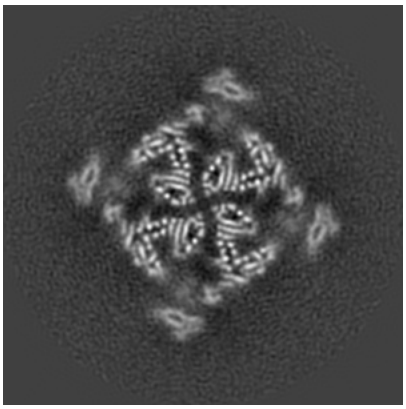
6.2.1 Primary map



X Index: 200

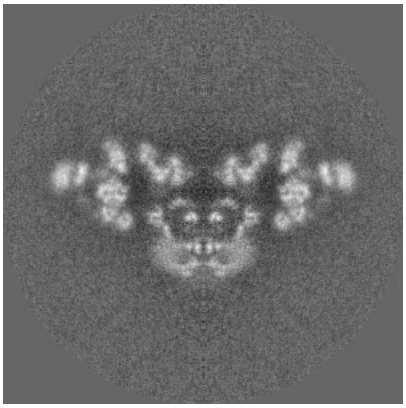


Y Index: 200

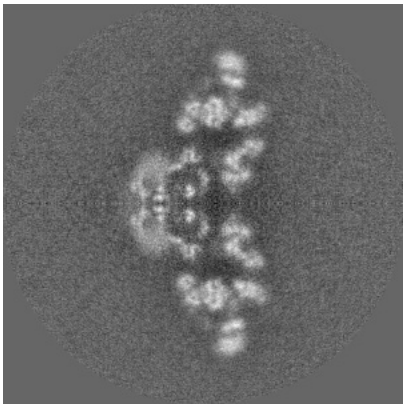


Z Index: 200

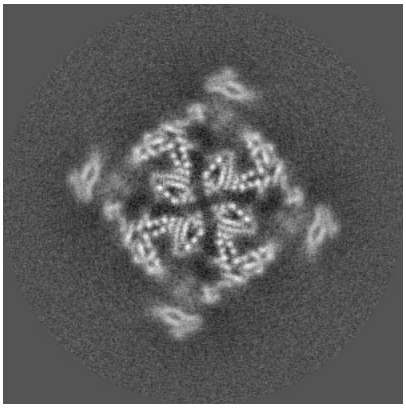
6.2.2 Raw map



X Index: 200



Y Index: 200

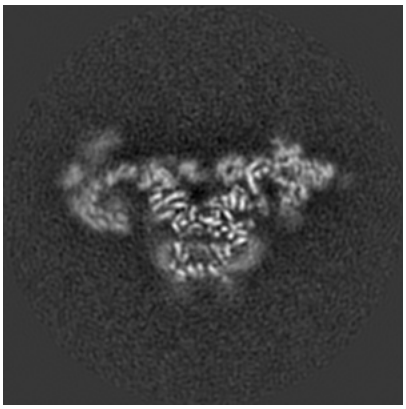


Z Index: 200

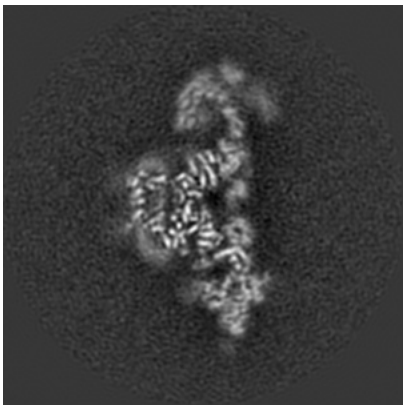
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

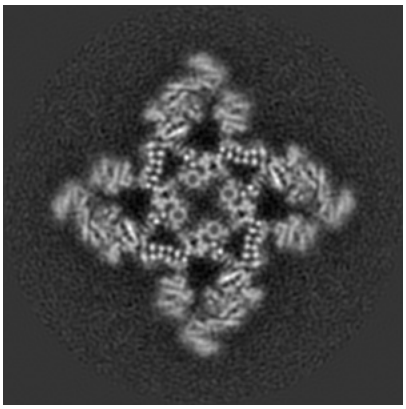
6.3.1 Primary map



X Index: 183

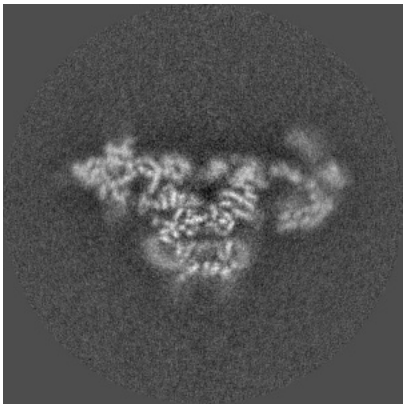


Y Index: 183

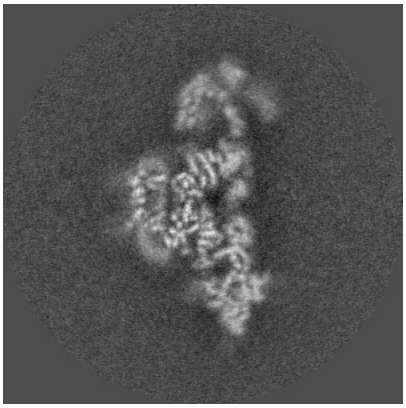


Z Index: 226

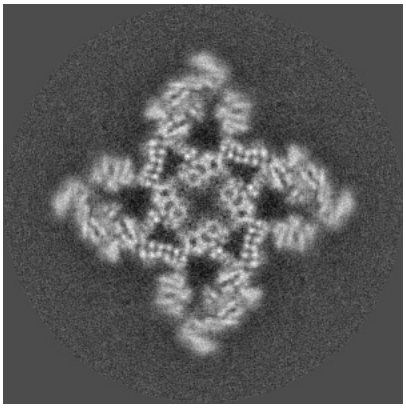
6.3.2 Raw map



X Index: 217



Y Index: 183

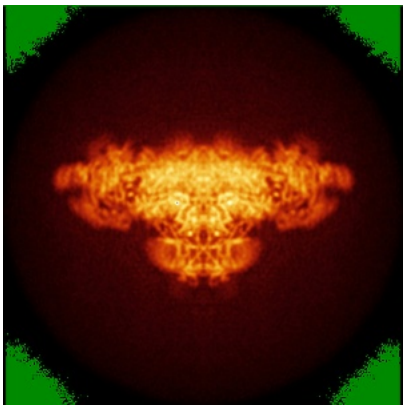


Z Index: 227

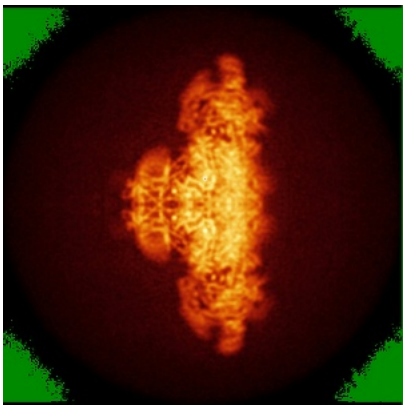
The images above show the largest variance slices of the map in three orthogonal directions.

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

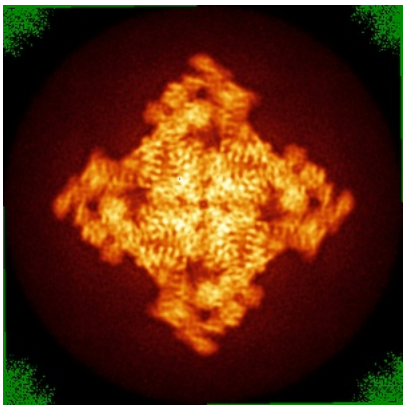
6.4.1 Primary map



X

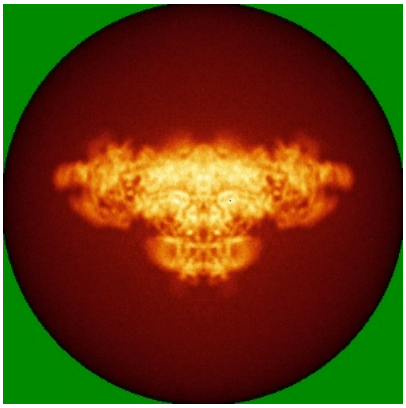


Y

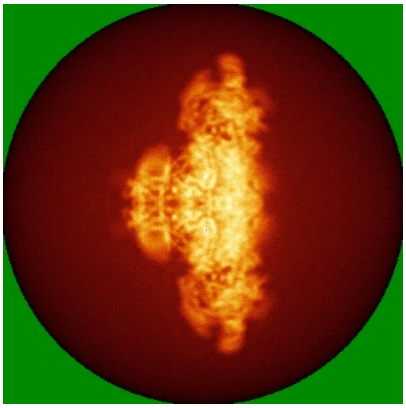


Z

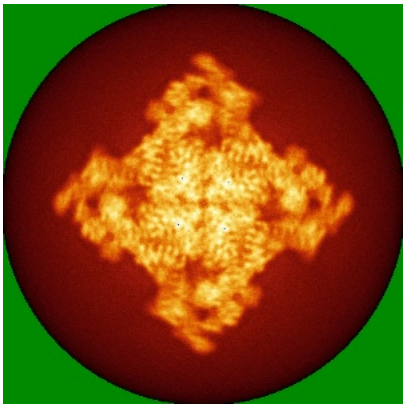
6.4.2 Raw map



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.

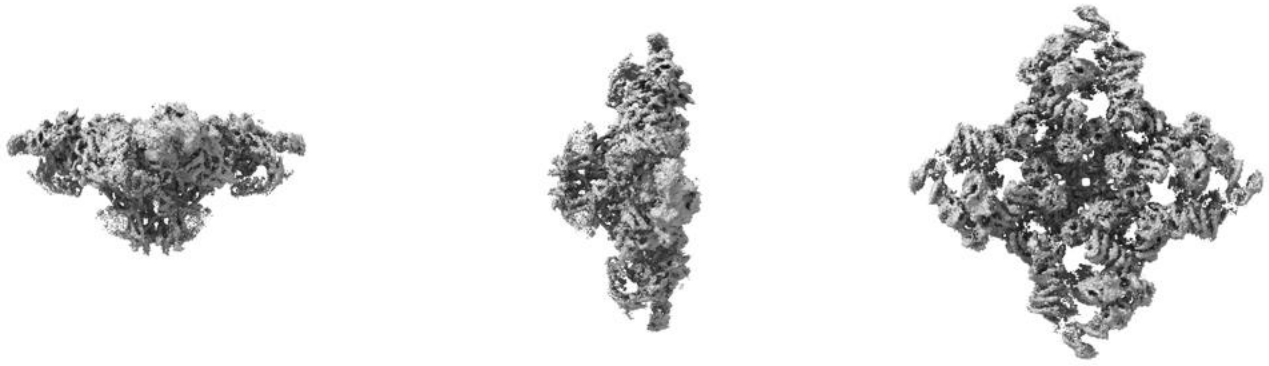
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

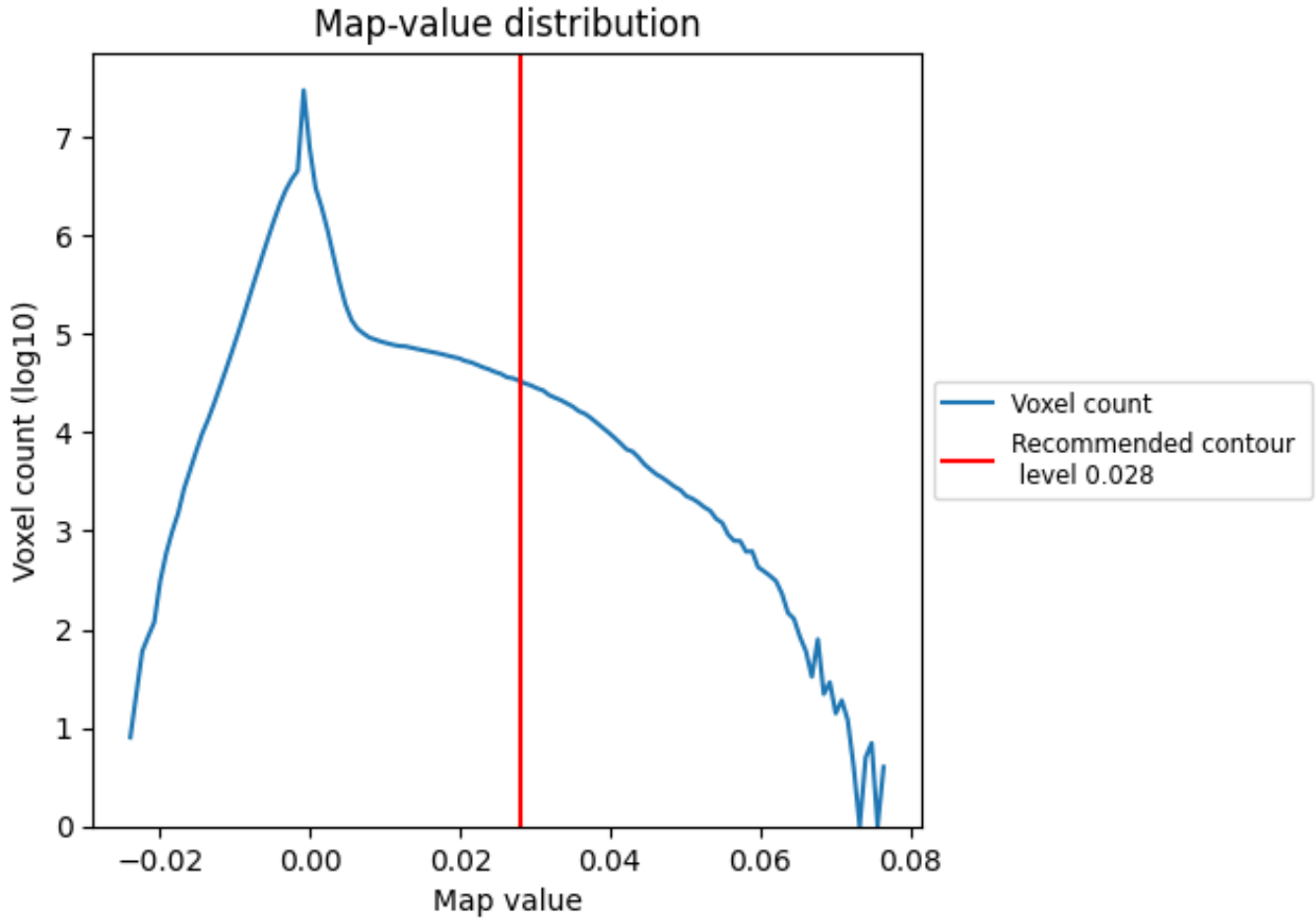
6.6 Mask visualisation (i)

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

7 Map analysis

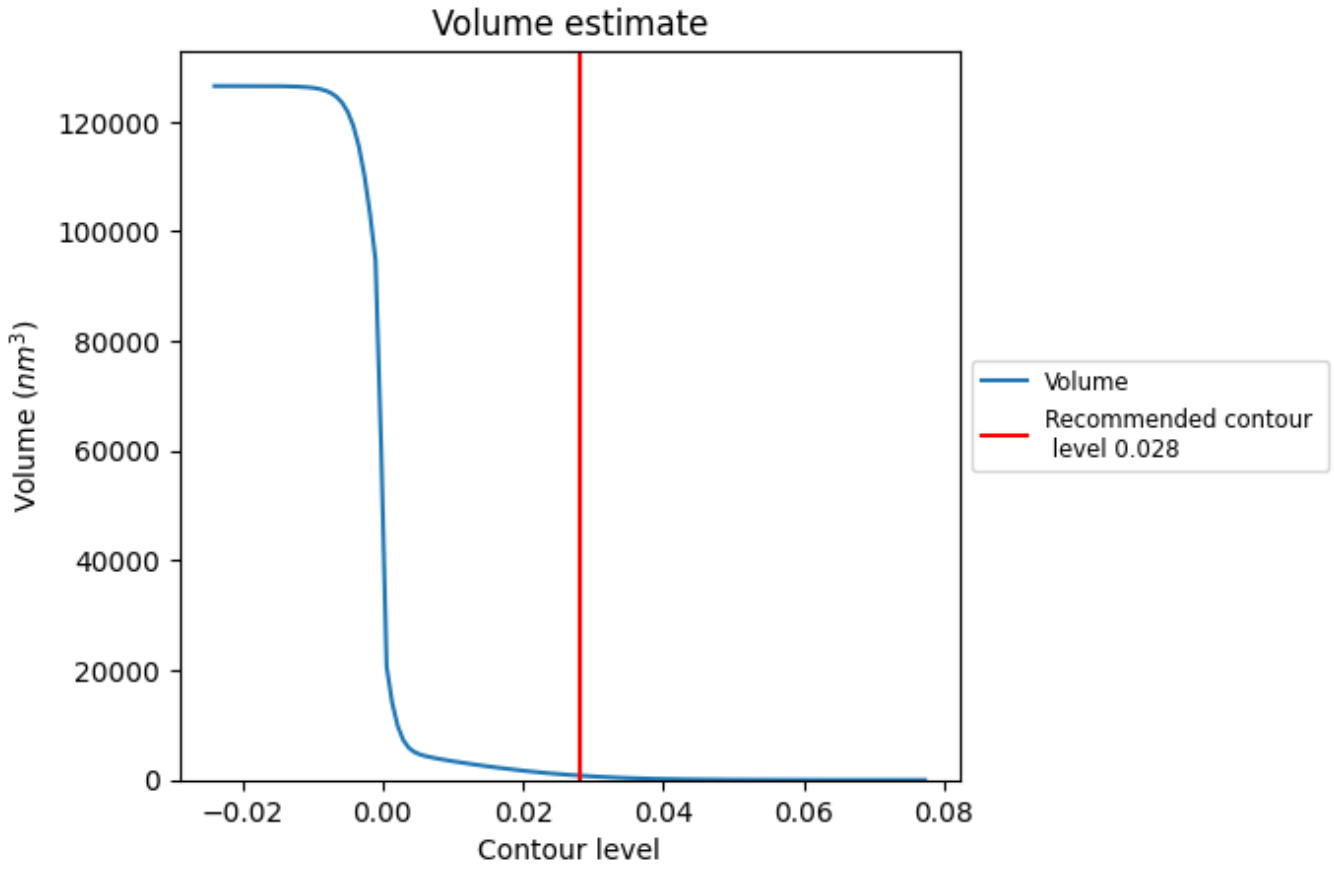
This section contains the results of statistical analysis of the map.

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.

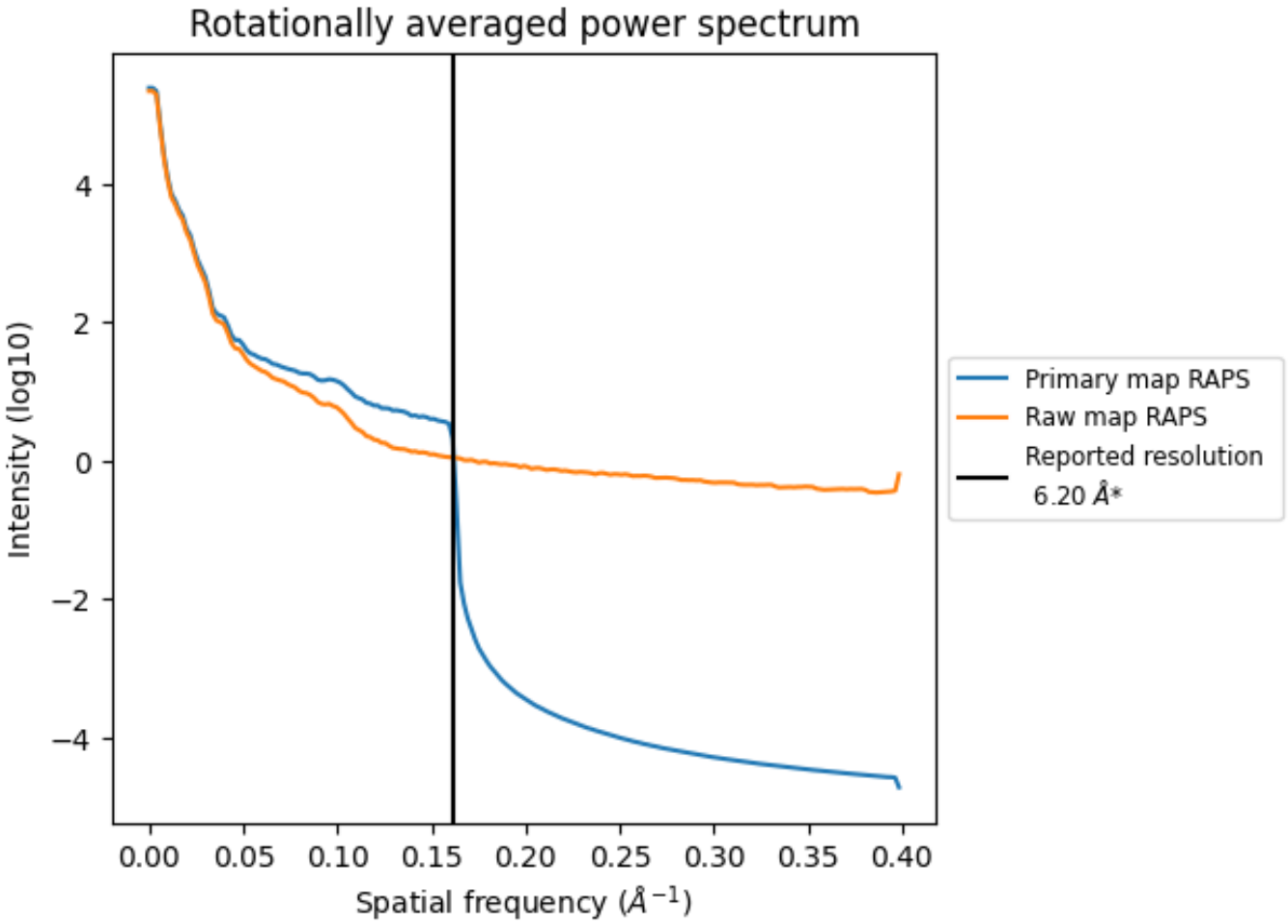
7.2 Volume estimate (i)



The volume at the recommended contour level is 804 nm^3; this corresponds to an approximate mass of 726 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)

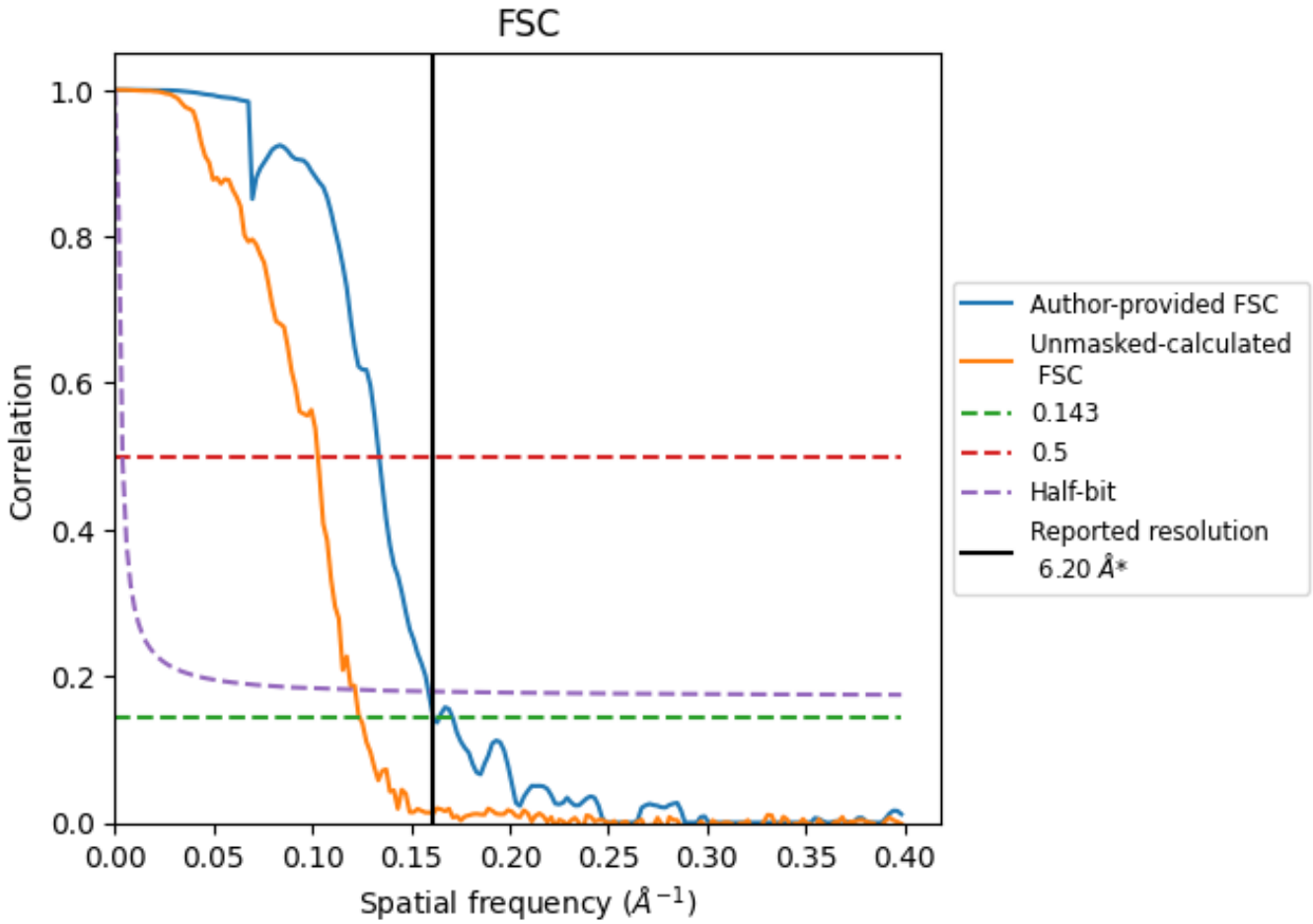


*Reported resolution corresponds to spatial frequency of 0.161 Å^{-1}

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 0.161 Å^{-1}

8.2 Resolution estimates (i)

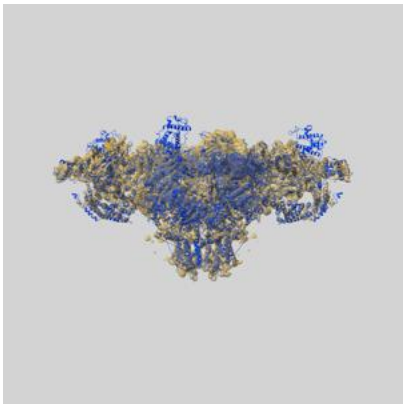
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.19	7.47	6.29
Unmasked-calculated*	8.06	9.72	8.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.06 differs from the reported value 6.2 by more than 10 %

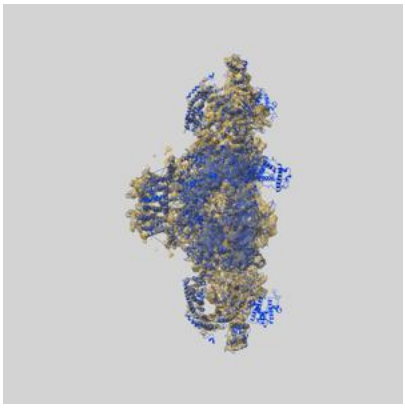
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8383 and PDB model 5TAS. Per-residue inclusion information can be found in section 3 on page 6.

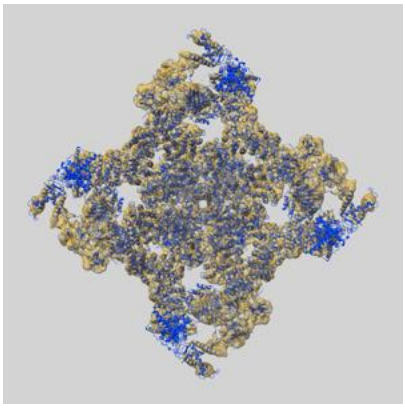
9.1 Map-model overlay



X



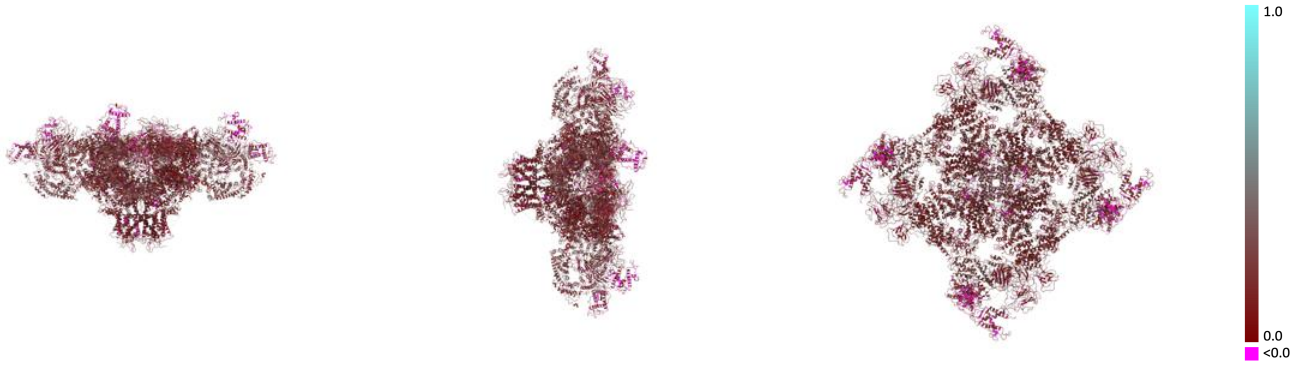
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

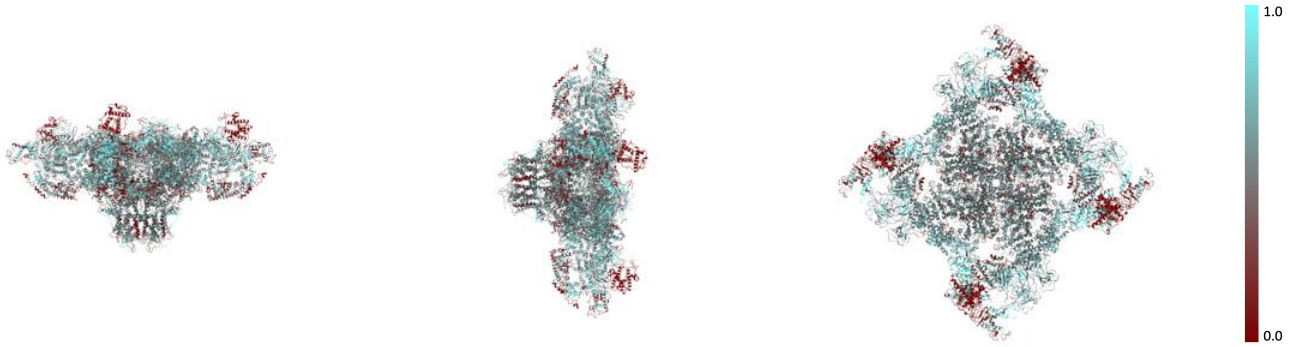
9.2 Q-score mapped to coordinate model



X Y Z

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

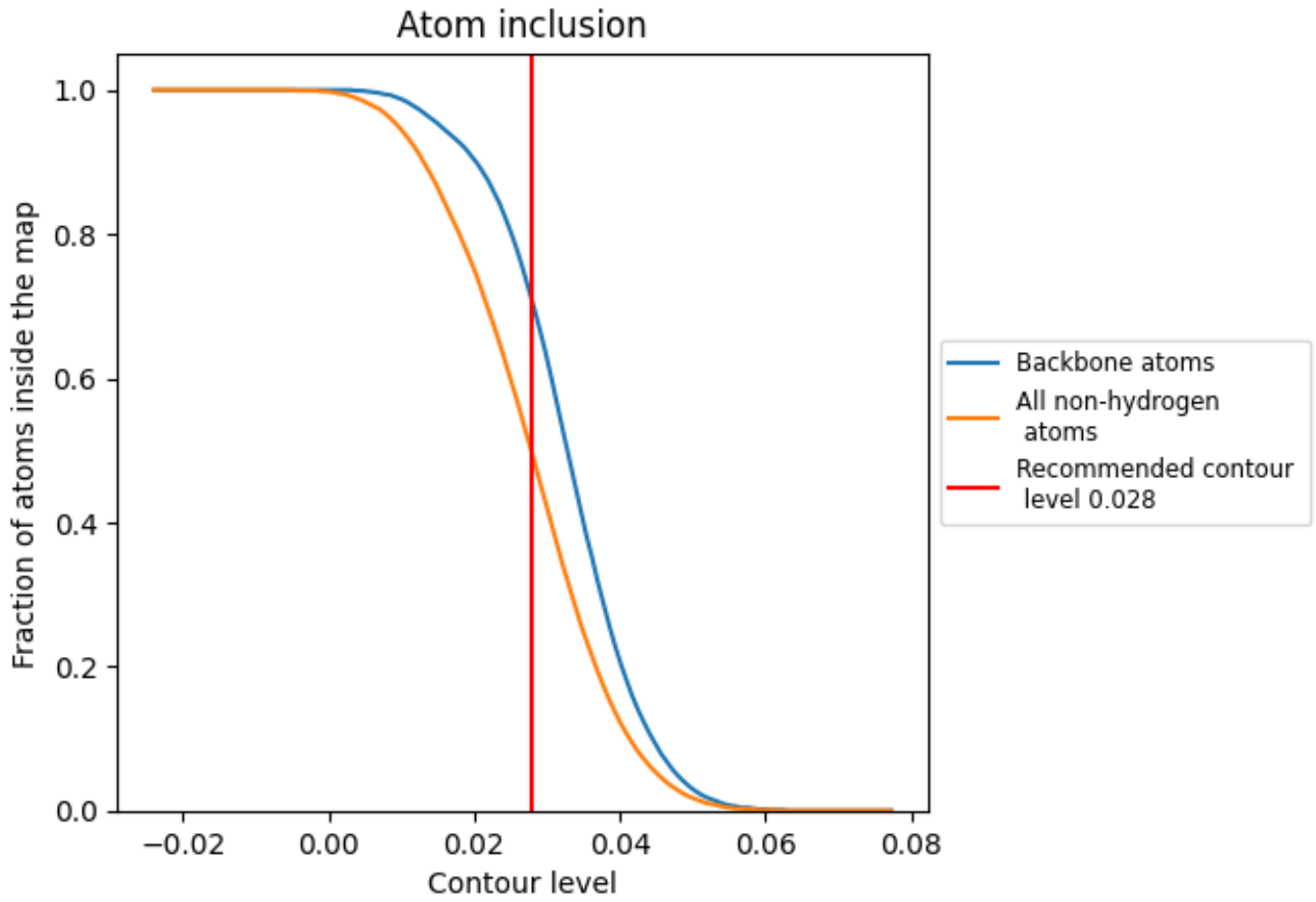
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 49% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4930	0.1830
A	0.5400	0.1700
B	0.4910	0.1840
E	0.4910	0.1830
F	0.5470	0.1750
G	0.4930	0.1840
H	0.5450	0.1730
I	0.4920	0.1830
J	0.5450	0.1720