wwPDB EM Validation Summary Report (i)

Apr 29, 2024 – 03:26 pm BST

PDB ID	:	4UWE
EMDB ID	:	EMD-2752
Title	:	Structure of the ryanodine receptor at resolution of 8.5 A in partially open state
Authors	:	Efremov, R.G.; Leitner, A.; Aebersold, R.; Raunser, S.
Deposited on	:	2014-08-11
Resolution	:	8.50 Å(reported)
Based on initial model	:	2UWA

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

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

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

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

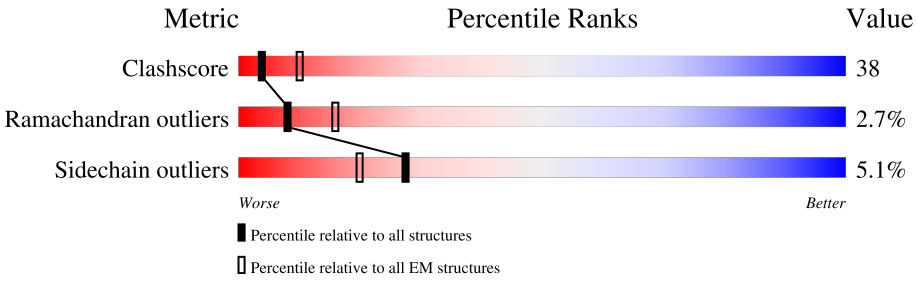
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 8.50 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	5037	7% 52% 13% · 34%
1	B	5037	7% 51% 13% · 34%
1	C	5037	7% 52% 13% · 34%
1	D	5037	7% 52% 13% · 34%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 81600 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RYANODINE RECEPTOR 1.

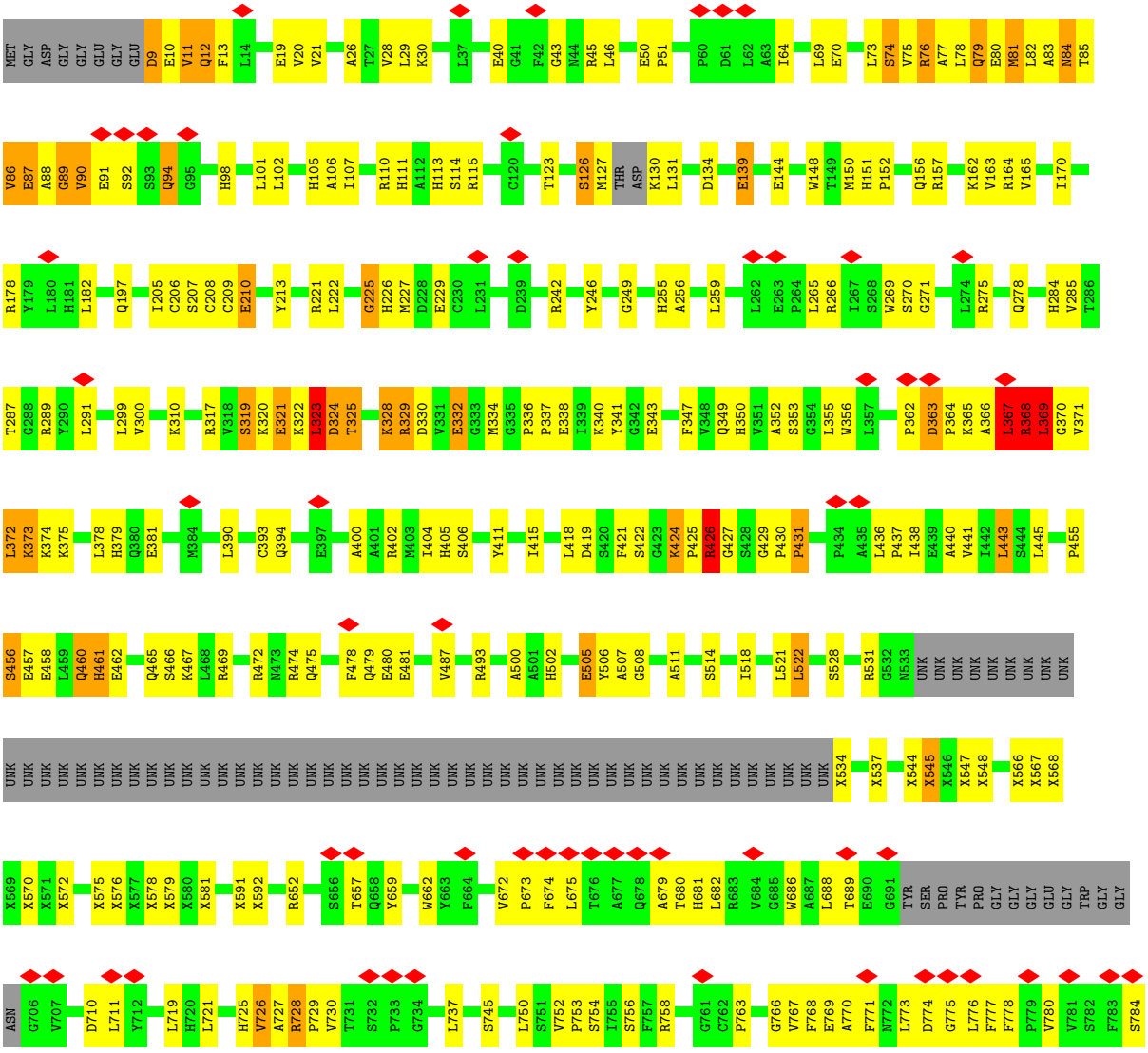
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3322	Total	C	N	O	S	0	0
			20400	12584	3816	3944	56		
1	B	3322	Total	C	N	O	S	0	0
			20400	12584	3816	3944	56		
1	C	3322	Total	C	N	O	S	0	0
			20400	12584	3816	3944	56		
1	D	3322	Total	C	N	O	S	0	0
			20400	12584	3816	3944	56		

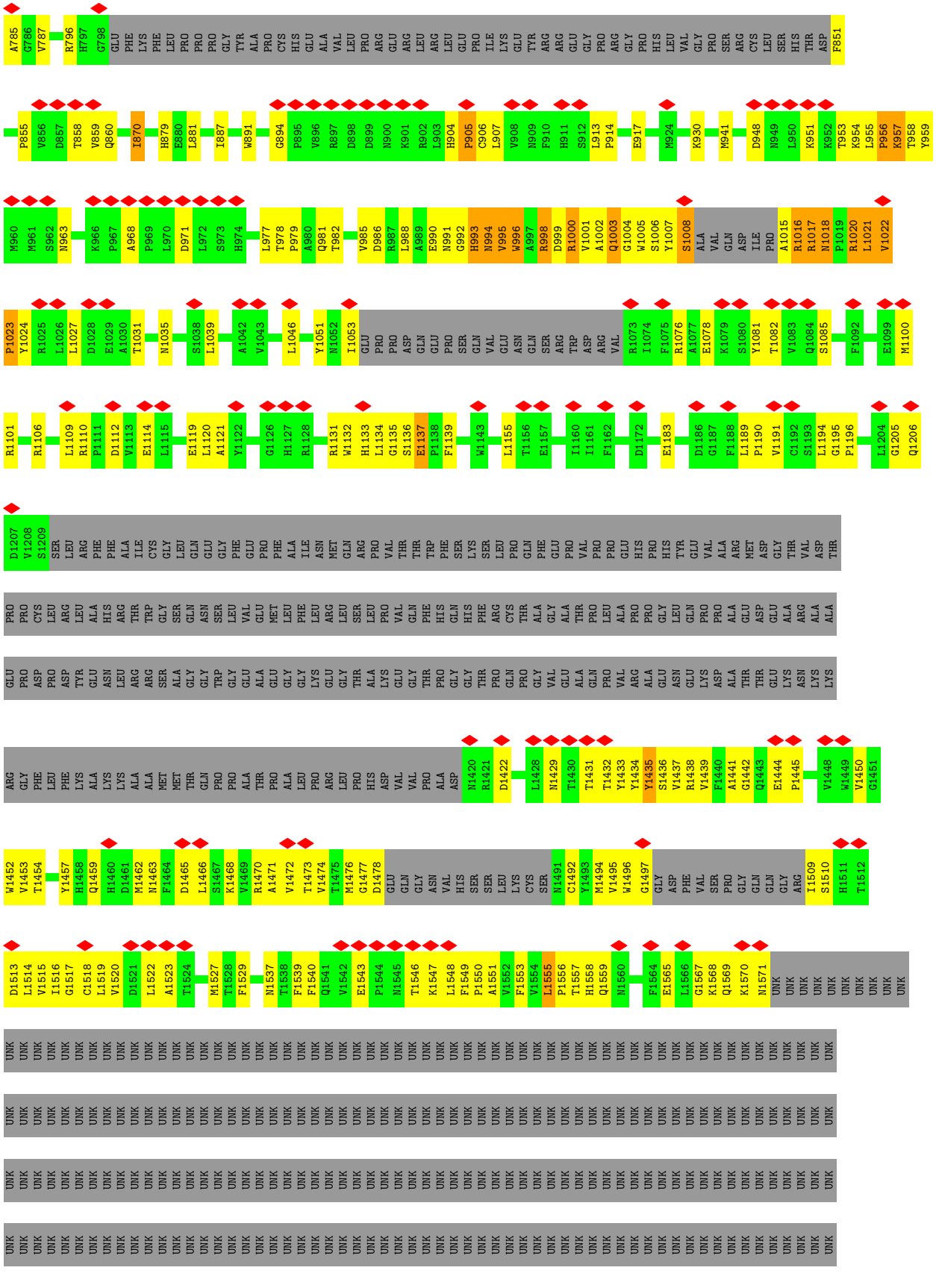
3 Residue-property plots (i)

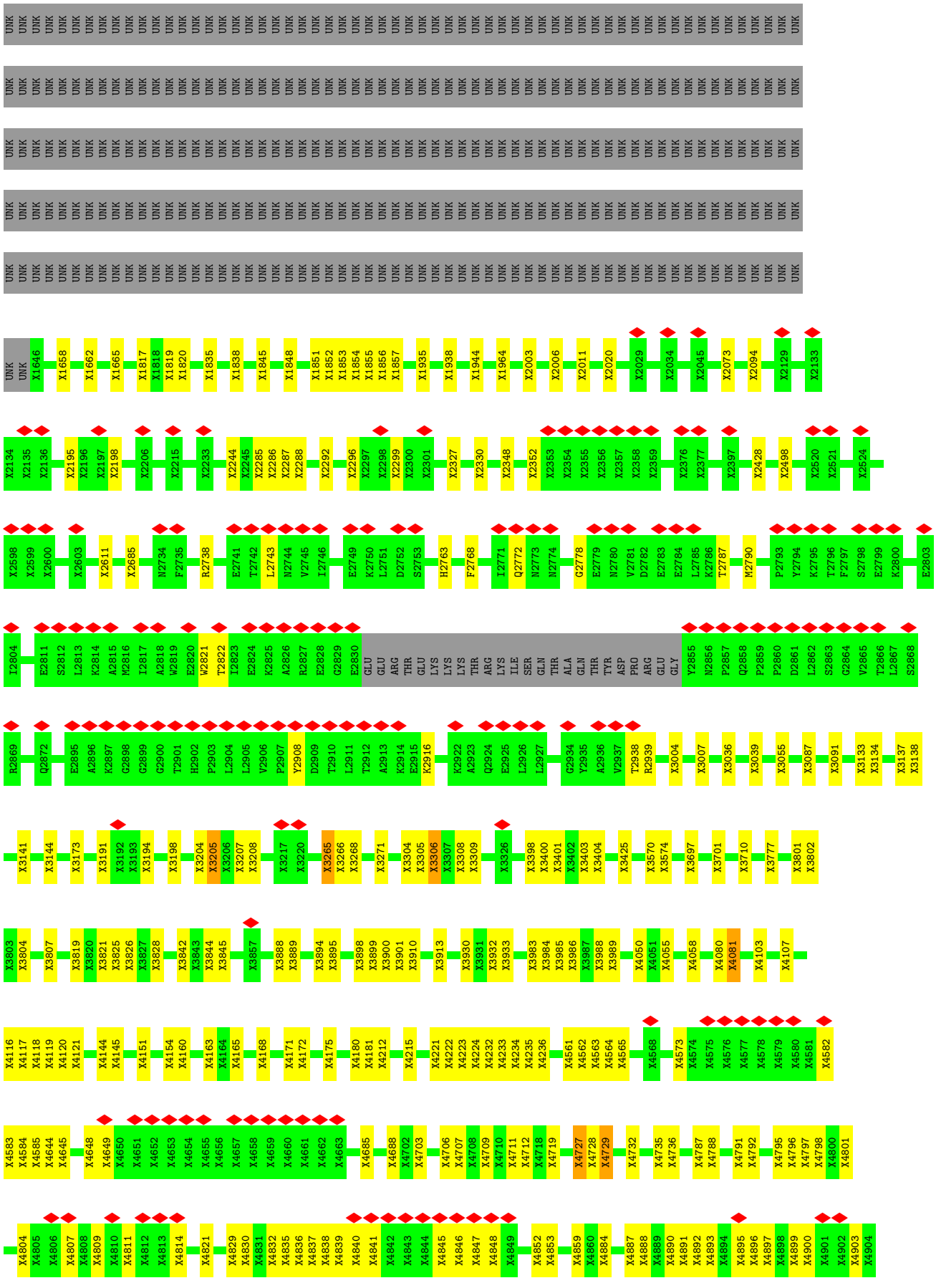
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: RYANODINE RECEPTOR 1

Chain A:



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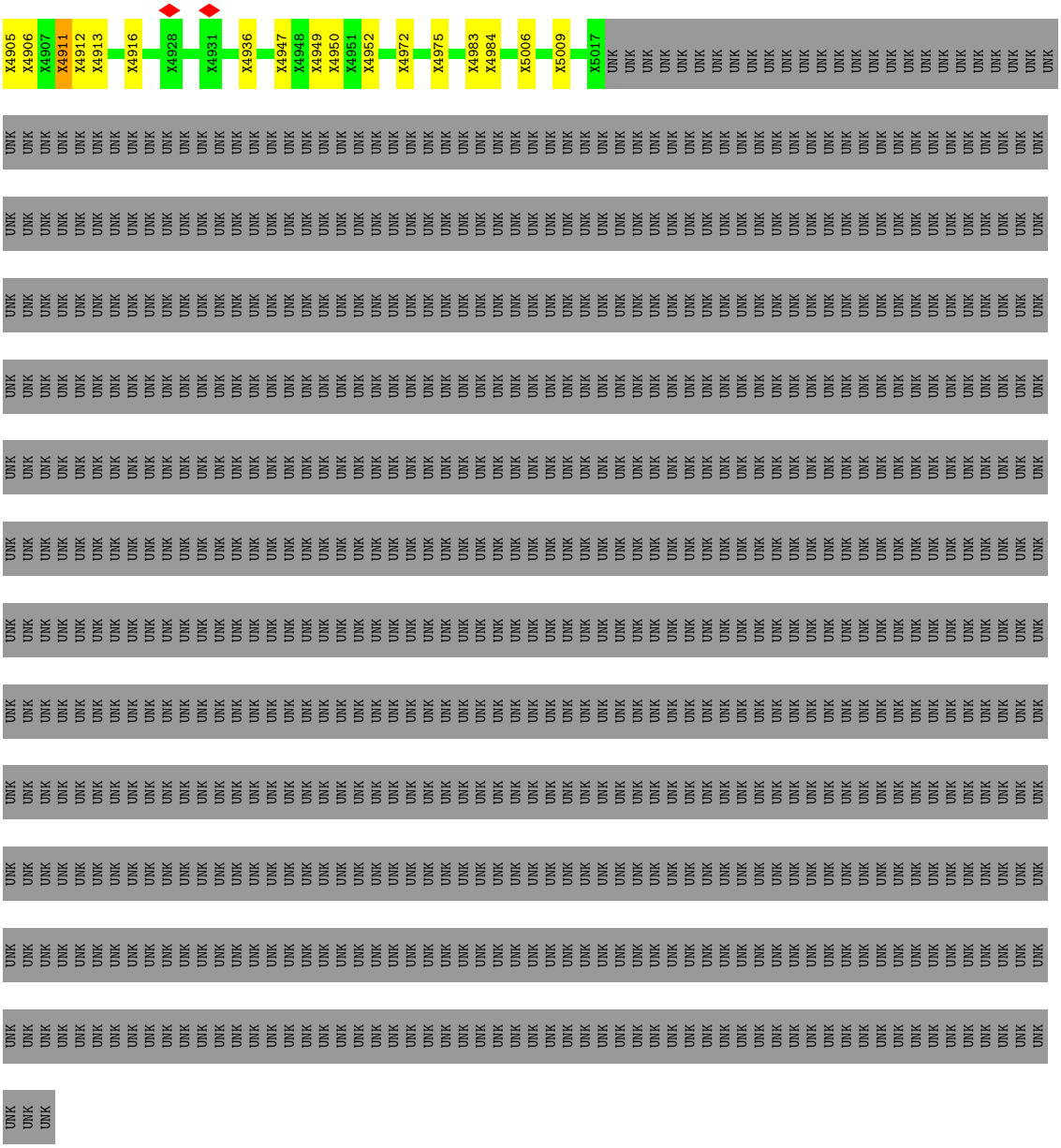
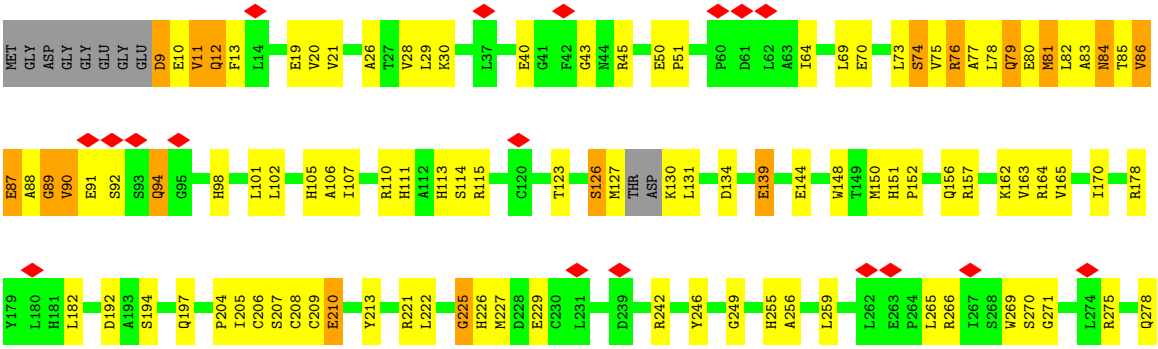
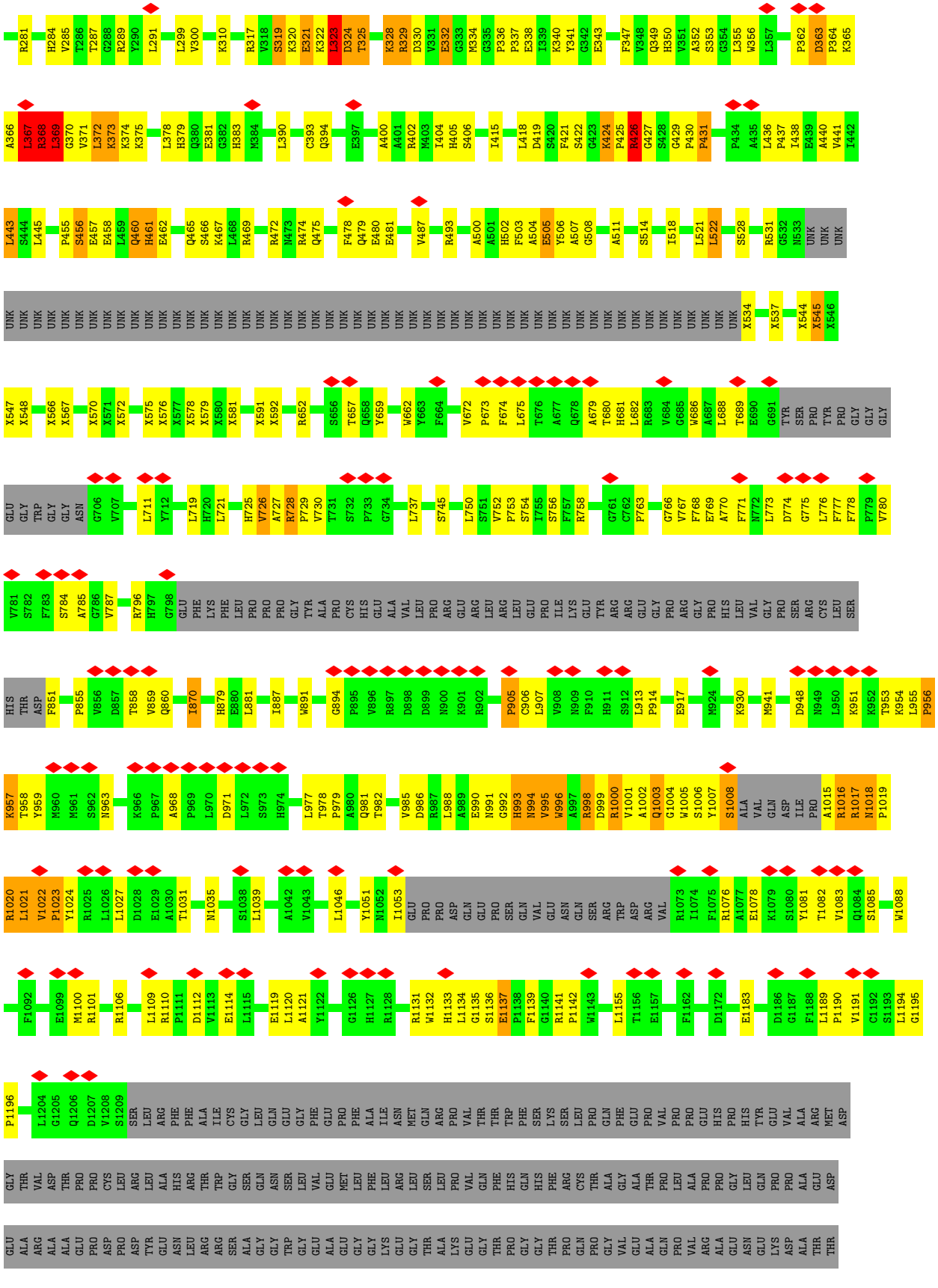
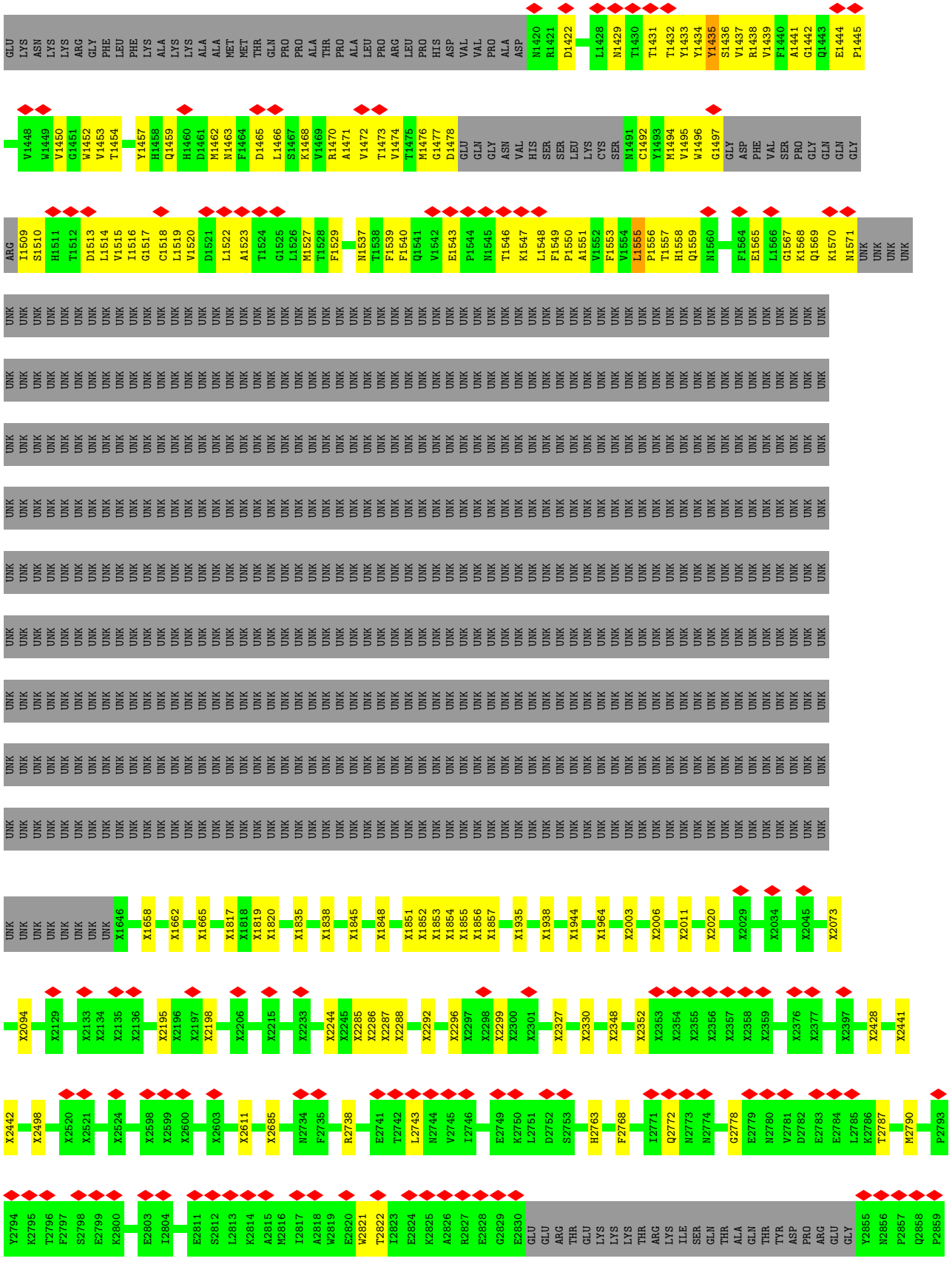


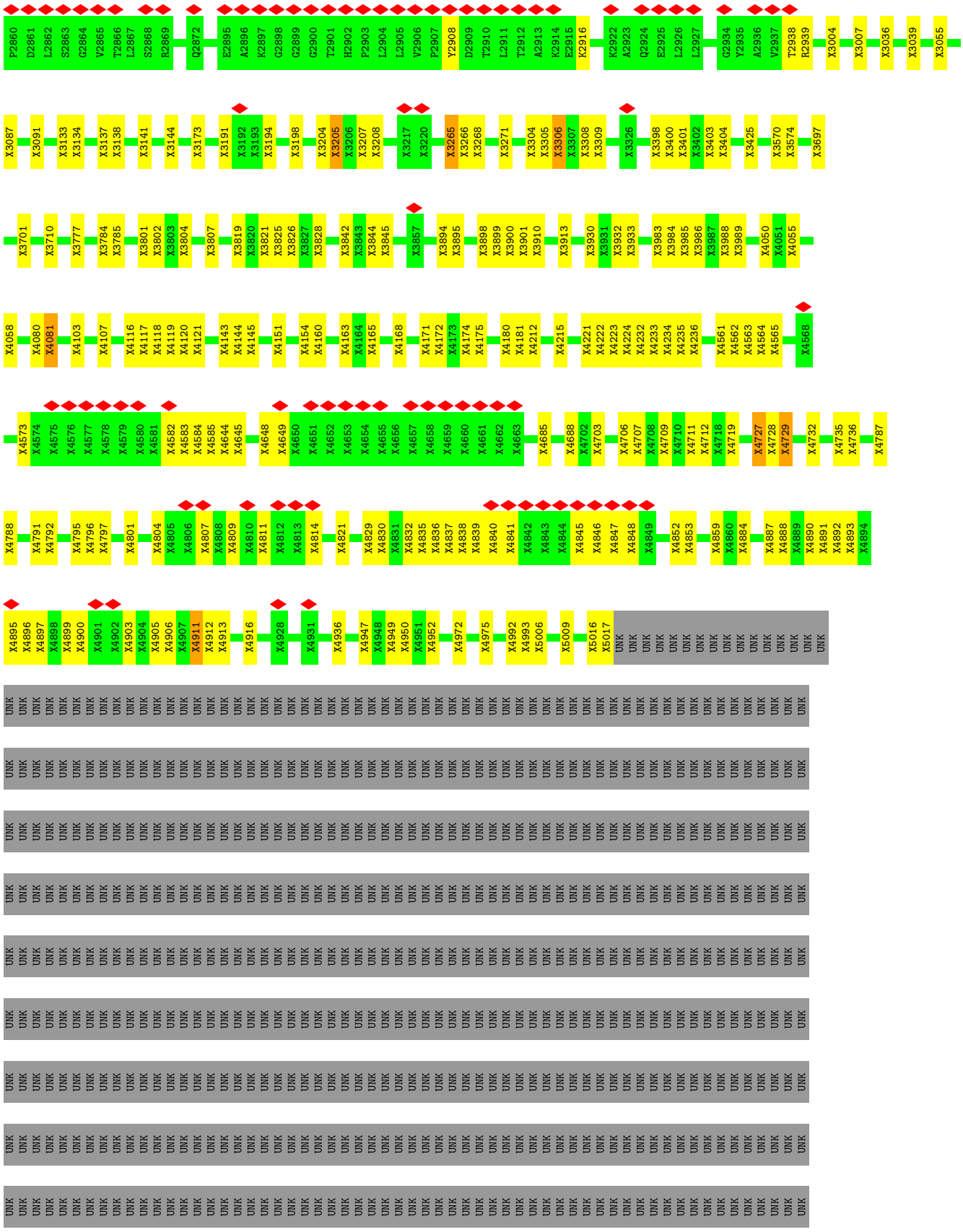
• Molecule 1: RYANODINE RECEPTOR 1

Chain B:





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X3087 X3091 X3133 X3134 X3137 X3138 X3141 X3144 X3173 X3191 X3192 X3193 X3194 X3198 X3204 X3205 X3206 X3207 X3208 X3217 X3220 X3265 X3266 X3268 X3271 X3304 X3305 X3306 X3307 X3308 X3309 X3326 X3398 X3400 X3401 X3402 X3403 X3404 X3425 X3570 X3574 X3697
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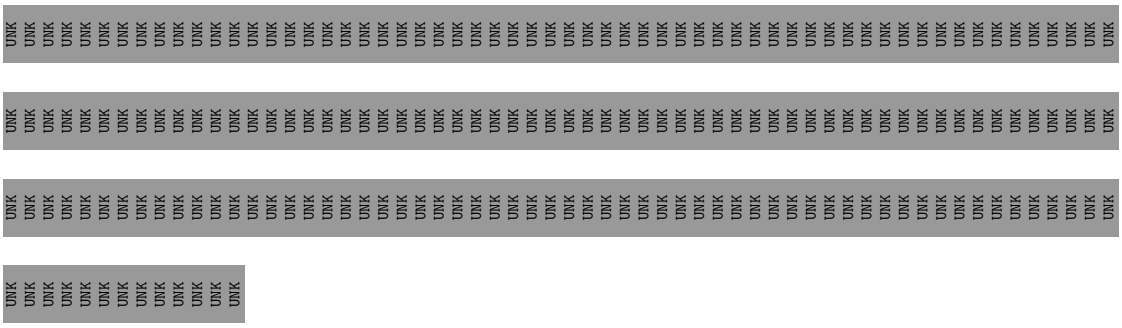
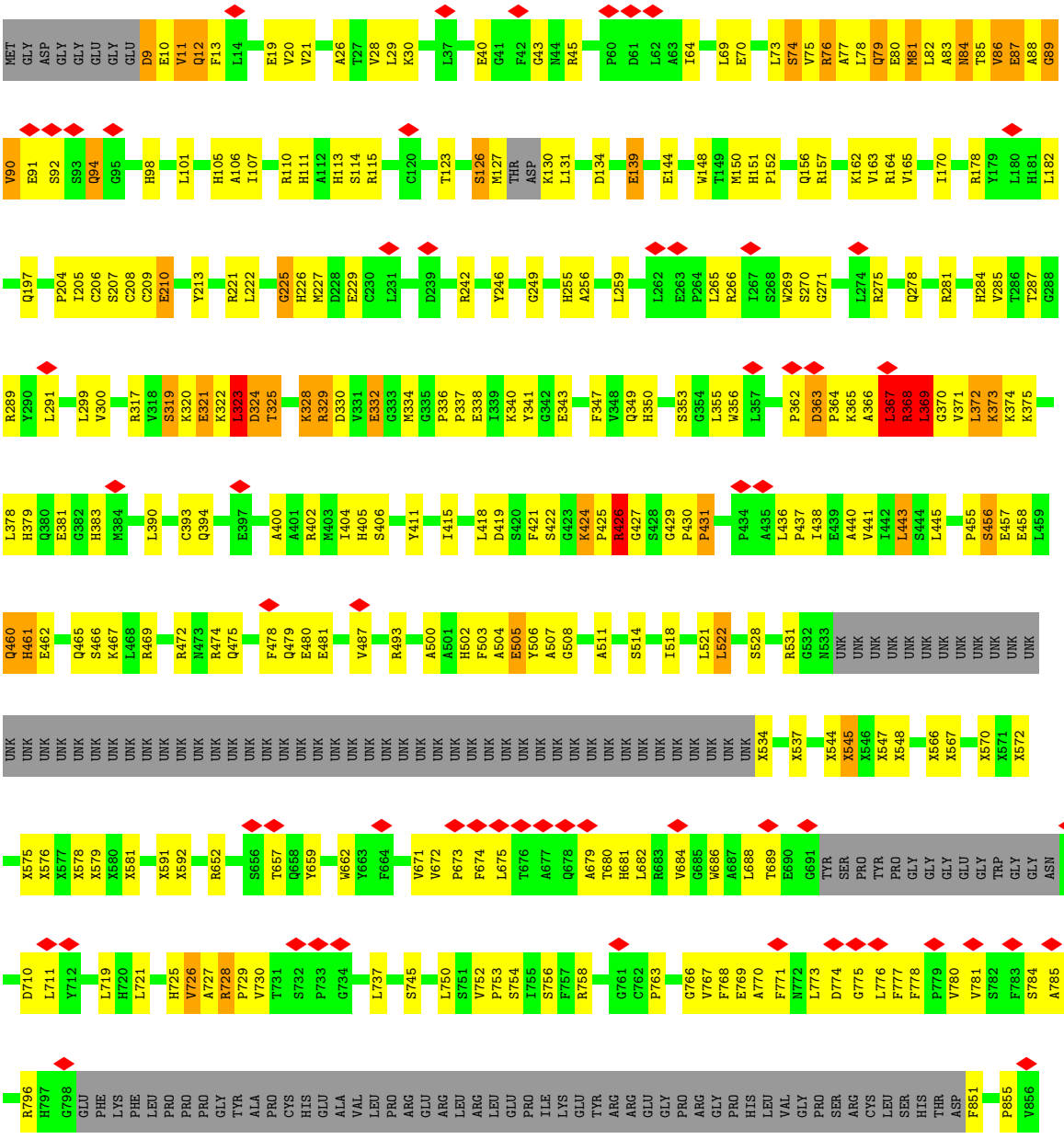
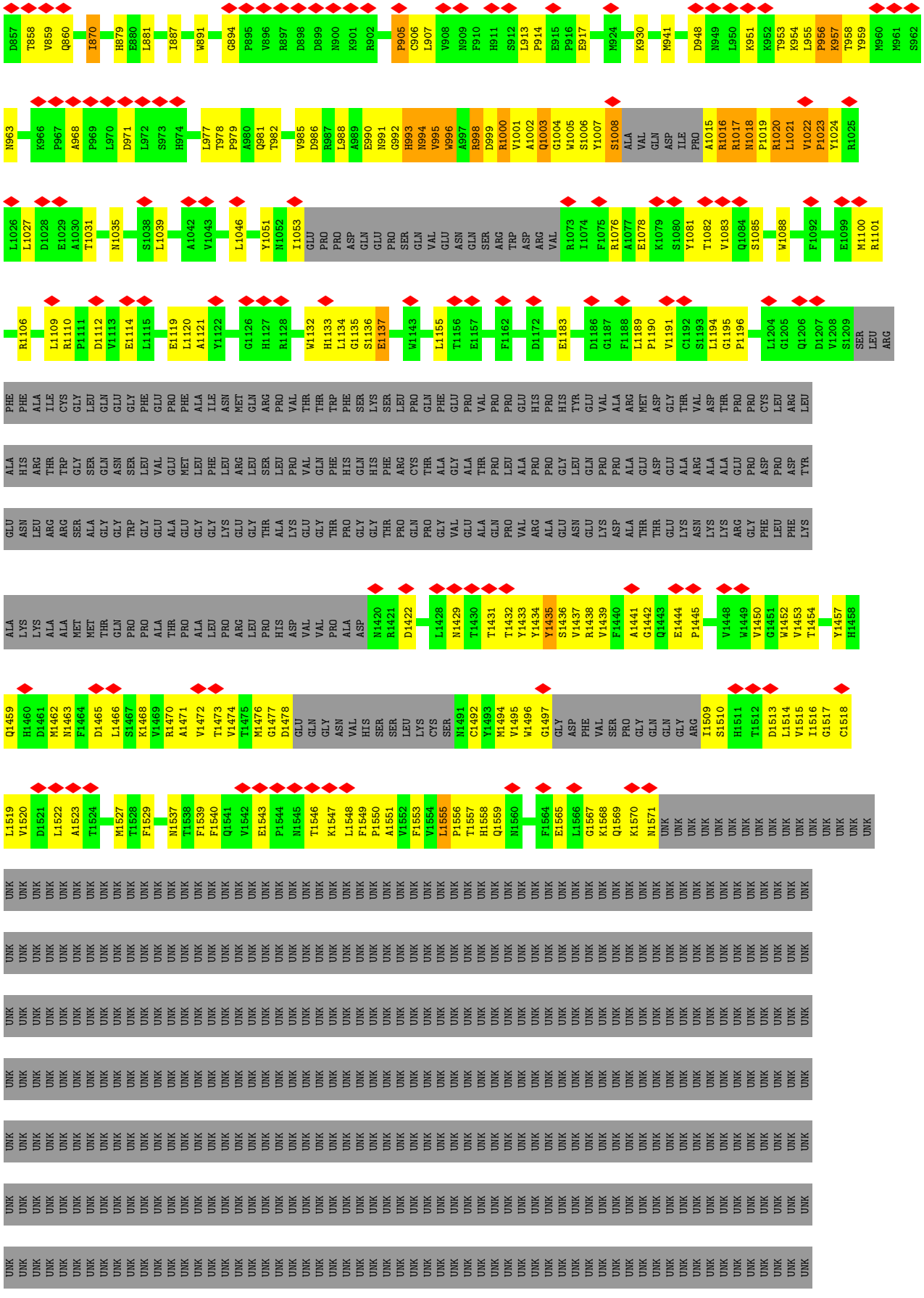


• Molecule 1: RYANODINE RECEPTOR 1

Chain C:

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N963 K966 P967 A968 P969 L970 D971 L972 S973 H974 L977 T978 P979 A980 Q981 T982 V985 D986 R987 L988 A989 E990 N991 G992 H993 N994 V995 W996 A997 R998 D999 R1000 V1001 A1002 Q1003 G1004 W1005 S1006 Y1007 S1008 ALA VAL GLN ASP ILE PRO A1015 R1016 R1017 N1018 P1019 R1020 L1021 V1022 P1023 Y1024 R1025
L1026 L1027 D1028 E1029 A1030 T1031 N1035 S1038 L1039 A1042 V1043 L1046 Y1051 N1052 I1053 GLU PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP ASP ARG VAL R1073 I1074 F1075 R1076 A1077 E1078 K1079 S1080 Y1081 T1082 V1083 Q1084 S1085 W1088 F1092 E1099 M1100 R1101
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PHE PHE ALA ILE CYS GLY LEU GLN GLU GLY PHE GLU PRO PHE ALA ILE ASN MET GLN ARG PRO VAL THR THR TRP PHE SER LYS SER LEU PRO GLN PHE GLU PRO VAL PRO PRO GLU HIS PRO HIS TYR GLU VAL ALA ARG MET ASP GLY THR VAL ASP THR PRO PRO CYS LEU ARG LEU
ALA HIS ARG THR TRP GLY SER GLN ASN SER LEU VAL GLU MET LEU PHE LEU ARG LEU SER LEU PRO VAL GLN PHE HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR
GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLN PRO GLY GLY THR 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 N1429 T1430 T1431 T1432 Y1433 Y1434 Y1435 S1436 V1437 R1438 V1439 F1440 A1441 G1442 Q1443 E1444 P1445 V1448 W1449 V1450 G1451 W1452 V1453 T1454 Y1457 H1458
Q1459 H1460 D1461 M1462 N1463 F1464 D1465 L1466 S1467 K1468 V1469 R1470 A1471 V1472 T1473 V1474 T1475 M1476 G1477 D1478 GLU GLN GLY ASN VAL HIS SER SER LEU LYS CYS SER N1491 C1492 Y1493 M1494 V1495 W1496 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG I1509 S1510 H1511 T1512 D1513 L1514 V1515 I1516 G1517 C1518
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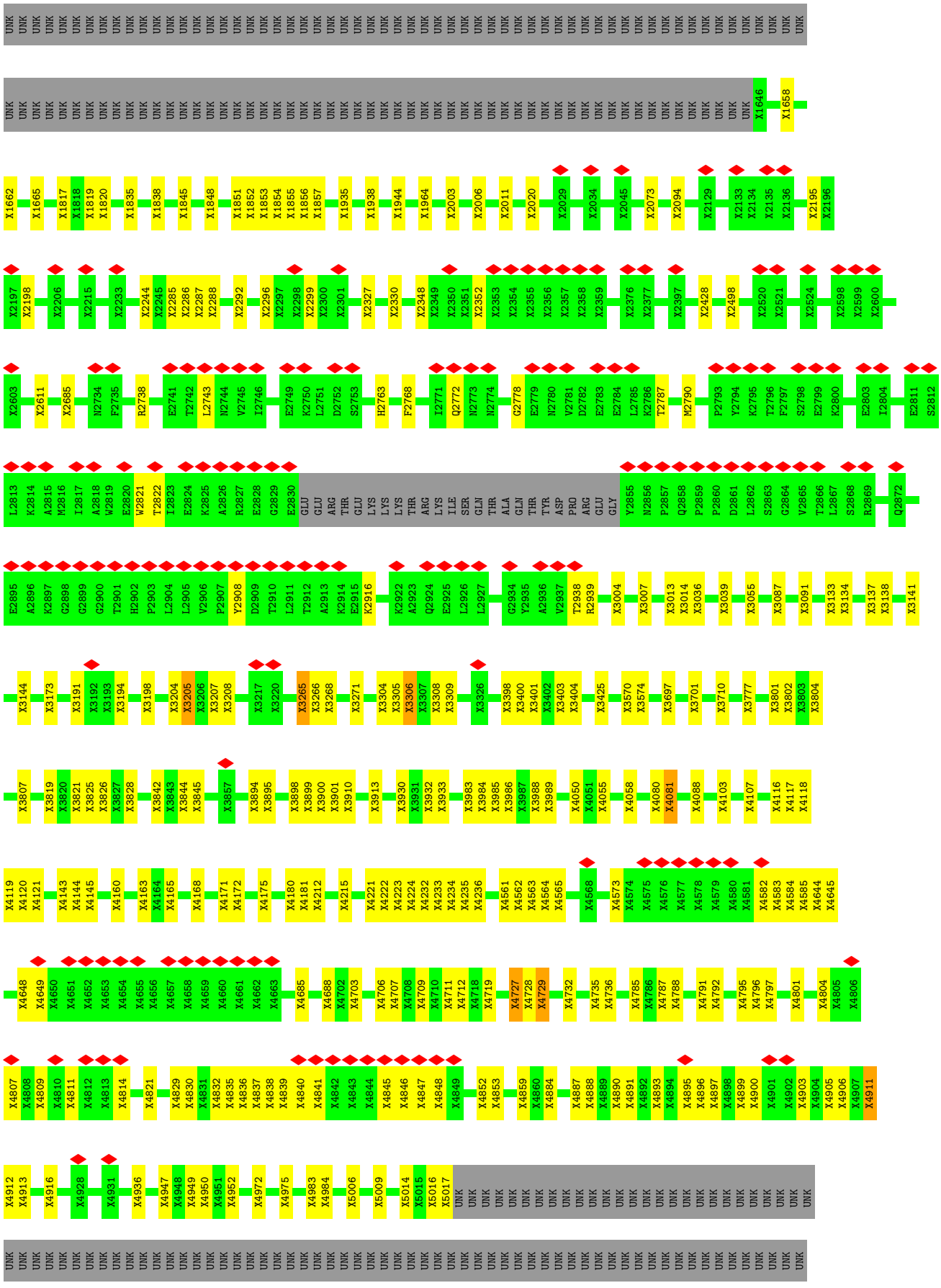
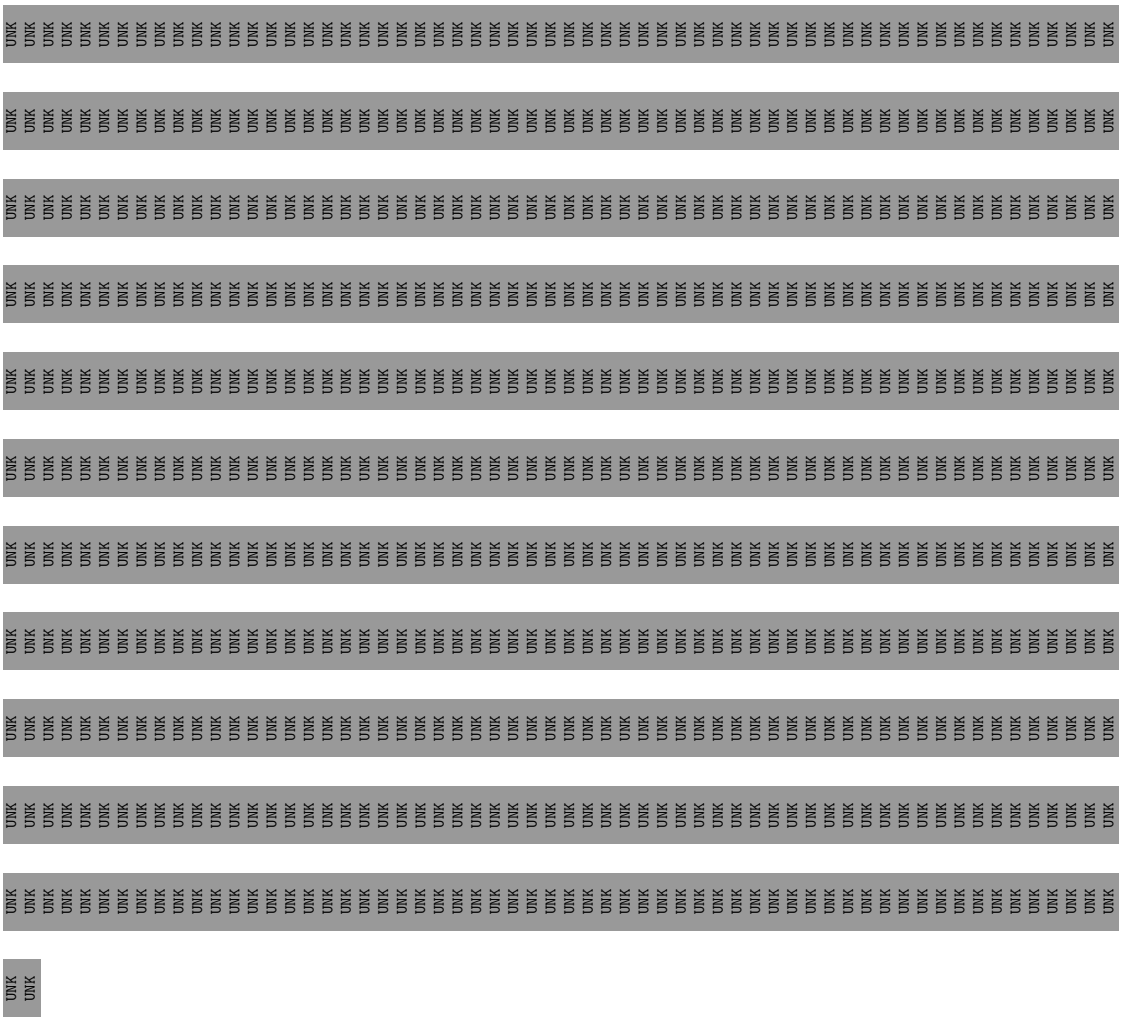
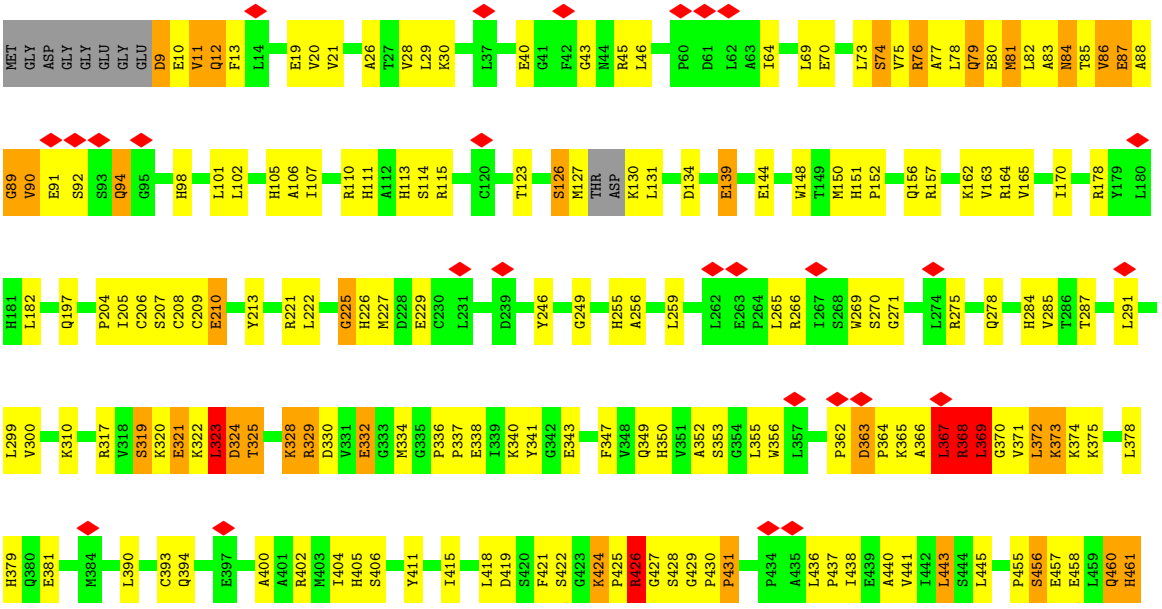
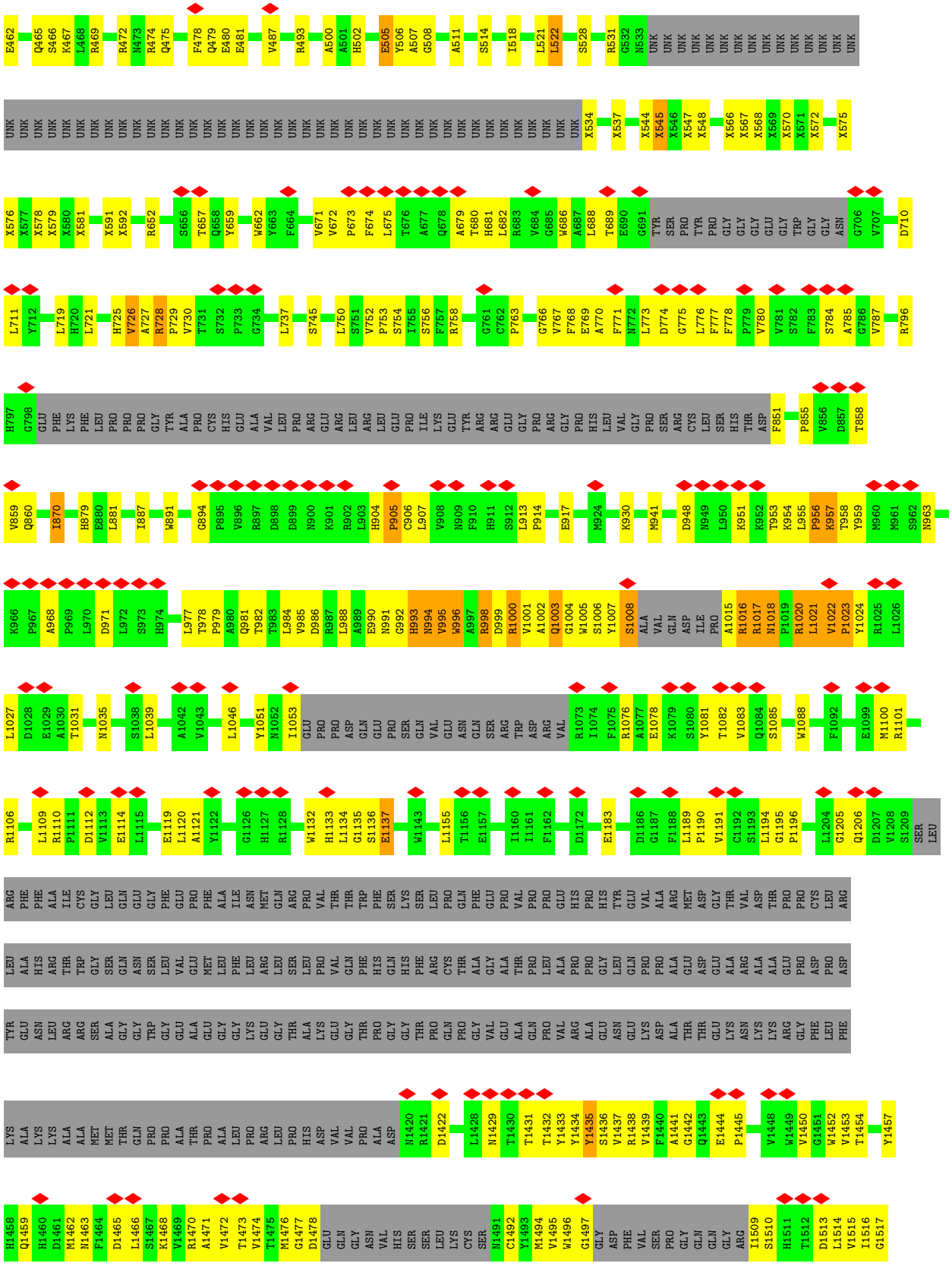




• Molecule 1: RYANODINE RECEPTOR 1

Chain D:

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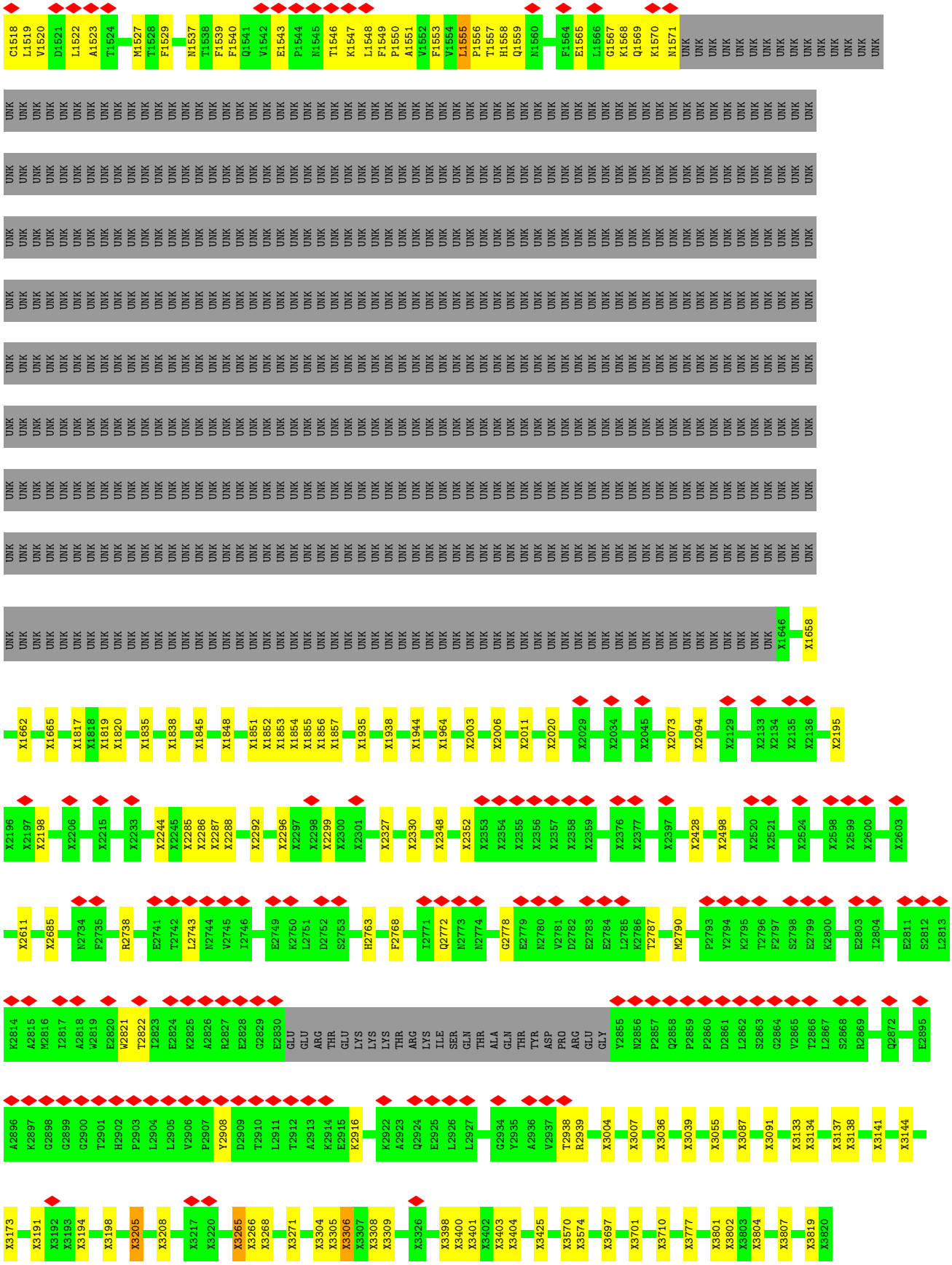
X534 X537 X544 X545 X546 X547 X548 X566 X567 X568 X569 X570 X571 X572 X575
X576 X577 X578 X579 X580 X581 X591 X592 R652 S656 T657 Q658 Y659 W662 Y663 F664 V671 V672 P673 F674 L675 T676 A677 Q678 A679 T680 H681 L682 R683 V684 G685 W686 A687 L688 T689 E690 G691 TYR SER PRO TYR PRO GLY GLY GLU GLU GLY TRP GLY GLY ASN G706 V707 D710
L711 Y712 L719 H720 L721 H725 V726 A727 R728 P729 V730 T731 S732 P733 G734 L737 S745 L750 S751 V752 P753 S754 I755 S756 F757 R758 G761 C762 P763 G766 V767 F768 E769 A770 F771 N772 L773 D774 G775 L776 F777 F778 P779 V780 V781 S782 F783 S784 A785 G786 V787 R796
H797 G798 GLU PHE LYS PHE LEU PRO PRO PRO GLY TYR ALA PRO CYS HIS GLU ALA VAL LEU PRO ARG GLU ARG LEU ARG LEU GLU PRO ILE LYS GLU TYR ARG ARG GLU GLY PRO ARG GLY PRO HIS LEU VAL GLY PRO SER ARG CYS LEU SER HIS THR ASP F851 P855 V856 D857 T858
V859 Q860 I870 H879 E880 L881 I887 W891 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E917 M924 K930 M941 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963
K966 P967 A968 P969 L970 D971 L972 S973 H974 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 A989 E990 N991 G992 H993 N994 V995 W996 A997 R998 D999 R1000 V1001 A1002 Q1003 G1004 W1005 S1006 Y1007 S1008 ALA VAL GLN ASP ILE PRO A1015 R1016 R1017 N1018 P1019 R1020 L1021 V1022 P1023 Y1024 R1025 L1026
L1027 D1028 E1029 A1030 T1031 N1035 S1038 L1039 A1042 V1043 L1046 Y1051 N1052 I1053 GLU PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP ASP ARG VAL R1073 I1074 F1075 R1076 A1077 E1078 K1079 S1080 Y1081 T1082 V1083 Q1084 S1085 W1088 F1092 E1099 M1100 R1101
R1106 L1109 R1110 P1111 D1112 Y1113 E1114 L1115 E1119 L1120 A1121 Y1122 G1126 H1127 R1128 W1132 H1133 L1134 G1135 S1136 E1137 W1143 L1155 T1156 E1157 I1160 I1161 F1162 D1172 E1183 D1186 G1187 F1188 L1189 P1190 V1191 C1192 S1193 L1194 G1195 P1196 L1204 G1205 Q1206 D1207 V1208 S1209 SER LEU
ARG PHE PHE ALA ILE CYS GLY LEU GLN GLU GLY PHE GLU PRO PHE ALA ILE ASN MET GLN ARG PRO VAL THR THR TRP PHE SER LYS SER LEU PRO GLN PHE GLU PRO VAL PRO PRO GLU HIS PRO HIS TYR GLU VAL ALA ARG MET ASP GLY THR VAL ASP THR PRO PRO CYS LEU ARG
LEU ALA HIS ARG THR TRP GLY SER GLN ASN SER LEU VAL GLU MET LEU PHE LEU ARG LEU SER LEU PRO VAL GLN PHE HIS GLN HIS PHE ARG CYS THR ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN LEU ALA PRO PRO ALA 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 PRO ALA THR PRO ALA ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 R1421 D1422 L1428 N1429 T1430 T1431 T1432 Y1433 Y1434 Y1435 S1436 V1437 R1438 V1439 F1440 A1441 G1442 Q1443 E1444 P1445 V1448 W1449 V1450 G1451 W1452 V1453 T1454 Y1457
H1458 Q1459 H1460 D1461 M1462 N1463 F1464 D1465 L1466 S1467 K1468 V1469 R1470 A1471 V1472 T1473 V1474 T1475 M1476 G1477 D1478 GLU GLN GLY ASN VAL HIS SER SER LEU LYS CYS SER N1491 C1492 Y1493 M1494 V1495 W1496 G1497 GLY ASP PHE VAL SER PRO GLY GLN GLN GLY ARG I1509 S1510 H1511 T1512 D1513 L1514 V1515 I1516 G1517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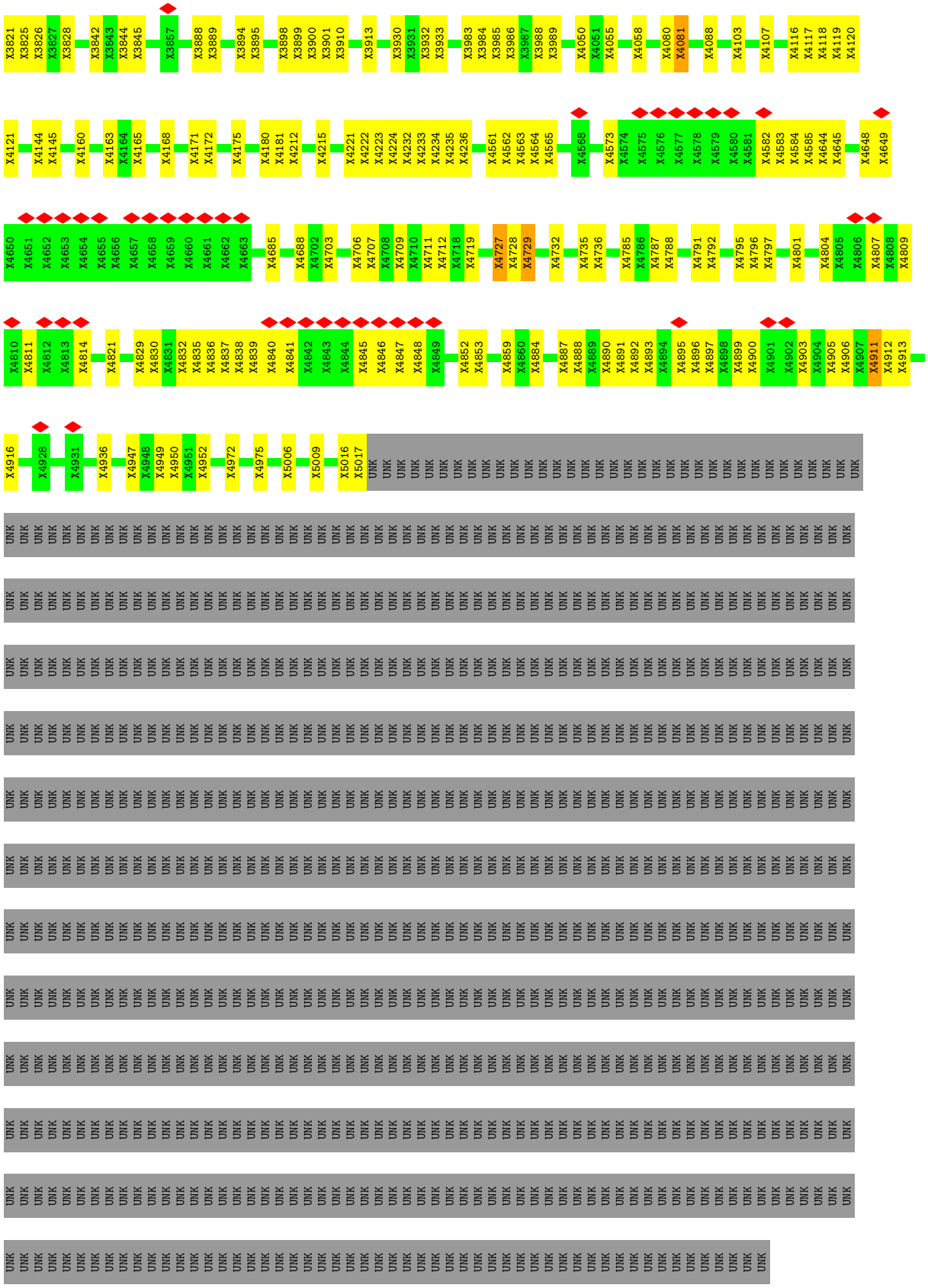
UNK
X1646 X1658
X1662 X1665 X1817 X1818 X1819 X1820 X1835 X1838 X1845 X1848 X1851 X1852 X1853 X1854 X1855 X1856 X1857 X1935 X1938 X1944 X1964 X2003 X2006 X2011 X2020 X2029 X2034 X2045 X2073 X2094 X2129 X2133 X2134 X2135 X2136 X2195
X2196 X2197 X2198 X2206 X2215 X2233 X2244 X2245 X2285 X2286 X2287 X2288 X2292 X2296 X2297 X2298 X2299 X2300 X2301 X2327 X2330 X2348 X2352 X2353 X2354 X2355 X2356 X2357 X2358 X2359 X2376 X2377 X2397 X2428 X2498 X2520 X2521 X2524 X2598 X2599 X2600 X2603
X2611 X2685 N2734 F2735 R2738 E2741 T2742 L2743 N2744 V2745 I2746 E2749 K2750 L2751 D2752 S2753 H2763 F2768 I2771 Q2772 N2773 N2774 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 M2790 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 E2803 I2804 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 Q2872 E2895
A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 K2922 A2923 Q2924 E2925 L2926 L2927 G2934 Y2935 A2936 V2937 T2938 R2939 X3004 X3007 X3036 X3039 X3055 X3087 X3091 X3133 X3134 X3137 X3138 X3141 X3144
X3173 X3191 X3192 X3193 X3194 X3198 X3205 X3208 X3217 X3220 X3265 X3266 X3268 X3271 X3304 X3305 X3306 X3307 X3308 X3309 X3326 X3398 X3400 X3401 X3402 X3403 X3404 X3425 X3570 X3574 X3697 X3701 X3710 X3777 X3801 X3802 X3803 X3804 X3807 X3819 X3820


X3821 X3825 X3826 X3827 X3828 X3842 X3843 X3844 X3845 X3867 X3888 X3889 X3894 X3895 X3898 X3899 X3900 X3901 X3910 X3913 X3930 X3931 X3932 X3933 X3983 X3984 X3985 X3986 X3987 X3988 X3989 X4050 X4051 X4055 X4058 X4080 X4081 X4088 X4103 X4107 X4116 X4117 X4118 X4119 X4120
X4121 X4144 X4145 X4160 X4163 X4164 X4165 X4168 X4171 X4172 X4175 X4180 X4181 X4212 X4215 X4221 X4222 X4223 X4224 X4232 X4233 X4234 X4235 X4236 X4561 X4562 X4563 X4564 X4565 X4568 X4573 X4574 X4575 X4576 X4577 X4578 X4579 X4580 X4581 X4582 X4583 X4584 X4585 X4644 X4645 X4648 X4649
X4650 X4651 X4652 X4653 X4654 X4655 X4656 X4657 X4658 X4659 X4660 X4661 X4662 X4663 X4685 X4688 X4702 X4703 X4706 X4707 X4708 X4709 X4710 X4711 X4712 X4718 X4719 X4727 X4728 X4729 X4732 X4735 X4736 X4785 X4786 X4787 X4788 X4791 X4792 X4795 X4796 X4797 X4801 X4804 X4805 X4806 X4807 X4808 X4809
X4810 X4811 X4812 X4813 X4814 X4821 X4829 X4830 X4831 X4832 X4835 X4836 X4837 X4838 X4839 X4840 X4841 X4842 X4843 X4844 X4845 X4846 X4847 X4848 X4849 X4852 X4853 X4859 X4860 X4884 X4887 X4888 X4889 X4890 X4891 X4892 X4893 X4894 X4895 X4896 X4897 X4898 X4899 X4900 X4901 X4902 X4903 X4904 X4905 X4906 X4907 X4911 X4912 X4913
X4916 X4928 X4931 X4936 X4947 X4948 X4949 X4950 X4951 X4952 X4972 X4975 X5006 X5009 X5016 X5017 UNK
UNK

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	94354	Depositor
Resolution determination method	Not provided	
CTF correction method	FULL CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	58610	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	9.766	Depositor
Minimum map value	-8.403	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.324	Depositor
Recommended contour level	1.31	Depositor
Map size (Å)	580.16, 580.16, 580.16	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.59, 2.59, 2.59	Depositor

5 Model quality

5.1 Standard geometry

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	0.40	2/10556 (0.0%)	0.61	11/14313 (0.1%)
1	B	0.40	2/10556 (0.0%)	0.61	11/14313 (0.1%)
1	C	0.40	2/10556 (0.0%)	0.61	11/14313 (0.1%)
1	D	0.40	2/10556 (0.0%)	0.61	11/14313 (0.1%)
All	All	0.40	8/42224 (0.0%)	0.61	44/57252 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	12
1	C	0	13
1	D	0	13
All	All	0	50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	CYS	C-N	13.92	1.66	1.34
1	C	209	CYS	C-N	13.92	1.66	1.34
1	D	209	CYS	C-N	13.92	1.66	1.34
1	B	209	CYS	C-N	13.90	1.66	1.34
1	A	394	GLN	C-N	11.34	1.60	1.34

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	367	LEU	CA-CB-CG	11.70	142.21	115.30
1	A	367	LEU	CA-CB-CG	11.68	142.16	115.30
1	D	367	LEU	CA-CB-CG	11.68	142.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	CYS	O-C-N	-11.67	104.02	122.70
1	B	367	LEU	CA-CB-CG	11.66	142.11	115.30

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3055	UNK	Peptide
1	A	3205	UNK	Peptide
1	A	3265	UNK	Mainchain
1	A	545	UNK	Peptide
1	A	88	ALA	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	20400	0	12256	1263	0
1	B	20400	0	12257	1265	0
1	C	20400	0	12256	1268	0
1	D	20400	0	12255	1263	0
All	All	81600	0	49024	4945	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 38.

The worst 5 of 4945 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:956:PRO:HG3	1:D:959:TYR:CZ	1.25	1.70
1:A:657:THR:HG21	1:A:662:TRP:CE3	1.15	1.68
1:C:956:PRO:HG3	1:C:959:TYR:CZ	1.25	1.65
1:D:657:THR:HG21	1:D:662:TRP:CD2	1.31	1.65
1:B:956:PRO:CD	1:B:959:TYR:CD2	1.74	1.64

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	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	5	31
1	B	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	5	31
1	C	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	5	31
1	D	1280/5037 (25%)	1175 (92%)	71 (6%)	34 (3%)	5	31
All	All	5120/20148 (25%)	4700 (92%)	284 (6%)	136 (3%)	8	31

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	368	ARG
1	A	393	CYS
1	A	425	PRO
1	A	426	ARG

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	1112/1410 (79%)	1055 (95%)	57 (5%)	24	48
1	B	1112/1410 (79%)	1055 (95%)	57 (5%)	24	48
1	C	1112/1410 (79%)	1055 (95%)	57 (5%)	24	48
1	D	1112/1410 (79%)	1055 (95%)	57 (5%)	24	48
All	All	4448/5640 (79%)	4220 (95%)	228 (5%)	27	48

5 of 228 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	10	GLU
1	D	1017	ARG
1	C	369	LEU
1	D	1008	SER
1	D	368	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	151	HIS
1	C	963	ASN
1	D	1558	HIS
1	C	226	HIS
1	C	412	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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
1	A	96
1	B	96
1	D	96
1	C	96

The worst 5 of 384 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1863:UNK	C	1935:UNK	N	104.73
1	B	1863:UNK	C	1935:UNK	N	104.73
1	D	1863:UNK	C	1935:UNK	N	104.73
1	C	1863:UNK	C	1935:UNK	N	104.72
1	A	2939:ARG	C	2953:UNK	N	48.34

6 Map visualisation

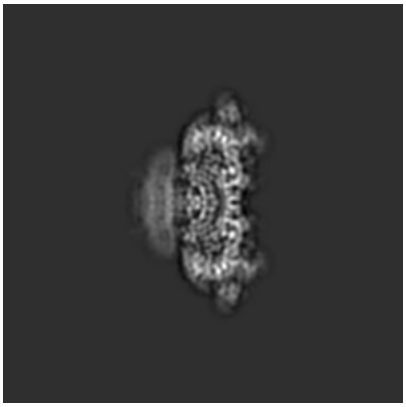
This section contains visualisations of the EMDB entry EMD-2752. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

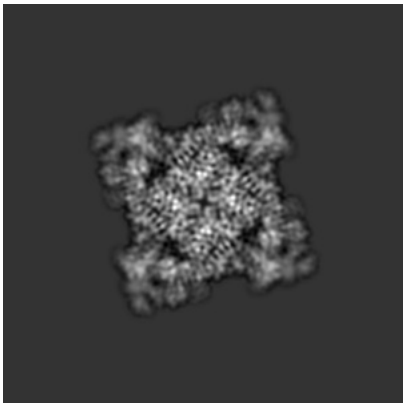
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



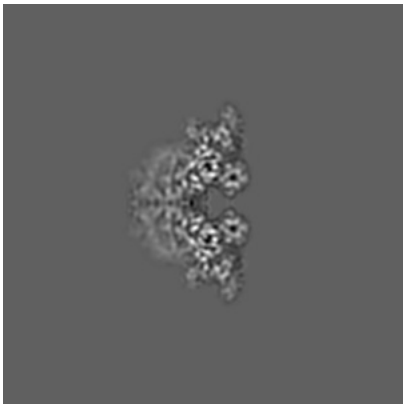
Z

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

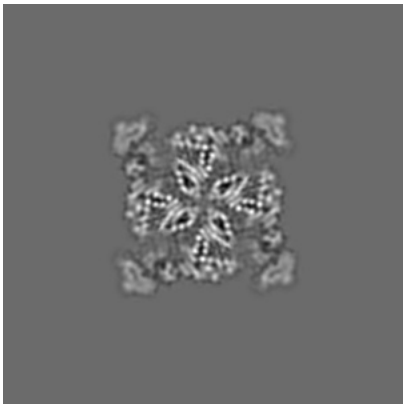
6.2 Central slices

6.2.1 Primary map

X Index: 112



Y Index: 112



Z Index: 112

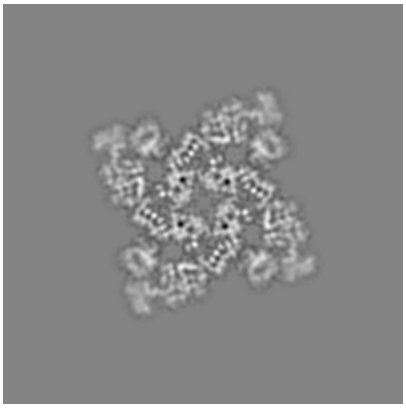
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 99

Y Index: 125

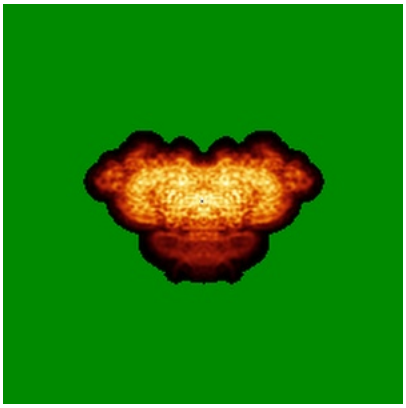


Z Index: 123

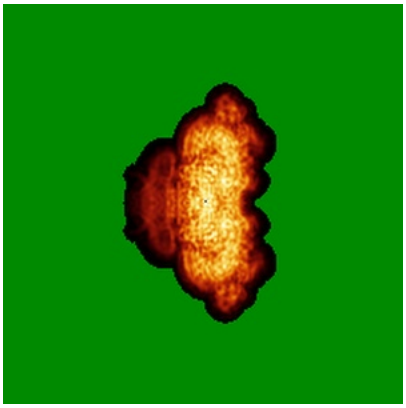
The images above show the largest variance slices of the map in three orthogonal directions.

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

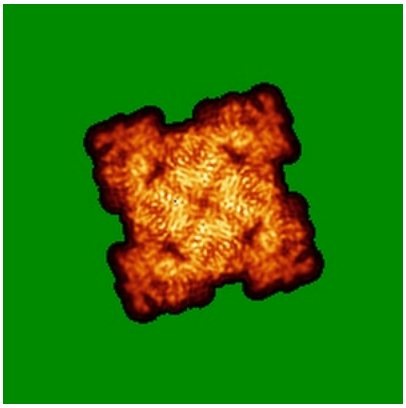
6.4.1 Primary map



X



Y

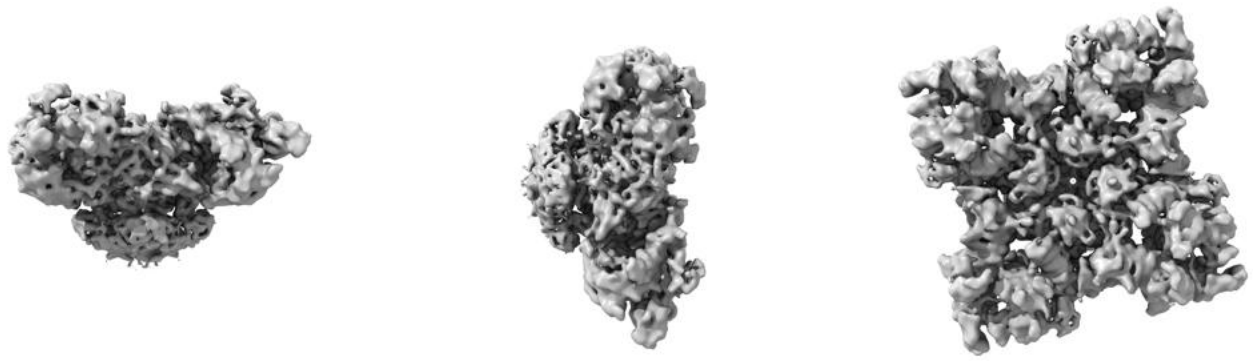


Z

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

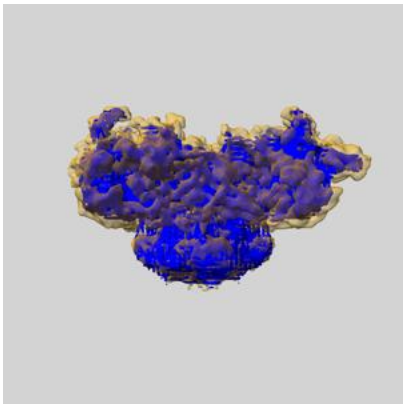
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

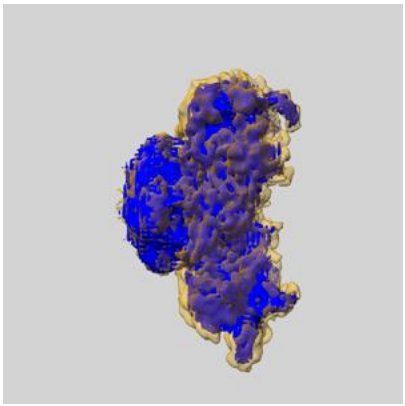
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

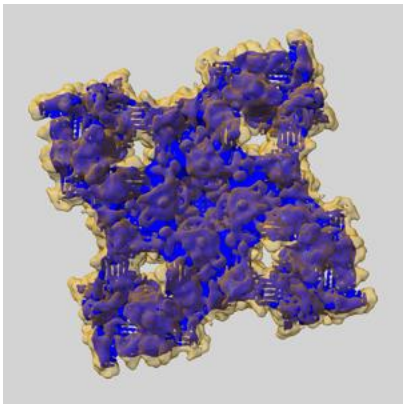
6.6.1 emd_2752_msk_1.map (i)



X



Y

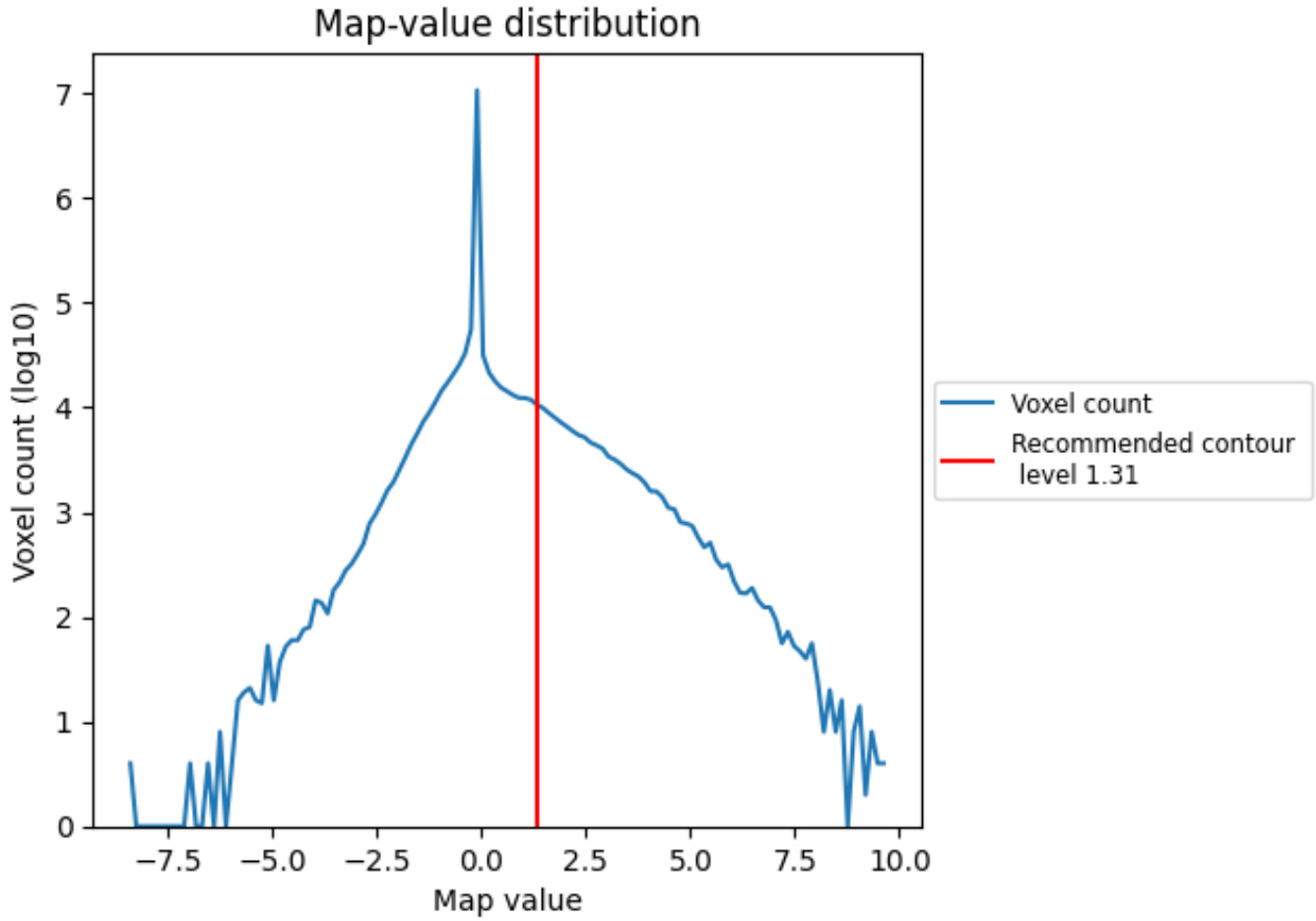


Z

7 Map analysis

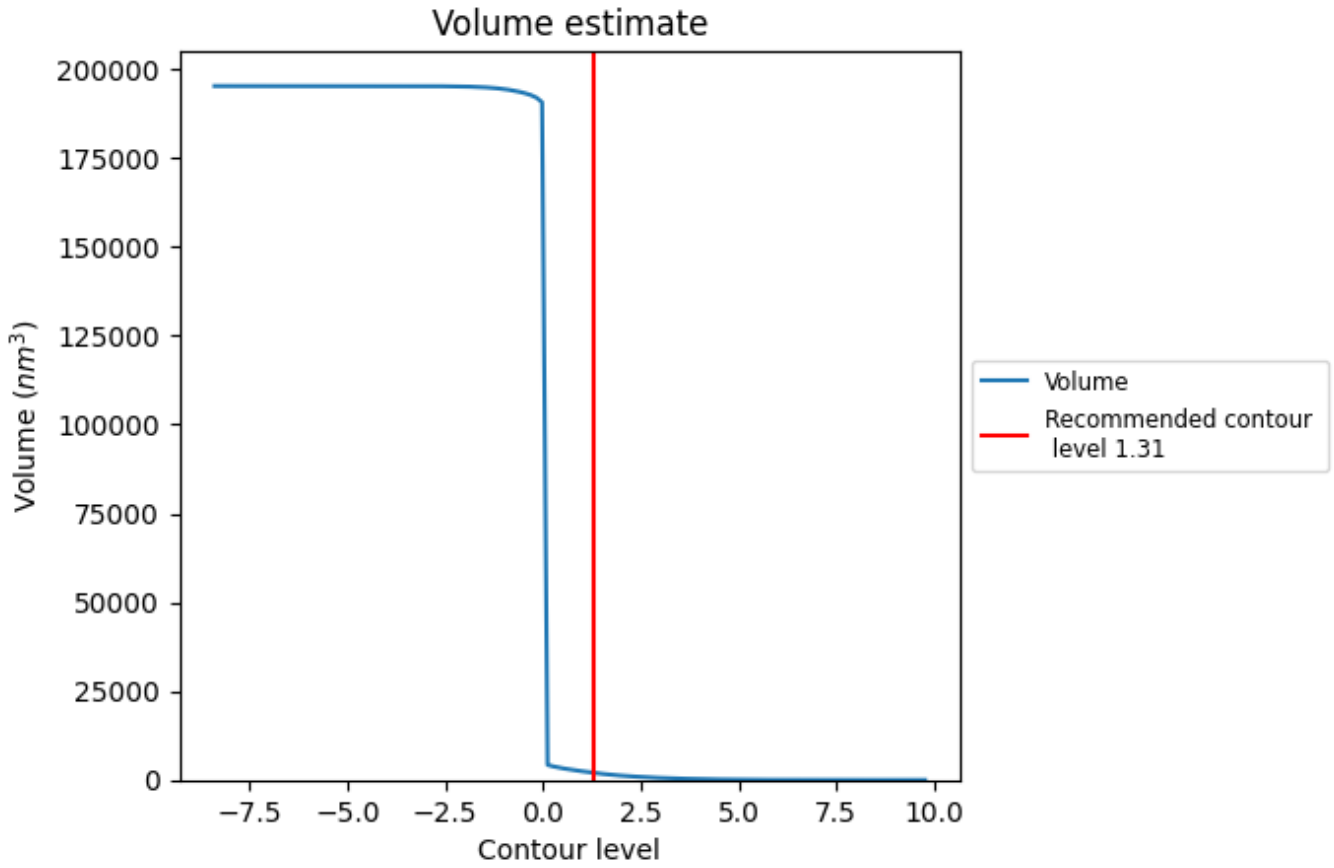
This section contains the results of statistical analysis of the map.

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.

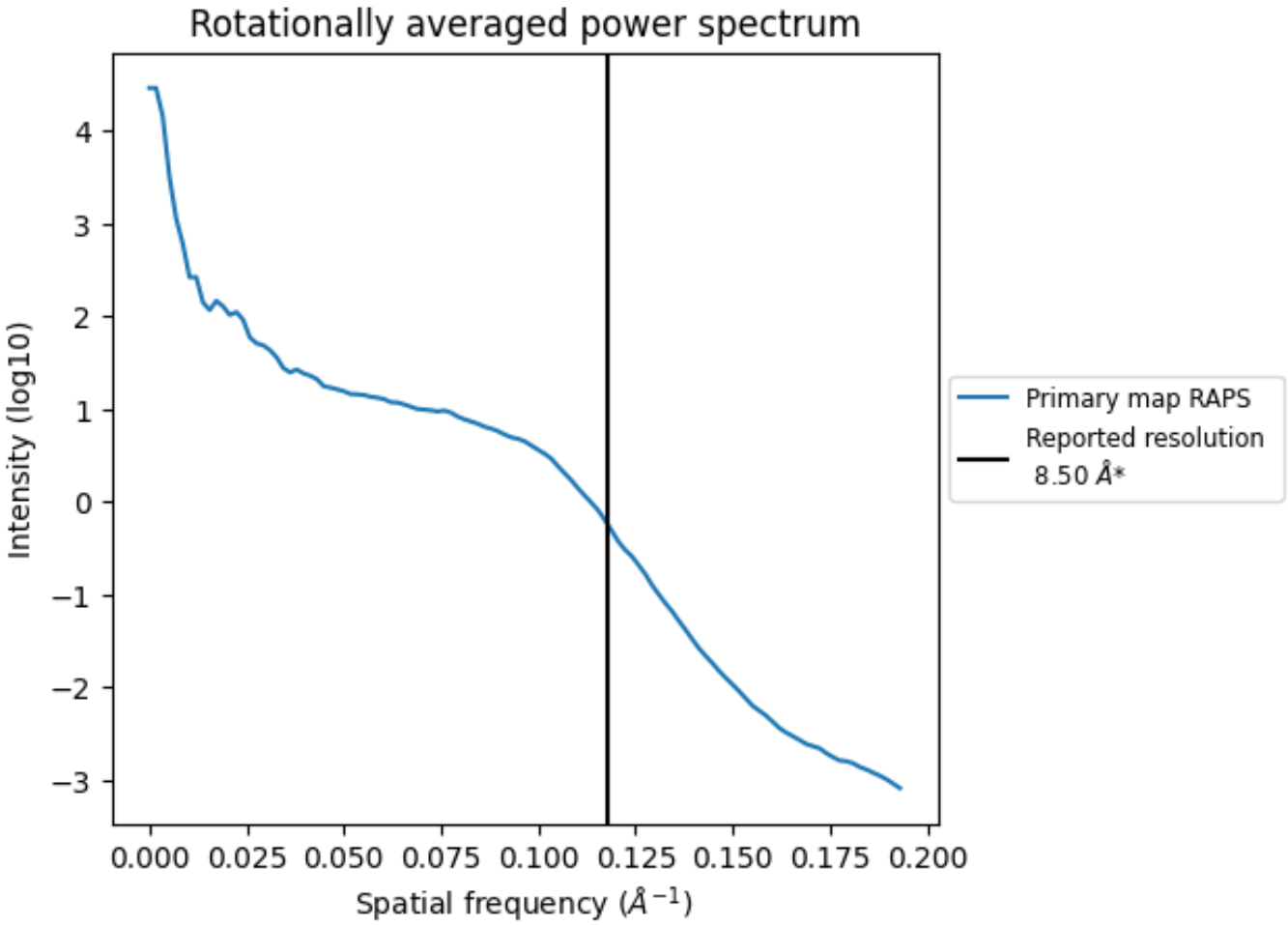
7.2 Volume estimate (i)



The volume at the recommended contour level is 1985 nm^3; this corresponds to an approximate mass of 1793 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)

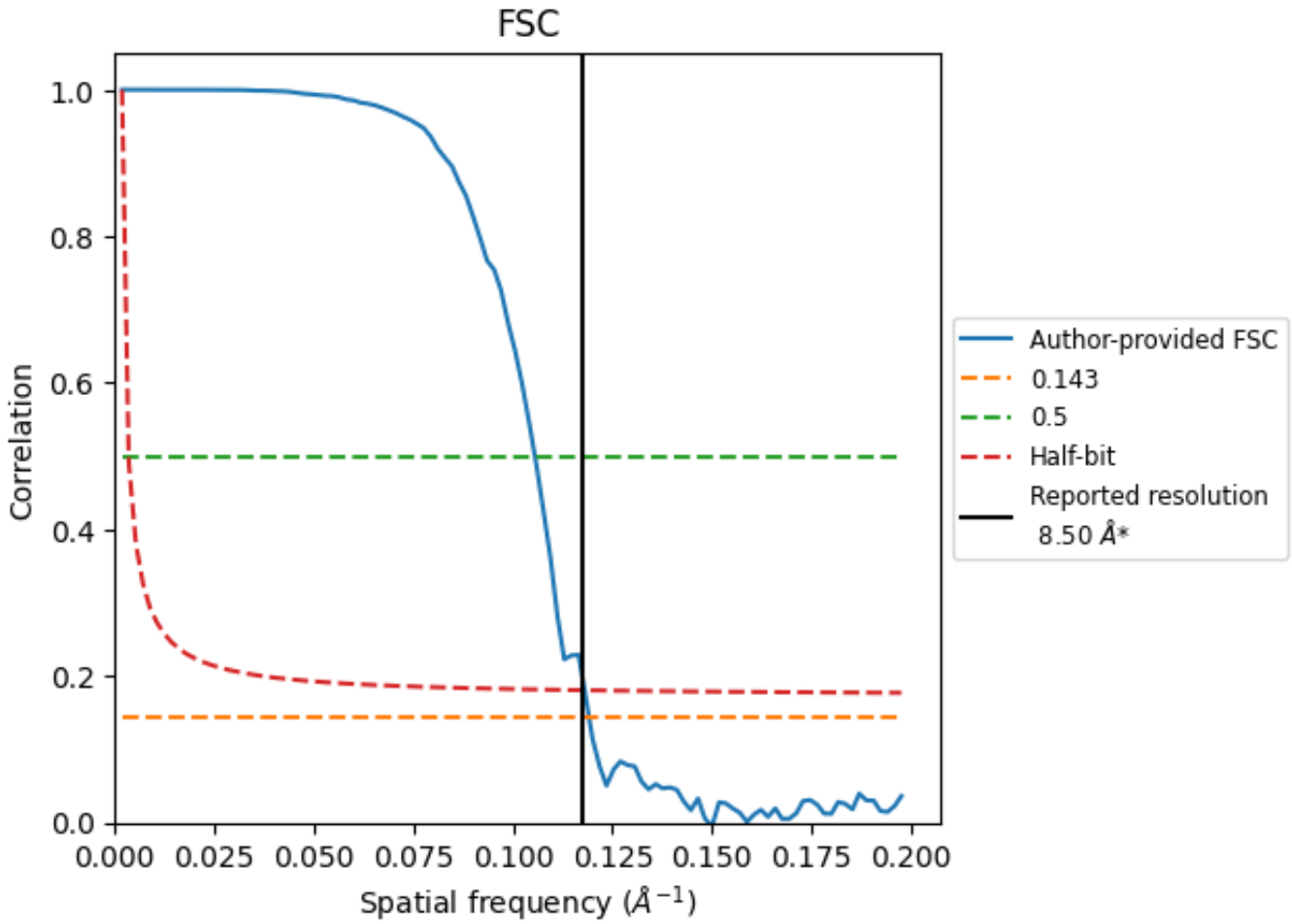


*Reported resolution corresponds to spatial frequency of 0.118 Å^{-1}

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 0.118 Å^{-1}

8.2 Resolution estimates (i)

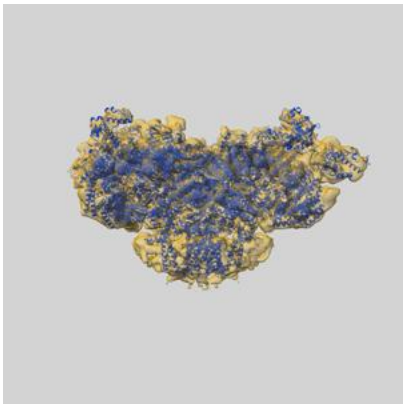
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	8.40	9.48	8.47
Unmasked-calculated*	-	-	-

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

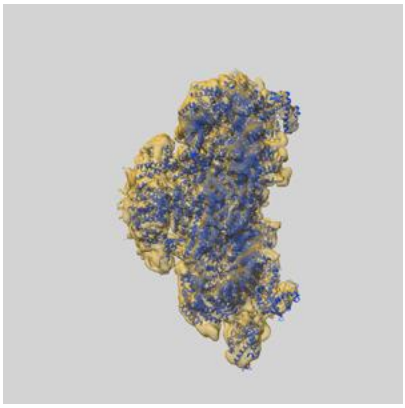
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2752 and PDB model 4UWE. Per-residue inclusion information can be found in section 3 on page 4.

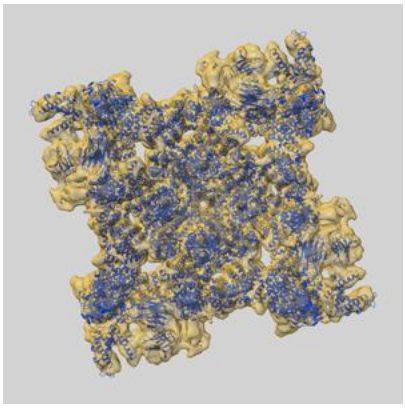
9.1 Map-model overlay



X



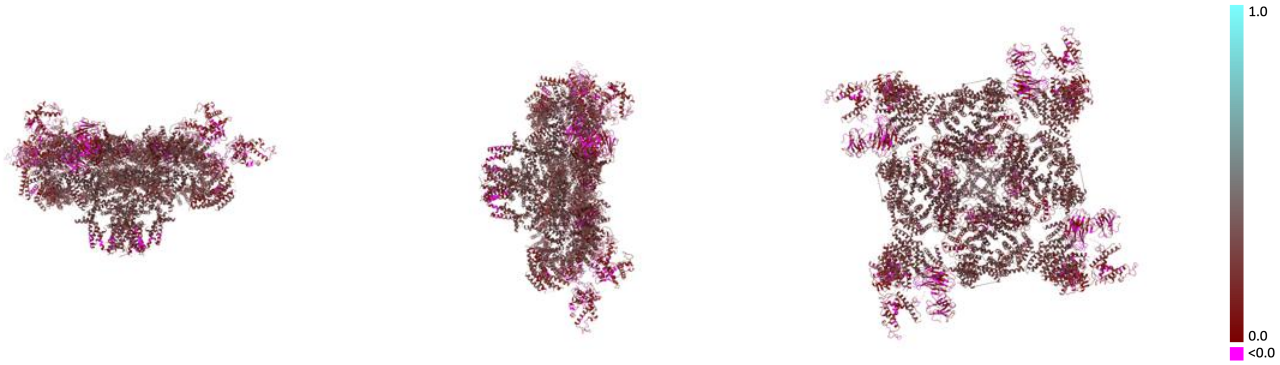
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.31 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.

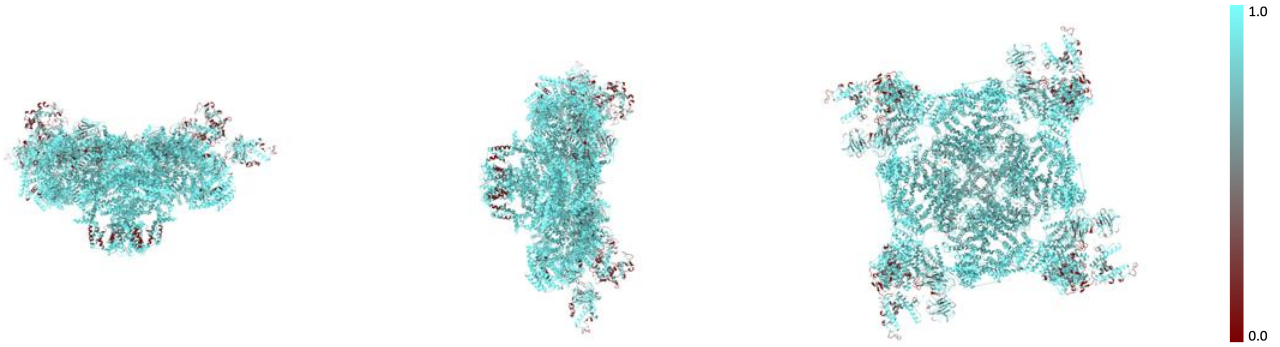
9.2 Q-score mapped to coordinate model (i)



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.

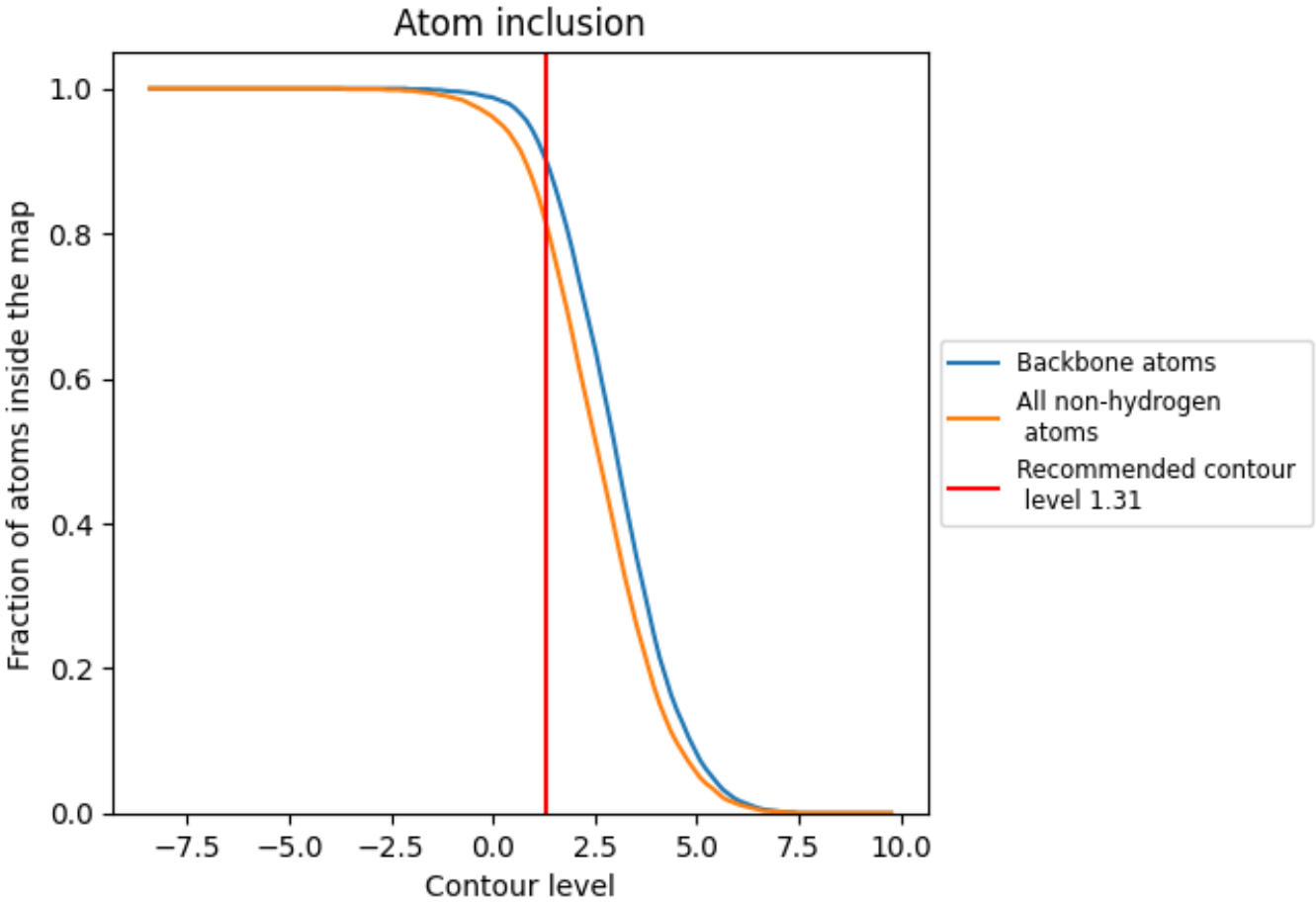
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.31).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (1.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8130	0.1850
A	0.8130	0.1850
B	0.8130	0.1850
C	0.8130	0.1850
D	0.8130	0.1850