wwPDB EM Validation Summary Report ⓘ

May 15, 2024 – 05:19 PM EDT

PDB ID	:	7K0S
EMDB ID	:	EMD-22615
Title	:	Cryo-EM structure of rabbit RyR1 in the presence of Mg2+ and AMP-PCP in nanodisc
Authors	:	Nayak, A.R.; Samso, M.
Deposited on	:	2020-09-05
Resolution	:	4.50 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:

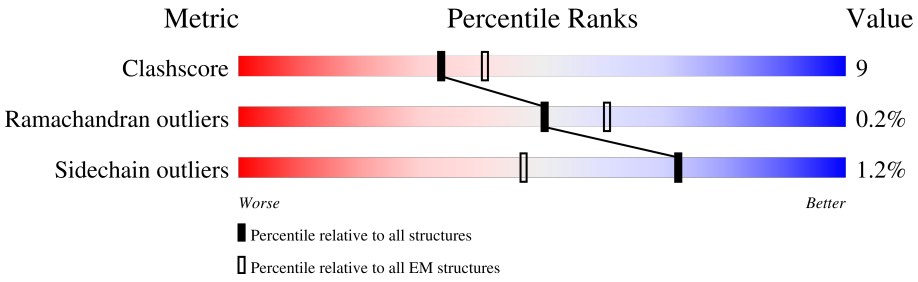
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.50 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	69% 12% 18%
1	B	5037	68% 13% 18%
1	C	5037	68% 13% 18%
1	D	5037	69% 13% 18%

2 Entry composition

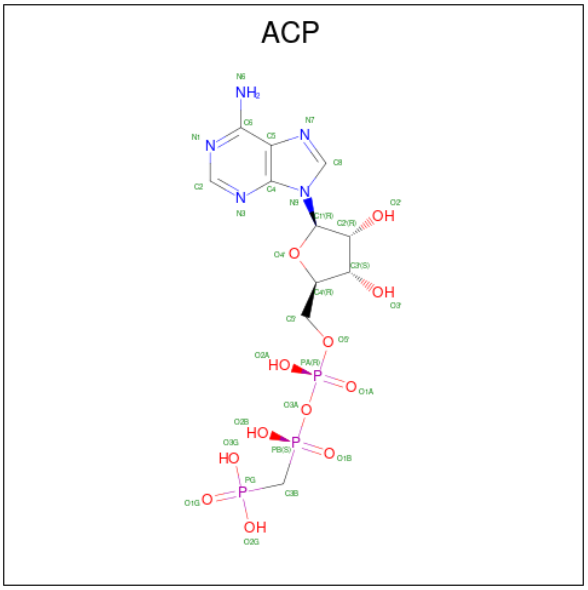
There are 4 unique types of molecules in this entry. The entry contains 115935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RyR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4110	Total	C	N	O	S	0	0
			28941	18335	5131	5318	157		
1	B	4110	Total	C	N	O	S	0	0
			28940	18334	5135	5315	156		
1	D	4110	Total	C	N	O	S	0	0
			28963	18348	5134	5324	157		
1	C	4110	Total	C	N	O	S	0	0
			28958	18354	5132	5317	155		

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	B	1	Total	C	N	O	P	0
			31	11	5	12	3	

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Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	N	O	P	0
			31	11	5	12	3	
2	C	1	Total	C	N	O	P	0
			31	11	5	12	3	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

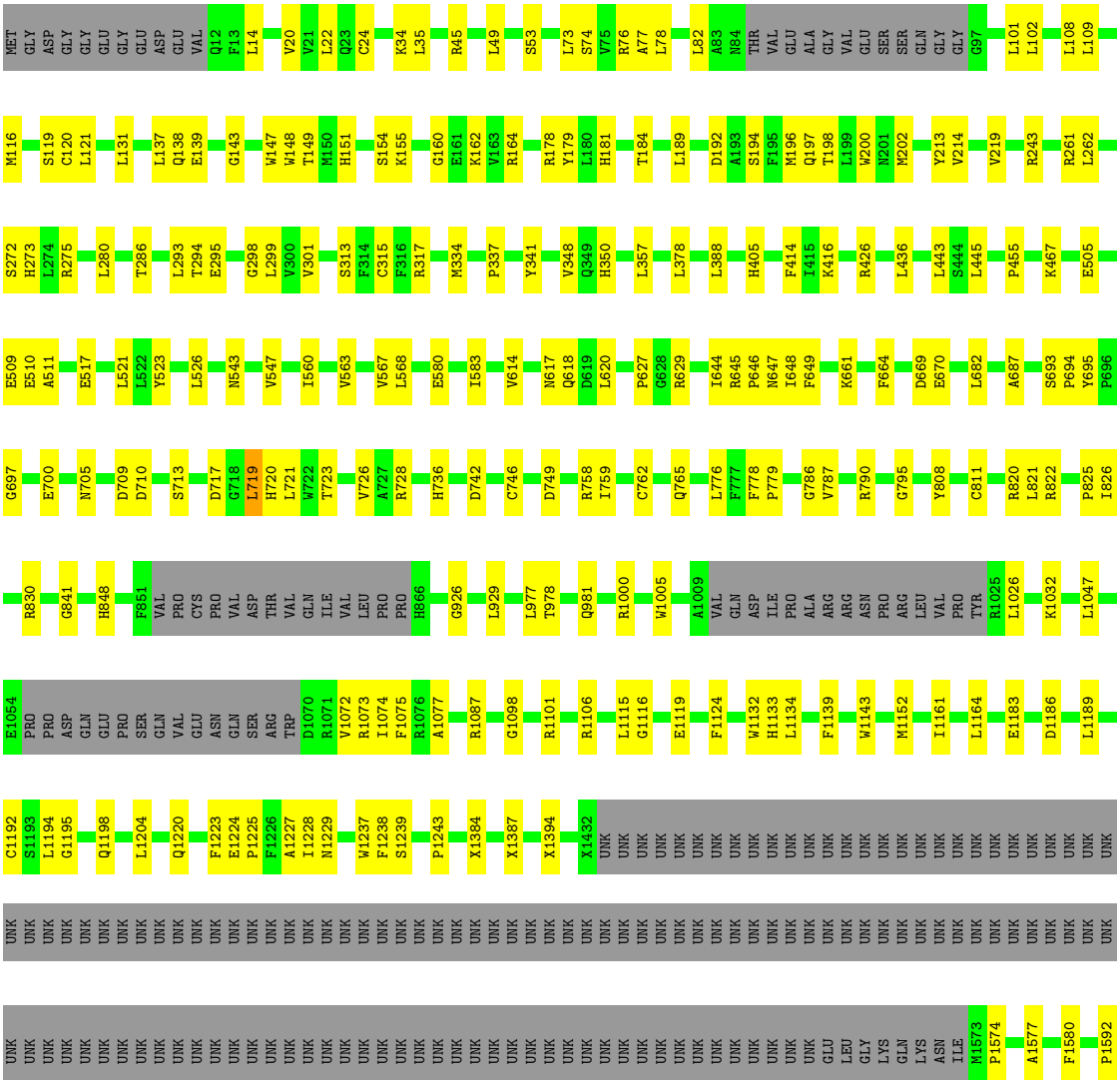
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	2	Total	Mg	0
			2	2	
4	D	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	

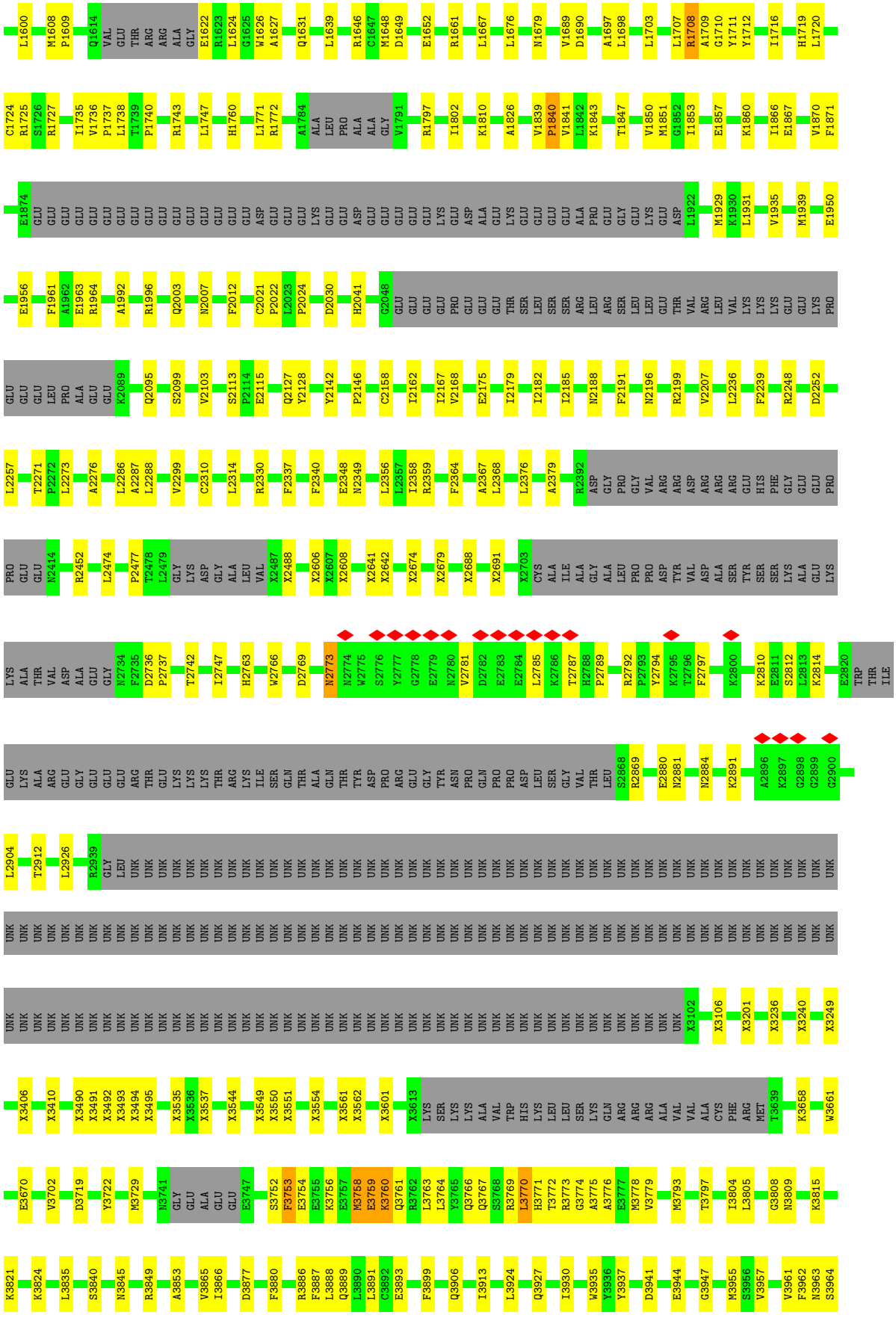
3 Residue-property plots (i)

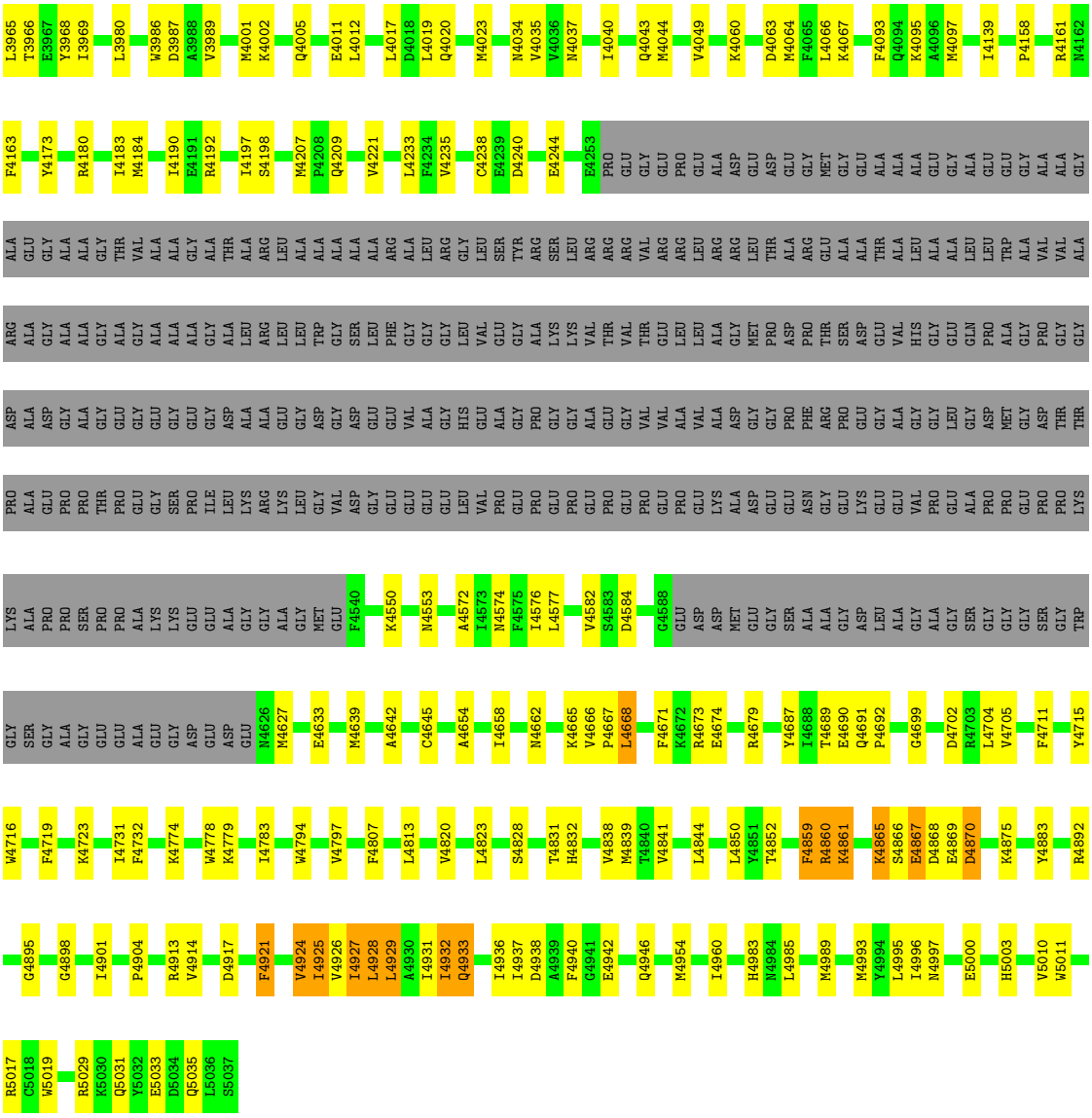
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RyR1

Chain A:

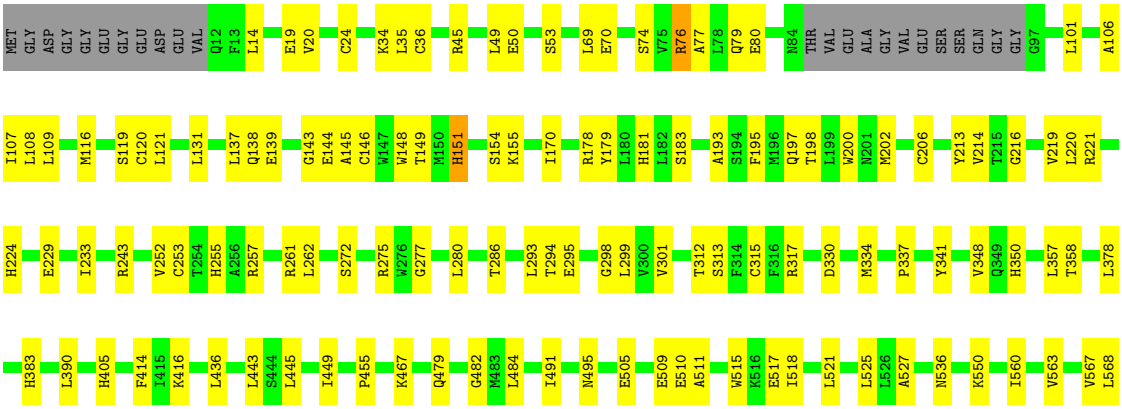


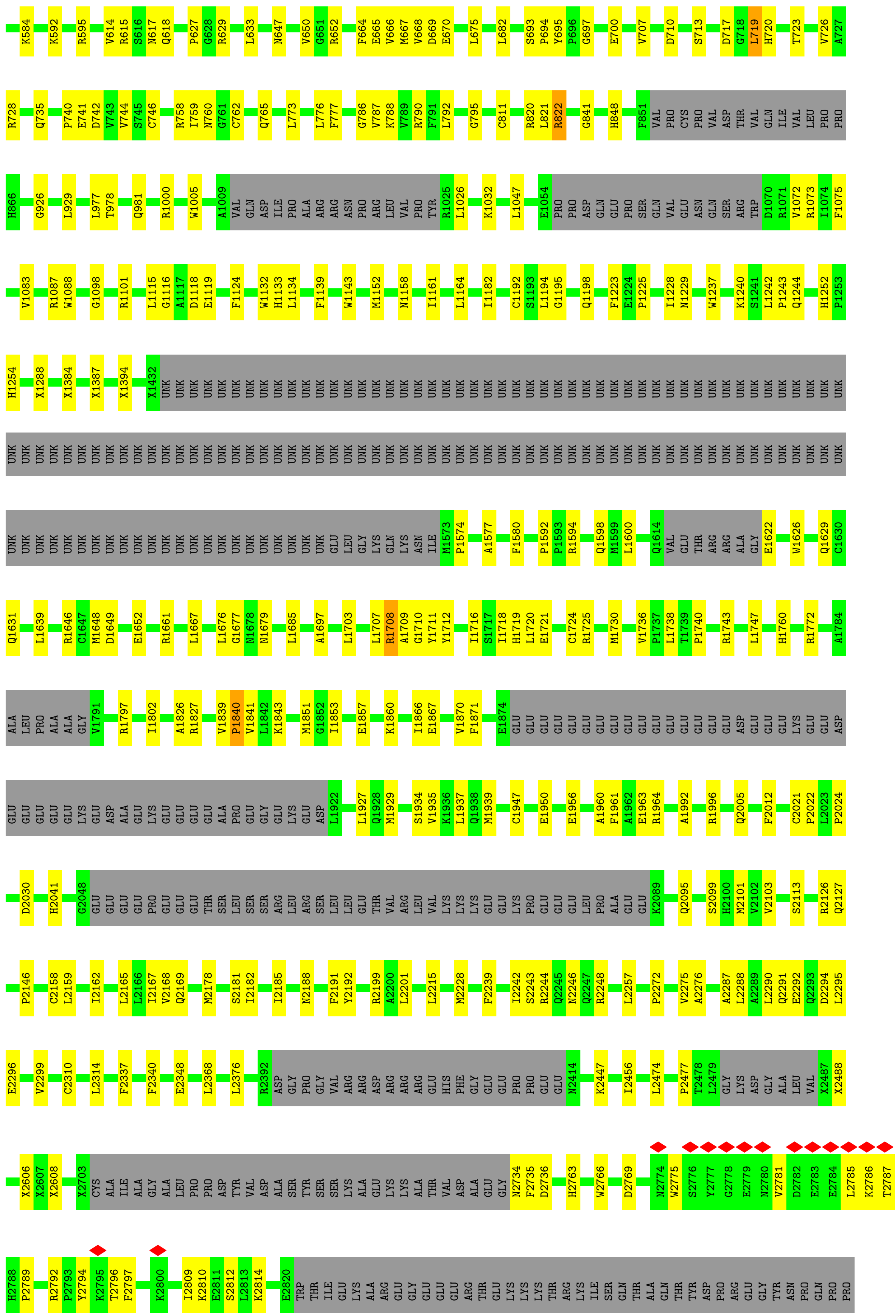




• Molecule 1: RyR1

Chain B:




K584 K592 R595 V614 R615 S616 N617 Q618 P627 G628 R629 L633 N647 V650 G651 R652 F664 E665 V666 M667 V668 D669 E670 L675 L682 S693 P694 Y695 P696 G697 E700 V707 D710 S713 D717 G718 L719 H720 T723 V726 A727
R728 Q735 P740 E741 D742 V743 V744 S745 C746 R758 I759 N760 G761 C762 Q765 L773 L776 F777 G786 V787 K788 V789 R790 F791 L792 G795 C811 R820 L821 R822 G841 H848 F851 VAL PRO CYS PRO VAL ASP THR VAL GLN ILE VAL LEU PRO PRO
H866 G926 L929 L977 T978 Q981 R1000 W1005 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO ARG LEU VAL PRO TYR R1025 L1026 K1032 L1047 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 I1074 F1075
V1083 R1087 W1088 G1098 R1101 L1115 G1116 A1117 D1118 E1119 F1124 W1132 H1133 L1134 F1139 W1143 M1152 N1158 I1161 L1164 I1182 C1192 S1193 L1194 G1195 Q1198 F1223 E1224 P1225 I1228 N1229 W1237 K1240 S1241 L1242 P1243 Q1244 H1252 P1253
H1254 X1288 X1384 X1387 X1394 X1432 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
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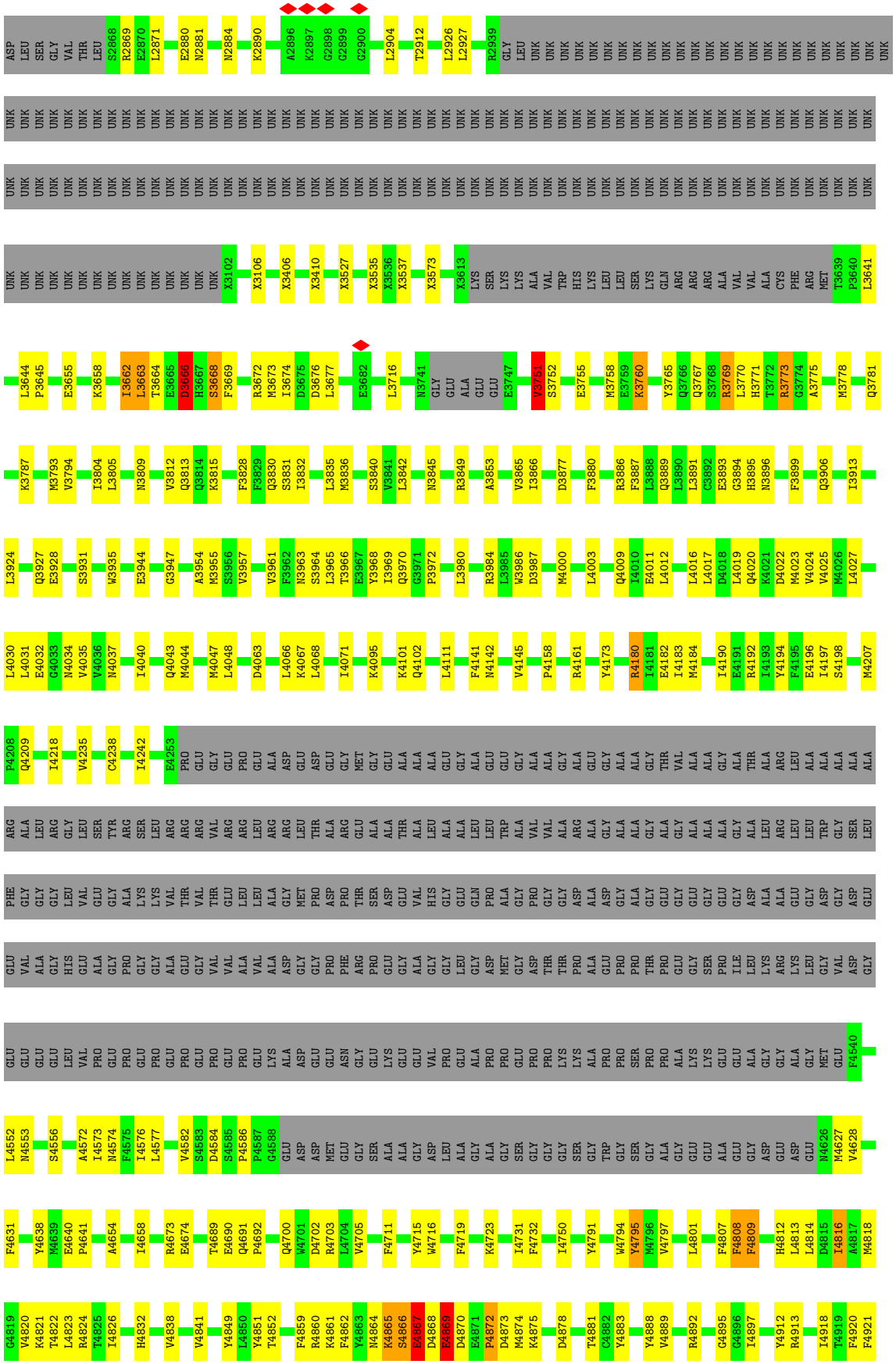
Q1631 L1639 R1646 C1647 M1648 D1649 E1652 R1661 L1667 L1676 G1677 N1678 N1679 L1685 A1697 L1703 L1707 R1708 A1709 G1710 Y1711 Y1712 I1716 S1717 I1718 H1719 L1720 E1721 C1724 R1725 M1730 V1736 P1737 L1738 T1739 P1740 R1743 L1747 H1760 R1772 A1784
ALA LEU PRO ALA ALA GLY V1791 R1797 I1802 A1826 R1827 V1839 P1840 V1841 L1842 K1843 M1851 G1852 I1853 E1857 K1860 I1866 E1867 V1870 F1871 E1874 GLU 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 L1927 Q1928 M1929 S1934 V1935 K1936 L1937 Q1938 M1939 C1947 E1950 E1956 A1960 F1961 A1962 E1963 R1964 A1992 R1996 Q2005 F2012 C2021 P2022 L2023 P2024
D2030 H2041 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089 Q2095 S2099 H2100 M2101 V2102 V2103 S2113 R2126 Q2127
P2146 C2158 L2159 I2162 L2165 L2166 I2167 V2168 Q2169 M2178 S2181 I2182 I2185 N2188 F2191 Y2192 R2199 A2200 L2201 L2215 M2228 F2239 I2242 S2243 R2244 Q2245 N2246 Q2247 R2248 L2257 P2272 V2275 A2276 A2287 L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295
E2296 V2299 C2310 L2314 F2337 F2340 E2348 L2368 L2376 R2392 ASP GLY PRO GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 K2447 I2456 L2474 P2477 T2478 L2479 GLY LYS ASP GLY ALA LEU VAL X2487 X2488
X2606 X2607 X2608 X2703 CYS ALA ILE ALA GLY ALA LEU PRO PRO ASP TYR VAL ASP ALA SER TYR SER SER LYS ALA GLU LYS LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 H2763 W2766 D2769 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787
H2788 P2789 R2792 P2793 Y2794 K2795 T2796 F2797 K2800 I2809 K2810 E2811 S2812 L2813 K2814 E2820 TRP THR ILE GLU LYS ALA ARG GLU GLY GLU GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY TYR ASN PRO GLN PRO PRO



F4922 F4923 V4924 I4925 L4928 L4935 I4936 I4937 D4938 A4939 F4940 G4941 E4942 L4943 R4944 D4945 Q4946 Q4949 K4957 C4958 D4966 H4978 E4982 H4983 N4984 L4985 F4990 M4993 Y4994 L4995 I4996 N4997 K4998 D4999 E5000 H5003 V5010 W5011 R5017 C5018 W5019 R5029 K5030 Q5031 Y5032 E5033 D5034

Q5035 L5036 S5037

• Molecule 1: RyR1

Chain D: 69% 13% 18%

MET GLY ASP GLY GLY GLU GLY GLU ASP GLU VAL Q12 F13 L14 R15 D18 E19 V20 C24 K34 L35 C36 R45 E50 S53 T68 R76 E80 N84 THR VAL GLU ALA GLY VAL GLU SER SER GLN GLY GLY G97 L101 L102 L108 L109 R110

M116 Y117 L118 S119 C120 D134 L137 Q138 E139 W147 W148 T149 M150 H151 S154 K155 G160 E161 K162 V163 R164 V165 S175 S176 E177 R178 Y179 L180 H181 D192 A193 S194 F195 M196 Q197 T198 M202 Y213 V214 T215 G216 V219 L220 E229 R243 Y247 E248

V252 R257 W260 R261 L262 S272 R275 L280 H284 T294 E295 L299 V300 V301 T312 S313 F314 C315 F316 R317 D330 M334 P337 Y341 V348 Q349 H350 L357 T358 L372 K373 K374 L378 H383 K416 F421 R426

L436 L443 P455 K467 Q479 M483 L486 E505 Y523 L526 N536 L539 L551 I560 V563 V567 L568 E573 I577 L589 K592 R595 V614 R615 S616 N617 Q618 P627 G628 R629 L633 Q634 T635 I644 R645 P646

N647 I648 F649 R652 G660 K661 F664 E665 V666 M667 V668 D669 E670 L682 W686 S693 P694 Y695 P696 G697 E700 D710 S713 F716 D717 G718 L719 H720 L721 W722 T723 V726 A727 R728 P740 E741 D742 V743 V744 S745 C746 C747 L750 S756 F757 R758

I759 N760 G761 C762 Q765 L773 L776 F777 F778 P779 G786 V787 L792 Y808 R820 L821 R822 P825 I826 R830 L839 V840 G841 H848 F851 VAL PRO CYS PRO VAL ASP THR VAL GLN ILE VAL LEU PRO PRO H866 G926 L929 L977 T978

Q981 R1000 W1005 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO ARG LEU VAL PRO TYR R1025 L1026 K1032 L1047 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 I1074 F1075 R1076 A1077 G1098 R1101 R1106

L1115 G1116 A1117 D1118 E1119 F1124 N1125 G1126 W1132 H1133 F1139 W1143 M1152 N1158 I1161 L1164 N1165 G1166 T1177 I1182 E1183 L1189 C1192 S1193 L1194 G1195 Q1198 N1203 S1210 I1216 P1225 I1228 N1229 W1237 F1238 S1239 K1240 S1241 L1242 P1243

X1288 X1384 X1387 X1394 X1432 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK

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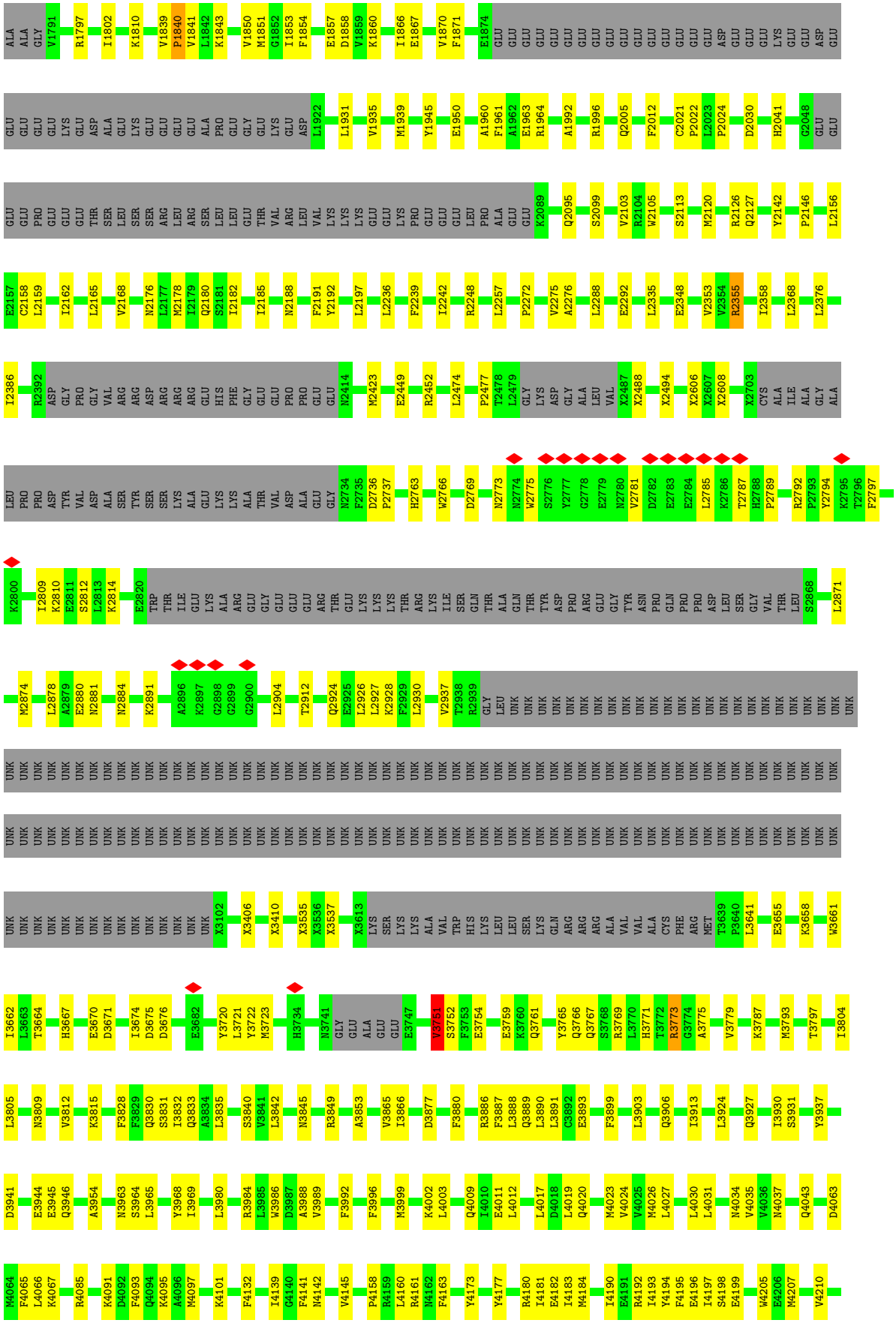
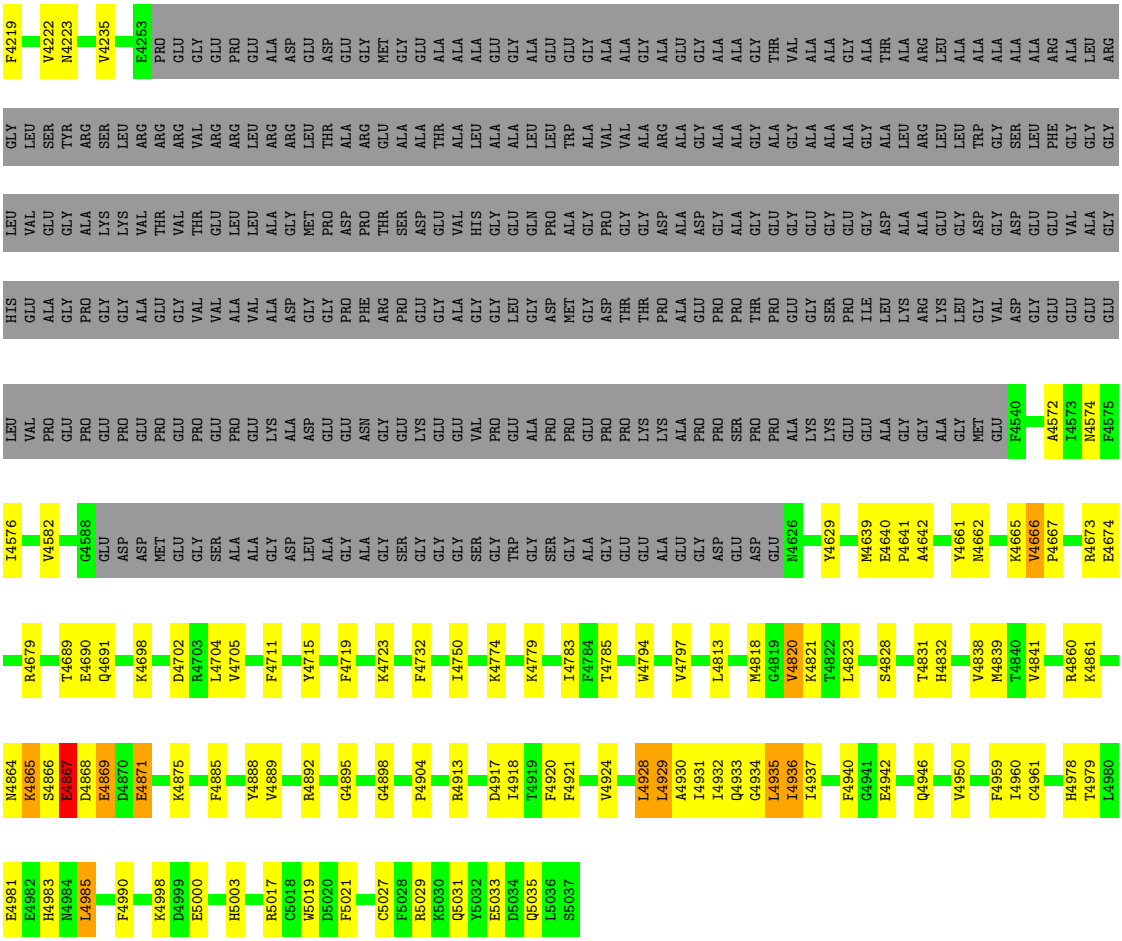
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK GLU LEU GLY LYS GLN LYS ASN ILE M1573 F1580 P1592 P1593 R1594 Q1598 M1599 L1600 Q1614 VAL GLU THR ARG ARG ALA GLY E1622 R1623 L1624 G1625 W1626 Q1631 L1639 R1646

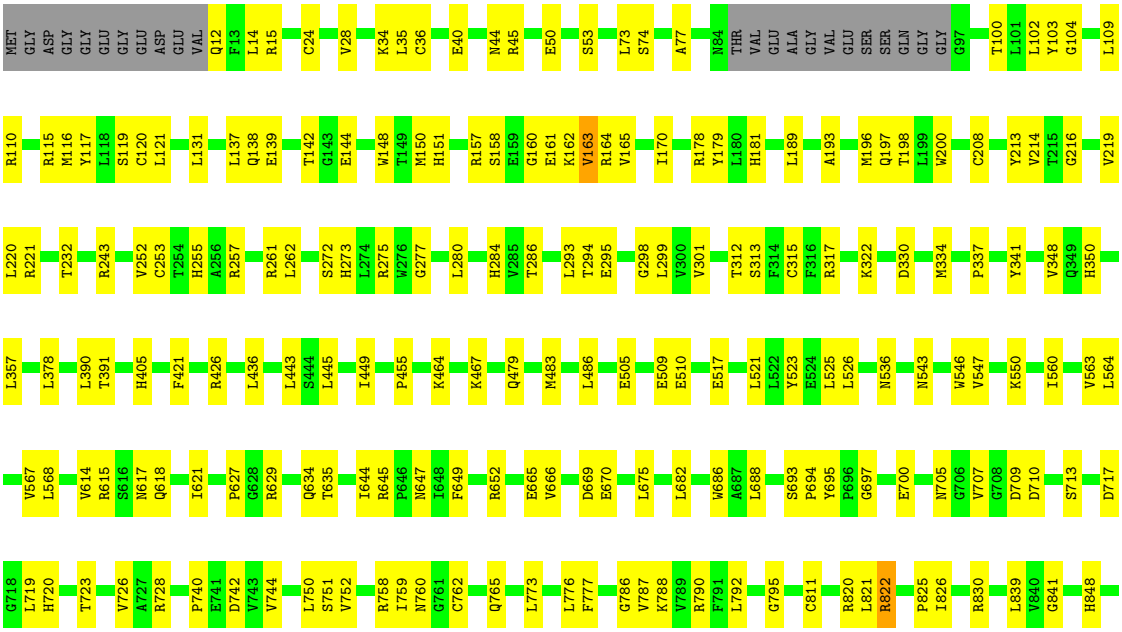
C1647 M1648 D1649 E1652 D1658 L1667 L1676 G1677 N1678 N1679 L1685 V1689 D1690 A1697 L1698 L1703 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 L1714 L1715 I1716 S1717 I1718 H1719 L1720 C1724 R1725 L1738 T1739 P1740 R1743 L1747 F1748 P1749 P1750 H1760 A1784 ALA LEU PRO

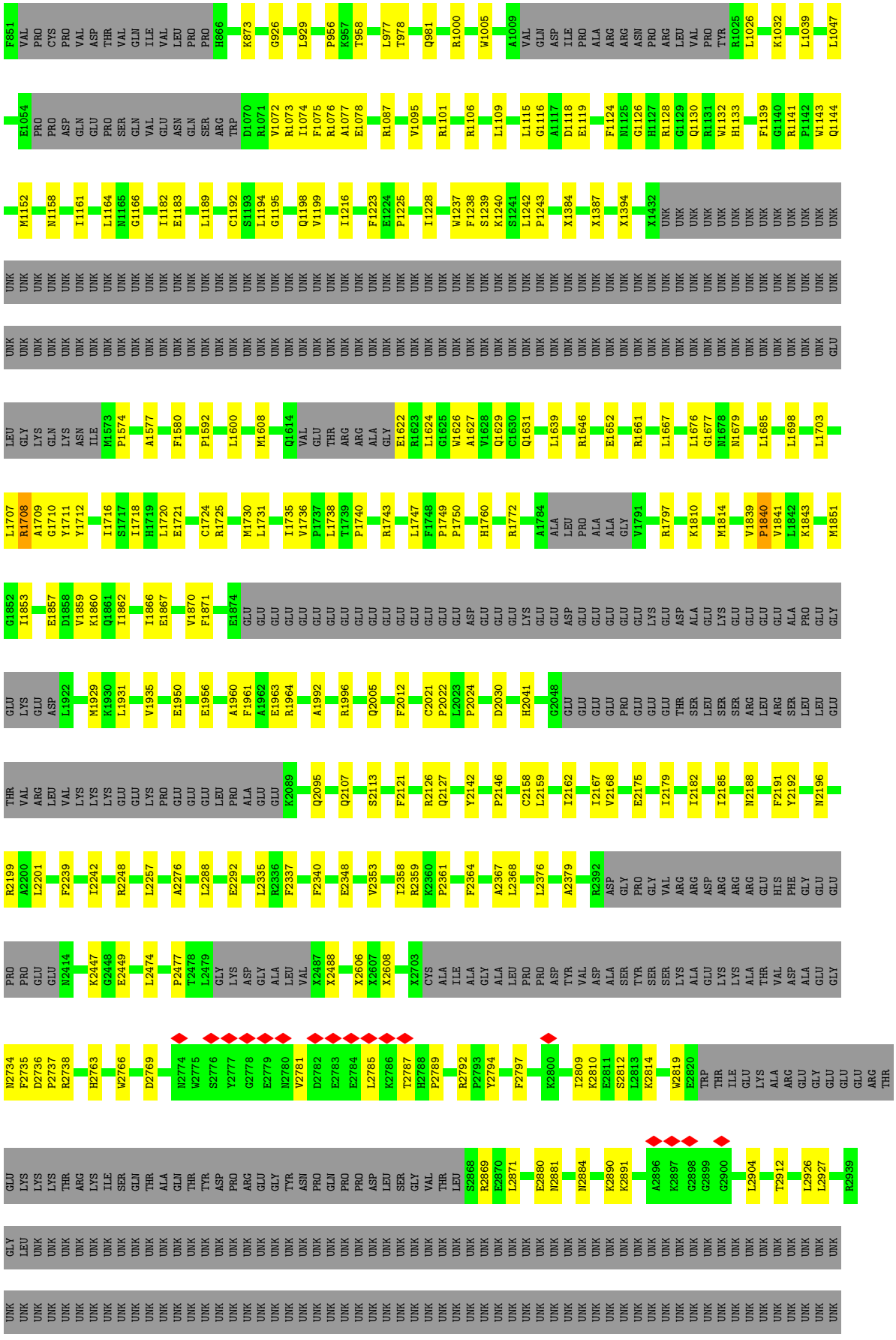


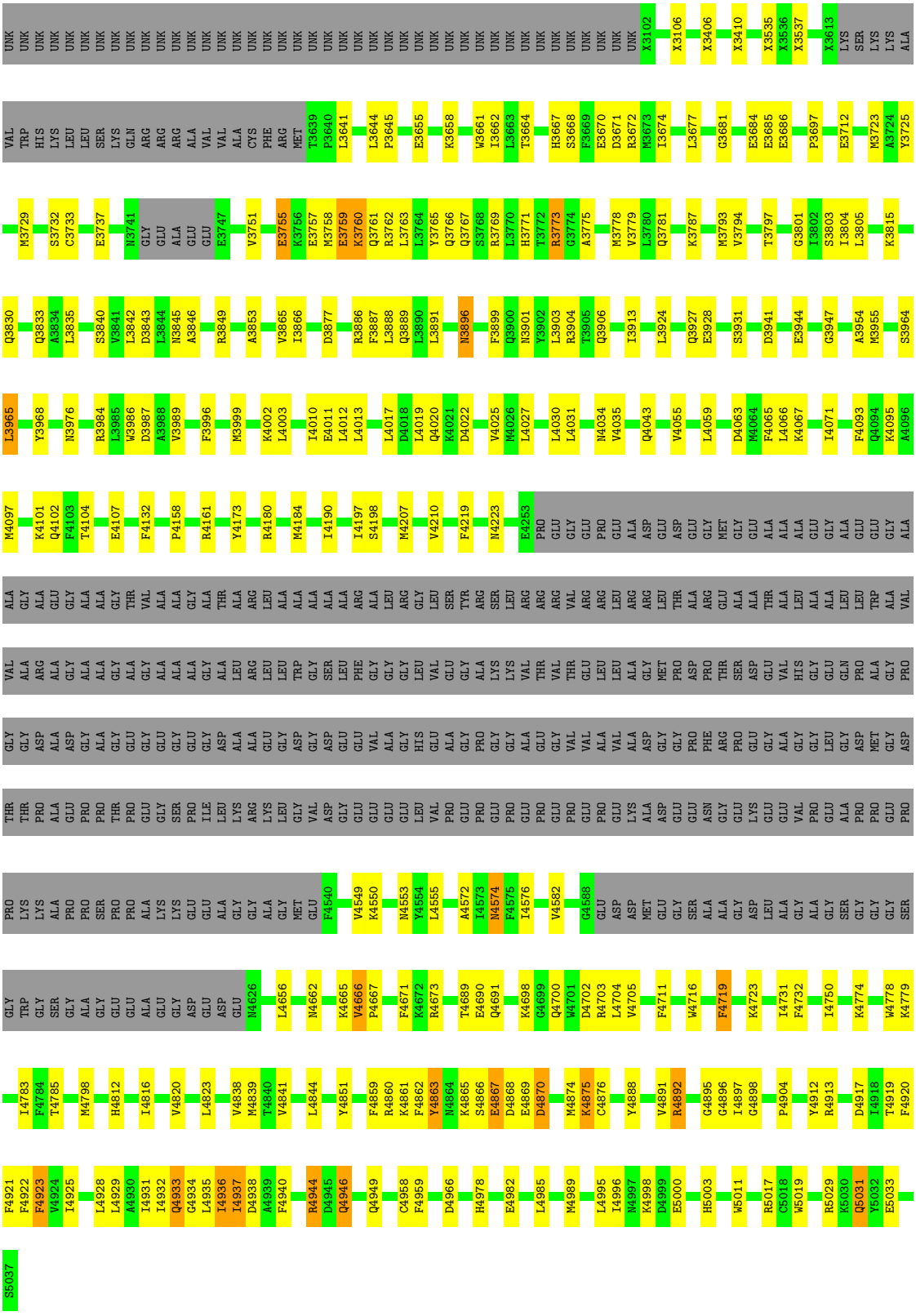


• Molecule 1: RyR1

Chain C:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	68155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	478.72, 478.72, 478.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/25057	0.50	1/34021 (0.0%)
1	B	0.27	0/25055	0.50	3/34016 (0.0%)
1	C	0.26	0/25076	0.50	2/34047 (0.0%)
1	D	0.26	0/25078	0.50	2/34045 (0.0%)
All	All	0.26	0/100266	0.50	8/136129 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3751	VAL	C-N-CA	-5.77	107.27	121.70
1	B	719	LEU	CA-CB-CG	5.62	128.23	115.30
1	D	3751	VAL	C-N-CA	-5.62	107.66	121.70
1	D	719	LEU	CA-CB-CG	5.56	128.08	115.30
1	C	4891	VAL	O-C-N	5.30	131.18	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	4892	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	28941	0	24397	483	0
1	B	28940	0	24404	519	0
1	C	28958	0	24429	510	0
1	D	28963	0	24439	493	0
2	A	31	0	14	7	0
2	B	31	0	14	4	0
2	C	31	0	14	3	0
2	D	31	0	14	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	115935	0	97725	1937	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1937 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:A:3773:ARG:CB	1:A:3815:LYS:HE3	1.46	1.45
1:C:3765:TYR:CE1	1:C:4750:ILE:HG23	1.52	1.40
1:A:4921:PHE:O	1:A:4925:ILE:HG22	1.27	1.30
1:A:3767:GLN:O	1:A:3772:THR:HB	1.29	1.28
1:D:3674:ILE:HG12	1:D:3769:ARG:CD	1.64	1.28

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	3191/5037 (63%)	2943 (92%)	243 (8%)	5 (0%)	47 81
1	B	3191/5037 (63%)	2934 (92%)	247 (8%)	10 (0%)	41 76
1	C	3191/5037 (63%)	2929 (92%)	254 (8%)	8 (0%)	41 76
1	D	3191/5037 (63%)	2932 (92%)	253 (8%)	6 (0%)	47 81
All	All	12764/20148 (63%)	11738 (92%)	997 (8%)	29 (0%)	50 81

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4866	SER
1	A	4870	ASP
1	B	3662	ILE
1	B	3666	ASP
1	B	4867	GLU

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	2452/3264 (75%)	2421 (99%)	31 (1%)	69 82
1	B	2452/3264 (75%)	2419 (99%)	33 (1%)	69 82
1	C	2455/3264 (75%)	2425 (99%)	30 (1%)	71 84
1	D	2458/3264 (75%)	2431 (99%)	27 (1%)	73 85
All	All	9817/13056 (75%)	9696 (99%)	121 (1%)	72 84

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4936	ILE
1	C	4875	LYS
1	D	3759	GLU
1	C	4868	ASP
1	C	4944	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	151	HIS
1	C	4946	GLN
1	D	3761	GLN
1	C	4223	ASN
1	D	2180	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	$\#\|Z\|>2$
2	ACP	A	5101	4	27,33,33	1.35	5 (18%)	32,52,52	1.51	5 (15%)
2	ACP	B	5101	4	27,33,33	0.89	1 (3%)	32,52,52	0.84	2 (6%)
2	ACP	D	5101	4	27,33,33	1.37	5 (18%)	32,52,52	1.46	4 (12%)
2	ACP	C	5101	4	27,33,33	1.33	5 (18%)	32,52,52	1.50	4 (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
2	ACP	A	5101	4	-	5/15/38/38	0/3/3/3
2	ACP	B	5101	4	-	8/15/38/38	0/3/3/3
2	ACP	D	5101	4	-	9/15/38/38	0/3/3/3
2	ACP	C	5101	4	-	7/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5101	ACP	PG-O3G	2.87	1.61	1.54
2	C	5101	ACP	PG-O3G	2.86	1.61	1.54
2	C	5101	ACP	PG-O2G	2.85	1.61	1.54
2	D	5101	ACP	PG-O3G	2.83	1.61	1.54
2	D	5101	ACP	PG-O2G	2.83	1.61	1.54

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5101	ACP	PB-O3A-PA	-4.14	119.42	132.56
2	A	5101	ACP	PB-O3A-PA	-4.07	119.65	132.56
2	D	5101	ACP	PB-O3A-PA	-3.87	120.27	132.56
2	A	5101	ACP	N3-C2-N1	-3.70	122.90	128.68
2	C	5101	ACP	N3-C2-N1	-3.65	122.98	128.68

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5101	ACP	C5'-O5'-PA-O1A
2	A	5101	ACP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	5101	ACP	PG-C3B-PB-O1B
2	B	5101	ACP	PG-C3B-PB-O3A
2	B	5101	ACP	C5'-O5'-PA-O2A

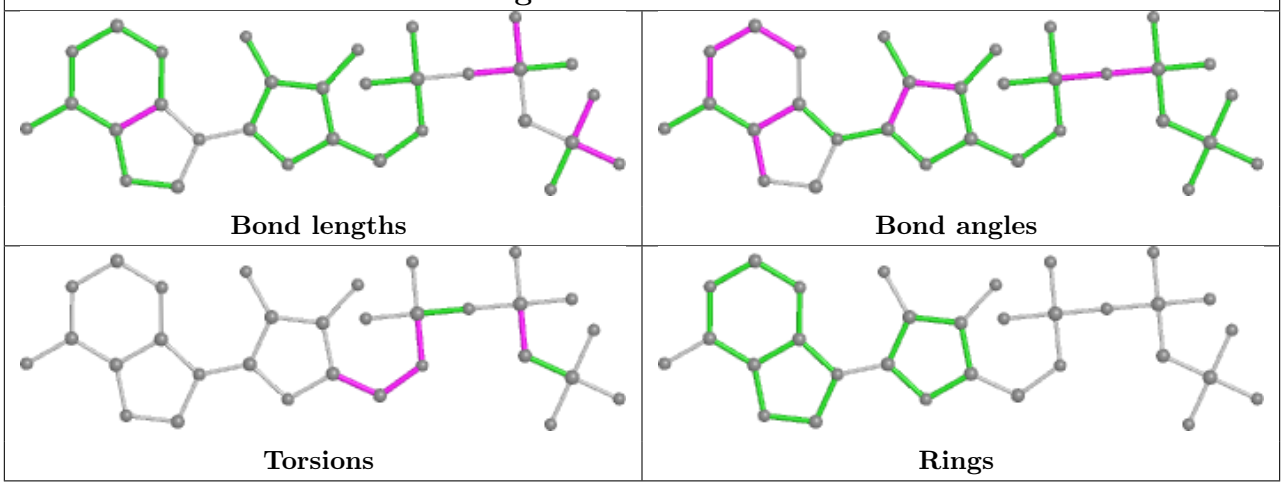
There are no ring outliers.

4 monomers are involved in 22 short contacts:

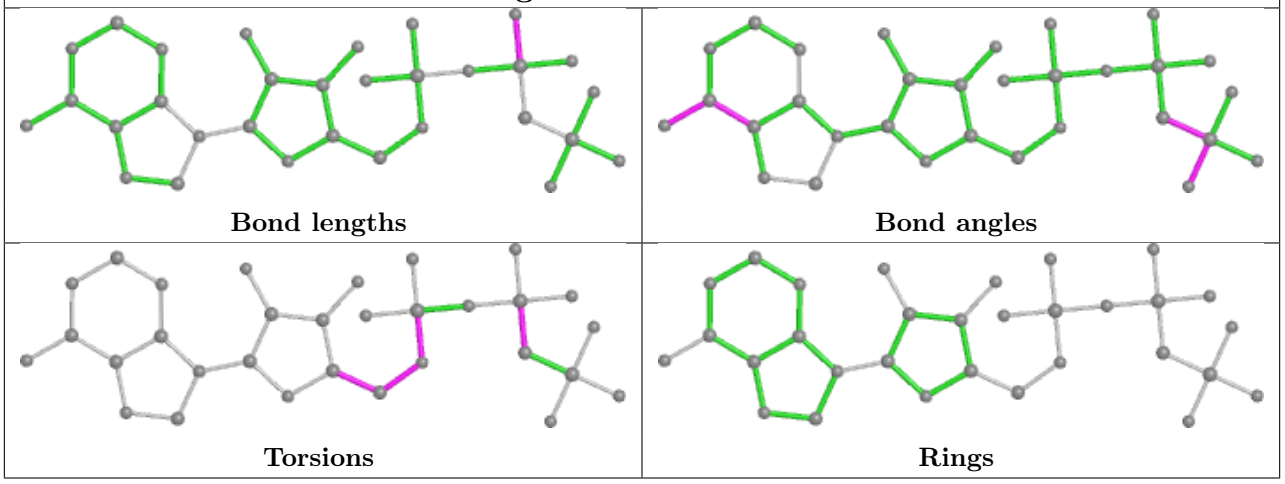
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5101	ACP	7	0
2	B	5101	ACP	4	0
2	D	5101	ACP	8	0
2	C	5101	ACP	3	0

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.

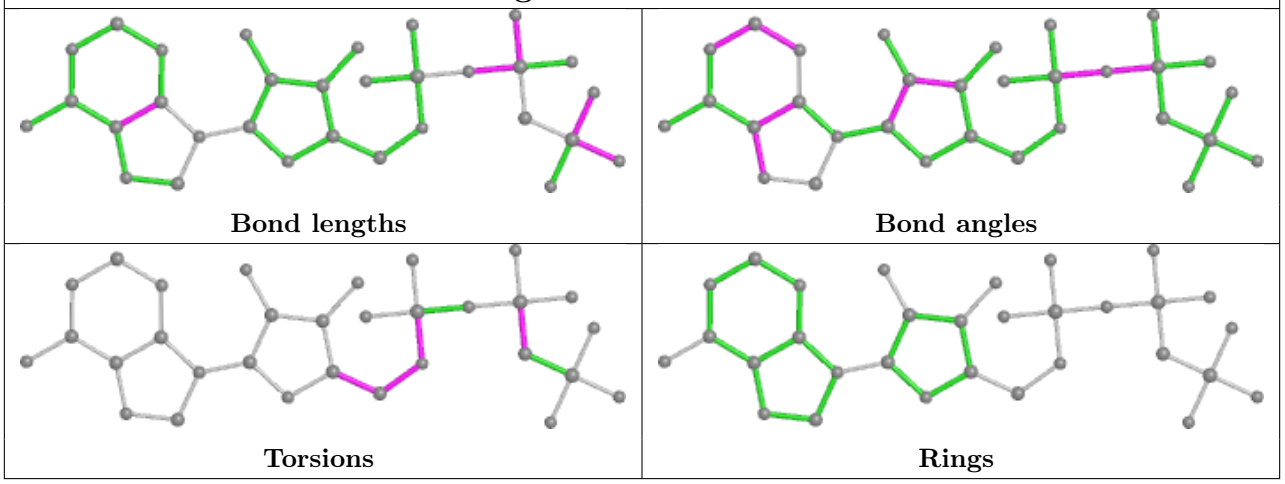
Ligand ACP A 5101



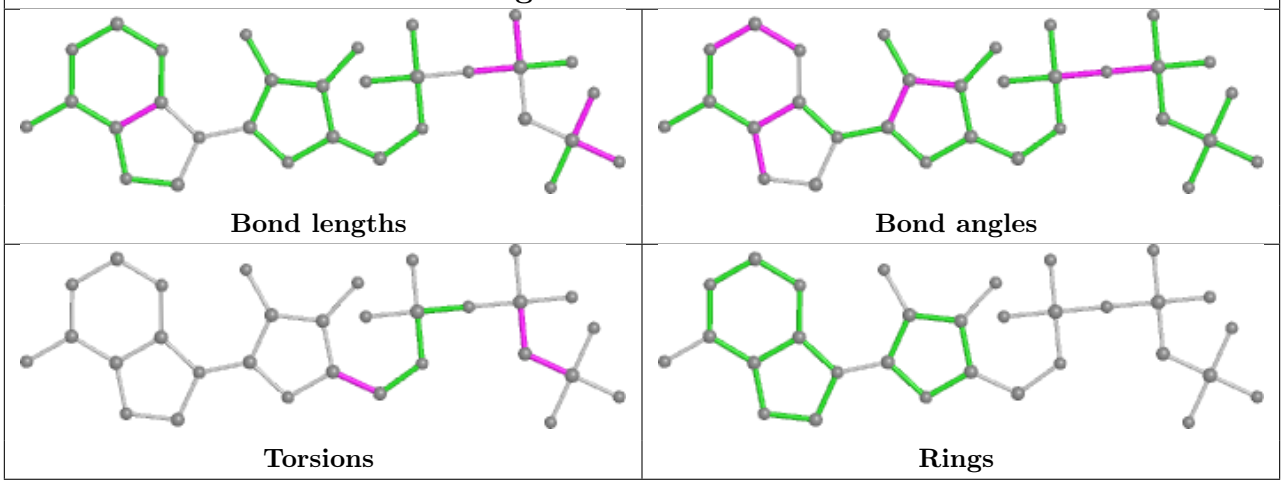
Ligand ACP B 5101



Ligand ACP D 5101



Ligand ACP C 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
1	D	6
1	B	6
1	C	6
1	A	6

The worst 5 of 24 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	3302:UNK	C	3303:UNK	N	17.16
1	B	3302:UNK	C	3303:UNK	N	17.15
1	C	3302:UNK	C	3303:UNK	N	17.10
1	A	3302:UNK	C	3303:UNK	N	17.01
1	A	3510:UNK	C	3511:UNK	N	16.97

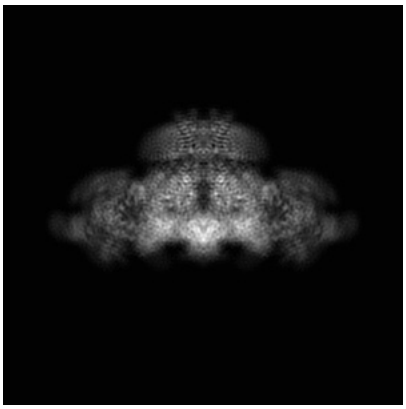
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22615. These allow visual inspection of the internal detail of the map and identification of artifacts.

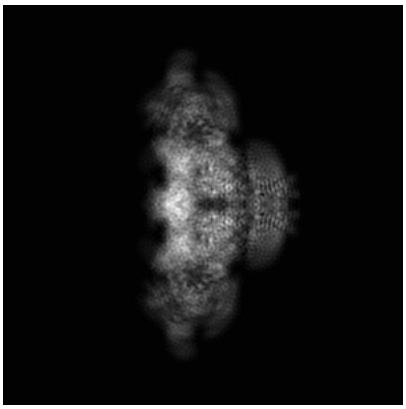
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

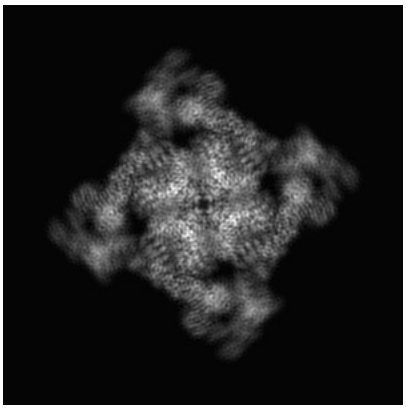
6.1.1 Primary map



X

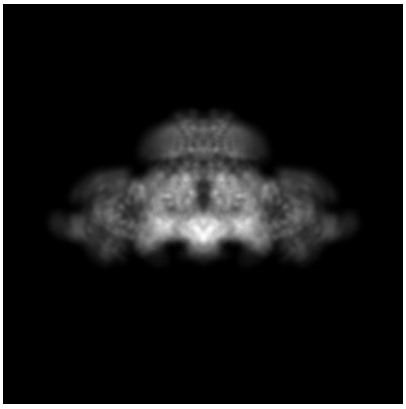


Y

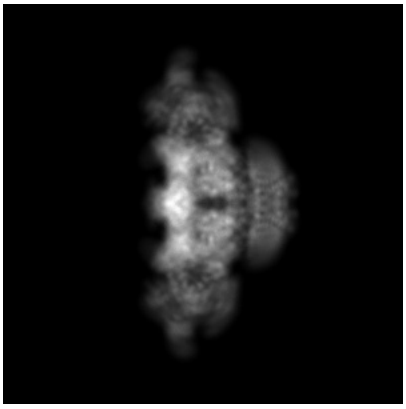


Z

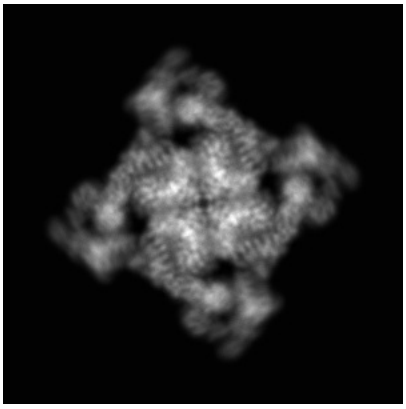
6.1.2 Raw map



X



Y

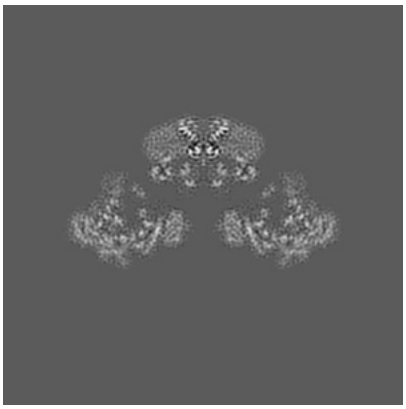


Z

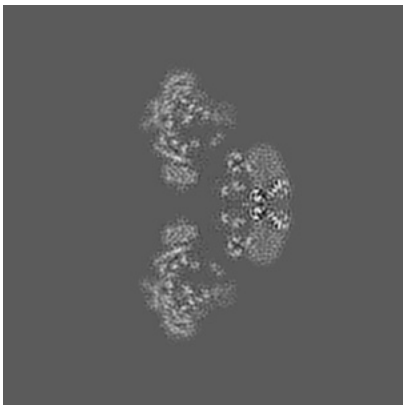
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



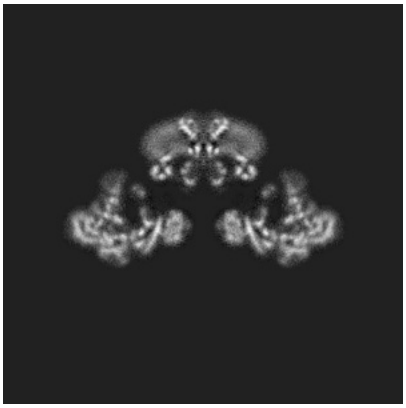
X Index: 176



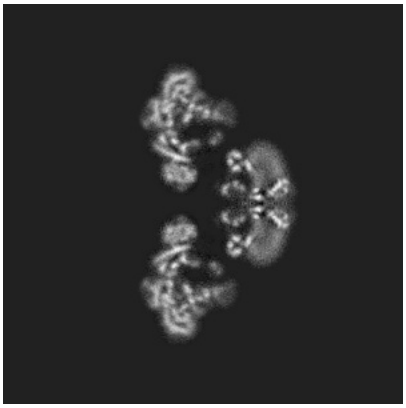
Y Index: 176

Z Index: 176

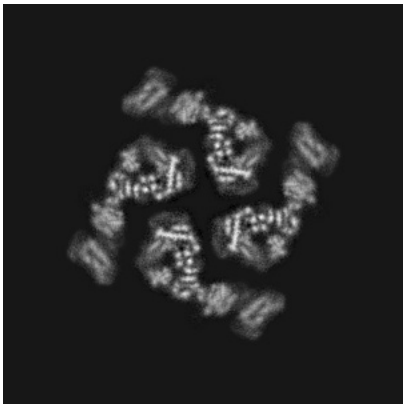
6.2.2 Raw map



X Index: 176



Y Index: 176

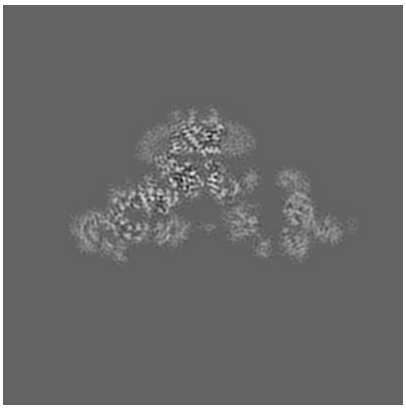


Z Index: 176

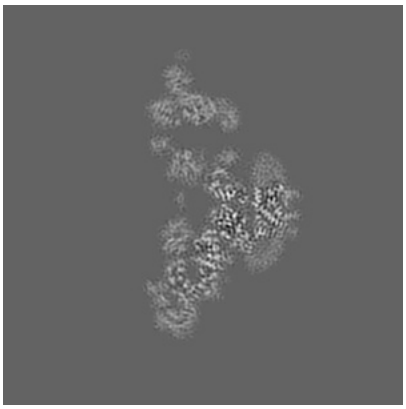
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

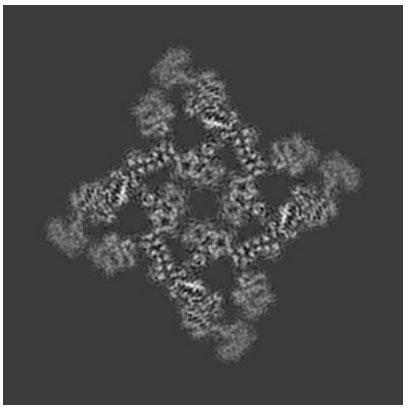
6.3.1 Primary map



X Index: 165

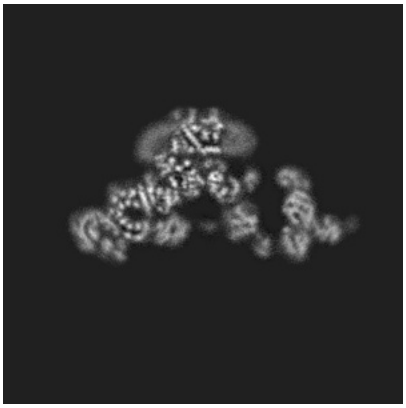


Y Index: 187

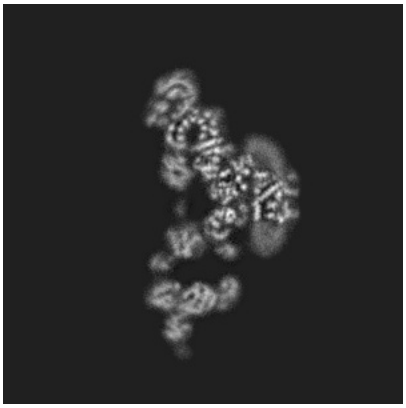


Z Index: 160

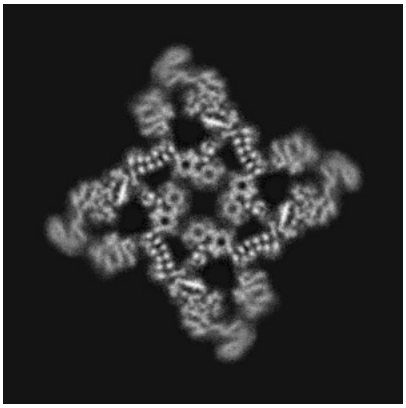
6.3.2 Raw map



X Index: 165



Y Index: 165

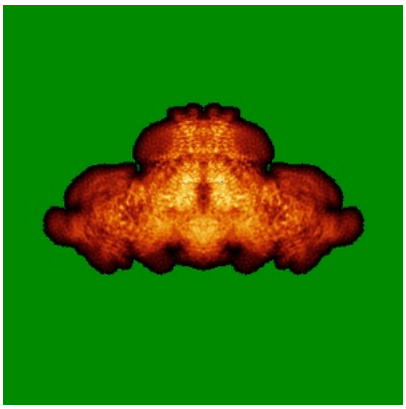


Z Index: 160

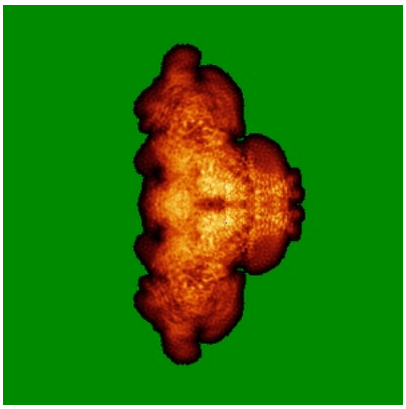
The images above show the largest variance slices of the map in three orthogonal directions.

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

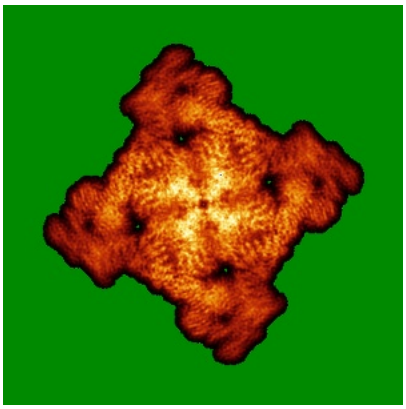
6.4.1 Primary map



X

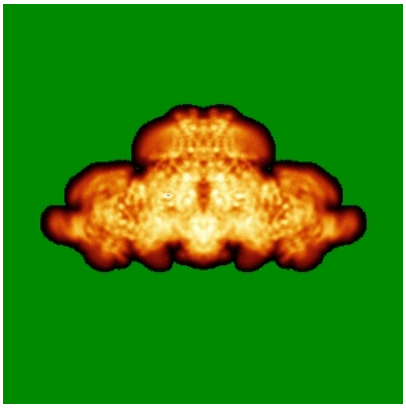


Y

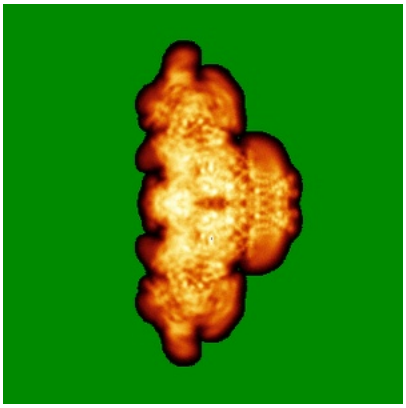


Z

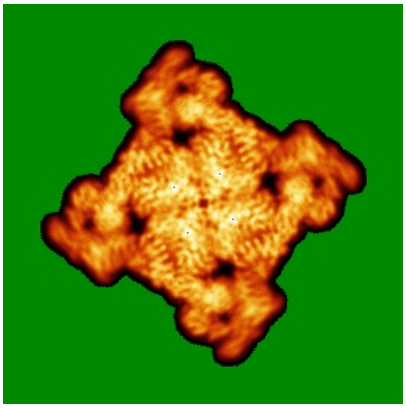
6.4.2 Raw map



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 0.006. 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.

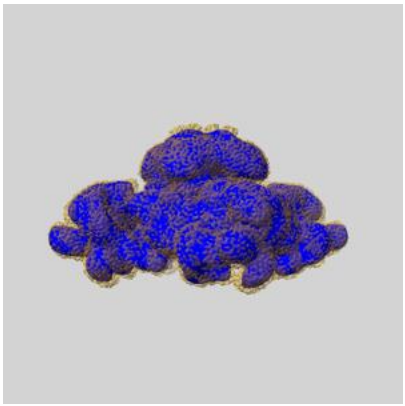
6.6 Mask visualisation (i)

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

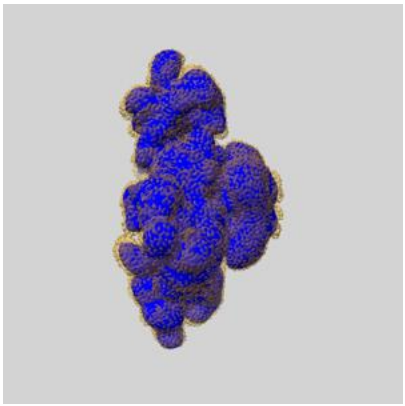
A mask typically either:

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

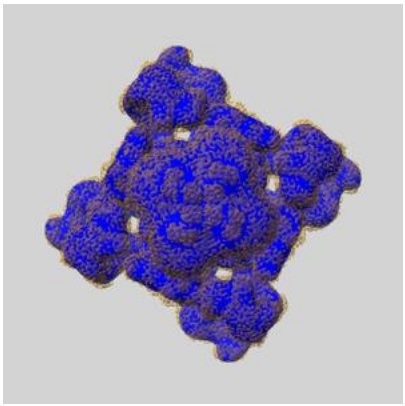
6.6.1 emd_22615_msk_1.map (i)



X



Y

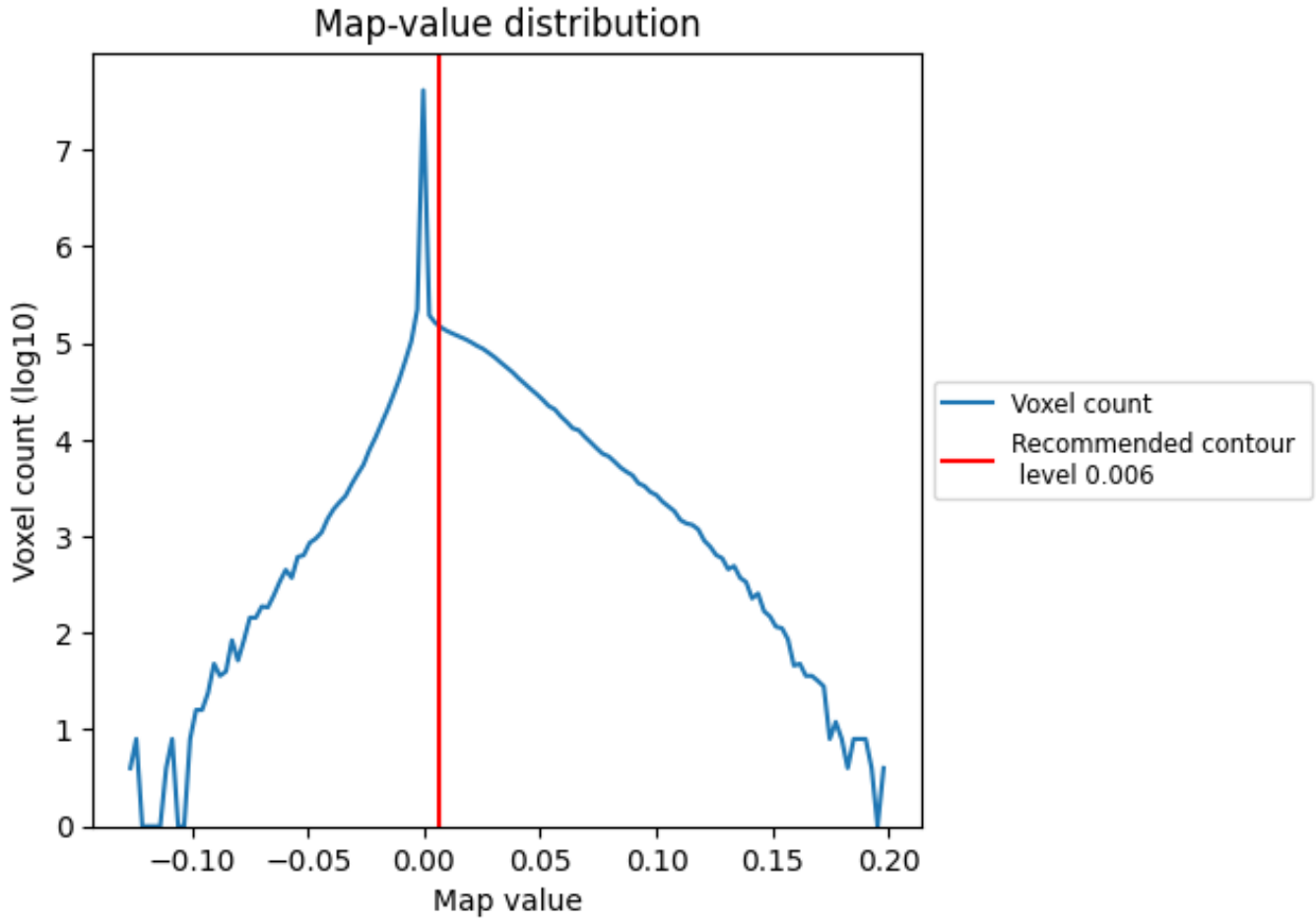


Z

7 Map analysis

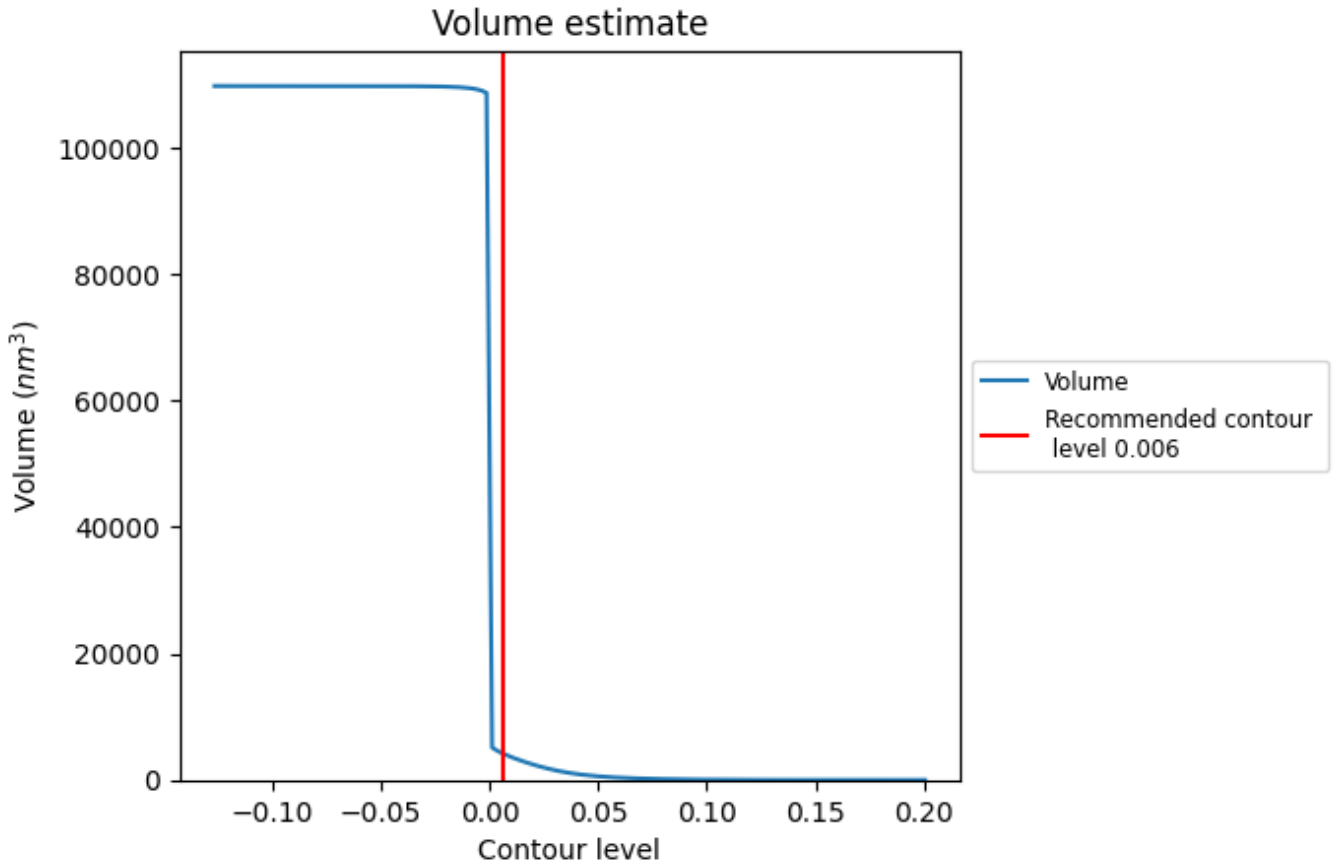
This section contains the results of statistical analysis of the map.

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.

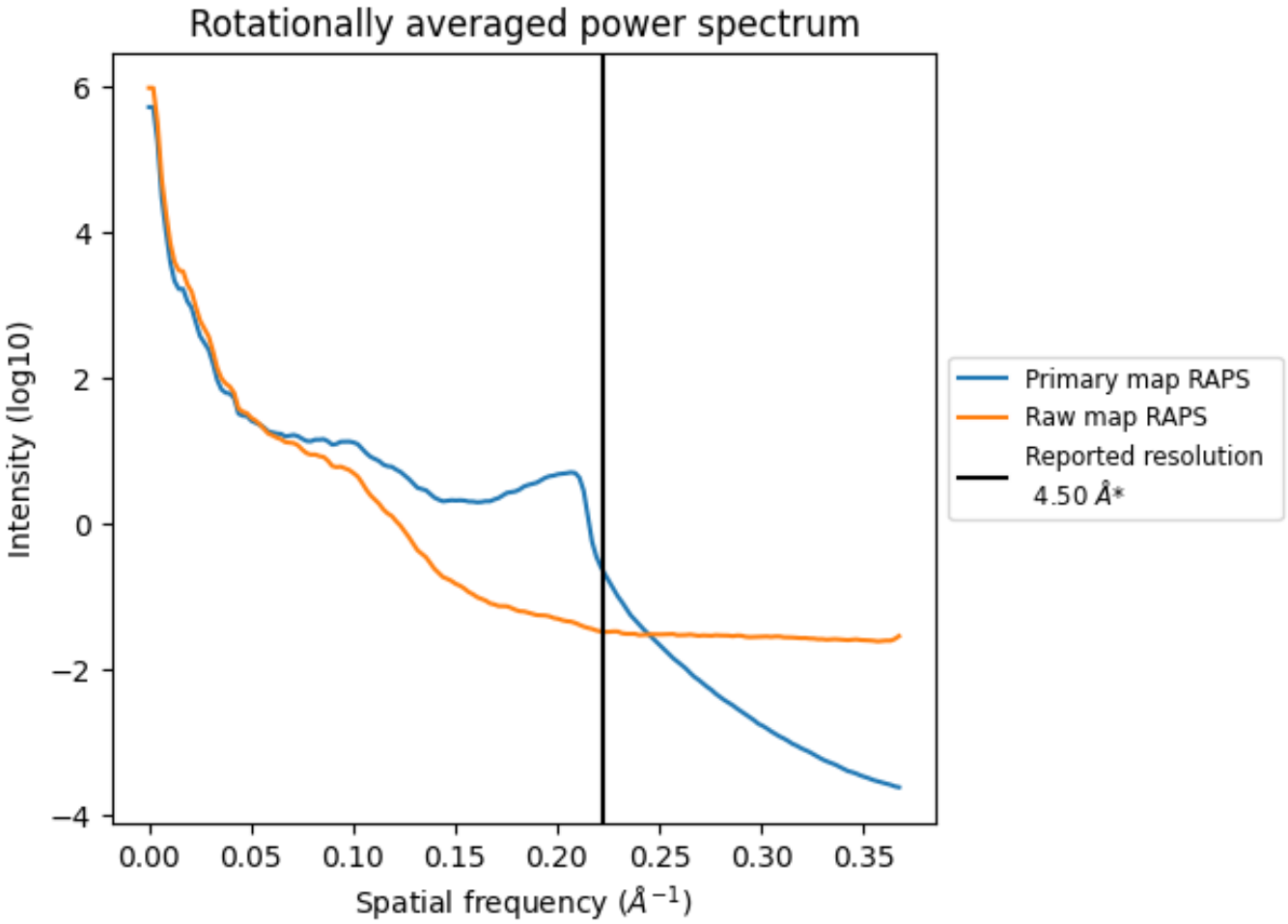
7.2 Volume estimate (i)



The volume at the recommended contour level is 4210 nm^3; this corresponds to an approximate mass of 3803 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)

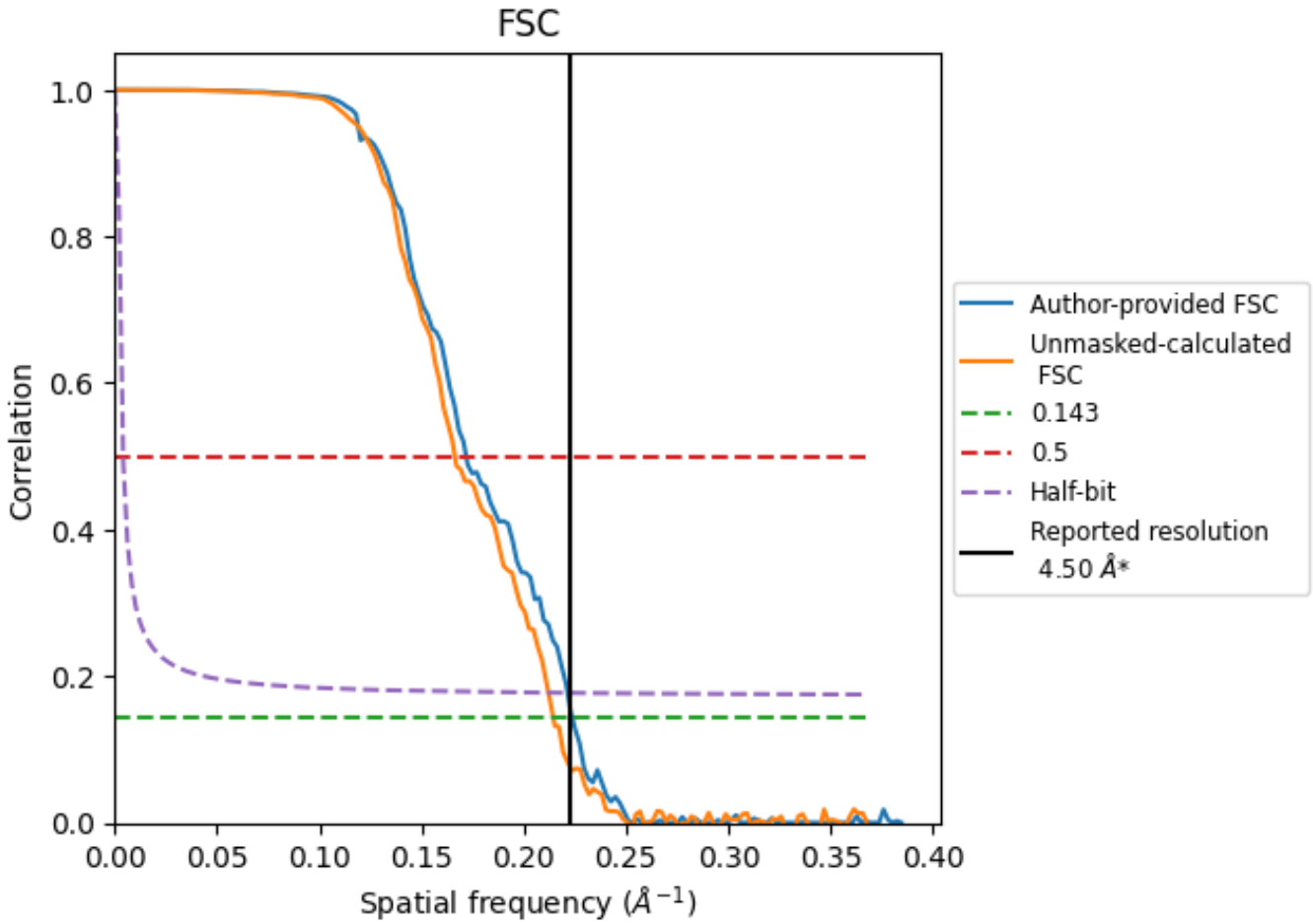


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

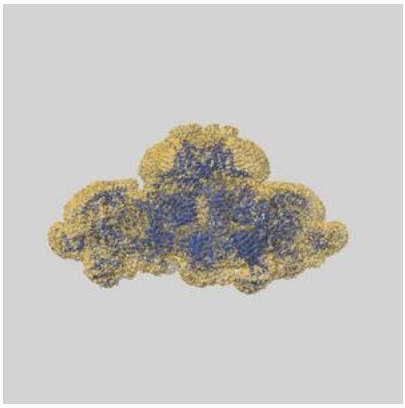
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.47	5.82	4.52
Unmasked-calculated*	4.66	6.01	4.71

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

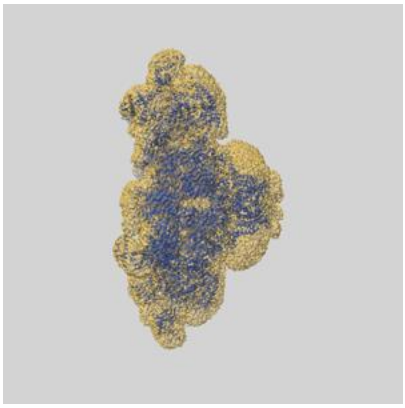
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22615 and PDB model 7K0S. Per-residue inclusion information can be found in section 3 on page 5.

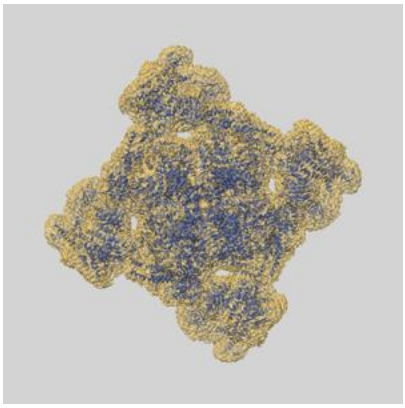
9.1 Map-model overlay



X



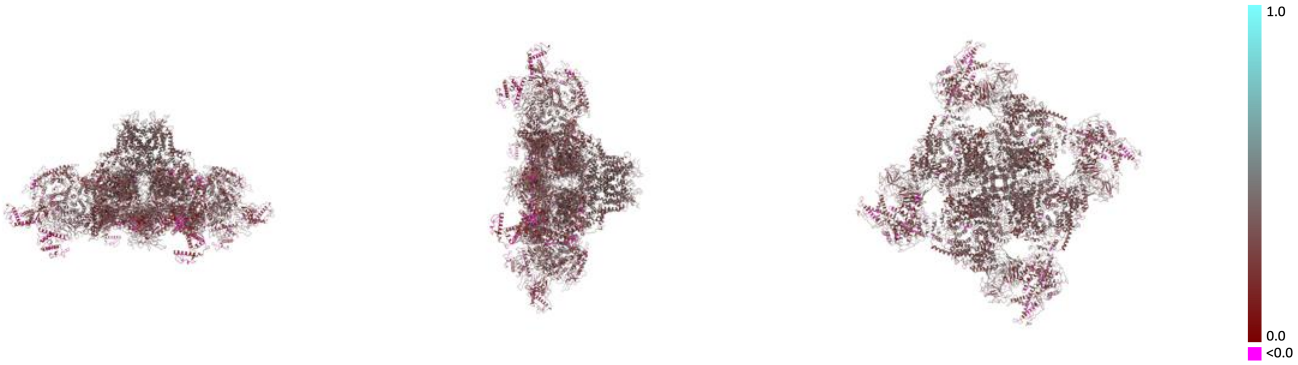
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

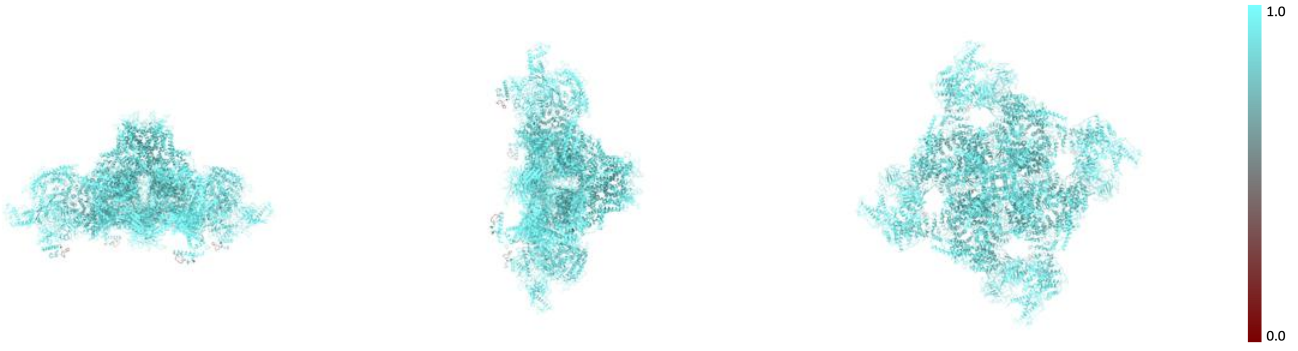
9.2 Q-score mapped to coordinate model



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.

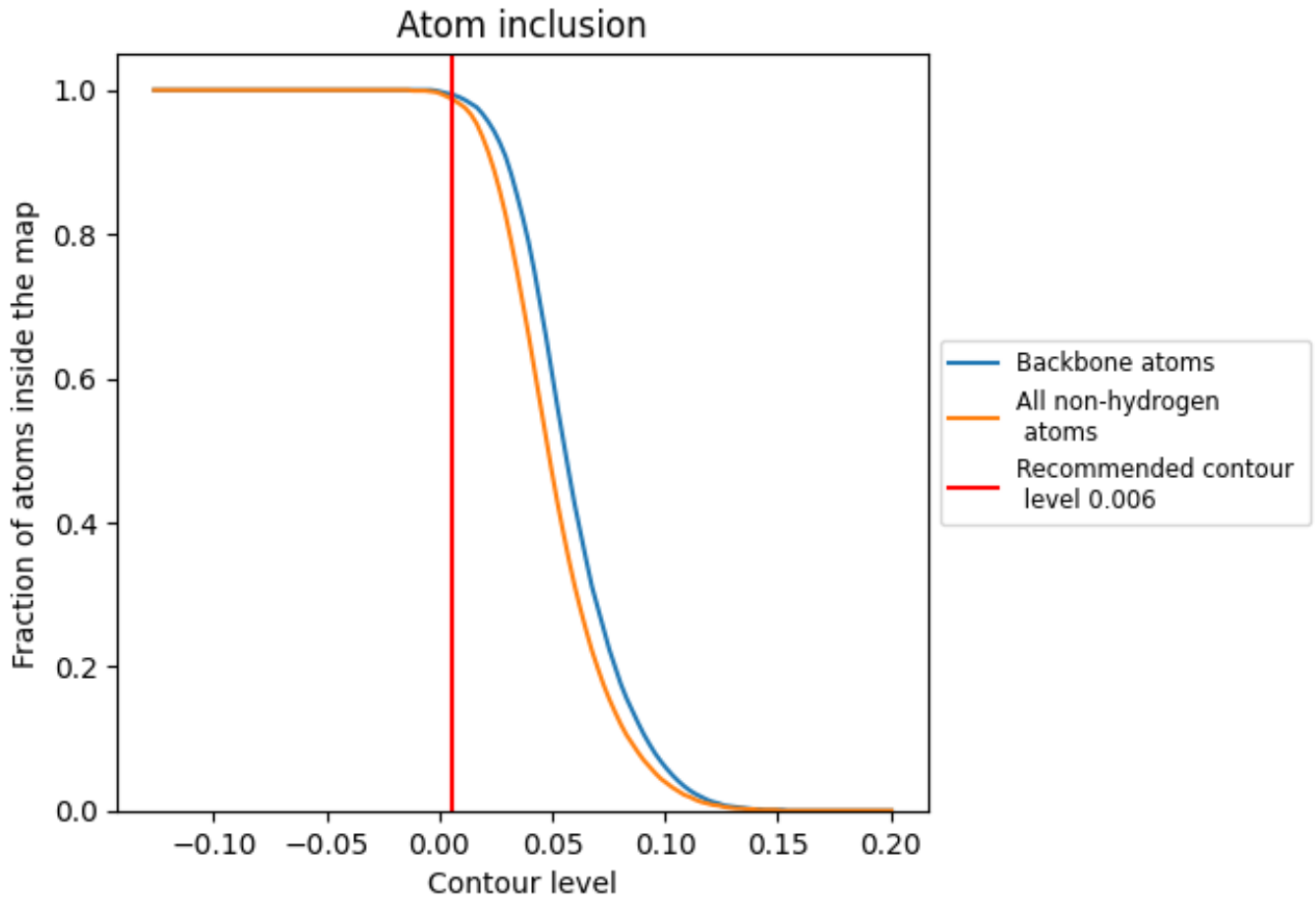
9.3 Atom inclusion mapped to coordinate model



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9870	0.3120
A	0.9870	0.3110
B	0.9870	0.3120
C	0.9870	0.3120
D	0.9870	0.3110