wwPDB EM Validation Summary Report (i)

Mar 3, 2025 – 07:35 PM JST

PDB ID	:	8X4E
EMDB ID	:	EMD-38048
Title	:	Cryo-EM structure of Ryanodine receptor 1 (TM helix S0, 5 mM Ca2+)
Authors	:	Chen, Q.; Hu, H.
Deposited on	:	2023-11-15
Resolution	:	3.30 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 (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:

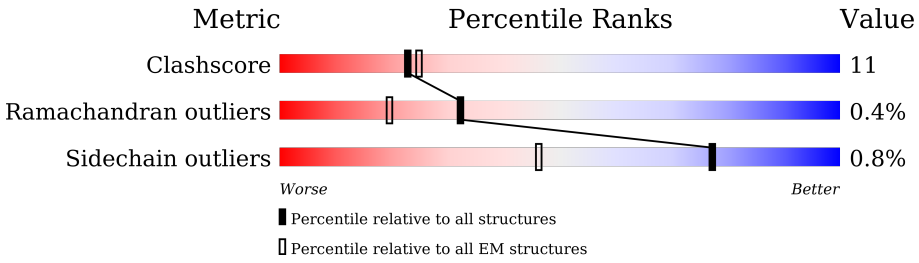
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 3.30 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	5037	62% 17% 21%
1	B	5037	61% 17% 21%
1	C	5037	61% 17% 21%
1	D	5037	61% 17% 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 118280 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	3982	Total 29568	C 18816	N 5133	O 5431	S 188	0	0
1	B	3982	Total 29568	C 18816	N 5133	O 5431	S 188	0	0
1	C	3982	Total 29568	C 18816	N 5133	O 5431	S 188	0	0
1	D	3982	Total 29568	C 18816	N 5133	O 5431	S 188	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

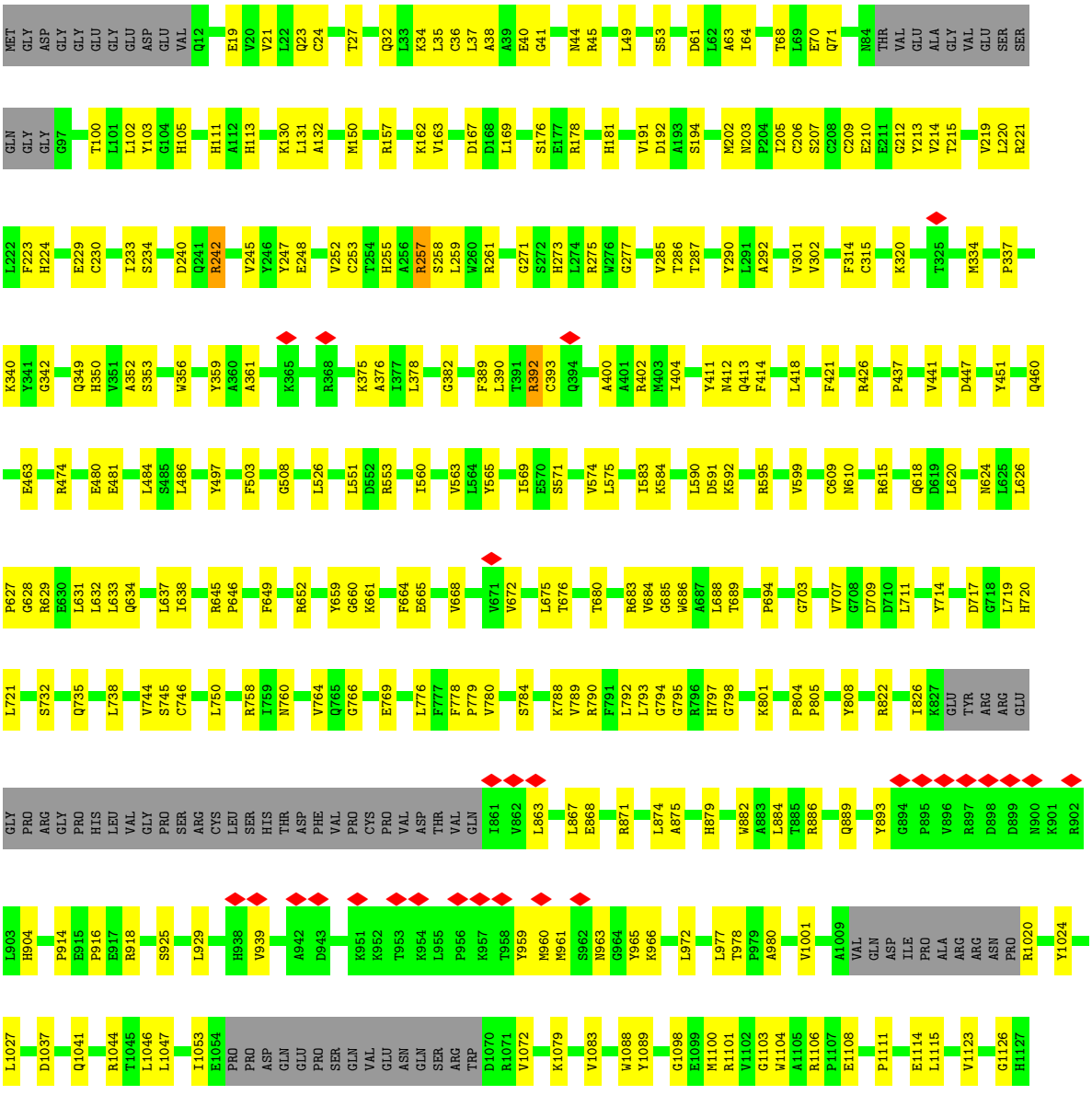
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Ca 1	0
3	B	1	Total 1	Ca 1	0
3	C	1	Total 1	Ca 1	0
3	D	1	Total 1	Ca 1	0

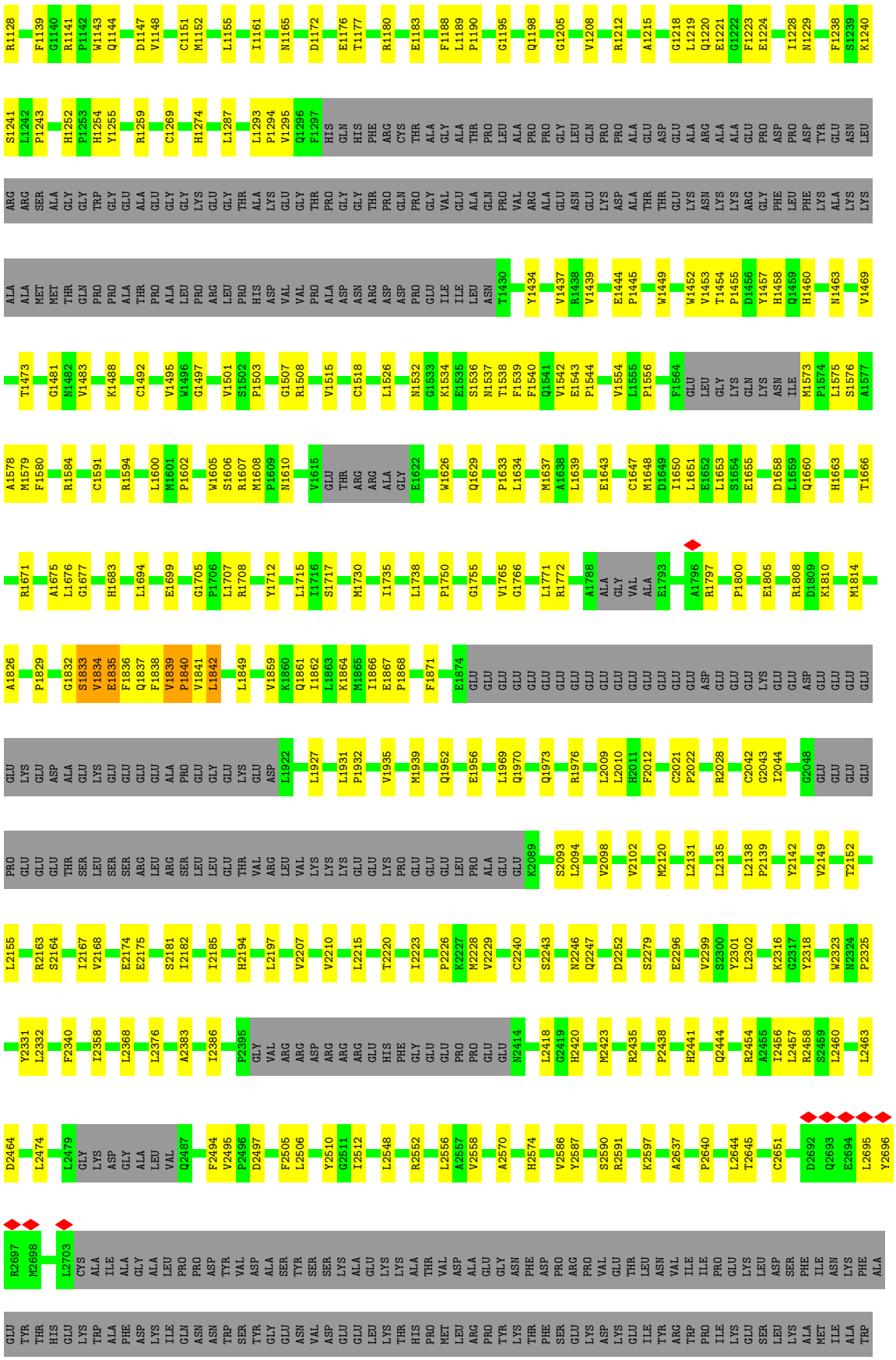
3 Residue-property plots (i)

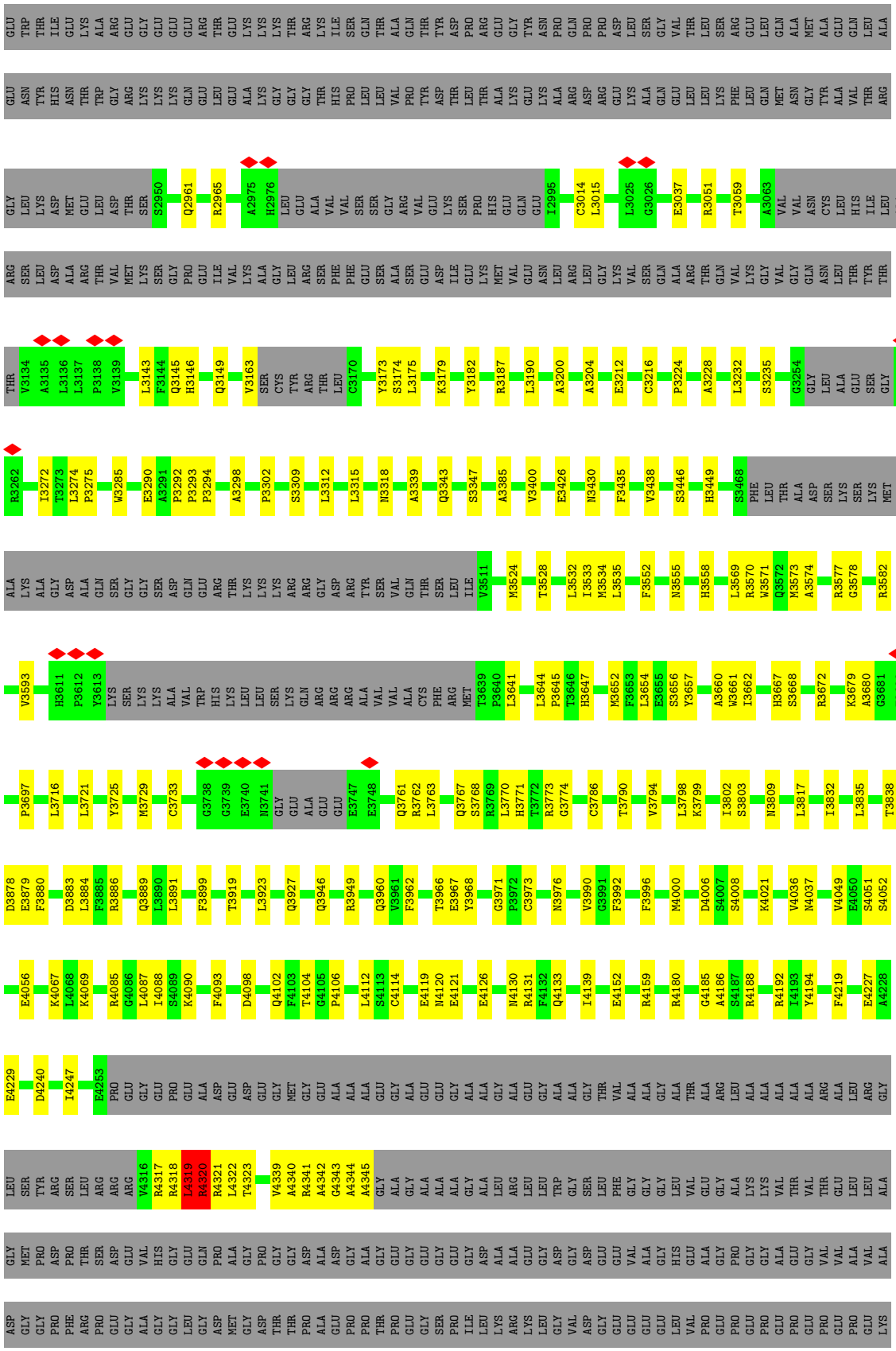
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

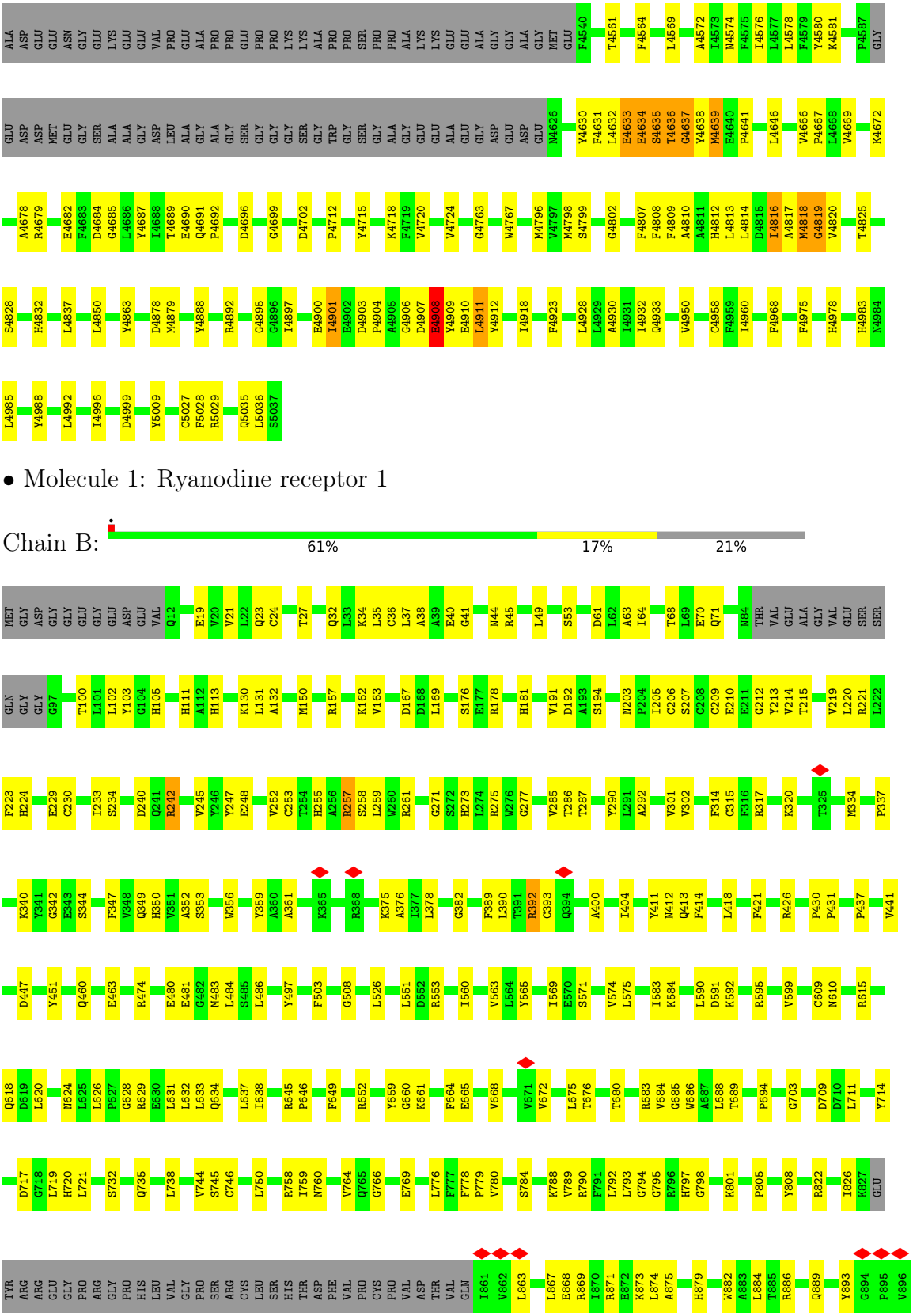
- Molecule 1: Ryanodine receptor 1

Chain A:



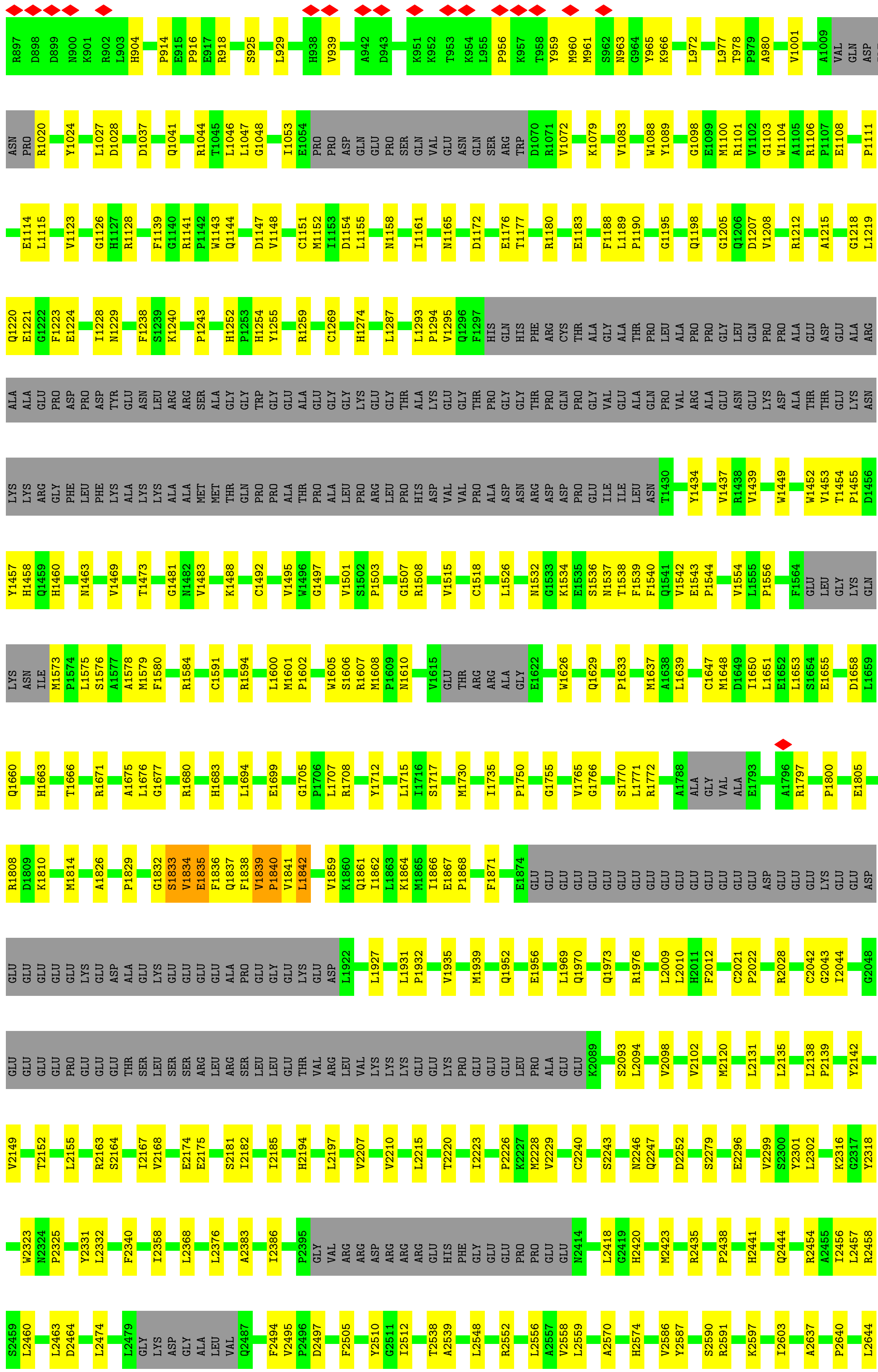


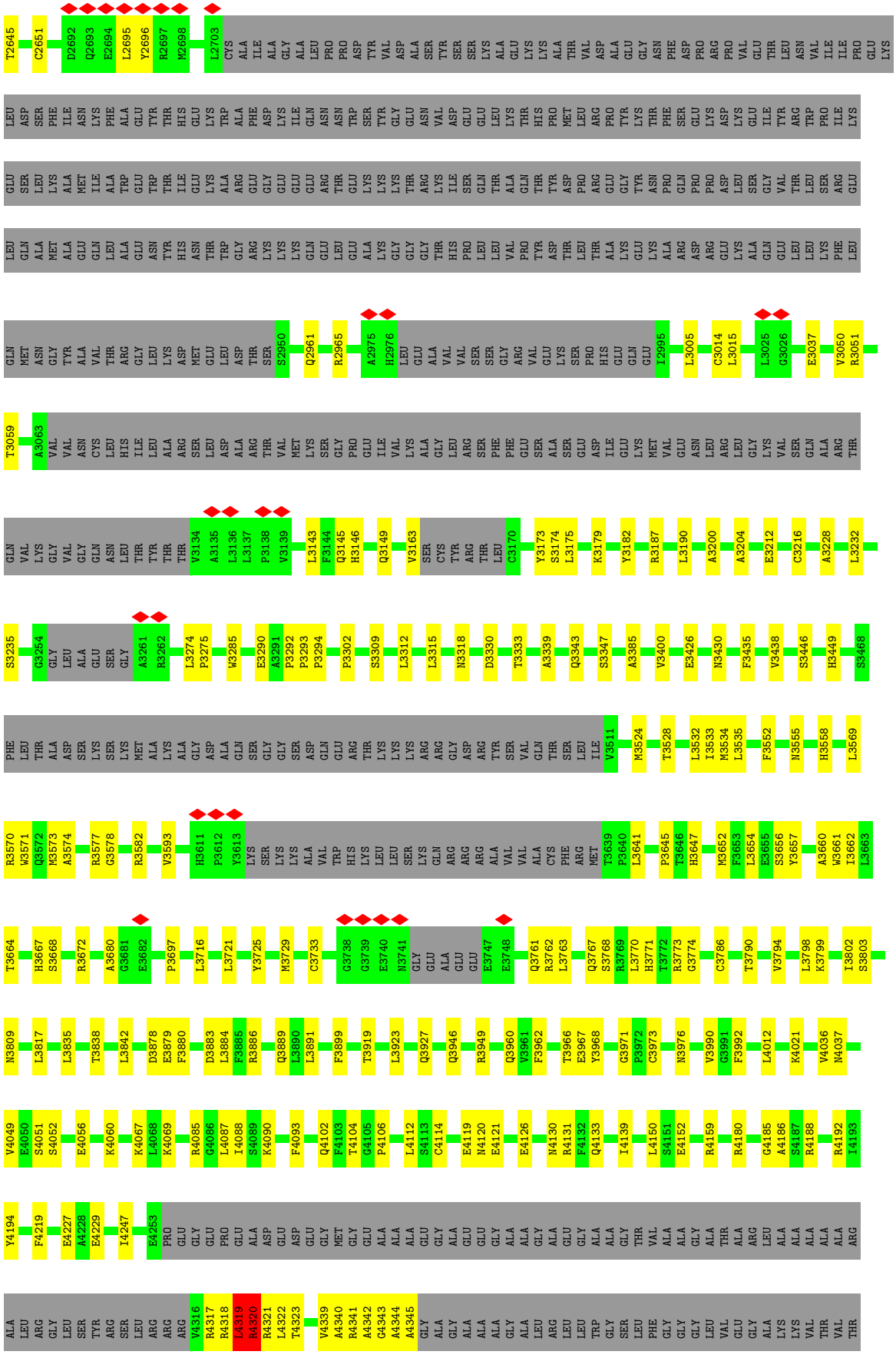




• Molecule 1: Ryanodine receptor 1

Chain B:


R897 D898 D899 N900 K901 R902 L903 H904 P914 E915 P916 E917 R918 S925 L929 H938 V939 A942 D943 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 L972 L977 T978 P979 A980 V1001 A1009 VAL GLN ASP ILE PRO ALA ARG ARG
ASN PRO R1020 Y1024 L1027 D1028 D1037 Q1041 R1044 T1045 L1046 L1047 G1048 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 K1079 V1083 W1088 Y1089 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 P1111
E1114 L1115 V1123 G1126 H1127 R1128 F1139 G1140 R1141 P1142 W1143 Q1144 D1147 V1148 C1151 M1152 I1153 D1154 L1155 N1158 I1161 N1165 D1172 E1176 T1177 R1180 E1183 F1188 L1189 P1190 G1195 Q1198 G1205 Q1206 D1207 V1208 R1212 A1215 G1218 L1219
Q1220 E1221 G1222 F1223 E1224 I1228 N1229 F1238 S1239 K1240 P1243 H1252 P1253 H1254 Y1255 R1259 C1269 H1274 L1287 L1293 P1294 V1295 Q1296 F1297 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 GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN
LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP ASN ARG ASP ASP PRO GLU ILE ILE LEU ASN T1430 Y1434 V1437 R1438 V1439 W1449 W1452 V1453 T1454 P1455 D1456
Y1457 H1458 Q1459 H1460 N1463 V1469 T1473 G1481 N1482 V1483 K1488 C1492 V1495 W1496 G1497 V1501 S1502 P1503 G1507 R1508 V1515 C1518 L1526 N1532 G1533 K1534 E1535 S1536 N1537 T1538 F1539 F1540 Q1541 V1542 E1543 P1544 V1554 L1555 P1556 F1564 GLU LEU GLY LYS GLN
LYS ASN ILE M1573 P1574 L1575 S1576 A1577 A1578 M1579 F1580 R1584 C1591 R1594 L1600 M1601 P1602 W1605 S1606 R1607 M1608 P1609 N1610 V1615 GLU THR ARG ARG ALA GLY E1622 W1626 Q1629 P1633 M1637 A1638 L1639 C1647 M1648 D1649 I1650 L1651 E1652 L1653 S1654 E1655 D1658 L1659
Q1660 H1663 T1666 R1671 A1675 L1676 G1677 R1680 H1683 L1694 E1699 G1705 P1706 L1707 R1708 Y1712 L1715 I1716 S1717 M1730 I1735 P1750 G1755 V1765 G1766 S1770 L1771 R1772 A1788 ALA GLY VAL ALA E1793 A1796 R1797 P1800 E1805
R1808 D1809 K1810 M1814 A1826 P1829 G1832 S1833 V1834 E1835 F1836 Q1837 F1838 V1839 P1840 V1841 L1842 V1859 K1860 Q1861 I1862 L1863 K1864 M1865 I1866 E1867 P1868 F1871 E1874 GLU 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 L1931 P1932 V1935 M1939 Q1952 E1956 L1969 Q1970 Q1973 R1976 L2009 L2010 H2011 F2012 C2021 P2022 R2028 C2042 G2043 I2044 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 S2093 L2094 V2098 V2102 M2120 L2131 L2135 L2138 P2139 Y2142
V2149 T2152 L2155 R2163 S2164 I2167 V2168 E2174 E2175 S2181 I2182 I2185 H2194 L2197 V2207 V2210 L2215 T2220 I2223 P2226 K2227 M2228 V2229 C2240 S2243 N2246 Q2247 D2252 S2279 E2296 V2299 S2300 Y2301 L2302 K2316 G2317 Y2318
W2323 N2324 P2325 Y2331 L2332 F2340 I2358 L2368 L2376 A2383 I2386 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 L2418 G2419 H2420 M2423 R2435 P2438 H2441 Q2444 R2454 A2455 I2456 L2457 R2458
S2459 L2460 L2463 D2464 L2474 L2479 GLY LYS ASP GLY ALA LEU VAL Q2487 F2494 V2495 P2496 D2497 F2505 Y2510 G2511 I2512 T2538 A2539 L2548 R2552 L2556 A2557 V2558 L2559 A2570 H2574 V2586 Y2587 S2590 R2591 K2597 I2603 A2637 P2640 L2644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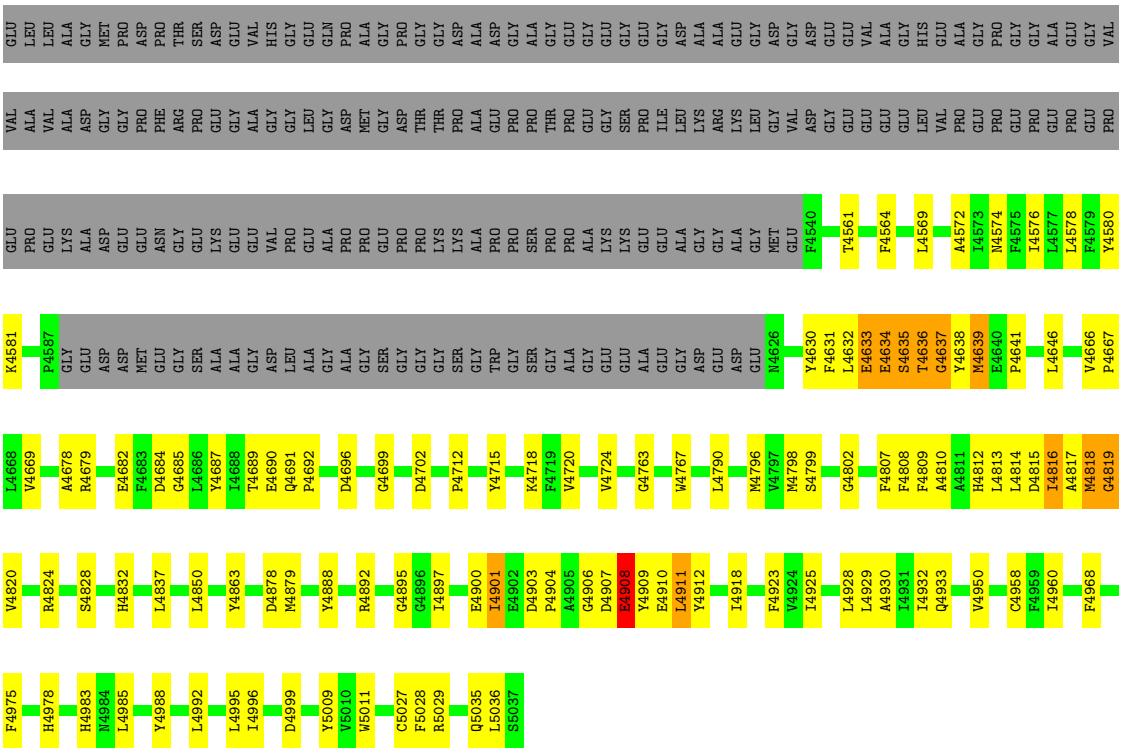
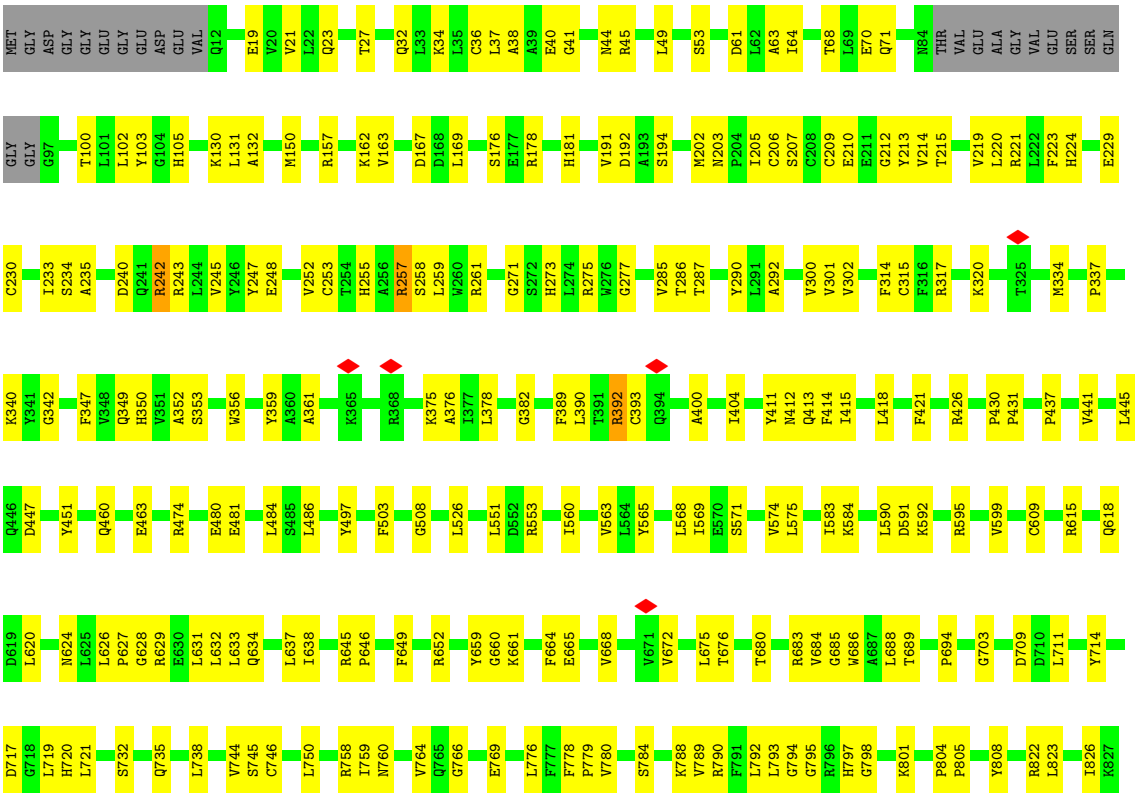
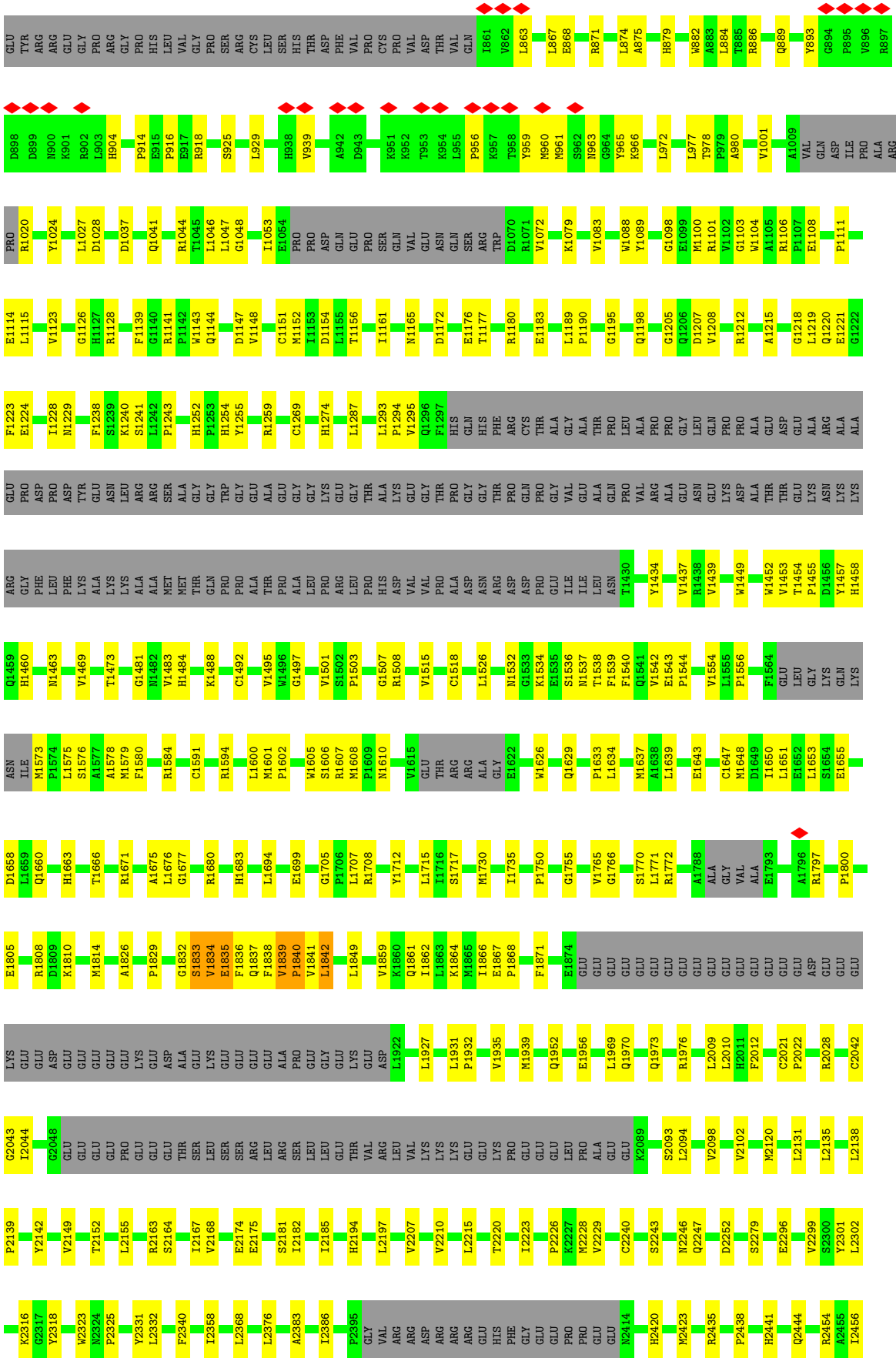
LEU ASP SER PHE ILE ASN LYS PHE ALA GLU TYR THR HIS GLU LYS TRP ALA PHE ASP LYS ILE GLN ASN ASN TRP SER TYR GLY GLU ASN VAL ASP GLU GLU LEU LYS THR HIS PRO MET LEU ARG PRO TYR LYS THR PHE SER GLU LYS GLU ILE TYR ARG TRP PRO ILE LYS
GLU SER LEU LYS ALA MET ILE ALA TRP GLU TRP THR ILE GLU LYS ALA ARG GLU 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 ASP ARG GLU LYS ASP LEU SER SER GLY VAL THR LEU SER ARG GLU
LEU GLN ALA MET ALA GLU GLN LEU ALA GLU ASN TYR HIS ASN THR TRP GLY ARG LYS LYS LYS GLN GLU LEU GLU ALA LYS GLY GLY THR HIS PRO LEU LEU VAL PRO TYR ASP THR LEU THR ALA LYS LYS GLU LYS ALA GLN GLU LEU LEU LEU LYS PHE LEU
GLN MET ASN GLY TYR ALA VAL THR ARG GLY LEU LEU LYS ASP MET GLU LEU ASP THR SER S2950 Q2961 R2965 A2975 H2976 LEU GLU ALA VAL VAL SER SER GLY ARG VAL GLU LYS SER PRO HIS GLU GLN GLU I2995 L3005 C3014 L3015 L3025 G3026 E3037 V3050 R3051
T3059 A3063 VAL VAL ASN CYS LEU HIS ILE LEU ALA ARG SER LEU ASP ALA ARG THR VAL VAL MET LYS SER GLY PRO GLU ILE VAL LYS ALA GLY LEU ARG SER PHE PHE GLU SER ALA SER GLU ASP ILE GLU LYS MET VAL GLU ASN LEU ARG LEU GLY LYS VAL SER GLN ALA ARG THR
GLN VAL LYS GLY VAL GLY GLN ASN LEU THR TYR THR THR V3134 A3135 L3136 L3137 P3138 V3139 L3143 F3144 Q3145 H3146 Q3149 V3163 SER CYS TYR ARG THR LEU C3170 Y3173 S3174 L3175 K3179 Y3182 R3187 L3190 A3200 A3204 E3212 C3216 A3228 L3232
S3235 G3254 GLY LEU ALA GLU SER GLY A3261 R3262 L3274 P3275 W3285 E3290 A3291 P3292 P3293 P3294 P3302 S3309 L3312 L3315 N3318 D3330 T3333 A3339 Q3343 S3347 A3385 V3400 E3426 N3430 F3435 V3438 S3446 H3449 S3468
PHE LEU THR ALA ASP SER LYS SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG TYR SER VAL GLN THR SER LEU ILE V3511 M3524 T3528 L3532 I3533 M3534 L3535 F3552 N3555 H3558 L3569
R3570 W3571 Q3572 M3573 A3574 R3577 G3578 R3582 V3593 H3611 P3612 Y3613 LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3640 L3641 P3645 T3646 H3647 M3652 F3653 L3654 E3655 S3656 Y3657 A3660 W3661 I3662 L3663
T3664 H3667 S3668 R3672 A3680 G3681 E3682 P3697 L3716 L3721 Y3725 M3729 C3733 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 Q3761 R3762 L3763 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 C3786 T3790 V3794 L3798 K3799 I3802 S3803
N3809 L3817 L3835 T3838 L3842 D3878 E3879 F3880 D3883 L3884 F3885 R3886 Q3889 L3890 L3891 F3899 T3919 L3923 Q3927 Q3946 R3949 Q3960 V3961 F3962 T3966 E3967 Y3968 G3971 P3972 C3973 N3976 V3990 G3991 F3992 L4012 K4021 V4036 N4037
V4049 E4050 S4051 S4052 E4056 K4060 K4067 L4068 K4069 R4085 G4086 L4087 I4088 S4089 K4090 F4093 Q4102 F4103 T4104 G4105 P4106 L4112 S4113 C4114 E4119 N4120 E4121 E4126 N4130 R4131 F4132 Q4133 I4139 L4150 S4151 E4152 R4159 R4180 G4185 A4186 S4187 R4188 R4192 I4193
Y4194 F4219 E4227 A4228 E4229 I4247 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA GLU GLY GLY ALA GLU GLU GLY GLY ALA ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ARG
ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG V4316 R4317 R4318 L4319 R4320 R4321 L4322 T4323 V4339 A4340 R4341 A4342 G4343 A4344 A4345 GLY ALA GLY ALA ALA ALA GLY ALA ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR

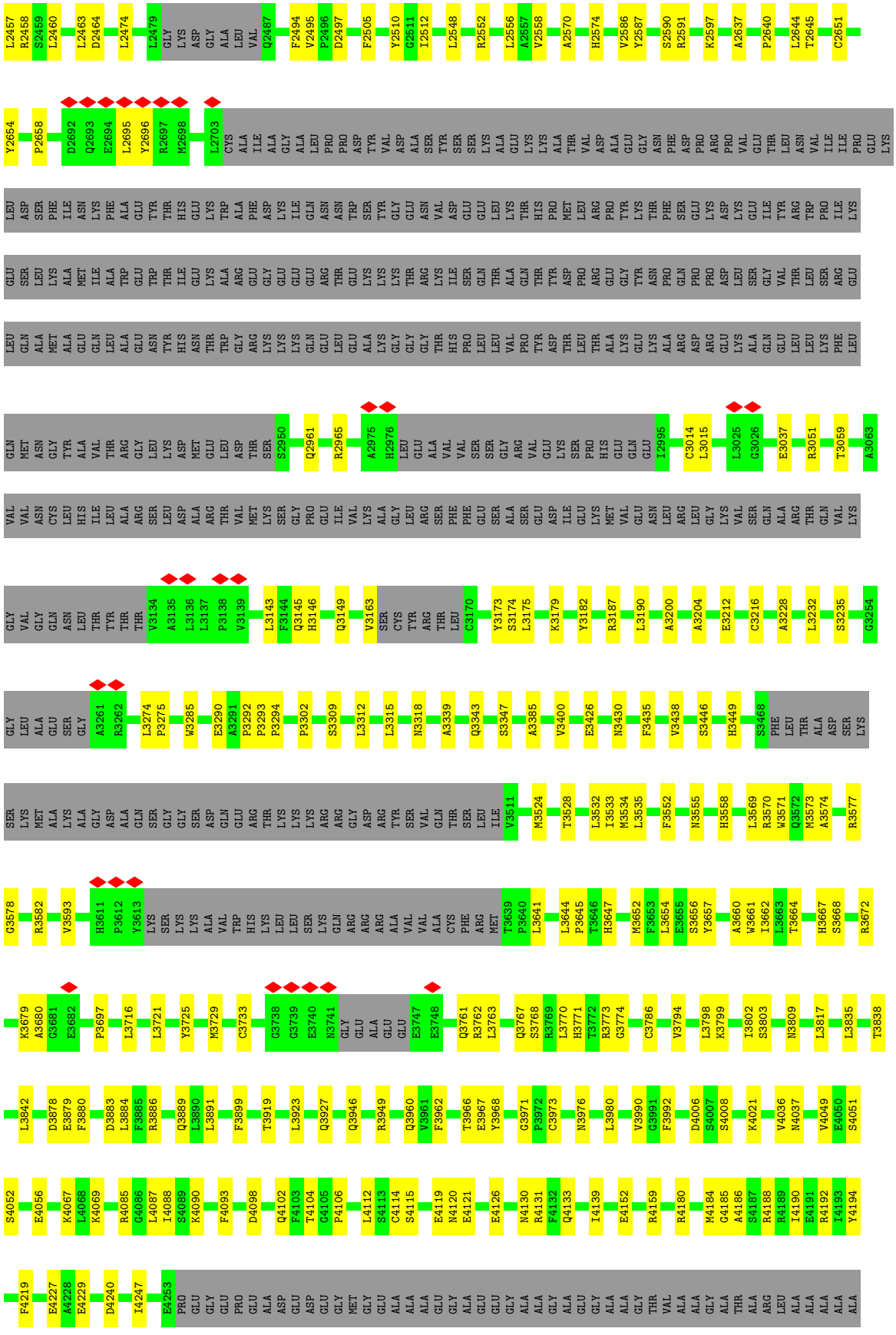


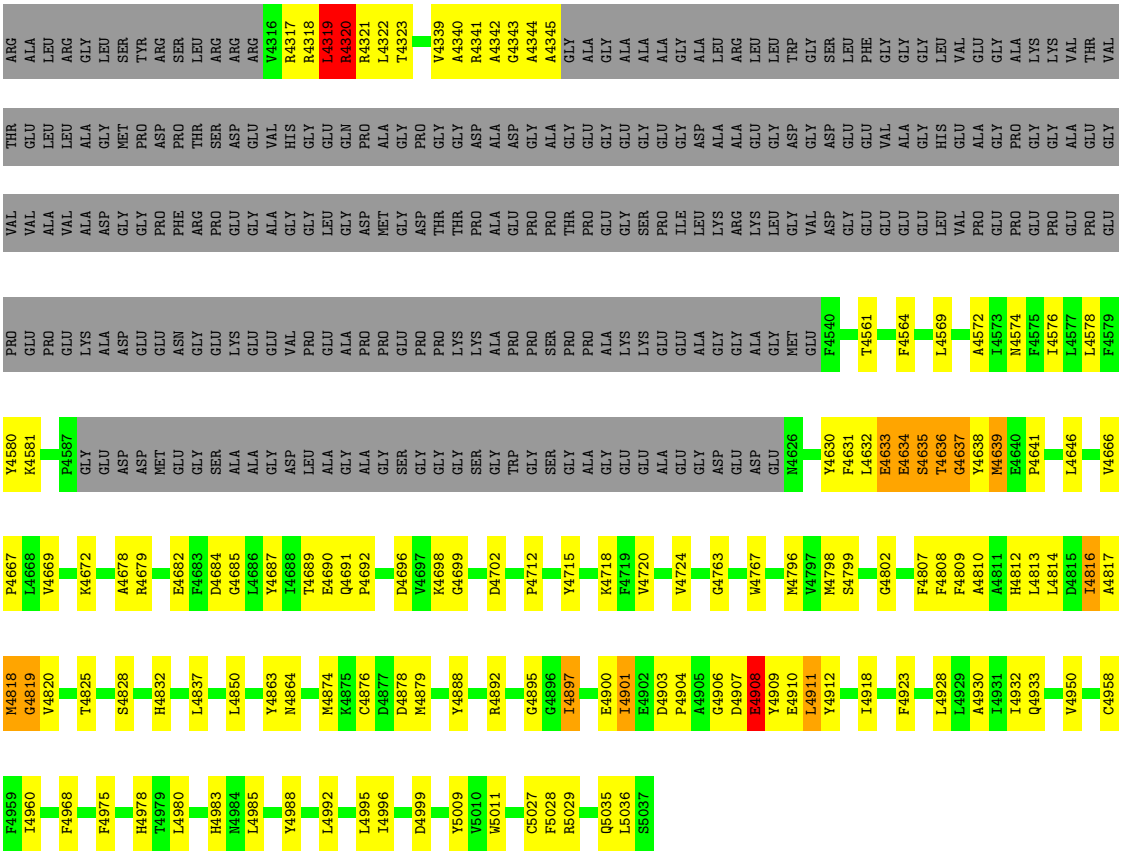
• Molecule 1: Ryanodine receptor 1

Chain C:



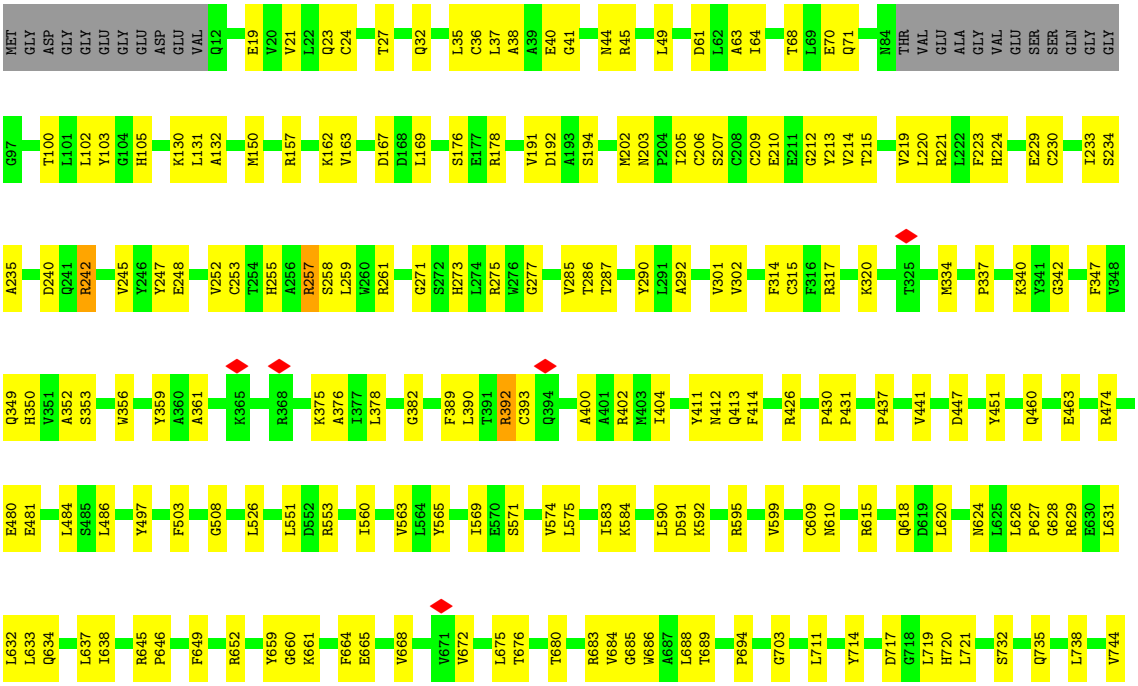


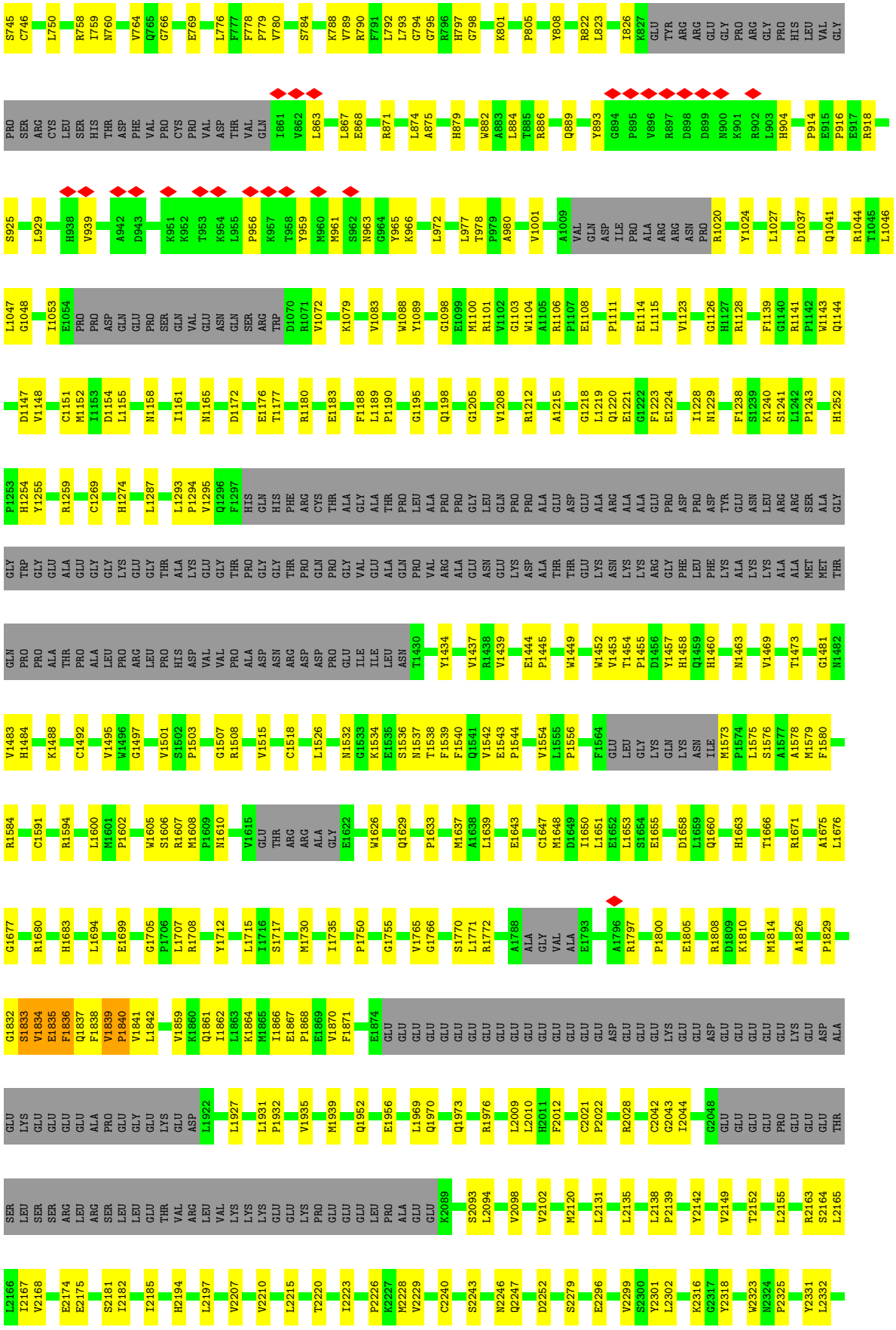


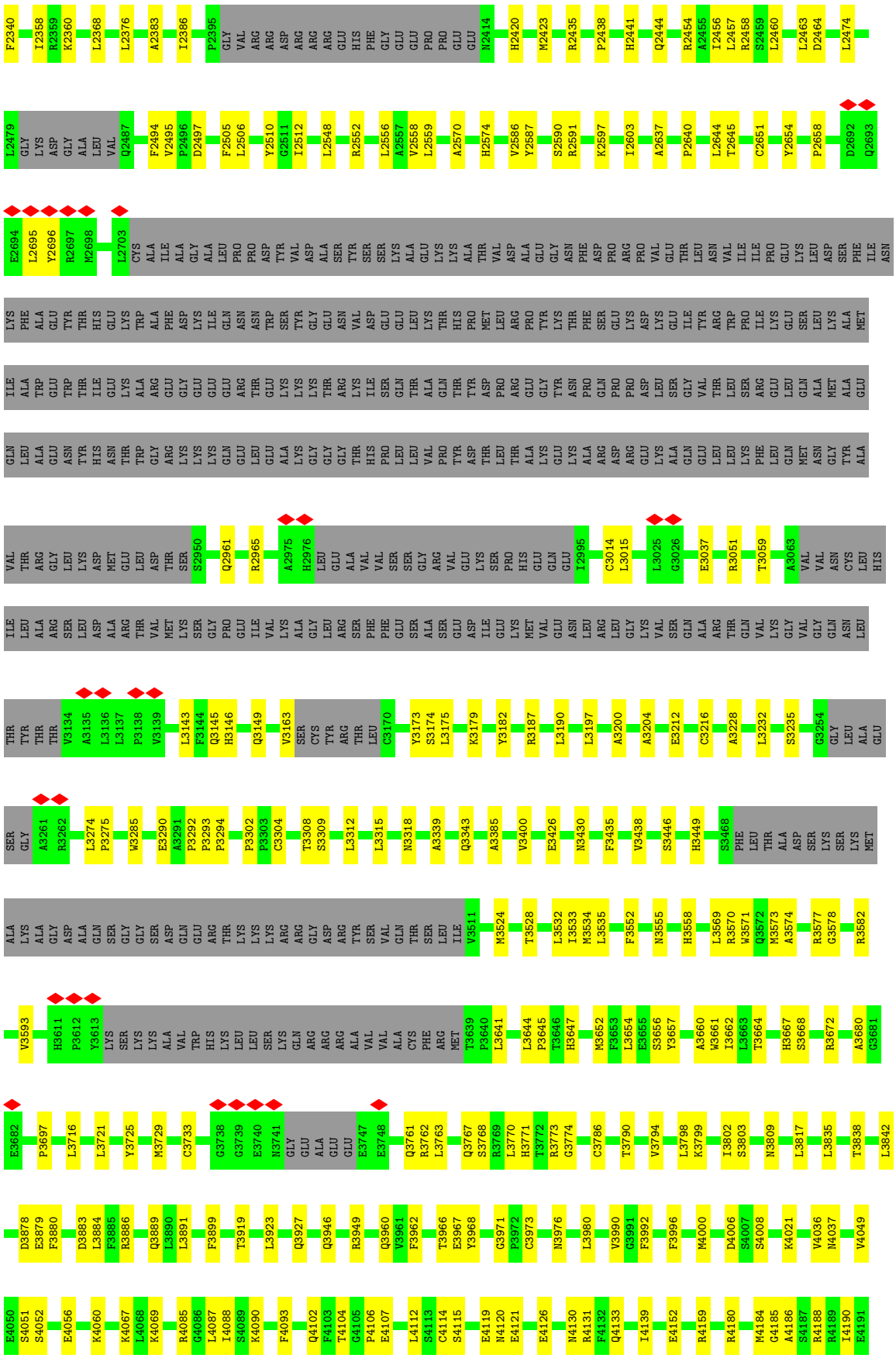


• Molecule 1: Ryanodine receptor 1

Chain D:



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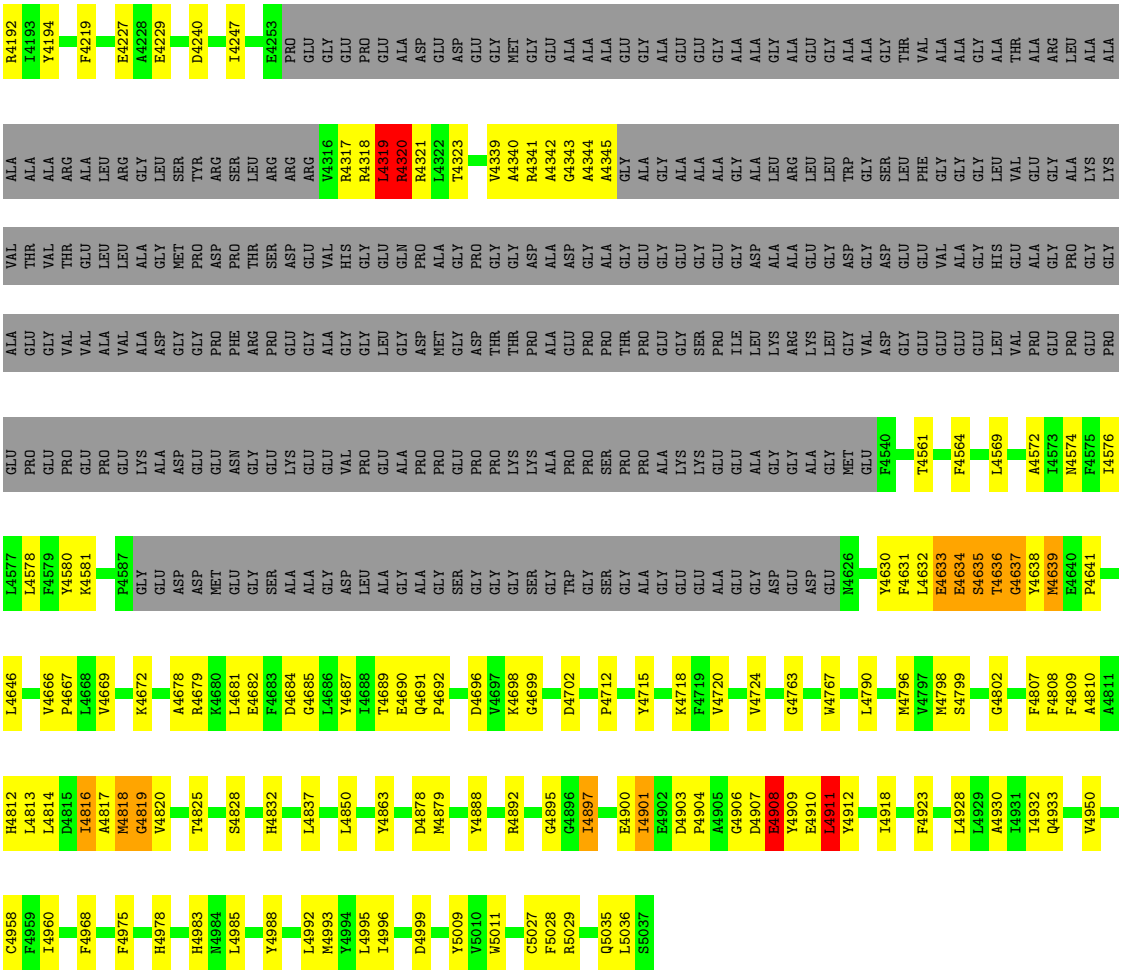
E2694 L2695 Y2696 R2697 M2698 L2703
S2950 Q2961 R2965 A2975 H2976 I2995 C3014 L3015 L3025 G3026 E3037 R3051 T3059 A3063
V3134 A3135 L3136 L3137 P3138 V3139 L3143 F3144 Q3145 H3146 Q3149 V3163 C3170 Y3173 S3174 L3175 K3179 Y3182 R3187 L3190 L3197 A3200 A3204 E3212 C3216 A3228 L3232 S3235 G3254
A3261 R3262 L3274 P3275 W3285 E3290 A3291 P3292 P3293 P3294 P3302 P3303 C3304 T3308 S3309 L3312 L3315 N3318 A3339 Q3343 A3385 V3400 E3426 N3430 F3435 V3438 S3446 H3449 S3468
V3511 M3524 T3528 L3532 I3533 M3534 L3535 F3552 N3555 H3558 L3569 R3570 W3571 Q3572 M3573 A3574 R3577 G3578 R3582
V3593 H3611 P3612 Y3613 T3639 P3640 L3641 L3644 P3645 T3646 H3647 M3652 F3653 L3654 E3655 S3656 Y3657 A3660 W3661 I3662 L3663 T3664 H3667 S3668 R3672 A3680 G3681
E3682 P3697 L3716 L3721 Y3725 M3729 C3733 G3738 G3739 E3740 N3741 E3747 E3748 Q3761 R3762 L3763 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 C3786 T3790 V3794 L3798 K3799 I3802 S3803 N3809 L3817 L3835 T3838 L3842
D3878 E3879 F3880 D3883 L3884 F3885 R3886 Q3889 L3890 L3891 F3899 T3919 L3923 Q3927 Q3946 R3949 Q3960 V3961 F3962 T3966 E3967 Y3968 G3971 P3972 C3973 N3976 L3980 V3990 G3991 F3992 F3996 M4000 D4006 S4007 S4008 K4021 V4036 N4037 V4049
E4050 S4051 S4052 E4056 K4060 K4067 L4068 K4069 R4085 G4086 L4087 I4088 S4089 K4090 F4093 Q4102 F4103 T4104 G4105 P4106 E4107 L4112 S4113 C4114 S4115 E4119 N4120 E4121 E4126 N4130 R4131 F4132 Q4133 I4139 E4152 R4159 R4180 M4184 G4185 A4186 S4187 R4188 R4189 I4190 E4191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ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG V4316 R4317 R4318 L4319 R4320 R4321 L4322 T4323 V4339 A4340 R4341 A4342 G4343 A4344 A4345 GLY
VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY GLU GLU VAL ALA ALA GLY HIS GLU ALA GLY PRO GLU GLY
ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO
GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 T4561 F4564 L4569 A4572 I4573 N4574 F4575 I4576
L4577 L4578 F4579 Y4580 K4581 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLY ASP GLU ASP GLU M4626 Y4630 F4631 L4632 E4633 E4634 S4635 T4636 G4637 Y4638 M4639 E4640 P4641
L4646 V4666 P4667 L4668 V4669 K4672 A4678 R4679 K4680 L4681 E4682 F4683 D4684 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 D4696 V4697 K4698 G4699 D4702 P4712 Y4715 K4718 F4719 V4720 V4724 G4763 W4767 L4790 M4796 V4797 M4798 S4799 G4802 F4807 F4808 F4809 A4810 A4811
H4812 L4813 L4814 D4815 I4816 A4817 M4818 G4819 V4820 T4825 S4828 H4832 L4837 L4850 Y4863 D4878 M4879 Y4888 R4892 G4895 G4896 I4897 E4900 I4901 F4902 D4903 P4904 A4905 G4906 D4907 E4908 Y4909 E4910 L4911 Y4912 I4918 F4923 L4928 L4929 A4930 I4931 I4932 Q4933 V4950
C4958 F4959 I4960 F4968 F4975 H4978 H4983 N4984 L4985 Y4988 L4992 M4993 Y4994 L4995 I4996 D4999 Y5009 V5010 W5011 C5027 F5028 R5029 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	279704	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.162	Depositor
Minimum map value	-1.419	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	643.2, 643.2, 643.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.072, 1.072, 1.072	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, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.32	0/30188	0.46	0/41084
1	B	0.32	0/30188	0.46	0/41084
1	C	0.32	0/30188	0.46	0/41084
1	D	0.32	0/30188	0.46	0/41084
All	All	0.32	0/120752	0.46	0/164336

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	29568	0	27784	634	0
1	B	29568	0	27784	641	0
1	C	29568	0	27784	643	0
1	D	29568	0	27784	647	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	118280	0	111136	2512	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 11.

The worst 5 of 2512 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:B:4634:GLU:HG3	1:B:4636:THR:HG22	1.46	0.97
1:C:4634:GLU:HG3	1:C:4636:THR:HG22	1.46	0.97
1:A:4634:GLU:HG3	1:A:4636:THR:HG22	1.46	0.94
1:D:4634:GLU:HG3	1:D:4636:THR:HG22	1.46	0.94
1:D:4069:LYS:HB2	1:D:4133:GLN:HE22	1.41	0.85

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	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
1	B	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
1	C	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
1	D	3934/5037 (78%)	3496 (89%)	423 (11%)	15 (0%)	30	61
All	All	15736/20148 (78%)	13984 (89%)	1692 (11%)	60 (0%)	32	61

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4808	PHE
1	B	4808	PHE
1	C	4808	PHE
1	D	4808	PHE
1	A	1835	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	2905/4276 (68%)	2882 (99%)	23 (1%)	79 87
1	B	2905/4276 (68%)	2882 (99%)	23 (1%)	79 87
1	C	2905/4276 (68%)	2882 (99%)	23 (1%)	79 87
1	D	2905/4276 (68%)	2882 (99%)	23 (1%)	79 87
All	All	11620/17104 (68%)	11528 (99%)	92 (1%)	77 87

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4633	GLU
1	D	392	ARG
1	C	4635	SER
1	C	4901	ILE
1	D	4120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1041	GLN
1	C	3976	ASN
1	D	3976	ASN
1	C	1165	ASN
1	C	3146	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

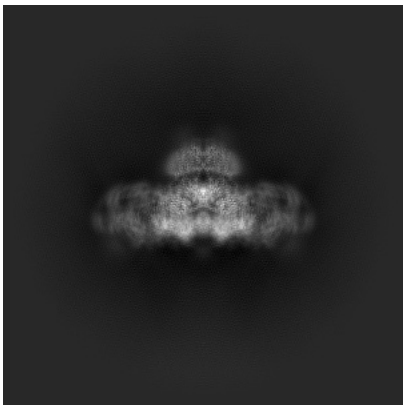
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38048. These allow visual inspection of the internal detail of the map and identification of artifacts.

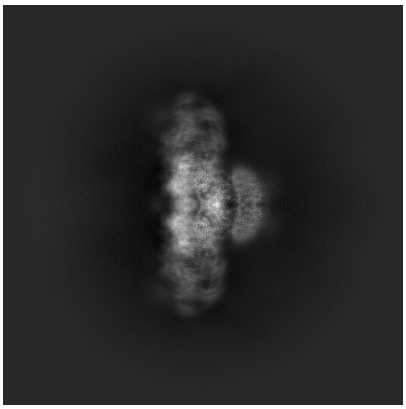
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

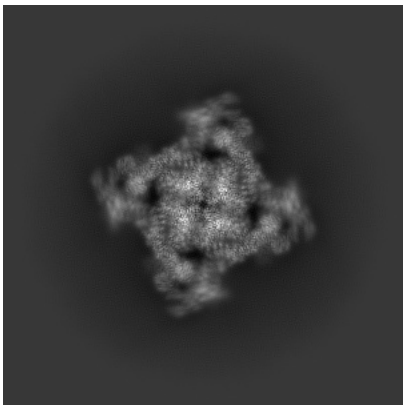
6.1.1 Primary map



X

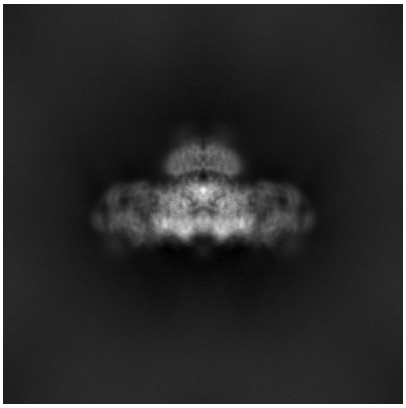


Y

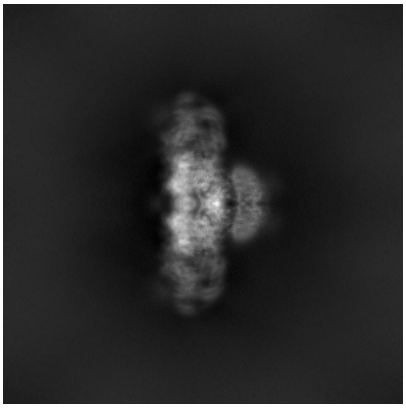


Z

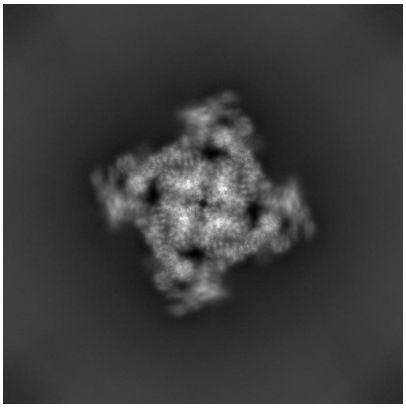
6.1.2 Raw map



X



Y

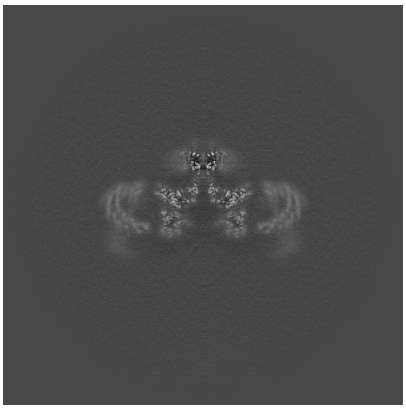


Z

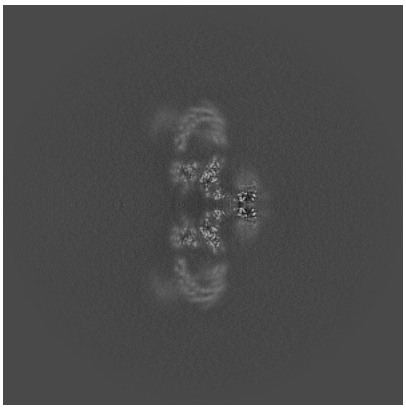
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

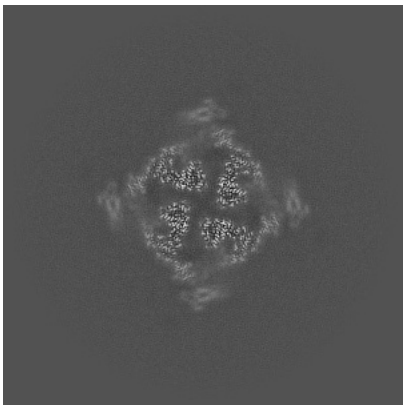
6.2.1 Primary map



X Index: 300

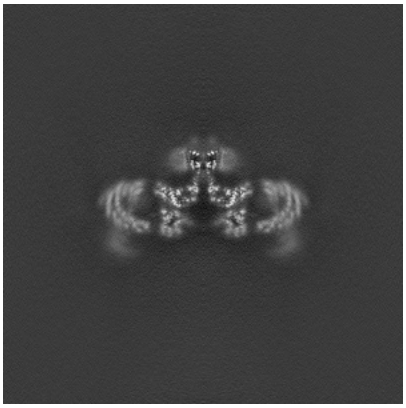


Y Index: 300

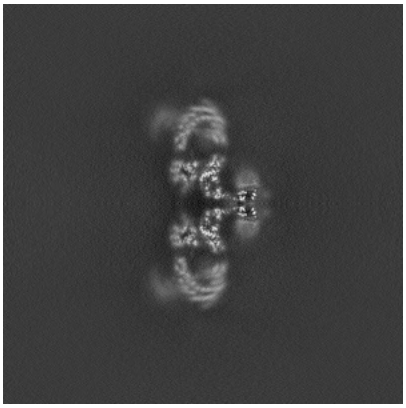


Z Index: 300

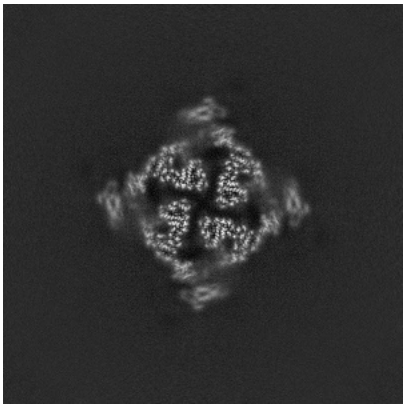
6.2.2 Raw map



X Index: 300



Y Index: 300

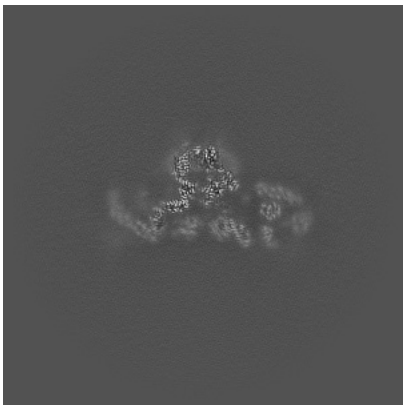


Z Index: 300

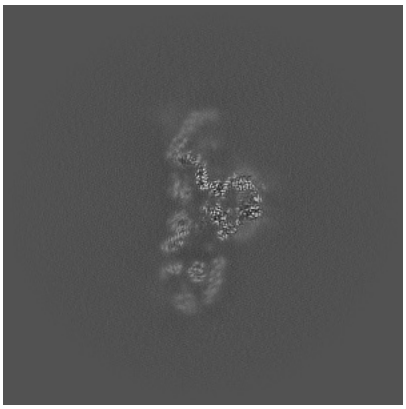
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

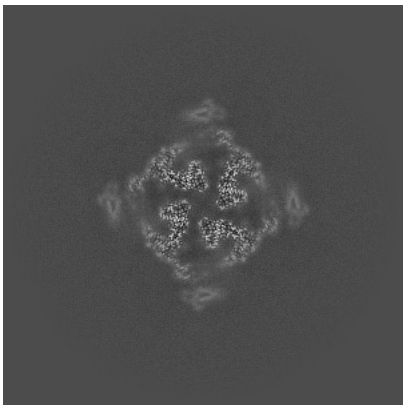
6.3.1 Primary map



X Index: 321

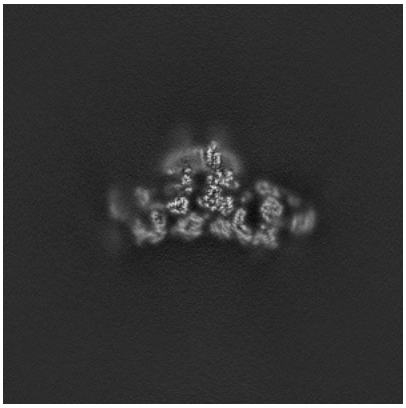


Y Index: 321

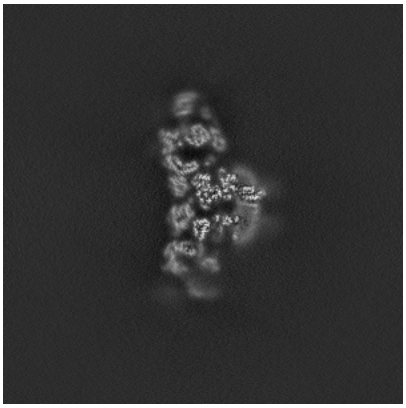


Z Index: 302

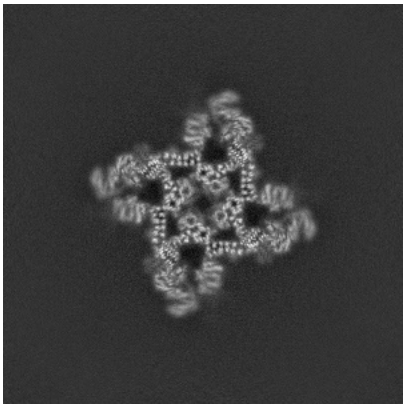
6.3.2 Raw map



X Index: 329



Y Index: 271

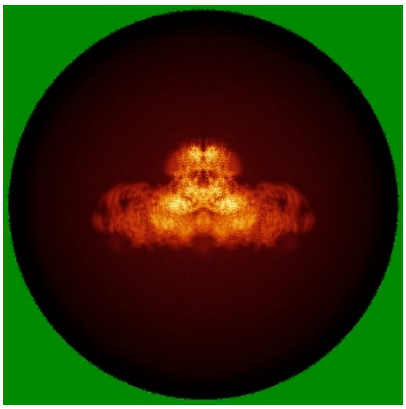


Z Index: 273

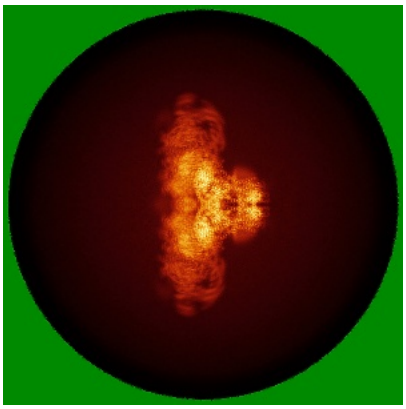
The images above show the largest variance slices of the map in three orthogonal directions.

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

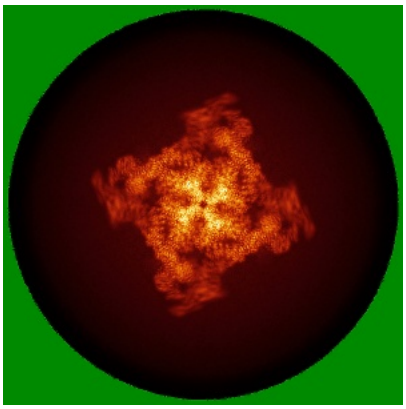
6.4.1 Primary map



X

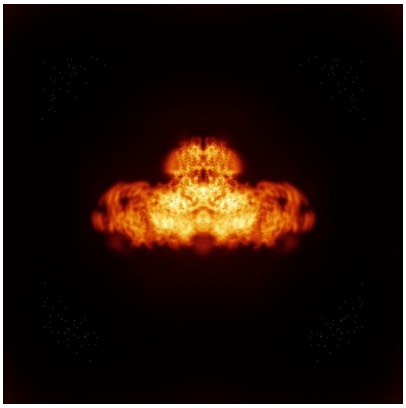


Y

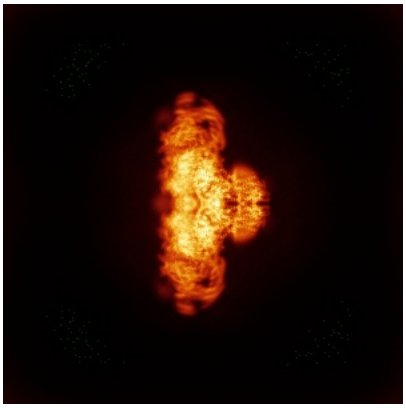


Z

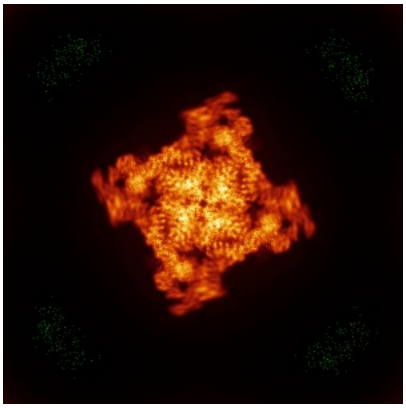
6.4.2 Raw map



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 0.182. 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.

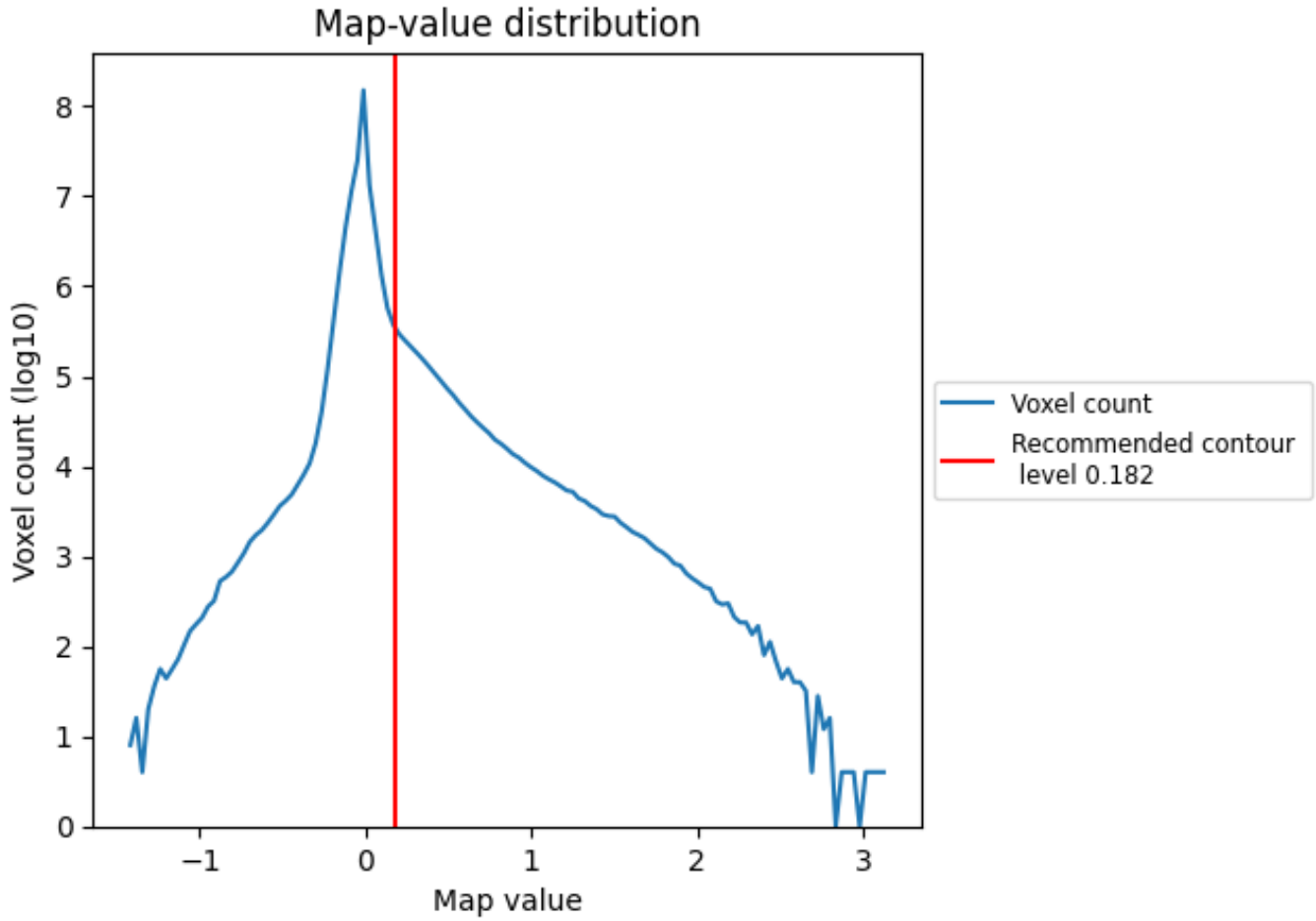
6.6 Mask visualisation (i)

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

7 Map analysis

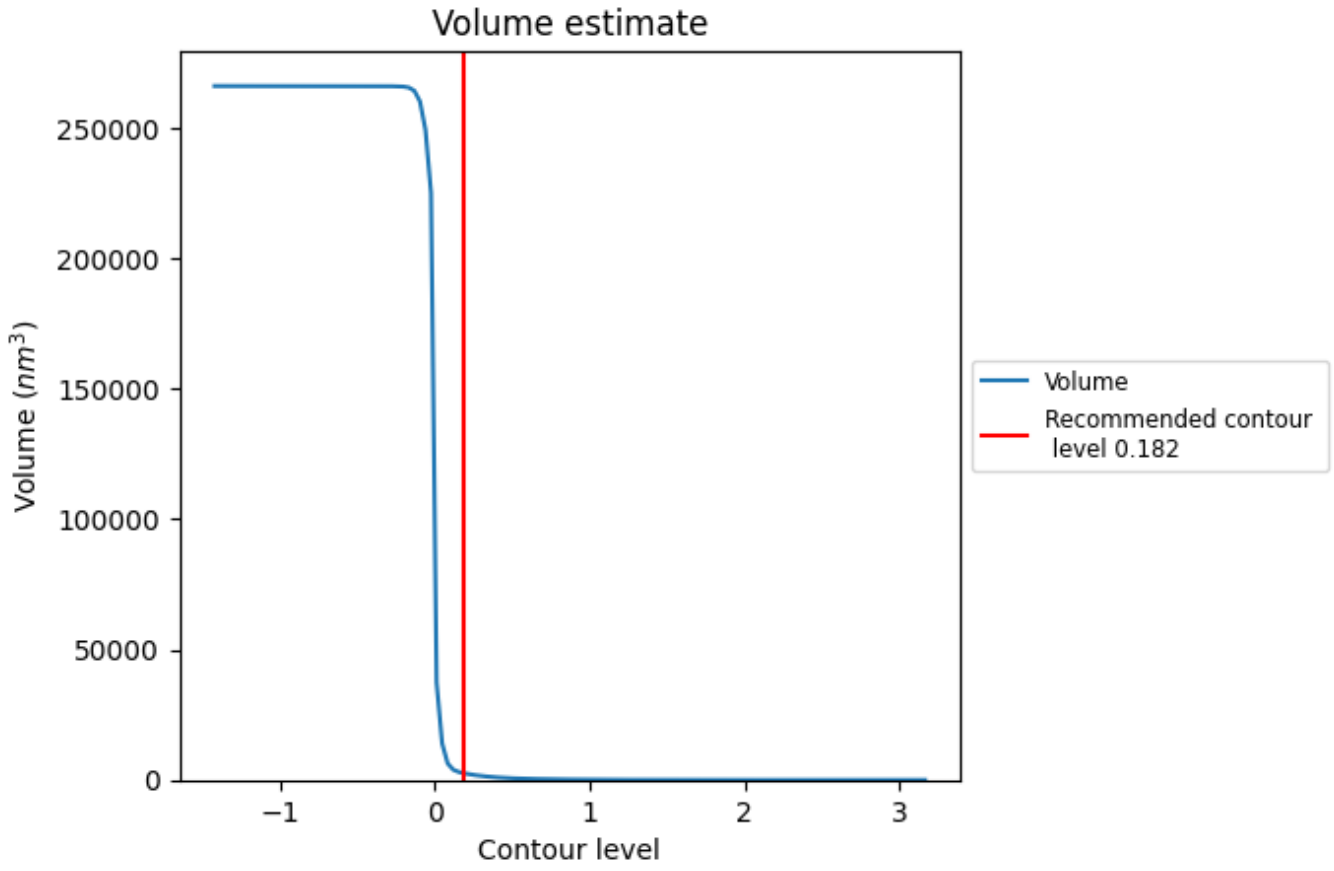
This section contains the results of statistical analysis of the map.

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.

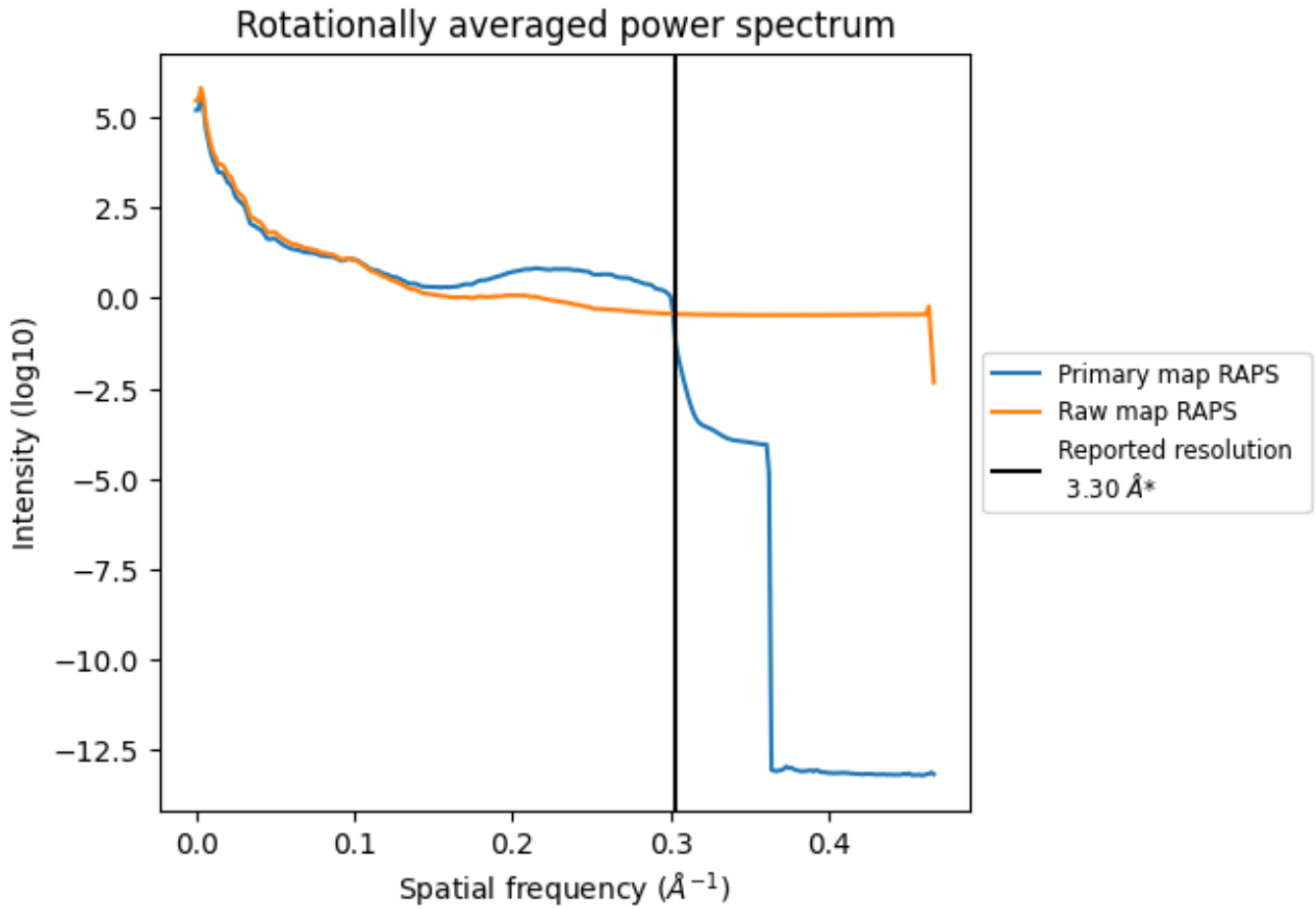
7.2 Volume estimate (i)



The volume at the recommended contour level is 2676 nm^3; this corresponds to an approximate mass of 2418 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)

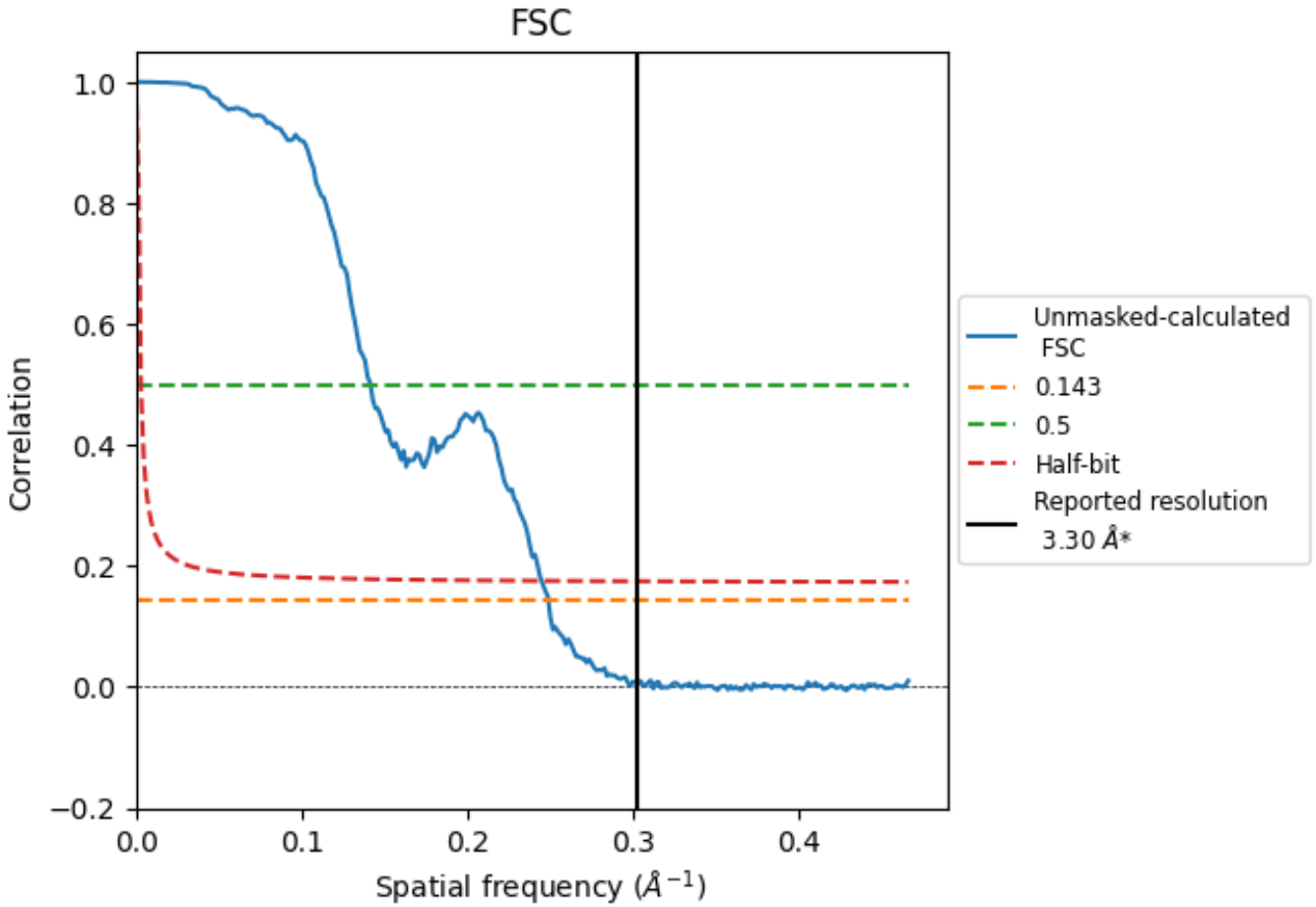


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

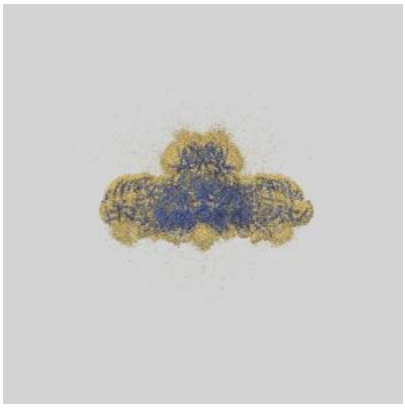
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.02	7.06	4.08

*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 4.02 differs from the reported value 3.3 by more than 10 %

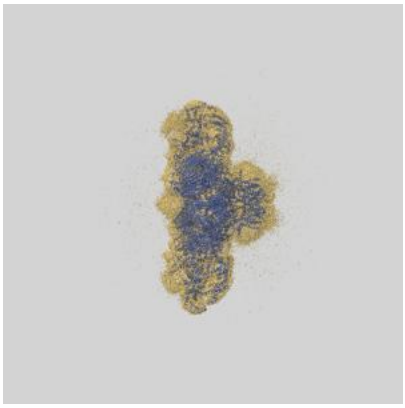
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38048 and PDB model 8X4E. Per-residue inclusion information can be found in section 3 on page 4.

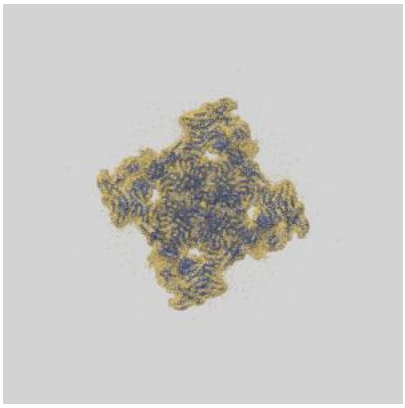
9.1 Map-model overlay



X



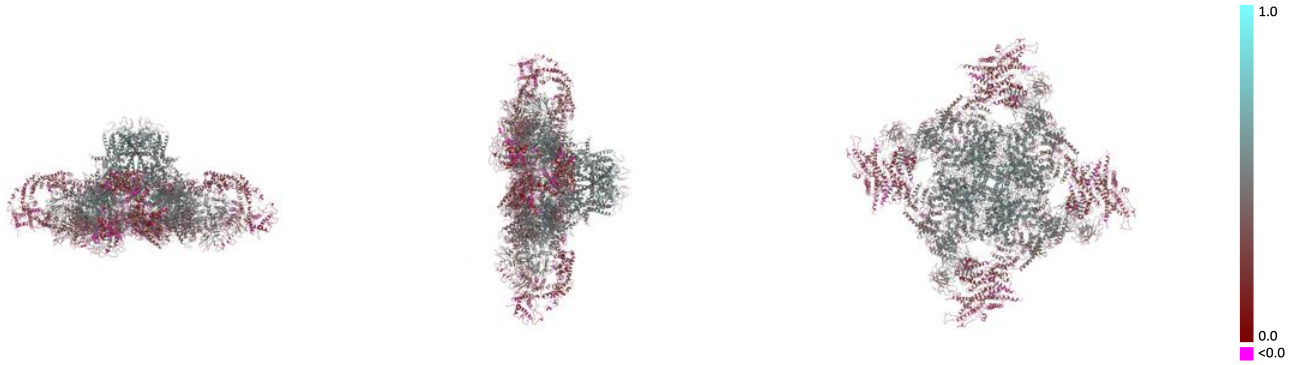
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.182 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.

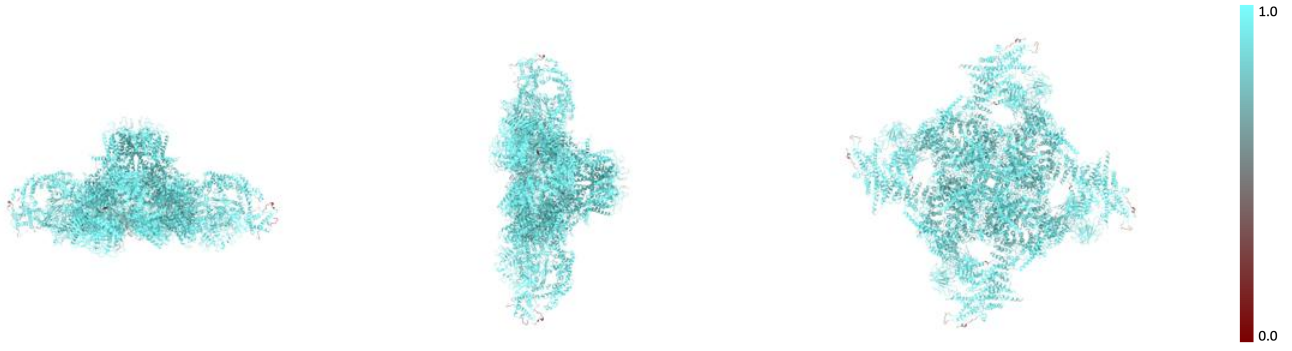
9.2 Q-score mapped to coordinate model



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.

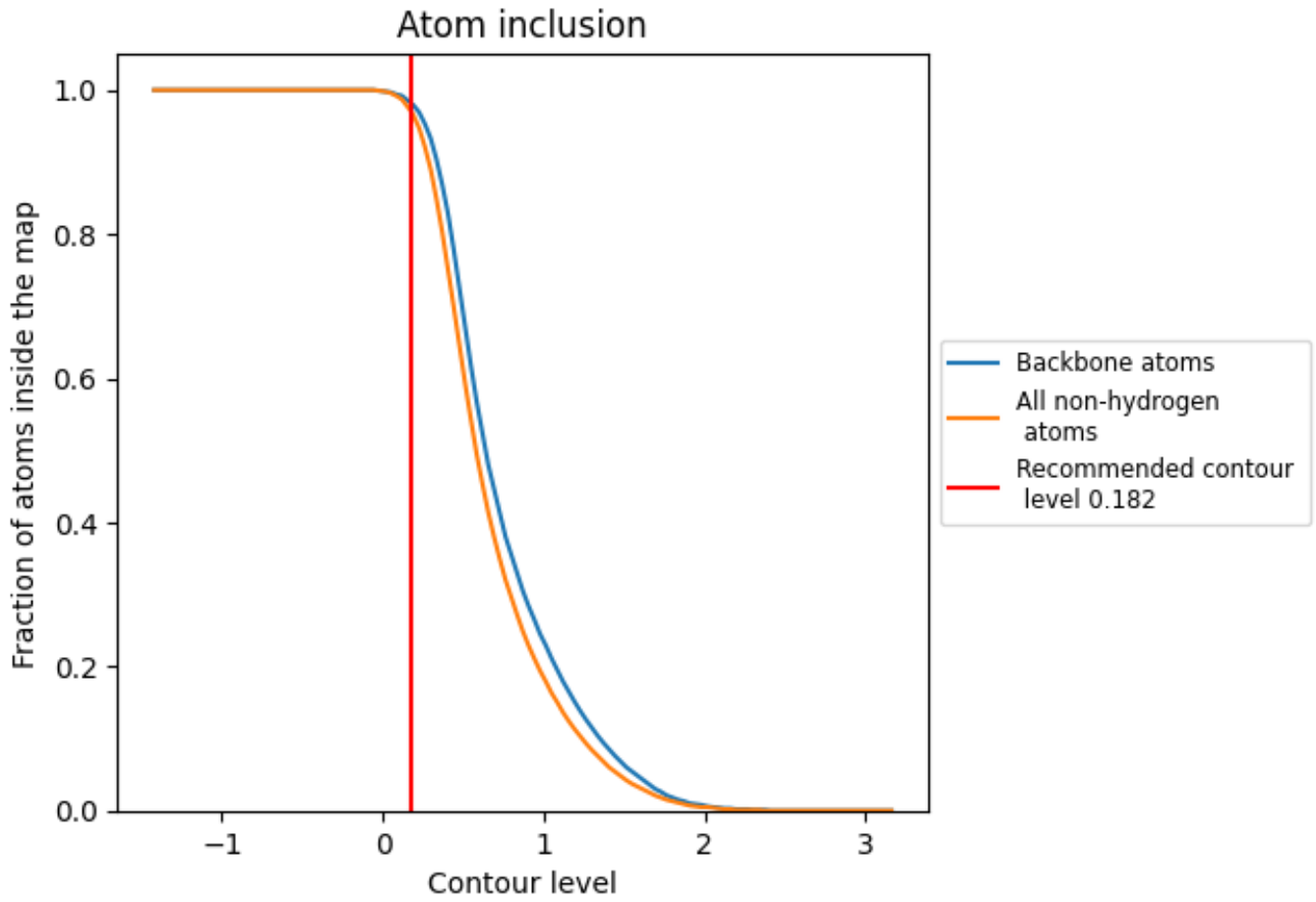
9.3 Atom inclusion mapped to coordinate model



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 (0.182).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9690	0.3850
A	0.9690	0.3840
B	0.9690	0.3850
C	0.9690	0.3850
D	0.9690	0.3850