wwPDB EM Validation Summary Report (i)

Feb 25, 2024 – 09:47 AM EST

PDB ID	:	7JMI
EMDB ID	:	EMD-22395
Title	:	Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots - Frame 29 - State 3 (S3)
Authors	:	Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on	:	2020-07-31
Resolution	:	4.50 Å(reported)
Based on initial model	:	5TB4

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:

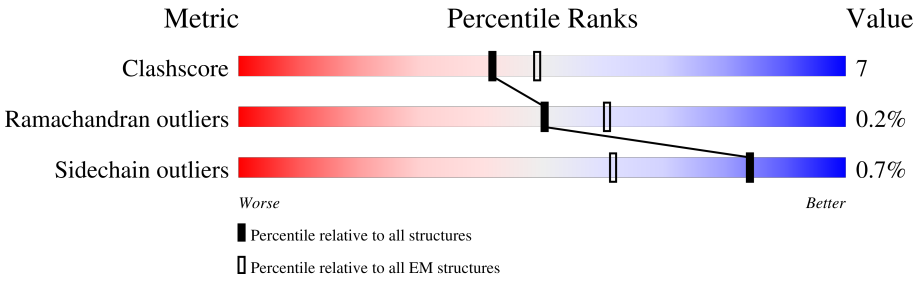
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	107	18% 74% 26%
1	F	107	21% 74% 26%
1	H	107	33% 77% 23%
1	J	107	27% 73% 27%
2	B	4687	21% 74% 14% 11%
2	E	4687	23% 74% 15% 11%
2	G	4687	27% 74% 14% 11%
2	I	4687	26% 74% 14% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called ryanodine receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

Interest" by depositor).

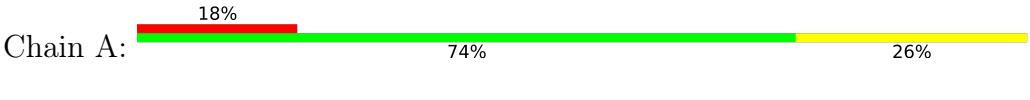
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0

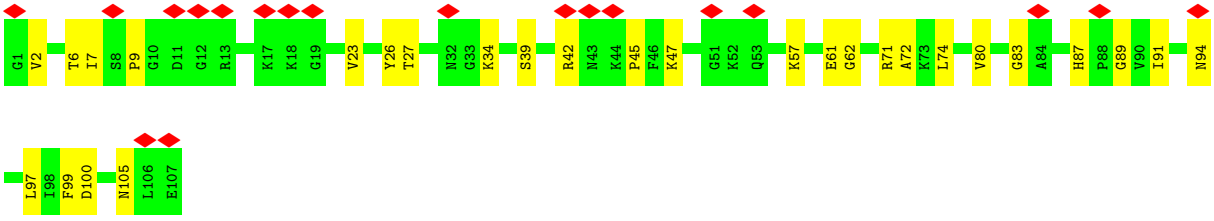
3 Residue-property plots (i)

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

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

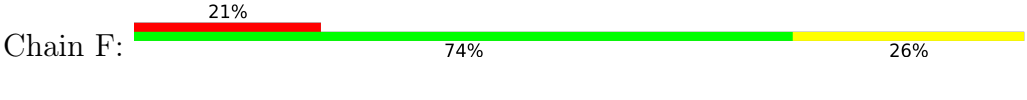
Chain A:

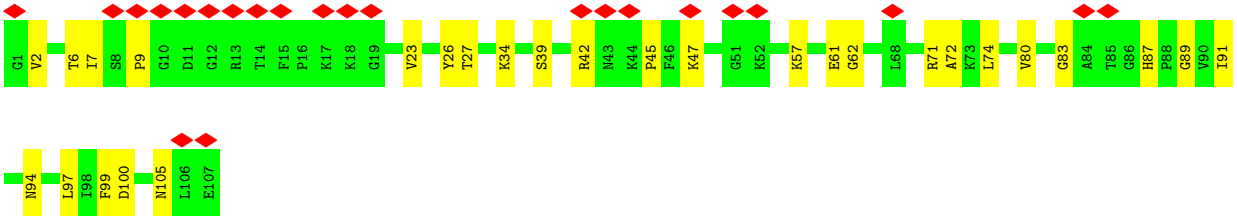




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

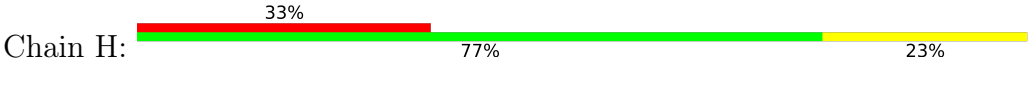
Chain F:

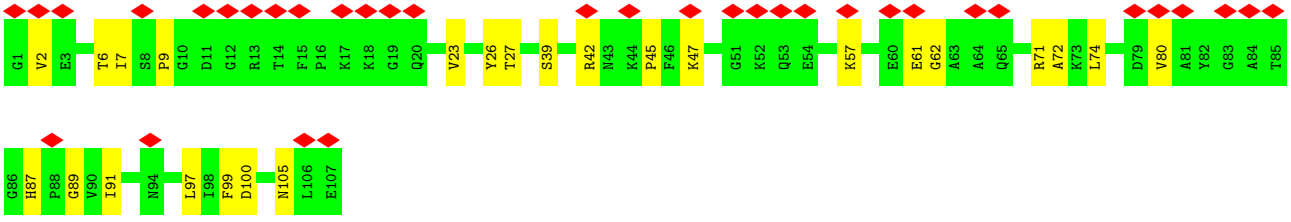




• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

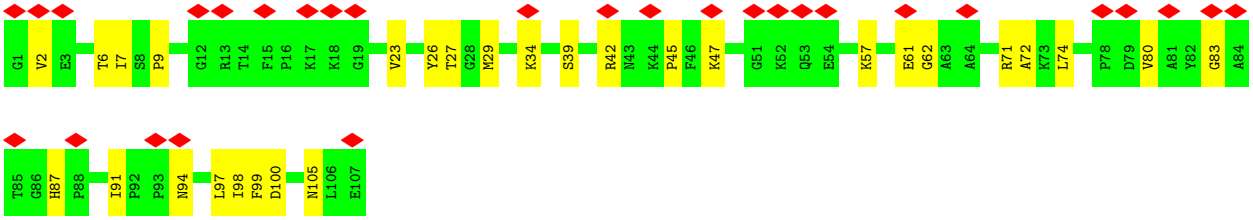
Chain H:





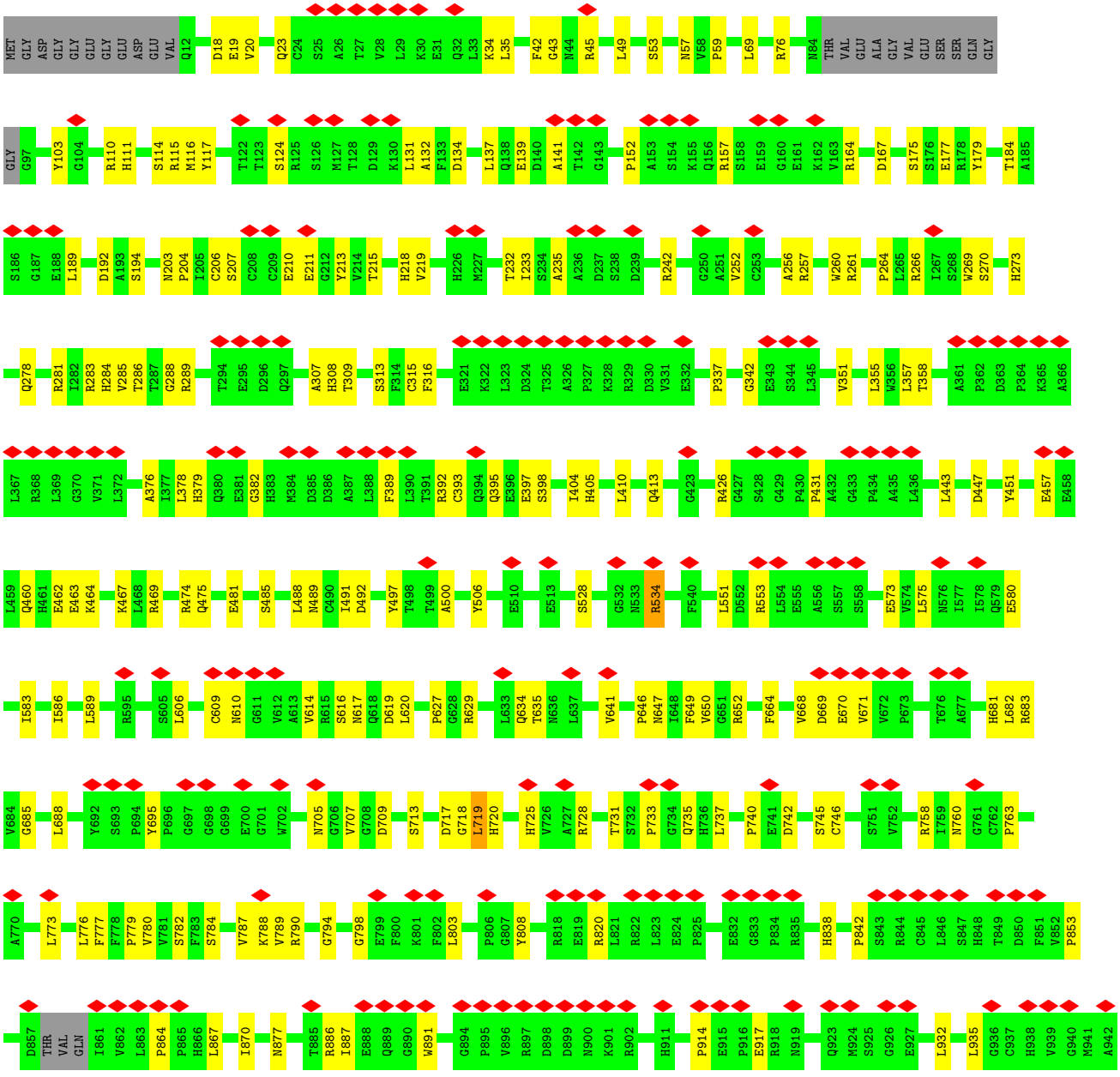
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

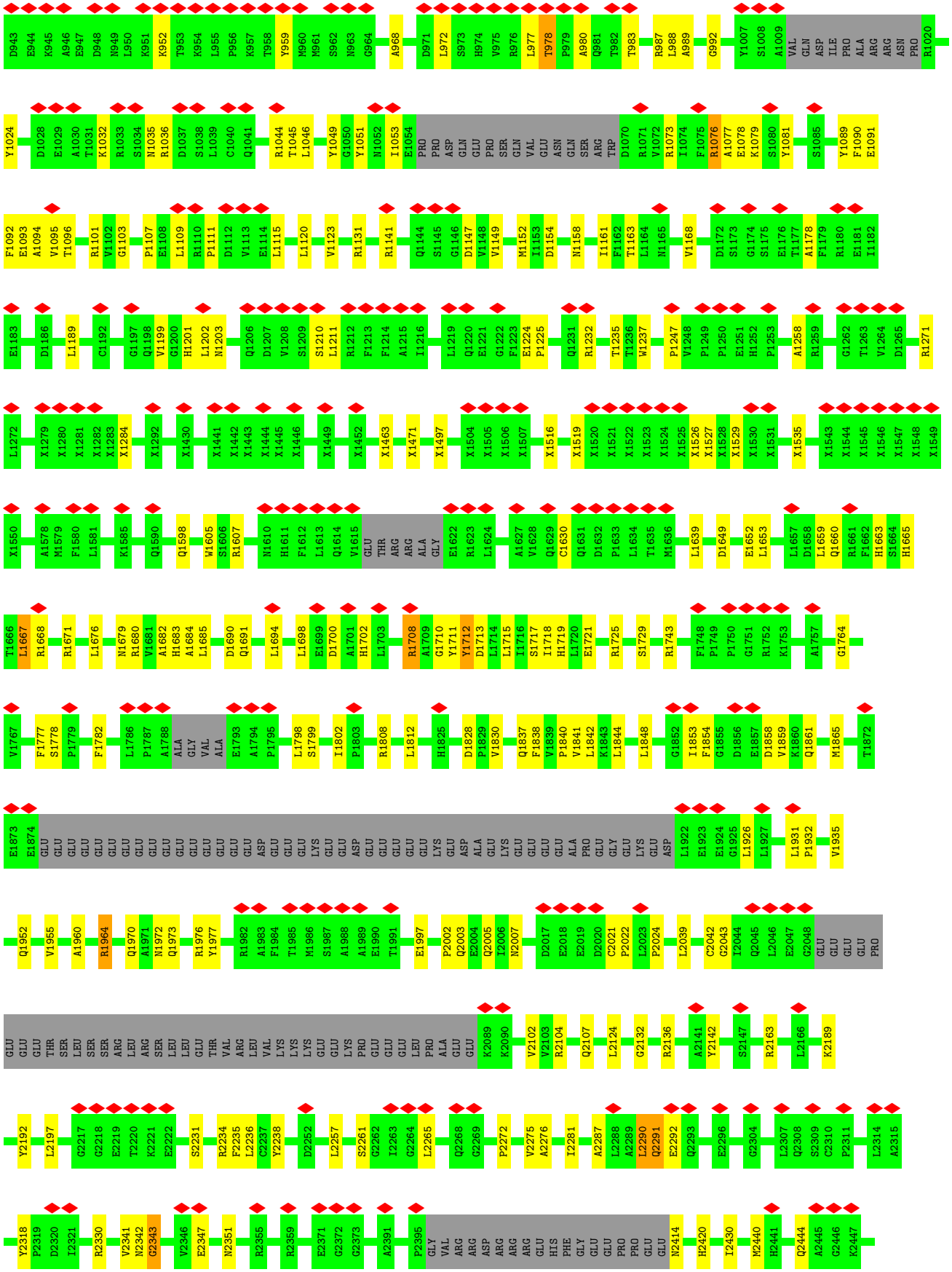
Chain J:



• Molecule 2: ryanodine receptor type 1

Chain B:

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Y1024 D1028 E1029 A1030 T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 R1044 T1045 L1046 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 I1074 F1075 R1076 A1077 E1078 K1079 S1080 Y1081 S1085 Y1089 F1090 E1091
F1092 E1093 A1094 V1095 T1096 R1101 Y1102 G1103 P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 L1120 V1123 R1131 R1141 Q1144 S1145 G1146 D1147 V1148 V1149 M1152 I1153 D1154 N1158 I1161 F1162 T1163 L1164 N1165 V1168 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1182
E1183 D1186 L1189 C1192 G1197 Q1198 V1199 G1200 H1201 L1202 N1203 Q1206 D1207 V1208 S1209 S1210 L1211 R1212 F1213 F1214 A1215 I1216 L1219 Q1220 E1221 G1222 F1223 E1224 P1225 Q1231 R1232 T1235 T1236 W1237 P1247 V1248 P1249 P1250 E1251 H1252 P1253 A1258 R1259 G1262 T1263 V1264 D1265 R1271
L1272 X1279 X1280 X1281 X1282 X1283 X1284 X1292 X1430 X1441 X1442 X1443 X1444 X1445 X1446 X1449 X1452 X1463 X1471 X1497 X1504 X1505 X1506 X1507 X1516 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1535 X1543 X1544 X1545 X1546 X1547 X1548 X1549
X1550 A1578 M1579 F1580 L1581 K1585 Q1590 Q1598 W1605 S1606 R1607 N1610 H1611 F1612 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 T1635 M1636 L1639 D1649 E1652 L1653 L1657 D1658 L1659 Q1660 R1661 F1662 H1663 S1664 H1665
T1666 L1667 R1668 R1671 L1676 N1679 R1680 Y1681 A1682 H1683 A1684 L1685 D1690 Q1691 L1694 L1698 E1699 D1700 A1701 H1702 L1703 R1708 A1709 G1710 Y1711 Y1712 D1713 L1714 L1715 I1716 S1717 I1718 H1719 L1720 E1721 R1725 S1729 R1743 F1748 P1749 P1750 G1751 R1752 K1753 A1757 G1764
V1767 F1777 S1778 P1779 F1782 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 L1798 S1799 I1802 P1803 R1808 L1812 H1825 D1828 P1829 V1830 Q1837 F1838 V1839 P1840 V1841 L1842 K1843 L1844 L1848 G1852 I1853 F1854 G1855 D1856 E1857 D1858 V1859 K1860 Q1861 M1865 T1872
E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 L1931 P1932 V1935
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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 K2090 V2102 V2103 R2104 Q2107 L2124 G2132 R2136 A2141 Y2142 S2147 R2163 L2166 K2189
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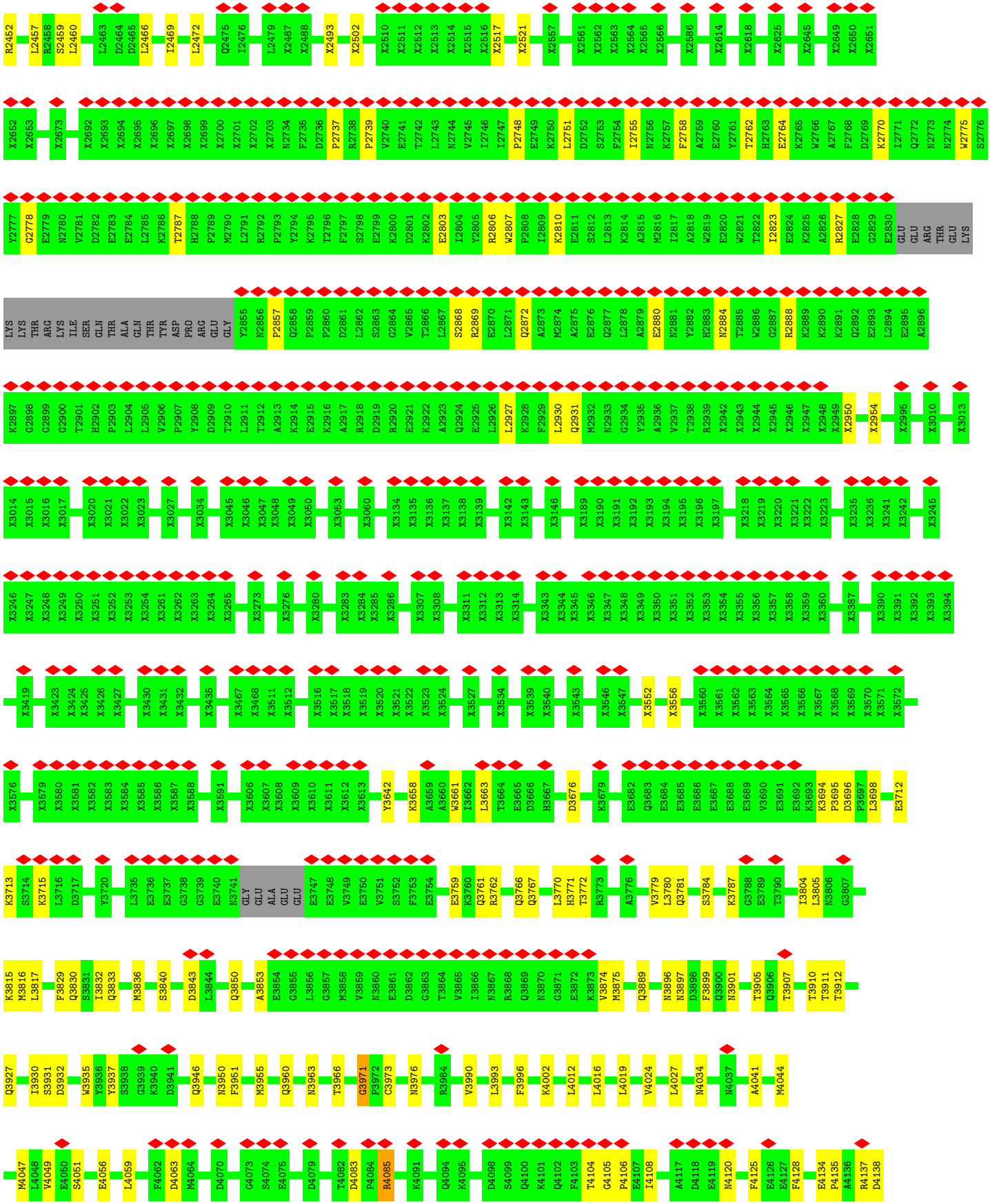
Y2318 P2319 D2320 I2321 R2330 V2341 N2342 G2343 V2346 E2347 N2351 R2355 R2359 E2371 G2372 G2373 A2391 P2396 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2420 I2430 M2440 H2441 Q2444 A2445 G2446 K2447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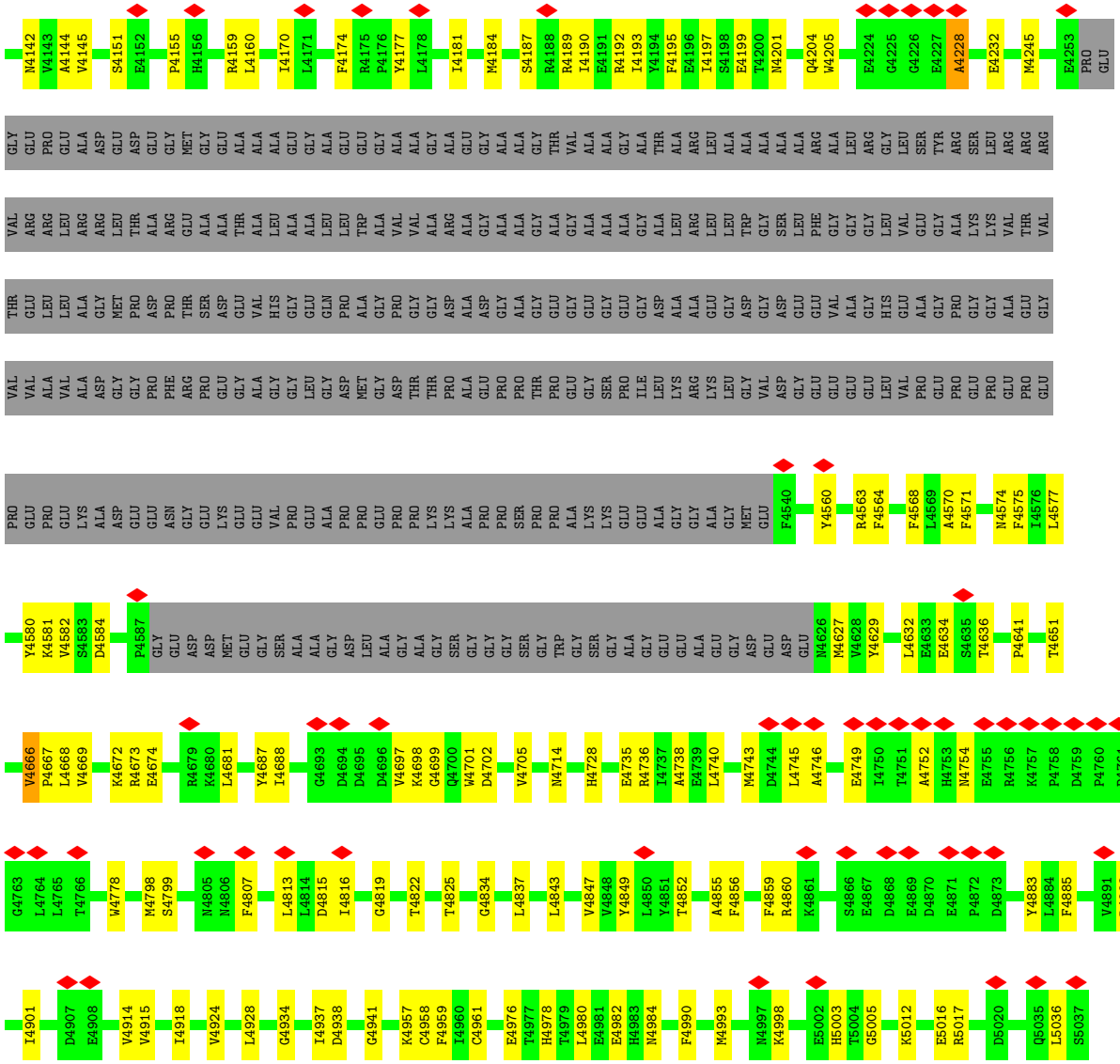
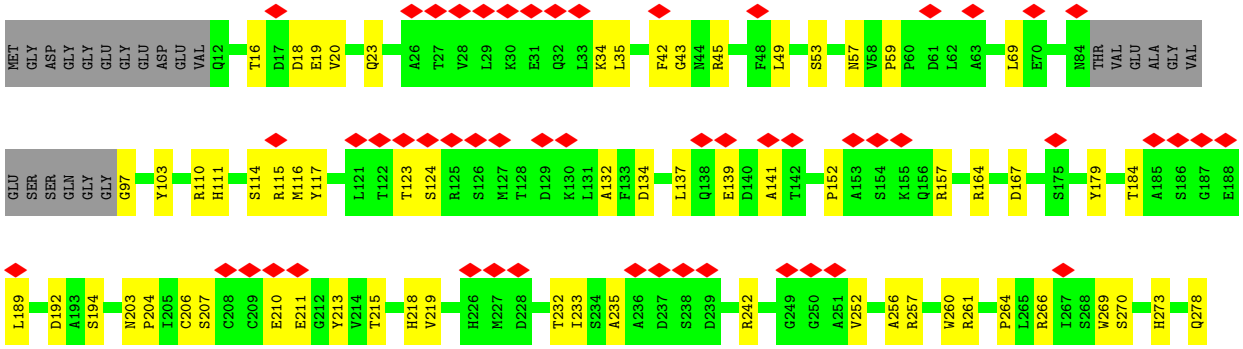
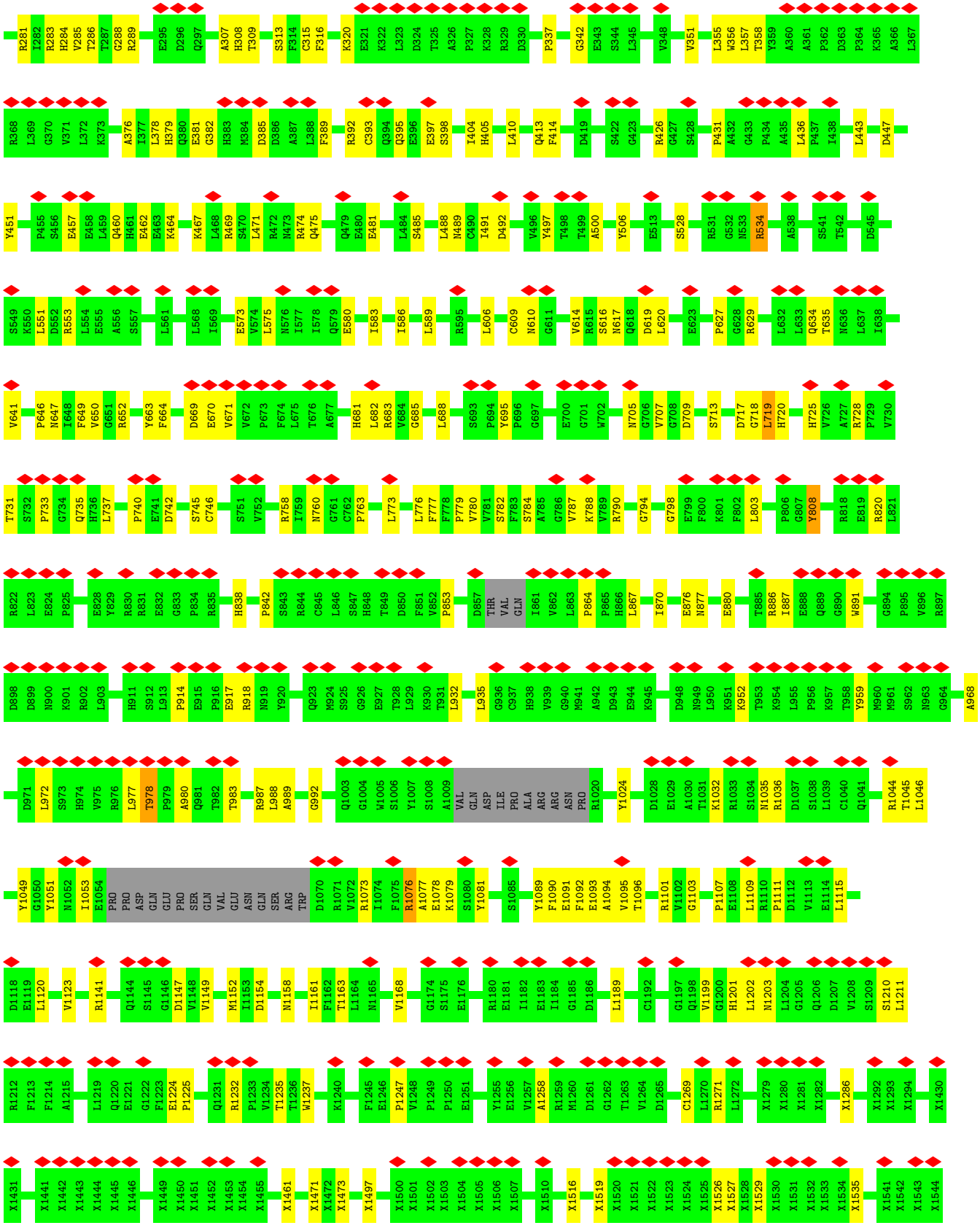


• Molecule 2: ryanodine receptor type 1

Chain E:

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P337
G342 E343 S344 L345
V348
V351
L355 W356 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366 L367
R368 L369 G370 V371 L372 K373
A376 I377 L378 H379 Q380 E381 G382
H383 M384 D385 D386 A387 L388 F389
R392 C393 Q394 Q395 E396 E397 S398
I404 H405 L410
Q413 F414
D419
S422 G423
R426 G427 S428
P431 A432 G433 P434 A435 L436 P437 I438 L443 D447
Y451
P455 S456 E457 E458 L459 Q460 H461 E462 F463 K464
K467 L468 R469 S470 L471 R472 N473 R474 Q475
Q479 E480 E481
L484 S485
L488 N489 C490 I491 D492
V496 Y497 T498 T499 A500
Y506
E513
S528
R531 G532 N533 R534
A538
S541 T542
D545
S549 K550 L551 D552 R553 L554 E555 A556 S557
L561
L568 I569
E573 V574 L575 N576 I577 I578 Q579 E580
I583
I586
L589
R595
L606
C609 N610 G611
V614 R615 S616 N617 Q618 D619 L620
E623
P627 G628 R629
L632 L633 Q634 T635 N636 L637 I638
V641 P646 N647 I648 F649 V650 G651 R652
Y663 F664
D669 E670 V671 V672 P673 F674 L675 T676 A677
H681 L682 R683 V684 G685
L688
S693 P694 Y695 P696 G697
E700 G701 W702
N705 G706 V707 G708 D709
S713
D717 G718 L719 H720
H725 V726 A727 R728 P729 V730
T731 S732 P733 G734 Q735 H736 L737
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S751 V752
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L773
L776 F777 F778 P779 V780 V781 S782 F783 S784 A785 G786 V787 K788 V789 R790
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R822 L823 E824 P825
E828 Y829 R830 R831 E832 G833 P834 R835
H838
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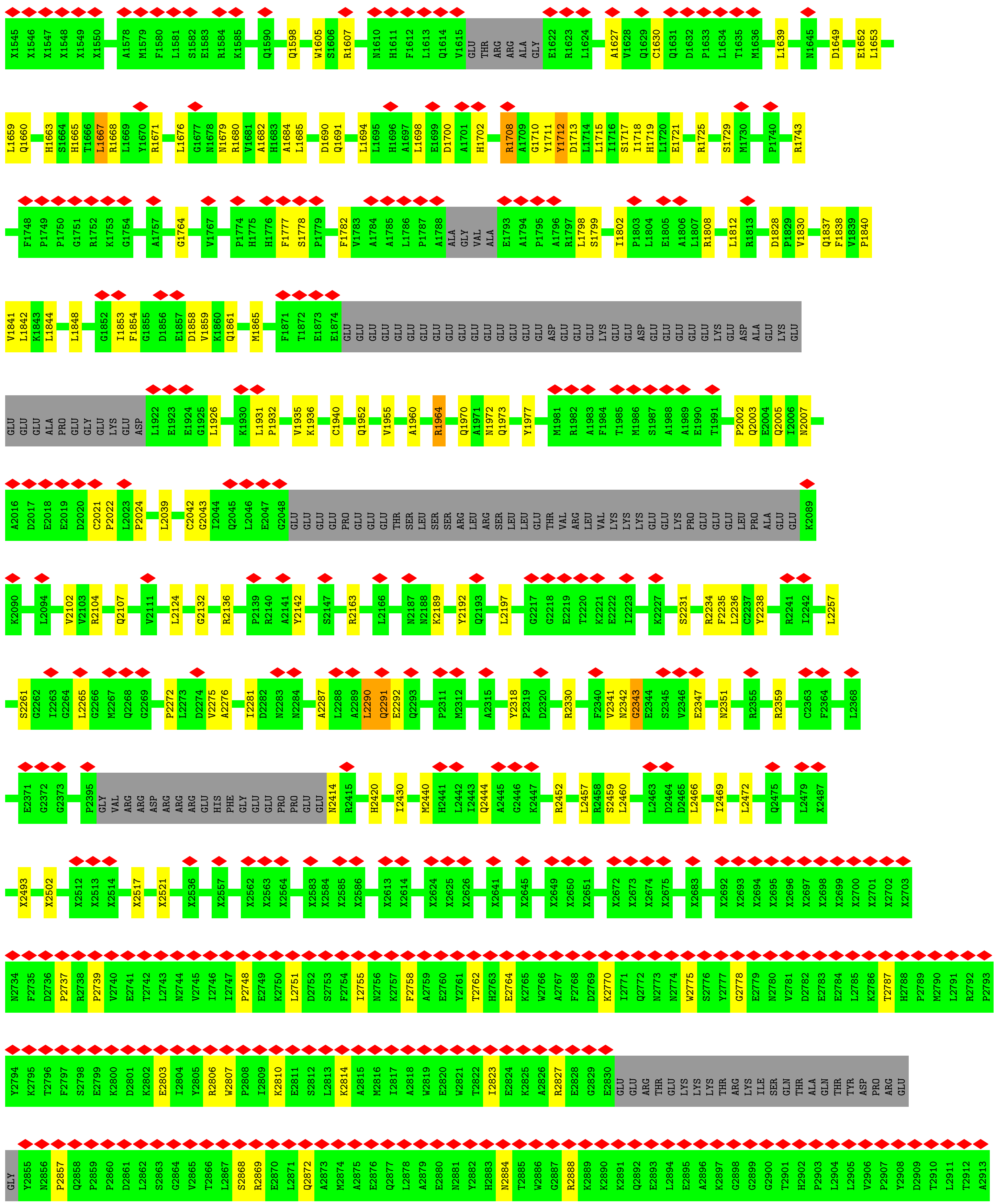
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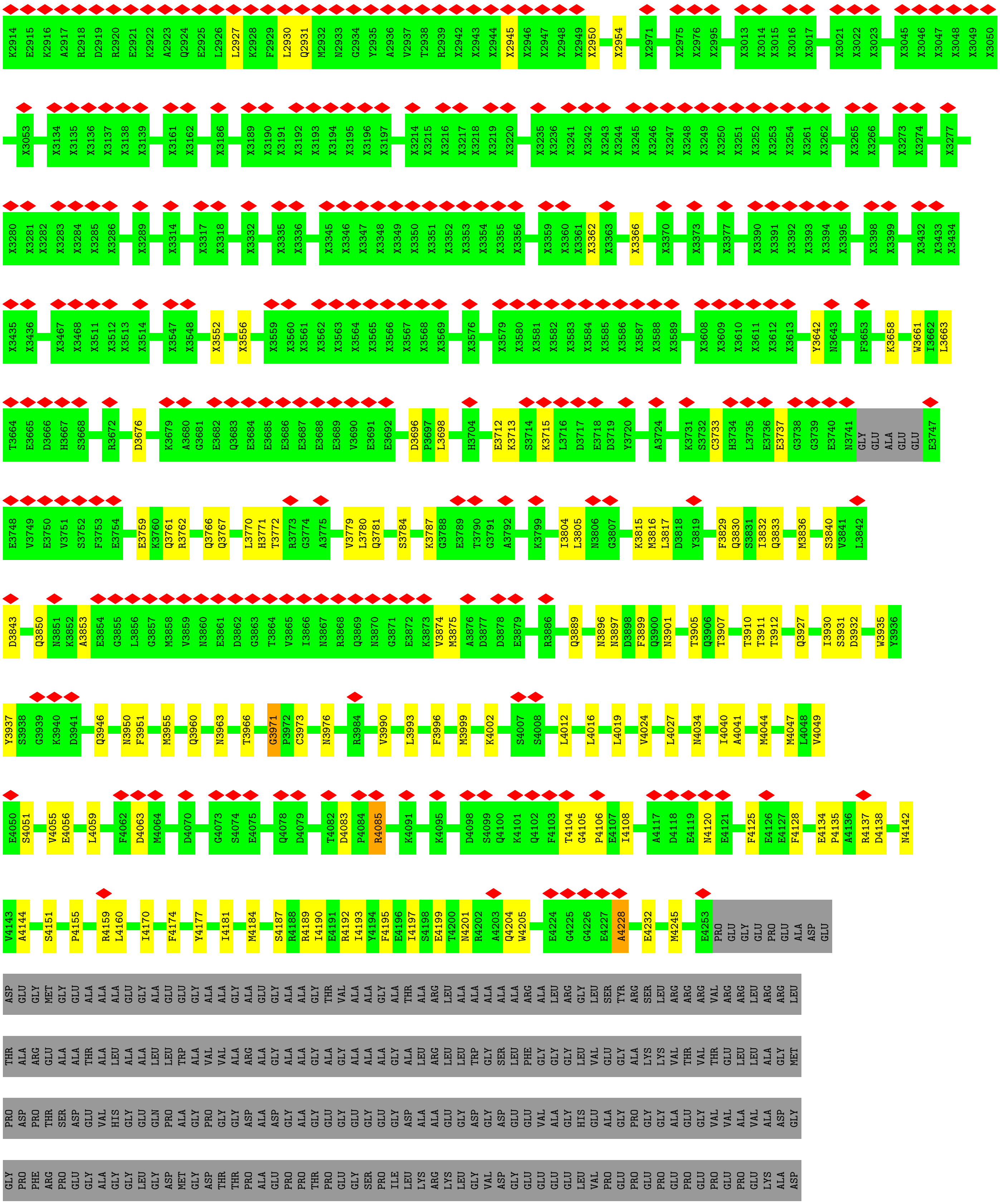
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PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY
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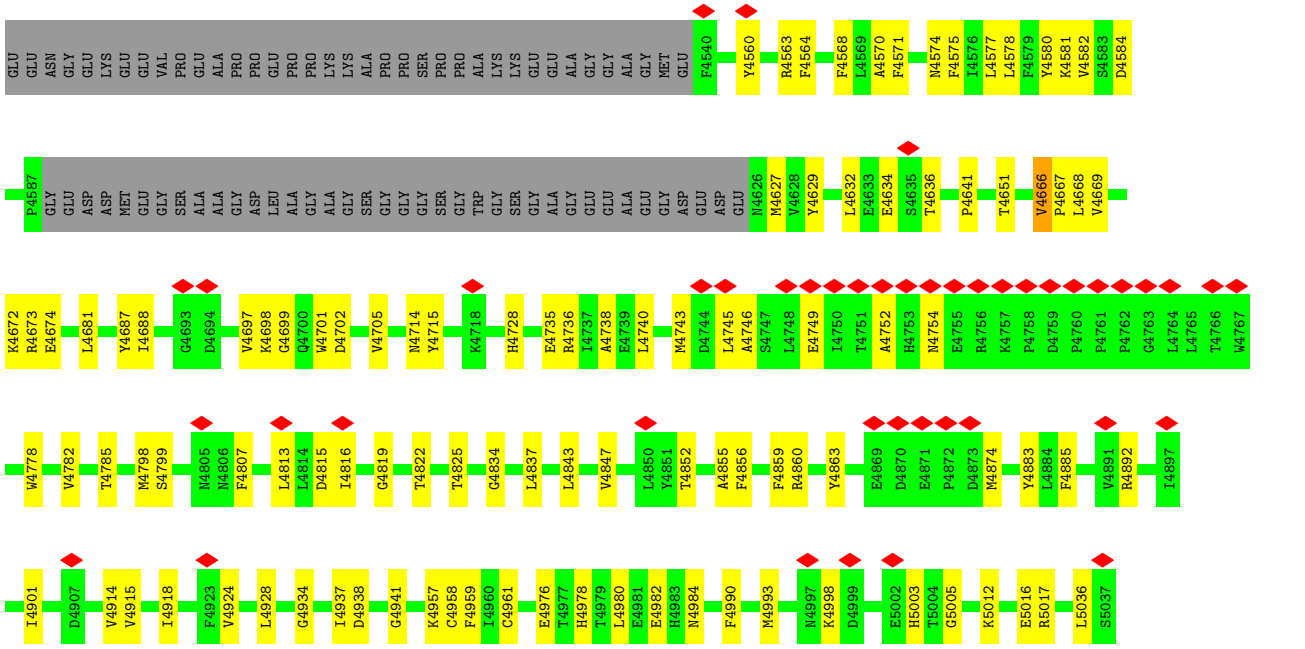
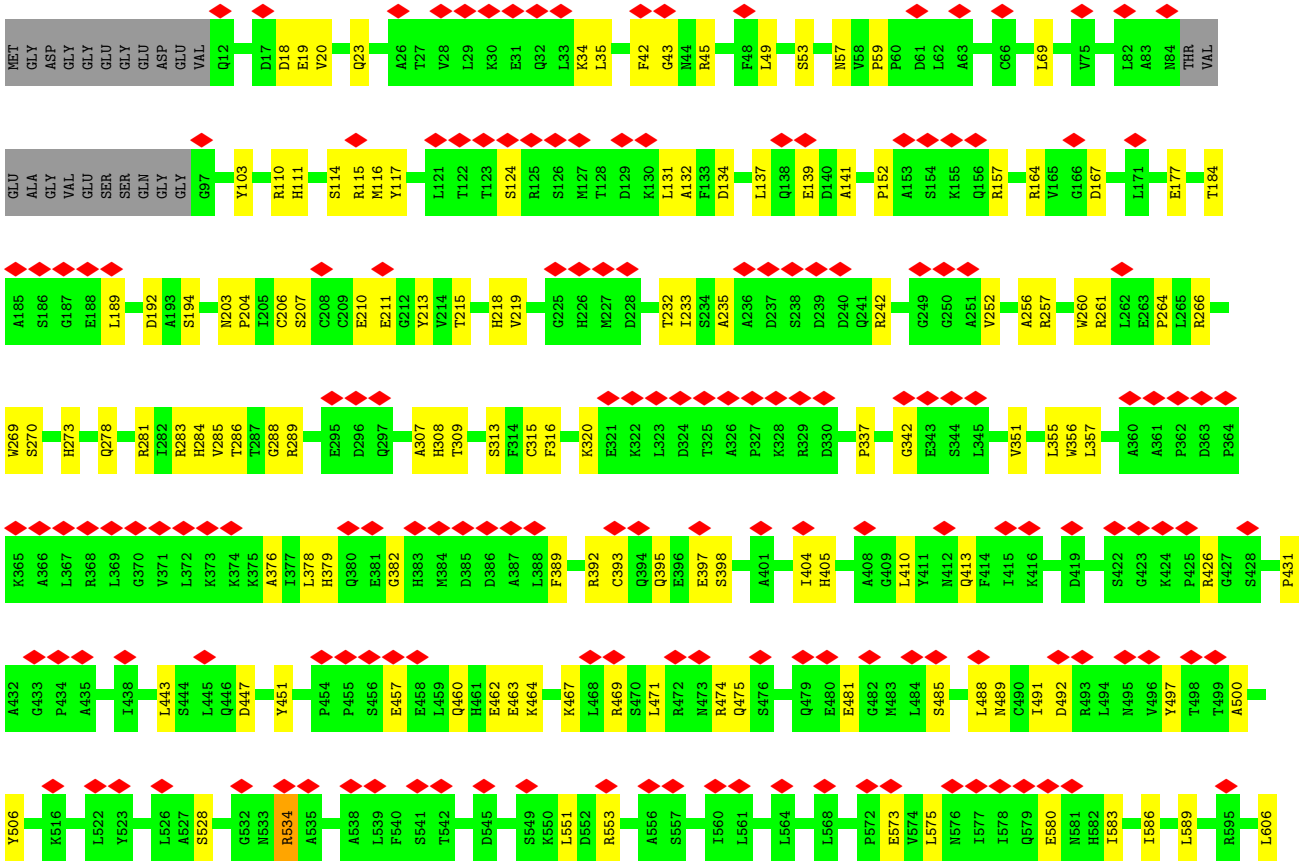
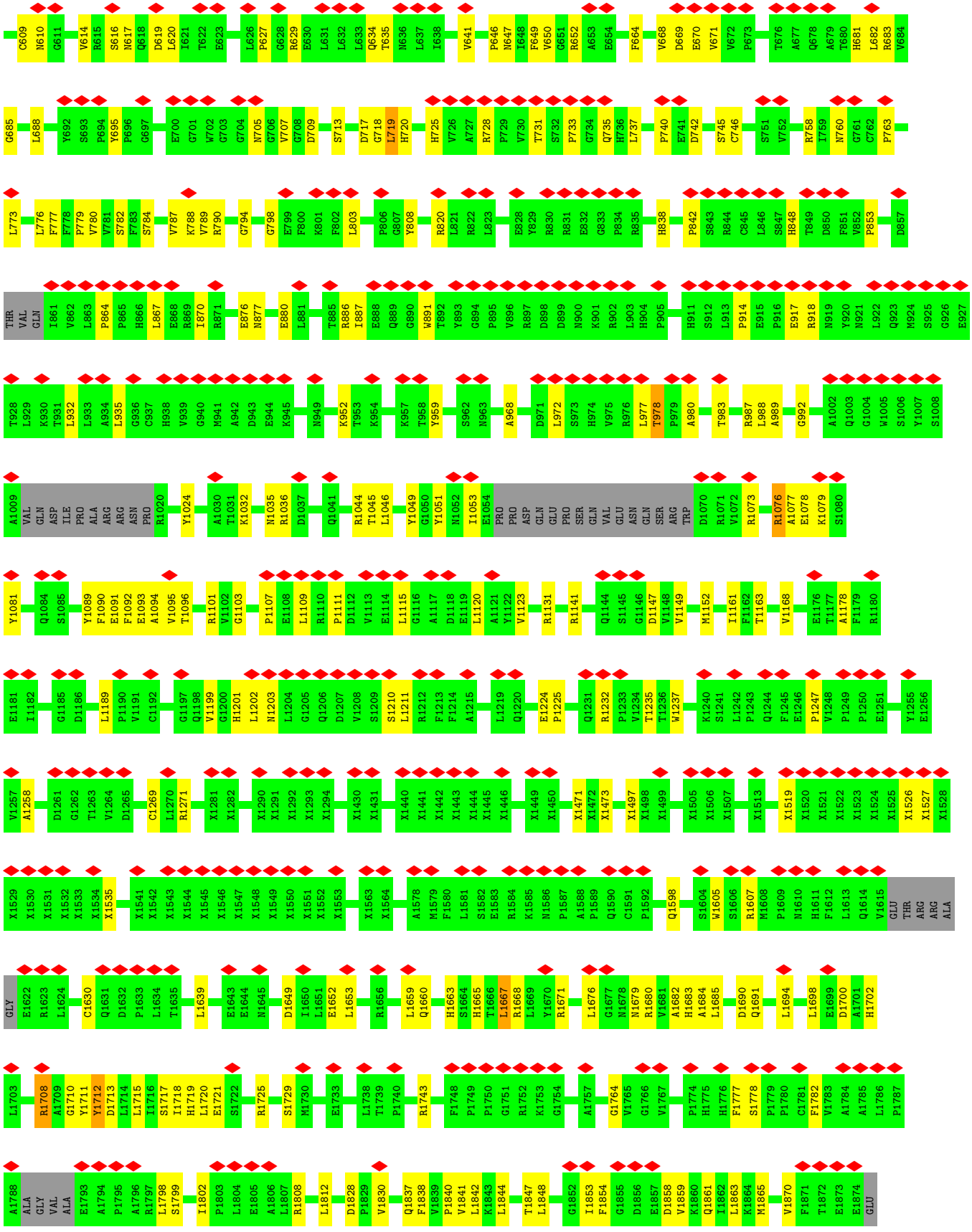


• Molecule 2: ryanodine receptor type 1

Chain G:

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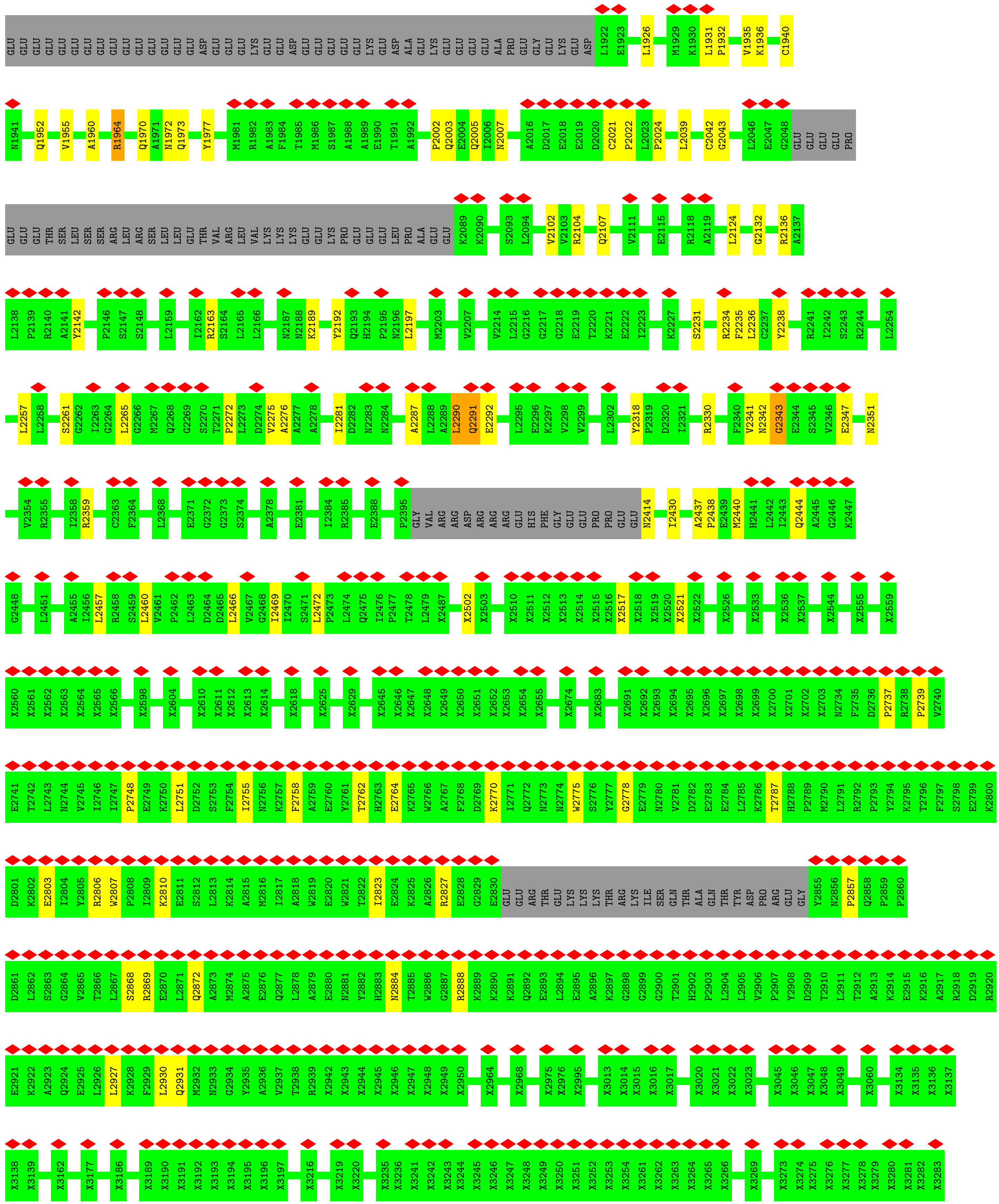
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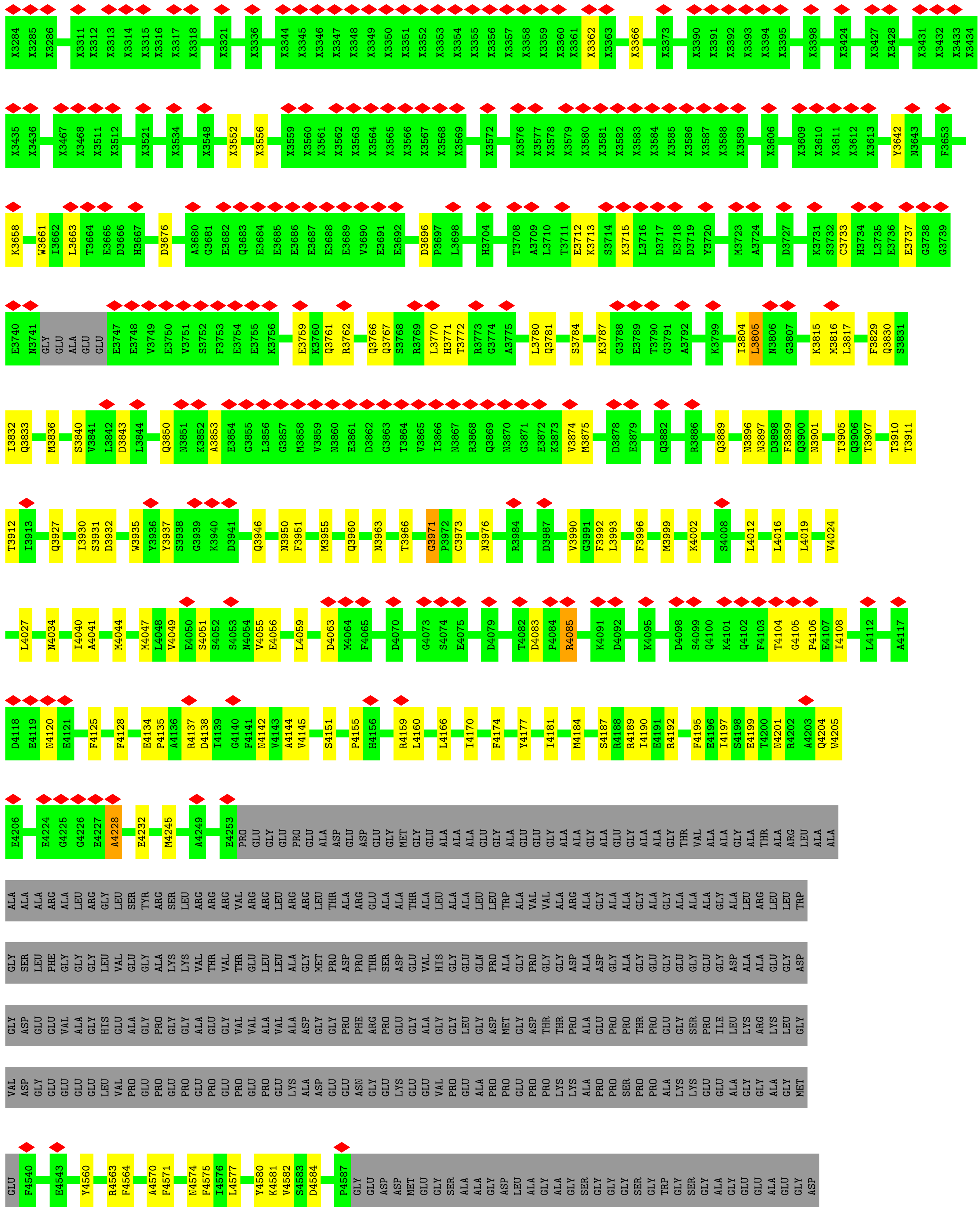
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ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP
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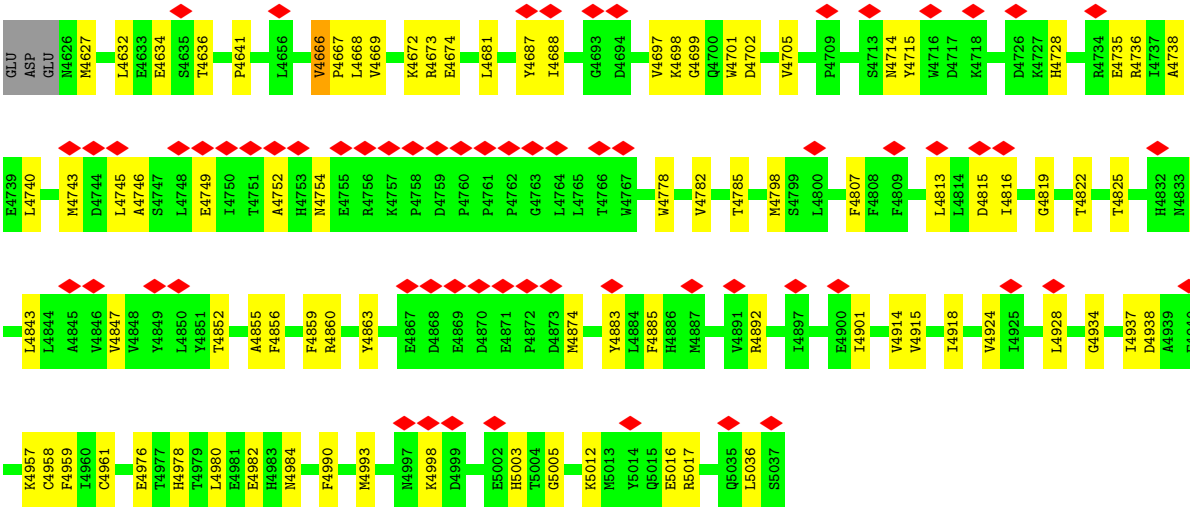
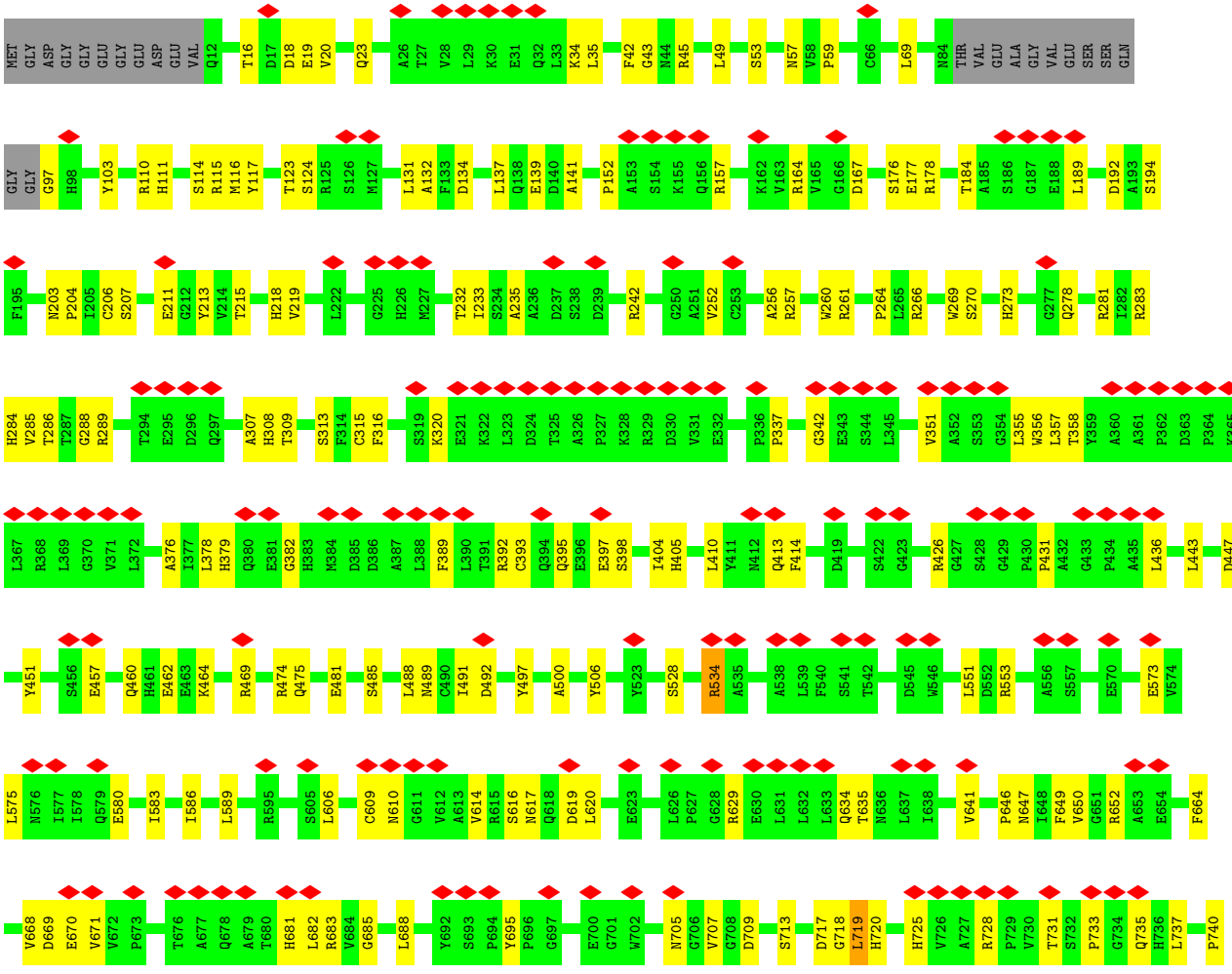
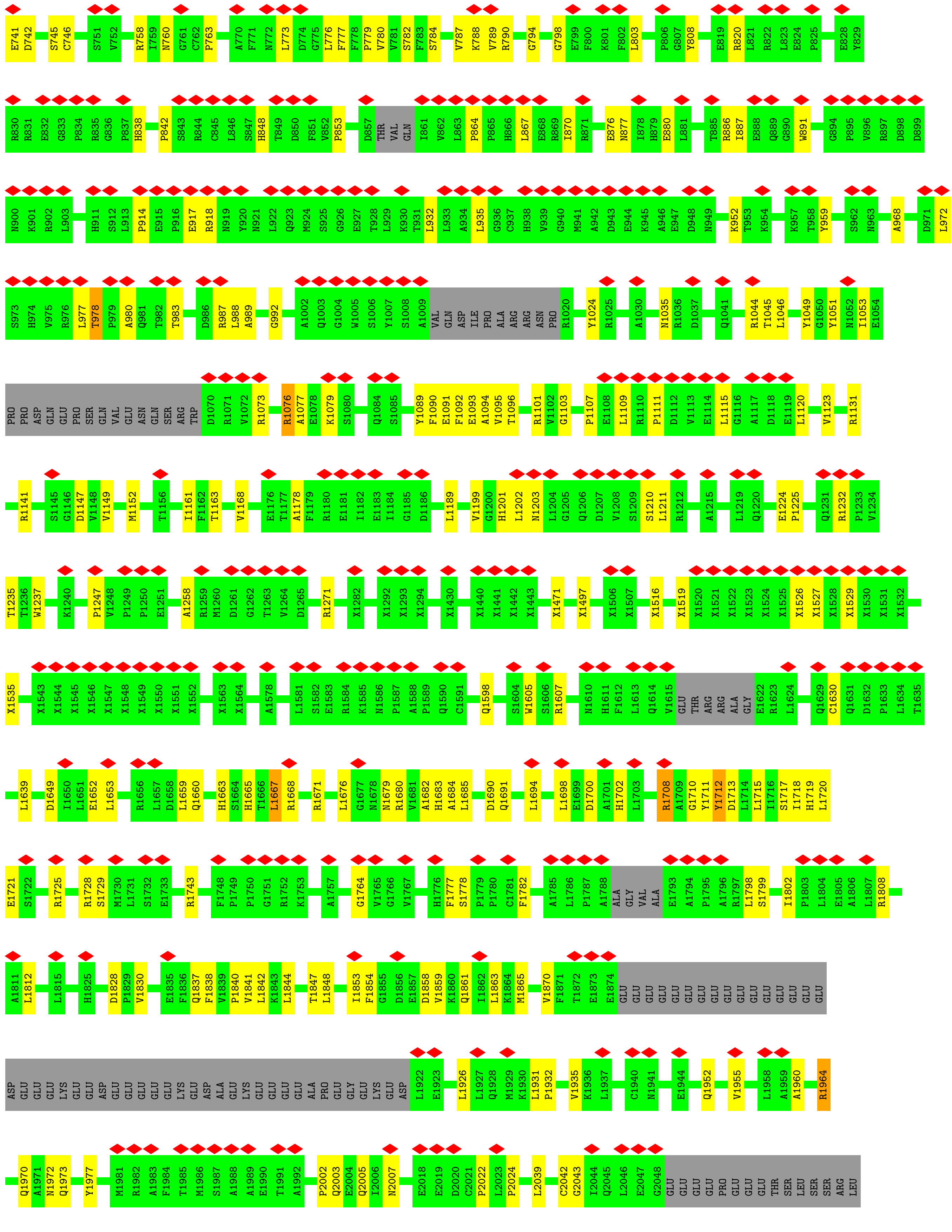
VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET
GLU F4540 E4543 Y4560 R4563 F4564 A4570 F4571 N4574 F4575 I4576 L4577 Y4580 K4581 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP



• Molecule 2: ryanodine receptor type 1

Chain I:

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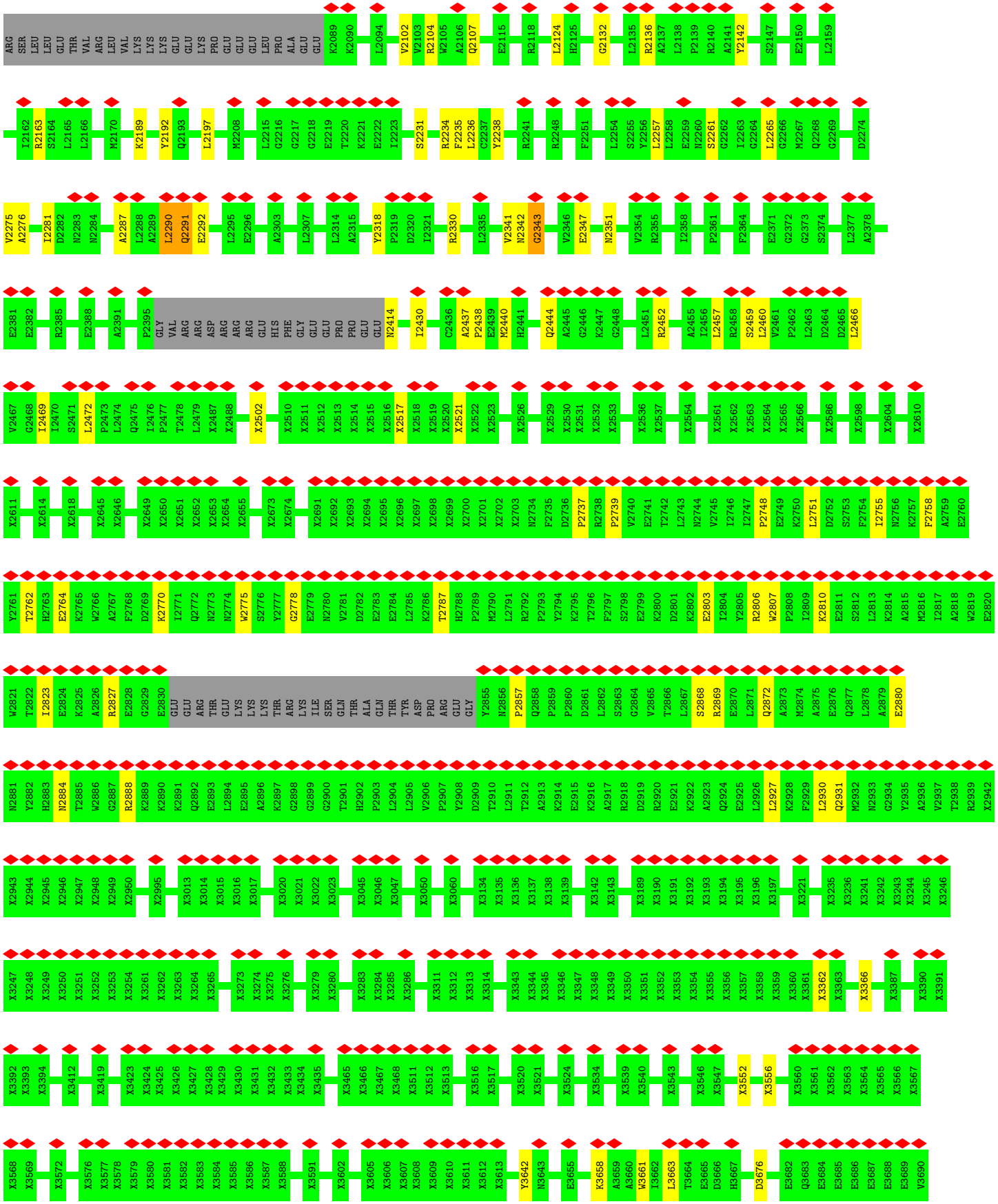
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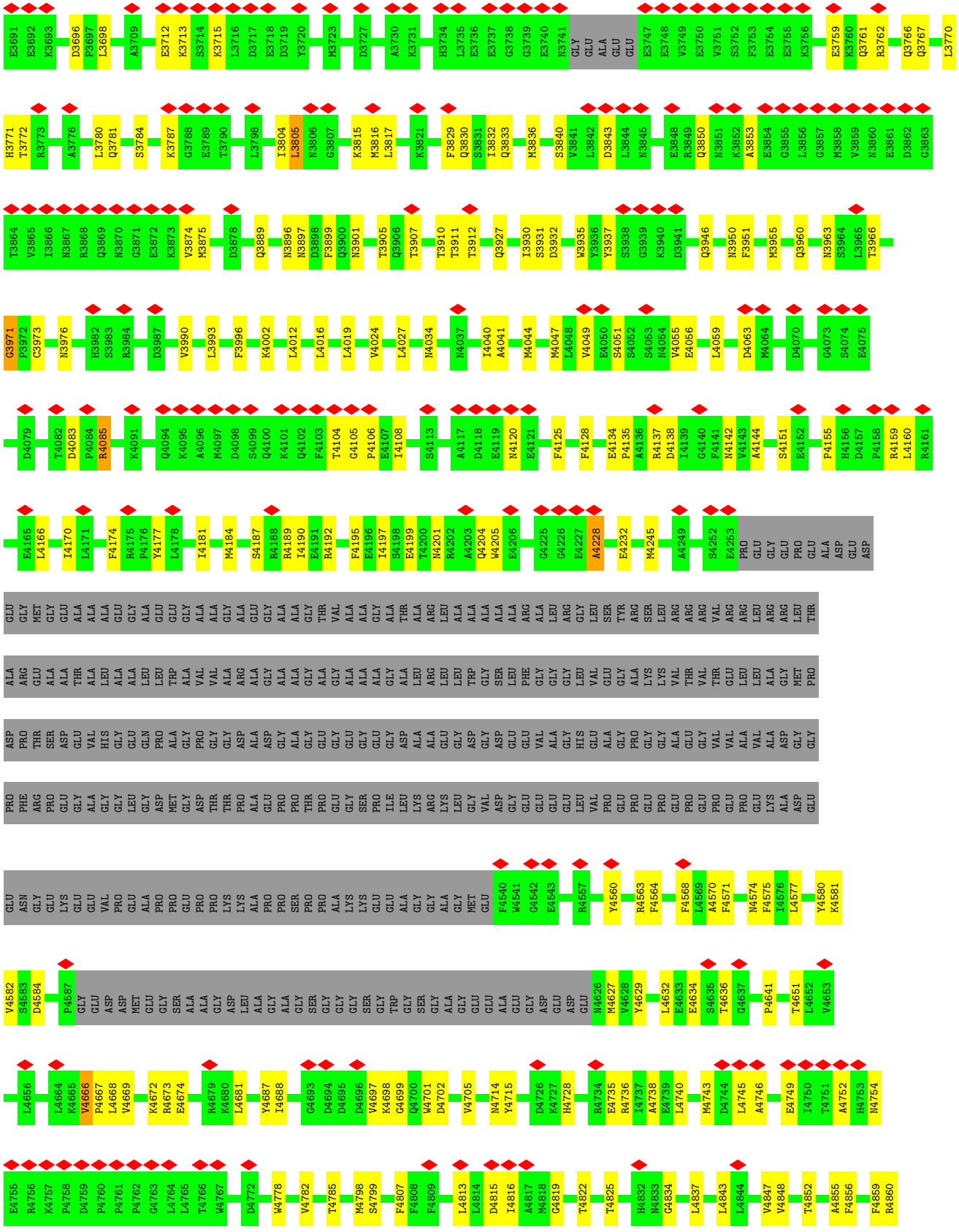
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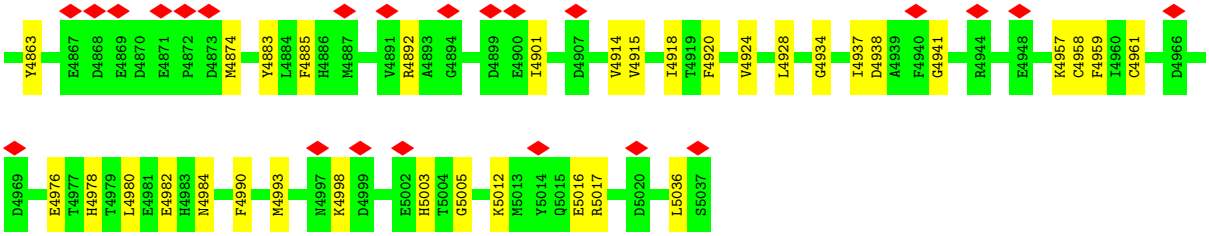
G3971 P3972 C3973 N3976 H3982 S3983 R3984 D3987 V3990 L3993 F3996 K4002 L4012 L4016 L4019 V4024 L4027 N4034 N4037 I4040 A4041 M4044 M4047 L4048 V4049 E4050 S4051 S4052 S4053 N4054 V4055 E4056 L4059 D4063 M4064 D4070 G4073 S4074 E4075
D4079 T4082 D4083 P4084 R4085 K4091 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 E4107 I4108 S4113 A4117 D4118 E4119 N4120 E4121 F4125 F4128 E4134 P4135 A4136 R4137 D4138 I4139 G4140 F4141 N4142 V4143 A4144 S4151 E4152 P4155 H4156 D4157 P4158 R4159 L4160 R4161
E4165 L4166 I4170 L4171 F4174 R4175 P4176 Y4177 L4178 I4181 M4184 S4187 R4188 R4189 I4190 E4191 R4192 F4195 E4196 I4197 S4198 E4199 T4200 N4201 R4202 A4203 Q4204 W4205 E4206 G4225 G4226 E4227 A4228 E4232 M4245 A4249 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP
GLU GLY MET GLY GLU ALA ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLY GLY THR VAL ALA ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR
ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA ALA GLY GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA ALA LYS LYS VAL THR VAL THR GLU LEU 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 GLY GLU GLU GLY ALA ALA GLU GLY GLY GLU VAL ALA ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY
PRO PHE ARG PRO GLU GLY ALA 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 GLY VAL ASP GLY GLU GLU GLU GLU GLU LEU VAL PRO GLU PRO PRO GLU PRO GLU PRO GLU GLU PRO GLU LYS ALA ASP 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 GLU F4540 W4541 G4542 E4543 R4557 Y4560 R4563 F4564 F4568 L4569 A4570 F4571 N4574 F4575 T4576 L4577 Y4580 K4581
V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLY ALA GLU GLY ASP GLU ASP GLU N4626 M4627 V4628 Y4629 L4632 E4633 E4634 S4635 T4636 G4637 P4641 T4651 L4652 V4653
L4656 L4664 K4665 V4666 P4667 L4668 V4669 K4672 R4673 E4674 R4679 K4680 L4681 Y4687 I4688 G4693 D4694 D4695 D4696 V4697 K4698 G4699 Q4700 W4701 D4702 V4705 N4714 Y4715 D4726 K4727 H4728 R4734 E4735 R4736 I4737 A4738 E4739 L4740 M4743 D4744 L4745 A4746 E4749 I4750 T4751 A4752 H4753 N4754
E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 D4772 W4778 V4782 T4785 M4798 S4799 F4807 F4808 F4809 L4813 L4814 D4815 I4816 A4617 M4818 G4819 T4822 T4825 H4832 N4833 G4834 L4837 L4843 L4844 V4847 V4848 T4852 A4855 F4856 F4859 R4860


Y4863
E4867
D4868
E4869
D4870
E4871
P4872
D4873
M4874
Y4883
L4884
F4885
H4886
M4887
V4891
R4892
A4893
G4894
D4899
E4900
I4901
D4907
V4914
V4915
I4918
T4919
F4920
V4924
L4928
G4934
I4937
D4938
A4939
F4940
G4941
R4944
E4948
K4957
C4958
F4959
I4960
C4961
D4966
D4969
E4976
T4977
H4978
T4979
L4980
E4981
E4982
H4983
N4984
F4990
M4993
N4997
K4998
D4999
E5002
H5003
T5004
G5005
K5012
M5013
Y5014
Q5015
E5016
R5017
D5020
L5036
S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.549	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

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	0.31	0/834	0.56	0/1123
1	F	0.31	0/834	0.56	0/1123
1	H	0.31	0/834	0.56	0/1123
1	J	0.31	0/834	0.56	0/1123
2	B	0.30	0/25428	0.55	5/34534 (0.0%)
2	E	0.30	0/25428	0.55	5/34534 (0.0%)
2	G	0.30	0/25428	0.55	5/34534 (0.0%)
2	I	0.30	0/25428	0.55	5/34534 (0.0%)
All	All	0.30	0/105048	0.55	20/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	64

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	719	LEU	CA-CB-CG	6.09	129.30	115.30
2	G	719	LEU	CA-CB-CG	6.08	129.29	115.30
2	E	719	LEU	CA-CB-CG	6.08	129.28	115.30
2	I	719	LEU	CA-CB-CG	6.07	129.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1667	LEU	CA-CB-CG	5.71	128.43	115.30

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	808	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	18	0
1	F	818	0	824	17	0
1	H	818	0	824	17	0
1	J	818	0	824	18	0
2	B	29369	0	24711	395	0
2	E	29369	0	24713	406	0
2	G	29369	0	24713	395	0
2	I	29369	0	24712	397	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102145	1629	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 7.

The worst 5 of 1629 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.88	0.72
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.88	0.71
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.88	0.71
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.56	0.71
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.56	0.70

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
1	F	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
1	H	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
1	J	105/107 (98%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4687 (69%)	2890 (89%)	339 (10%)	6 (0%)	47	81
2	E	3235/4687 (69%)	2887 (89%)	342 (11%)	6 (0%)	47	81
2	G	3235/4687 (69%)	2892 (89%)	337 (10%)	6 (0%)	47	81
2	I	3235/4687 (69%)	2889 (89%)	340 (10%)	6 (0%)	47	81
All	All	13360/19176 (70%)	11926 (89%)	1410 (11%)	24 (0%)	50	81

5 of 24 Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
2	B	1932	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/88 (100%)	88 (100%)	0	100	100
1	F	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	J	88/88 (100%)	88 (100%)	0	100	100
2	B	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3209 (78%)	2476 (99%)	17 (1%)	84	90
All	All	10324/13188 (78%)	10256 (99%)	68 (1%)	84	90

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	1964	ARG
2	I	3787	LYS
2	I	4137	ARG
2	E	3663	LEU
2	E	1964	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 147 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	224	HIS
2	I	4142	ASN
2	I	395	GLN
2	I	1972	ASN

Continued on next page...

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Mol	Chain	Res	Type
2	E	479	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 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	12
2	B	12

Continued on next page...

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Mol	Chain	Number of breaks
2	I	12
2	E	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	3613:UNK	C	3639:THR	N	44.80
1	B	3613:UNK	C	3639:THR	N	44.74
1	I	3613:UNK	C	3639:THR	N	44.65
1	E	3613:UNK	C	3639:THR	N	44.57
1	B	3163:UNK	C	3170:UNK	N	16.54

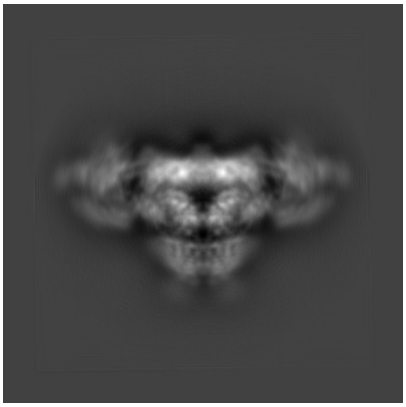
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22395. These allow visual inspection of the internal detail of the map and identification of artifacts.

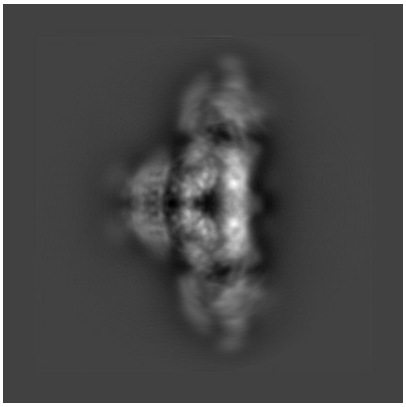
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

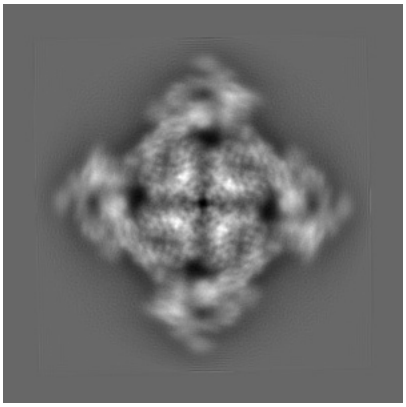
6.1.1 Primary map



X



Y

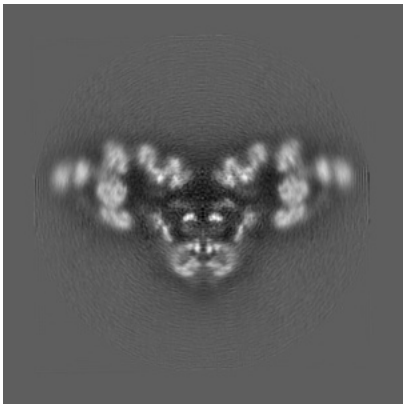


Z

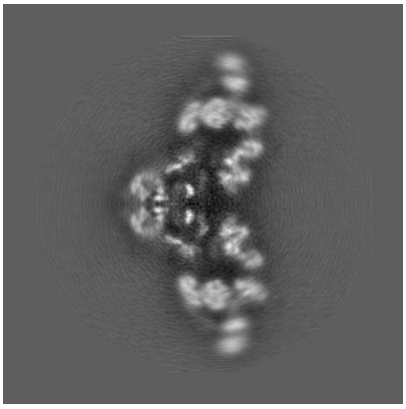
The images above show the map projected in three orthogonal directions.

6.2 Central slices

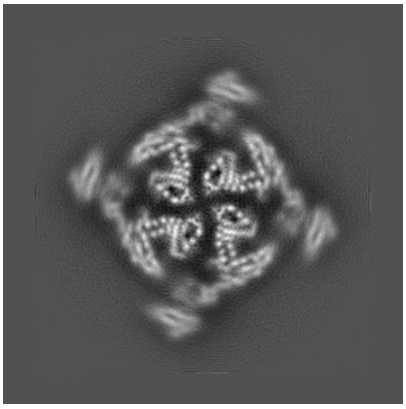
6.2.1 Primary map



X Index: 200



Y Index: 200

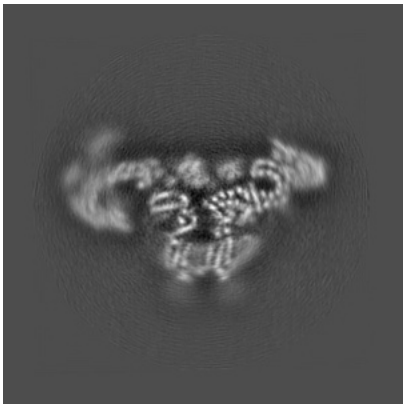


Z Index: 200

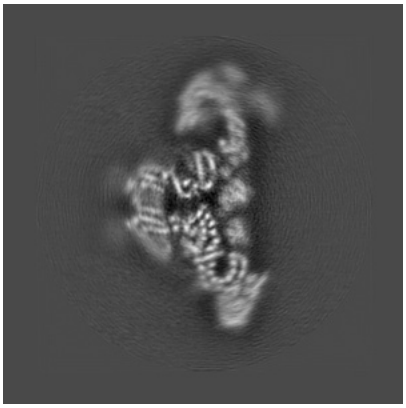
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

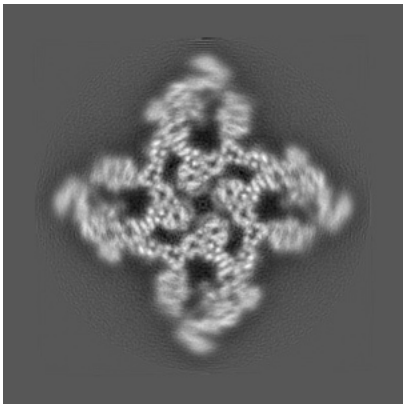
6.3.1 Primary map



X Index: 177



Y Index: 177



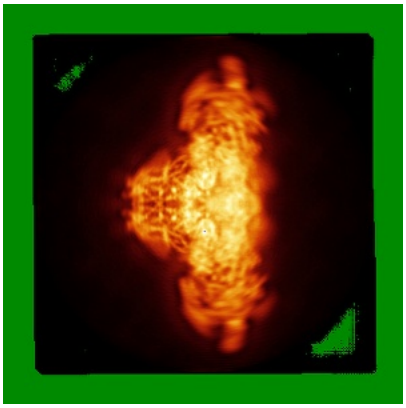
Z Index: 230

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

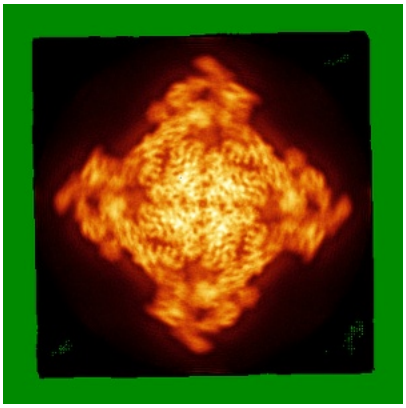
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

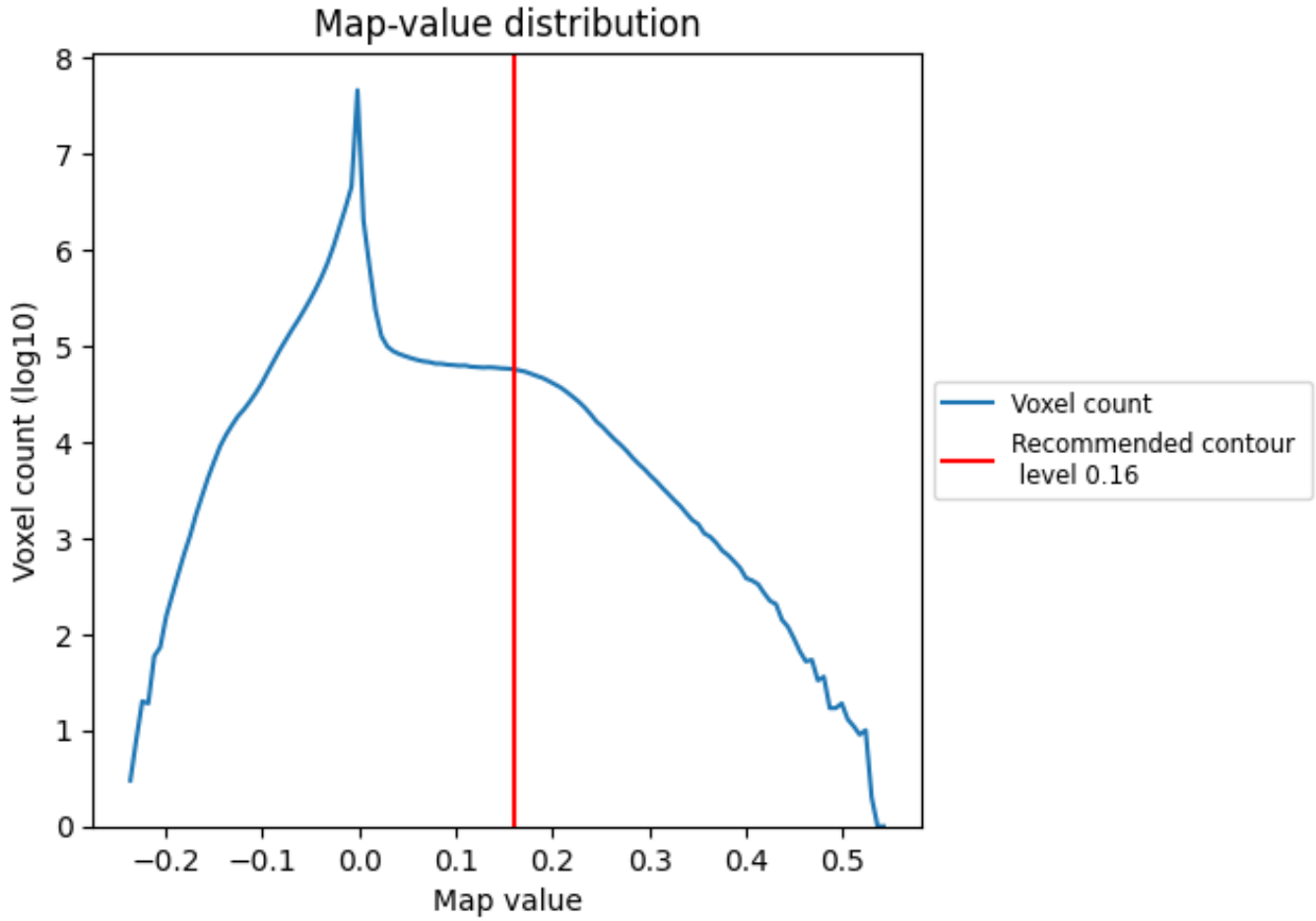
6.6 Mask visualisation (i)

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

7 Map analysis

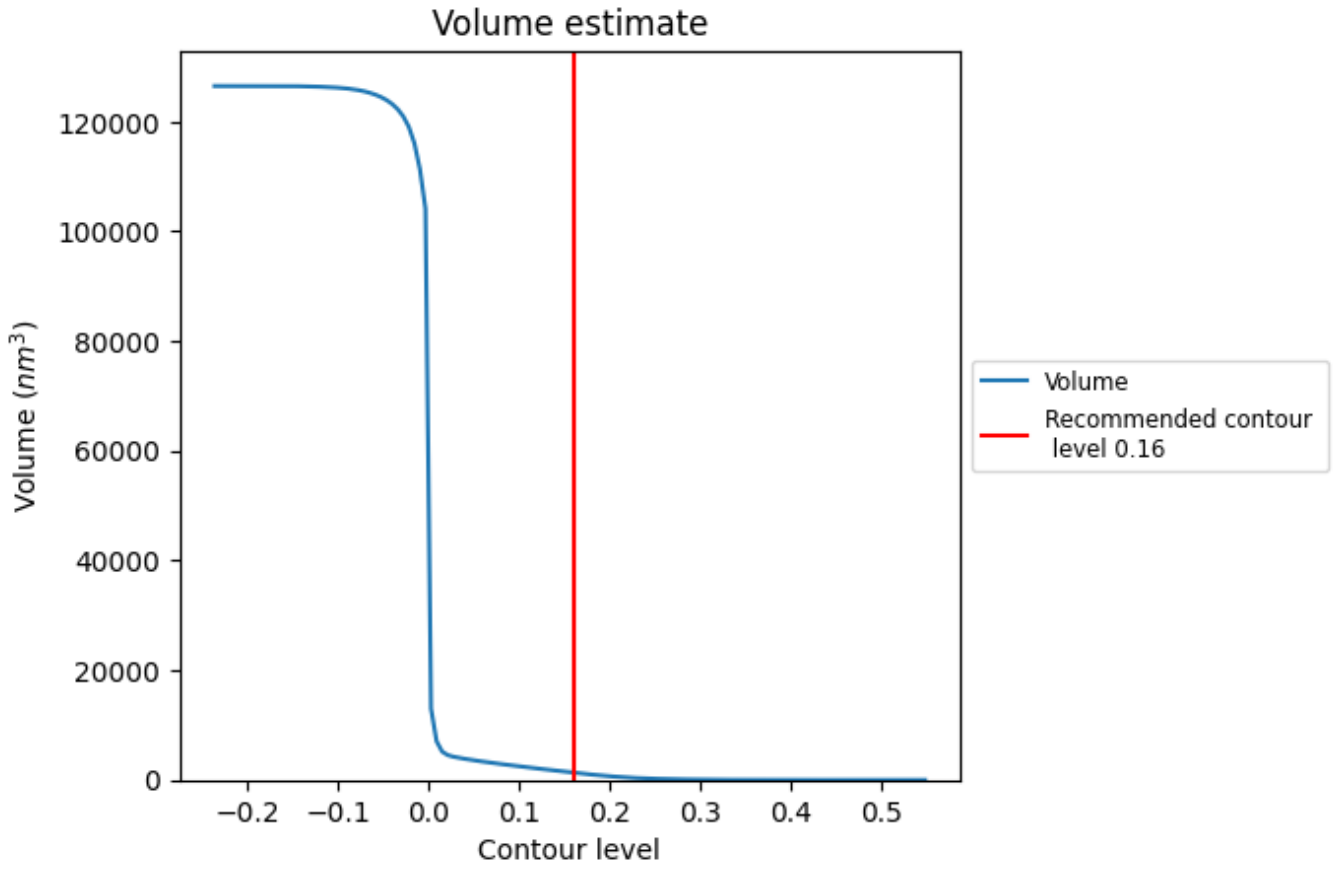
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

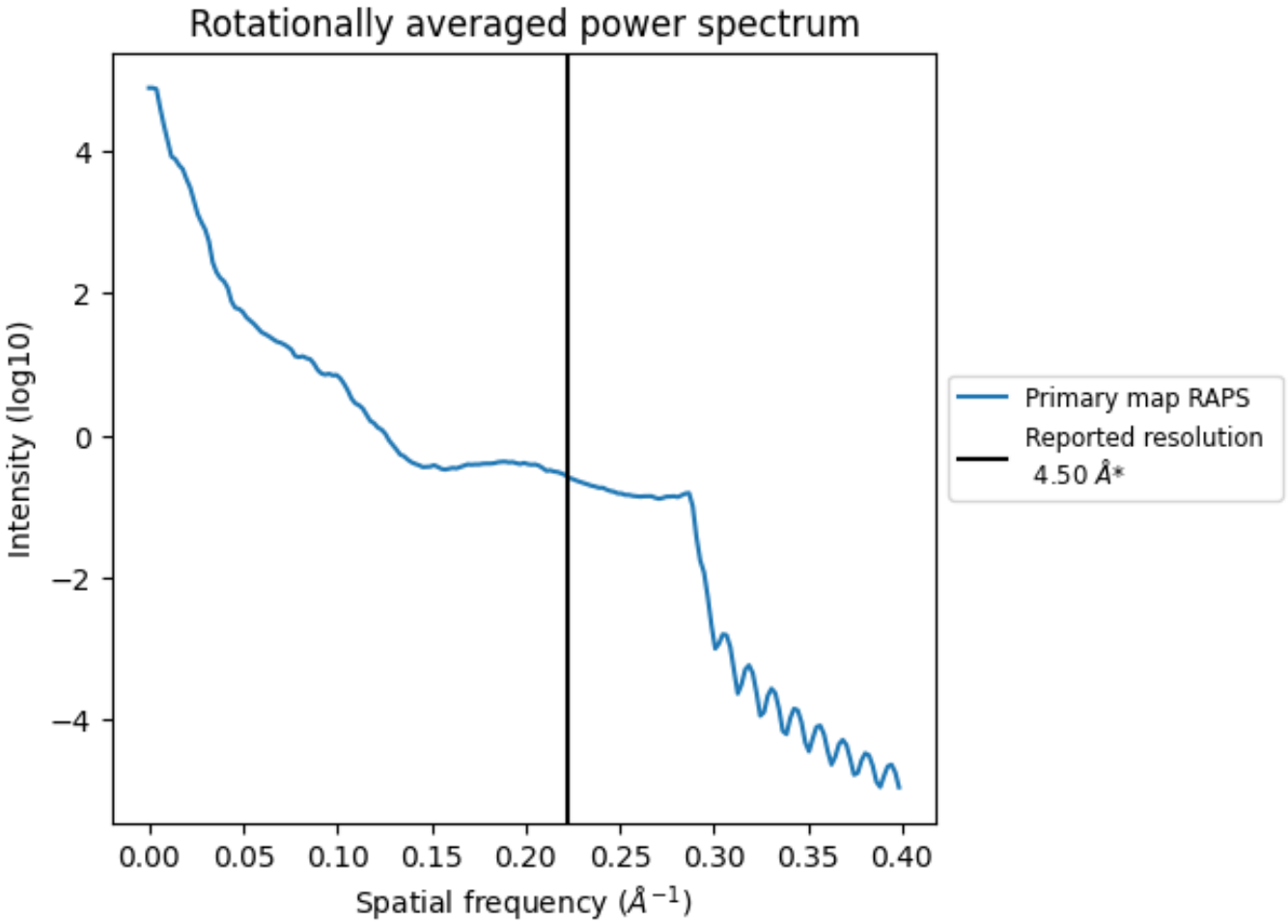
7.2 Volume estimate (i)



The volume at the recommended contour level is 1337 nm^3; this corresponds to an approximate mass of 1208 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}

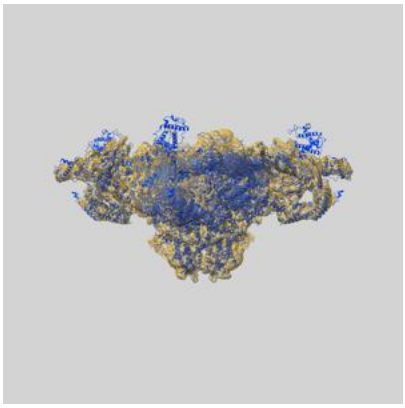
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

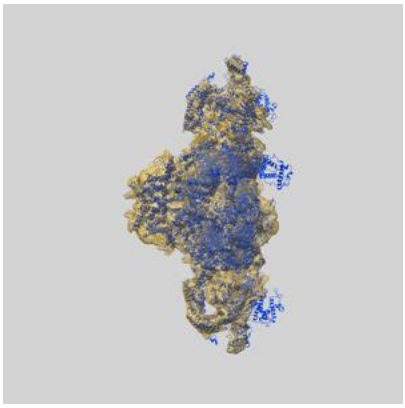
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22395 and PDB model 7JMI. Per-residue inclusion information can be found in section 3 on page 5.

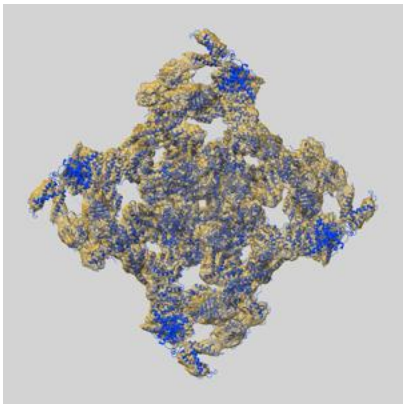
9.1 Map-model overlay



X



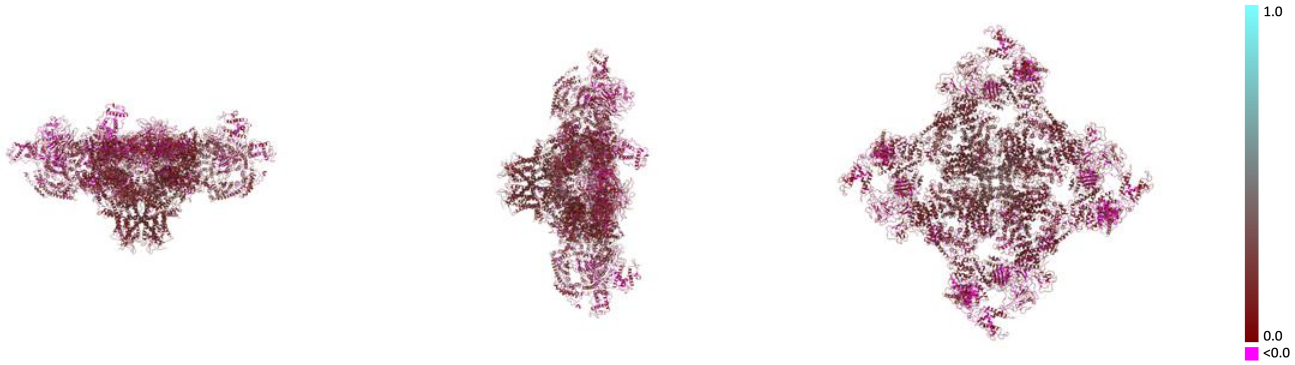
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

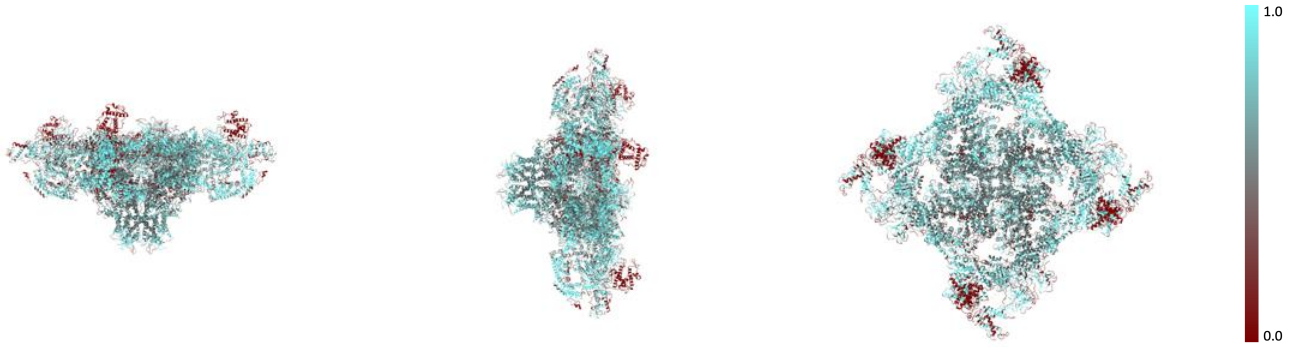
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

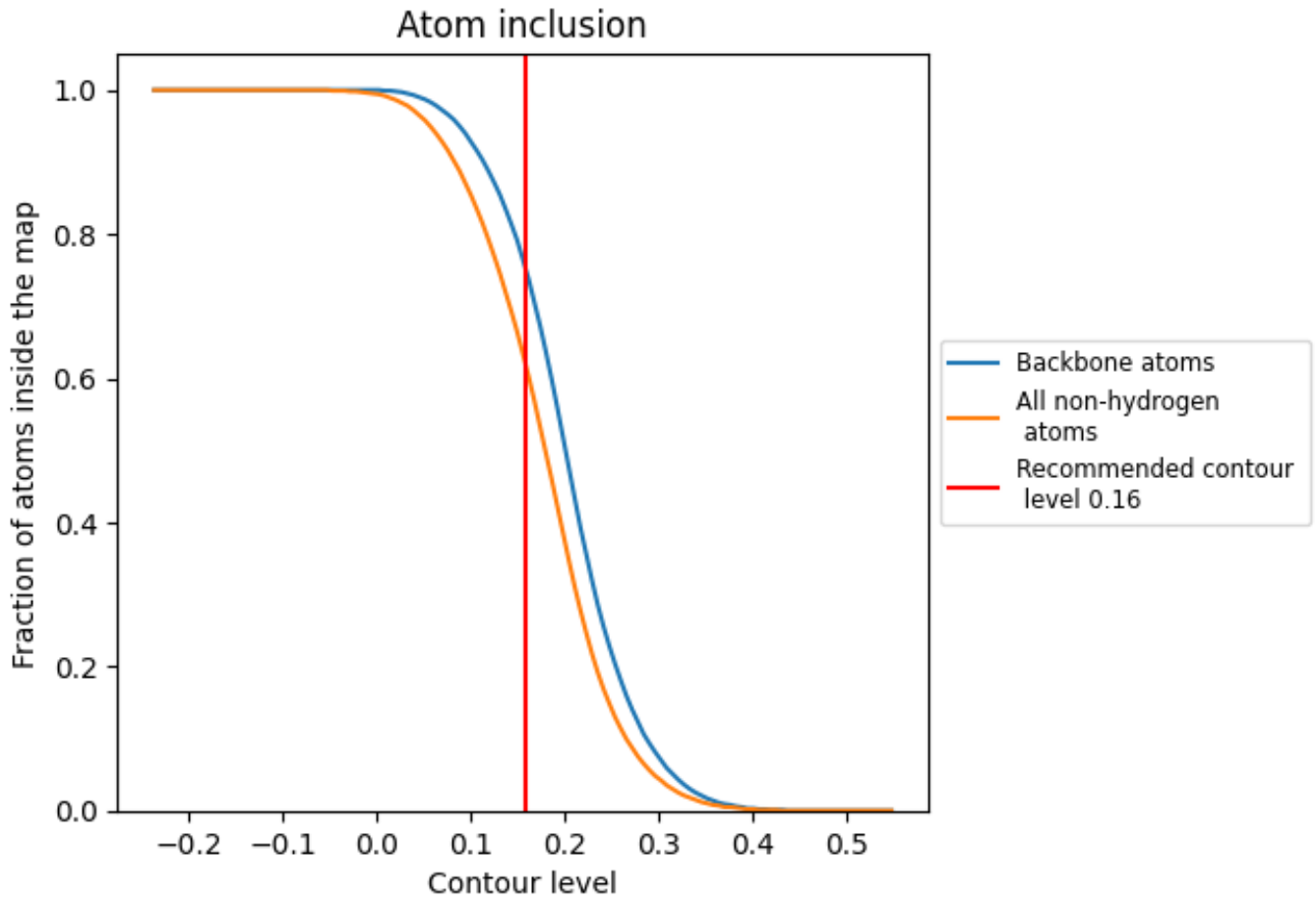
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 61% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6140	0.1530
A	0.7020	0.1430
B	0.6330	0.1730
E	0.6190	0.1580
F	0.6700	0.1150
G	0.5960	0.1340
H	0.6220	0.1130
I	0.6040	0.1490
J	0.6440	0.1220