Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 08:03 AM EDT

PDB ID	:	5TB3
EMDB ID	:	EMD-8394
Title	:	Structure of rabbit RyR1 (EGTA-only dataset, class 3)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-11
Resolution	:	4.70 Å(reported)

This is a Full wwPDB EM Validation 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:

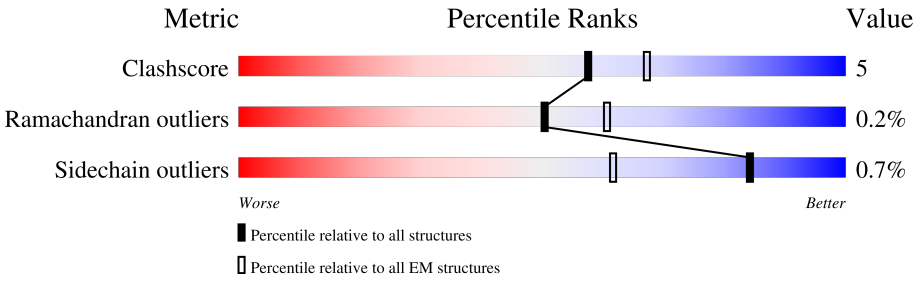
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	108	80% 81% 18% ·
1	F	108	80% 81% 18% ·
1	H	108	80% 81% 18% ·
1	J	108	80% 81% 18% ·
2	B	4416	66% 84% 11% 5%
2	E	4416	67% 84% 11% 5%
2	G	4416	66% 84% 11% 5%
2	I	4416	67% 84% 11% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 121312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	E	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	I	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		
2	G	4196	Total	C	N	O	S	0	0
			29509	18692	5230	5430	157		

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

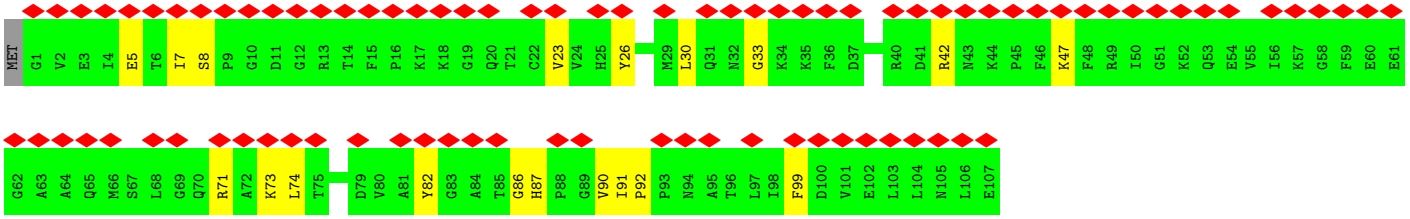
Mol	Chain	Residues	Atoms		AltConf
3	B	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

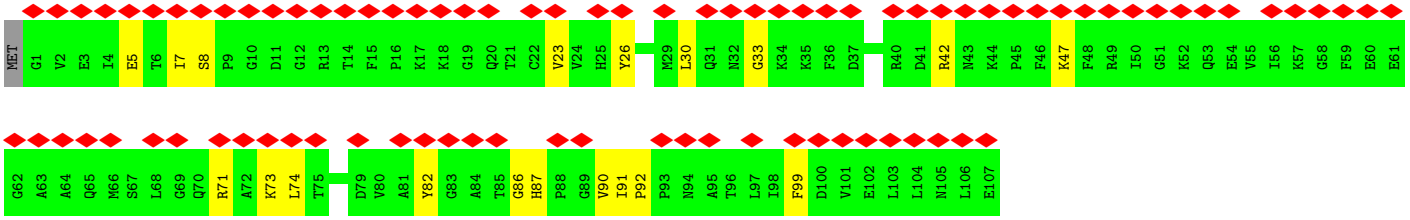
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



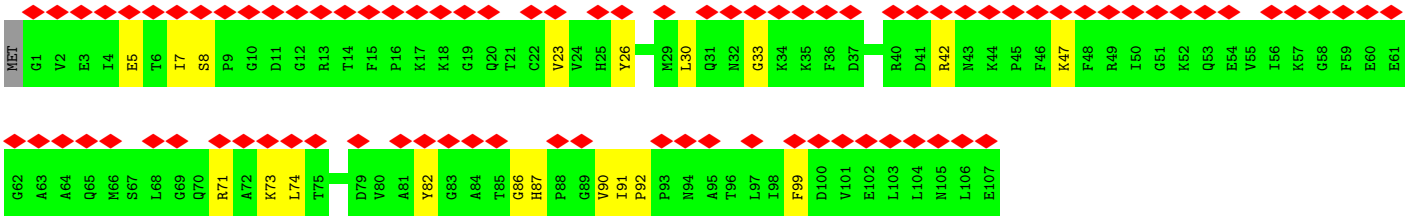
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



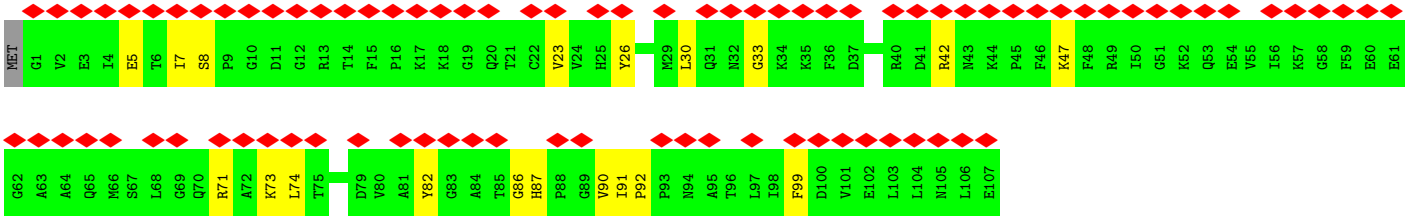
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



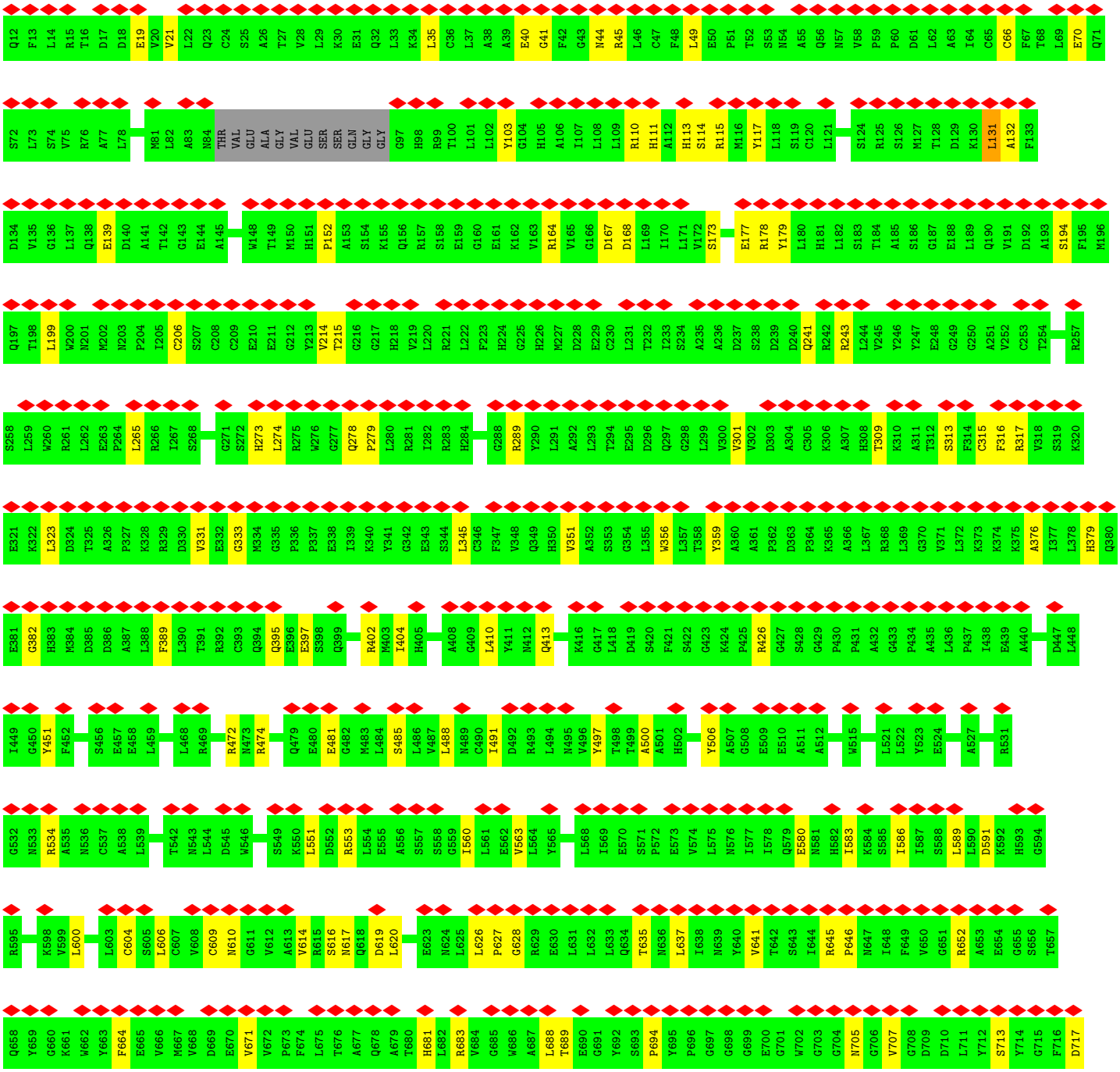
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

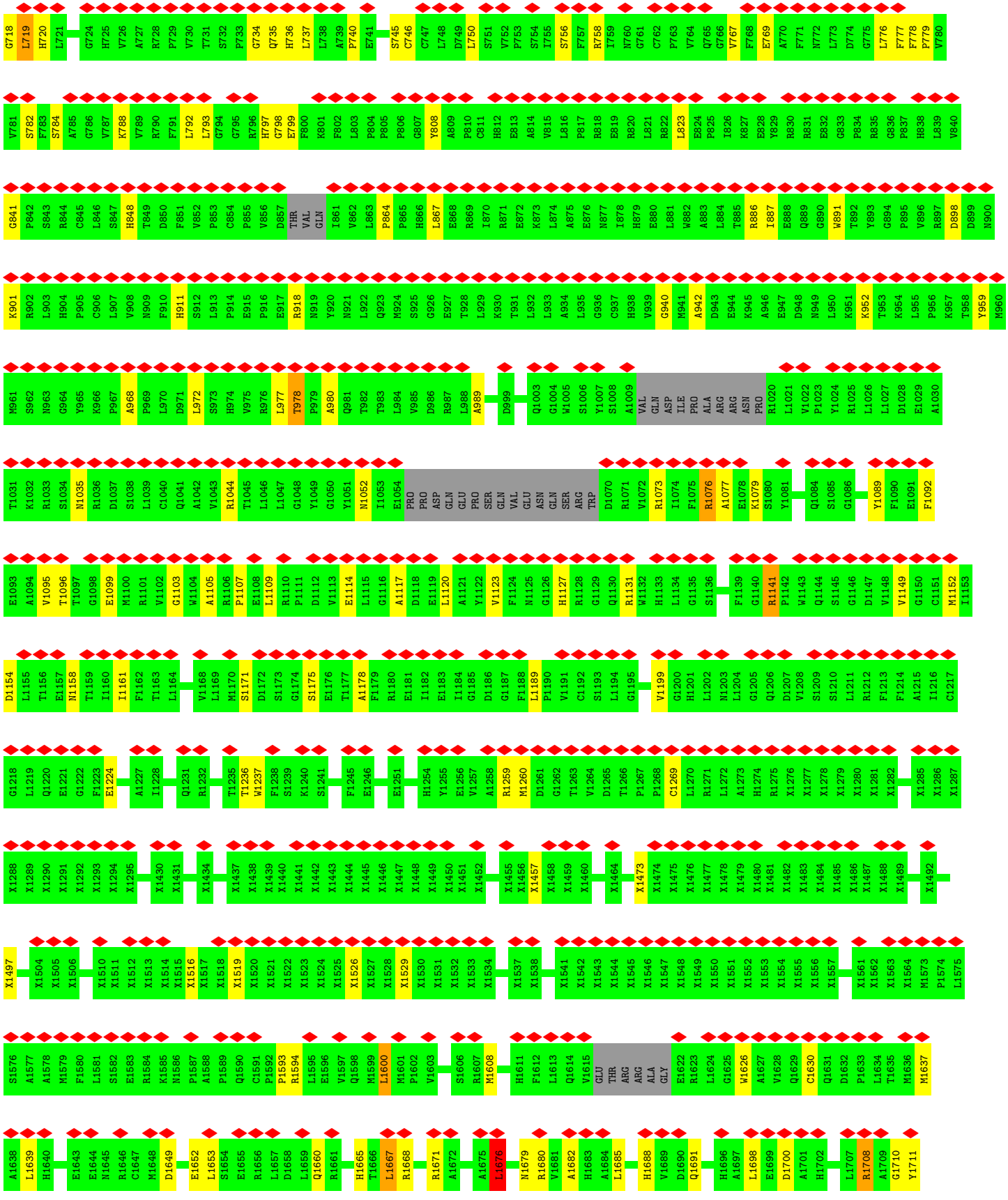
Chain J:



• Molecule 2: Ryanodine receptor 1

Chain B:

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V781 S782 F783 S784 A785 G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 H797 G798 E799 F800 K801 F802 L803 P804 P805 P806 G807 Y808 A809 P810 C811 H812 E813 A814 V815 L816 P817 R818 E819 R820 L821 R822 L823 E824 F825 I826 K827 E828 Y829 R830 R831 E832 G833 P834 R835 G836 P837 H838 L839 Y840
G841 P842 S843 R844 C845 L846 S847 H848 T849 D850 F851 V852 P853 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900
K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 L923 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960
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T1031 K1032 R1033 S1034 N1035 R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 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 Q1084 S1085 G1086 Y1089 F1090 E1091 F1092
E1093 A1094 V1095 T1096 T1097 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 G1116 A1117 D1118 E1119 L1120 A1121 Y1122 V1123 F1124 N1125 G1126 H1127 R1128 G1129 Q1130 R1131 W1132 H1133 L1134 G1135 S1136 F1139 G1140 R1141 P1142 W1143 Q1144 S1145 G1146 D1147 V1148 V1149 G1150 C1151 M1152 I1153
D1154 L1155 T1156 E1157 N1158 T1159 I1160 I1161 F1162 T1163 L1164 V1168 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1182 E1183 I1184 G1185 D1186 G1187 F1188 L1189 P1190 V1191 C1192 S1193 L1194 G1195 V1199 G1200 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 V1208 S1209 S1210 L1211 R1212 F1213 F1214 A1215 I1216 C1217
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X1497 X1504 X1505 X1506 X1510 X1511 X1512 X1513 X1514 X1515 X1516 X1517 X1518 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1532 X1533 X1534 X1537 X1538 X1541 X1542 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 X1551 X1552 X1553 X1554 X1555 X1556 X1557 X1561 X1562 X1563 X1564 M1573 P1574 L1575
S1576 A1577 A1578 M1579 F1580 L1581 S1582 E1583 R1584 K1585 N1586 P1587 A1588 P1589 Q1590 C1591 P1592 P1593 R1594 L1595 E1596 V1597 Q1598 M1599 L1600 M1601 P1602 V1603 S1606 R1607 M1608 H1611 F1612 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624 G1625 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 T1635 M1636 M1637
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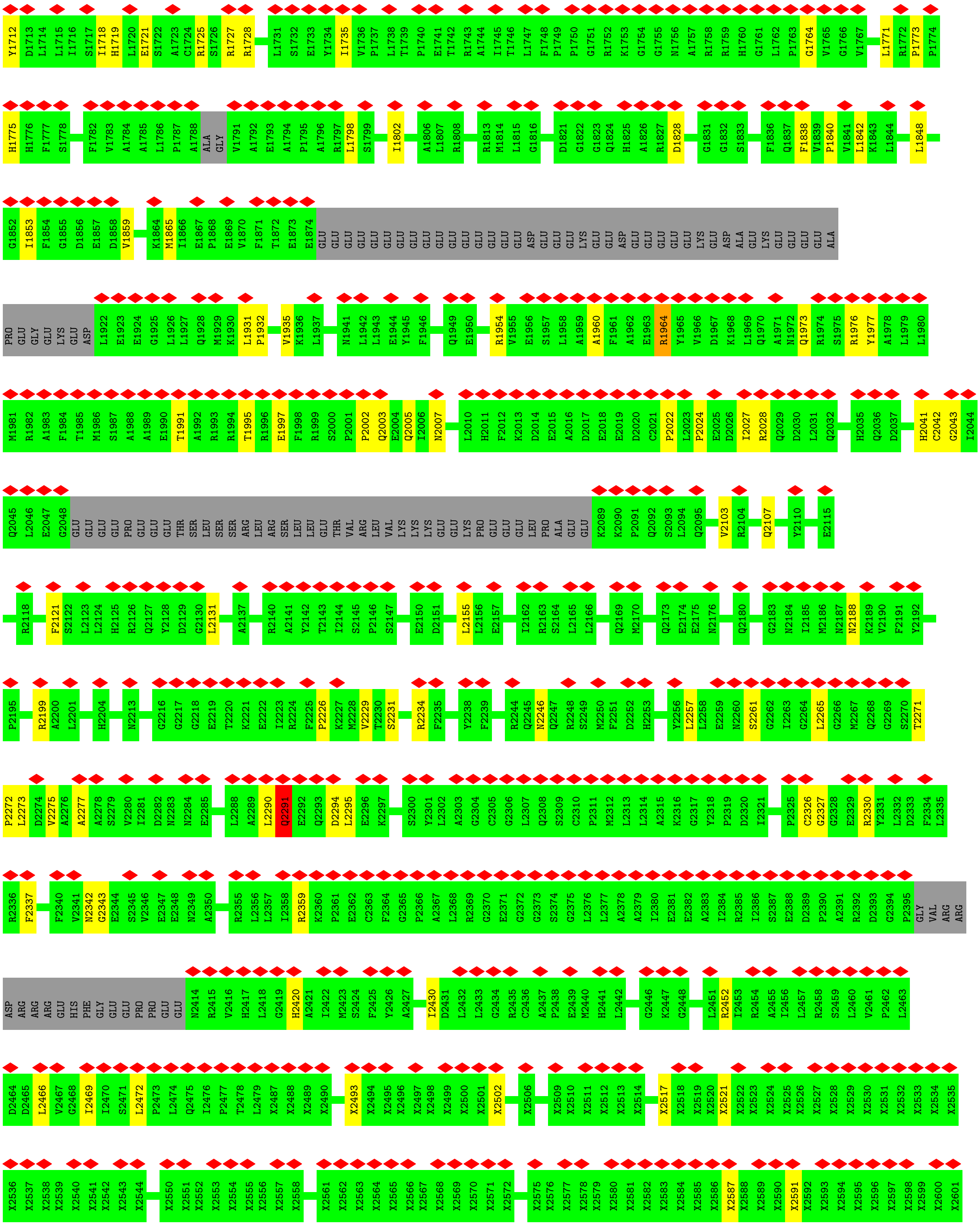
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H1775 H1776 F1777 S1778 F1782 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY V1791 A1792 E1793 A1794 P1795 A1796 R1797 L1798 S1799 I1802 A1806 L1807 R1808 R1813 M1814 L1815 G1816 D1821 G1822 G1823 Q1824 H1825 A1826 R1827 D1828 G1831 G1832 S1833 F1836 Q1837 F1838 V1839 P1840 V1841 L1842 K1843 L1844 L1848
G1852 I1853 F1854 G1855 D1856 E1857 D1858 V1859 K1864 M1865 I1866 E1867 P1868 E1869 V1870 F1871 T1872 E1873 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
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R2336 F2337 F2340 V2341 N2342 G2343 E2344 S2345 V2346 E2347 E2348 N2349 A2350 R2355 L2356 L2357 I2358 R2359 K2360 P2361 E2362 C2363 F2364 G2365 P2366 A2367 L2368 R2369 G2370 E2371 G2372 G2373 S2374 G2375 L2376 L2377 A2378 A2379 I2380 E2381 E2382 A2383 I2384 R2385 I2386 S2387 E2388 D2389 P2390 A2391 R2392 D2393 G2394 P2395 GLY VAL ARG ARG
ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 H2417 L2418 G2419 H2420 A2421 I2422 M2423 S2424 F2425 Y2426 A2427 I2430 D2431 L2432 L2433 G2434 R2435 C2436 A2437 P2438 E2439 M2440 H2441 L2442 G2446 K2447 G2448 L2451 R2452 I2453 R2454 A2455 I2456 L2457 R2458 S2459 L2460 V2461 P2462 L2463
D2464 D2465 L2466 V2467 G2468 I2469 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479 X2487 X2488 X2489 X2490 X2493 X2494 X2495 X2496 X2497 X2498 X2499 X2500 X2501 X2502 X2506 X2509 X2510 X2511 X2512 X2513 X2514 X2517 X2518 X2519 X2520 X2521 X2522 X2523 X2524 X2525 X2526 X2527 X2528 X2529 X2530 X2531 X2532 X2533 X2534 X2535
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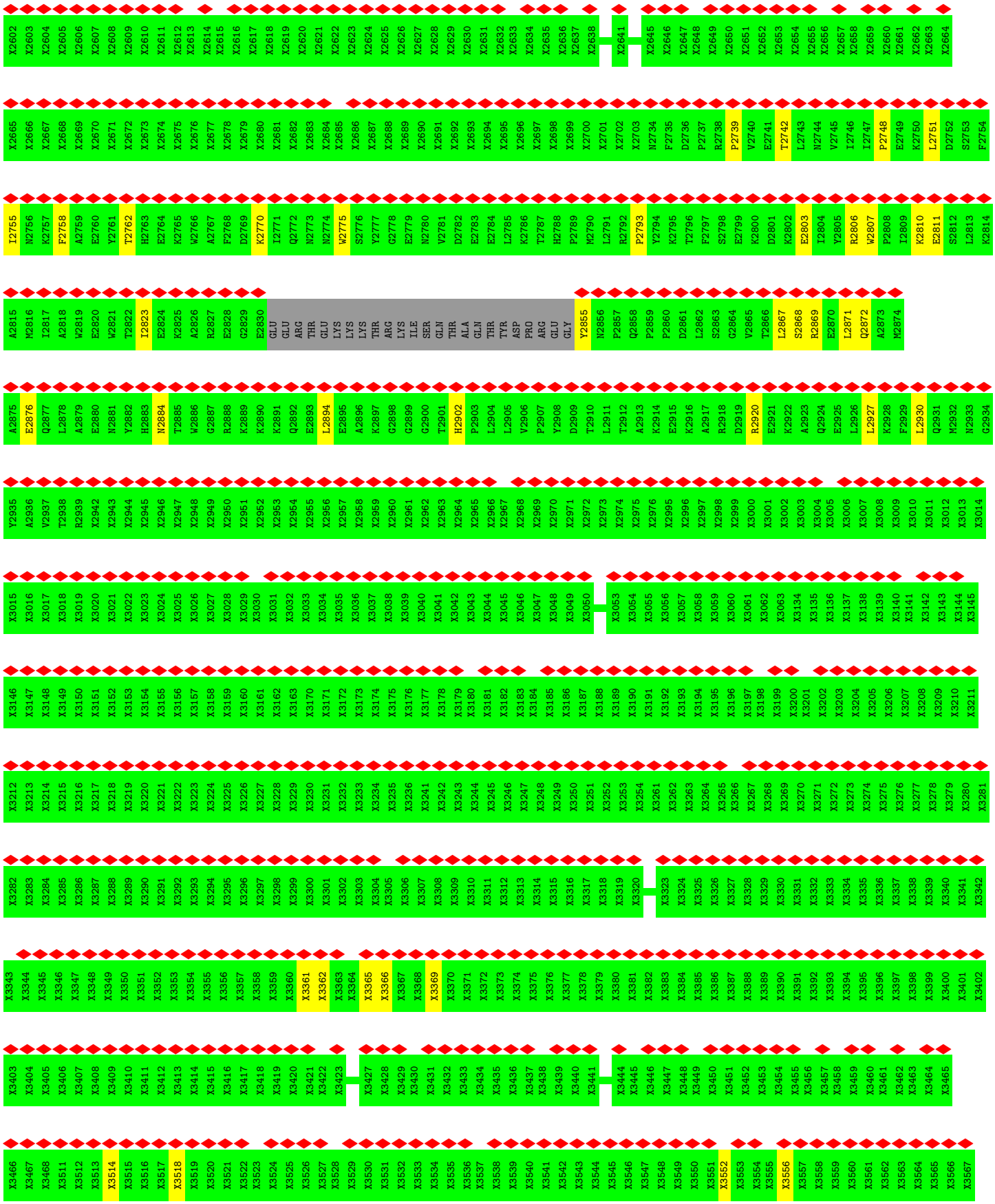
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A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874
A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934
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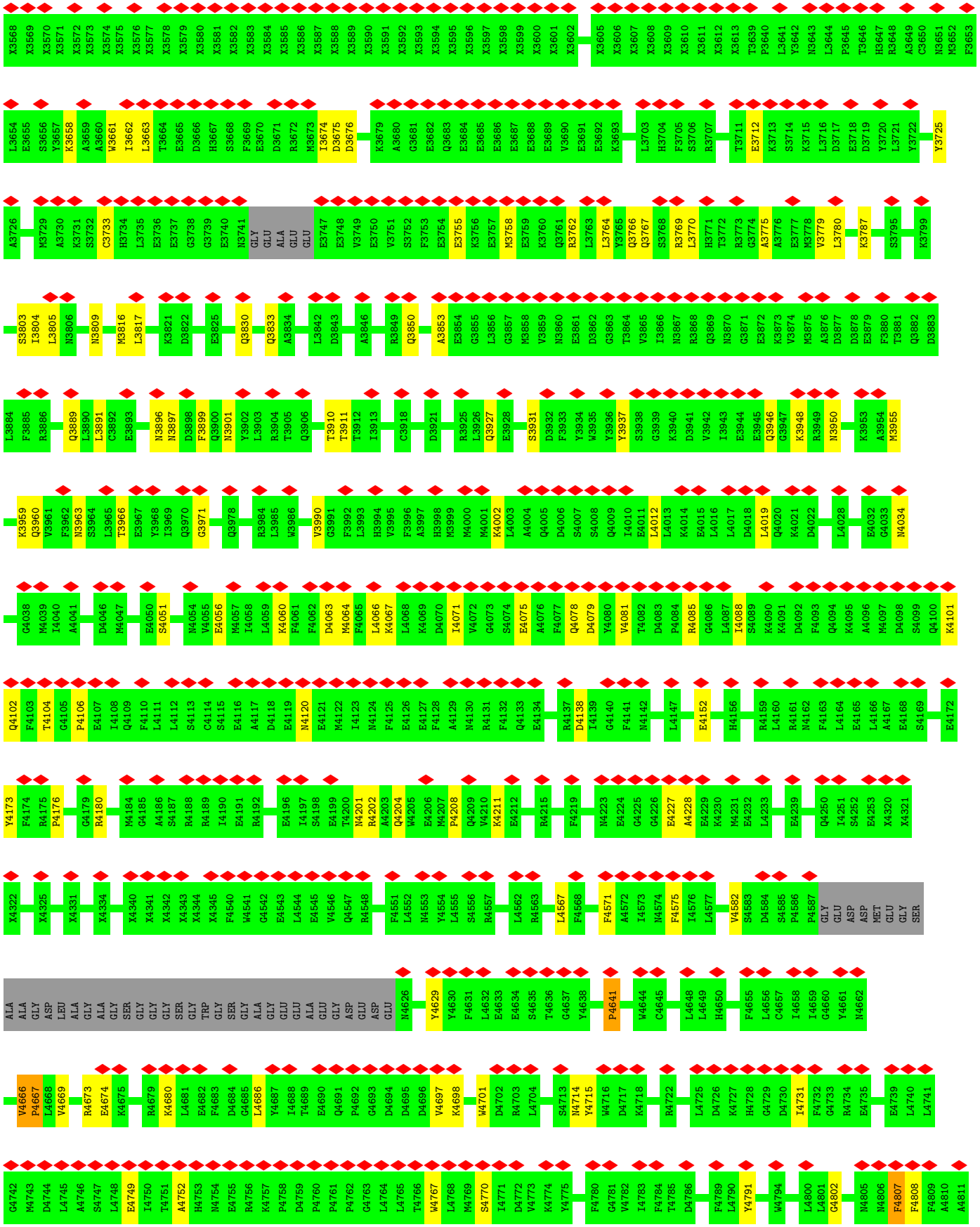
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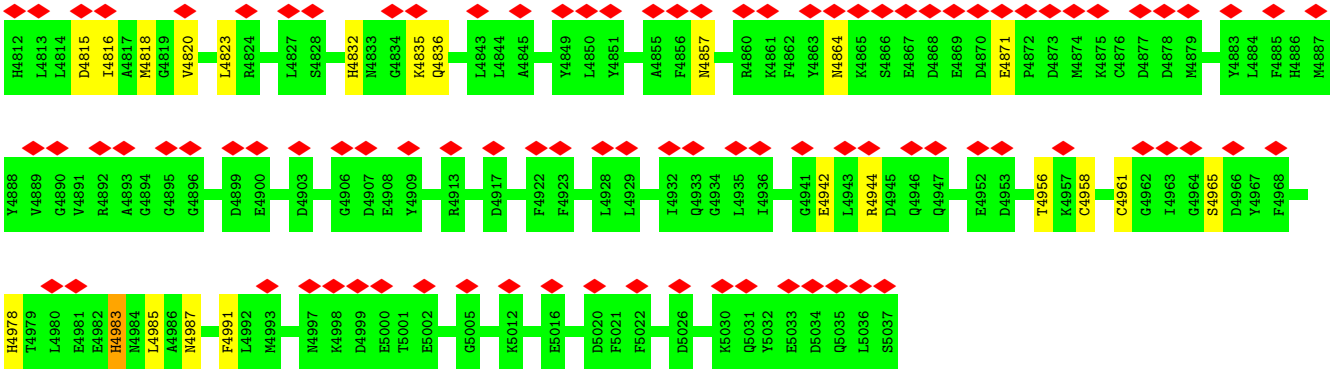
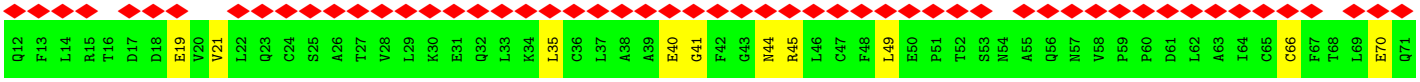
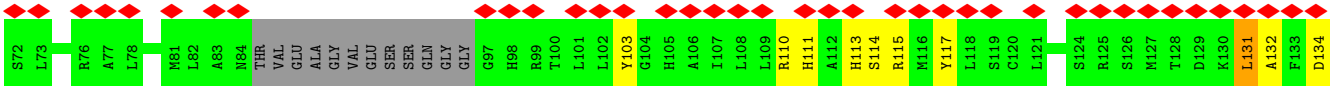
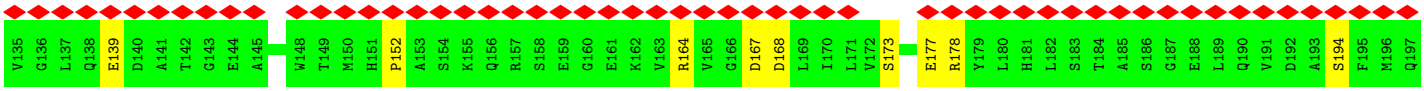


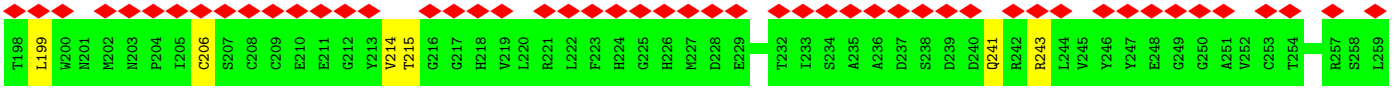
• Molecule 2: Ryanodine receptor 1

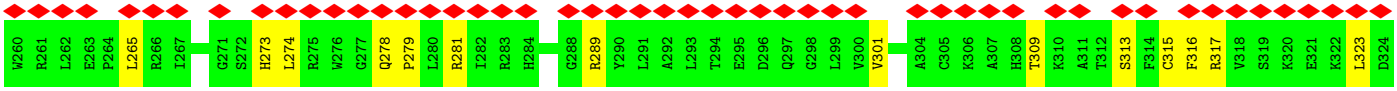
Chain E:

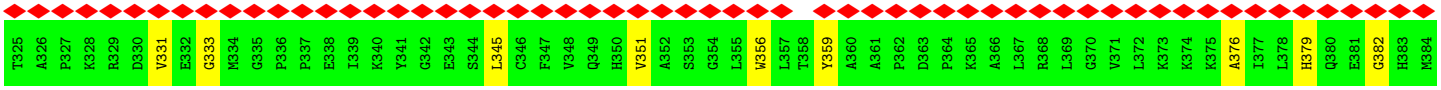


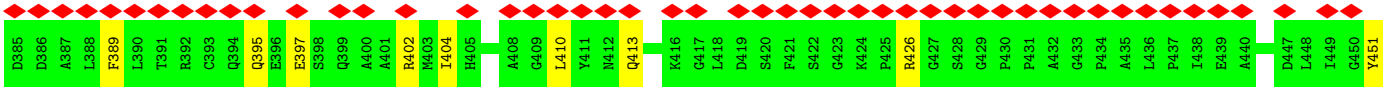


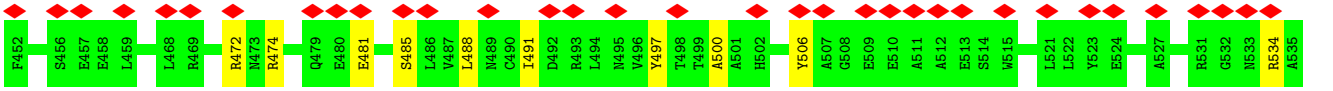


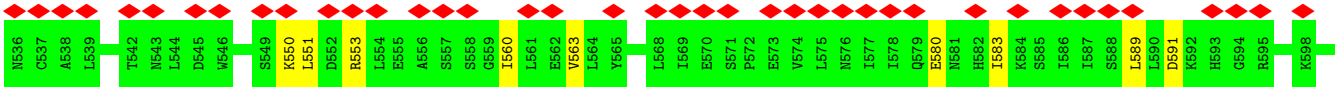


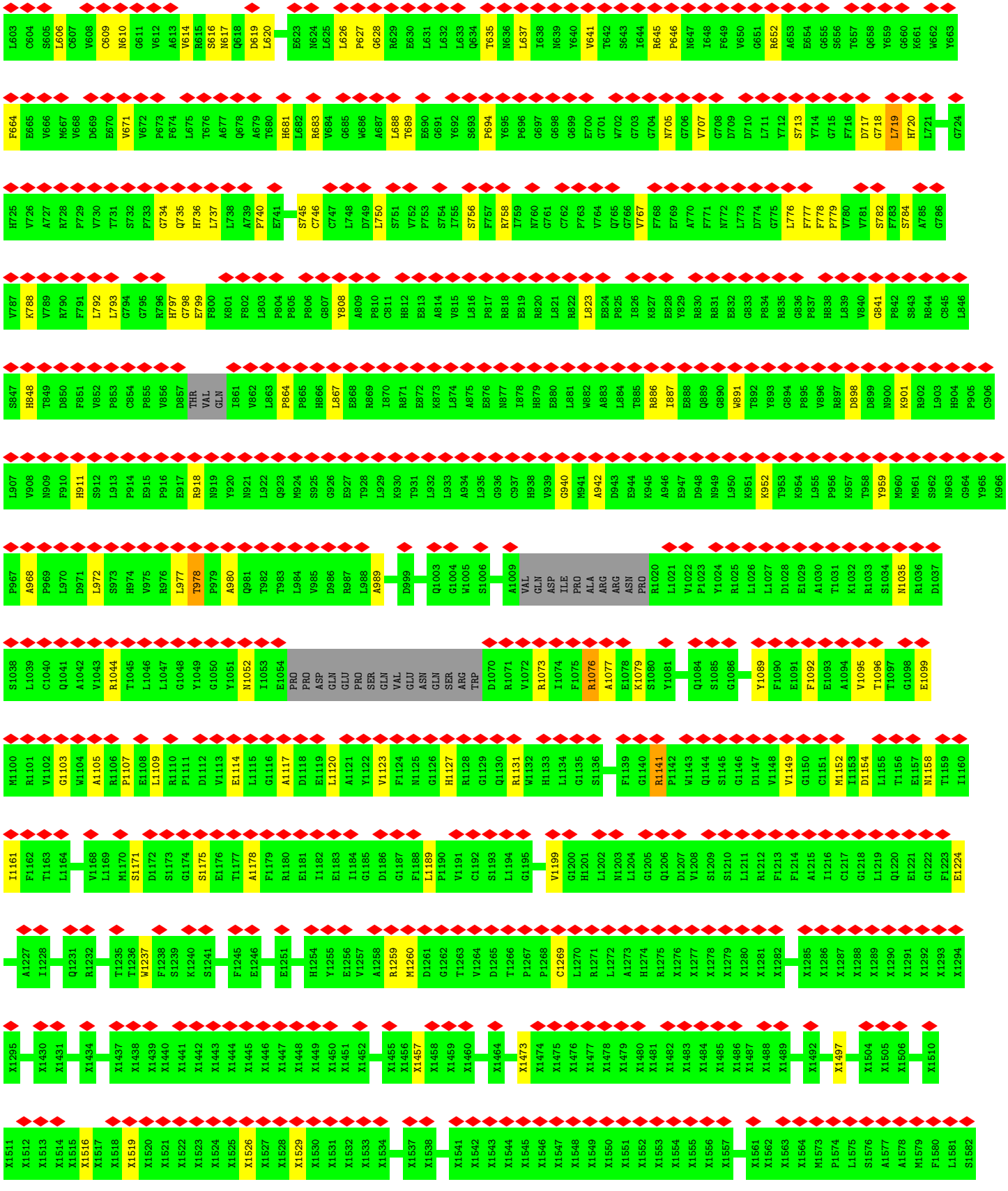








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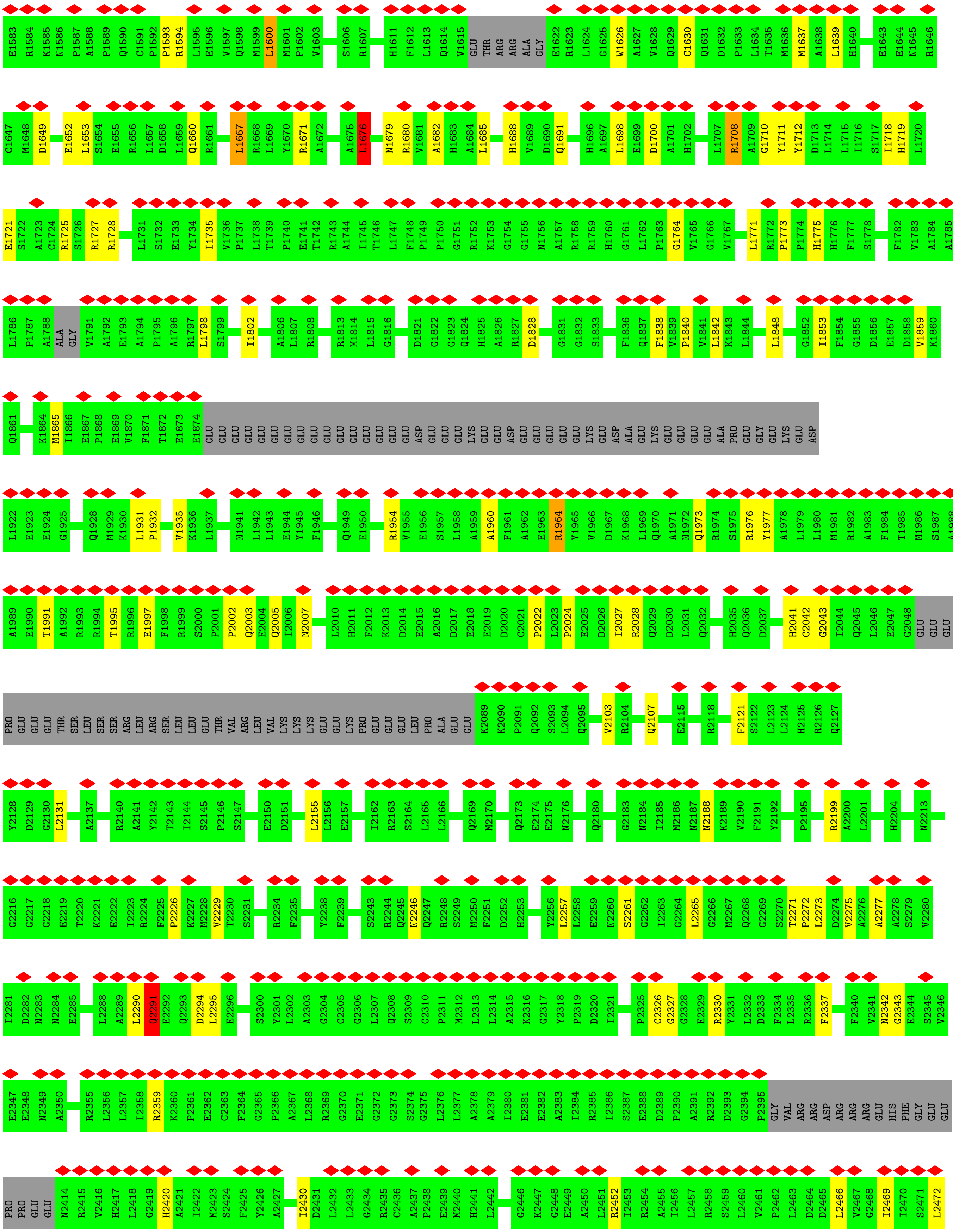
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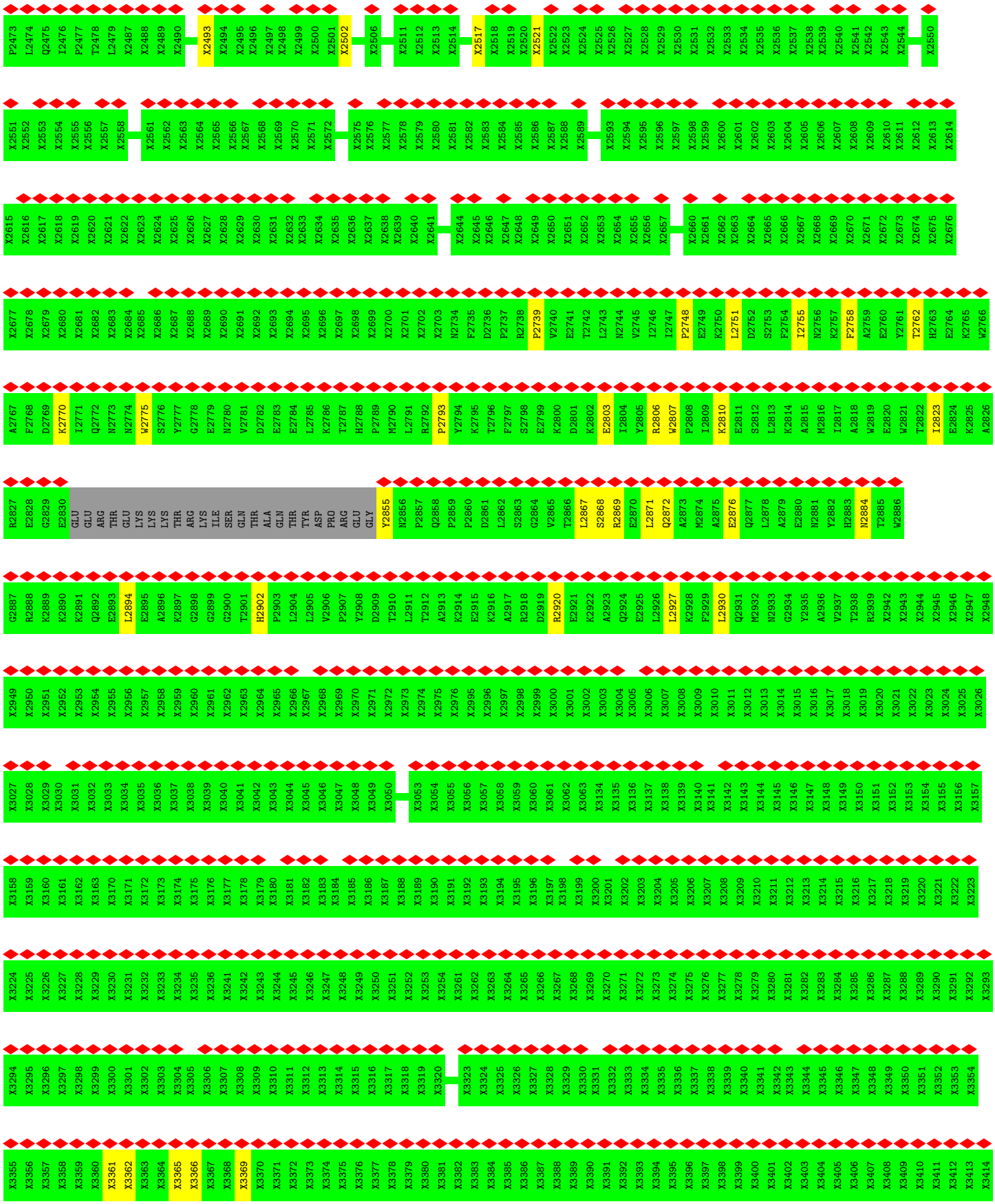
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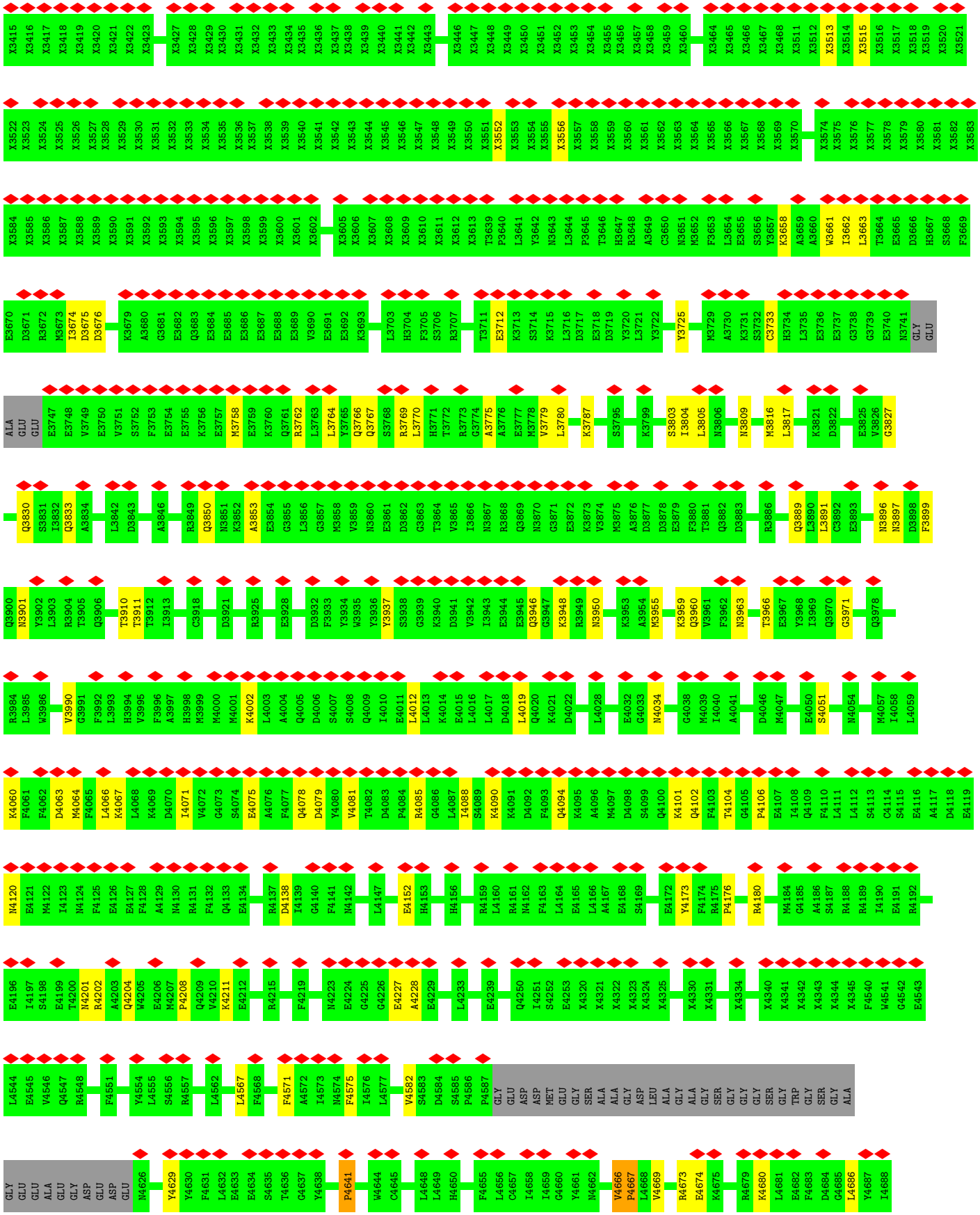
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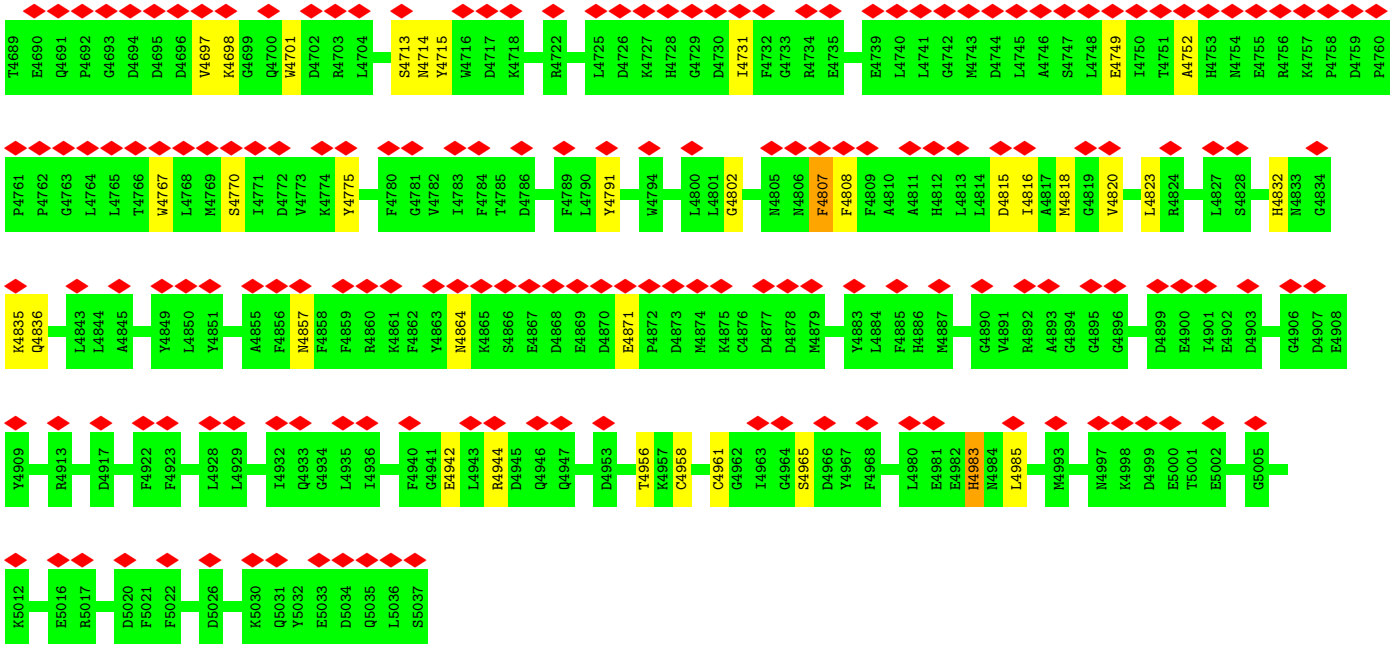

• Molecule 2: Ryanodine receptor 1

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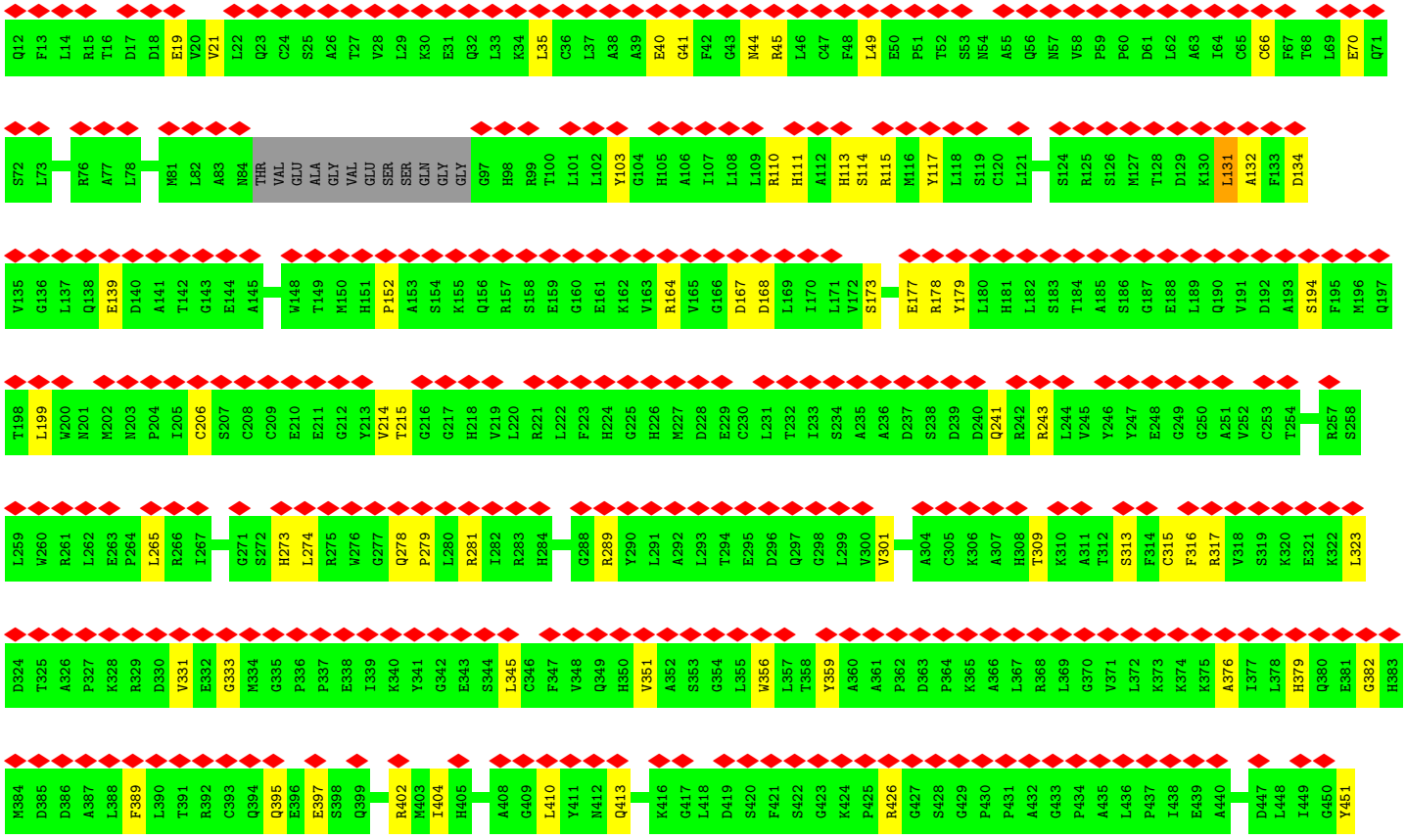

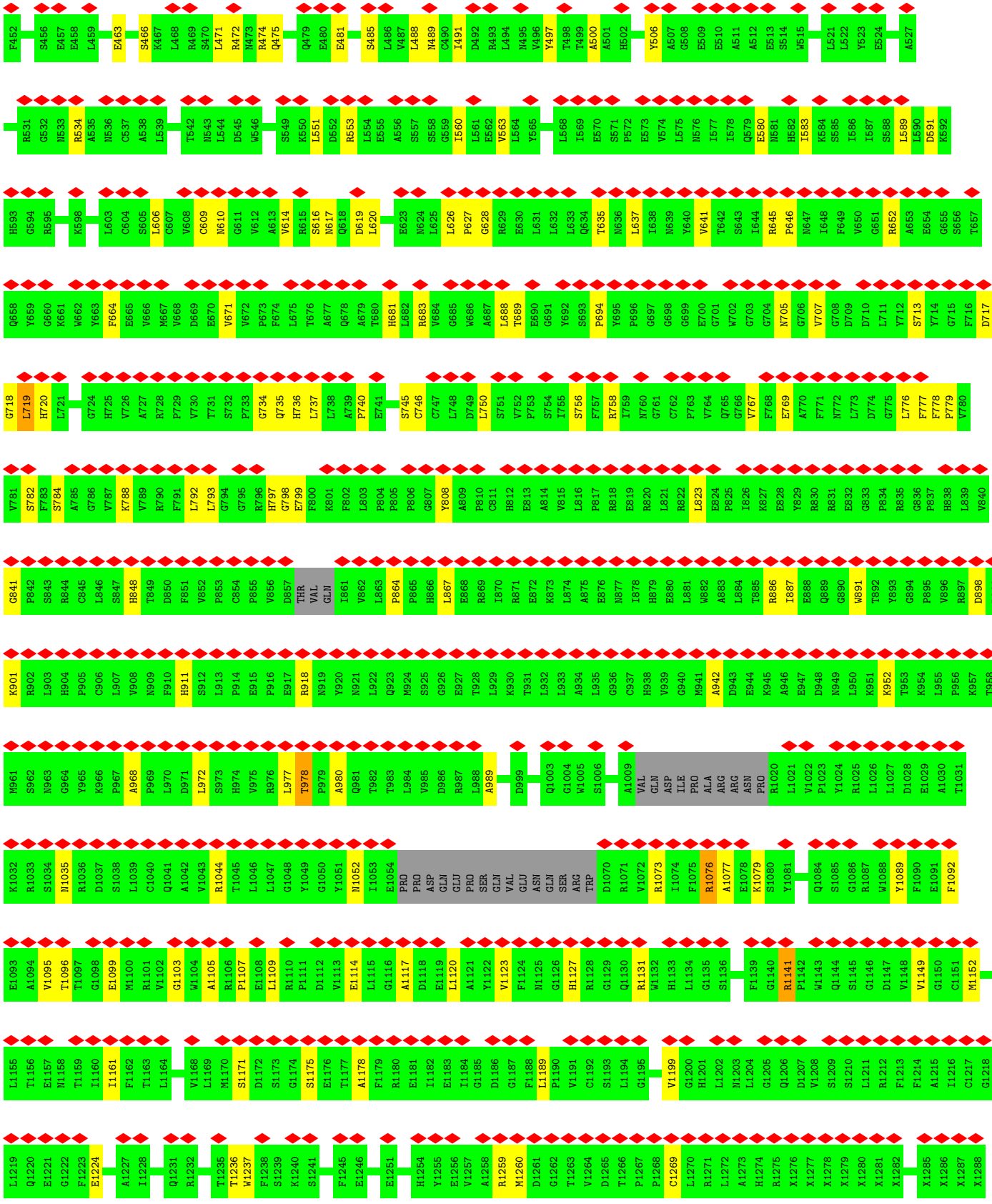
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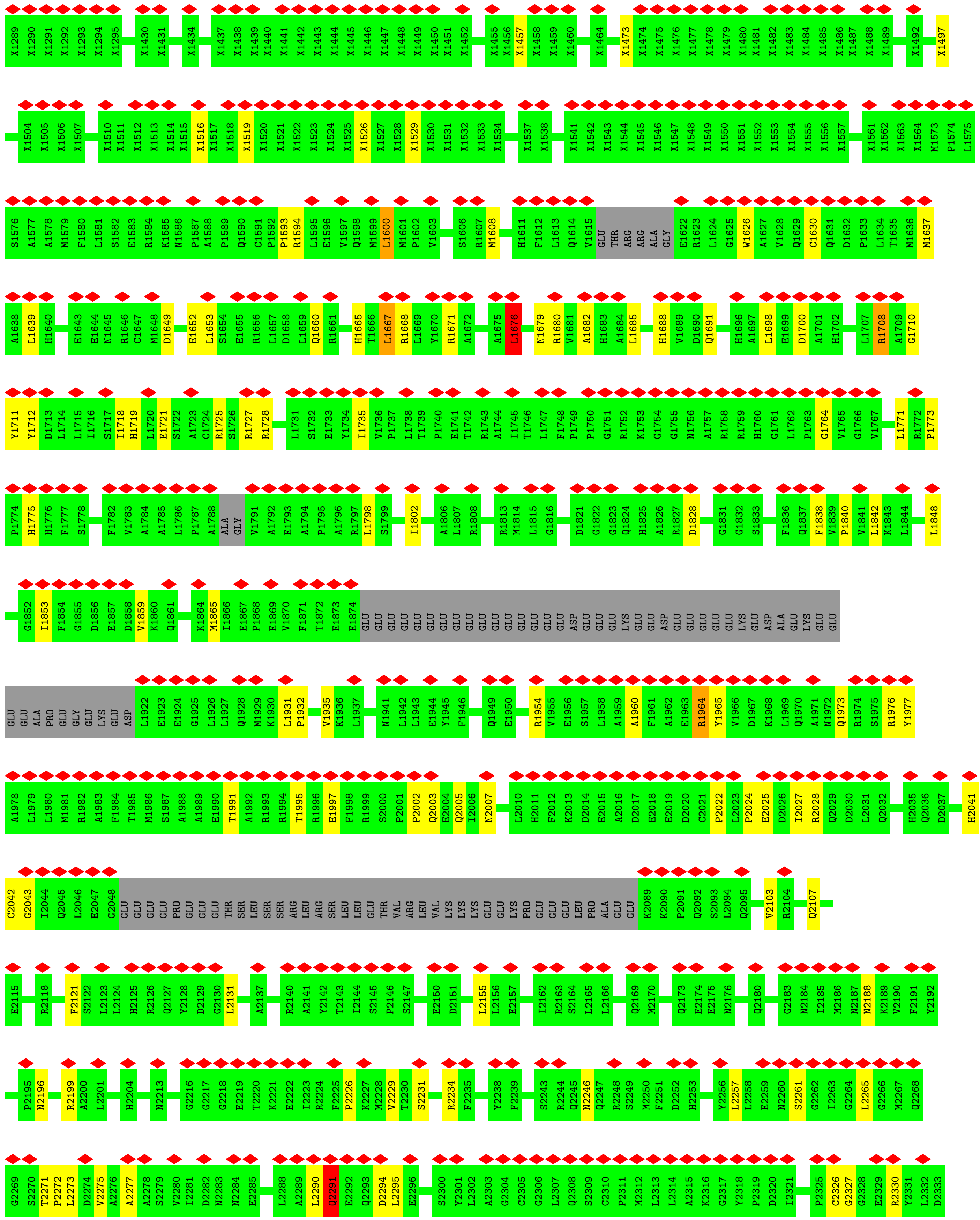
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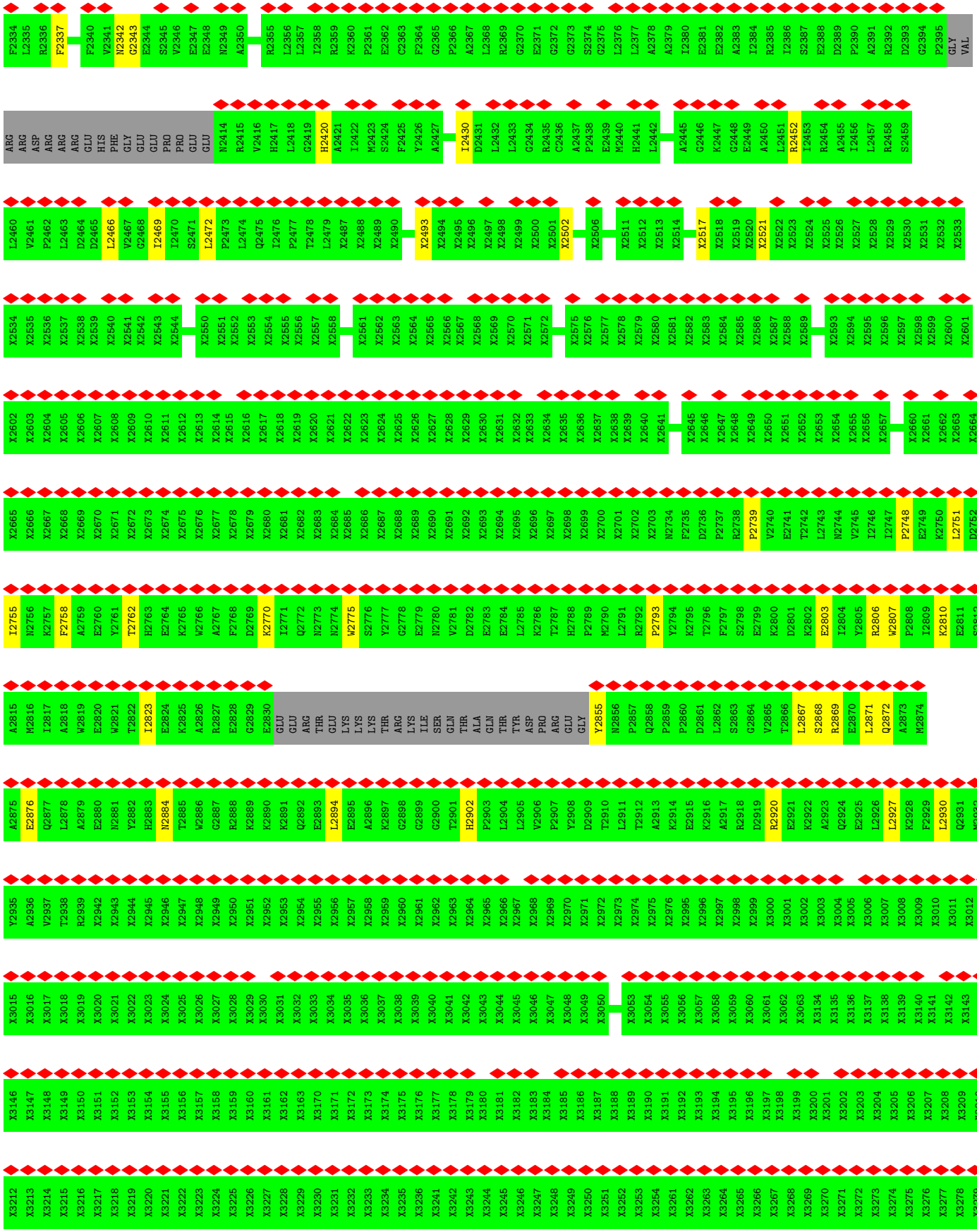
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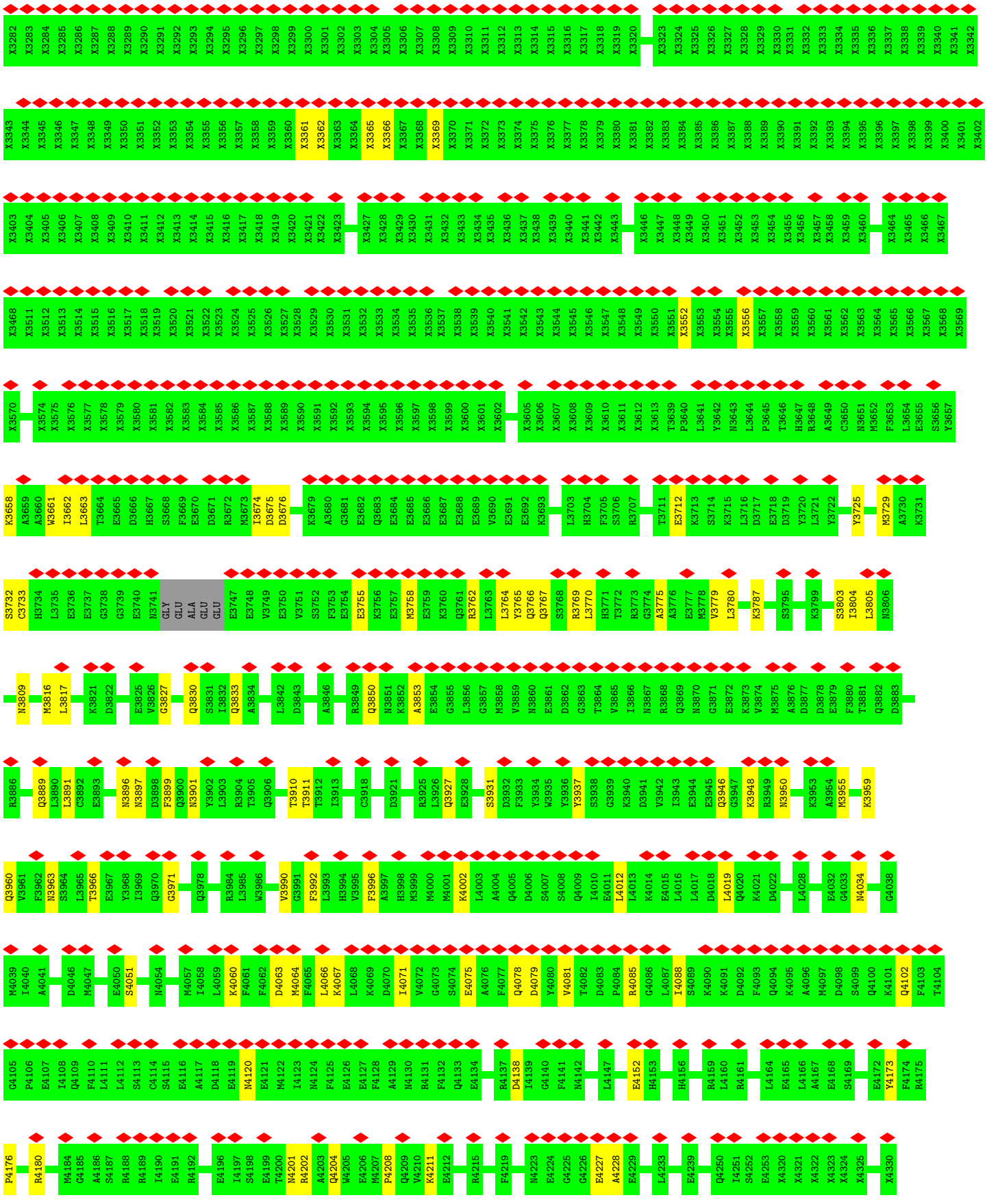
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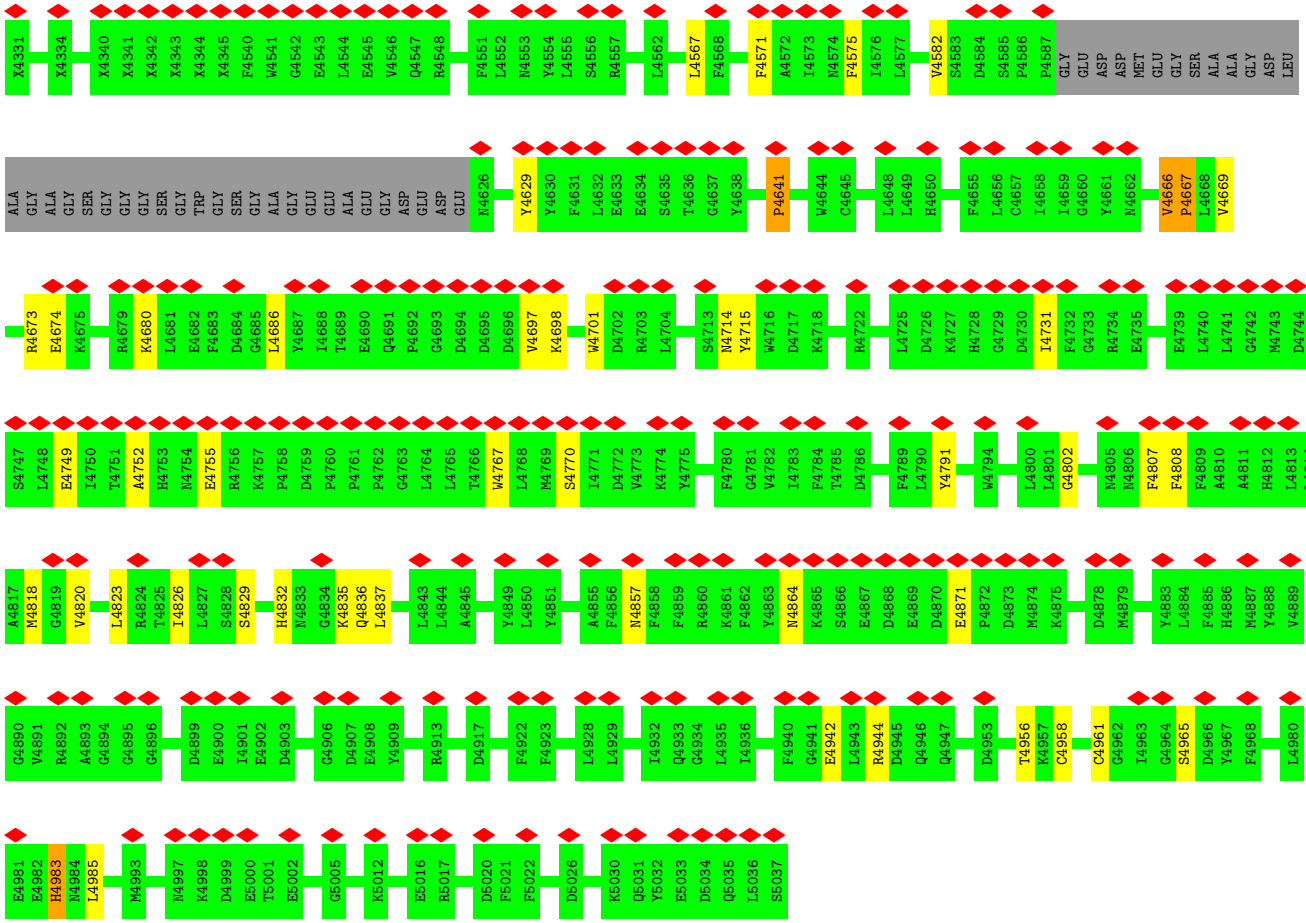
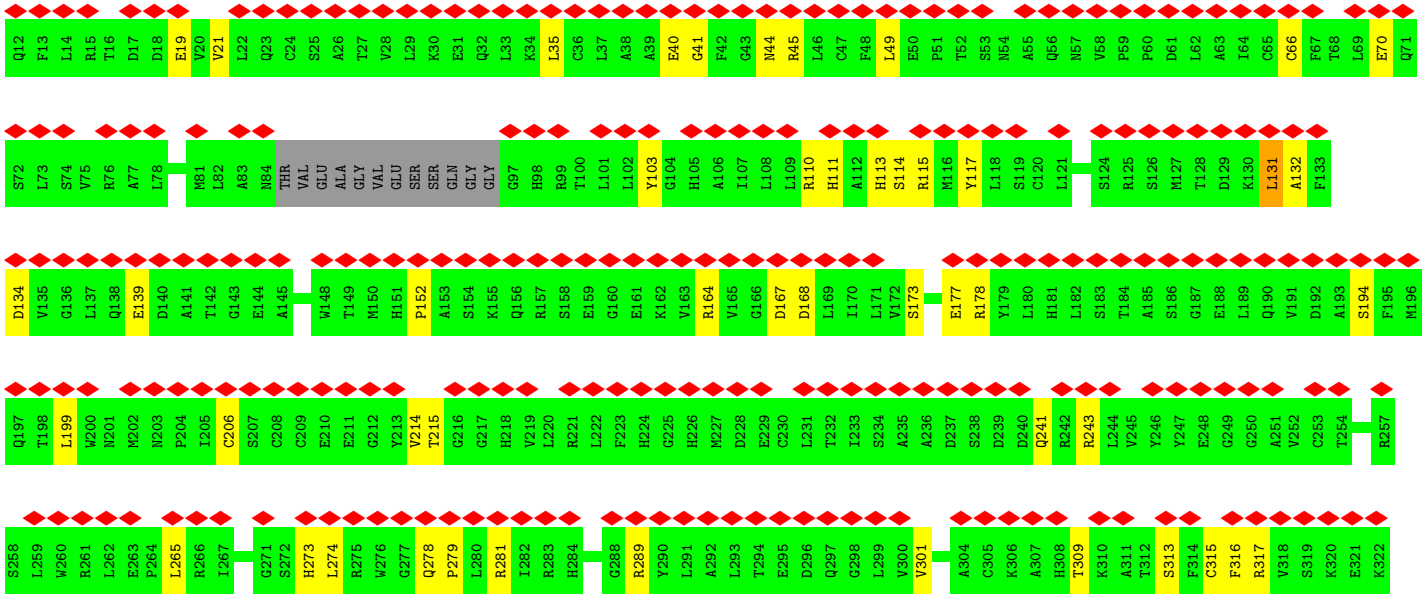
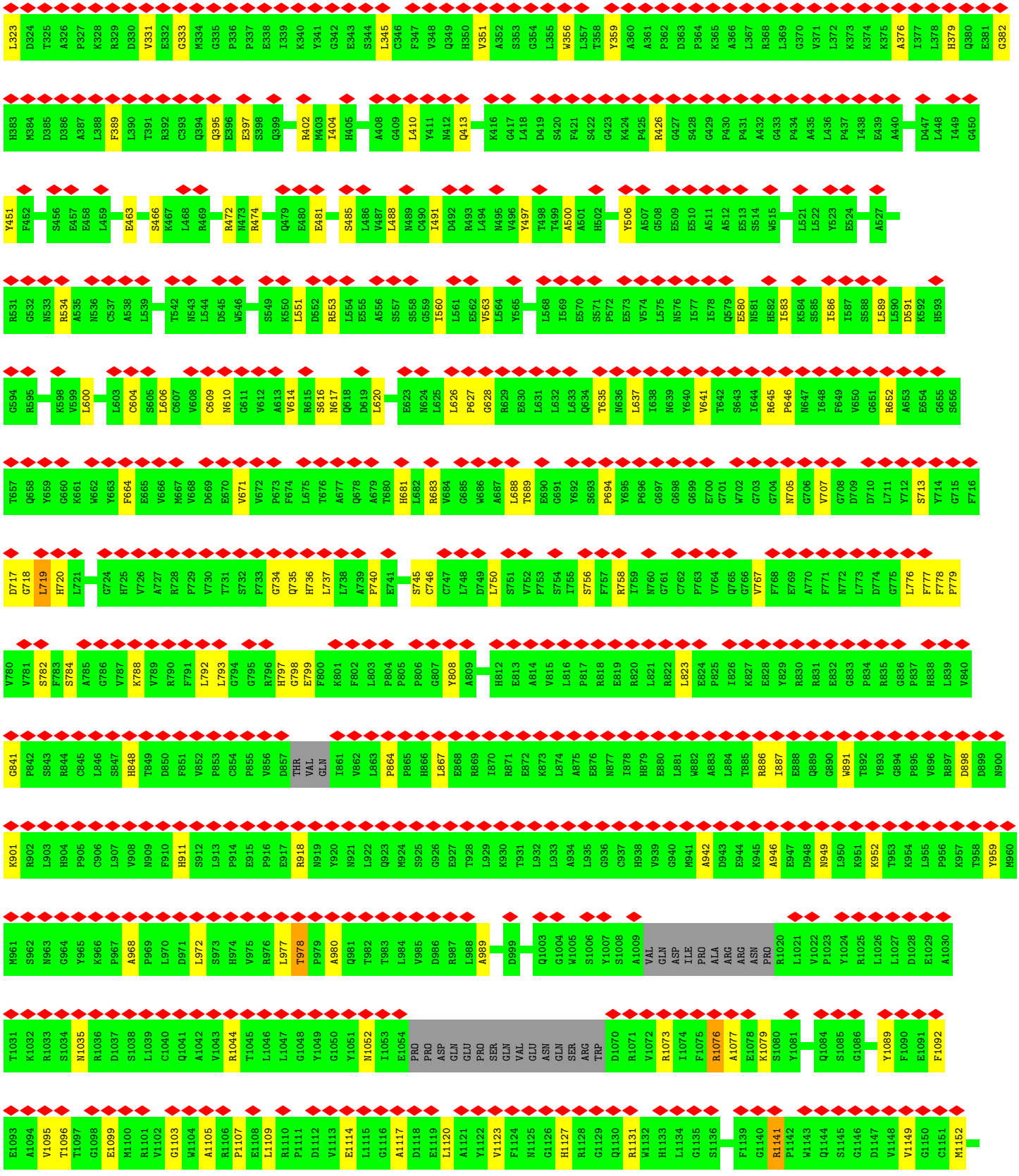


• Molecule 2: Ryanodine receptor 1

Chain G:

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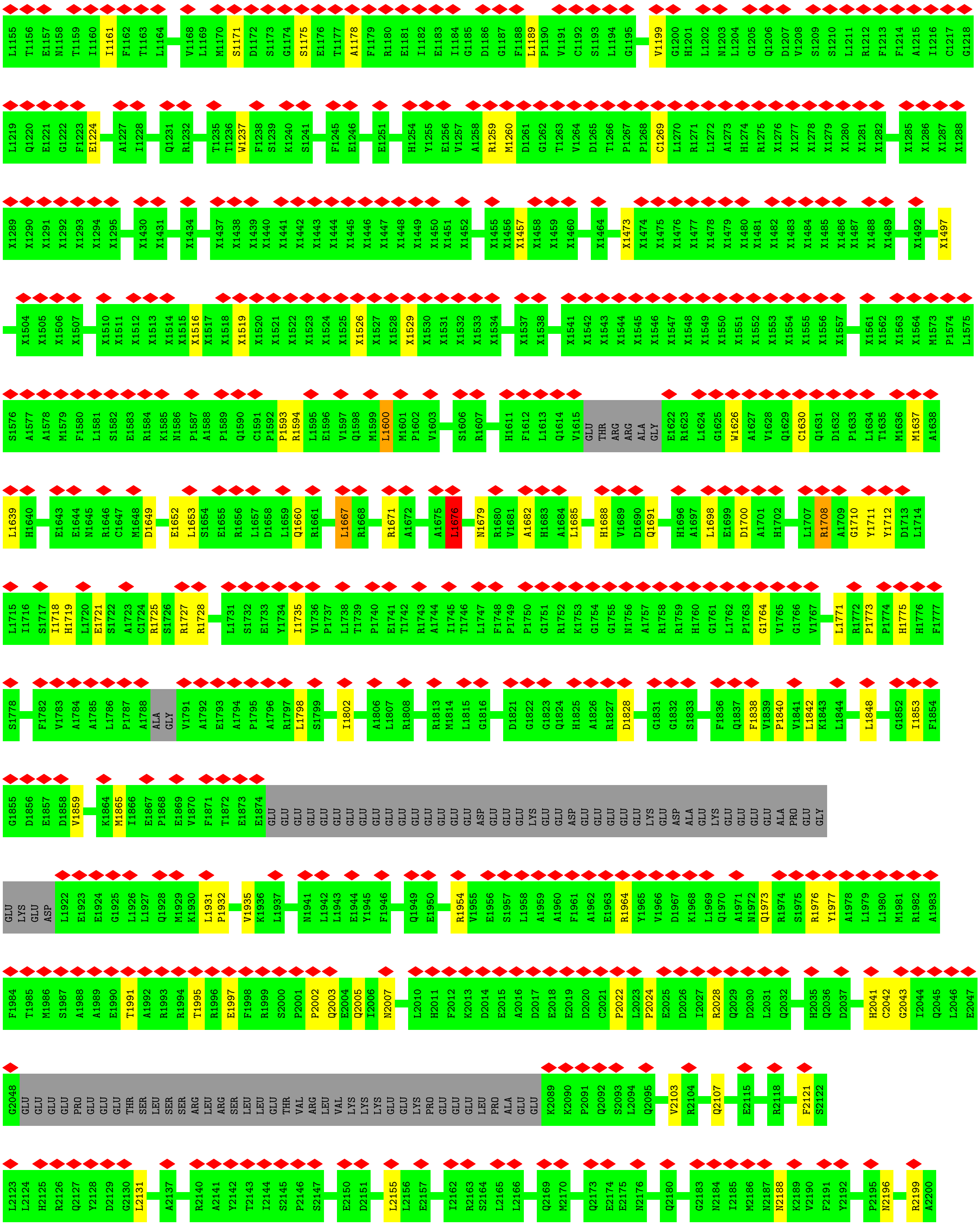
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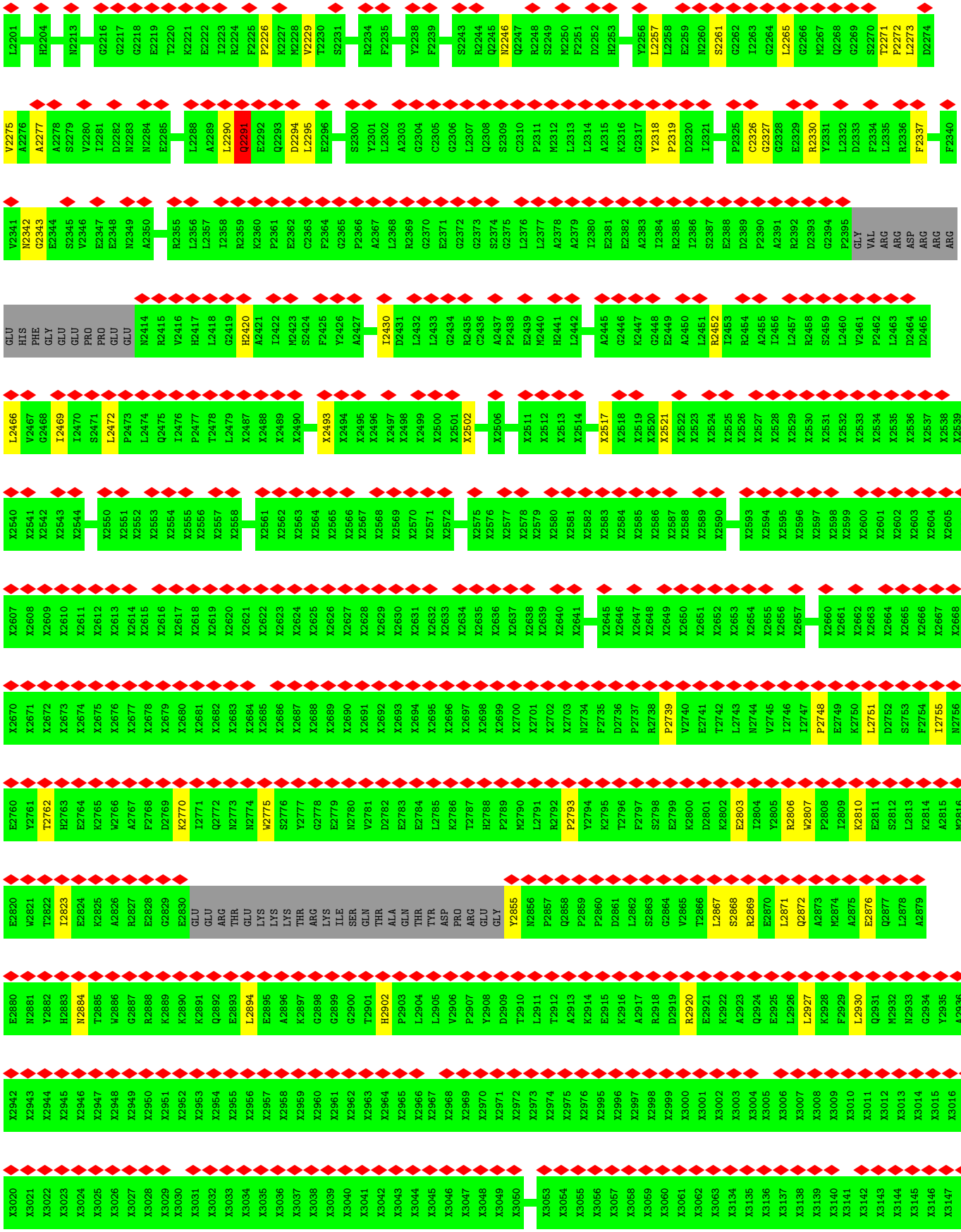
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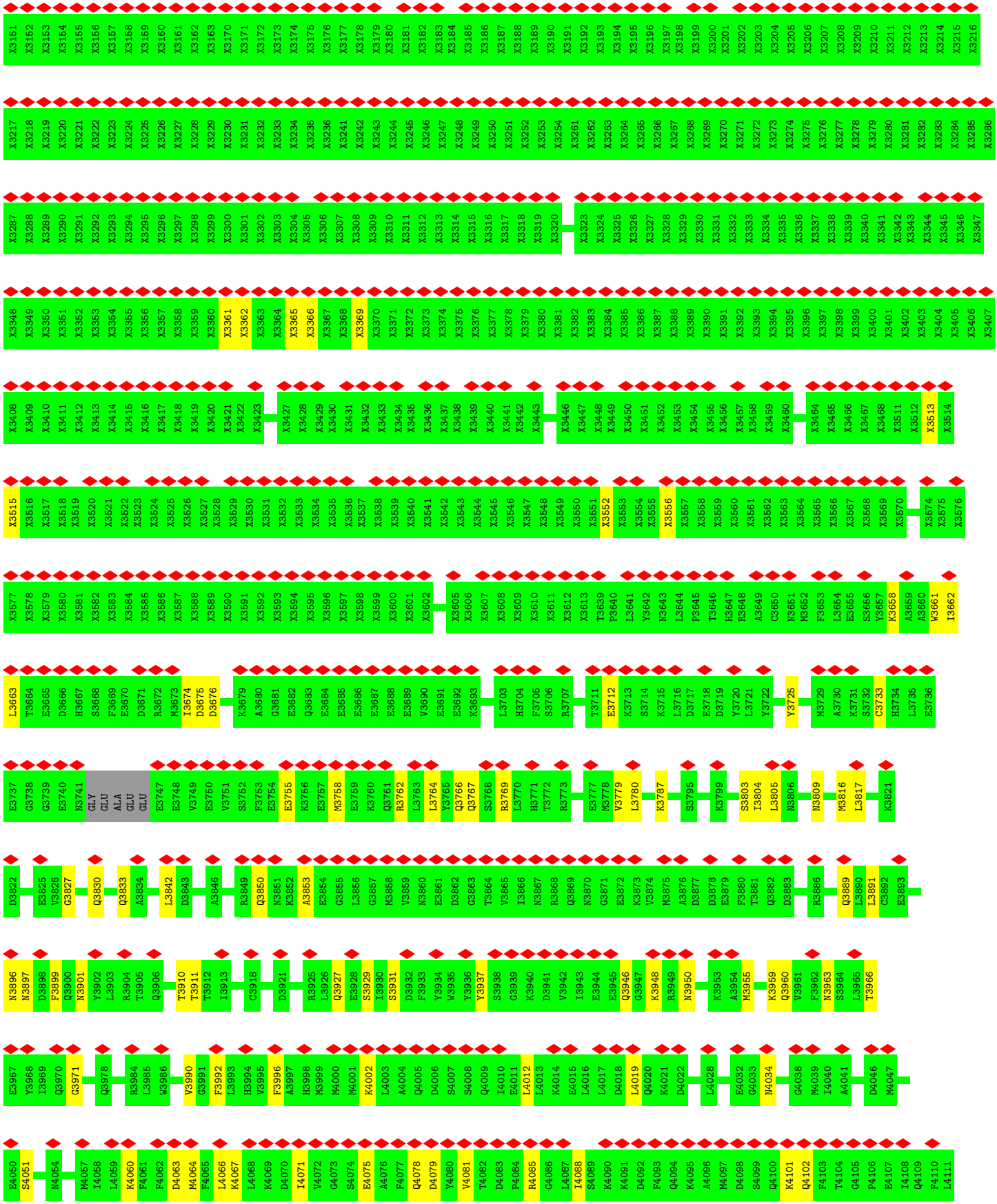
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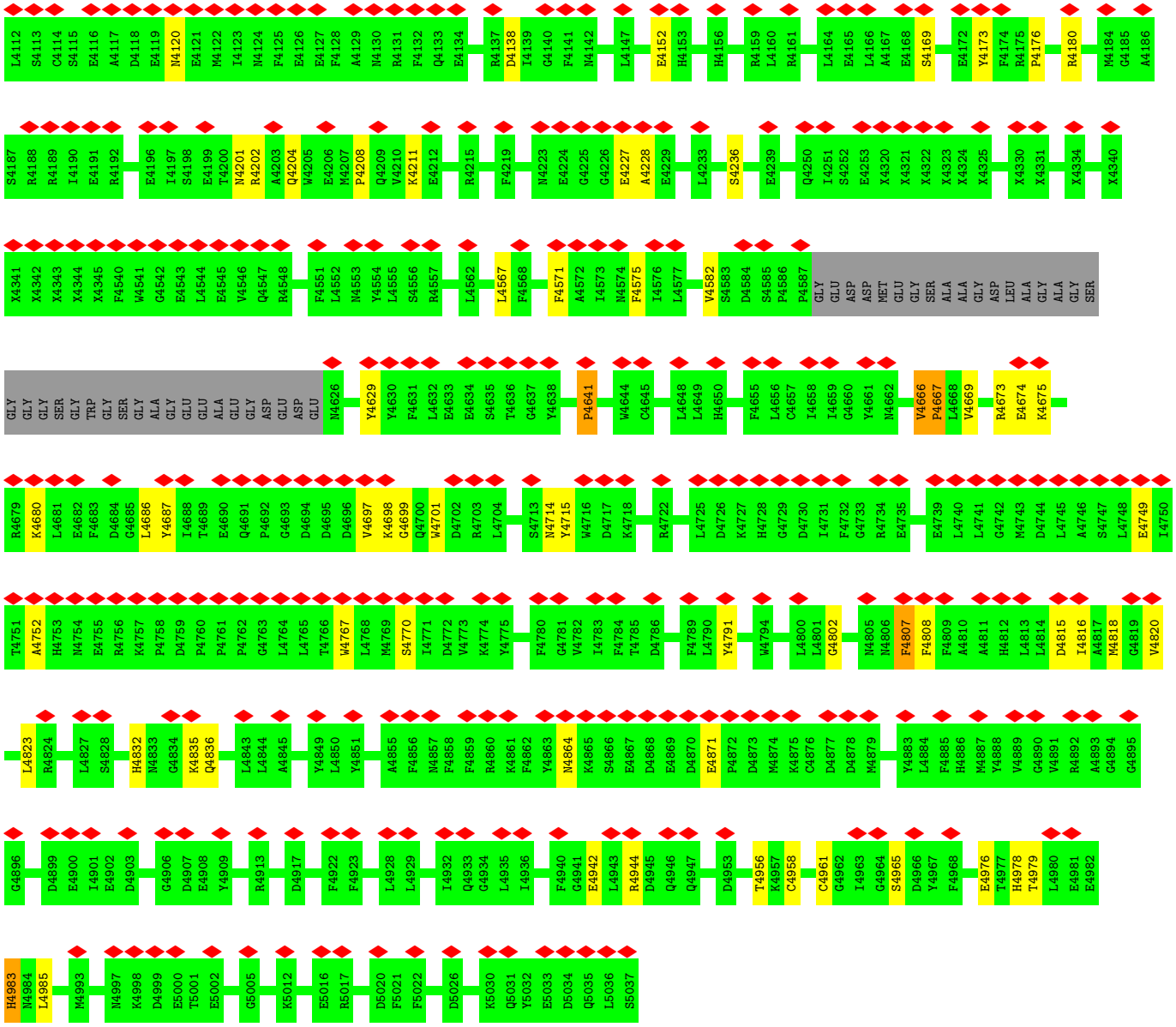
E4050 S4051 M4054 M4057 I4058 L4059 K4060 F4061 F4062 D4063 M4064 F4065 L4066 K4067 L4068 K4069 D4070 I4071 V4072 G4073 S4074 E4075 A4076 F4077 Q4078 D4079 Y4080 V4081 T4082 D4083 P4084 R4085 G4086 L4087 I4088 S4089 K4090 K4091 D4092 F4093 Q4094 K4095 A4096 M4097 D4098 S4099 Q4100 K4101 Q4102 F4103 T4104 G4105 P4106 E4107 I4108 Q4109 F4110 L4111


L4112 S4113 C4114 S4115 E4116 A4117 D4118 E4119 N4120 E4121 M4122 I4123 N4124 F4125 E4126 E4127 F4128 A4129 N4130 R4131 F4132 Q4133 E4134 R4137 D4138 I4139 G4140 F4141 N4142 L4147 E4152 H4153 H4156 R4159 L4160 R4161 L4164 E4165 L4166 A4167 E4168 S4169 E4172 Y4173 F4174 R4175 P4176 R4180 M4184 G4185 A4186
S4187 R4188 R4189 I4190 E4191 R4192 E4196 I4197 S4198 E4199 T4200 N4201 R4202 A4203 Q4204 W4205 E4206 M4207 P4208 Q4209 V4210 K4211 E4212 R4215 F4219 N4223 E4224 G4225 G4226 E4227 A4228 E4229 L4233 S4236 E4239 Q4250 I4251 S4252 E4253 X4320 X4321 X4322 X4323 X4324 X4325 X4330 X4331 X4334 X4340
X4341 X4342 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547 R4548 F4551 L4552 N4553 Y4554 L4555 S4556 R4557 L4562 L4567 F4568 F4571 A4572 I4573 N4574 F4575 I4576 L4577 V4582 S4583 D4584 S4585 P4586 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 GLU GLU N4626 Y4629 Y4630 F4631 L4632 E4633 E4634 S4635 T4636 G4637 Y4638 P4641 W4644 C4645 L4648 L4649 H4650 F4655 L4656 C4657 I4658 I4659 G4660 Y4661 N4662 V4666 P4667 L4668 V4669 R4673 E4674 K4675
R4679 K4680 L4681 E4682 F4683 D4684 L4686 G4685 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 D4696 V4697 K4698 G4699 Q4700 W4701 D4702 R4703 L4704 S4713 N4714 Y4715 W4716 D4717 K4718 R4722 L4725 D4726 K4727 H4728 G4729 D4730 I4731 F4732 G4733 R4734 E4735 E4739 L4740 L4741 G4742 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750
T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 S4770 I4771 D4772 V4773 K4774 Y4775 F4780 G4781 V4782 I4783 F4784 T4785 D4786 F4789 L4790 Y4791 W4794 L4800 L4801 G4802 N4805 N4806 P4807 F4808 F4809 A4810 A4811 H4812 L4813 L4814 D4815 I4816 A4817 M4818 G4819 V4820
L4823 R4824 L4827 S4828 H4832 N4833 G4834 K4835 Q4836 L4843 L4844 A4845 Y4849 L4850 Y4851 A4855 F4856 N4857 F4858 F4859 R4860 K4861 F4862 Y4863 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876 D4877 D4878 M4879 Y4883 L4884 F4885 H4886 M4887 Y4888 V4889 G4890 V4891 R4892 A4893 G4894 G4895
G4896 D4899 E4900 I4901 E4902 D4903 G4906 D4907 E4908 Y4909 R4913 D4917 F4922 F4923 L4928 L4929 I4932 Q4933 G4934 L4935 I4936 F4940 G4941 E4942 L4943 R4944 D4945 Q4946 Q4947 D4953 T4956 K4957 C4958 C4961 G4962 I4963 G4964 S4965 D4966 Y4967 F4968 E4976 T4977 H4978 T4979 L4980 E4981 E4982
H4983 N4984 L4985 M4993 N4997 K4998 D4999 E5000 T5001 E5002 G5005 K5012 E5016 R5017 D5020 F5021 F5022 D5026 K5030 Q5031 Y5032 E5033 D5034 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	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	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

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	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.30	0/25438	0.54	8/34548 (0.0%)
2	E	0.30	0/25438	0.54	8/34548 (0.0%)
2	G	0.30	0/25438	0.54	8/34548 (0.0%)
2	I	0.30	0/25438	0.54	8/34548 (0.0%)
All	All	0.30	0/105088	0.54	32/142684 (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	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	56

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	7.74	133.11	115.30
2	B	131	LEU	CA-CB-CG	7.73	133.09	115.30
2	I	131	LEU	CA-CB-CG	7.73	133.08	115.30
2	G	131	LEU	CA-CB-CG	7.73	133.08	115.30
2	E	1600	LEU	CA-CB-CG	7.38	132.27	115.30
2	B	1600	LEU	CA-CB-CG	7.37	132.24	115.30
2	G	1600	LEU	CA-CB-CG	7.36	132.23	115.30
2	I	1600	LEU	CA-CB-CG	7.35	132.20	115.30
2	E	1676	LEU	CA-CB-CG	6.49	130.24	115.30
2	B	1676	LEU	CA-CB-CG	6.49	130.22	115.30
2	G	1676	LEU	CA-CB-CG	6.48	130.20	115.30
2	I	1676	LEU	CA-CB-CG	6.48	130.19	115.30
2	E	4985	LEU	CA-CB-CG	6.27	129.73	115.30
2	G	4985	LEU	CA-CB-CG	6.27	129.73	115.30
2	I	4985	LEU	CA-CB-CG	6.27	129.71	115.30
2	B	4985	LEU	CA-CB-CG	6.26	129.71	115.30
2	B	977	LEU	CA-CB-CG	5.85	128.76	115.30
2	G	977	LEU	CA-CB-CG	5.85	128.75	115.30
2	E	977	LEU	CA-CB-CG	5.84	128.72	115.30
2	I	977	LEU	CA-CB-CG	5.83	128.70	115.30
2	I	2290	LEU	CA-CB-CG	5.72	128.47	115.30
2	B	2290	LEU	CA-CB-CG	5.72	128.45	115.30
2	E	2290	LEU	CA-CB-CG	5.71	128.44	115.30
2	G	2290	LEU	CA-CB-CG	5.71	128.42	115.30
2	B	1667	LEU	CA-CB-CG	5.48	127.90	115.30
2	I	1667	LEU	CA-CB-CG	5.47	127.89	115.30
2	G	1667	LEU	CA-CB-CG	5.47	127.89	115.30
2	E	1667	LEU	CA-CB-CG	5.46	127.85	115.30
2	I	688	LEU	CA-CB-CG	5.18	127.21	115.30
2	B	688	LEU	CA-CB-CG	5.18	127.20	115.30
2	E	688	LEU	CA-CB-CG	5.17	127.20	115.30
2	G	688	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1828	ASP	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1828	ASP	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1828	ASP	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1828	ASP	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	I	2807	TRP	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	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	11	0
1	F	818	0	824	11	0
1	H	818	0	824	11	0
1	J	818	0	824	11	0
2	B	29509	0	24752	277	0
2	E	29509	0	24753	269	0
2	G	29509	0	24753	269	0
2	I	29509	0	24753	276	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
All	All	121312	0	102307	1111	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 5.

All (1111) 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:B:4983:HIS:CD2	2:B:4983:HIS:H	2.10	0.70
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.10	0.70
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.10	0.67
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.61	0.65
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.61	0.65
2:E:111:HIS:HD2	2:E:114:SER:H	1.45	0.64
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.61	0.64
2:B:111:HIS:HD2	2:B:114:SER:H	1.45	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.61	0.64
2:E:4958:CYS:SG	2:E:4961:CYS:HB2	2.38	0.64
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.80	0.63
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.79	0.63
2:I:4958:CYS:SG	2:I:4961:CYS:HB2	2.38	0.63
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.63	0.63
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.63	0.63
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.81	0.63
2:G:4958:CYS:SG	2:G:4961:CYS:HB2	2.38	0.63
2:B:4958:CYS:SG	2:B:4961:CYS:HB2	2.38	0.63
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.81	0.62
2:I:379:HIS:HD2	2:I:382:GLY:H	1.47	0.62
2:G:111:HIS:HD2	2:G:114:SER:H	1.45	0.62
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.62
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.63	0.62
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.64	0.62
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.80	0.62
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.63	0.62
2:I:4958:CYS:SG	2:I:4961:CYS:CB	2.88	0.62
2:I:111:HIS:HD2	2:I:114:SER:H	1.45	0.62
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.82	0.62
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.64	0.62
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.81	0.61
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.61
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.61
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.82	0.61
2:B:4958:CYS:SG	2:B:4961:CYS:CB	2.88	0.61
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.82	0.61
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.82	0.61
2:B:379:HIS:HD2	2:B:382:GLY:H	1.47	0.61
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.64	0.61
2:E:4958:CYS:SG	2:E:4961:CYS:CB	2.88	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.81	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.80	0.61
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.61
2:E:379:HIS:HD2	2:E:382:GLY:H	1.47	0.61
2:G:379:HIS:HD2	2:G:382:GLY:H	1.47	0.61
2:G:4958:CYS:SG	2:G:4961:CYS:CB	2.88	0.60
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.35	0.60
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.35	0.60
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.35	0.60
2:B:173:SER:HB3	2:B:178:ARG:H	1.67	0.60
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.84	0.60
2:I:173:SER:HB3	2:I:178:ARG:H	1.67	0.60
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.35	0.60
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.84	0.60
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.84	0.59
2:G:173:SER:HB3	2:G:178:ARG:H	1.67	0.59
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.35	0.59
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.35	0.59
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.84	0.59
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.59
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.59
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.85	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.85	0.59
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.85	0.59
2:G:4176:PRO:O	2:G:4202:ARG:NH1	2.35	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.59
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.36	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.59
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.35	0.59
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.84	0.59
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.85	0.59
2:I:4176:PRO:O	2:I:4202:ARG:NH1	2.35	0.59
2:I:241:GLN:O	2:I:289:ARG:NH1	2.34	0.59
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.59
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.36	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.59
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.84	0.59
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.36	0.59
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.36	0.59
2:E:4176:PRO:O	2:E:4202:ARG:NH1	2.35	0.59
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.35	0.59
2:B:4176:PRO:O	2:B:4202:ARG:NH1	2.35	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.85	0.59
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.36	0.59
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.36	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.84	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.59
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.84	0.58
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.36	0.58
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.58
2:G:3733:CYS:HA	2:G:3766:GLN:HG3	1.85	0.58
2:E:173:SER:HB3	2:E:178:ARG:H	1.67	0.58
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.36	0.58
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.85	0.58
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.84	0.58
2:I:3733:CYS:HA	2:I:3766:GLN:HG3	1.85	0.58
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.85	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:B:3733:CYS:HA	2:B:3766:GLN:HG3	1.85	0.58
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.58
2:G:241:GLN:O	2:G:289:ARG:NH1	2.34	0.58
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.37	0.58
2:E:3733:CYS:HA	2:E:3766:GLN:HG3	1.84	0.58
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.85	0.58
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.85	0.58
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.58
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.85	0.58
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.85	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.85	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.69	0.57
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.85	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.38	0.57
2:G:614:VAL:HG22	2:G:616:SER:H	1.69	0.57
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.37	0.57
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.37	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.36	0.57
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.85	0.57
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.37	0.57
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.37	0.57
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.38	0.57
2:I:614:VAL:HG22	2:I:616:SER:H	1.69	0.57
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.38	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.36	0.57
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.87	0.57
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.37	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.87	0.57
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.78	0.57
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.57
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.78	0.57
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.57
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.57
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.38	0.56
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.37	0.56
2:I:359:TYR:HA	2:I:376:ALA:HA	1.87	0.56
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.87	0.56
2:B:241:GLN:O	2:B:289:ARG:NH1	2.34	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.87	0.56
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.87	0.56
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.78	0.56
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.38	0.56
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.85	0.56
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.87	0.56
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.87	0.56
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.73	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.69	0.56
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.38	0.56
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.37	0.56
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.70	0.56
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.87	0.56
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.78	0.56
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.38	0.56
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.38	0.56
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.70	0.56
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.87	0.56
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.87	0.56
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.88	0.56
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.88	0.56
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.37	0.56
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.89	0.55
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.39	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.70	0.55
2:G:359:TYR:HA	2:G:376:ALA:HA	1.87	0.55
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.87	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.55
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.87	0.55
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.39	0.55
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.87	0.55
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.73	0.55
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.39	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.88	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.88	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.70	0.55
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.89	0.55
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.89	0.55
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.89	0.55
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.89	0.55
2:E:241:GLN:O	2:E:289:ARG:NH1	2.34	0.55
2:E:978:THR:HB	2:E:980:ALA:H	1.72	0.55
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.89	0.55
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.89	0.55
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.89	0.55
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.89	0.55
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.88	0.55
2:B:978:THR:HB	2:B:980:ALA:H	1.72	0.54
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.89	0.54
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.54
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.41	0.54
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.41	0.54
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.90	0.54
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.89	0.54
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.73	0.54
2:E:132:ALA:HA	2:E:194:SER:HB2	1.90	0.54
2:E:451:TYR:O	2:E:474:ARG:NH1	2.41	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.90	0.54
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.90	0.54
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.73	0.54
2:E:315:CYS:SG	2:E:316:PHE:N	2.81	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.54
1:F:87:HIS:H	1:F:91:ILE:HB	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.90	0.54
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.89	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.81	0.54
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.41	0.54
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.73	0.54
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.41	0.54
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.39	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.90	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.90	0.54
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.73	0.53
2:I:978:THR:HB	2:I:980:ALA:H	1.72	0.53
2:G:315:CYS:SG	2:G:316:PHE:N	2.81	0.53
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.39	0.53
2:B:313:SER:HB3	2:B:351:VAL:HB	1.90	0.53
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.41	0.53
2:G:978:THR:HB	2:G:980:ALA:H	1.72	0.53
1:H:87:HIS:H	1:H:91:ILE:HB	1.73	0.53
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.90	0.53
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.90	0.53
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.91	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.53
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.90	0.53
1:J:87:HIS:H	1:J:91:ILE:HB	1.73	0.53
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.37	0.53
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.91	0.53
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.90	0.53
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.91	0.53
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.57	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.41	0.53
1:A:87:HIS:H	1:A:91:ILE:HB	1.73	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.90	0.53
2:G:451:TYR:O	2:G:474:ARG:NH1	2.41	0.53
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.57	0.53
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.91	0.53
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.74	0.53
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.52
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.91	0.52
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.91	0.52
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.91	0.52
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.74	0.52
2:I:315:CYS:SG	2:I:316:PHE:N	2.81	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.74	0.52
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.37	0.52
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.90	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.52
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.92	0.52
2:B:683:ARG:NH1	2:B:707:VAL:O	2.40	0.52
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.90	0.52
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.74	0.52
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.74	0.52
2:G:776:LEU:HG	2:G:848:HIS:HA	1.91	0.52
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.91	0.52
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.57	0.52
2:B:776:LEU:HG	2:B:848:HIS:HA	1.91	0.52
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.92	0.52
2:E:776:LEU:HG	2:E:848:HIS:HA	1.91	0.52
2:I:4063:ASP:O	2:I:4067:LYS:NZ	2.37	0.52
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.28	0.52
2:B:4063:ASP:O	2:B:4067:LYS:NZ	2.37	0.52
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.91	0.52
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.28	0.52
2:I:776:LEU:HG	2:I:848:HIS:HA	1.91	0.52
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.74	0.52
2:E:313:SER:HB3	2:E:351:VAL:HB	1.90	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.92	0.52
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.91	0.52
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.28	0.52
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.41	0.52
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.57	0.51
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.37	0.51
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.90	0.51
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.51
2:B:1685:LEU:HD22	2:B:1718:ILE:HG21	1.92	0.51
2:I:1865:MET:SD	2:I:1865:MET:N	2.84	0.51
2:G:683:ARG:NH1	2:G:707:VAL:O	2.40	0.51
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.44	0.51
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.28	0.51
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.92	0.51
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.51
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.74	0.51
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.74	0.51
2:B:451:TYR:O	2:B:474:ARG:NH1	2.41	0.51
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.92	0.51
2:B:689:THR:H	2:B:778:PHE:HE2	1.59	0.51
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.93	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.91	0.51
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.92	0.51
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.93	0.51
2:E:1865:MET:SD	2:E:1865:MET:N	2.84	0.51
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.74	0.51
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.51
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.92	0.51
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.93	0.51
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.73	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.51
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.93	0.51
2:I:1685:LEU:HD22	2:I:1718:ILE:HG21	1.92	0.51
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.41	0.51
2:B:4820:VAL:HB	2:B:4823:LEU:HD23	1.93	0.51
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.41	0.51
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.92	0.51
2:I:451:TYR:O	2:I:474:ARG:NH1	2.41	0.51
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.93	0.51
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.93	0.51
2:G:4820:VAL:HB	2:G:4823:LEU:HD23	1.93	0.51
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.50
2:B:1865:MET:SD	2:B:1865:MET:N	2.84	0.50
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.91	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.45	0.50
2:E:1991:THR:O	2:E:1995:THR:OG1	2.29	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.45	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.50
2:E:689:THR:H	2:E:778:PHE:HE2	1.59	0.50
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.93	0.50
2:E:4820:VAL:HB	2:E:4823:LEU:HD23	1.93	0.50
2:I:4820:VAL:HB	2:I:4823:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.93	0.50
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.92	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.44	0.50
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.94	0.50
2:I:689:THR:H	2:I:778:PHE:HE2	1.59	0.50
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.93	0.50
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.92	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.45	0.50
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.92	0.50
2:G:265:LEU:HD12	2:G:279:PRO:HB2	1.94	0.50
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.94	0.50
2:G:1457:UNK:N	2:G:1497:UNK:O	2.44	0.50
2:G:1865:MET:SD	2:G:1865:MET:N	2.84	0.50
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.92	0.50
2:B:3733:CYS:HB2	2:B:3803:SER:HB3	1.94	0.50
2:E:41:GLY:O	2:E:45:ARG:NH1	2.45	0.50
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.93	0.50
2:E:911:HIS:O	2:E:918:ARG:NH2	2.45	0.50
2:I:243:ARG:NH1	2:I:301:VAL:O	2.38	0.50
2:G:1991:THR:O	2:G:1995:THR:OG1	2.29	0.50
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.92	0.50
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.93	0.50
2:E:265:LEU:HD12	2:E:279:PRO:HB2	1.94	0.50
2:I:41:GLY:O	2:I:45:ARG:NH1	2.45	0.50
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.93	0.50
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.39	0.50
2:G:41:GLY:O	2:G:45:ARG:NH1	2.45	0.50
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.93	0.50
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.93	0.50
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.41	0.50
2:E:4571:PHE:O	2:E:4575:PHE:N	2.45	0.50
2:I:683:ARG:NH1	2:I:707:VAL:O	2.40	0.50
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.77	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.45	0.50
2:I:1991:THR:O	2:I:1995:THR:OG1	2.29	0.50
2:G:1685:LEU:HD22	2:G:1718:ILE:HG21	1.92	0.50
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.93	0.50
2:B:265:LEU:HD12	2:B:279:PRO:HB2	1.94	0.50
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.94	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4832:HIS:NE2	2:E:4942:GLU:OE2	2.45	0.50
2:I:265:LEU:HD12	2:I:279:PRO:HB2	1.94	0.50
2:G:911:HIS:O	2:G:918:ARG:NH2	2.45	0.50
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.77	0.50
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.94	0.49
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.93	0.49
2:B:41:GLY:O	2:B:45:ARG:NH1	2.45	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.44	0.49
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.94	0.49
2:E:3733:CYS:HB2	2:E:3803:SER:HB3	1.94	0.49
2:G:689:THR:H	2:G:778:PHE:HE2	1.59	0.49
2:B:1991:THR:O	2:B:1995:THR:OG1	2.29	0.49
2:B:4571:PHE:O	2:B:4575:PHE:N	2.45	0.49
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.45	0.49
2:I:4832:HIS:NE2	2:I:4942:GLU:OE2	2.45	0.49
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.45	0.49
2:B:1973:GLN:O	2:B:1977:TYR:N	2.40	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.94	0.49
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.46	0.49
2:G:4063:ASP:O	2:G:4067:LYS:NZ	2.37	0.49
2:B:4832:HIS:NE2	2:B:4942:GLU:OE2	2.45	0.49
2:G:4571:PHE:O	2:G:4575:PHE:N	2.45	0.49
2:B:911:HIS:O	2:B:918:ARG:NH2	2.45	0.49
2:B:1171:SER:OG	2:B:1175:SER:N	2.43	0.49
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.46	0.49
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.77	0.49
2:E:1685:LEU:HD22	2:E:1718:ILE:HG21	1.93	0.49
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.46	0.49
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	1.94	0.49
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.49
2:B:243:ARG:NH1	2:B:301:VAL:O	2.38	0.49
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.94	0.49
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.45	0.49
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.77	0.49
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.95	0.49
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.95	0.49
2:G:4832:HIS:NE2	2:G:4942:GLU:OE2	2.45	0.49
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.46	0.49
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.93	0.49
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.94	0.49
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.94	0.49
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.95	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.95	0.49
2:I:4571:PHE:O	2:I:4575:PHE:N	2.45	0.49
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.48
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.46	0.48
2:E:4063:ASP:O	2:E:4067:LYS:NZ	2.37	0.48
2:I:911:HIS:O	2:I:918:ARG:NH2	2.45	0.48
2:I:2758:PHE:O	2:I:2762:THR:N	2.43	0.48
1:J:5:GLU:HB2	1:J:73:LYS:HB3	1.95	0.48
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.46	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.94	0.48
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.94	0.48
2:I:3755:GLU:O	2:I:3762:ARG:NH2	2.44	0.48
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.46	0.48
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	1.94	0.48
1:A:5:GLU:HB2	1:A:73:LYS:HB3	1.95	0.48
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.48
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.96	0.48
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.46	0.48
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.96	0.48
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.96	0.48
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.94	0.48
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.96	0.48
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.96	0.48
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.95	0.48
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.96	0.48
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.96	0.48
1:F:5:GLU:HB2	1:F:73:LYS:HB3	1.95	0.48
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.96	0.48
2:B:792:LEU:HB3	2:B:798:GLY:HA2	1.95	0.48
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	1.96	0.48
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.41	0.48
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	1.96	0.48
1:H:5:GLU:HB2	1:H:73:LYS:HB3	1.95	0.48
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.48
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.46	0.48
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.96	0.48
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.94	0.48
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.46	0.48
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.79	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.95	0.48
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.95	0.48
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.79	0.48
2:E:243:ARG:NH1	2:E:301:VAL:O	2.38	0.48
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.79	0.48
2:G:243:ARG:NH1	2:G:301:VAL:O	2.38	0.48
2:G:2103:VAL:O	2:G:2107:GLN:N	2.43	0.48
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.95	0.48
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.79	0.48
2:E:4582:VAL:HG23	2:E:4629:TYR:HA	1.96	0.48
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.47	0.48
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.47	0.48
2:B:345:LEU:HD23	2:B:389:PHE:HB3	1.96	0.47
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.78	0.47
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.95	0.47
2:B:756:SER:HB3	2:B:767:VAL:HG22	1.96	0.47
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.96	0.47
2:I:1171:SER:OG	2:I:1175:SER:N	2.43	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.47
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.46	0.47
2:B:177:GLU:HG3	2:E:2452:ARG:HH12	1.79	0.47
2:E:606:LEU:O	2:E:617:ASN:ND2	2.47	0.47
2:G:756:SER:HB3	2:G:767:VAL:HG22	1.96	0.47
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.97	0.47
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.39	0.47
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.96	0.47
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.79	0.47
2:G:345:LEU:HD23	2:G:389:PHE:HB3	1.96	0.47
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.79	0.47
2:B:4582:VAL:HG23	2:B:4629:TYR:HA	1.96	0.47
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.97	0.47
2:G:792:LEU:HB3	2:G:798:GLY:HA2	1.95	0.47
2:B:4673:ARG:HH22	2:B:4698:LYS:HE3	1.80	0.47
2:E:331:VAL:HG12	2:E:333:GLY:H	1.79	0.47
2:I:756:SER:HB3	2:I:767:VAL:HG22	1.96	0.47
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.97	0.47
2:G:606:LEU:O	2:G:617:ASN:ND2	2.48	0.47
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.80	0.47
2:B:331:VAL:HG12	2:B:333:GLY:H	1.79	0.47
2:B:606:LEU:O	2:B:617:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2758:PHE:O	2:B:2762:THR:N	2.43	0.47
2:E:345:LEU:HD23	2:E:389:PHE:HB3	1.96	0.47
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.97	0.47
2:E:792:LEU:HB3	2:E:798:GLY:HA2	1.95	0.47
2:E:4673:ARG:HH22	2:E:4698:LYS:HE3	1.80	0.47
2:I:331:VAL:HG12	2:I:333:GLY:H	1.79	0.47
2:I:345:LEU:HD23	2:I:389:PHE:HB3	1.96	0.47
2:I:606:LEU:O	2:I:617:ASN:ND2	2.47	0.47
2:G:331:VAL:HG12	2:G:333:GLY:H	1.79	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.50	0.47
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.79	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.50	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.80	0.47
2:I:792:LEU:HB3	2:I:798:GLY:HA2	1.95	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.50	0.47
2:I:4673:ARG:HH22	2:I:4698:LYS:HE3	1.80	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.50	0.47
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	1.96	0.47
2:G:4152:GLU:OE2	2:G:4180:ARG:NH1	2.48	0.47
2:E:756:SER:HB3	2:E:767:VAL:HG22	1.96	0.47
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	1.96	0.47
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.97	0.46
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.47	0.46
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.98	0.46
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.98	0.46
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.98	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.43	0.46
2:E:4152:GLU:OE2	2:E:4180:ARG:NH1	2.48	0.46
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.80	0.46
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.98	0.46
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.79	0.46
2:I:1976:ARG:NH1	2:I:1997:GLU:OE2	2.49	0.46
2:I:2103:VAL:O	2:I:2107:GLN:N	2.43	0.46
2:G:1171:SER:OG	2:G:1175:SER:N	2.43	0.46
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.47	0.46
2:B:1976:ARG:NH1	2:B:1997:GLU:OE2	2.49	0.46
2:B:4101:LYS:HE3	2:I:4731:ILE:HA	1.97	0.46
2:E:683:ARG:NH1	2:E:707:VAL:O	2.40	0.46
2:E:1976:ARG:NH1	2:E:1997:GLU:OE2	2.49	0.46
1:F:82:TYR:O	1:F:86:GLY:N	2.46	0.46
2:B:792:LEU:HD22	2:B:799:GLU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:LEU:HD12	2:E:413:GLN:HE21	1.80	0.46
2:E:792:LEU:HD22	2:E:799:GLU:H	1.81	0.46
2:I:1965:TYR:OH	2:I:2027:ILE:O	2.29	0.46
2:I:4582:VAL:HG23	2:I:4629:TYR:HA	1.96	0.46
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.98	0.46
2:G:4582:VAL:HG23	2:G:4629:TYR:HA	1.96	0.46
2:B:1099:GLU:OE2	2:B:1127:HIS:ND1	2.35	0.46
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.98	0.46
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.97	0.46
2:I:164:ARG:N	2:I:167:ASP:OD2	2.49	0.46
2:I:410:LEU:HD12	2:I:413:GLN:HE21	1.80	0.46
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.96	0.46
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.81	0.46
2:G:1976:ARG:NH1	2:G:1997:GLU:OE2	2.49	0.46
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.98	0.46
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.98	0.46
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.80	0.46
2:I:792:LEU:HD22	2:I:799:GLU:H	1.81	0.46
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.98	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.40	0.46
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.96	0.46
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.80	0.46
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.81	0.46
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.98	0.46
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.98	0.46
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.98	0.46
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.98	0.46
2:G:4673:ARG:HH22	2:G:4698:LYS:HE3	1.80	0.46
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.98	0.46
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.98	0.46
2:B:164:ARG:N	2:B:167:ASP:OD2	2.49	0.46
2:B:410:LEU:HD12	2:B:413:GLN:HE21	1.80	0.46
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	1.98	0.46
2:B:4152:GLU:OE2	2:B:4180:ARG:NH1	2.48	0.46
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.80	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.98	0.46
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.49	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.97	0.46
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.37	0.46
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.99	0.46
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.97	0.46
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.80	0.46
2:G:164:ARG:N	2:G:167:ASP:OD2	2.49	0.46
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.98	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.80	0.45
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.97	0.45
2:E:3362:UNK:O	2:E:3366:UNK:N	2.49	0.45
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.81	0.45
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.80	0.45
2:I:3362:UNK:O	2:I:3366:UNK:N	2.49	0.45
2:G:410:LEU:HD12	2:G:413:GLN:HE21	1.81	0.45
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.98	0.45
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.97	0.45
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.98	0.45
2:B:215:THR:HG22	2:B:273:HIS:HA	1.99	0.45
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.98	0.45
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.49	0.45
2:E:164:ARG:N	2:E:167:ASP:OD2	2.49	0.45
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.98	0.45
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.49	0.45
2:I:4081:VAL:HB	2:I:4088:ILE:HD12	1.98	0.45
2:I:4152:GLU:OE2	2:I:4180:ARG:NH1	2.48	0.45
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.81	0.45
1:H:30:LEU:HD23	1:H:33:GLY:HA3	1.99	0.45
2:B:626:LEU:HG	2:B:628:GLY:H	1.82	0.45
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.98	0.45
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.98	0.45
2:I:278:GLN:N	2:I:315:CYS:SG	2.90	0.45
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.98	0.45
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.35	0.45
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.98	0.45
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.98	0.45
2:G:3362:UNK:O	2:G:3366:UNK:N	2.49	0.45
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.98	0.45
2:B:3362:UNK:O	2:B:3366:UNK:N	2.49	0.45
2:B:4697:VAL:O	2:B:4701:TRP:N	2.49	0.45
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.45
2:E:626:LEU:HG	2:E:628:GLY:H	1.82	0.45
2:E:2103:VAL:O	2:E:2107:GLN:N	2.43	0.45
2:E:4835:LYS:HG3	2:E:4836:GLN:HG3	1.98	0.45
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.98	0.45
2:E:1105:ALA:N	2:E:1189:LEU:O	2.50	0.45
2:E:1973:GLN:O	2:E:1977:TYR:N	2.40	0.45
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.49	0.45
2:I:463:GLU:O	2:I:466:SER:OG	2.30	0.45
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	1.98	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.97	0.45
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	1.98	0.45
2:G:1105:ALA:N	2:G:1189:LEU:O	2.50	0.45
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.99	0.45
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.98	0.45
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.99	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.98	0.45
2:B:4081:VAL:HB	2:B:4088:ILE:HD12	1.98	0.45
2:E:278:GLN:N	2:E:315:CYS:SG	2.90	0.45
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.98	0.45
2:E:4081:VAL:HB	2:E:4088:ILE:HD12	1.98	0.45
2:G:395:GLN:HG3	2:G:397:GLU:H	1.82	0.45
2:G:792:LEU:HD22	2:G:799:GLU:H	1.81	0.45
2:G:2758:PHE:O	2:G:2762:THR:N	2.43	0.45
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.80	0.45
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.98	0.45
2:B:823:LEU:HD23	2:B:1626:TRP:HB3	1.99	0.45
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.99	0.45
2:E:21:VAL:HG12	2:E:66:CYS:HA	1.99	0.45
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.99	0.45
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.98	0.45
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.98	0.45
2:G:168:ASP:HB3	2:G:199:LEU:HD22	1.99	0.45
2:G:4081:VAL:HB	2:G:4088:ILE:HD12	1.98	0.45
2:B:21:VAL:HG12	2:B:66:CYS:HA	1.99	0.45
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.80	0.45
2:B:4956:THR:O	2:B:4965:SER:N	2.48	0.45
2:E:215:THR:HG22	2:E:273:HIS:HA	1.99	0.45
2:E:823:LEU:HD23	2:E:1626:TRP:HB3	1.99	0.45
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.98	0.45
2:I:215:THR:HG22	2:I:273:HIS:HA	1.99	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.99	0.45
2:I:1114:GLU:HG3	2:I:1117:ALA:HB2	1.99	0.45
2:G:70:GLU:HG3	2:G:117:TYR:HE1	1.80	0.45
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4835:LYS:HG3	2:G:4836:GLN:HG3	1.98	0.45
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.50	0.45
2:B:1105:ALA:N	2:B:1189:LEU:O	2.50	0.45
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.99	0.45
2:E:168:ASP:HB3	2:E:199:LEU:HD22	1.99	0.45
2:E:4201:ASN:ND2	2:E:4204:GLN:OE1	2.49	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.50	0.45
2:G:1269:CYS:HA	2:G:1473:UNK:HA	1.99	0.45
2:G:4201:ASN:ND2	2:G:4204:GLN:OE1	2.49	0.45
1:F:30:LEU:HD23	1:F:33:GLY:HA3	1.99	0.45
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	1.98	0.45
2:B:1114:GLU:HG3	2:B:1117:ALA:HB2	1.99	0.45
2:B:1269:CYS:HA	2:B:1473:UNK:HA	1.99	0.45
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.45
2:B:4201:ASN:ND2	2:B:4204:GLN:OE1	2.49	0.45
2:B:4835:LYS:HG3	2:B:4836:GLN:HG3	1.98	0.45
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.99	0.45
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.98	0.45
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.99	0.45
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.35	0.45
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.99	0.45
2:B:2257:LEU:O	2:B:2261:SER:N	2.50	0.44
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.44
2:B:3755:GLU:O	2:B:3762:ARG:NH2	2.44	0.44
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	1.98	0.44
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.44
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.99	0.44
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.98	0.44
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.98	0.44
2:I:3992:PHE:O	2:I:3996:PHE:N	2.40	0.44
2:G:278:GLN:N	2:G:315:CYS:SG	2.90	0.44
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.98	0.44
1:J:82:TYR:O	1:J:86:GLY:N	2.46	0.44
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.98	0.44
2:E:3758:MET:HE2	2:E:3762:ARG:HH21	1.82	0.44
2:I:1269:CYS:HA	2:I:1473:UNK:HA	1.99	0.44
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.99	0.44
2:I:4835:LYS:HG3	2:I:4836:GLN:HG3	1.98	0.44
2:I:4956:THR:O	2:I:4965:SER:N	2.48	0.44
2:G:21:VAL:HG12	2:G:66:CYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.44
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.98	0.44
2:B:168:ASP:HB3	2:B:199:LEU:HD22	1.99	0.44
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.99	0.44
2:E:395:GLN:HG3	2:E:397:GLU:H	1.82	0.44
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.50	0.44
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.99	0.44
2:E:1114:GLU:HG3	2:E:1117:ALA:HB2	1.99	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44
2:E:4697:VAL:O	2:E:4701:TRP:N	2.49	0.44
2:E:4802:GLY:HA2	2:E:4808:PHE:HB2	1.99	0.44
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.44
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.50	0.44
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.99	0.44
2:I:1973:GLN:O	2:I:1977:TYR:N	2.40	0.44
2:G:4697:VAL:O	2:G:4701:TRP:N	2.49	0.44
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.99	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.44
2:B:3758:MET:HE2	2:B:3762:ARG:HH21	1.83	0.44
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.82	0.44
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	1.98	0.44
2:I:21:VAL:HG12	2:I:66:CYS:HA	1.99	0.44
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.99	0.44
2:I:4201:ASN:ND2	2:I:4204:GLN:OE1	2.50	0.44
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.99	0.44
2:G:823:LEU:HD23	2:G:1626:TRP:HB3	1.99	0.44
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	1.98	0.44
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.44
2:B:3764:LEU:HD21	2:B:3809:ASN:HD21	1.82	0.44
2:E:2257:LEU:O	2:E:2261:SER:N	2.50	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.44
2:I:168:ASP:HB3	2:I:199:LEU:HD22	1.99	0.44
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.53	0.44
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.99	0.44
2:G:626:LEU:HG	2:G:628:GLY:H	1.82	0.44
2:G:1114:GLU:HG3	2:G:1117:ALA:HB2	1.99	0.44
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.98	0.44
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.00	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:G:4667:PRO:O	2:G:4714:ASN:ND2	2.48	0.44
2:B:179:TYR:OH	2:E:2359:ARG:NH1	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.44
2:B:395:GLN:HG3	2:B:397:GLU:H	1.82	0.44
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.99	0.44
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.53	0.44
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.98	0.44
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.99	0.44
2:E:1269:CYS:HA	2:E:1473:UNK:HA	1.99	0.44
2:I:626:LEU:HG	2:I:628:GLY:H	1.82	0.44
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.35	0.44
2:I:2517:UNK:O	2:I:2521:UNK:N	2.51	0.44
2:I:3764:LEU:HD21	2:I:3809:ASN:HD21	1.82	0.44
2:I:4075:GLU:O	2:I:4079:ASP:N	2.51	0.44
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.00	0.44
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.99	0.44
2:G:2257:LEU:O	2:G:2261:SER:N	2.50	0.44
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.99	0.44
1:J:30:LEU:HD23	1:J:33:GLY:HA3	1.99	0.44
2:B:719:LEU:HD22	2:B:735:GLN:HG2	2.00	0.44
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.99	0.44
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.99	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:I:4826:ILE:O	2:I:4829:SER:OG	2.29	0.44
2:G:719:LEU:HD22	2:G:735:GLN:HG2	2.00	0.44
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.44
2:G:3758:MET:HE2	2:G:3762:ARG:HH21	1.83	0.44
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.00	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.44
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.99	0.44
2:I:823:LEU:HD23	2:I:1626:TRP:HB3	1.99	0.44
2:I:1105:ALA:N	2:I:1189:LEU:O	2.50	0.44
2:I:2257:LEU:O	2:I:2261:SER:N	2.50	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:I:3729:MET:O	2:I:3732:SER:OG	2.32	0.44
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.99	0.44
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.44
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.00	0.44
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.99	0.44
2:B:356:TRP:O	2:B:379:HIS:N	2.51	0.44
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.44
2:B:4667:PRO:O	2:B:4714:ASN:ND2	2.48	0.44
2:B:4802:GLY:HA2	2:B:4808:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2517:UNK:O	2:E:2521:UNK:N	2.51	0.44
2:E:3959:LYS:O	2:E:3963:ASN:ND2	2.51	0.44
2:E:4075:GLU:O	2:E:4079:ASP:N	2.50	0.44
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.83	0.44
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.00	0.44
2:I:4802:GLY:HA2	2:I:4808:PHE:HB2	1.99	0.44
2:G:215:THR:HG22	2:G:273:HIS:HA	1.99	0.44
2:G:2517:UNK:O	2:G:2521:UNK:N	2.51	0.44
2:G:3755:GLU:O	2:G:3762:ARG:NH2	2.44	0.44
2:G:3764:LEU:HD21	2:G:3809:ASN:HD21	1.83	0.44
2:G:3959:LYS:O	2:G:3963:ASN:ND2	2.51	0.44
2:G:4075:GLU:O	2:G:4079:ASP:N	2.51	0.44
1:A:30:LEU:HD23	1:A:33:GLY:HA3	1.99	0.43
2:B:560:ILE:HA	2:B:563:VAL:HG12	2.00	0.43
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.99	0.43
2:B:3552:UNK:O	2:B:3556:UNK:N	2.51	0.43
2:E:1171:SER:OG	2:E:1175:SER:N	2.43	0.43
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.53	0.43
2:E:4956:THR:O	2:E:4965:SER:N	2.48	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.98	0.43
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.83	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.43
2:I:4697:VAL:O	2:I:4701:TRP:N	2.49	0.43
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.41	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.43
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.43
2:I:560:ILE:HA	2:I:563:VAL:HG12	2.00	0.43
2:I:719:LEU:HD22	2:I:735:GLN:HG2	2.00	0.43
2:I:3552:UNK:O	2:I:3556:UNK:N	2.51	0.43
2:I:4667:PRO:O	2:I:4714:ASN:ND2	2.48	0.43
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.83	0.43
2:G:3963:ASN:O	2:G:3966:THR:OG1	2.33	0.43
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.52	0.43
1:H:82:TYR:O	1:H:86:GLY:N	2.46	0.43
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.00	0.43
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.99	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	2.01	0.43
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.43
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3927:GLN:O	2:I:3931:SER:N	2.51	0.43
2:I:4066:LEU:HD11	2:I:4173:TYR:CG	2.53	0.43
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.53	0.43
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.84	0.43
2:B:278:GLN:N	2:B:315:CYS:SG	2.90	0.43
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.52	0.43
2:B:2517:UNK:O	2:B:2521:UNK:N	2.51	0.43
2:B:4075:GLU:O	2:B:4079:ASP:N	2.51	0.43
2:E:3552:UNK:O	2:E:3556:UNK:N	2.51	0.43
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.52	0.43
2:I:3758:MET:HE2	2:I:3762:ARG:HH21	1.83	0.43
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.00	0.43
2:G:4956:THR:O	2:G:4965:SER:N	2.48	0.43
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.00	0.43
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.00	0.43
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.00	0.43
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.35	0.43
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.52	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.43
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.43
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.01	0.43
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.52	0.43
2:B:3674:ILE:HB	2:B:3769:ARG:HH21	1.84	0.43
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	2.01	0.43
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.99	0.43
2:E:793:LEU:HB2	2:E:797:HIS:H	1.84	0.43
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.00	0.43
2:I:3963:ASN:O	2:I:3966:THR:OG1	2.33	0.43
2:G:4802:GLY:HA2	2:G:4808:PHE:HB2	1.99	0.43
2:G:4976:GLU:O	2:G:4979:THR:OG1	2.35	0.43
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.84	0.43
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.99	0.43
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.83	0.43
2:I:395:GLN:HG3	2:I:397:GLU:H	1.82	0.43
2:I:734:GLY:O	2:I:736:HIS:ND1	2.52	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.43
2:E:356:TRP:O	2:E:379:HIS:N	2.51	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.01	0.43
2:I:3765:TYR:OH	2:I:4755:GLU:O	2.34	0.43
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.84	0.43
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.84	0.43
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.83	0.43
2:B:4066:LEU:HD11	2:B:4173:TYR:CG	2.53	0.43
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.00	0.43
2:I:3959:LYS:O	2:I:3963:ASN:ND2	2.51	0.43
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.99	0.43
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.84	0.43
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.52	0.43
2:G:3674:ILE:HB	2:G:3769:ARG:HH21	1.84	0.43
2:G:4066:LEU:HD11	2:G:4173:TYR:CG	2.53	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.43
2:B:4857:ASN:HB2	2:E:4807:PHE:HZ	1.84	0.43
2:E:719:LEU:HD22	2:E:735:GLN:HG2	2.00	0.43
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.84	0.43
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.00	0.43
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.52	0.43
2:I:2452:ARG:HH12	2:G:177:GLU:HG3	1.84	0.43
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.83	0.43
2:G:356:TRP:O	2:G:379:HIS:N	2.51	0.43
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.52	0.43
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	2.01	0.43
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.84	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.42
2:B:3959:LYS:O	2:B:3963:ASN:ND2	2.51	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.42
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.52	0.42
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.52	0.42
2:E:3361:UNK:O	2:E:3365:UNK:N	2.52	0.42
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.00	0.42
2:E:4713:SER:HG	2:E:4775:TYR:HH	1.67	0.42
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.01	0.42
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.52	0.42
2:G:1954:ARG:HE	2:G:2041:HIS:HD2	1.67	0.42
2:E:1954:ARG:HE	2:E:2041:HIS:HD2	1.67	0.42
2:I:356:TRP:O	2:I:379:HIS:N	2.51	0.42
2:I:793:LEU:HB2	2:I:797:HIS:H	1.84	0.42
2:I:1954:ARG:HE	2:I:2041:HIS:HD2	1.68	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.00	0.42
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	2.01	0.42
2:G:793:LEU:HB2	2:G:797:HIS:H	1.84	0.42
2:G:3552:UNK:O	2:G:3556:UNK:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:LEU:O	2:B:604:CYS:N	2.50	0.42
2:B:793:LEU:HB2	2:B:797:HIS:H	1.84	0.42
2:E:1089:TYR:N	2:E:1224:GLU:O	2.52	0.42
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.83	0.42
2:E:3764:LEU:HD21	2:E:3809:ASN:HD21	1.83	0.42
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.52	0.42
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.84	0.42
2:I:3674:ILE:HB	2:I:3769:ARG:HH21	1.84	0.42
2:G:600:LEU:O	2:G:604:CYS:N	2.50	0.42
2:G:3992:PHE:O	2:G:3996:PHE:N	2.40	0.42
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.52	0.42
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.01	0.42
2:E:560:ILE:HA	2:E:563:VAL:HG12	2.00	0.42
2:E:4066:LEU:HD11	2:E:4173:TYR:CG	2.53	0.42
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.42
2:B:1089:TYR:N	2:B:1224:GLU:O	2.52	0.42
2:B:4978:HIS:CE1	2:B:4983:HIS:NE2	2.87	0.42
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.42
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.01	0.42
2:I:1089:TYR:N	2:I:1224:GLU:O	2.52	0.42
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.02	0.42
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.01	0.42
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.00	0.42
2:G:3361:UNK:O	2:G:3365:UNK:N	2.52	0.42
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.02	0.42
2:B:3361:UNK:O	2:B:3365:UNK:N	2.52	0.42
2:B:4060:LYS:NZ	2:B:4064:MET:SD	2.93	0.42
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.35	0.42
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.02	0.42
2:E:3805:LEU:H	2:E:3805:LEU:HG	1.77	0.42
2:G:560:ILE:HA	2:G:563:VAL:HG12	2.00	0.42
2:G:3927:GLN:O	2:G:3931:SER:N	2.51	0.42
1:A:82:TYR:O	1:A:86:GLY:N	2.46	0.42
2:B:1954:ARG:HE	2:B:2041:HIS:HD2	1.67	0.42
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.52	0.42
2:B:3927:GLN:O	2:B:3931:SER:N	2.51	0.42
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.02	0.42
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.85	0.42
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.01	0.42
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.52	0.42
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.01	0.42
2:E:3674:ILE:HB	2:E:3769:ARG:HH21	1.84	0.42
2:G:1089:TYR:N	2:G:1224:GLU:O	2.52	0.42
2:G:1099:GLU:OE2	2:G:1127:HIS:ND1	2.35	0.42
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.02	0.42
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.85	0.42
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.01	0.42
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	2.02	0.42
2:B:4056:GLU:O	2:B:4060:LYS:N	2.51	0.42
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.02	0.42
2:E:4060:LYS:NZ	2:E:4064:MET:SD	2.93	0.42
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.02	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.02	0.42
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.01	0.42
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	2.02	0.42
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.02	0.42
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.02	0.41
2:G:40:GLU:HB3	2:G:44:ASN:HB3	2.02	0.41
2:B:4071:ILE:HD11	2:B:4102:GLN:HE21	1.85	0.41
2:E:40:GLU:HB3	2:E:44:ASN:HB3	2.02	0.41
2:E:3963:ASN:O	2:E:3966:THR:OG1	2.33	0.41
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.01	0.41
2:I:317:ARG:HE	2:I:323:LEU:HD22	1.86	0.41
2:I:4060:LYS:NZ	2:I:4064:MET:SD	2.93	0.41
2:I:4071:ILE:HD11	2:I:4102:GLN:HE21	1.85	0.41
2:G:2867:LEU:HB3	2:G:2871:LEU:HB2	2.02	0.41
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.02	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.41
2:I:2196:ASN:OD1	2:I:2199:ARG:NH1	2.41	0.41
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.02	0.41
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.02	0.41
2:B:2359:ARG:NH1	2:I:179:TYR:OH	2.41	0.41
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.02	0.41
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	2.02	0.41
2:B:2867:LEU:HB3	2:B:2871:LEU:HB2	2.03	0.41
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.53	0.41
2:E:940:GLY:O	2:E:1052:ASN:N	2.53	0.41
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.02	0.41
2:E:4071:ILE:HD11	2:E:4102:GLN:HE21	1.85	0.41
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.49	0.41
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.02	0.41
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.02	0.41
2:E:2867:LEU:HB3	2:E:2871:LEU:HB2	2.02	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:2867:LEU:HB3	2:I:2871:LEU:HB2	2.02	0.41
2:G:317:ARG:HE	2:G:323:LEU:HD22	1.86	0.41
2:G:4060:LYS:NZ	2:G:4064:MET:SD	2.93	0.41
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.35	0.41
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	2.03	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.02	0.41
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.39	0.41
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.02	0.41
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.39	0.41
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.02	0.41
2:E:4731:ILE:HA	2:G:4101:LYS:HE3	2.02	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.03	0.41
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.86	0.41
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	2.02	0.41
2:G:2265:LEU:HD22	2:G:2330:ARG:HB3	2.02	0.41
2:G:4071:ILE:HD11	2:G:4102:GLN:HE21	1.85	0.41
2:B:317:ARG:HE	2:B:323:LEU:HD22	1.86	0.41
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	2.02	0.41
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	2.03	0.41
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.85	0.41
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.37	0.41
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.86	0.41
2:G:583:ILE:HA	2:G:586:ILE:HD12	2.03	0.41
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.36	0.41
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.41
2:B:583:ILE:HA	2:B:586:ILE:HD12	2.03	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.78	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.03	0.41
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.52	0.41
2:B:2103:VAL:O	2:B:2107:GLN:N	2.43	0.41
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.56	0.41
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.85	0.41
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.02	0.41
2:B:3963:ASN:O	2:B:3966:THR:OG1	2.33	0.41
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.03	0.41
2:B:4807:PHE:HZ	2:I:4857:ASN:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.01	0.41
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.03	0.41
2:E:1154:ASP:O	2:E:1158:ASN:N	2.54	0.41
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.39	0.41
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.52	0.41
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.02	0.41
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	2.02	0.41
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.03	0.41
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	2.03	0.41
2:I:4837:LEU:HD13	2:I:4837:LEU:HA	1.96	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.54	0.41
2:G:485:SER:HA	2:G:488:LEU:HB2	2.03	0.41
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.03	0.41
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.56	0.41
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.86	0.41
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.37	0.41
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.53	0.41
2:G:4236:SER:OG	2:G:4675:LYS:NZ	2.53	0.41
2:B:1154:ASP:O	2:B:1158:ASN:N	2.54	0.41
2:E:134:ASP:OD1	2:E:134:ASP:N	2.54	0.41
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.56	0.41
2:E:4090:LYS:O	2:E:4094:GLN:N	2.49	0.41
2:I:40:GLU:HB3	2:I:44:ASN:HB3	2.03	0.41
2:I:485:SER:O	2:I:489:ASN:N	2.43	0.41
2:I:485:SER:HA	2:I:488:LEU:HB2	2.03	0.41
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.02	0.41
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.03	0.41
2:G:4978:HIS:CE1	2:G:4983:HIS:NE2	2.87	0.41
2:B:40:GLU:HB3	2:B:44:ASN:HB3	2.02	0.40
2:B:767:VAL:HG12	2:B:769:GLU:HG3	2.03	0.40
2:E:485:SER:HA	2:E:488:LEU:HB2	2.03	0.40
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.86	0.40
2:I:471:LEU:O	2:I:475:GLN:N	2.53	0.40
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.03	0.40
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.03	0.40
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.56	0.40
2:G:2318:TYR:HA	2:G:2319:PRO:HD3	1.95	0.40
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.86	0.40
2:B:940:GLY:O	2:B:1052:ASN:N	2.53	0.40
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.86	0.40
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4731:ILE:HA	2:E:4101:LYS:HE3	2.03	0.40
2:E:317:ARG:HE	2:E:323:LEU:HD22	1.85	0.40
2:E:3513:UNK:O	2:E:3515:UNK:N	2.55	0.40
2:E:4667:PRO:O	2:E:4714:ASN:ND2	2.48	0.40
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.40
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	2.02	0.40
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.03	0.40
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	2.03	0.40
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	2.02	0.40
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.86	0.40
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	2.03	0.40
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.03	0.40
2:I:2231:SER:HA	2:I:2234:ARG:HG2	2.04	0.40
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.56	0.40
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.39	0.40
2:G:3513:UNK:O	2:G:3515:UNK:N	2.55	0.40
2:B:2231:SER:HA	2:B:2234:ARG:HG2	2.04	0.40
2:B:2587:UNK:O	2:B:2591:UNK:N	2.54	0.40
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.40
2:B:3514:UNK:O	2:B:3518:UNK:N	2.55	0.40
2:B:4987:ASN:O	2:B:4991:PHE:N	2.55	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:550:LYS:HD3	2:E:550:LYS:HA	1.93	0.40
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.04	0.40
2:I:134:ASP:N	2:I:134:ASP:OD1	2.54	0.40
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.78	0.40
2:G:463:GLU:O	2:G:466:SER:OG	2.30	0.40
2:G:946:ALA:HA	2:G:949:ASN:HB2	2.03	0.40
2:G:3842:LEU:O	2:G:3929:SER:OG	2.40	0.40
2:B:485:SER:HA	2:B:488:LEU:HB2	2.03	0.40
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.03	0.40
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.04	0.40
2:B:2742:THR:OG1	2:B:2811:GLU:OE1	2.34	0.40
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.49	0.40
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.53	0.40
2:E:4857:ASN:HB2	2:G:4807:PHE:HZ	1.86	0.40
2:I:113:HIS:CE1	2:I:402:ARG:HB3	2.56	0.40
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.49	0.40
2:I:767:VAL:HG12	2:I:769:GLU:HG3	2.03	0.40
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	2.03	0.40
2:I:2025:GLU:HA	2:I:2028:ARG:NE	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	47	81
2	E	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	47	81
2	G	3237/4416 (73%)	2887 (89%)	344 (11%)	6 (0%)	47	81
2	I	3237/4416 (73%)	2890 (89%)	341 (10%)	6 (0%)	47	81
All	All	13368/18096 (74%)	11931 (89%)	1413 (11%)	24 (0%)	50	81

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	B	4641	PRO
2	E	1932	PRO
2	E	4641	PRO
2	I	1932	PRO

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Mol	Chain	Res	Type
2	I	4641	PRO
2	G	1932	PRO
2	G	4641	PRO
2	B	1840	PRO
2	B	2291	GLN
2	E	2291	GLN
2	I	1840	PRO
2	I	2291	GLN
2	G	1840	PRO
2	G	2291	GLN
2	E	1840	PRO
2	B	4667	PRO
2	E	4667	PRO
2	I	4667	PRO
2	G	4667	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/89 (99%)	88 (100%)	0	100 100
1	F	88/89 (99%)	88 (100%)	0	100 100
1	H	88/89 (99%)	88 (100%)	0	100 100
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3022 (82%)	2475 (99%)	18 (1%)	84 90
2	E	2493/3022 (82%)	2475 (99%)	18 (1%)	84 90
2	G	2493/3022 (82%)	2475 (99%)	18 (1%)	84 90
2	I	2493/3022 (82%)	2475 (99%)	18 (1%)	84 90
All	All	10324/12444 (83%)	10252 (99%)	72 (1%)	84 90

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	719	LEU
2	B	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3663	LEU
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4818	MET
2	B	4983	HIS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	719	LEU
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3663	LEU
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4818	MET
2	E	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	719	LEU
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG

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Mol	Chain	Res	Type
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3663	LEU
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4818	MET
2	I	4983	HIS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	719	LEU
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4818	MET
2	G	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	71	GLN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS

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Mol	Chain	Res	Type
2	B	379	HIS
2	B	413	GLN
2	B	479	GLN
2	B	520	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2127	GLN
2	B	3766	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4054	ASN
2	B	4102	GLN
2	B	4120	ASN
2	B	4553	ASN
2	B	4946	GLN
2	E	57	ASN
2	E	71	GLN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	413	GLN
2	E	479	GLN
2	E	520	ASN
2	E	797	HIS
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2127	GLN
2	E	3766	GLN

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Mol	Chain	Res	Type
2	E	3809	ASN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4054	ASN
2	E	4102	GLN
2	E	4120	ASN
2	E	4553	ASN
2	E	4946	GLN
2	I	57	ASN
2	I	71	GLN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	413	GLN
2	I	479	GLN
2	I	520	ASN
2	I	797	HIS
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	3766	GLN
2	I	3809	ASN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4054	ASN
2	I	4102	GLN
2	I	4120	ASN

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Mol	Chain	Res	Type
2	I	4553	ASN
2	I	4946	GLN
2	G	57	ASN
2	G	71	GLN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	413	GLN
2	G	479	GLN
2	G	520	ASN
2	G	797	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	3766	GLN
2	G	3809	ASN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4054	ASN
2	G	4102	GLN
2	G	4120	ASN
2	G	4553	ASN
2	G	4946	GLN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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	B	14
2	E	14
2	I	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.38
1	E	4345:UNK	C	4540:PHE	N	73.38
1	I	4345:UNK	C	4540:PHE	N	73.38
1	G	4345:UNK	C	4540:PHE	N	73.38
1	B	3613:UNK	C	3639:THR	N	48.21
1	E	3613:UNK	C	3639:THR	N	48.21
1	I	3613:UNK	C	3639:THR	N	48.21
1	G	3613:UNK	C	3639:THR	N	48.21
1	B	4253:GLU	C	4320:UNK	N	27.50

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4253:GLU	C	4320:UNK	N	27.50
1	I	4253:GLU	C	4320:UNK	N	27.50
1	G	4253:GLU	C	4320:UNK	N	27.50
1	B	3163:UNK	C	3170:UNK	N	16.06
1	E	3163:UNK	C	3170:UNK	N	16.06
1	I	3163:UNK	C	3170:UNK	N	16.06
1	G	3163:UNK	C	3170:UNK	N	16.06
1	B	3063:UNK	C	3134:UNK	N	14.88
1	E	3063:UNK	C	3134:UNK	N	14.88
1	I	3063:UNK	C	3134:UNK	N	14.88
1	G	3063:UNK	C	3134:UNK	N	14.88
1	B	3468:UNK	C	3511:UNK	N	14.29
1	E	3468:UNK	C	3511:UNK	N	14.29
1	I	3468:UNK	C	3511:UNK	N	14.29
1	G	3468:UNK	C	3511:UNK	N	14.29
1	B	2703:UNK	C	2734:ASN	N	13.58
1	E	2703:UNK	C	2734:ASN	N	13.58
1	I	2703:UNK	C	2734:ASN	N	13.58
1	G	2703:UNK	C	2734:ASN	N	13.58
1	B	3236:UNK	C	3241:UNK	N	13.52
1	E	3236:UNK	C	3241:UNK	N	13.52
1	I	3236:UNK	C	3241:UNK	N	13.52
1	G	3236:UNK	C	3241:UNK	N	13.52
1	B	1564:UNK	C	1573:MET	N	12.58
1	E	1564:UNK	C	1573:MET	N	12.58
1	I	1564:UNK	C	1573:MET	N	12.58
1	G	1564:UNK	C	1573:MET	N	12.58
1	B	2976:UNK	C	2995:UNK	N	12.37
1	E	2976:UNK	C	2995:UNK	N	12.37
1	I	2976:UNK	C	2995:UNK	N	12.37
1	G	2976:UNK	C	2995:UNK	N	12.37
1	B	3254:UNK	C	3261:UNK	N	8.09
1	E	3254:UNK	C	3261:UNK	N	8.09
1	I	3254:UNK	C	3261:UNK	N	8.09
1	G	3254:UNK	C	3261:UNK	N	8.09
1	B	1297:UNK	C	1430:UNK	N	5.89
1	I	1297:UNK	C	1430:UNK	N	5.89
1	E	1297:UNK	C	1430:UNK	N	5.88
1	G	1297:UNK	C	1430:UNK	N	5.88
1	B	2479:LEU	C	2487:UNK	N	3.66
1	E	2479:LEU	C	2487:UNK	N	3.66
1	I	2479:LEU	C	2487:UNK	N	3.66

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	2479:LEU	C	2487:UNK	N	3.66
1	B	2939:ARG	C	2942:UNK	N	3.38
1	E	2939:ARG	C	2942:UNK	N	3.38
1	I	2939:ARG	C	2942:UNK	N	3.38
1	G	2939:ARG	C	2942:UNK	N	3.38

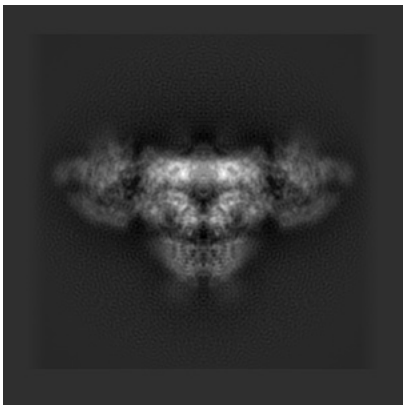
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8394. These allow visual inspection of the internal detail of the map and identification of artifacts.

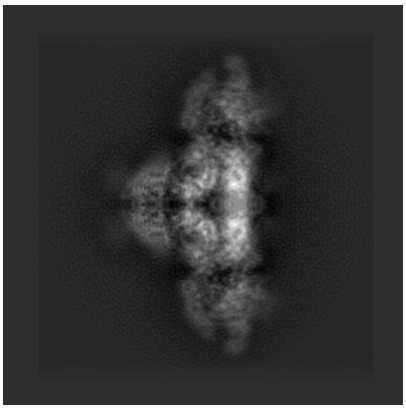
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

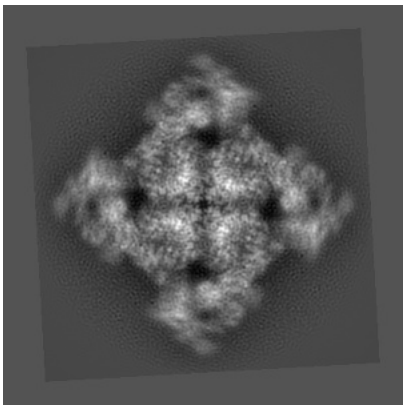
6.1.1 Primary map



X

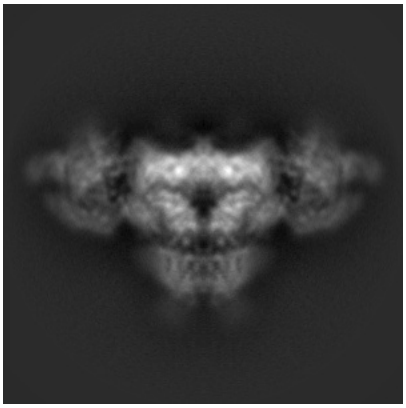


Y

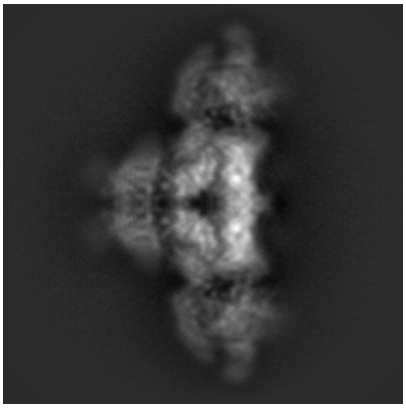


Z

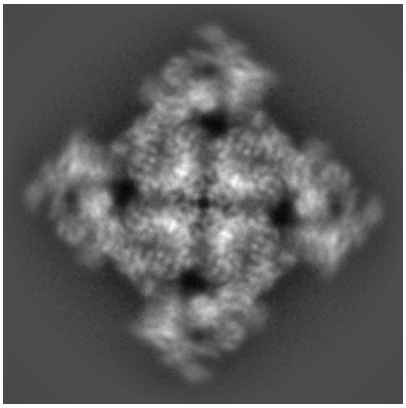
6.1.2 Raw map



X



Y

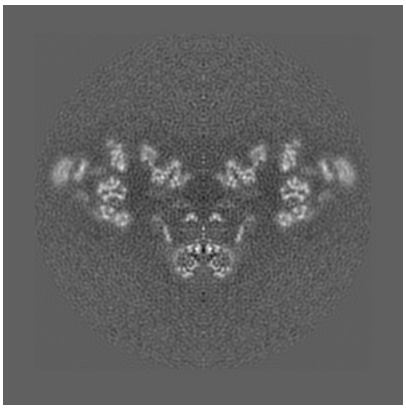


Z

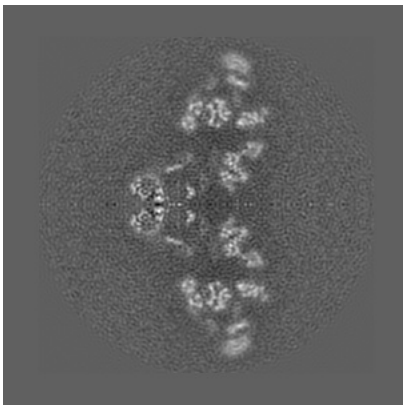
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

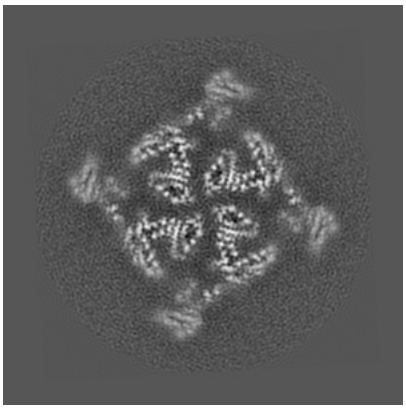
6.2.1 Primary map



X Index: 200

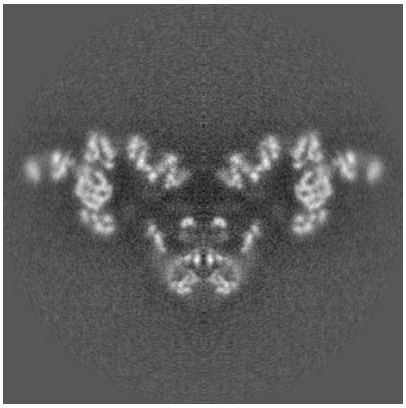


Y Index: 200

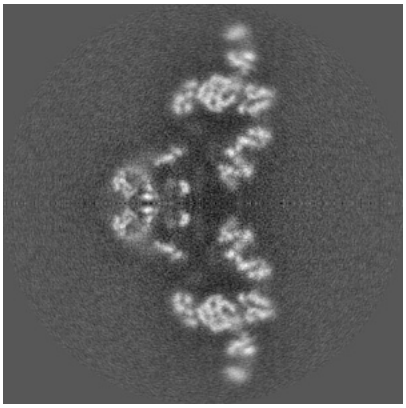


Z Index: 200

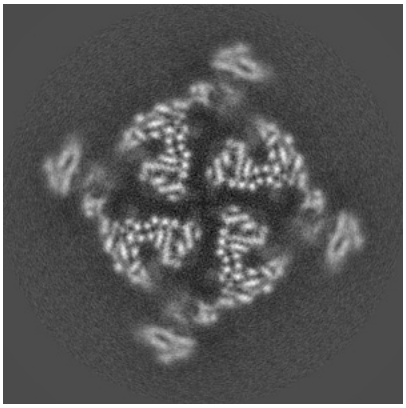
6.2.2 Raw map



X Index: 168



Y Index: 168

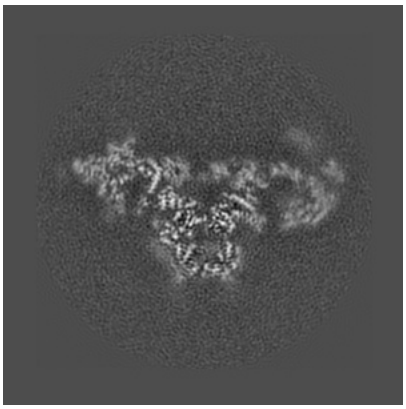


Z Index: 168

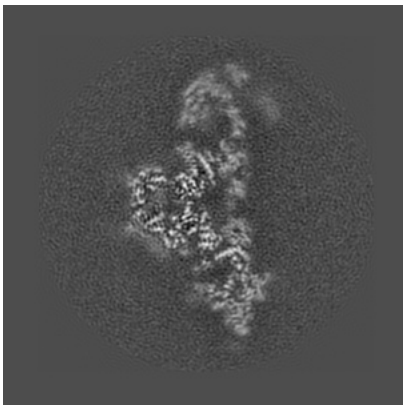
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

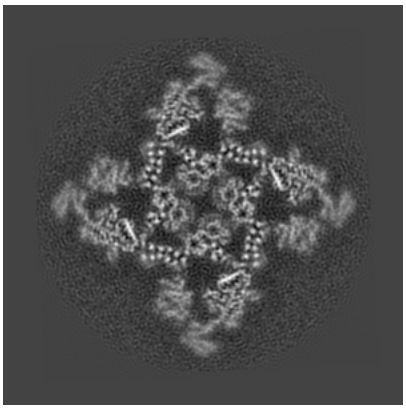
6.3.1 Primary map



X Index: 217

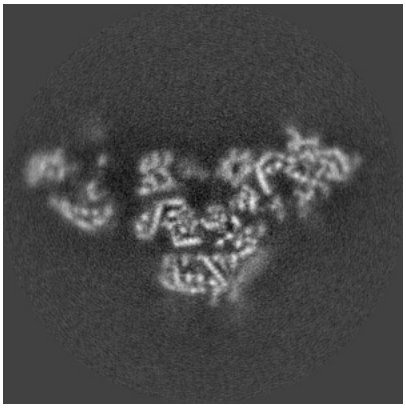


Y Index: 183

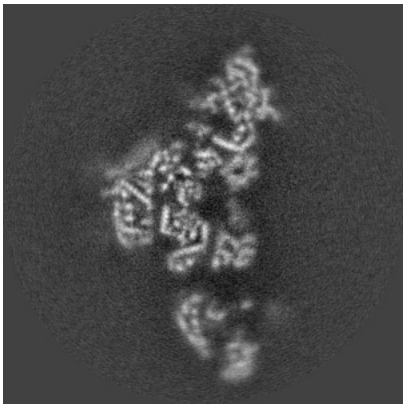


Z Index: 227

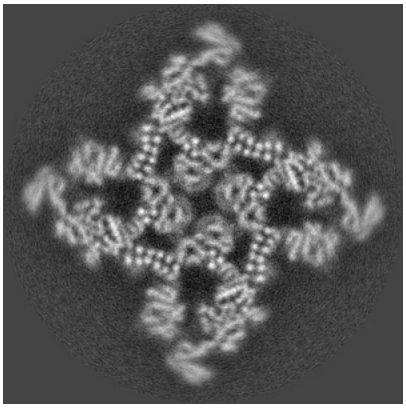
6.3.2 Raw map



X Index: 154



Y Index: 182



Z Index: 193

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

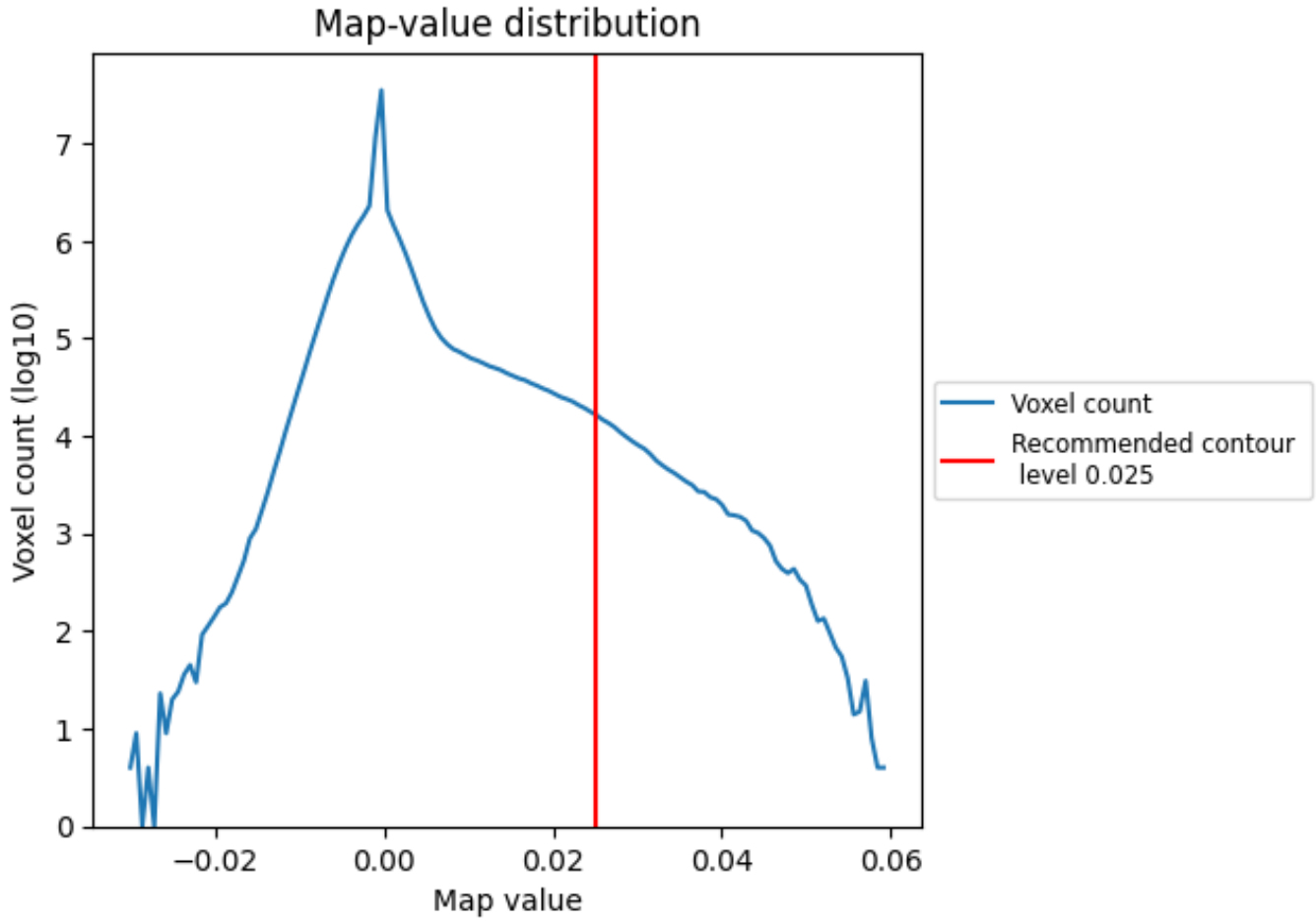
6.5 Mask visualisation (i)

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

7 Map analysis

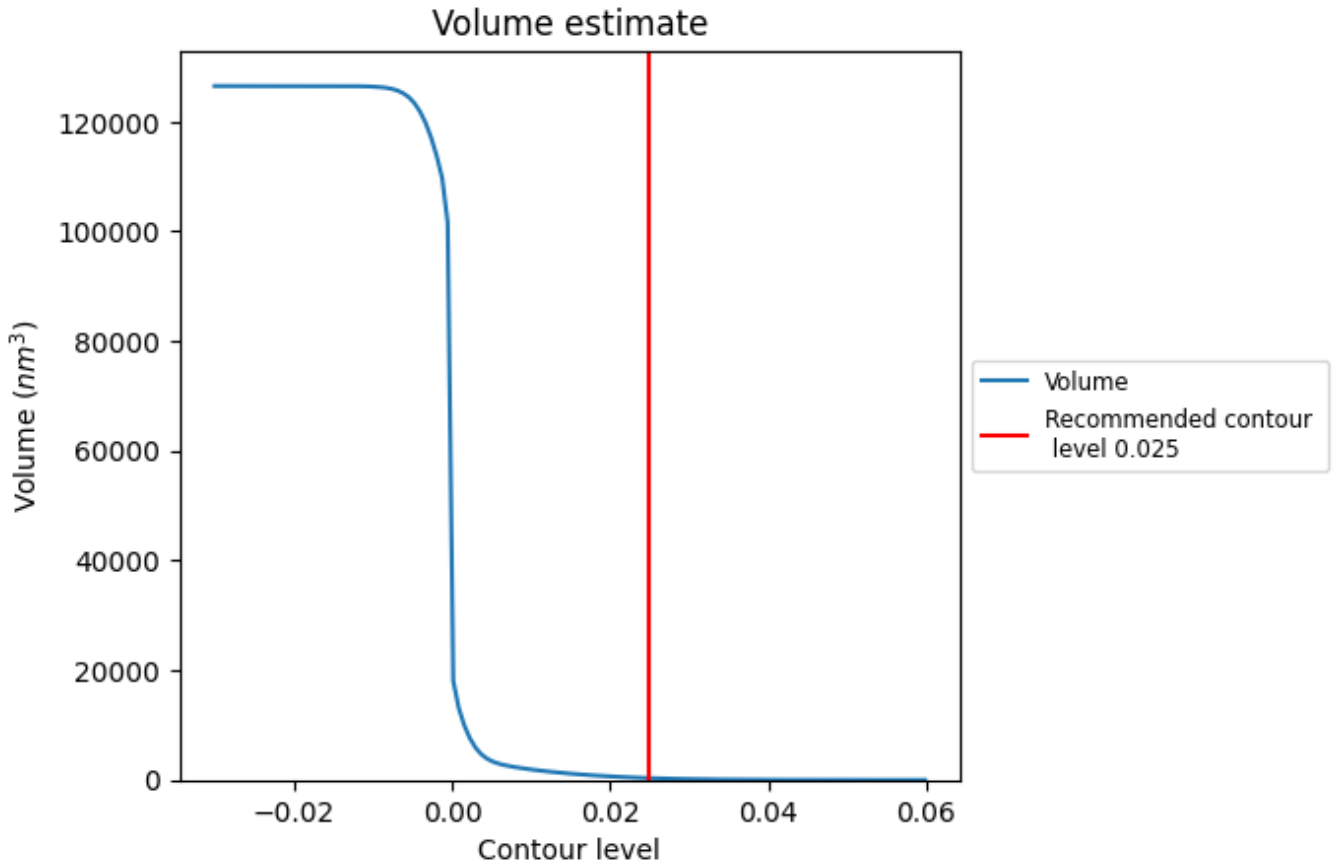
This section contains the results of statistical analysis of the map.

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.

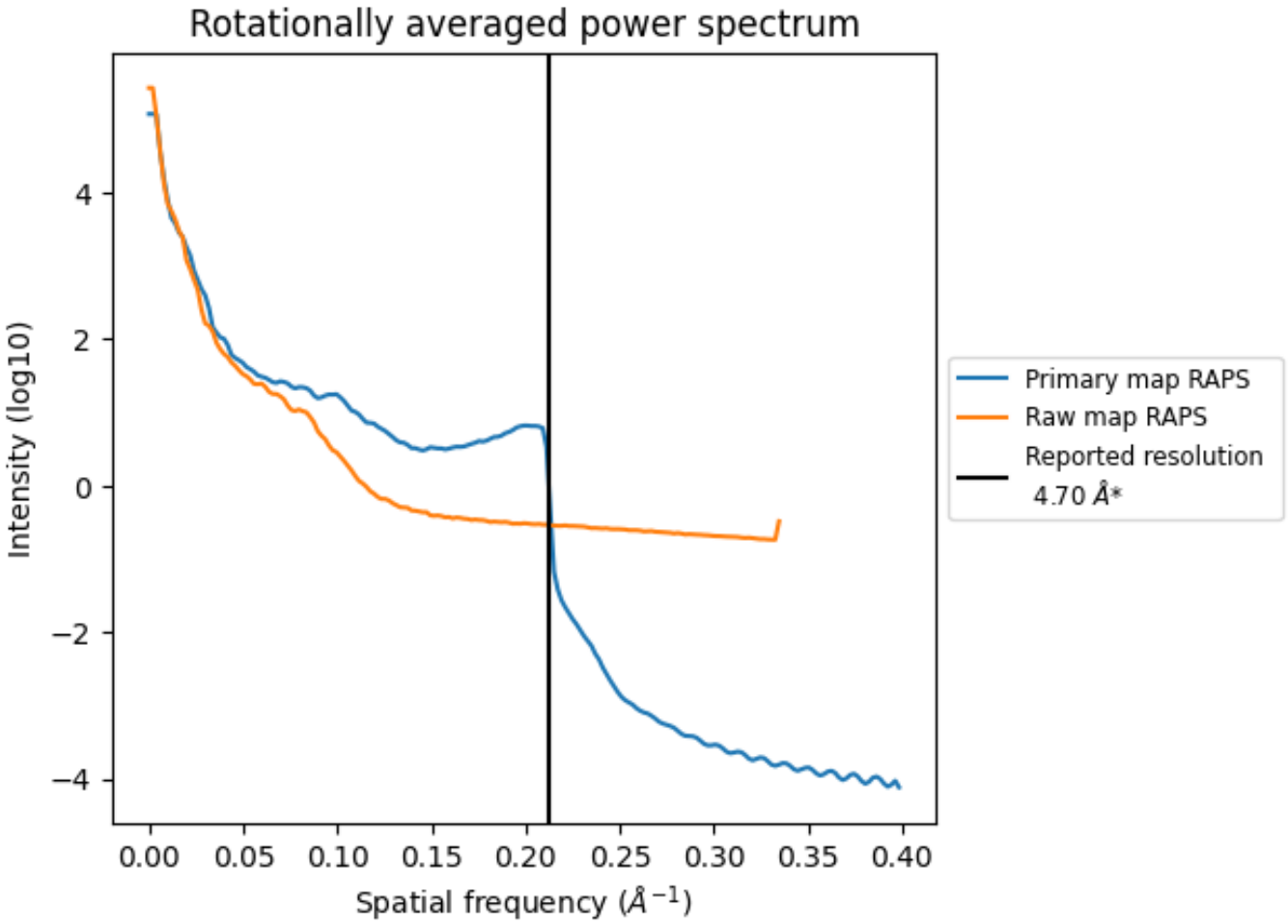
7.2 Volume estimate



The volume at the recommended contour level is 330 nm^3; this corresponds to an approximate mass of 299 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)

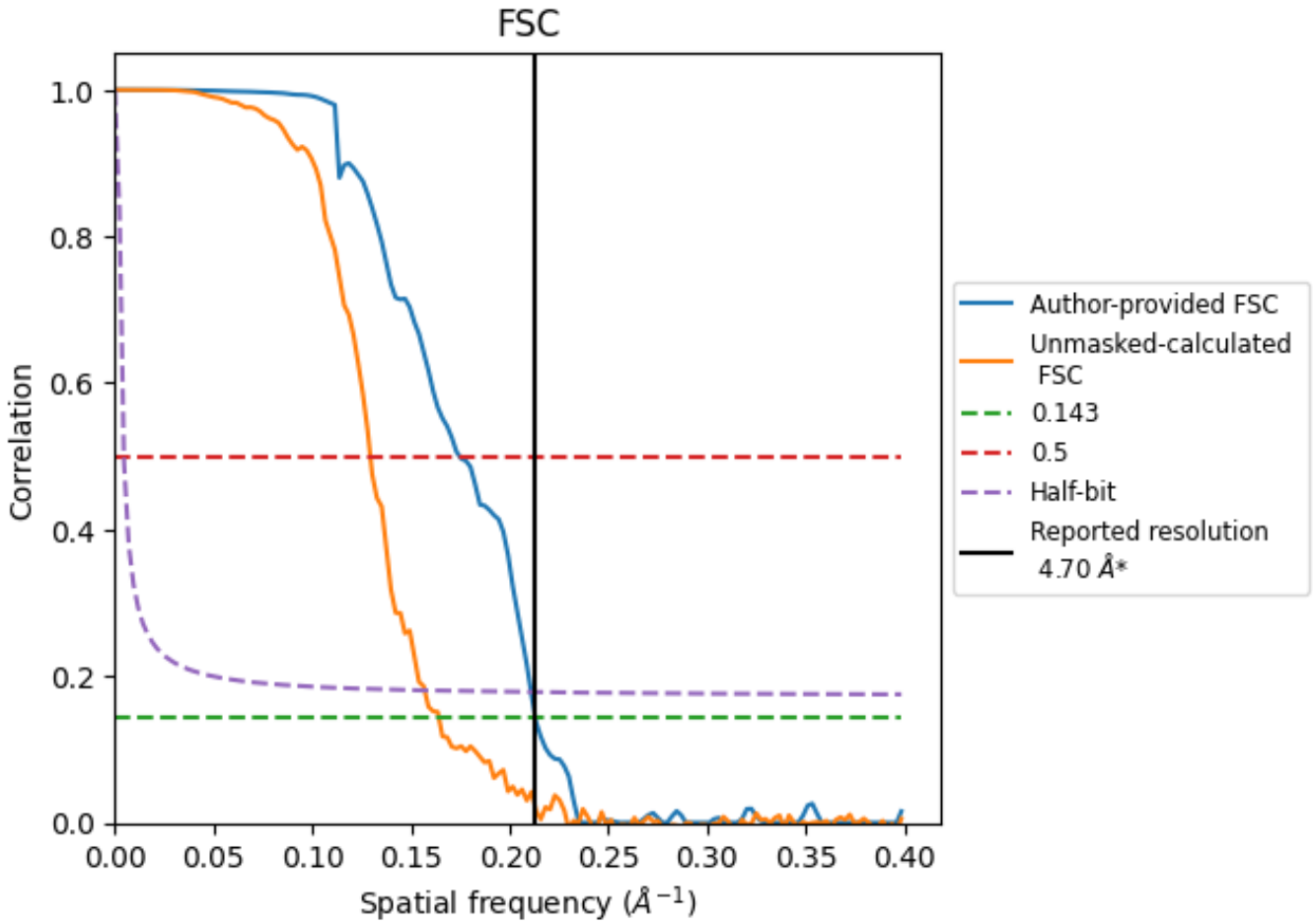


*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

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 0.213 Å^{-1}

8.2 Resolution estimates (i)

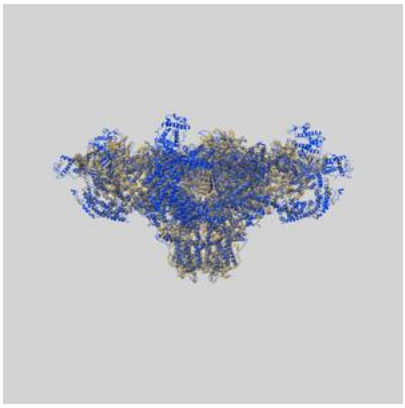
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.69	5.73	4.74
Unmasked-calculated*	6.09	7.73	6.37

*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 6.09 differs from the reported value 4.7 by more than 10 %

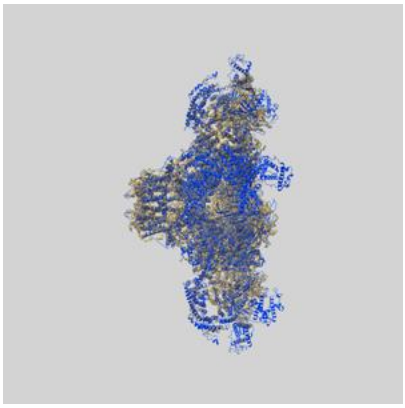
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8394 and PDB model 5TB3. Per-residue inclusion information can be found in section 3 on page 4.

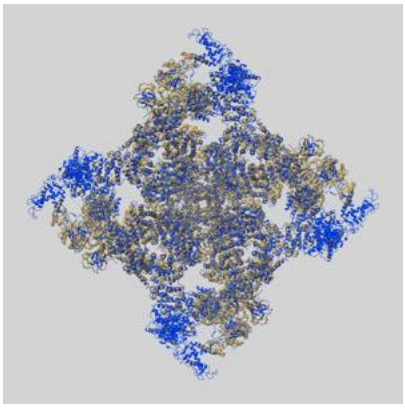
9.1 Map-model overlay



X



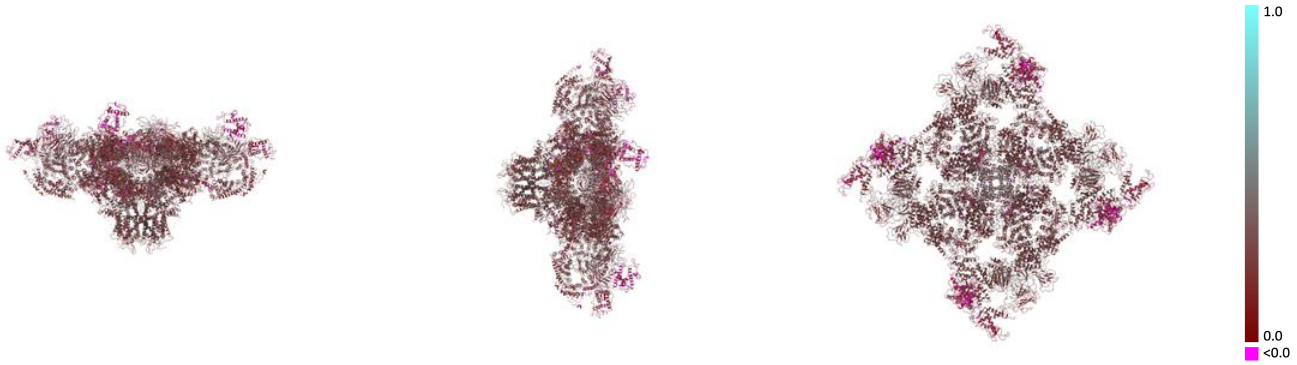
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

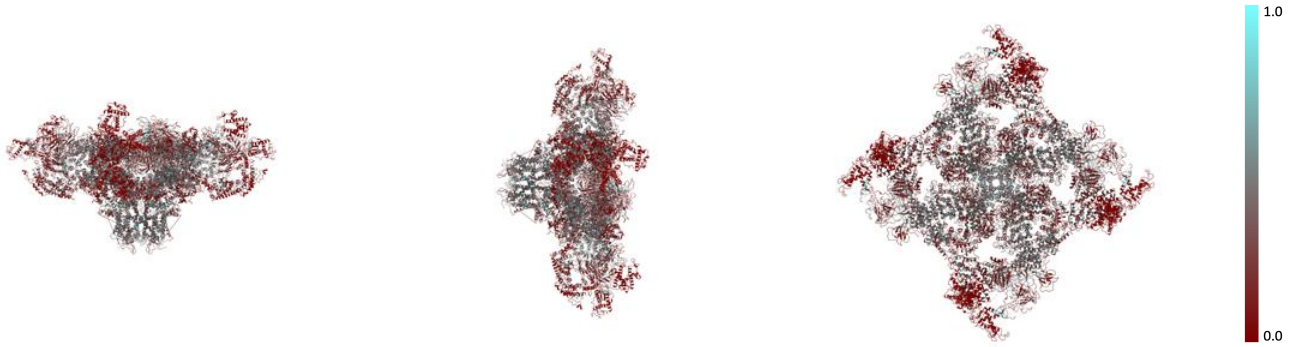
9.2 Q-score mapped to coordinate model



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.

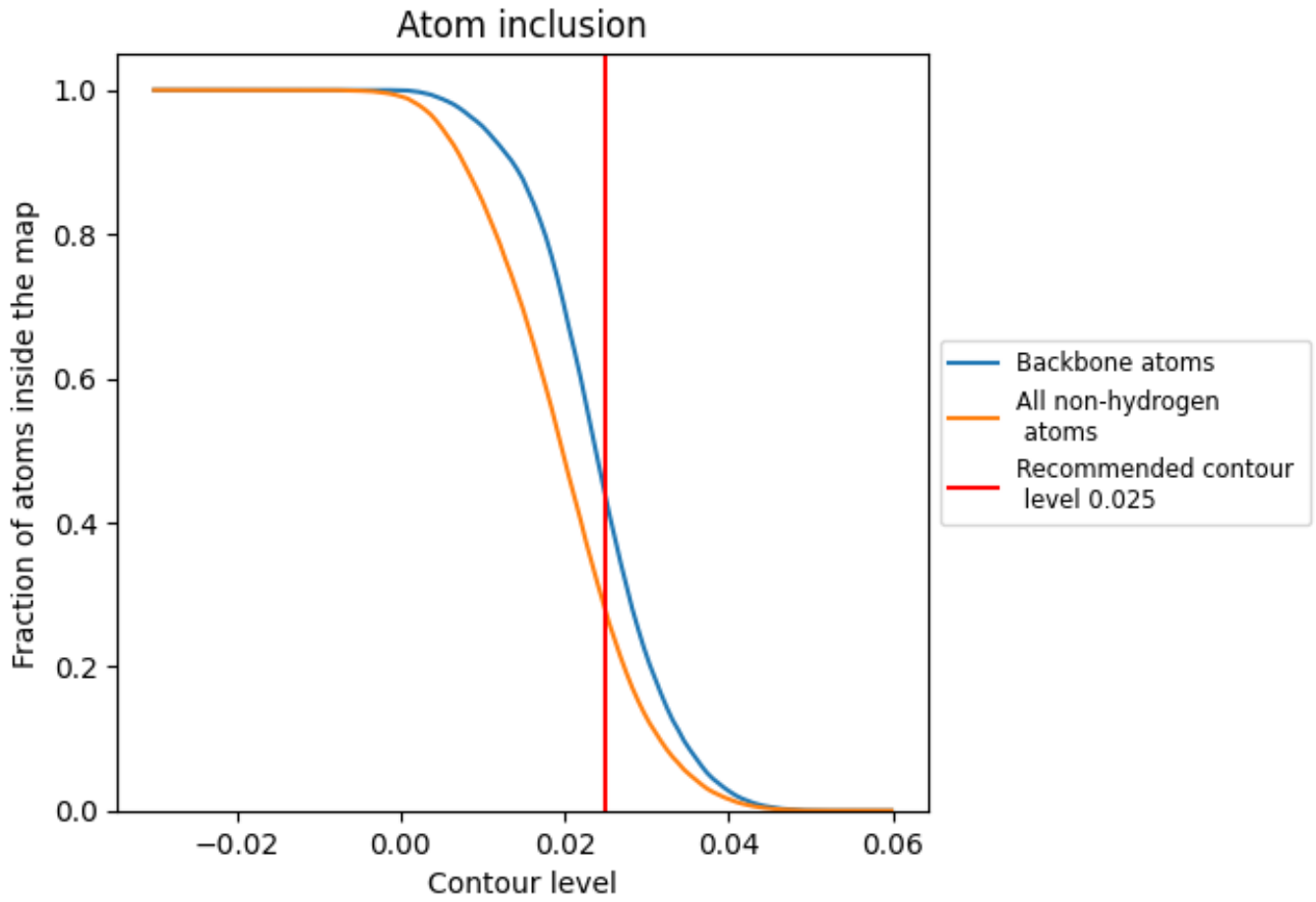
9.3 Atom inclusion mapped to coordinate model



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 28% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2764	0.2630
A	0.2395	0.2880
B	0.2777	0.2620
E	0.2772	0.2620
F	0.2382	0.2900
G	0.2774	0.2620
H	0.2395	0.2920
I	0.2774	0.2620
J	0.2395	0.2900