# Full wwPDB EM Validation Report (i)

Nov 2, 2022 – 03:37 AM EDT

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|---|---|---|
| PDB ID | : | 5TAM |
| EMDB ID | : | EMD-8379 |
| Title | : | Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 4) |
| Authors | : | Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J. |
| Deposited on | : | 2016-09-10 |
| Resolution | : | 4.30 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

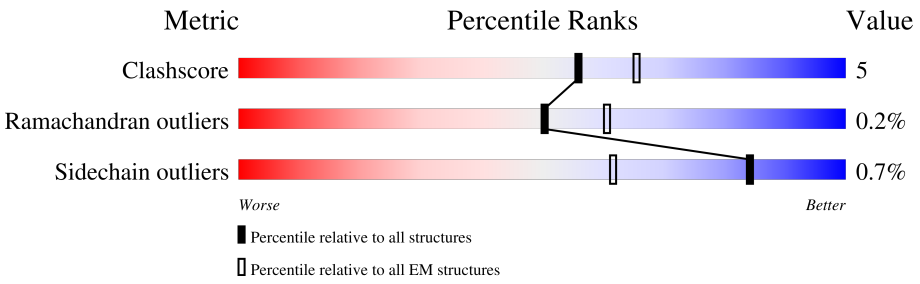
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev43 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| 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 (i)

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

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 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 | 56% 79% 20% • |
| 1 | F | 108 | 56% 81% 19% • |
| 1 | H | 108 | 57% 81% 19% • |
| 1 | J | 108 | 56% 81% 19% • |
| 2 | B | 4416 | 49% 83% 11% 5% |
| 2 | E | 4416 | 49% 84% 11% 5% |
| 2 | G | 4416 | 50% 83% 11% 5% |
| 2 | I | 4416 | 50% 84% 11% 5% |

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 121456 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.

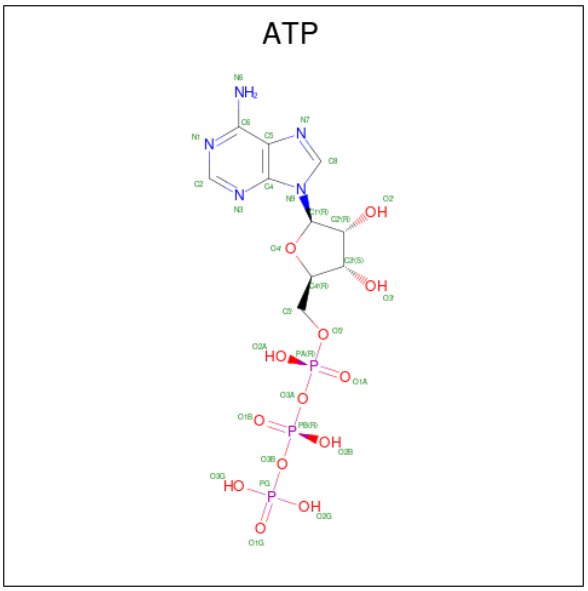
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

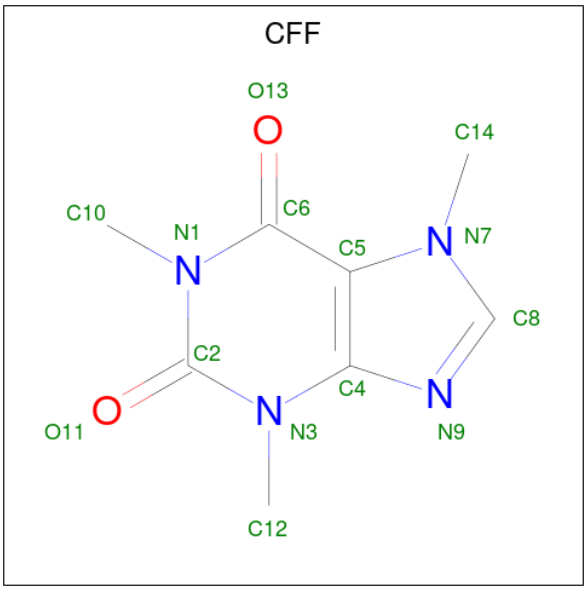
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 4194 | 29499 | 18686 | 5228 | 5428 | 157 | 0 | 0 |
| 2 | E | 4194 | 29499 | 18686 | 5228 | 5428 | 157 | 0 | 0 |
| 2 | I | 4194 | 29499 | 18686 | 5228 | 5428 | 157 | 0 | 0 |
| 2 | G | 4194 | 29499 | 18686 | 5228 | 5428 | 157 | 0 | 0 |

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 3 | B | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |
| 3 | E | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |
| 3 | I | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |
| 3 | G | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | |
| 4 | B | 1 | 14 | 8 | 4 | 2 | 0 |
| 4 | E | 1 | 14 | 8 | 4 | 2 | 0 |
| 4 | I | 1 | 14 | 8 | 4 | 2 | 0 |
| 4 | G | 1 | 14 | 8 | 4 | 2 | 0 |

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 5 | B | 1 | 1 | 1 | 0 |
| 5 | E | 1 | 1 | 1 | 0 |
| 5 | I | 1 | 1 | 1 | 0 |
| 5 | G | 1 | 1 | 1 | 0 |

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

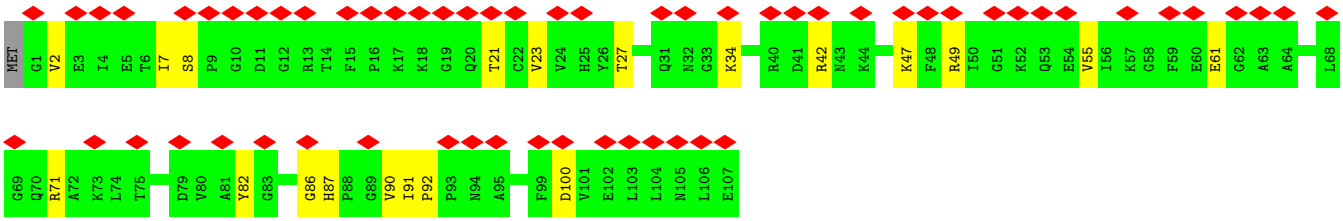
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Ca | |
| 6 | B | 1 | 1 | 1 | 0 |
| 6 | E | 1 | 1 | 1 | 0 |
| 6 | I | 1 | 1 | 1 | 0 |
| 6 | G | 1 | 1 | 1 | 0 |

# 3 Residue-property plots (i)

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

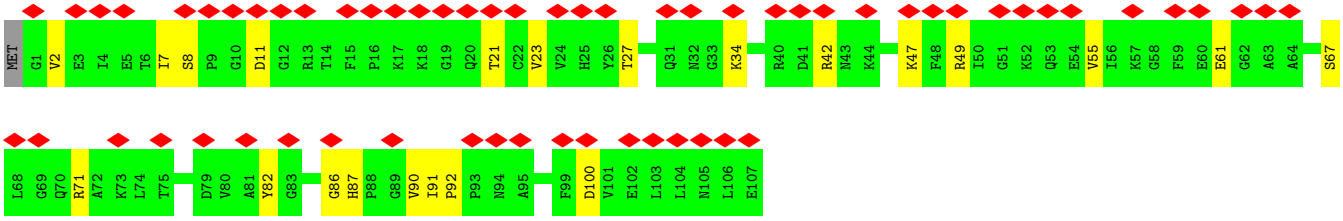
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



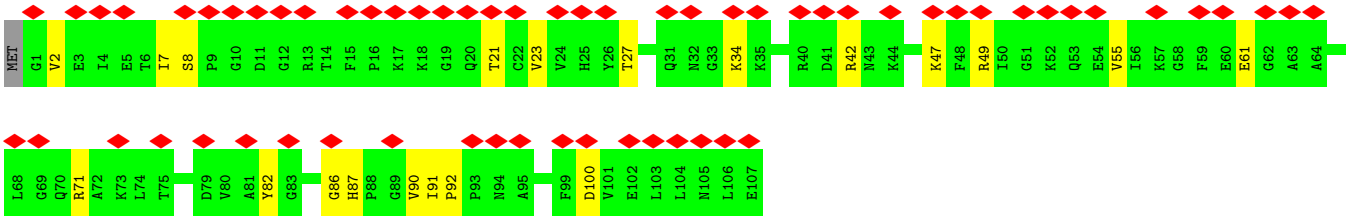

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



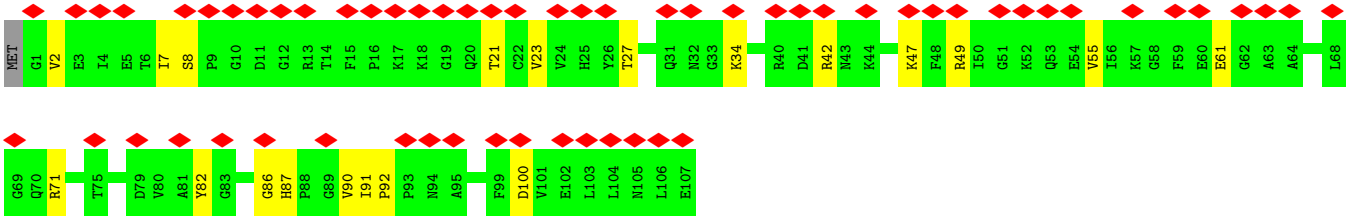

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



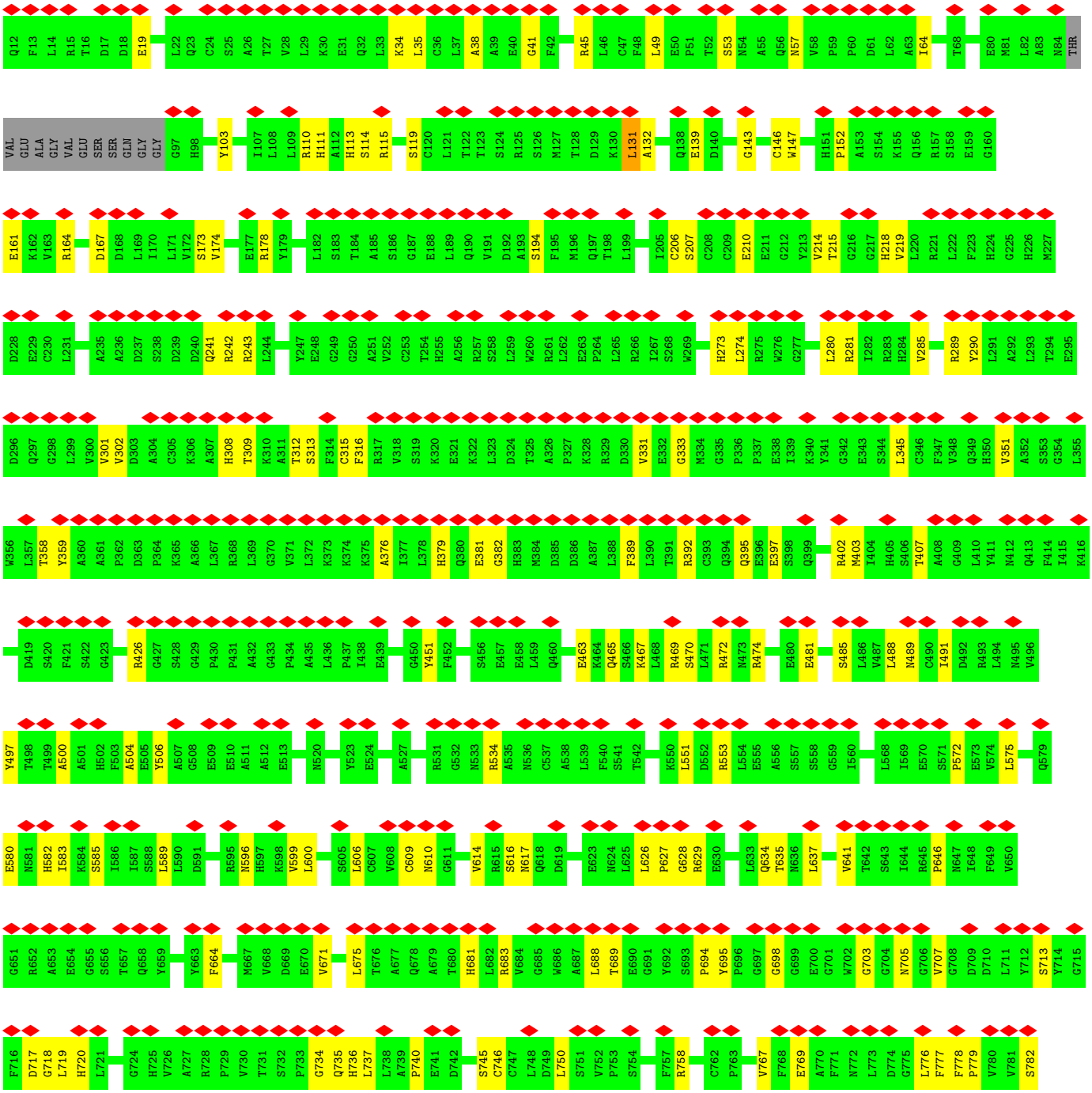

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

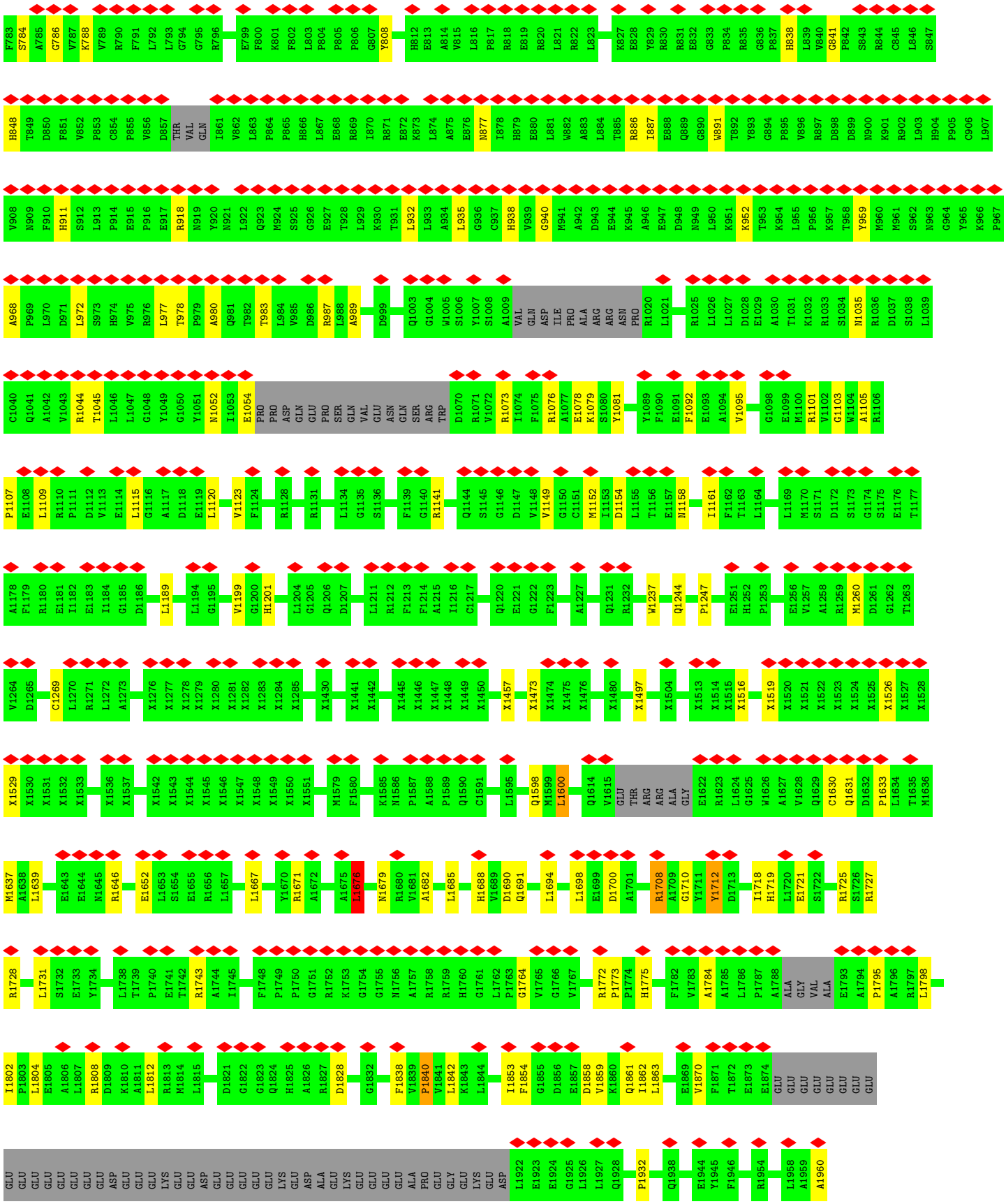
Chain J:

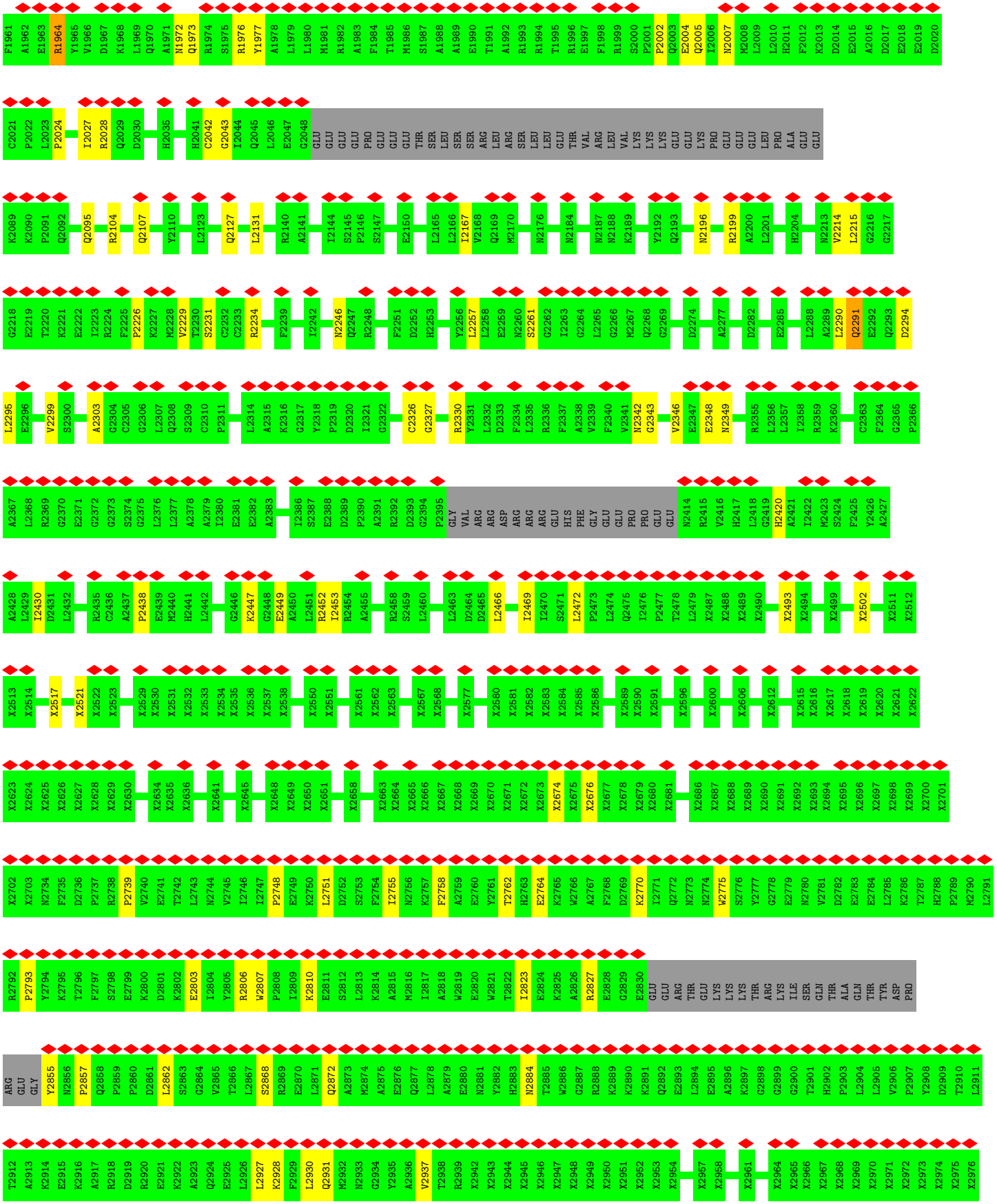



• Molecule 2: Ryanodine receptor 1

Chain B:




F783 S784 A785 G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 E799 F800 K801 F802 L803 P804 P805 P806 G807 Y808 H812 E813 A814 V815 L816 P817 R818 E819 R820 L821 R822 L823 K827 E828 Y829 R830 R831 E832 G833 P834 R835 G836 P837 H838 L839 V840 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 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 M961 S962 N963 G964 Y965 K966 P967
A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 A989 D999 Q1003 G1004 W1005 S1006 Y1007 S1008 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 R1025 L1026 L1027 D1028 E1029 A1030 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 Y1089 F1090 E1091 F1092 E1093 A1094 V1095 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106
P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 G1116 A1117 D1118 E1119 L1120 V1123 F1124 R1128 R1131 L1134 G1135 S1136 F1139 G1140 R1141 Q1144 S1145 G1146 D1147 V1148 V1149 G1150 C1151 M1152 I1153 D1154 L1155 T1156 E1157 N1158 I1161 F1162 T1163 L1164 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177
A1178 F1179 R1180 E1181 I1182 E1183 I1184 G1185 D1186 L1189 L1194 G1195 V1199 G1200 H1201 L1204 G1205 Q1206 D1207 L1211 R1212 F1213 F1214 A1215 I1216 C1217 Q1220 E1221 G1222 F1223 A1227 Q1231 R1232 W1237 Q1244 P1247 E1251 H1252 P1253 E1256 V1257 A1258 R1259 M1260 D1261 G1262 T1263
V1264 D1265 C1269 L1270 R1271 L1272 A1273 X1276 X1277 X1278 X1279 X1280 X1281 X1282 X1283 X1284 X1285 X1430 X1441 X1442 X1445 X1446 X1447 X1448 X1449 X1450 X1457 X1473 X1474 X1475 X1476 X1480 X1497 X1504 X1513 X1514 X1515 X1516 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528
X1529 X1530 X1531 X1532 X1533 X1536 X1537 X1542 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 X1551 M1579 F1580 K1585 N1586 P1587 A1588 P1589 Q1590 C1591 L1595 Q1598 M1599 L1600 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624 G1625 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 T1635 M1636
M1637 A1638 L1639 E1643 E1644 N1645 R1646 E1652 L1653 S1654 E1655 R1656 L1657 L1667 Y1670 R1671 A1672 A1675 L1676 N1679 R1680 V1681 A1682 L1685 H1688 V1689 D1690 Q1691 L1694 L1698 E1699 D1700 A1701 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 S1722 R1725 S1726 R1727
R1728 L1731 S1732 E1733 Y1734 L1738 T1739 P1740 E1741 T1742 R1743 A1744 I1745 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1761 L1762 P1763 G1764 V1765 G1766 V1767 R1772 P1773 P1774 H1775 F1782 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798
I1802 P1803 L1804 E1805 A1806 A1807 R1808 D1809 K1810 A1811 L1812 R1813 M1814 L1815 D1821 G1822 G1823 Q1824 H1825 A1826 R1827 D1828 G1832 F1838 V1839 P1840 V1841 L1842 K1843 L1844 I1853 F1854 G1855 D1856 E1857 D1858 V1859 K1860 Q1861 I1862 L1863 E1869 V1870 F1871 T1872 E1873 E1874 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 GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 P1932 Q1938 E1944 Y1945 F1946 R1964 L1968 A1959 A1960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C2021 P2022 L2023 P2024 I2027 R2028 Q2029 D2030 H2035 H2041 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU
K2089 K2090 P2091 Q2092 Q2095 R2104 Q2107 Y2110 L2123 Q2127 L2131 R2140 A2141 I2144 S2145 P2146 S2147 E2150 L2165 L2166 I2167 V2168 Q2169 M2170 N2176 N2184 N2187 N2188 K2189 Y2192 Q2193 N2196 R2199 A2200 L2201 H2204 N2213 V2214 L2215 G2216 G2217
G2218 E2219 T2220 K2221 E2222 I2223 R2224 F2225 P2226 K2227 M2228 V2229 T2230 S2231 C2232 C2233 R2234 F2239 I2242 N2246 Q2247 R2248 F2251 D2252 H2253 Y2256 L2257 L2258 E2259 N2260 S2261 G2262 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 D2274 A2277 D2282 E2285 L2288 A2289 L2290 Q2291 E2292 Q2293 D2294
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A2428 L2429 I2430 D2431 L2432 R2435 C2436 A2437 P2438 E2439 M2440 H2441 L2442 G2446 K2447 G2448 E2449 A2450 L2451 R2452 I2453 R2454 A2455 R2458 S2459 L2460 L2463 D2464 D2465 L2466 I2469 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479 X2487 X2488 X2489 X2490 X2493 X2494 X2499 X2502 X2511 X2512
X2513 X2514 X2517 X2521 X2522 X2523 X2529 X2530 X2531 X2532 X2533 X2534 X2535 X2536 X2537 X2538 X2550 X2551 X2561 X2562 X2563 X2567 X2568 X2577 X2580 X2581 X2582 X2583 X2584 X2585 X2586 X2589 X2590 X2591 X2596 X2600 X2606 X2612 X2615 X2616 X2617 X2618 X2619 X2620 X2621 X2622
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X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 P2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791
R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO
ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 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
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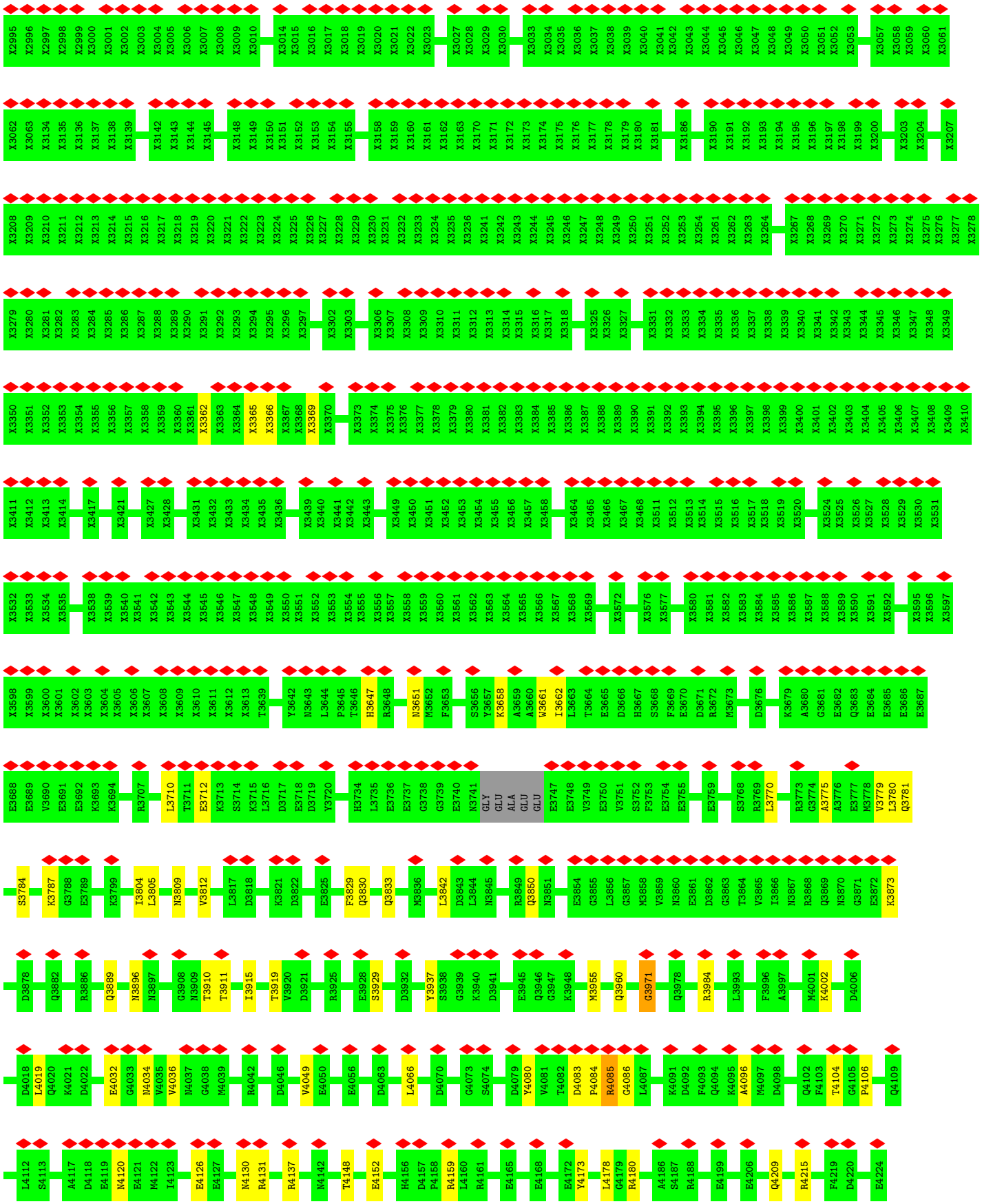
X2995 X2996 X2997 X2998 X2999 X3000 X3001 X3002 X3003 X3004 X3005 X3006 X3007 X3008 X3009 X3010
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X3027 X3028 X3029 X3030
X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040 X3041 X3042 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3051 X3052 X3053
X3057 X3058 X3059 X3060 X3061
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X3142 X3143 X3144 X3145
X3148 X3149 X3150 X3151 X3152 X3153 X3154 X3155
X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3180 X3181
X3186
X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3198 X3199 X3200
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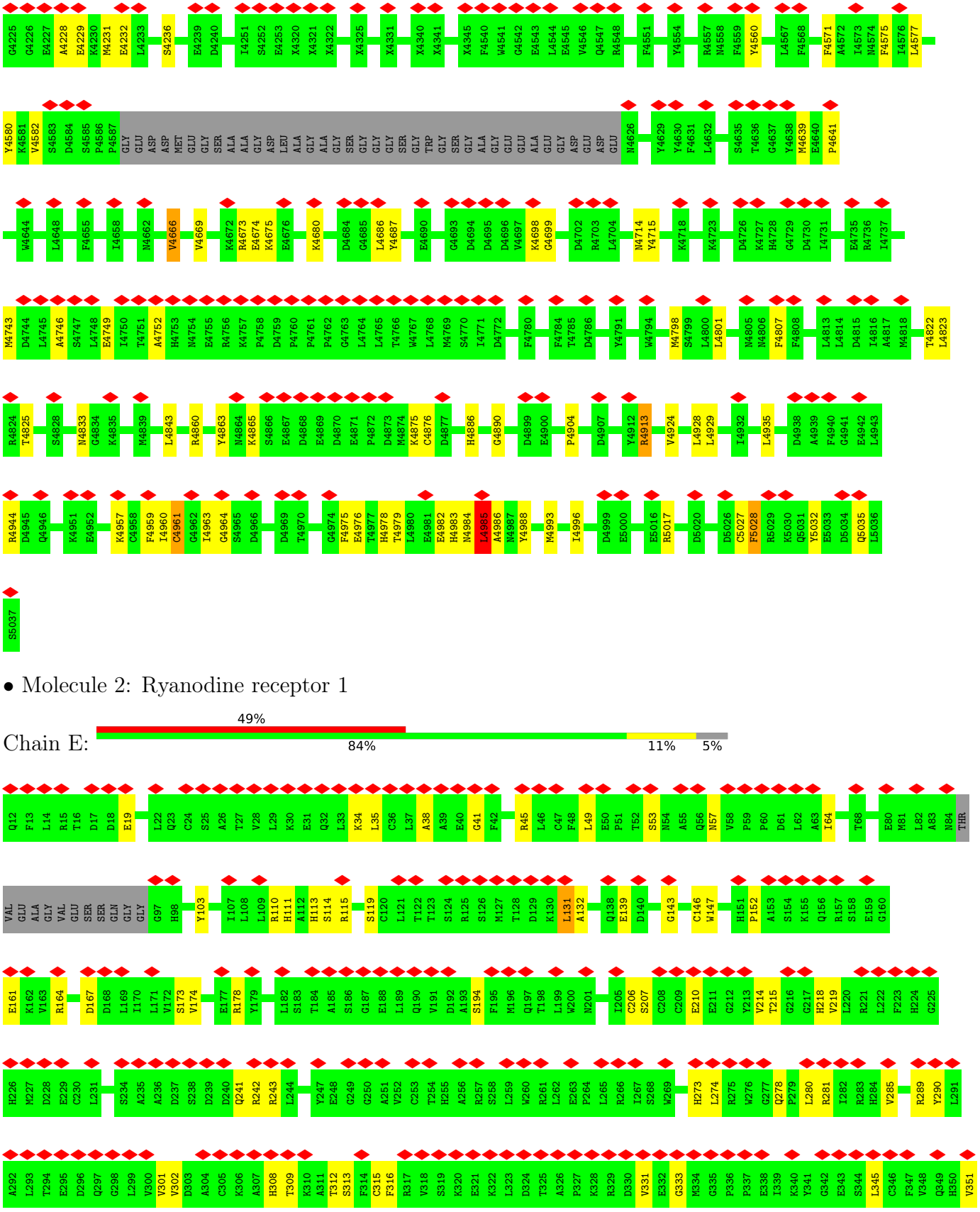


- Molecule 2: Ryanodine receptor 1

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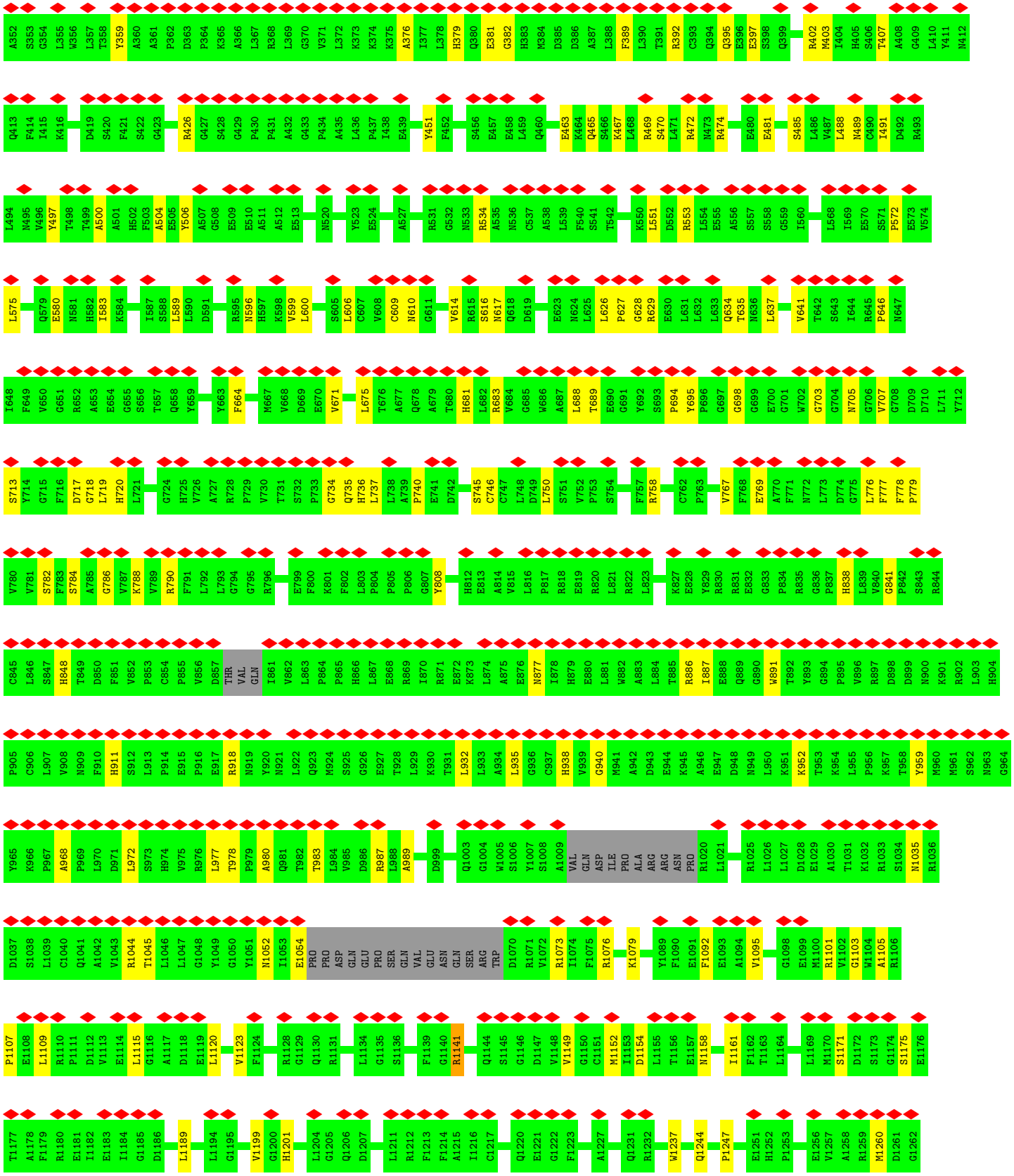
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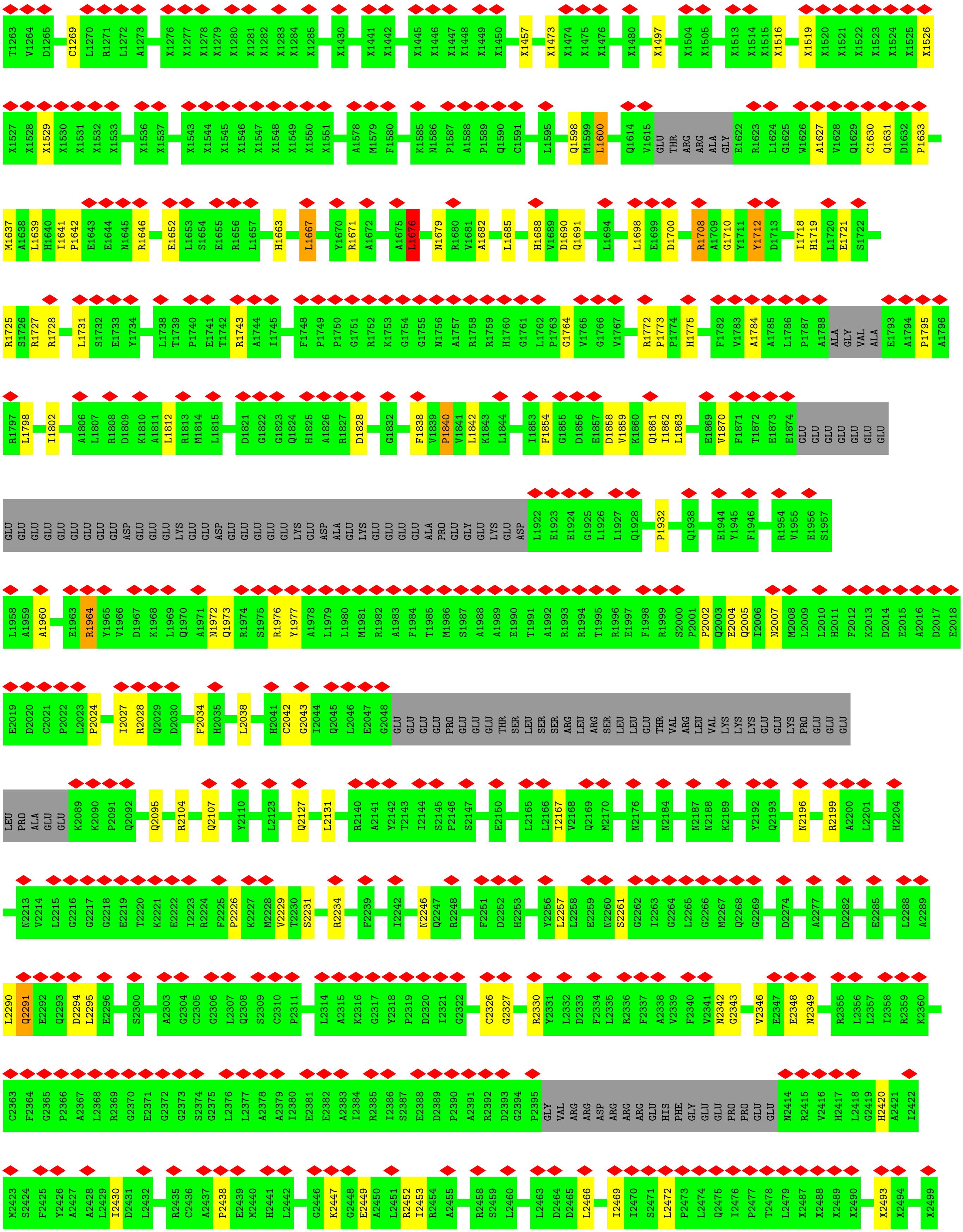
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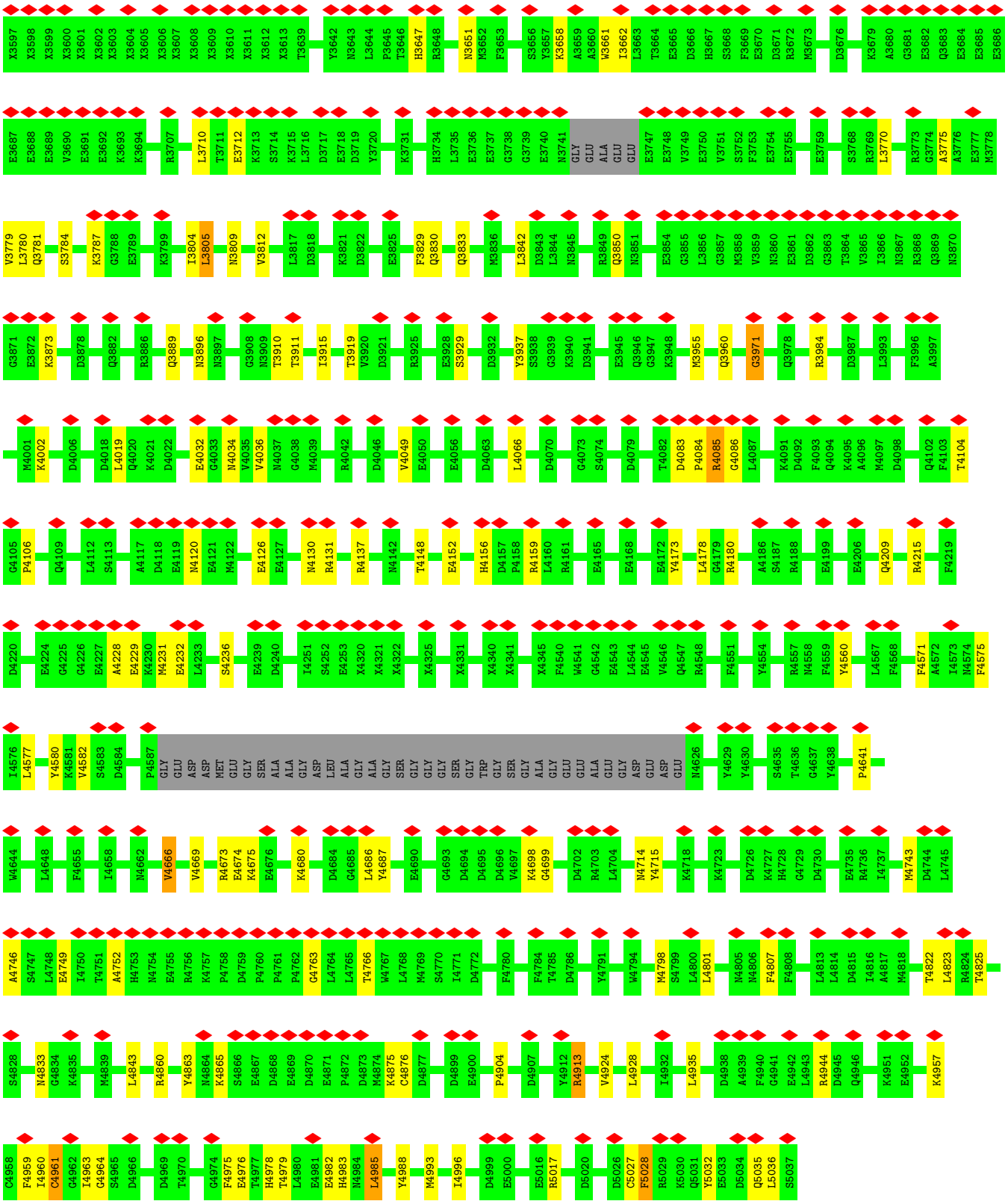

- Molecule 2: Ryanodine receptor 1

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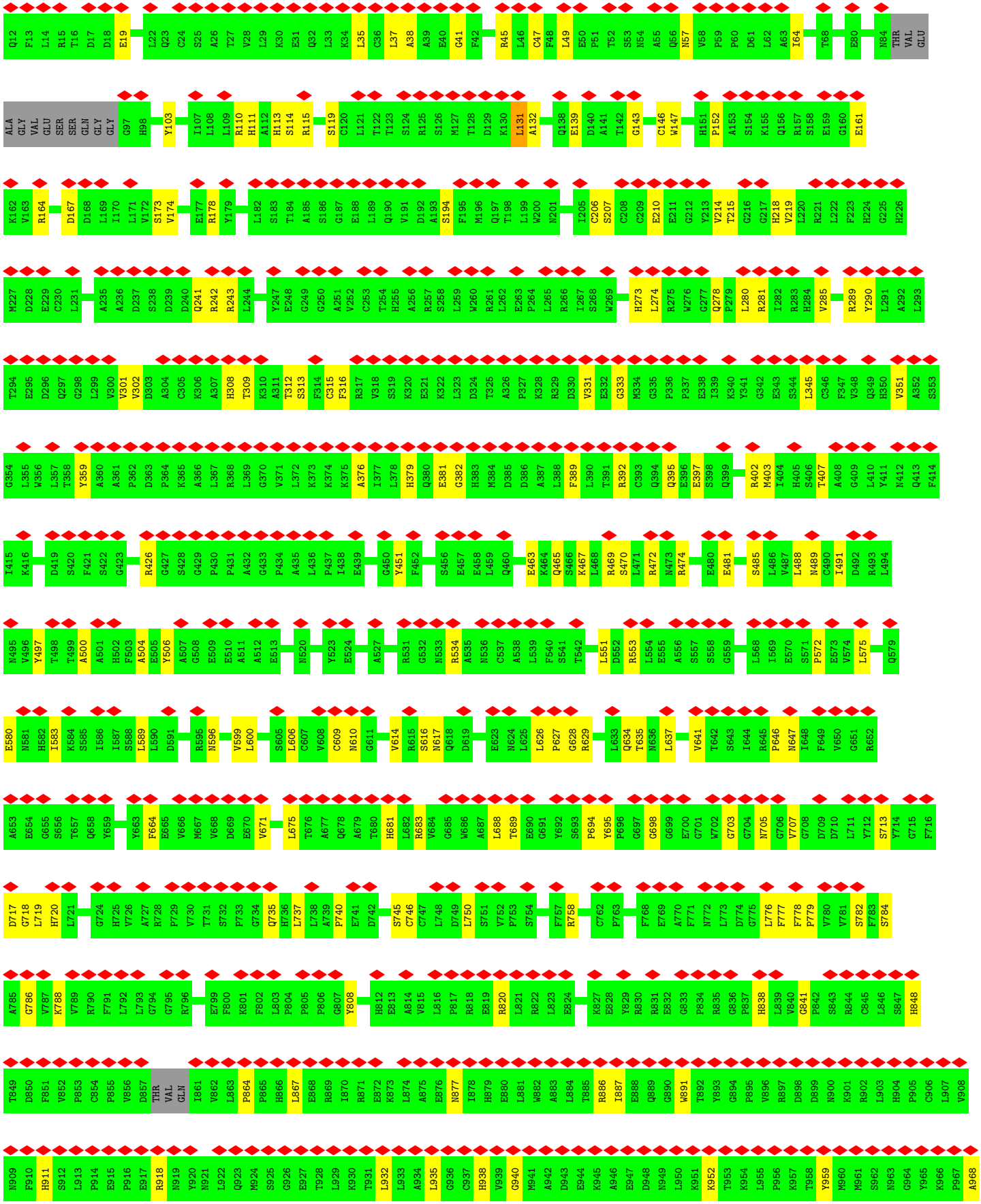
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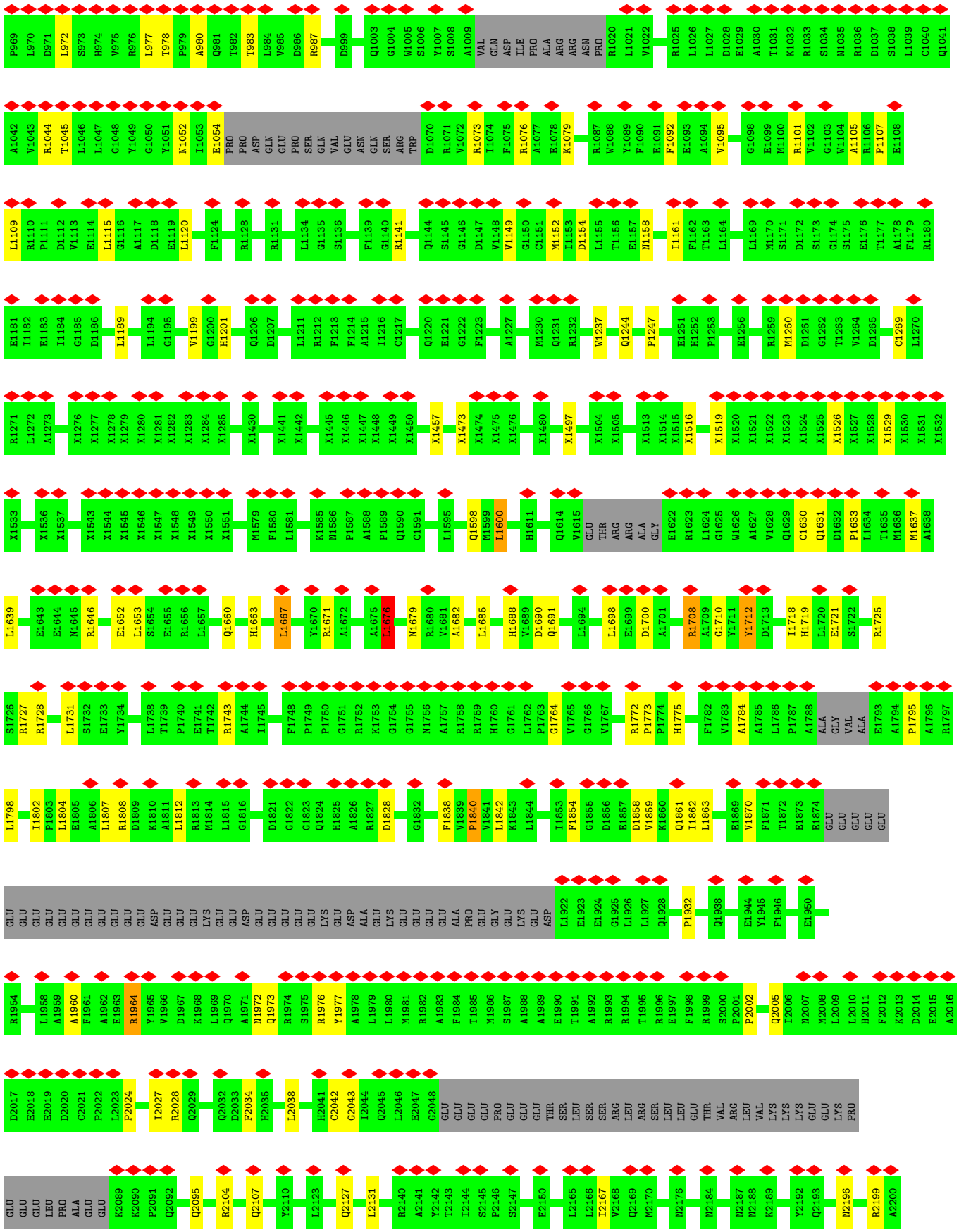
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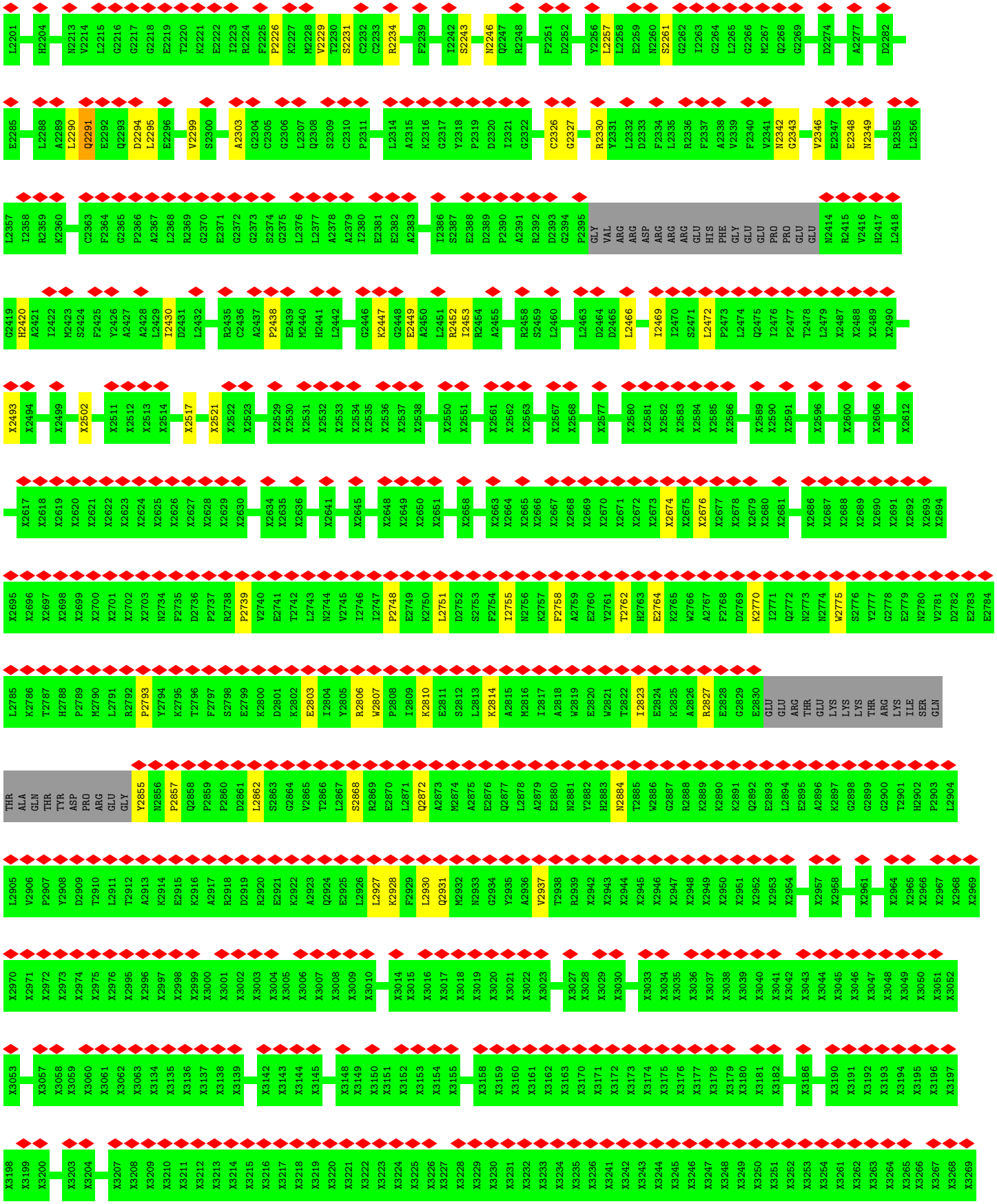
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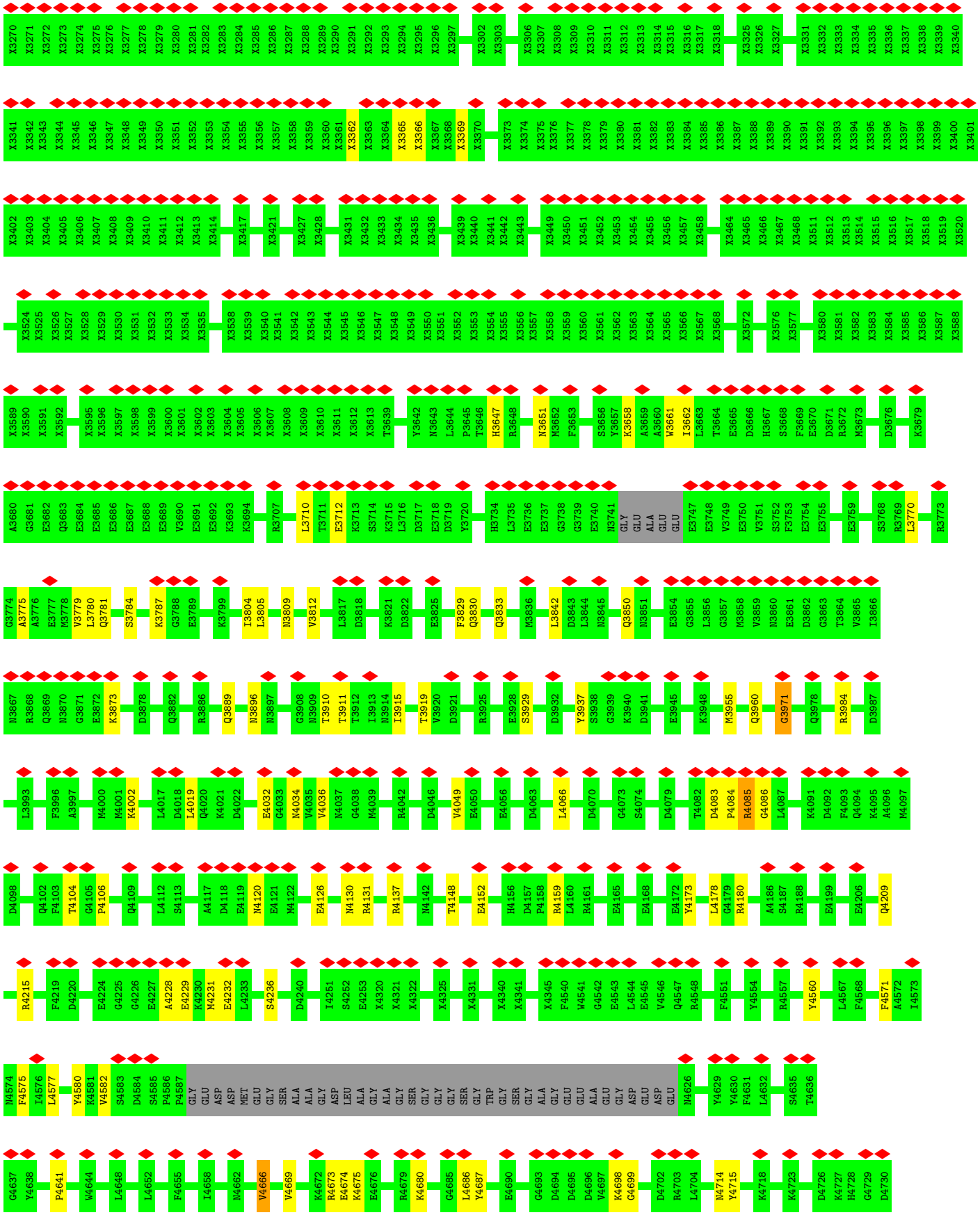
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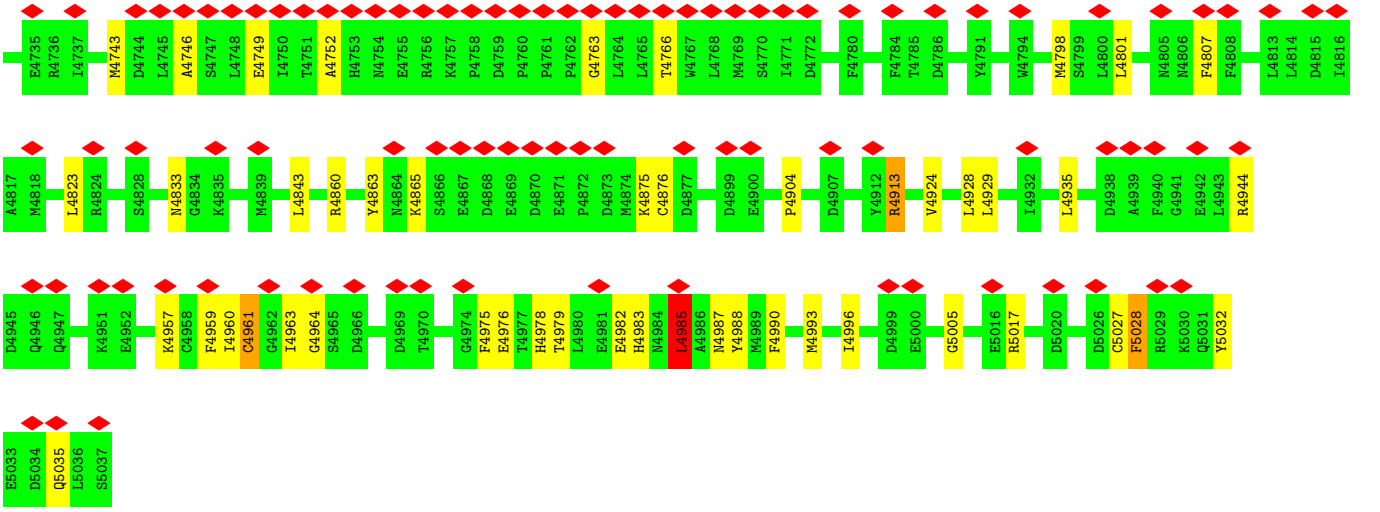


- Molecule 2: Ryanodine receptor 1

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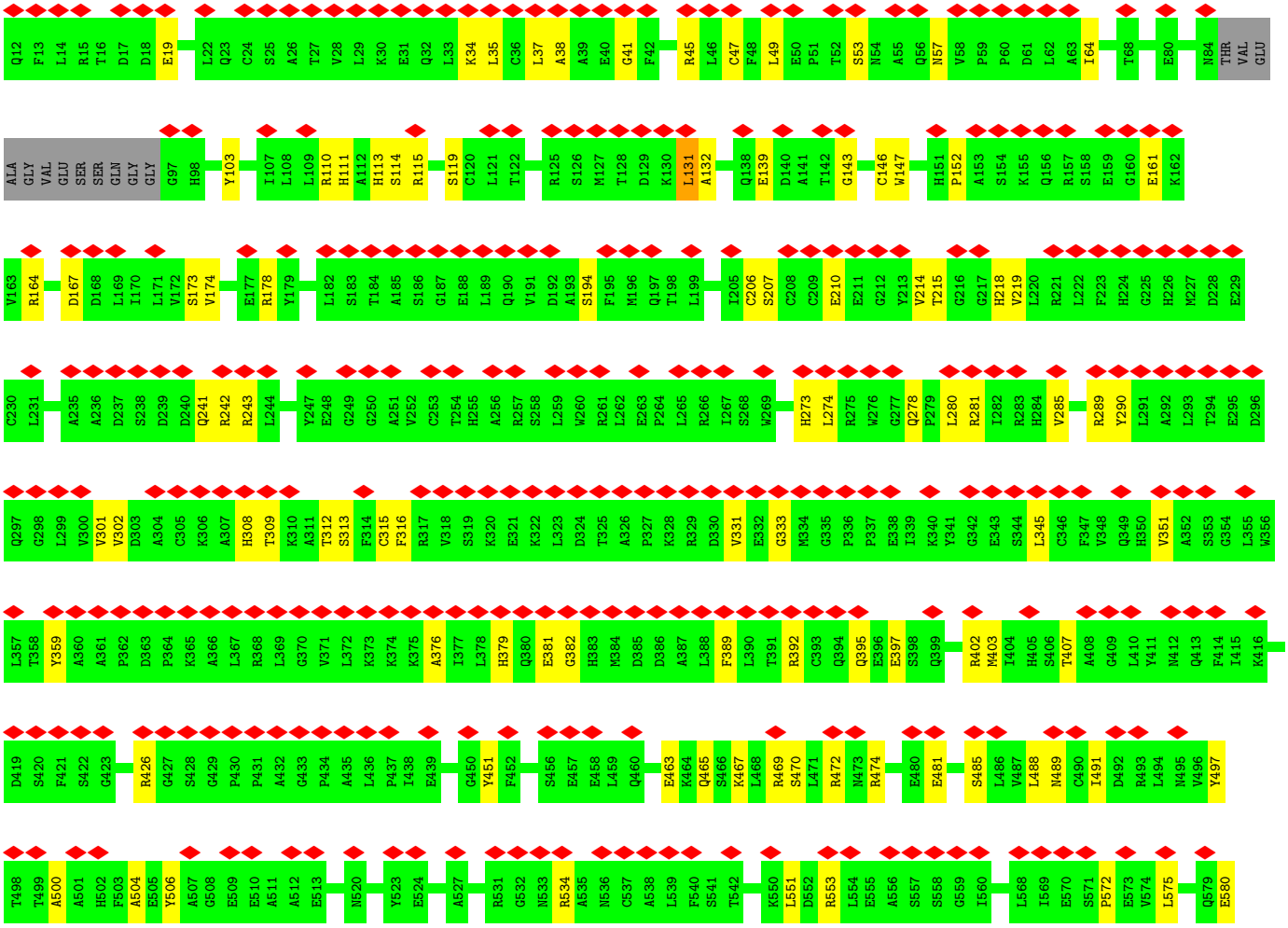

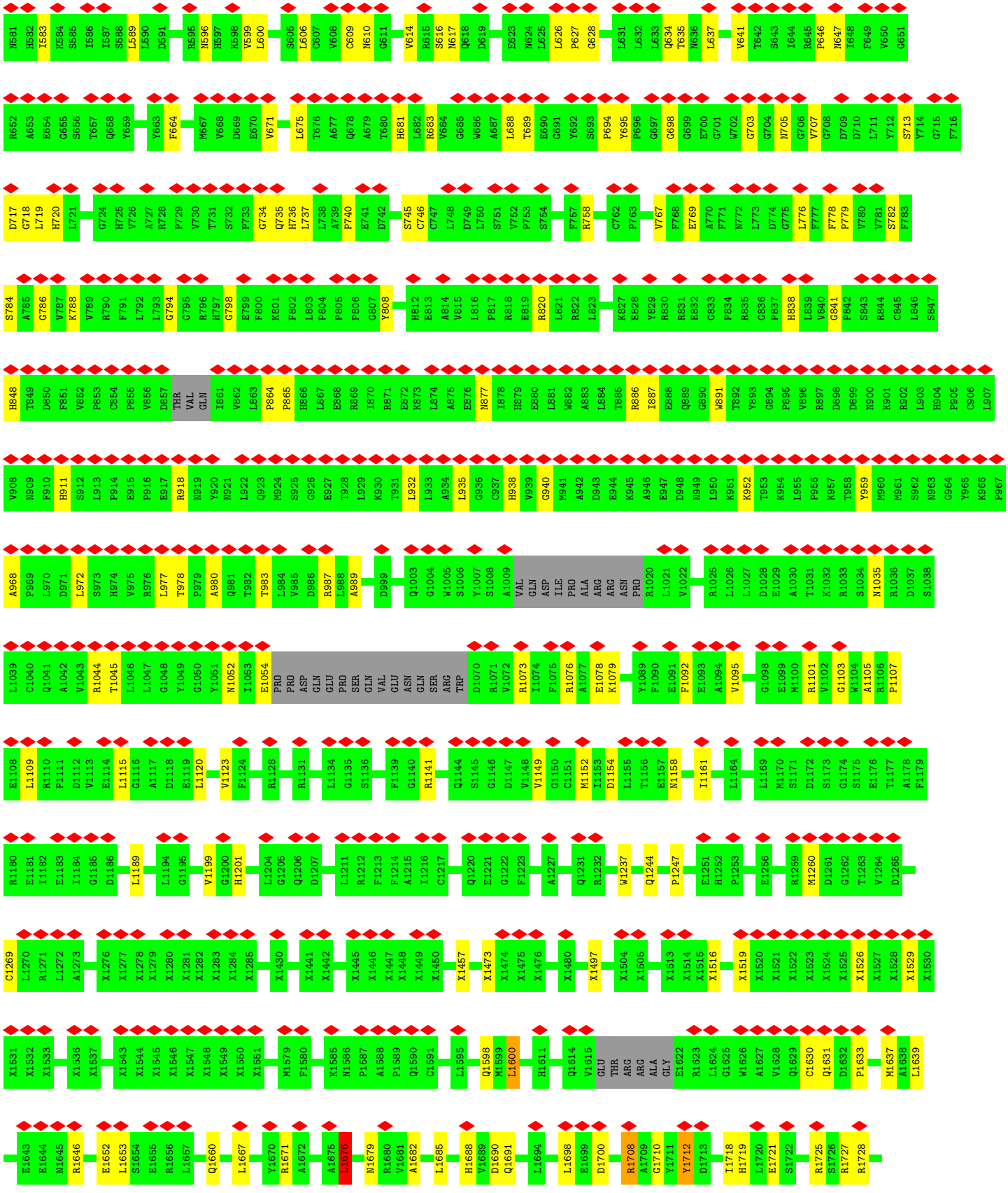
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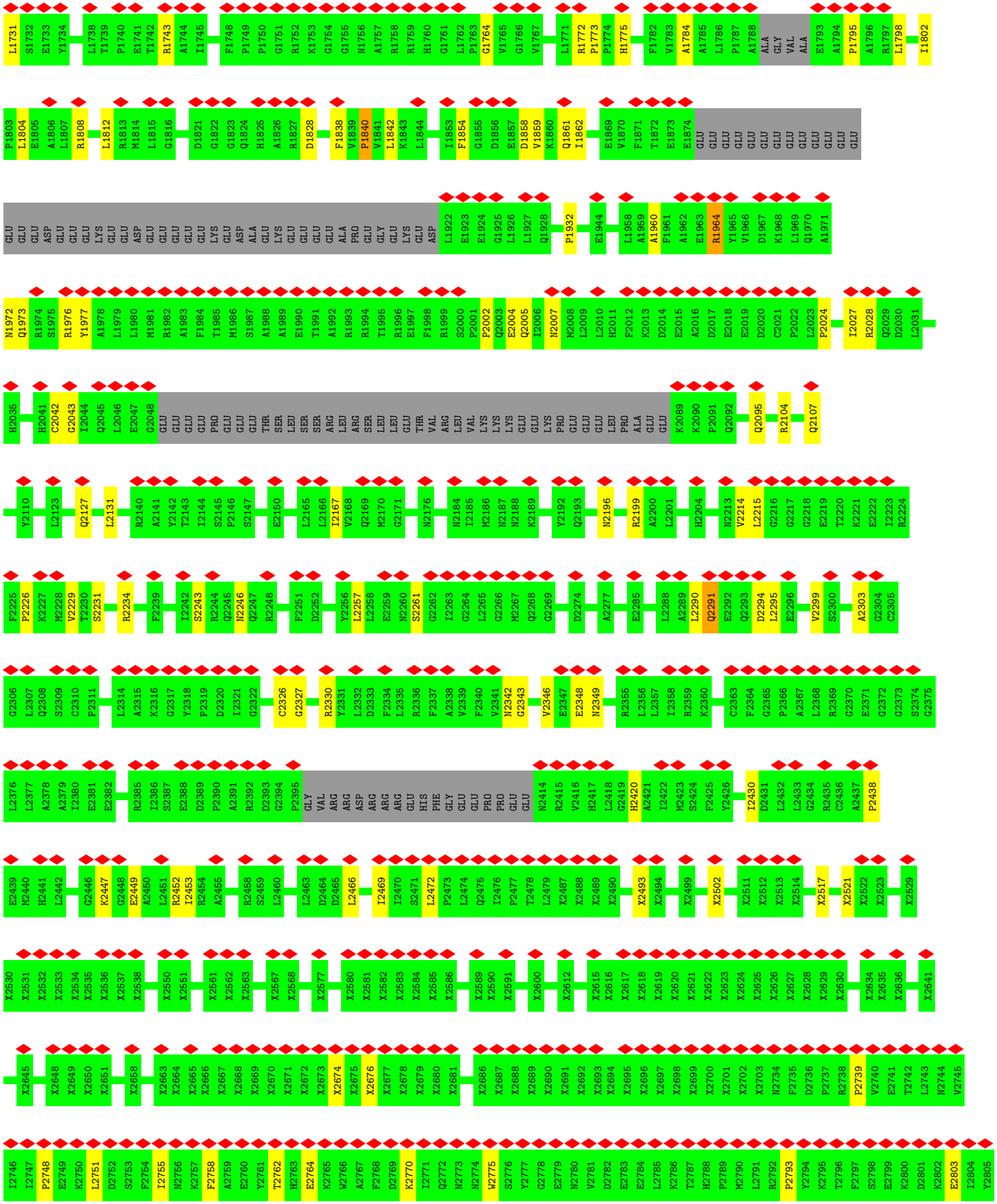
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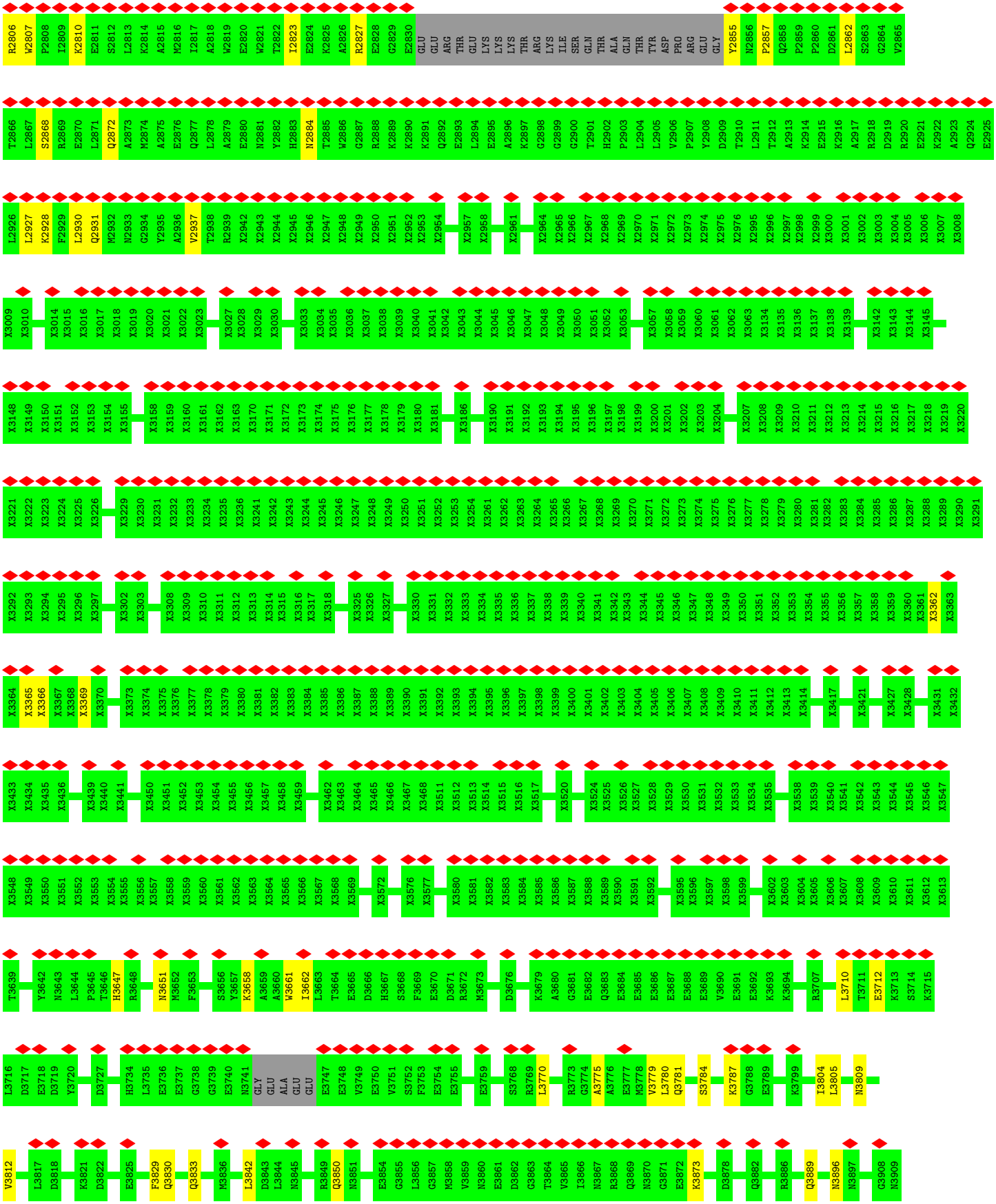
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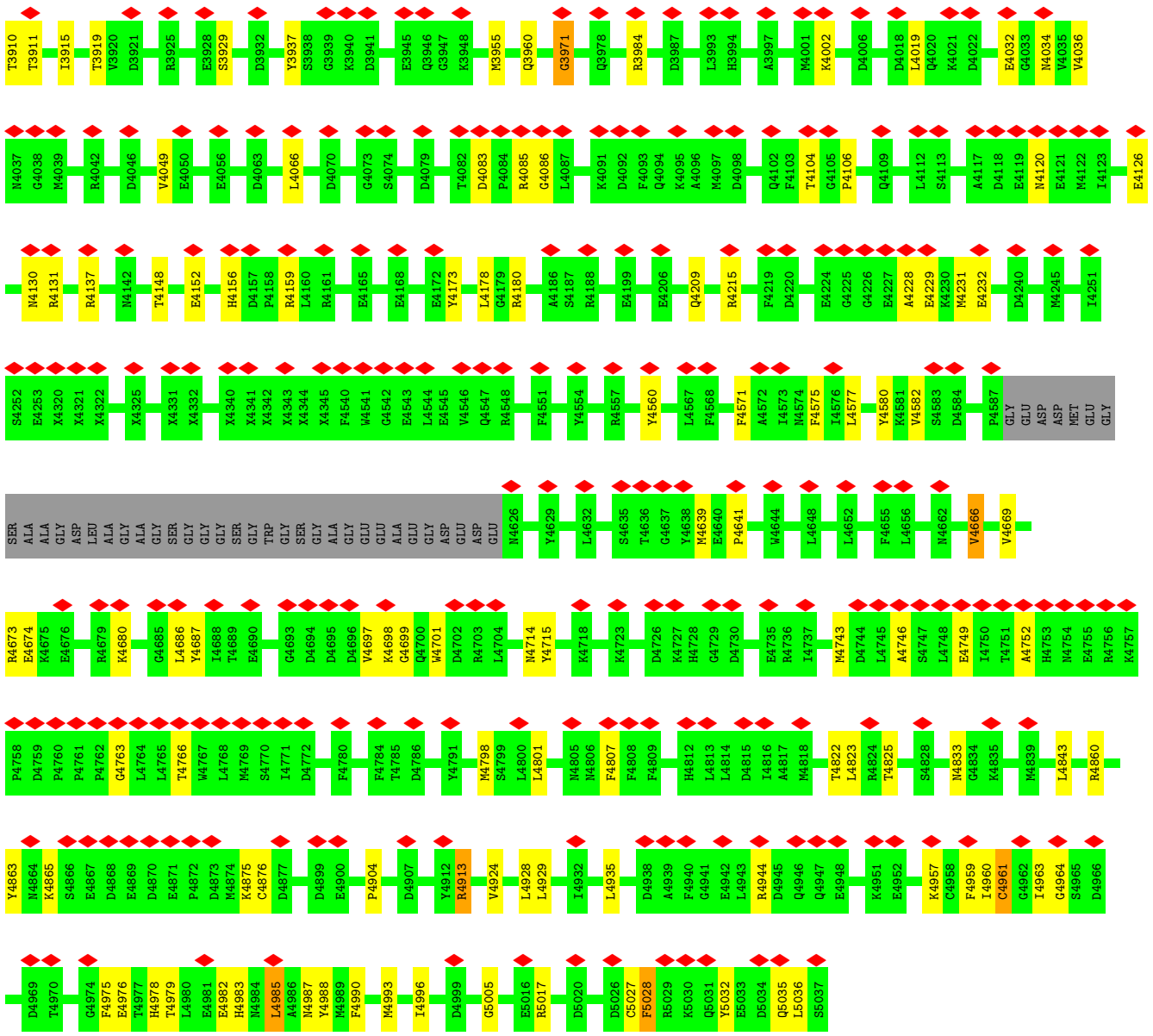
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S4252 E4253 X4320 X4321 X4322 X4325 X4331 X4332 X4340 X4341 X4342 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 V4546 Q4547 R4548 F4551 Y4554 R4557 Y4560 L4567 F4568 F4571 A4572 I4573 N4574 F4575 I4576 L4577 Y4580 K4581 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY
SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 Y4629 L4632 S4635 T4636 G4637 Y4638 M4639 E4640 P4641 W4644 L4648 L4652 F4655 L4656 N4662 V4666 V4669
R4673 E4674 K4675 E4676 R4679 K4680 G4685 L4686 Y4687 I4688 T4689 E4690 G4693 D4694 D4695 D4696 V4697 K4698 G4699 Q4700 W4701 D4702 R4703 L4704 N4714 Y4715 K4718 K4723 D4726 K4727 H4728 G4729 D4730 E4735 R4736 I4737 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 F4780 F4784 T4785 D4786 Y4791 M4798 S4799 L4800 L4801 N4805 M4806 F4807 F4808 F4809 H4812 L4813 L4814 D4815 I4816 A4817 M4818 T4822 L4823 R4824 T4825 S4828 N4833 G4834 K4835 M4839 L4843 R4860
Y4863 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876 D4877 D4899 E4900 P4904 D4907 Y4912 R4913 V4924 L4928 L4929 I4932 L4935 D4938 A4939 F4940 G4941 E4942 L4943 R4944 D4945 Q4946 Q4947 E4948 K4951 E4952 K4957 C4958 F4959 I4960 C4961 G4962 I4963 G4964 S4965 D4966
D4969 T4970 G4974 F4975 E4976 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 N4987 Y4988 M4989 F4990 M4993 I4996 D4999 G5005 E5016 R5017 D5020 D5026 C5027 F5028 R5029 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 | 0.065 | Depositor |
| Minimum map value | -0.034 | 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 (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, CFF, ATP

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | A | 0.31 | 0/834 | 0.52 | 0/1123 |
| 1 | F | 0.31 | 0/834 | 0.52 | 0/1123 |
| 1 | H | 0.31 | 0/834 | 0.52 | 0/1123 |
| 1 | J | 0.31 | 0/834 | 0.52 | 0/1123 |
| 2 | B | 0.31 | 0/25428 | 0.55 | 9/34534 (0.0%) |
| 2 | E | 0.31 | 0/25428 | 0.55 | 8/34534 (0.0%) |
| 2 | G | 0.31 | 0/25428 | 0.55 | 9/34534 (0.0%) |
| 2 | I | 0.31 | 0/25428 | 0.55 | 8/34534 (0.0%) |
| All | All | 0.31 | 0/105048 | 0.55 | 34/142628 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | F | 0 | 1 |
| 1 | H | 0 | 1 |
| 1 | J | 0 | 1 |
| 2 | B | 0 | 17 |
| 2 | E | 0 | 17 |
| 2 | G | 0 | 17 |
| 2 | I | 0 | 17 |
| All | All | 0 | 72 |

There are no bond length outliers.

All (34) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | E | 131 | LEU | CA-CB-CG | 8.16 | 134.07 | 115.30 |
| 2 | G | 131 | LEU | CA-CB-CG | 8.16 | 134.07 | 115.30 |
| 2 | B | 131 | LEU | CA-CB-CG | 8.15 | 134.04 | 115.30 |
| 2 | I | 131 | LEU | CA-CB-CG | 8.13 | 133.99 | 115.30 |
| 2 | E | 4985 | LEU | CA-CB-CG | 7.48 | 132.50 | 115.30 |
| 2 | G | 4985 | LEU | CA-CB-CG | 7.47 | 132.47 | 115.30 |
| 2 | B | 4985 | LEU | CA-CB-CG | 7.46 | 132.47 | 115.30 |
| 2 | I | 4985 | LEU | CA-CB-CG | 7.45 | 132.44 | 115.30 |
| 2 | I | 1600 | LEU | CA-CB-CG | 6.83 | 131.00 | 115.30 |
| 2 | G | 1600 | LEU | CA-CB-CG | 6.82 | 130.98 | 115.30 |
| 2 | B | 1600 | LEU | CA-CB-CG | 6.81 | 130.97 | 115.30 |
| 2 | E | 1600 | LEU | CA-CB-CG | 6.81 | 130.97 | 115.30 |
| 2 | B | 1676 | LEU | CA-CB-CG | 6.66 | 130.62 | 115.30 |
| 2 | G | 1676 | LEU | CA-CB-CG | 6.65 | 130.60 | 115.30 |
| 2 | E | 1676 | LEU | CA-CB-CG | 6.64 | 130.57 | 115.30 |
| 2 | I | 1676 | LEU | CA-CB-CG | 6.64 | 130.56 | 115.30 |
| 2 | G | 2290 | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 2 | B | 2290 | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 2 | E | 2290 | LEU | CA-CB-CG | 6.02 | 129.14 | 115.30 |
| 2 | I | 2290 | LEU | CA-CB-CG | 6.00 | 129.10 | 115.30 |
| 2 | G | 688 | LEU | CA-CB-CG | 5.72 | 128.46 | 115.30 |
| 2 | G | 977 | LEU | CA-CB-CG | 5.72 | 128.45 | 115.30 |
| 2 | E | 977 | LEU | CA-CB-CG | 5.71 | 128.44 | 115.30 |
| 2 | B | 688 | LEU | CA-CB-CG | 5.71 | 128.44 | 115.30 |
| 2 | E | 688 | LEU | CA-CB-CG | 5.71 | 128.44 | 115.30 |
| 2 | B | 977 | LEU | CA-CB-CG | 5.71 | 128.43 | 115.30 |
| 2 | I | 977 | LEU | CA-CB-CG | 5.71 | 128.43 | 115.30 |
| 2 | I | 688 | LEU | CA-CB-CG | 5.70 | 128.41 | 115.30 |
| 2 | I | 1667 | LEU | CA-CB-CG | 5.34 | 127.57 | 115.30 |
| 2 | G | 1667 | LEU | CA-CB-CG | 5.33 | 127.57 | 115.30 |
| 2 | B | 1667 | LEU | CA-CB-CG | 5.32 | 127.53 | 115.30 |
| 2 | E | 1667 | LEU | CA-CB-CG | 5.32 | 127.53 | 115.30 |
| 2 | G | 4639 | MET | C-N-CA | 5.00 | 134.21 | 121.70 |
| 2 | B | 4639 | MET | C-N-CA | 5.00 | 134.21 | 121.70 |

There are no chirality outliers.

All (72) 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 | 1690 | ASP | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | B | 1712 | TYR | Peptide |
| 2 | B | 1795 | PRO | Peptide |
| 2 | B | 1828 | ASP | Peptide |
| 2 | B | 1840 | PRO | Peptide |
| 2 | B | 2291 | GLN | Peptide |
| 2 | B | 2343 | GLY | Peptide |
| 2 | B | 2472 | LEU | Peptide |
| 2 | B | 2807 | TRP | Peptide |
| 2 | B | 312 | THR | Peptide |
| 2 | B | 3971 | GLY | 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 | 1690 | ASP | Peptide |
| 2 | E | 1712 | TYR | Peptide |
| 2 | E | 1795 | PRO | Peptide |
| 2 | E | 1828 | ASP | Peptide |
| 2 | E | 1840 | PRO | Peptide |
| 2 | E | 2291 | GLN | Peptide |
| 2 | E | 2343 | GLY | Peptide |
| 2 | E | 2472 | LEU | Peptide |
| 2 | E | 2807 | TRP | Peptide |
| 2 | E | 312 | THR | Peptide |
| 2 | E | 3971 | GLY | 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 | 1690 | ASP | Peptide |
| 2 | G | 1712 | TYR | Peptide |
| 2 | G | 1795 | PRO | Peptide |
| 2 | G | 1828 | ASP | Peptide |
| 2 | G | 1840 | PRO | Peptide |
| 2 | G | 2291 | GLN | Peptide |
| 2 | G | 2343 | GLY | Peptide |
| 2 | G | 2472 | LEU | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | G | 2807 | TRP | Peptide |
| 2 | G | 312 | THR | Peptide |
| 2 | G | 3971 | GLY | 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 | 1690 | ASP | Peptide |
| 2 | I | 1712 | TYR | Peptide |
| 2 | I | 1795 | PRO | Peptide |
| 2 | I | 1828 | ASP | Peptide |
| 2 | I | 1840 | PRO | Peptide |
| 2 | I | 2291 | GLN | Peptide |
| 2 | I | 2343 | GLY | Peptide |
| 2 | I | 2472 | LEU | Peptide |
| 2 | I | 2807 | TRP | Peptide |
| 2 | I | 312 | THR | Peptide |
| 2 | I | 3971 | GLY | 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 | 15 | 0 |
| 1 | F | 818 | 0 | 824 | 13 | 0 |
| 1 | H | 818 | 0 | 824 | 12 | 0 |
| 1 | J | 818 | 0 | 824 | 14 | 0 |
| 2 | B | 29499 | 0 | 24747 | 289 | 0 |
| 2 | E | 29499 | 0 | 24747 | 286 | 0 |
| 2 | G | 29499 | 0 | 24747 | 288 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | I | 29499 | 0 | 24748 | 285 | 0 |
| 3 | B | 31 | 0 | 12 | 2 | 0 |
| 3 | E | 31 | 0 | 12 | 2 | 0 |
| 3 | G | 31 | 0 | 12 | 2 | 0 |
| 3 | I | 31 | 0 | 12 | 2 | 0 |
| 4 | B | 14 | 0 | 10 | 1 | 0 |
| 4 | E | 14 | 0 | 10 | 1 | 0 |
| 4 | G | 14 | 0 | 10 | 1 | 0 |
| 4 | I | 14 | 0 | 10 | 1 | 0 |
| 5 | B | 1 | 0 | 0 | 0 | 0 |
| 5 | E | 1 | 0 | 0 | 0 | 0 |
| 5 | G | 1 | 0 | 0 | 0 | 0 |
| 5 | I | 1 | 0 | 0 | 0 | 0 |
| 6 | B | 1 | 0 | 0 | 0 | 0 |
| 6 | E | 1 | 0 | 0 | 0 | 0 |
| 6 | G | 1 | 0 | 0 | 0 | 0 |
| 6 | I | 1 | 0 | 0 | 0 | 0 |
| All | All | 121456 | 0 | 102373 | 1167 | 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 (1167) 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:4975:PHE:O | 2:B:4979:THR:HG23 | 1.85 | 0.77 |
| 2:I:4975:PHE:O | 2:I:4979:THR:HG23 | 1.85 | 0.76 |
| 2:E:4975:PHE:O | 2:E:4979:THR:HG23 | 1.86 | 0.76 |
| 2:G:4975:PHE:O | 2:G:4979:THR:HG23 | 1.86 | 0.76 |
| 2:I:5028:PHE:CE1 | 2:I:5032:TYR:CD2 | 2.78 | 0.71 |
| 2:G:5028:PHE:CE1 | 2:G:5032:TYR:CD2 | 2.78 | 0.71 |
| 2:B:5028:PHE:CE1 | 2:B:5032:TYR:CD2 | 2.78 | 0.71 |
| 2:E:5028:PHE:CE1 | 2:E:5032:TYR:CD2 | 2.78 | 0.70 |
| 2:E:2291:GLN:HB3 | 2:E:2294:ASP:H | 1.57 | 0.70 |
| 2:G:2291:GLN:HB3 | 2:G:2294:ASP:H | 1.57 | 0.70 |
| 2:I:2291:GLN:HB3 | 2:I:2294:ASP:H | 1.57 | 0.68 |
| 2:B:2291:GLN:HB3 | 2:B:2294:ASP:H | 1.57 | 0.67 |
| 2:G:788:LYS:HG2 | 2:G:1630:CYS:H | 1.60 | 0.67 |
| 2:I:788:LYS:HG2 | 2:I:1630:CYS:H | 1.60 | 0.66 |
| 2:E:788:LYS:HG2 | 2:E:1630:CYS:H | 1.60 | 0.66 |
| 2:I:745:SER:HB2 | 2:I:758:ARG:HB3 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:745:SER:HB2 | 2:G:758:ARG:HB3 | 1.78 | 0.66 |
| 2:B:745:SER:HB2 | 2:B:758:ARG:HB3 | 1.78 | 0.66 |
| 2:E:745:SER:HB2 | 2:E:758:ARG:HB3 | 1.78 | 0.66 |
| 2:G:173:SER:HB3 | 2:G:178:ARG:H | 1.61 | 0.65 |
| 2:B:173:SER:HB3 | 2:B:178:ARG:H | 1.61 | 0.65 |
| 2:I:173:SER:HB3 | 2:I:178:ARG:H | 1.61 | 0.65 |
| 2:B:788:LYS:HG2 | 2:B:1630:CYS:H | 1.60 | 0.65 |
| 2:B:4860:ARG:HD2 | 2:E:4582:VAL:HG11 | 1.78 | 0.65 |
| 2:B:641:VAL:HG21 | 2:B:705:ASN:HA | 1.79 | 0.65 |
| 2:E:641:VAL:HG21 | 2:E:705:ASN:HA | 1.79 | 0.65 |
| 2:I:5028:PHE:CE1 | 2:I:5032:TYR:CE2 | 2.86 | 0.64 |
| 2:G:379:HIS:HD2 | 2:G:382:GLY:H | 1.46 | 0.64 |
| 2:B:5028:PHE:CE1 | 2:B:5032:TYR:CE2 | 2.86 | 0.64 |
| 2:I:331:VAL:HG12 | 2:I:333:GLY:H | 1.62 | 0.64 |
| 2:I:379:HIS:HD2 | 2:I:382:GLY:H | 1.46 | 0.64 |
| 2:E:938:HIS:HB2 | 2:E:1054:GLU:HB2 | 1.79 | 0.64 |
| 2:E:379:HIS:HD2 | 2:E:382:GLY:H | 1.46 | 0.63 |
| 2:E:4674:GLU:HG3 | 2:E:4714:ASN:HB3 | 1.81 | 0.63 |
| 2:G:664:PHE:HB2 | 2:G:746:CYS:HB2 | 1.80 | 0.63 |
| 2:G:5028:PHE:CE1 | 2:G:5032:TYR:CE2 | 2.86 | 0.63 |
| 2:B:938:HIS:HB2 | 2:B:1054:GLU:HB2 | 1.79 | 0.63 |
| 2:E:173:SER:HB3 | 2:E:178:ARG:H | 1.61 | 0.63 |
| 2:I:2291:GLN:HB2 | 2:I:2295:LEU:HG | 1.80 | 0.63 |
| 2:I:4582:VAL:HG11 | 2:G:4860:ARG:HD2 | 1.79 | 0.63 |
| 2:B:2291:GLN:HB2 | 2:B:2295:LEU:HG | 1.80 | 0.63 |
| 2:B:4674:GLU:HG3 | 2:B:4714:ASN:HB3 | 1.81 | 0.63 |
| 2:E:5028:PHE:CE1 | 2:E:5032:TYR:CE2 | 2.86 | 0.63 |
| 2:I:938:HIS:HB2 | 2:I:1054:GLU:HB2 | 1.79 | 0.63 |
| 2:E:2291:GLN:HB2 | 2:E:2295:LEU:HG | 1.80 | 0.63 |
| 2:G:641:VAL:HG21 | 2:G:705:ASN:HA | 1.79 | 0.63 |
| 2:G:938:HIS:HB2 | 2:G:1054:GLU:HB2 | 1.79 | 0.63 |
| 2:G:4674:GLU:HG3 | 2:G:4714:ASN:HB3 | 1.81 | 0.63 |
| 2:G:331:VAL:HG12 | 2:G:333:GLY:H | 1.62 | 0.63 |
| 2:E:174:VAL:O | 2:G:2452:ARG:NH1 | 2.31 | 0.63 |
| 2:E:3937:TYR:O | 2:E:4002:LYS:NZ | 2.32 | 0.63 |
| 2:I:664:PHE:HB2 | 2:I:746:CYS:HB2 | 1.80 | 0.63 |
| 2:G:2291:GLN:HB2 | 2:G:2295:LEU:HG | 1.80 | 0.63 |
| 2:I:641:VAL:HG21 | 2:I:705:ASN:HA | 1.79 | 0.63 |
| 2:B:664:PHE:HB2 | 2:B:746:CYS:HB2 | 1.80 | 0.62 |
| 2:G:4957:LYS:HG2 | 2:G:4964:GLY:HA2 | 1.81 | 0.62 |
| 2:E:664:PHE:HB2 | 2:E:746:CYS:HB2 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:379:HIS:HD2 | 2:B:382:GLY:H | 1.46 | 0.62 |
| 2:E:4957:LYS:HG2 | 2:E:4964:GLY:HA2 | 1.81 | 0.62 |
| 2:E:331:VAL:HG12 | 2:E:333:GLY:H | 1.63 | 0.62 |
| 2:B:331:VAL:HG12 | 2:B:333:GLY:H | 1.62 | 0.62 |
| 2:B:4582:VAL:HG11 | 2:I:4860:ARG:HD2 | 1.80 | 0.62 |
| 2:I:111:HIS:HD2 | 2:I:114:SER:H | 1.48 | 0.62 |
| 2:B:3937:TYR:O | 2:B:4002:LYS:NZ | 2.32 | 0.62 |
| 2:I:3937:TYR:O | 2:I:4002:LYS:NZ | 2.32 | 0.62 |
| 2:I:4674:GLU:HG3 | 2:I:4714:ASN:HB3 | 1.81 | 0.62 |
| 2:G:111:HIS:HD2 | 2:G:114:SER:H | 1.48 | 0.62 |
| 2:I:4957:LYS:HG2 | 2:I:4964:GLY:HA2 | 1.81 | 0.62 |
| 2:G:3937:TYR:O | 2:G:4002:LYS:NZ | 2.32 | 0.62 |
| 2:B:111:HIS:HD2 | 2:B:114:SER:H | 1.48 | 0.61 |
| 2:B:4957:LYS:HG2 | 2:B:4964:GLY:HA2 | 1.81 | 0.61 |
| 2:E:281:ARG:NH2 | 2:E:309:THR:OG1 | 2.34 | 0.61 |
| 2:G:281:ARG:NH2 | 2:G:309:THR:OG1 | 2.34 | 0.61 |
| 2:E:472:ARG:NH2 | 2:E:3712:GLU:OE2 | 2.34 | 0.61 |
| 2:E:4985:LEU:HB2 | 3:E:5101:ATP:HN61 | 1.66 | 0.61 |
| 2:G:1700:ASP:OD2 | 2:G:1708:ARG:NH2 | 2.34 | 0.61 |
| 2:I:2755:ILE:HD13 | 2:I:2810:LYS:HG2 | 1.83 | 0.61 |
| 2:G:472:ARG:NH2 | 2:G:3712:GLU:OE2 | 2.34 | 0.60 |
| 2:B:2755:ILE:HD13 | 2:B:2810:LYS:HG2 | 1.83 | 0.60 |
| 2:E:111:HIS:HD2 | 2:E:114:SER:H | 1.48 | 0.60 |
| 2:B:4985:LEU:HB2 | 3:B:5101:ATP:HN61 | 1.66 | 0.60 |
| 2:B:281:ARG:NH2 | 2:B:309:THR:OG1 | 2.34 | 0.60 |
| 2:B:472:ARG:NH2 | 2:B:3712:GLU:OE2 | 2.34 | 0.60 |
| 2:E:1700:ASP:OD2 | 2:E:1708:ARG:NH2 | 2.34 | 0.60 |
| 2:I:4985:LEU:HB2 | 3:I:5101:ATP:HN61 | 1.66 | 0.60 |
| 2:G:4985:LEU:HB2 | 3:G:5101:ATP:HN61 | 1.66 | 0.60 |
| 2:B:1700:ASP:OD2 | 2:B:1708:ARG:NH2 | 2.34 | 0.60 |
| 2:I:472:ARG:NH2 | 2:I:3712:GLU:OE2 | 2.34 | 0.60 |
| 2:I:1700:ASP:OD2 | 2:I:1708:ARG:NH2 | 2.34 | 0.60 |
| 2:E:2755:ILE:HD13 | 2:E:2810:LYS:HG2 | 1.83 | 0.59 |
| 2:B:110:ARG:HH21 | 2:B:115:ARG:HB3 | 1.67 | 0.59 |
| 2:G:646:PRO:HD2 | 2:G:779:PRO:HB2 | 1.84 | 0.59 |
| 2:G:2755:ILE:HD13 | 2:G:2810:LYS:HG2 | 1.83 | 0.59 |
| 2:E:4049:VAL:HG21 | 2:E:4159:ARG:HD2 | 1.85 | 0.59 |
| 2:B:4049:VAL:HG21 | 2:B:4159:ARG:HD2 | 1.85 | 0.59 |
| 2:I:646:PRO:HD2 | 2:I:779:PRO:HB2 | 1.84 | 0.59 |
| 2:B:497:TYR:HB3 | 2:B:500:ALA:HB2 | 1.85 | 0.59 |
| 2:E:3955:MET:HG3 | 2:E:4019:LEU:HD22 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:4049:VAL:HG21 | 2:G:4159:ARG:HD2 | 1.85 | 0.59 |
| 2:I:497:TYR:HB3 | 2:I:500:ALA:HB2 | 1.85 | 0.59 |
| 2:I:4049:VAL:HG21 | 2:I:4159:ARG:HD2 | 1.85 | 0.59 |
| 2:G:671:VAL:HG22 | 2:G:740:PRO:HG3 | 1.85 | 0.58 |
| 2:B:3805:LEU:HA | 2:B:3809:ASN:HD22 | 1.68 | 0.58 |
| 2:E:646:PRO:HD2 | 2:E:779:PRO:HB2 | 1.84 | 0.58 |
| 2:I:281:ARG:NH2 | 2:I:309:THR:OG1 | 2.34 | 0.58 |
| 2:G:1637:MET:SD | 2:G:1708:ARG:NH1 | 2.77 | 0.58 |
| 1:F:42:ARG:HG2 | 2:E:1691:GLN:HG2 | 1.85 | 0.58 |
| 2:B:1637:MET:SD | 2:B:1708:ARG:NH1 | 2.77 | 0.58 |
| 2:E:110:ARG:HH21 | 2:E:115:ARG:HB3 | 1.67 | 0.58 |
| 2:E:1519:UNK:HA | 2:E:1526:UNK:HA | 1.86 | 0.58 |
| 2:E:3805:LEU:HA | 2:E:3809:ASN:HD22 | 1.68 | 0.58 |
| 2:B:646:PRO:HD2 | 2:B:779:PRO:HB2 | 1.84 | 0.58 |
| 2:B:1519:UNK:HA | 2:B:1526:UNK:HA | 1.86 | 0.58 |
| 2:I:1637:MET:SD | 2:I:1708:ARG:NH1 | 2.77 | 0.58 |
| 2:B:671:VAL:HG22 | 2:B:740:PRO:HG3 | 1.85 | 0.58 |
| 2:B:3955:MET:HG3 | 2:B:4019:LEU:HD22 | 1.84 | 0.58 |
| 2:I:110:ARG:HH21 | 2:I:115:ARG:HB3 | 1.67 | 0.58 |
| 2:G:110:ARG:HH21 | 2:G:115:ARG:HB3 | 1.67 | 0.58 |
| 2:G:2748:PRO:HD2 | 2:G:2751:LEU:HD12 | 1.86 | 0.58 |
| 2:E:671:VAL:HG22 | 2:E:740:PRO:HG3 | 1.85 | 0.58 |
| 2:E:5028:PHE:CE1 | 2:E:5032:TYR:HD2 | 2.21 | 0.58 |
| 2:G:3955:MET:HG3 | 2:G:4019:LEU:HD22 | 1.84 | 0.58 |
| 2:E:1637:MET:SD | 2:E:1708:ARG:NH1 | 2.77 | 0.58 |
| 2:I:1691:GLN:HE22 | 2:I:1802:ILE:HG12 | 1.69 | 0.58 |
| 2:I:2748:PRO:HD2 | 2:I:2751:LEU:HD12 | 1.86 | 0.58 |
| 2:B:1691:GLN:HE22 | 2:B:1802:ILE:HG12 | 1.69 | 0.58 |
| 2:B:2452:ARG:NH1 | 2:I:174:VAL:O | 2.37 | 0.58 |
| 2:B:5028:PHE:CE1 | 2:B:5032:TYR:HD2 | 2.21 | 0.58 |
| 2:I:609:CYS:SG | 2:I:610:ASN:N | 2.77 | 0.58 |
| 2:G:497:TYR:HB3 | 2:G:500:ALA:HB2 | 1.85 | 0.58 |
| 1:H:92:PRO:HD3 | 2:G:627:PRO:HB2 | 1.86 | 0.58 |
| 2:B:1079:LYS:NZ | 2:B:1107:PRO:O | 2.37 | 0.58 |
| 2:E:2748:PRO:HD2 | 2:E:2751:LEU:HD12 | 1.86 | 0.58 |
| 2:I:3955:MET:HG3 | 2:I:4019:LEU:HD22 | 1.84 | 0.58 |
| 2:E:1812:LEU:HD21 | 2:E:1861:GLN:HG2 | 1.85 | 0.58 |
| 2:I:5028:PHE:CE1 | 2:I:5032:TYR:HD2 | 2.21 | 0.58 |
| 2:G:5028:PHE:CE1 | 2:G:5032:TYR:HD2 | 2.21 | 0.58 |
| 2:E:609:CYS:SG | 2:E:610:ASN:N | 2.77 | 0.57 |
| 2:I:426:ARG:HB2 | 2:I:506:TYR:HA | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1079:LYS:NZ | 2:I:1107:PRO:O | 2.37 | 0.57 |
| 2:G:609:CYS:SG | 2:G:610:ASN:N | 2.77 | 0.57 |
| 2:G:3805:LEU:HA | 2:G:3809:ASN:HD22 | 1.68 | 0.57 |
| 2:E:952:LYS:HB3 | 2:E:968:ALA:HB1 | 1.86 | 0.57 |
| 2:B:174:VAL:O | 2:E:2452:ARG:NH1 | 2.37 | 0.57 |
| 2:B:609:CYS:SG | 2:B:610:ASN:N | 2.77 | 0.57 |
| 2:B:952:LYS:HB3 | 2:B:968:ALA:HB1 | 1.87 | 0.57 |
| 2:B:1812:LEU:HD21 | 2:B:1861:GLN:HG2 | 1.85 | 0.57 |
| 2:E:1079:LYS:NZ | 2:E:1107:PRO:O | 2.37 | 0.57 |
| 2:I:3805:LEU:HA | 2:I:3809:ASN:HD22 | 1.68 | 0.57 |
| 2:I:4232:GLU:OE2 | 2:I:5017:ARG:NH1 | 2.38 | 0.57 |
| 2:G:1691:GLN:HE22 | 2:G:1802:ILE:HG12 | 1.69 | 0.57 |
| 2:G:2751:LEU:HD11 | 2:G:2823:ILE:HG21 | 1.86 | 0.57 |
| 2:B:683:ARG:NH1 | 2:B:707:VAL:O | 2.37 | 0.57 |
| 2:B:2751:LEU:HD11 | 2:B:2823:ILE:HG21 | 1.86 | 0.57 |
| 2:E:497:TYR:HB3 | 2:E:500:ALA:HB2 | 1.85 | 0.57 |
| 2:G:1519:UNK:HA | 2:G:1526:UNK:HA | 1.86 | 0.57 |
| 2:E:426:ARG:HB2 | 2:E:506:TYR:HA | 1.86 | 0.57 |
| 2:G:1812:LEU:HD21 | 2:G:1861:GLN:HG2 | 1.85 | 0.57 |
| 2:I:1812:LEU:HD21 | 2:I:1861:GLN:HG2 | 1.85 | 0.57 |
| 2:I:2452:ARG:NH1 | 2:G:174:VAL:O | 2.36 | 0.57 |
| 2:B:2748:PRO:HD2 | 2:B:2751:LEU:HD12 | 1.86 | 0.57 |
| 2:E:1743:ARG:O | 2:E:1964:ARG:NH2 | 2.38 | 0.57 |
| 2:E:4860:ARG:HD2 | 2:G:4582:VAL:HG11 | 1.86 | 0.57 |
| 2:I:2751:LEU:HD11 | 2:I:2823:ILE:HG21 | 1.86 | 0.57 |
| 2:G:1079:LYS:NZ | 2:G:1107:PRO:O | 2.37 | 0.57 |
| 2:B:1743:ARG:O | 2:B:1964:ARG:NH2 | 2.38 | 0.57 |
| 2:I:1519:UNK:HA | 2:I:1526:UNK:HA | 1.86 | 0.57 |
| 2:B:426:ARG:HB2 | 2:B:506:TYR:HA | 1.86 | 0.57 |
| 2:E:2751:LEU:HD11 | 2:E:2823:ILE:HG21 | 1.86 | 0.57 |
| 2:I:671:VAL:HG22 | 2:I:740:PRO:HG3 | 1.85 | 0.57 |
| 2:B:4232:GLU:OE2 | 2:B:5017:ARG:NH1 | 2.38 | 0.57 |
| 2:G:426:ARG:HB2 | 2:G:506:TYR:HA | 1.86 | 0.57 |
| 2:G:1743:ARG:O | 2:G:1964:ARG:NH2 | 2.38 | 0.57 |
| 2:G:952:LYS:HB3 | 2:G:968:ALA:HB1 | 1.87 | 0.56 |
| 2:E:1691:GLN:HE22 | 2:E:1802:ILE:HG12 | 1.69 | 0.56 |
| 2:I:2420:HIS:ND1 | 2:I:2493:UNK:O | 2.38 | 0.56 |
| 2:G:2420:HIS:ND1 | 2:G:2493:UNK:O | 2.38 | 0.56 |
| 2:B:1721:GLU:OE2 | 2:B:1725:ARG:NH2 | 2.39 | 0.56 |
| 2:I:952:LYS:HB3 | 2:I:968:ALA:HB1 | 1.87 | 0.56 |
| 2:I:1743:ARG:O | 2:I:1964:ARG:NH2 | 2.38 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:4673:ARG:HH22 | 2:G:4698:LYS:HB2 | 1.71 | 0.56 |
| 2:E:2420:HIS:ND1 | 2:E:2493:UNK:O | 2.38 | 0.56 |
| 2:E:2770:LYS:HB3 | 2:E:2775:TRP:HB2 | 1.88 | 0.56 |
| 2:I:315:CYS:SG | 2:I:316:PHE:N | 2.79 | 0.56 |
| 1:F:55:VAL:HA | 2:E:1784:ALA:HA | 1.88 | 0.56 |
| 2:E:717:ASP:OD1 | 2:E:720:HIS:ND1 | 2.39 | 0.56 |
| 2:G:345:LEU:HD23 | 2:G:389:PHE:HB3 | 1.88 | 0.56 |
| 2:B:2770:LYS:HB3 | 2:B:2775:TRP:HB2 | 1.88 | 0.56 |
| 2:E:1721:GLU:OE2 | 2:E:1725:ARG:NH2 | 2.38 | 0.56 |
| 2:E:345:LEU:HD23 | 2:E:389:PHE:HB3 | 1.88 | 0.55 |
| 2:G:683:ARG:NH1 | 2:G:707:VAL:O | 2.37 | 0.55 |
| 2:G:1721:GLU:OE2 | 2:G:1725:ARG:NH2 | 2.39 | 0.55 |
| 2:B:111:HIS:CD2 | 2:B:114:SER:H | 2.25 | 0.55 |
| 2:B:4673:ARG:HH22 | 2:B:4698:LYS:HB2 | 1.71 | 0.55 |
| 2:E:683:ARG:NH1 | 2:E:707:VAL:O | 2.37 | 0.55 |
| 2:E:4232:GLU:OE2 | 2:E:5017:ARG:NH1 | 2.38 | 0.55 |
| 2:G:717:ASP:OD1 | 2:G:720:HIS:ND1 | 2.39 | 0.55 |
| 2:B:463:GLU:OE2 | 2:B:467:LYS:NZ | 2.40 | 0.55 |
| 2:E:4673:ARG:HH22 | 2:E:4698:LYS:HB2 | 1.71 | 0.55 |
| 2:I:111:HIS:CD2 | 2:I:114:SER:H | 2.25 | 0.55 |
| 2:I:4231:MET:HE1 | 2:I:4960:ILE:HA | 1.88 | 0.55 |
| 2:G:4232:GLU:OE2 | 2:G:5017:ARG:NH1 | 2.38 | 0.55 |
| 2:I:1685:LEU:HA | 2:I:1688:HIS:HD2 | 1.72 | 0.55 |
| 2:G:315:CYS:SG | 2:G:316:PHE:N | 2.79 | 0.55 |
| 2:G:1685:LEU:HA | 2:G:1688:HIS:HD2 | 1.72 | 0.55 |
| 2:G:4983:HIS:HB2 | 2:G:4988:TYR:HE2 | 1.72 | 0.55 |
| 2:I:4666:VAL:HG23 | 2:I:4669:VAL:HB | 1.89 | 0.55 |
| 2:G:4104:THR:HG22 | 2:G:4106:PRO:HD2 | 1.89 | 0.55 |
| 2:G:4666:VAL:HG23 | 2:G:4669:VAL:HB | 1.89 | 0.55 |
| 2:I:345:LEU:HD23 | 2:I:389:PHE:HB3 | 1.88 | 0.55 |
| 2:I:463:GLU:OE2 | 2:I:467:LYS:NZ | 2.40 | 0.55 |
| 2:I:683:ARG:NH1 | 2:I:707:VAL:O | 2.37 | 0.55 |
| 2:I:4104:THR:HG22 | 2:I:4106:PRO:HD2 | 1.89 | 0.55 |
| 2:G:111:HIS:CD2 | 2:G:114:SER:H | 2.25 | 0.55 |
| 2:G:2770:LYS:HB3 | 2:G:2775:TRP:HB2 | 1.88 | 0.55 |
| 2:B:2420:HIS:ND1 | 2:B:2493:UNK:O | 2.38 | 0.55 |
| 2:E:3889:GLN:OE1 | 2:E:3960:GLN:NE2 | 2.40 | 0.55 |
| 2:I:635:THR:HB | 2:I:1639:LEU:HD23 | 1.88 | 0.55 |
| 2:B:717:ASP:OD1 | 2:B:720:HIS:ND1 | 2.39 | 0.55 |
| 2:E:1671:ARG:NH2 | 2:E:1710:GLY:O | 2.40 | 0.55 |
| 2:E:2002:PRO:HA | 2:E:2005:GLN:HB3 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:4673:ARG:HH22 | 2:I:4698:LYS:HB2 | 1.71 | 0.55 |
| 2:B:635:THR:HB | 2:B:1639:LEU:HD23 | 1.88 | 0.55 |
| 2:B:2326:CYS:SG | 2:B:2327:GLY:N | 2.80 | 0.55 |
| 2:B:4104:THR:HG22 | 2:B:4106:PRO:HD2 | 1.89 | 0.55 |
| 2:I:675:LEU:HD11 | 2:I:1633:PRO:HB3 | 1.89 | 0.55 |
| 2:I:717:ASP:OD1 | 2:I:720:HIS:ND1 | 2.39 | 0.55 |
| 2:I:2770:LYS:HB3 | 2:I:2775:TRP:HB2 | 1.88 | 0.55 |
| 2:I:3889:GLN:OE1 | 2:I:3960:GLN:NE2 | 2.40 | 0.55 |
| 2:I:4983:HIS:HB2 | 2:I:4988:TYR:HE2 | 1.72 | 0.55 |
| 2:G:2326:CYS:SG | 2:G:2327:GLY:N | 2.80 | 0.55 |
| 2:B:345:LEU:HD23 | 2:B:389:PHE:HB3 | 1.88 | 0.54 |
| 2:B:972:LEU:O | 2:B:1044:ARG:NH2 | 2.40 | 0.54 |
| 2:E:4983:HIS:HB2 | 2:E:4988:TYR:HE2 | 1.72 | 0.54 |
| 2:I:1721:GLU:OE2 | 2:I:1725:ARG:NH2 | 2.39 | 0.54 |
| 2:I:2002:PRO:HA | 2:I:2005:GLN:HB3 | 1.89 | 0.54 |
| 2:G:635:THR:HB | 2:G:1639:LEU:HD23 | 1.88 | 0.54 |
| 2:G:675:LEU:HD11 | 2:G:1633:PRO:HB3 | 1.89 | 0.54 |
| 2:B:614:VAL:HG22 | 2:B:616:SER:H | 1.73 | 0.54 |
| 2:B:3889:GLN:OE1 | 2:B:3960:GLN:NE2 | 2.40 | 0.54 |
| 2:B:1685:LEU:HA | 2:B:1688:HIS:HD2 | 1.72 | 0.54 |
| 2:E:19:GLU:HB2 | 2:E:206:CYS:HB3 | 1.90 | 0.54 |
| 2:E:4228:ALA:O | 2:E:4232:GLU:N | 2.40 | 0.54 |
| 2:I:972:LEU:O | 2:I:1044:ARG:NH2 | 2.40 | 0.54 |
| 2:G:3889:GLN:OE1 | 2:G:3960:GLN:NE2 | 2.40 | 0.54 |
| 2:B:4209:GLN:HE22 | 2:B:4560:TYR:HE2 | 1.56 | 0.54 |
| 2:G:463:GLU:OE2 | 2:G:467:LYS:NZ | 2.40 | 0.54 |
| 2:B:315:CYS:SG | 2:B:316:PHE:N | 2.79 | 0.54 |
| 2:B:4983:HIS:HB2 | 2:B:4988:TYR:HE2 | 1.72 | 0.54 |
| 2:E:614:VAL:HG22 | 2:E:616:SER:H | 1.73 | 0.54 |
| 2:E:4104:THR:HG22 | 2:E:4106:PRO:HD2 | 1.89 | 0.54 |
| 2:I:19:GLU:HB2 | 2:I:206:CYS:HB3 | 1.90 | 0.54 |
| 2:I:1671:ARG:NH2 | 2:I:1710:GLY:O | 2.40 | 0.54 |
| 2:G:695:TYR:OH | 2:G:1073:ARG:NH1 | 2.40 | 0.54 |
| 2:G:1764:GLY:HA3 | 2:G:1859:VAL:HG11 | 1.90 | 0.54 |
| 2:B:1671:ARG:NH2 | 2:B:1710:GLY:O | 2.40 | 0.54 |
| 2:E:463:GLU:OE2 | 2:E:467:LYS:NZ | 2.40 | 0.54 |
| 2:E:2326:CYS:SG | 2:E:2327:GLY:N | 2.80 | 0.54 |
| 2:I:2326:CYS:SG | 2:I:2327:GLY:N | 2.80 | 0.54 |
| 2:B:580:GLU:HG2 | 2:B:583:ILE:HD11 | 1.89 | 0.54 |
| 2:E:395:GLN:HG3 | 2:E:397:GLU:H | 1.73 | 0.54 |
| 2:I:4924:VAL:HA | 2:I:4928:LEU:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:395:GLN:HG3 | 2:G:397:GLU:H | 1.73 | 0.54 |
| 2:B:4666:VAL:HG23 | 2:B:4669:VAL:HB | 1.89 | 0.54 |
| 2:E:1685:LEU:HA | 2:E:1688:HIS:HD2 | 1.72 | 0.54 |
| 2:G:19:GLU:HB2 | 2:G:206:CYS:HB3 | 1.90 | 0.54 |
| 2:G:689:THR:H | 2:G:778:PHE:HE2 | 1.55 | 0.54 |
| 2:G:4982:GLU:OE1 | 2:G:4982:GLU:HA | 2.08 | 0.54 |
| 2:B:689:THR:H | 2:B:778:PHE:HE2 | 1.55 | 0.54 |
| 2:E:1764:GLY:HA3 | 2:E:1859:VAL:HG11 | 1.90 | 0.54 |
| 2:G:1671:ARG:NH2 | 2:G:1710:GLY:O | 2.40 | 0.54 |
| 2:G:4209:GLN:HE22 | 2:G:4560:TYR:HE2 | 1.56 | 0.54 |
| 2:B:19:GLU:HB2 | 2:B:206:CYS:HB3 | 1.90 | 0.53 |
| 2:I:606:LEU:HG | 2:I:617:ASN:HD22 | 1.73 | 0.53 |
| 2:I:637:LEU:HD23 | 2:I:1637:MET:HB3 | 1.90 | 0.53 |
| 2:I:4674:GLU:HB3 | 2:I:4715:TYR:HB2 | 1.90 | 0.53 |
| 2:G:2002:PRO:HA | 2:G:2005:GLN:HB3 | 1.89 | 0.53 |
| 2:E:635:THR:HB | 2:E:1639:LEU:HD23 | 1.88 | 0.53 |
| 2:E:4152:GLU:OE2 | 2:E:4180:ARG:NH1 | 2.42 | 0.53 |
| 2:E:4666:VAL:HG23 | 2:E:4669:VAL:HB | 1.89 | 0.53 |
| 2:G:637:LEU:HD23 | 2:G:1637:MET:HB3 | 1.90 | 0.53 |
| 2:B:1764:GLY:HA3 | 2:B:1859:VAL:HG11 | 1.90 | 0.53 |
| 2:E:313:SER:HB3 | 2:E:351:VAL:HB | 1.91 | 0.53 |
| 2:E:580:GLU:HG2 | 2:E:583:ILE:HD11 | 1.89 | 0.53 |
| 2:E:972:LEU:O | 2:E:1044:ARG:NH2 | 2.41 | 0.53 |
| 2:G:606:LEU:HG | 2:G:617:ASN:HD22 | 1.73 | 0.53 |
| 2:G:4924:VAL:HA | 2:G:4928:LEU:HB2 | 1.90 | 0.53 |
| 2:B:675:LEU:HD11 | 2:B:1633:PRO:HB3 | 1.89 | 0.53 |
| 2:E:111:HIS:CD2 | 2:E:114:SER:H | 2.25 | 0.53 |
| 2:I:689:THR:H | 2:I:778:PHE:HE2 | 1.55 | 0.53 |
| 2:I:1152:MET:HB2 | 2:I:1161:ILE:HB | 1.91 | 0.53 |
| 2:I:4152:GLU:OE2 | 2:I:4180:ARG:NH1 | 2.42 | 0.53 |
| 2:B:4152:GLU:OE2 | 2:B:4180:ARG:NH1 | 2.42 | 0.53 |
| 2:G:972:LEU:O | 2:G:1044:ARG:NH2 | 2.40 | 0.53 |
| 2:B:1247:PRO:HA | 2:B:1598:GLN:HA | 1.91 | 0.53 |
| 2:E:675:LEU:HD11 | 2:E:1633:PRO:HB3 | 1.89 | 0.53 |
| 2:I:313:SER:HB3 | 2:I:351:VAL:HB | 1.91 | 0.53 |
| 2:I:614:VAL:HG22 | 2:I:616:SER:H | 1.73 | 0.53 |
| 2:B:4674:GLU:HB3 | 2:B:4715:TYR:HB2 | 1.90 | 0.53 |
| 2:B:4982:GLU:OE1 | 2:B:4982:GLU:HA | 2.08 | 0.53 |
| 2:E:4982:GLU:OE1 | 2:E:4982:GLU:HA | 2.08 | 0.53 |
| 2:I:1764:GLY:HA3 | 2:I:1859:VAL:HG11 | 1.90 | 0.53 |
| 1:J:7:ILE:HB | 1:J:71:ARG:HB3 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:315:CYS:SG | 2:E:316:PHE:N | 2.79 | 0.53 |
| 2:I:395:GLN:HG3 | 2:I:397:GLU:H | 1.73 | 0.53 |
| 2:I:695:TYR:OH | 2:I:1073:ARG:NH1 | 2.40 | 0.53 |
| 2:I:4209:GLN:HE22 | 2:I:4560:TYR:HE2 | 1.56 | 0.53 |
| 2:G:4152:GLU:OE2 | 2:G:4180:ARG:NH1 | 2.42 | 0.53 |
| 1:A:7:ILE:HB | 1:A:71:ARG:HB3 | 1.91 | 0.53 |
| 2:B:4924:VAL:HA | 2:B:4928:LEU:HB2 | 1.90 | 0.53 |
| 2:B:4960:ILE:HD11 | 2:B:4985:LEU:HD23 | 1.91 | 0.53 |
| 2:B:4961:CYS:HB3 | 2:B:4983:HIS:CE1 | 2.44 | 0.53 |
| 2:E:1092:PHE:HB3 | 2:E:1149:VAL:HB | 1.90 | 0.53 |
| 2:E:1247:PRO:HA | 2:E:1598:GLN:HA | 1.91 | 0.53 |
| 2:E:4961:CYS:HB3 | 2:E:4983:HIS:CE1 | 2.44 | 0.53 |
| 2:G:580:GLU:HG2 | 2:G:583:ILE:HD11 | 1.89 | 0.53 |
| 2:G:1092:PHE:HB3 | 2:G:1149:VAL:HB | 1.90 | 0.53 |
| 2:G:3781:GLN:HA | 2:G:3784:SER:HB3 | 1.91 | 0.53 |
| 1:F:92:PRO:HD3 | 2:E:627:PRO:HB2 | 1.90 | 0.53 |
| 2:B:313:SER:HB3 | 2:B:351:VAL:HB | 1.91 | 0.53 |
| 2:B:395:GLN:HG3 | 2:B:397:GLU:H | 1.73 | 0.53 |
| 2:B:606:LEU:HG | 2:B:617:ASN:HD22 | 1.73 | 0.53 |
| 2:E:4231:MET:HE1 | 2:E:4960:ILE:HA | 1.91 | 0.53 |
| 2:I:4960:ILE:HD11 | 2:I:4985:LEU:HD23 | 1.91 | 0.53 |
| 2:I:4961:CYS:HB3 | 2:I:4983:HIS:CE1 | 2.44 | 0.53 |
| 2:E:4924:VAL:HA | 2:E:4928:LEU:HB2 | 1.90 | 0.52 |
| 2:I:911:HIS:O | 2:I:918:ARG:NH2 | 2.42 | 0.52 |
| 2:G:313:SER:HB3 | 2:G:351:VAL:HB | 1.91 | 0.52 |
| 2:G:1152:MET:HB2 | 2:G:1161:ILE:HB | 1.91 | 0.52 |
| 2:G:4961:CYS:HB3 | 2:G:4983:HIS:CE1 | 2.44 | 0.52 |
| 1:F:7:ILE:HB | 1:F:71:ARG:HB3 | 1.91 | 0.52 |
| 2:B:911:HIS:O | 2:B:918:ARG:NH2 | 2.42 | 0.52 |
| 2:E:3781:GLN:HA | 2:E:3784:SER:HB3 | 1.91 | 0.52 |
| 2:I:580:GLU:HG2 | 2:I:583:ILE:HD11 | 1.89 | 0.52 |
| 2:I:4743:MET:HB3 | 2:I:4746:ALA:HB3 | 1.92 | 0.52 |
| 2:I:4860:ARG:HG3 | 2:I:4876:CYS:HB3 | 1.91 | 0.52 |
| 2:G:4978:HIS:HA | 2:G:4982:GLU:HB2 | 1.91 | 0.52 |
| 2:B:683:ARG:HB2 | 2:B:782:SER:HB3 | 1.92 | 0.52 |
| 2:B:1152:MET:HB2 | 2:B:1161:ILE:HB | 1.91 | 0.52 |
| 2:B:2002:PRO:HA | 2:B:2005:GLN:HB3 | 1.89 | 0.52 |
| 2:I:1092:PHE:HB3 | 2:I:1149:VAL:HB | 1.90 | 0.52 |
| 2:G:1247:PRO:HA | 2:G:1598:GLN:HA | 1.91 | 0.52 |
| 2:B:132:ALA:HA | 2:B:194:SER:HB2 | 1.91 | 0.52 |
| 2:I:143:GLY:HA3 | 2:I:147:TRP:HE1 | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:683:ARG:HB2 | 2:I:782:SER:HB3 | 1.92 | 0.52 |
| 2:G:143:GLY:HA3 | 2:G:147:TRP:HE1 | 1.75 | 0.52 |
| 1:A:34:LYS:HD3 | 2:B:629:ARG:HD2 | 1.92 | 0.52 |
| 2:B:637:LEU:HD23 | 2:B:1637:MET:HB3 | 1.90 | 0.52 |
| 2:B:4860:ARG:HG3 | 2:B:4876:CYS:HB3 | 1.92 | 0.52 |
| 2:I:4982:GLU:OE1 | 2:I:4982:GLU:HA | 2.08 | 0.52 |
| 2:E:143:GLY:HA3 | 2:E:147:TRP:HE1 | 1.75 | 0.52 |
| 2:E:1152:MET:HB2 | 2:E:1161:ILE:HB | 1.91 | 0.52 |
| 2:I:488:LEU:HD23 | 2:I:491:ILE:HD12 | 1.92 | 0.52 |
| 2:I:3781:GLN:HA | 2:I:3784:SER:HB3 | 1.91 | 0.52 |
| 2:E:606:LEU:HG | 2:E:617:ASN:HD22 | 1.73 | 0.52 |
| 2:E:637:LEU:HD23 | 2:E:1637:MET:HB3 | 1.90 | 0.52 |
| 2:E:4674:GLU:HB3 | 2:E:4715:TYR:HB2 | 1.90 | 0.52 |
| 2:G:614:VAL:HG22 | 2:G:616:SER:H | 1.73 | 0.52 |
| 2:G:683:ARG:HB2 | 2:G:782:SER:HB3 | 1.92 | 0.52 |
| 2:G:1698:LEU:N | 2:G:1712:TYR:OH | 2.43 | 0.52 |
| 2:G:4674:GLU:HB3 | 2:G:4715:TYR:HB2 | 1.90 | 0.52 |
| 2:G:4960:ILE:HD11 | 2:G:4985:LEU:HD23 | 1.91 | 0.52 |
| 2:B:1092:PHE:HB3 | 2:B:1149:VAL:HB | 1.90 | 0.52 |
| 2:E:465:GLN:HG3 | 2:E:3710:LEU:HB3 | 1.92 | 0.52 |
| 2:E:4743:MET:HB3 | 2:E:4746:ALA:HB3 | 1.91 | 0.52 |
| 2:E:4960:ILE:HD11 | 2:E:4985:LEU:HD23 | 1.91 | 0.52 |
| 2:G:465:GLN:HG3 | 2:G:3710:LEU:HB3 | 1.92 | 0.52 |
| 2:E:132:ALA:HA | 2:E:194:SER:HB2 | 1.91 | 0.52 |
| 2:G:4860:ARG:HG3 | 2:G:4876:CYS:HB3 | 1.91 | 0.52 |
| 1:H:55:VAL:HA | 2:G:1784:ALA:HA | 1.92 | 0.51 |
| 2:B:4749:GLU:HA | 2:B:4752:ALA:HB3 | 1.93 | 0.51 |
| 2:B:4978:HIS:HA | 2:B:4982:GLU:HB2 | 1.91 | 0.51 |
| 2:E:683:ARG:HB2 | 2:E:782:SER:HB3 | 1.92 | 0.51 |
| 2:E:689:THR:H | 2:E:778:PHE:HE2 | 1.55 | 0.51 |
| 2:E:4209:GLN:HE22 | 2:E:4560:TYR:HE2 | 1.56 | 0.51 |
| 2:E:4798:MET:HA | 2:E:4801:LEU:HB2 | 1.91 | 0.51 |
| 2:E:4865:LYS:HG3 | 2:E:4875:LYS:HZ3 | 1.76 | 0.51 |
| 2:E:4978:HIS:HA | 2:E:4982:GLU:HB2 | 1.91 | 0.51 |
| 2:I:707:VAL:HG23 | 2:I:713:SER:HB2 | 1.92 | 0.51 |
| 2:G:707:VAL:HG23 | 2:G:713:SER:HB2 | 1.92 | 0.51 |
| 2:B:143:GLY:HA3 | 2:B:147:TRP:HE1 | 1.75 | 0.51 |
| 2:B:707:VAL:HG23 | 2:B:713:SER:HB2 | 1.92 | 0.51 |
| 2:E:470:SER:O | 2:E:474:ARG:NE | 2.40 | 0.51 |
| 2:E:695:TYR:OH | 2:E:1073:ARG:NH1 | 2.40 | 0.51 |
| 2:I:465:GLN:HG3 | 2:I:3710:LEU:HB3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1247:PRO:HA | 2:I:1598:GLN:HA | 1.91 | 0.51 |
| 2:I:1516:UNK:N | 2:I:1529:UNK:O | 2.43 | 0.51 |
| 2:G:309:THR:O | 2:G:313:SER:OG | 2.28 | 0.51 |
| 2:G:4743:MET:HB3 | 2:G:4746:ALA:HB3 | 1.91 | 0.51 |
| 2:G:4798:MET:HA | 2:G:4801:LEU:HB2 | 1.91 | 0.51 |
| 2:B:465:GLN:HG3 | 2:B:3710:LEU:HB3 | 1.92 | 0.51 |
| 2:B:695:TYR:OH | 2:B:1073:ARG:NH1 | 2.40 | 0.51 |
| 2:E:309:THR:O | 2:E:313:SER:OG | 2.28 | 0.51 |
| 2:E:488:LEU:HD23 | 2:E:491:ILE:HD12 | 1.92 | 0.51 |
| 2:I:164:ARG:N | 2:I:167:ASP:OD2 | 2.44 | 0.51 |
| 2:I:1698:LEU:N | 2:I:1712:TYR:OH | 2.43 | 0.51 |
| 2:G:911:HIS:O | 2:G:918:ARG:NH2 | 2.42 | 0.51 |
| 2:G:4749:GLU:HA | 2:G:4752:ALA:HB3 | 1.93 | 0.51 |
| 2:G:5028:PHE:HE1 | 2:G:5032:TYR:CE2 | 2.29 | 0.51 |
| 2:B:3781:GLN:HA | 2:B:3784:SER:HB3 | 1.91 | 0.51 |
| 2:B:4798:MET:HA | 2:B:4801:LEU:HB2 | 1.91 | 0.51 |
| 2:B:4865:LYS:HG3 | 2:B:4875:LYS:HZ3 | 1.76 | 0.51 |
| 2:E:4749:GLU:HA | 2:E:4752:ALA:HB3 | 1.93 | 0.51 |
| 2:G:132:ALA:HA | 2:G:194:SER:HB2 | 1.91 | 0.51 |
| 1:A:42:ARG:HG2 | 2:B:1691:GLN:HG2 | 1.92 | 0.51 |
| 2:B:1698:LEU:N | 2:B:1712:TYR:OH | 2.43 | 0.51 |
| 2:E:485:SER:O | 2:E:489:ASN:N | 2.37 | 0.51 |
| 2:E:1698:LEU:N | 2:E:1712:TYR:OH | 2.43 | 0.51 |
| 2:I:4749:GLU:HA | 2:I:4752:ALA:HB3 | 1.92 | 0.51 |
| 2:I:4798:MET:HA | 2:I:4801:LEU:HB2 | 1.91 | 0.51 |
| 2:I:4978:HIS:HA | 2:I:4982:GLU:HB2 | 1.91 | 0.51 |
| 2:B:309:THR:O | 2:B:313:SER:OG | 2.29 | 0.51 |
| 2:B:488:LEU:HD23 | 2:B:491:ILE:HD12 | 1.92 | 0.51 |
| 2:B:5028:PHE:HE1 | 2:B:5032:TYR:CE2 | 2.29 | 0.51 |
| 2:E:707:VAL:HG23 | 2:E:713:SER:HB2 | 1.92 | 0.51 |
| 2:E:1516:UNK:N | 2:E:1529:UNK:O | 2.43 | 0.51 |
| 2:G:1516:UNK:N | 2:G:1529:UNK:O | 2.43 | 0.51 |
| 1:H:7:ILE:HB | 1:H:71:ARG:HB3 | 1.91 | 0.51 |
| 2:E:718:GLY:HA3 | 2:E:737:LEU:HA | 1.93 | 0.51 |
| 2:E:1095:VAL:HB | 2:E:1199:VAL:HG23 | 1.93 | 0.51 |
| 2:I:4865:LYS:HG3 | 2:I:4875:LYS:HZ3 | 1.76 | 0.51 |
| 2:G:1095:VAL:HB | 2:G:1199:VAL:HG23 | 1.93 | 0.51 |
| 1:H:42:ARG:HG2 | 2:G:1691:GLN:HG2 | 1.92 | 0.51 |
| 2:E:2196:ASN:OD1 | 2:E:2199:ARG:NH1 | 2.40 | 0.51 |
| 2:G:4231:MET:HE1 | 2:G:4960:ILE:HA | 1.93 | 0.51 |
| 2:E:4860:ARG:HG3 | 2:E:4876:CYS:HB3 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:718:GLY:HA3 | 2:G:737:LEU:HA | 1.93 | 0.51 |
| 2:B:4743:MET:HB3 | 2:B:4746:ALA:HB3 | 1.92 | 0.51 |
| 2:I:132:ALA:HA | 2:I:194:SER:HB2 | 1.91 | 0.51 |
| 2:B:1516:UNK:N | 2:B:1529:UNK:O | 2.43 | 0.50 |
| 2:B:4231:MET:HE1 | 2:B:4960:ILE:HA | 1.92 | 0.50 |
| 2:G:2868:SER:O | 2:G:2872:GLN:N | 2.45 | 0.50 |
| 2:B:1095:VAL:HB | 2:B:1199:VAL:HG23 | 1.93 | 0.50 |
| 2:G:1679:ASN:ND2 | 2:G:1798:LEU:O | 2.45 | 0.50 |
| 1:A:21:THR:HA | 1:A:49:ARG:HA | 1.94 | 0.50 |
| 1:A:82:TYR:O | 1:A:86:GLY:N | 2.45 | 0.50 |
| 2:B:164:ARG:N | 2:B:167:ASP:OD2 | 2.44 | 0.50 |
| 2:I:1095:VAL:HB | 2:I:1199:VAL:HG23 | 1.93 | 0.50 |
| 1:F:21:THR:HA | 1:F:49:ARG:HA | 1.94 | 0.50 |
| 1:J:34:LYS:HD3 | 2:I:629:ARG:HD2 | 1.93 | 0.50 |
| 2:E:241:GLN:O | 2:E:289:ARG:NH1 | 2.38 | 0.50 |
| 2:E:359:TYR:HA | 2:E:376:ALA:HA | 1.94 | 0.50 |
| 2:E:2868:SER:O | 2:E:2872:GLN:N | 2.45 | 0.50 |
| 2:I:242:ARG:NH1 | 2:I:481:GLU:OE1 | 2.45 | 0.50 |
| 2:I:470:SER:O | 2:I:474:ARG:NE | 2.40 | 0.50 |
| 2:G:359:TYR:HA | 2:G:376:ALA:HA | 1.93 | 0.50 |
| 2:G:488:LEU:HD23 | 2:G:491:ILE:HD12 | 1.92 | 0.50 |
| 1:J:82:TYR:O | 1:J:86:GLY:N | 2.45 | 0.50 |
| 2:B:242:ARG:NH1 | 2:B:481:GLU:OE1 | 2.45 | 0.50 |
| 2:E:911:HIS:O | 2:E:918:ARG:NH2 | 2.42 | 0.50 |
| 2:I:1679:ASN:ND2 | 2:I:1798:LEU:O | 2.45 | 0.50 |
| 2:E:5028:PHE:HE1 | 2:E:5032:TYR:CE2 | 2.29 | 0.50 |
| 2:I:309:THR:O | 2:I:313:SER:OG | 2.29 | 0.50 |
| 2:E:242:ARG:NH1 | 2:E:481:GLU:OE1 | 2.45 | 0.50 |
| 2:E:1679:ASN:ND2 | 2:E:1798:LEU:O | 2.45 | 0.50 |
| 2:I:2042:CYS:SG | 2:I:2043:GLY:N | 2.83 | 0.50 |
| 2:B:4996:ILE:HG12 | 4:B:5102:CFF:H123 | 1.94 | 0.50 |
| 2:I:243:ARG:NH1 | 2:I:301:VAL:O | 2.39 | 0.50 |
| 2:I:1727:ARG:NH2 | 2:I:1773:PRO:O | 2.44 | 0.50 |
| 2:E:4996:ILE:HG12 | 4:E:5102:CFF:H123 | 1.94 | 0.50 |
| 1:J:21:THR:HA | 1:J:49:ARG:HA | 1.94 | 0.49 |
| 2:B:1679:ASN:ND2 | 2:B:1798:LEU:O | 2.45 | 0.49 |
| 2:B:4976:GLU:HA | 2:B:4979:THR:HG23 | 1.94 | 0.49 |
| 2:E:243:ARG:NH1 | 2:E:301:VAL:O | 2.39 | 0.49 |
| 2:E:3850:GLN:HB3 | 2:E:3873:LYS:HD3 | 1.94 | 0.49 |
| 2:I:572:PRO:HA | 2:I:575:LEU:HD13 | 1.94 | 0.49 |
| 2:I:886:ARG:HB3 | 2:I:891:TRP:HB2 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:470:SER:O | 2:G:474:ARG:NE | 2.40 | 0.49 |
| 2:G:3850:GLN:HB3 | 2:G:3873:LYS:HD3 | 1.94 | 0.49 |
| 1:H:82:TYR:O | 1:H:86:GLY:N | 2.45 | 0.49 |
| 2:B:572:PRO:HA | 2:B:575:LEU:HD13 | 1.94 | 0.49 |
| 2:B:718:GLY:HA3 | 2:B:737:LEU:HA | 1.93 | 0.49 |
| 2:B:2196:ASN:OD1 | 2:B:2199:ARG:NH1 | 2.40 | 0.49 |
| 2:E:41:GLY:O | 2:E:45:ARG:NH1 | 2.45 | 0.49 |
| 2:G:2438:PRO:HB3 | 2:G:2453:ILE:HB | 1.95 | 0.49 |
| 2:G:4865:LYS:HG3 | 2:G:4875:LYS:HZ3 | 1.76 | 0.49 |
| 1:J:92:PRO:HD3 | 2:I:627:PRO:HB2 | 1.93 | 0.49 |
| 2:B:886:ARG:HB3 | 2:B:891:TRP:HB2 | 1.94 | 0.49 |
| 2:E:886:ARG:HB3 | 2:E:891:TRP:HB2 | 1.94 | 0.49 |
| 2:I:2131:LEU:HD23 | 2:I:3662:ILE:HB | 1.94 | 0.49 |
| 2:I:4228:ALA:O | 2:I:4232:GLU:N | 2.40 | 0.49 |
| 2:G:164:ARG:N | 2:G:167:ASP:OD2 | 2.44 | 0.49 |
| 2:G:2196:ASN:OD1 | 2:G:2199:ARG:NH1 | 2.40 | 0.49 |
| 1:A:55:VAL:HA | 2:B:1784:ALA:HA | 1.94 | 0.49 |
| 2:B:241:GLN:O | 2:B:289:ARG:NH1 | 2.38 | 0.49 |
| 2:B:470:SER:O | 2:B:474:ARG:NE | 2.40 | 0.49 |
| 2:E:1727:ARG:NH2 | 2:E:1773:PRO:O | 2.44 | 0.49 |
| 2:I:718:GLY:HA3 | 2:I:737:LEU:HA | 1.93 | 0.49 |
| 2:I:2438:PRO:HB3 | 2:I:2453:ILE:HB | 1.94 | 0.49 |
| 2:I:4996:ILE:HG12 | 4:I:5102:CFF:H123 | 1.94 | 0.49 |
| 2:G:886:ARG:HB3 | 2:G:891:TRP:HB2 | 1.94 | 0.49 |
| 2:B:41:GLY:O | 2:B:45:ARG:NH1 | 2.45 | 0.49 |
| 2:B:2438:PRO:HB3 | 2:B:2453:ILE:HB | 1.94 | 0.49 |
| 2:I:596:ASN:HB3 | 2:I:599:VAL:HG22 | 1.95 | 0.49 |
| 2:G:4976:GLU:HA | 2:G:4979:THR:HG23 | 1.94 | 0.49 |
| 2:B:596:ASN:HB3 | 2:B:599:VAL:HG22 | 1.95 | 0.49 |
| 2:B:2131:LEU:HD23 | 2:B:3662:ILE:HB | 1.94 | 0.49 |
| 2:E:161:GLU:HA | 2:G:3984:ARG:HH22 | 1.77 | 0.49 |
| 2:E:2438:PRO:HB3 | 2:E:2453:ILE:HB | 1.95 | 0.49 |
| 2:I:500:ALA:HB1 | 2:I:504:ALA:HB2 | 1.95 | 0.49 |
| 2:I:2196:ASN:OD1 | 2:I:2199:ARG:NH1 | 2.40 | 0.49 |
| 2:I:2868:SER:O | 2:I:2872:GLN:N | 2.44 | 0.49 |
| 2:I:4904:PRO:HB3 | 2:I:4913:ARG:HD2 | 1.95 | 0.49 |
| 2:G:4904:PRO:HB3 | 2:G:4913:ARG:HD2 | 1.95 | 0.49 |
| 1:H:21:THR:HA | 1:H:49:ARG:HA | 1.94 | 0.49 |
| 2:B:290:TYR:O | 2:B:302:VAL:N | 2.46 | 0.49 |
| 2:E:164:ARG:N | 2:E:167:ASP:OD2 | 2.44 | 0.49 |
| 2:G:500:ALA:HB1 | 2:G:504:ALA:HB2 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:2346:VAL:HG22 | 2:G:2348:GLU:H | 1.78 | 0.49 |
| 1:F:82:TYR:O | 1:F:86:GLY:N | 2.45 | 0.49 |
| 2:I:359:TYR:HA | 2:I:376:ALA:HA | 1.93 | 0.49 |
| 2:B:359:TYR:HA | 2:B:376:ALA:HA | 1.93 | 0.49 |
| 2:E:572:PRO:HA | 2:E:575:LEU:HD13 | 1.94 | 0.49 |
| 2:I:4976:GLU:HA | 2:I:4979:THR:HG23 | 1.94 | 0.49 |
| 2:B:2346:VAL:HG22 | 2:B:2348:GLU:H | 1.78 | 0.49 |
| 2:B:2827:ARG:HH21 | 2:B:2931:GLN:HG3 | 1.78 | 0.49 |
| 2:E:5028:PHE:HE1 | 2:E:5032:TYR:HE2 | 1.61 | 0.49 |
| 2:I:1109:LEU:HA | 2:I:1120:LEU:HD21 | 1.95 | 0.49 |
| 2:I:2346:VAL:HG22 | 2:I:2348:GLU:H | 1.78 | 0.49 |
| 2:G:41:GLY:O | 2:G:45:ARG:NH1 | 2.45 | 0.49 |
| 2:G:596:ASN:HB3 | 2:G:599:VAL:HG22 | 1.95 | 0.49 |
| 1:J:55:VAL:HA | 2:I:1784:ALA:HA | 1.95 | 0.48 |
| 2:E:1731:LEU:HA | 2:E:1772:ARG:HH12 | 1.78 | 0.48 |
| 2:E:1960:ALA:O | 2:E:1964:ARG:NE | 2.46 | 0.48 |
| 2:I:5028:PHE:HE1 | 2:I:5032:TYR:CE2 | 2.29 | 0.48 |
| 2:G:978:THR:HB | 2:G:980:ALA:H | 1.78 | 0.48 |
| 2:B:485:SER:O | 2:B:489:ASN:N | 2.37 | 0.48 |
| 2:B:2868:SER:O | 2:B:2872:GLN:N | 2.44 | 0.48 |
| 2:B:3850:GLN:HB3 | 2:B:3873:LYS:HD3 | 1.94 | 0.48 |
| 2:E:551:LEU:HD21 | 2:E:589:LEU:HD13 | 1.95 | 0.48 |
| 2:I:978:THR:HB | 2:I:980:ALA:H | 1.78 | 0.48 |
| 2:B:1960:ALA:O | 2:B:1964:ARG:NE | 2.46 | 0.48 |
| 2:B:2042:CYS:SG | 2:B:2043:GLY:N | 2.83 | 0.48 |
| 2:B:2226:PRO:HA | 2:B:2229:VAL:HG12 | 1.96 | 0.48 |
| 2:B:4904:PRO:HB3 | 2:B:4913:ARG:HD2 | 1.95 | 0.48 |
| 2:E:290:TYR:O | 2:E:302:VAL:N | 2.46 | 0.48 |
| 2:E:2827:ARG:HH21 | 2:E:2931:GLN:HG3 | 1.78 | 0.48 |
| 2:E:4976:GLU:HA | 2:E:4979:THR:HG23 | 1.94 | 0.48 |
| 2:G:551:LEU:HD21 | 2:G:589:LEU:HD13 | 1.95 | 0.48 |
| 2:G:4996:ILE:HG12 | 4:G:5102:CFF:H123 | 1.94 | 0.48 |
| 2:B:1731:LEU:HA | 2:B:1772:ARG:HH12 | 1.78 | 0.48 |
| 2:I:290:TYR:O | 2:I:302:VAL:N | 2.46 | 0.48 |
| 2:I:2346:VAL:HG13 | 2:I:2349:ASN:H | 1.79 | 0.48 |
| 2:I:4126:GLU:O | 2:I:4130:ASN:ND2 | 2.47 | 0.48 |
| 2:G:243:ARG:NH1 | 2:G:301:VAL:O | 2.39 | 0.48 |
| 2:G:4228:ALA:O | 2:G:4232:GLU:N | 2.40 | 0.48 |
| 2:G:5028:PHE:HE1 | 2:G:5032:TYR:HE2 | 1.61 | 0.48 |
| 2:B:978:THR:HB | 2:B:980:ALA:H | 1.78 | 0.48 |
| 2:B:2346:VAL:HG13 | 2:B:2349:ASN:H | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:4126:GLU:O | 2:B:4130:ASN:ND2 | 2.47 | 0.48 |
| 2:E:3910:THR:HG23 | 2:E:3911:THR:HG23 | 1.96 | 0.48 |
| 2:E:4126:GLU:O | 2:E:4130:ASN:ND2 | 2.47 | 0.48 |
| 2:E:4904:PRO:HB3 | 2:E:4913:ARG:HD2 | 1.95 | 0.48 |
| 2:I:1718:ILE:HG13 | 2:I:1719:HIS:CD2 | 2.49 | 0.48 |
| 2:I:3850:GLN:HB3 | 2:I:3873:LYS:HD3 | 1.94 | 0.48 |
| 2:G:1109:LEU:HA | 2:G:1120:LEU:HD21 | 1.95 | 0.48 |
| 2:G:1960:ALA:O | 2:G:1964:ARG:NE | 2.46 | 0.48 |
| 2:G:2131:LEU:HD23 | 2:G:3662:ILE:HB | 1.94 | 0.48 |
| 2:G:4577:LEU:HG | 2:G:4580:TYR:HE2 | 1.79 | 0.48 |
| 2:G:4963:ILE:HD13 | 2:G:5027:CYS:SG | 2.54 | 0.48 |
| 1:J:42:ARG:HG2 | 2:I:1691:GLN:HG2 | 1.94 | 0.48 |
| 2:B:698:GLY:HA2 | 2:B:703:GLY:HA2 | 1.96 | 0.48 |
| 2:I:551:LEU:HD21 | 2:I:589:LEU:HD13 | 1.95 | 0.48 |
| 2:G:1718:ILE:HG13 | 2:G:1719:HIS:CD2 | 2.49 | 0.48 |
| 2:B:4963:ILE:HD13 | 2:B:5027:CYS:SG | 2.54 | 0.48 |
| 2:E:978:THR:HB | 2:E:980:ALA:H | 1.78 | 0.48 |
| 2:E:2131:LEU:HD23 | 2:E:3662:ILE:HB | 1.94 | 0.48 |
| 2:E:4577:LEU:HG | 2:E:4580:TYR:HE2 | 1.79 | 0.48 |
| 2:G:572:PRO:HA | 2:G:575:LEU:HD13 | 1.94 | 0.48 |
| 2:G:3910:THR:HG23 | 2:G:3911:THR:HG23 | 1.96 | 0.48 |
| 2:G:4126:GLU:O | 2:G:4130:ASN:ND2 | 2.47 | 0.48 |
| 2:B:551:LEU:HD21 | 2:B:589:LEU:HD13 | 1.95 | 0.48 |
| 2:E:596:ASN:HB3 | 2:E:599:VAL:HG22 | 1.95 | 0.48 |
| 2:E:1109:LEU:HA | 2:E:1120:LEU:HD21 | 1.95 | 0.48 |
| 2:E:2346:VAL:HG22 | 2:E:2348:GLU:H | 1.78 | 0.48 |
| 2:I:3984:ARG:HH22 | 2:G:161:GLU:HA | 1.79 | 0.48 |
| 2:G:2346:VAL:HG13 | 2:G:2349:ASN:H | 1.79 | 0.48 |
| 2:B:161:GLU:HA | 2:E:3984:ARG:HH22 | 1.79 | 0.48 |
| 2:E:500:ALA:HB1 | 2:E:504:ALA:HB2 | 1.95 | 0.48 |
| 2:E:698:GLY:HA2 | 2:E:703:GLY:HA2 | 1.96 | 0.48 |
| 2:E:1718:ILE:HG13 | 2:E:1719:HIS:CD2 | 2.49 | 0.48 |
| 2:E:4963:ILE:HD13 | 2:E:5027:CYS:SG | 2.54 | 0.48 |
| 2:I:1960:ALA:O | 2:I:1964:ARG:NE | 2.46 | 0.48 |
| 2:I:4963:ILE:HD13 | 2:I:5027:CYS:SG | 2.54 | 0.48 |
| 2:G:3770:LEU:HD21 | 2:G:3775:ALA:HB3 | 1.96 | 0.48 |
| 2:G:4083:ASP:HB3 | 2:G:4086:GLY:H | 1.79 | 0.48 |
| 2:B:3915:ILE:O | 2:B:3919:THR:N | 2.45 | 0.48 |
| 2:I:2226:PRO:HA | 2:I:2229:VAL:HG12 | 1.95 | 0.48 |
| 2:G:698:GLY:HA2 | 2:G:703:GLY:HA2 | 1.96 | 0.48 |
| 2:B:500:ALA:HB1 | 2:B:504:ALA:HB2 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:4577:LEU:HG | 2:I:4580:TYR:HE2 | 1.79 | 0.47 |
| 2:I:41:GLY:O | 2:I:45:ARG:NH1 | 2.45 | 0.47 |
| 2:I:1731:LEU:HA | 2:I:1772:ARG:HH12 | 1.78 | 0.47 |
| 2:I:2827:ARG:HH21 | 2:I:2931:GLN:HG3 | 1.78 | 0.47 |
| 2:I:3910:THR:HG23 | 2:I:3911:THR:HG23 | 1.96 | 0.47 |
| 2:B:1109:LEU:HA | 2:B:1120:LEU:HD21 | 1.95 | 0.47 |
| 2:B:4577:LEU:HG | 2:B:4580:TYR:HE2 | 1.79 | 0.47 |
| 2:E:2226:PRO:HA | 2:E:2229:VAL:HG12 | 1.96 | 0.47 |
| 2:E:4083:ASP:HB3 | 2:E:4086:GLY:H | 1.79 | 0.47 |
| 2:G:3915:ILE:O | 2:G:3919:THR:N | 2.45 | 0.47 |
| 1:A:92:PRO:HD3 | 2:B:627:PRO:HB2 | 1.97 | 0.47 |
| 2:B:1718:ILE:HG13 | 2:B:1719:HIS:CD2 | 2.49 | 0.47 |
| 2:G:290:TYR:O | 2:G:302:VAL:N | 2.46 | 0.47 |
| 2:B:575:LEU:HD22 | 2:B:609:CYS:HB3 | 1.96 | 0.47 |
| 2:B:3910:THR:HG23 | 2:B:3911:THR:HG23 | 1.96 | 0.47 |
| 2:B:4228:ALA:O | 2:B:4232:GLU:N | 2.40 | 0.47 |
| 2:B:4822:THR:O | 2:B:4825:THR:OG1 | 2.27 | 0.47 |
| 2:E:3915:ILE:O | 2:E:3919:THR:N | 2.45 | 0.47 |
| 2:G:242:ARG:NH1 | 2:G:481:GLU:OE1 | 2.45 | 0.47 |
| 2:G:2042:CYS:SG | 2:G:2043:GLY:N | 2.83 | 0.47 |
| 2:B:2199:ARG:NH2 | 2:B:2246:ASN:OD1 | 2.48 | 0.47 |
| 2:B:4083:ASP:HB3 | 2:B:4086:GLY:H | 1.79 | 0.47 |
| 2:I:4236:SER:OG | 2:I:4675:LYS:NZ | 2.36 | 0.47 |
| 2:G:2827:ARG:HH21 | 2:G:2931:GLN:HG3 | 1.78 | 0.47 |
| 2:B:3971:GLY:N | 2:B:4032:GLU:OE2 | 2.47 | 0.47 |
| 2:B:5028:PHE:HE1 | 2:B:5032:TYR:HE2 | 1.61 | 0.47 |
| 2:E:2199:ARG:NH2 | 2:E:2246:ASN:OD1 | 2.48 | 0.47 |
| 2:I:698:GLY:HA2 | 2:I:703:GLY:HA2 | 1.96 | 0.47 |
| 2:I:2739:PRO:HB3 | 2:I:2884:ASN:HB3 | 1.97 | 0.47 |
| 2:I:4083:ASP:HB3 | 2:I:4086:GLY:H | 1.79 | 0.47 |
| 2:G:1731:LEU:HA | 2:G:1772:ARG:HH12 | 1.78 | 0.47 |
| 2:G:2199:ARG:NH2 | 2:G:2246:ASN:OD1 | 2.48 | 0.47 |
| 2:G:2226:PRO:HA | 2:G:2229:VAL:HG12 | 1.96 | 0.47 |
| 2:G:4863:TYR:HD2 | 2:G:4875:LYS:HB2 | 1.79 | 0.47 |
| 1:F:34:LYS:HE3 | 2:E:634:GLN:HB3 | 1.95 | 0.47 |
| 2:B:1727:ARG:NH2 | 2:B:1773:PRO:O | 2.44 | 0.47 |
| 2:B:4236:SER:OG | 2:B:4675:LYS:NZ | 2.36 | 0.47 |
| 2:E:4822:THR:O | 2:E:4825:THR:OG1 | 2.27 | 0.47 |
| 2:E:4863:TYR:HD2 | 2:E:4875:LYS:HB2 | 1.79 | 0.47 |
| 2:I:451:TYR:O | 2:I:474:ARG:NH1 | 2.47 | 0.47 |
| 2:G:241:GLN:O | 2:G:289:ARG:NH1 | 2.38 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:57:ASN:HD22 | 2:B:308:HIS:HB2 | 1.80 | 0.47 |
| 2:B:2739:PRO:HB3 | 2:B:2884:ASN:HB3 | 1.97 | 0.47 |
| 2:B:34:LYS:H | 2:B:53:SER:HG | 1.62 | 0.47 |
| 2:E:641:VAL:HG11 | 2:E:681:HIS:HD1 | 1.80 | 0.47 |
| 2:E:2739:PRO:HB3 | 2:E:2884:ASN:HB3 | 1.97 | 0.47 |
| 2:G:1727:ARG:NH2 | 2:G:1773:PRO:O | 2.44 | 0.47 |
| 1:H:87:HIS:HD2 | 1:H:90:VAL:HB | 1.80 | 0.46 |
| 1:J:87:HIS:HD2 | 1:J:90:VAL:HB | 1.80 | 0.46 |
| 2:B:403:MET:O | 2:B:407:THR:N | 2.49 | 0.46 |
| 2:B:719:LEU:HD22 | 2:B:735:GLN:HG2 | 1.97 | 0.46 |
| 2:B:4863:TYR:HD2 | 2:B:4875:LYS:HB2 | 1.79 | 0.46 |
| 2:E:57:ASN:HD22 | 2:E:308:HIS:HB2 | 1.80 | 0.46 |
| 2:E:719:LEU:HD22 | 2:E:735:GLN:HG2 | 1.97 | 0.46 |
| 2:E:3770:LEU:HD21 | 2:E:3775:ALA:HB3 | 1.96 | 0.46 |
| 2:B:683:ARG:HG2 | 2:B:717:ASP:HB3 | 1.98 | 0.46 |
| 2:I:4863:TYR:HD2 | 2:I:4875:LYS:HB2 | 1.78 | 0.46 |
| 2:G:451:TYR:O | 2:G:474:ARG:NH1 | 2.47 | 0.46 |
| 2:E:1244:GLN:OE1 | 2:E:1646:ARG:NH1 | 2.49 | 0.46 |
| 2:G:2739:PRO:HB3 | 2:G:2884:ASN:HB3 | 1.97 | 0.46 |
| 1:A:87:HIS:HD2 | 1:A:90:VAL:HB | 1.80 | 0.46 |
| 1:J:34:LYS:HE3 | 2:I:634:GLN:HB3 | 1.97 | 0.46 |
| 2:B:641:VAL:HG11 | 2:B:681:HIS:HD1 | 1.80 | 0.46 |
| 2:B:1260:MET:HB2 | 2:B:1269:CYS:H | 1.81 | 0.46 |
| 2:B:3770:LEU:HD21 | 2:B:3775:ALA:HB3 | 1.96 | 0.46 |
| 2:E:1105:ALA:N | 2:E:1189:LEU:O | 2.49 | 0.46 |
| 2:E:1260:MET:HB2 | 2:E:1269:CYS:H | 1.81 | 0.46 |
| 2:E:1727:ARG:HH21 | 2:E:1775:HIS:CE1 | 2.34 | 0.46 |
| 2:E:3658:LYS:HA | 2:E:3661:TRP:CD2 | 2.51 | 0.46 |
| 2:E:4036:VAL:HG11 | 2:E:5035:GLN:HB3 | 1.97 | 0.46 |
| 2:E:4571:PHE:O | 2:E:4575:PHE:N | 2.49 | 0.46 |
| 2:I:575:LEU:HD22 | 2:I:609:CYS:HB3 | 1.96 | 0.46 |
| 2:I:1244:GLN:OE1 | 2:I:1646:ARG:NH1 | 2.49 | 0.46 |
| 2:I:2803:GLU:OE2 | 2:I:2806:ARG:NH1 | 2.49 | 0.46 |
| 2:G:57:ASN:HD22 | 2:G:308:HIS:HB2 | 1.80 | 0.46 |
| 2:G:683:ARG:HG2 | 2:G:717:ASP:HB3 | 1.98 | 0.46 |
| 2:B:451:TYR:O | 2:B:474:ARG:NH1 | 2.47 | 0.46 |
| 2:B:2803:GLU:OE2 | 2:B:2806:ARG:NH1 | 2.49 | 0.46 |
| 2:B:3804:ILE:HG22 | 2:B:3812:VAL:HG21 | 1.98 | 0.46 |
| 2:I:403:MET:O | 2:I:407:THR:N | 2.49 | 0.46 |
| 2:I:2199:ARG:NH2 | 2:I:2246:ASN:OD1 | 2.48 | 0.46 |
| 2:I:3770:LEU:HD21 | 2:I:3775:ALA:HB3 | 1.96 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:35:LEU:HD13 | 2:G:49:LEU:HD13 | 1.98 | 0.46 |
| 2:G:641:VAL:HG11 | 2:G:681:HIS:HD1 | 1.80 | 0.46 |
| 2:G:1727:ARG:HH21 | 2:G:1775:HIS:CE1 | 2.34 | 0.46 |
| 2:G:3804:ILE:HG22 | 2:G:3812:VAL:HG21 | 1.98 | 0.46 |
| 2:G:4687:TYR:OH | 2:G:4699:GLY:O | 2.33 | 0.46 |
| 2:B:1244:GLN:OE1 | 2:B:1646:ARG:NH1 | 2.49 | 0.46 |
| 2:B:1727:ARG:HH21 | 2:B:1775:HIS:CE1 | 2.34 | 0.46 |
| 2:E:575:LEU:HD22 | 2:E:609:CYS:HB3 | 1.96 | 0.46 |
| 2:E:683:ARG:HG2 | 2:E:717:ASP:HB3 | 1.98 | 0.46 |
| 2:E:2346:VAL:HG13 | 2:E:2349:ASN:H | 1.79 | 0.46 |
| 2:G:575:LEU:HD22 | 2:G:609:CYS:HB3 | 1.96 | 0.46 |
| 2:B:4036:VAL:HG11 | 2:B:5035:GLN:HB3 | 1.97 | 0.46 |
| 2:I:1727:ARG:HH21 | 2:I:1775:HIS:CE1 | 2.34 | 0.46 |
| 2:I:3804:ILE:HG22 | 2:I:3812:VAL:HG21 | 1.98 | 0.46 |
| 2:G:1244:GLN:OE1 | 2:G:1646:ARG:NH1 | 2.49 | 0.46 |
| 2:G:3658:LYS:HA | 2:G:3661:TRP:CD2 | 2.51 | 0.46 |
| 1:F:87:HIS:HD2 | 1:F:90:VAL:HB | 1.80 | 0.46 |
| 1:H:87:HIS:H | 1:H:91:ILE:HB | 1.81 | 0.46 |
| 2:B:214:VAL:HG12 | 2:B:274:LEU:HD12 | 1.98 | 0.46 |
| 2:B:1105:ALA:N | 2:B:1189:LEU:O | 2.49 | 0.46 |
| 2:B:4687:TYR:OH | 2:B:4699:GLY:O | 2.33 | 0.46 |
| 2:E:35:LEU:HD13 | 2:E:49:LEU:HD13 | 1.98 | 0.46 |
| 2:E:3804:ILE:HG22 | 2:E:3812:VAL:HG21 | 1.98 | 0.46 |
| 2:E:4236:SER:OG | 2:E:4675:LYS:NZ | 2.36 | 0.46 |
| 2:I:57:ASN:HD22 | 2:I:308:HIS:HB2 | 1.80 | 0.46 |
| 2:I:681:HIS:HB3 | 2:I:784:SER:HB3 | 1.98 | 0.46 |
| 2:I:683:ARG:HG2 | 2:I:717:ASP:HB3 | 1.98 | 0.46 |
| 2:I:5028:PHE:HE1 | 2:I:5032:TYR:HE2 | 1.61 | 0.46 |
| 2:G:379:HIS:CD2 | 2:G:381:GLU:H | 2.34 | 0.46 |
| 2:G:4571:PHE:O | 2:G:4575:PHE:N | 2.49 | 0.46 |
| 2:B:606:LEU:O | 2:B:617:ASN:ND2 | 2.49 | 0.46 |
| 2:E:403:MET:O | 2:E:407:THR:N | 2.49 | 0.46 |
| 2:I:1260:MET:HB2 | 2:I:1269:CYS:H | 1.81 | 0.46 |
| 2:I:3658:LYS:HA | 2:I:3661:TRP:CD2 | 2.51 | 0.46 |
| 2:G:1260:MET:HB2 | 2:G:1269:CYS:H | 1.81 | 0.46 |
| 2:B:3842:LEU:O | 2:B:3929:SER:OG | 2.34 | 0.46 |
| 2:B:4571:PHE:O | 2:B:4575:PHE:N | 2.49 | 0.46 |
| 2:B:4680:LYS:HD3 | 2:B:4686:LEU:HD22 | 1.98 | 0.46 |
| 2:E:214:VAL:HG12 | 2:E:274:LEU:HD12 | 1.98 | 0.46 |
| 2:E:218:HIS:HB3 | 2:E:392:ARG:HD3 | 1.98 | 0.46 |
| 2:E:681:HIS:HB3 | 2:E:784:SER:HB3 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:2042:CYS:SG | 2:E:2043:GLY:N | 2.83 | 0.46 |
| 2:E:2803:GLU:OE2 | 2:E:2806:ARG:NH1 | 2.49 | 0.46 |
| 2:I:35:LEU:HD13 | 2:I:49:LEU:HD13 | 1.98 | 0.46 |
| 2:G:719:LEU:HD22 | 2:G:735:GLN:HG2 | 1.97 | 0.46 |
| 1:F:34:LYS:HD3 | 2:E:629:ARG:HD2 | 1.98 | 0.45 |
| 2:B:243:ARG:NH1 | 2:B:301:VAL:O | 2.39 | 0.45 |
| 2:E:983:THR:O | 2:E:987:ARG:N | 2.48 | 0.45 |
| 2:I:379:HIS:CD2 | 2:I:381:GLU:H | 2.34 | 0.45 |
| 2:I:641:VAL:HG11 | 2:I:681:HIS:HD1 | 1.80 | 0.45 |
| 2:I:719:LEU:HD22 | 2:I:735:GLN:HG2 | 1.97 | 0.45 |
| 1:F:87:HIS:H | 1:F:91:ILE:HB | 1.81 | 0.45 |
| 2:B:681:HIS:HB3 | 2:B:784:SER:HB3 | 1.98 | 0.45 |
| 2:B:4823:LEU:HD23 | 2:I:4843:LEU:HD12 | 1.98 | 0.45 |
| 2:E:3362:UNK:O | 2:E:3366:UNK:N | 2.50 | 0.45 |
| 2:E:4687:TYR:OH | 2:E:4699:GLY:O | 2.33 | 0.45 |
| 2:I:206:CYS:SG | 2:I:207:SER:N | 2.90 | 0.45 |
| 2:I:606:LEU:O | 2:I:617:ASN:ND2 | 2.49 | 0.45 |
| 2:I:4036:VAL:HG11 | 2:I:5035:GLN:HB3 | 1.97 | 0.45 |
| 2:E:1838:PHE:HB3 | 2:E:1842:LEU:HD11 | 1.99 | 0.45 |
| 2:I:1838:PHE:HB3 | 2:I:1842:LEU:HD11 | 1.99 | 0.45 |
| 2:I:3362:UNK:O | 2:I:3366:UNK:N | 2.50 | 0.45 |
| 2:I:4680:LYS:HD3 | 2:I:4686:LEU:HD22 | 1.98 | 0.45 |
| 2:G:403:MET:O | 2:G:407:THR:N | 2.49 | 0.45 |
| 2:G:3362:UNK:O | 2:G:3366:UNK:N | 2.50 | 0.45 |
| 2:B:218:HIS:HB3 | 2:B:392:ARG:HD3 | 1.98 | 0.45 |
| 2:B:1457:UNK:N | 2:B:1497:UNK:O | 2.49 | 0.45 |
| 2:B:1838:PHE:HB3 | 2:B:1842:LEU:HD11 | 1.99 | 0.45 |
| 2:E:1457:UNK:N | 2:E:1497:UNK:O | 2.49 | 0.45 |
| 2:I:218:HIS:HB3 | 2:I:392:ARG:HD3 | 1.98 | 0.45 |
| 2:I:4571:PHE:O | 2:I:4575:PHE:N | 2.49 | 0.45 |
| 2:G:2803:GLU:OE2 | 2:G:2806:ARG:NH1 | 2.49 | 0.45 |
| 2:B:206:CYS:SG | 2:B:207:SER:N | 2.89 | 0.45 |
| 2:B:379:HIS:CD2 | 2:B:381:GLU:H | 2.34 | 0.45 |
| 2:B:1973:GLN:O | 2:B:1977:TYR:N | 2.45 | 0.45 |
| 2:E:2327:GLY:HA2 | 2:E:2330:ARG:HD3 | 1.98 | 0.45 |
| 2:E:3842:LEU:O | 2:E:3929:SER:OG | 2.34 | 0.45 |
| 2:I:214:VAL:HG12 | 2:I:274:LEU:HD12 | 1.98 | 0.45 |
| 2:G:206:CYS:SG | 2:G:207:SER:N | 2.89 | 0.45 |
| 2:G:214:VAL:HG12 | 2:G:274:LEU:HD12 | 1.98 | 0.45 |
| 2:G:606:LEU:O | 2:G:617:ASN:ND2 | 2.49 | 0.45 |
| 2:G:1105:ALA:N | 2:G:1189:LEU:O | 2.49 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1838:PHE:HB3 | 2:G:1842:LEU:HD11 | 1.99 | 0.45 |
| 2:G:4822:THR:O | 2:G:4825:THR:OG1 | 2.27 | 0.45 |
| 2:E:206:CYS:SG | 2:E:207:SER:N | 2.90 | 0.45 |
| 2:I:1457:UNK:N | 2:I:1497:UNK:O | 2.49 | 0.45 |
| 2:G:1457:UNK:N | 2:G:1497:UNK:O | 2.49 | 0.45 |
| 2:G:4036:VAL:HG11 | 2:G:5035:GLN:HB3 | 1.97 | 0.45 |
| 2:G:4680:LYS:HD3 | 2:G:4686:LEU:HD22 | 1.98 | 0.45 |
| 2:B:35:LEU:HD13 | 2:B:49:LEU:HD13 | 1.98 | 0.45 |
| 2:B:3362:UNK:O | 2:B:3366:UNK:N | 2.50 | 0.45 |
| 2:B:3779:VAL:HG23 | 2:B:3780:LEU:HD12 | 1.98 | 0.45 |
| 2:E:3779:VAL:HG23 | 2:E:3780:LEU:HD12 | 1.98 | 0.45 |
| 2:G:681:HIS:HB3 | 2:G:784:SER:HB3 | 1.98 | 0.45 |
| 2:I:4687:TYR:OH | 2:I:4699:GLY:O | 2.33 | 0.45 |
| 2:G:218:HIS:HB3 | 2:G:392:ARG:HD3 | 1.98 | 0.45 |
| 1:A:87:HIS:H | 1:A:91:ILE:HB | 1.81 | 0.45 |
| 2:B:2327:GLY:HA2 | 2:B:2330:ARG:HD3 | 1.98 | 0.45 |
| 2:E:379:HIS:CD2 | 2:E:381:GLU:H | 2.34 | 0.45 |
| 2:E:4959:PHE:O | 2:E:4959:PHE:CG | 2.70 | 0.45 |
| 2:I:215:THR:HG22 | 2:I:273:HIS:HA | 1.99 | 0.45 |
| 2:I:3779:VAL:HG23 | 2:I:3780:LEU:HD12 | 1.98 | 0.45 |
| 2:G:469:ARG:HH21 | 2:G:3712:GLU:HB3 | 1.81 | 0.45 |
| 2:G:3779:VAL:HG23 | 2:G:3780:LEU:HD12 | 1.98 | 0.45 |
| 2:G:4959:PHE:O | 2:G:4959:PHE:CG | 2.70 | 0.45 |
| 1:A:23:VAL:HG22 | 1:A:47:LYS:HG2 | 1.99 | 0.45 |
| 2:B:219:VAL:HG13 | 2:B:285:VAL:HG21 | 1.99 | 0.45 |
| 2:E:451:TYR:O | 2:E:474:ARG:NH1 | 2.47 | 0.45 |
| 2:I:469:ARG:HH21 | 2:I:3712:GLU:HB3 | 1.81 | 0.45 |
| 2:I:626:LEU:HG | 2:I:628:GLY:H | 1.82 | 0.45 |
| 1:F:27:THR:HB | 1:F:100:ASP:HB3 | 1.99 | 0.44 |
| 1:A:27:THR:HB | 1:A:100:ASP:HB3 | 1.99 | 0.44 |
| 2:B:3984:ARG:HH22 | 2:I:161:GLU:HA | 1.82 | 0.44 |
| 2:E:1972:ASN:HD21 | 2:E:2024:PRO:HB3 | 1.83 | 0.44 |
| 2:I:5028:PHE:O | 2:I:5028:PHE:CG | 2.70 | 0.44 |
| 1:J:23:VAL:HG22 | 1:J:47:LYS:HG2 | 2.00 | 0.44 |
| 1:J:27:THR:HB | 1:J:100:ASP:HB3 | 1.99 | 0.44 |
| 2:B:3658:LYS:HA | 2:B:3661:TRP:CD2 | 2.51 | 0.44 |
| 2:E:215:THR:HG22 | 2:E:273:HIS:HA | 2.00 | 0.44 |
| 2:E:606:LEU:O | 2:E:617:ASN:ND2 | 2.49 | 0.44 |
| 2:E:841:GLY:HA2 | 2:E:1073:ARG:HD2 | 1.99 | 0.44 |
| 2:E:4680:LYS:HD3 | 2:E:4686:LEU:HD22 | 1.98 | 0.44 |
| 2:I:1972:ASN:HD21 | 2:I:2024:PRO:HB3 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:4959:PHE:O | 2:I:4959:PHE:CD1 | 2.70 | 0.44 |
| 2:G:215:THR:HG22 | 2:G:273:HIS:HA | 2.00 | 0.44 |
| 2:B:1972:ASN:HD21 | 2:B:2024:PRO:HB3 | 1.83 | 0.44 |
| 2:E:626:LEU:HG | 2:E:628:GLY:H | 1.82 | 0.44 |
| 2:I:1105:ALA:N | 2:I:1189:LEU:O | 2.49 | 0.44 |
| 2:I:3842:LEU:O | 2:I:3929:SER:OG | 2.34 | 0.44 |
| 2:E:2104:ARG:HA | 2:E:2107:GLN:HB3 | 1.99 | 0.44 |
| 2:E:2430:ILE:HG21 | 2:E:2502:UNK:HA | 1.99 | 0.44 |
| 2:E:3829:PHE:HD1 | 2:E:3915:ILE:HD11 | 1.82 | 0.44 |
| 2:I:3829:PHE:HD1 | 2:I:3915:ILE:HD11 | 1.82 | 0.44 |
| 2:G:210:GLU:H | 2:G:273:HIS:CE1 | 2.36 | 0.44 |
| 2:G:626:LEU:HG | 2:G:628:GLY:H | 1.82 | 0.44 |
| 2:G:3829:PHE:HD1 | 2:G:3915:ILE:HD11 | 1.82 | 0.44 |
| 1:J:87:HIS:H | 1:J:91:ILE:HB | 1.81 | 0.44 |
| 2:B:4843:LEU:HD12 | 2:E:4823:LEU:HD23 | 1.99 | 0.44 |
| 2:E:3971:GLY:N | 2:E:4032:GLU:OE2 | 2.47 | 0.44 |
| 2:I:838:HIS:HA | 2:I:1201:HIS:HB3 | 2.00 | 0.44 |
| 2:G:838:HIS:HA | 2:G:1201:HIS:HB3 | 2.00 | 0.44 |
| 2:G:1804:LEU:O | 2:G:1808:ARG:N | 2.49 | 0.44 |
| 2:G:2447:LYS:HG3 | 2:G:2449:GLU:H | 1.83 | 0.44 |
| 1:H:34:LYS:HE3 | 2:G:634:GLN:HB3 | 1.98 | 0.44 |
| 2:B:215:THR:HG22 | 2:B:273:HIS:HA | 1.99 | 0.44 |
| 2:B:395:GLN:NE2 | 2:B:397:GLU:OE1 | 2.51 | 0.44 |
| 2:B:626:LEU:HG | 2:B:628:GLY:H | 1.82 | 0.44 |
| 2:B:2104:ARG:HA | 2:B:2107:GLN:HB3 | 1.99 | 0.44 |
| 2:B:4959:PHE:O | 2:B:4959:PHE:CD1 | 2.71 | 0.44 |
| 2:B:4959:PHE:O | 2:B:4959:PHE:CG | 2.70 | 0.44 |
| 2:E:219:VAL:HG13 | 2:E:285:VAL:HG21 | 1.99 | 0.44 |
| 2:E:469:ARG:HH21 | 2:E:3712:GLU:HB3 | 1.81 | 0.44 |
| 2:E:4843:LEU:HD12 | 2:G:4823:LEU:HD23 | 2.00 | 0.44 |
| 2:I:2447:LYS:HG3 | 2:I:2449:GLU:H | 1.83 | 0.44 |
| 2:I:2764:GLU:HG3 | 2:I:2857:PRO:HB2 | 2.00 | 0.44 |
| 2:I:3915:ILE:O | 2:I:3919:THR:N | 2.45 | 0.44 |
| 2:G:1105:ALA:HB1 | 2:G:1109:LEU:HD21 | 2.00 | 0.44 |
| 2:B:5028:PHE:O | 2:B:5028:PHE:CG | 2.70 | 0.44 |
| 2:E:395:GLN:NE2 | 2:E:397:GLU:OE1 | 2.51 | 0.44 |
| 2:I:210:GLU:H | 2:I:273:HIS:CE1 | 2.36 | 0.44 |
| 2:I:2104:ARG:HA | 2:I:2107:GLN:HB3 | 1.99 | 0.44 |
| 2:I:2299:VAL:O | 2:I:2303:ALA:N | 2.50 | 0.44 |
| 2:I:2342:ASN:OD1 | 2:I:2342:ASN:N | 2.51 | 0.44 |
| 2:G:841:GLY:HA2 | 2:G:1073:ARG:HD2 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1973:GLN:HA | 2:G:1976:ARG:HB3 | 2.00 | 0.44 |
| 2:G:2327:GLY:HA2 | 2:G:2330:ARG:HD3 | 1.98 | 0.44 |
| 2:G:2927:LEU:HD23 | 2:G:2930:LEU:HD12 | 2.00 | 0.44 |
| 2:G:4959:PHE:O | 2:G:4959:PHE:CD1 | 2.70 | 0.44 |
| 2:G:5028:PHE:CG | 2:G:5028:PHE:O | 2.70 | 0.44 |
| 1:F:23:VAL:HG22 | 1:F:47:LYS:HG2 | 2.00 | 0.44 |
| 2:B:1101:ARG:HH21 | 2:B:1115:LEU:H | 1.66 | 0.44 |
| 2:E:210:GLU:H | 2:E:273:HIS:CE1 | 2.36 | 0.44 |
| 2:E:4215:ARG:NH2 | 3:E:5101:ATP:O1A | 2.51 | 0.44 |
| 2:I:485:SER:O | 2:I:489:ASN:N | 2.37 | 0.44 |
| 2:I:647:ASN:ND2 | 2:I:820:ARG:O | 2.50 | 0.44 |
| 2:I:2327:GLY:HA2 | 2:I:2330:ARG:HD3 | 1.98 | 0.44 |
| 2:I:2758:PHE:O | 2:I:2762:THR:N | 2.51 | 0.44 |
| 2:G:1972:ASN:HD21 | 2:G:2024:PRO:HB3 | 1.83 | 0.44 |
| 2:G:4229:GLU:HA | 2:G:4232:GLU:HB3 | 1.99 | 0.44 |
| 1:A:11:ASP:OD1 | 1:A:67:SER:OG | 2.29 | 0.44 |
| 2:B:34:LYS:N | 2:B:53:SER:OG | 2.40 | 0.44 |
| 2:E:4959:PHE:O | 2:E:4959:PHE:CD1 | 2.70 | 0.44 |
| 2:I:241:GLN:O | 2:I:289:ARG:NH1 | 2.38 | 0.44 |
| 2:I:1663:HIS:O | 2:I:1667:LEU:N | 2.49 | 0.44 |
| 2:I:2257:LEU:O | 2:I:2261:SER:N | 2.51 | 0.44 |
| 2:I:4959:PHE:O | 2:I:4959:PHE:CG | 2.70 | 0.44 |
| 2:G:2104:ARG:HA | 2:G:2107:GLN:HB3 | 1.99 | 0.44 |
| 2:G:2257:LEU:O | 2:G:2261:SER:N | 2.51 | 0.44 |
| 2:B:3365:UNK:O | 2:B:3369:UNK:N | 2.51 | 0.43 |
| 2:E:2927:LEU:HD23 | 2:E:2930:LEU:HD12 | 2.00 | 0.43 |
| 2:E:3365:UNK:O | 2:E:3369:UNK:N | 2.51 | 0.43 |
| 2:I:119:SER:HA | 2:I:146:CYS:HA | 2.00 | 0.43 |
| 2:I:395:GLN:NE2 | 2:I:397:GLU:OE1 | 2.51 | 0.43 |
| 2:I:2430:ILE:HG21 | 2:I:2502:UNK:HA | 1.99 | 0.43 |
| 2:I:3365:UNK:O | 2:I:3369:UNK:N | 2.51 | 0.43 |
| 2:I:4229:GLU:HA | 2:I:4232:GLU:HB3 | 1.99 | 0.43 |
| 2:G:2758:PHE:O | 2:G:2762:THR:N | 2.51 | 0.43 |
| 2:G:3971:GLY:N | 2:G:4032:GLU:OE2 | 2.47 | 0.43 |
| 2:G:4215:ARG:NH2 | 3:G:5101:ATP:O1A | 2.51 | 0.43 |
| 2:B:4215:ARG:NH2 | 3:B:5101:ATP:O1A | 2.51 | 0.43 |
| 2:E:34:LYS:N | 2:E:53:SER:OG | 2.40 | 0.43 |
| 2:E:2862:LEU:HB3 | 2:E:2928:LYS:HB3 | 2.00 | 0.43 |
| 2:G:379:HIS:NE2 | 2:G:381:GLU:OE1 | 2.52 | 0.43 |
| 2:G:2764:GLU:HG3 | 2:G:2857:PRO:HB2 | 2.00 | 0.43 |
| 1:H:23:VAL:HG22 | 1:H:47:LYS:HG2 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:27:THR:HB | 1:H:100:ASP:HB3 | 1.99 | 0.43 |
| 2:B:469:ARG:HH21 | 2:B:3712:GLU:HB3 | 1.81 | 0.43 |
| 2:B:2764:GLU:HG3 | 2:B:2857:PRO:HB2 | 2.00 | 0.43 |
| 2:B:3829:PHE:HD1 | 2:B:3915:ILE:HD11 | 1.82 | 0.43 |
| 2:E:1663:HIS:O | 2:E:1667:LEU:N | 2.49 | 0.43 |
| 2:E:4229:GLU:HA | 2:E:4232:GLU:HB3 | 1.99 | 0.43 |
| 2:I:219:VAL:HG13 | 2:I:285:VAL:HG21 | 1.99 | 0.43 |
| 2:I:4673:ARG:HH12 | 2:I:4698:LYS:HE3 | 1.84 | 0.43 |
| 2:G:3842:LEU:O | 2:G:3929:SER:OG | 2.34 | 0.43 |
| 2:B:210:GLU:H | 2:B:273:HIS:CE1 | 2.36 | 0.43 |
| 2:B:2342:ASN:OD1 | 2:B:2342:ASN:N | 2.51 | 0.43 |
| 2:B:2430:ILE:HG21 | 2:B:2502:UNK:HA | 1.99 | 0.43 |
| 2:B:2447:LYS:HG3 | 2:B:2449:GLU:H | 1.83 | 0.43 |
| 2:B:2758:PHE:O | 2:B:2762:THR:N | 2.51 | 0.43 |
| 2:B:4229:GLU:HA | 2:B:4232:GLU:HB3 | 1.99 | 0.43 |
| 2:E:2447:LYS:HG3 | 2:E:2449:GLU:H | 1.83 | 0.43 |
| 2:I:932:LEU:HA | 2:I:935:LEU:HD12 | 2.01 | 0.43 |
| 2:G:1101:ARG:HH21 | 2:G:1115:LEU:H | 1.65 | 0.43 |
| 1:A:34:LYS:HE3 | 2:B:634:GLN:HB3 | 2.00 | 0.43 |
| 2:B:838:HIS:HA | 2:B:1201:HIS:HB3 | 2.00 | 0.43 |
| 2:B:1105:ALA:HB1 | 2:B:1109:LEU:HD21 | 2.00 | 0.43 |
| 2:B:2231:SER:HA | 2:B:2234:ARG:HG2 | 2.01 | 0.43 |
| 2:E:119:SER:HA | 2:E:146:CYS:HA | 2.00 | 0.43 |
| 2:E:932:LEU:HA | 2:E:935:LEU:HD12 | 2.01 | 0.43 |
| 2:E:1973:GLN:HA | 2:E:1976:ARG:HB3 | 2.00 | 0.43 |
| 2:E:2231:SER:HA | 2:E:2234:ARG:HG2 | 2.01 | 0.43 |
| 2:I:379:HIS:NE2 | 2:I:381:GLU:OE1 | 2.52 | 0.43 |
| 2:G:776:LEU:HG | 2:G:848:HIS:HA | 2.01 | 0.43 |
| 2:G:864:PRO:HA | 2:G:865:PRO:HD3 | 1.92 | 0.43 |
| 2:G:1676:LEU:HD23 | 2:G:2167:ILE:HG23 | 2.01 | 0.43 |
| 2:G:3365:UNK:O | 2:G:3369:UNK:N | 2.51 | 0.43 |
| 2:B:1973:GLN:HA | 2:B:1976:ARG:HB3 | 2.00 | 0.43 |
| 2:E:887:ILE:HG21 | 2:E:959:TYR:HA | 2.01 | 0.43 |
| 2:E:2758:PHE:O | 2:E:2762:THR:N | 2.51 | 0.43 |
| 2:E:4673:ARG:HH12 | 2:E:4698:LYS:HE3 | 1.84 | 0.43 |
| 2:E:5028:PHE:O | 2:E:5028:PHE:CG | 2.70 | 0.43 |
| 2:I:1973:GLN:O | 2:I:1977:TYR:N | 2.45 | 0.43 |
| 2:I:2231:SER:HA | 2:I:2234:ARG:HG2 | 2.01 | 0.43 |
| 2:I:2793:PRO:HG3 | 2:I:2855:TYR:CZ | 2.54 | 0.43 |
| 2:G:219:VAL:HG13 | 2:G:285:VAL:HG21 | 1.99 | 0.43 |
| 2:G:4673:ARG:HH12 | 2:G:4698:LYS:HE3 | 1.84 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:119:SER:HA | 2:B:146:CYS:HA | 2.01 | 0.43 |
| 2:B:1854:PHE:HD1 | 2:B:1858:ASP:HB3 | 1.84 | 0.43 |
| 2:B:2024:PRO:O | 2:B:2028:ARG:NE | 2.49 | 0.43 |
| 2:I:103:TYR:HB3 | 2:I:152:PRO:HD3 | 2.01 | 0.43 |
| 2:I:1854:PHE:HD1 | 2:I:1858:ASP:HB3 | 1.84 | 0.43 |
| 2:I:4215:ARG:NH2 | 3:I:5101:ATP:O1A | 2.51 | 0.43 |
| 2:G:887:ILE:HG21 | 2:G:959:TYR:HA | 2.01 | 0.43 |
| 2:G:1269:CYS:HA | 2:G:1473:UNK:HA | 2.01 | 0.43 |
| 2:G:2231:SER:HA | 2:G:2234:ARG:HG2 | 2.01 | 0.43 |
| 2:B:841:GLY:HA2 | 2:B:1073:ARG:HD2 | 1.99 | 0.43 |
| 2:B:2862:LEU:HB3 | 2:B:2928:LYS:HB3 | 2.00 | 0.43 |
| 2:B:4983:HIS:CB | 2:B:4988:TYR:HE2 | 2.32 | 0.43 |
| 2:E:734:GLY:O | 2:E:736:HIS:ND1 | 2.51 | 0.43 |
| 2:I:599:VAL:HG23 | 2:I:600:LEU:HD12 | 2.00 | 0.43 |
| 2:I:1859:VAL:HA | 2:I:1862:ILE:HG12 | 2.01 | 0.43 |
| 2:G:932:LEU:HA | 2:G:935:LEU:HD12 | 2.01 | 0.43 |
| 2:G:2430:ILE:HG21 | 2:G:2502:UNK:HA | 1.99 | 0.43 |
| 2:G:2862:LEU:HB3 | 2:G:2928:LYS:HB3 | 2.00 | 0.43 |
| 2:B:932:LEU:HA | 2:B:935:LEU:HD12 | 2.01 | 0.43 |
| 2:I:841:GLY:HA2 | 2:I:1073:ARG:HD2 | 1.99 | 0.43 |
| 2:I:1105:ALA:HB1 | 2:I:1109:LEU:HD21 | 2.00 | 0.43 |
| 2:I:2927:LEU:HD23 | 2:I:2930:LEU:HD12 | 2.00 | 0.43 |
| 2:G:395:GLN:NE2 | 2:G:397:GLU:OE1 | 2.51 | 0.43 |
| 2:B:887:ILE:HG21 | 2:B:959:TYR:HA | 2.01 | 0.43 |
| 2:E:838:HIS:HA | 2:E:1201:HIS:HB3 | 2.00 | 0.43 |
| 2:E:1101:ARG:HH21 | 2:E:1115:LEU:H | 1.66 | 0.43 |
| 2:E:2257:LEU:O | 2:E:2261:SER:N | 2.51 | 0.43 |
| 2:I:776:LEU:HG | 2:I:848:HIS:HA | 2.01 | 0.43 |
| 2:I:4993:MET:HA | 2:I:4996:ILE:HD12 | 2.00 | 0.43 |
| 2:G:2024:PRO:O | 2:G:2028:ARG:NE | 2.49 | 0.43 |
| 2:G:2299:VAL:O | 2:G:2303:ALA:N | 2.50 | 0.43 |
| 2:G:4929:LEU:HD13 | 2:G:4929:LEU:HA | 1.91 | 0.43 |
| 2:B:103:TYR:HB3 | 2:B:152:PRO:HD3 | 2.01 | 0.42 |
| 2:B:2927:LEU:HD23 | 2:B:2930:LEU:HD12 | 2.00 | 0.42 |
| 2:E:1105:ALA:HB1 | 2:E:1109:LEU:HD21 | 2.00 | 0.42 |
| 2:E:2793:PRO:HG3 | 2:E:2855:TYR:CZ | 2.54 | 0.42 |
| 2:E:4983:HIS:CB | 2:E:4988:TYR:HE2 | 2.32 | 0.42 |
| 2:E:4993:MET:HA | 2:E:4996:ILE:HD12 | 2.01 | 0.42 |
| 2:I:887:ILE:HG21 | 2:I:959:TYR:HA | 2.01 | 0.42 |
| 2:I:1101:ARG:HH21 | 2:I:1115:LEU:H | 1.66 | 0.42 |
| 2:I:4983:HIS:CB | 2:I:4988:TYR:HE2 | 2.32 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:485:SER:O | 2:G:489:ASN:N | 2.37 | 0.42 |
| 2:G:2342:ASN:OD1 | 2:G:2342:ASN:N | 2.51 | 0.42 |
| 2:B:2793:PRO:HG3 | 2:B:2855:TYR:CZ | 2.54 | 0.42 |
| 2:E:2764:GLU:HG3 | 2:E:2857:PRO:HB2 | 2.00 | 0.42 |
| 2:I:2862:LEU:HB3 | 2:I:2928:LYS:HB3 | 2.00 | 0.42 |
| 2:G:599:VAL:HG23 | 2:G:600:LEU:HD12 | 2.00 | 0.42 |
| 2:G:4833:ASN:ND2 | 2:G:4935:LEU:O | 2.52 | 0.42 |
| 2:B:379:HIS:NE2 | 2:B:381:GLU:OE1 | 2.52 | 0.42 |
| 2:B:1725:ARG:HA | 2:B:1728:ARG:HG2 | 2.01 | 0.42 |
| 2:B:3830:GLN:HA | 2:B:3833:GLN:HG2 | 2.02 | 0.42 |
| 2:E:1859:VAL:HA | 2:E:1862:ILE:HG12 | 2.01 | 0.42 |
| 2:E:4763:GLY:O | 2:E:4766:THR:OG1 | 2.33 | 0.42 |
| 2:G:278:GLN:N | 2:G:315:CYS:SG | 2.92 | 0.42 |
| 2:B:38:ALA:HB1 | 2:B:64:ILE:HG13 | 2.02 | 0.42 |
| 2:B:599:VAL:HG23 | 2:B:600:LEU:HD12 | 2.00 | 0.42 |
| 2:B:1804:LEU:O | 2:B:1808:ARG:N | 2.49 | 0.42 |
| 2:B:2257:LEU:O | 2:B:2261:SER:N | 2.51 | 0.42 |
| 2:B:4673:ARG:HH12 | 2:B:4698:LYS:HE3 | 1.84 | 0.42 |
| 2:I:38:ALA:HB1 | 2:I:64:ILE:HG13 | 2.02 | 0.42 |
| 2:G:38:ALA:HB1 | 2:G:64:ILE:HG13 | 2.02 | 0.42 |
| 2:G:119:SER:HA | 2:G:146:CYS:HA | 2.01 | 0.42 |
| 2:G:2793:PRO:HG3 | 2:G:2855:TYR:CZ | 2.54 | 0.42 |
| 2:B:1269:CYS:HA | 2:B:1473:UNK:HA | 2.01 | 0.42 |
| 2:B:1694:LEU:O | 2:B:1712:TYR:OH | 2.27 | 0.42 |
| 2:B:4993:MET:HA | 2:B:4996:ILE:HD12 | 2.00 | 0.42 |
| 2:E:1679:ASN:HA | 2:E:1682:ALA:HB3 | 2.01 | 0.42 |
| 2:E:4833:ASN:ND2 | 2:E:4935:LEU:O | 2.52 | 0.42 |
| 2:I:1269:CYS:HA | 2:I:1473:UNK:HA | 2.01 | 0.42 |
| 2:G:1973:GLN:O | 2:G:1977:TYR:N | 2.45 | 0.42 |
| 2:B:2517:UNK:O | 2:B:2521:UNK:N | 2.53 | 0.42 |
| 2:E:1676:LEU:HD23 | 2:E:2167:ILE:HG23 | 2.01 | 0.42 |
| 2:I:3830:GLN:HA | 2:I:3833:GLN:HG2 | 2.02 | 0.42 |
| 2:I:4763:GLY:O | 2:I:4766:THR:OG1 | 2.32 | 0.42 |
| 2:G:940:GLY:O | 2:G:1052:ASN:N | 2.53 | 0.42 |
| 2:G:989:ALA:O | 2:G:1035:ASN:ND2 | 2.52 | 0.42 |
| 2:B:983:THR:O | 2:B:987:ARG:N | 2.48 | 0.42 |
| 2:I:983:THR:O | 2:I:987:ARG:N | 2.48 | 0.42 |
| 2:I:2024:PRO:O | 2:I:2028:ARG:NE | 2.49 | 0.42 |
| 2:G:34:LYS:N | 2:G:53:SER:OG | 2.40 | 0.42 |
| 2:G:103:TYR:HB3 | 2:G:152:PRO:HD3 | 2.01 | 0.42 |
| 2:G:1859:VAL:HA | 2:G:1862:ILE:HG12 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:4983:HIS:CB | 2:G:4988:TYR:HE2 | 2.32 | 0.42 |
| 2:G:4993:MET:HA | 2:G:4996:ILE:HD12 | 2.01 | 0.42 |
| 2:B:1859:VAL:HA | 2:B:1862:ILE:HG12 | 2.01 | 0.42 |
| 2:E:38:ALA:HB1 | 2:E:64:ILE:HG13 | 2.02 | 0.42 |
| 2:E:379:HIS:NE2 | 2:E:381:GLU:OE1 | 2.51 | 0.42 |
| 2:E:1725:ARG:HA | 2:E:1728:ARG:HG2 | 2.01 | 0.42 |
| 2:E:2024:PRO:HB2 | 2:E:2027:ILE:HG12 | 2.02 | 0.42 |
| 2:G:1725:ARG:HA | 2:G:1728:ARG:HG2 | 2.01 | 0.42 |
| 2:B:1676:LEU:HD23 | 2:B:2167:ILE:HG23 | 2.01 | 0.42 |
| 2:E:1237:TRP:HH2 | 2:E:1652:GLU:HA | 1.85 | 0.42 |
| 2:E:2024:PRO:O | 2:E:2028:ARG:NE | 2.49 | 0.42 |
| 2:E:3830:GLN:HA | 2:E:3833:GLN:HG2 | 2.02 | 0.42 |
| 2:I:940:GLY:O | 2:I:1052:ASN:N | 2.53 | 0.42 |
| 2:I:1804:LEU:O | 2:I:1808:ARG:N | 2.49 | 0.42 |
| 2:I:1973:GLN:HA | 2:I:1976:ARG:HB3 | 2.00 | 0.42 |
| 2:G:1854:PHE:HD1 | 2:G:1858:ASP:HB3 | 1.84 | 0.42 |
| 2:G:2024:PRO:HB2 | 2:G:2027:ILE:HG12 | 2.02 | 0.42 |
| 2:G:2517:UNK:O | 2:G:2521:UNK:N | 2.53 | 0.42 |
| 2:B:734:GLY:O | 2:B:736:HIS:ND1 | 2.51 | 0.42 |
| 2:B:776:LEU:HG | 2:B:848:HIS:HA | 2.01 | 0.42 |
| 2:B:4929:LEU:HD13 | 2:B:4929:LEU:HA | 1.91 | 0.42 |
| 2:E:599:VAL:HG23 | 2:E:600:LEU:HD12 | 2.00 | 0.42 |
| 2:E:1854:PHE:HD1 | 2:E:1858:ASP:HB3 | 1.84 | 0.42 |
| 2:E:2342:ASN:OD1 | 2:E:2342:ASN:N | 2.51 | 0.42 |
| 2:I:4066:LEU:HD11 | 2:I:4173:TYR:HB2 | 2.02 | 0.42 |
| 2:G:1679:ASN:HA | 2:G:1682:ALA:HB3 | 2.01 | 0.42 |
| 2:E:1269:CYS:HA | 2:E:1473:UNK:HA | 2.01 | 0.41 |
| 2:I:3647:HIS:O | 2:I:3651:ASN:ND2 | 2.53 | 0.41 |
| 2:G:734:GLY:O | 2:G:736:HIS:ND1 | 2.51 | 0.41 |
| 2:G:1103:GLY:HA3 | 2:G:1123:VAL:HA | 2.02 | 0.41 |
| 2:G:3830:GLN:HA | 2:G:3833:GLN:HG2 | 2.02 | 0.41 |
| 2:G:4066:LEU:HD11 | 2:G:4173:TYR:HB2 | 2.02 | 0.41 |
| 2:B:582:HIS:O | 2:B:585:SER:OG | 2.30 | 0.41 |
| 2:B:4066:LEU:HD11 | 2:B:4173:TYR:HB2 | 2.02 | 0.41 |
| 2:G:1154:ASP:O | 2:G:1158:ASN:N | 2.53 | 0.41 |
| 2:B:989:ALA:O | 2:B:1035:ASN:ND2 | 2.52 | 0.41 |
| 2:B:1237:TRP:HH2 | 2:B:1652:GLU:HA | 1.85 | 0.41 |
| 2:B:4833:ASN:ND2 | 2:B:4935:LEU:O | 2.52 | 0.41 |
| 2:E:1171:SER:OG | 2:E:1175:SER:N | 2.44 | 0.41 |
| 2:E:2517:UNK:O | 2:E:2521:UNK:N | 2.53 | 0.41 |
| 2:E:3647:HIS:O | 2:E:3651:ASN:ND2 | 2.53 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1676:LEU:HD23 | 2:I:2167:ILE:HG23 | 2.01 | 0.41 |
| 2:I:2674:UNK:O | 2:I:2676:UNK:N | 2.53 | 0.41 |
| 2:I:4084:PRO:HD2 | 2:I:4085:ARG:NH1 | 2.36 | 0.41 |
| 2:I:4823:LEU:HD23 | 2:G:4843:LEU:HD12 | 2.01 | 0.41 |
| 2:I:4929:LEU:HD13 | 2:I:4929:LEU:HA | 1.91 | 0.41 |
| 2:G:2674:UNK:O | 2:G:2676:UNK:N | 2.54 | 0.41 |
| 2:B:1103:GLY:HA3 | 2:B:1123:VAL:HA | 2.02 | 0.41 |
| 2:B:1679:ASN:HA | 2:B:1682:ALA:HB3 | 2.01 | 0.41 |
| 2:E:278:GLN:N | 2:E:315:CYS:SG | 2.92 | 0.41 |
| 2:E:776:LEU:HG | 2:E:848:HIS:HA | 2.01 | 0.41 |
| 2:E:2823:ILE:HG12 | 2:E:2937:VAL:HG22 | 2.03 | 0.41 |
| 2:I:1154:ASP:O | 2:I:1158:ASN:N | 2.53 | 0.41 |
| 2:I:2024:PRO:HB2 | 2:I:2027:ILE:HG12 | 2.02 | 0.41 |
| 2:G:280:LEU:HD21 | 2:G:316:PHE:HE2 | 1.86 | 0.41 |
| 1:A:2:VAL:HG21 | 1:A:61:GLU:HB2 | 2.02 | 0.41 |
| 2:B:280:LEU:HD21 | 2:B:316:PHE:HE2 | 1.86 | 0.41 |
| 2:B:2466:LEU:HD23 | 2:B:2469:ILE:HD12 | 2.03 | 0.41 |
| 2:B:4148:THR:HG21 | 2:B:4178:LEU:HD21 | 2.02 | 0.41 |
| 2:E:1973:GLN:O | 2:E:1977:TYR:N | 2.45 | 0.41 |
| 2:I:877:ASN:HD22 | 2:I:1045:THR:HG23 | 1.85 | 0.41 |
| 2:G:1237:TRP:HH2 | 2:G:1652:GLU:HA | 1.85 | 0.41 |
| 2:G:3647:HIS:O | 2:G:3651:ASN:ND2 | 2.53 | 0.41 |
| 2:E:113:HIS:CE1 | 2:E:402:ARG:HB3 | 2.55 | 0.41 |
| 2:E:280:LEU:HD21 | 2:E:316:PHE:HE2 | 1.86 | 0.41 |
| 2:E:4066:LEU:HD11 | 2:E:4173:TYR:HB2 | 2.02 | 0.41 |
| 2:E:4084:PRO:HD2 | 2:E:4085:ARG:NH1 | 2.36 | 0.41 |
| 2:E:4148:THR:HG21 | 2:E:4178:LEU:HD21 | 2.02 | 0.41 |
| 2:I:278:GLN:N | 2:I:315:CYS:SG | 2.92 | 0.41 |
| 2:I:1679:ASN:HA | 2:I:1682:ALA:HB3 | 2.01 | 0.41 |
| 2:G:113:HIS:CE1 | 2:G:402:ARG:HB3 | 2.55 | 0.41 |
| 2:G:2214:VAL:HG23 | 2:G:2215:LEU:HD12 | 2.03 | 0.41 |
| 2:B:113:HIS:CE1 | 2:B:402:ARG:HB3 | 2.55 | 0.41 |
| 2:B:786:GLY:HA2 | 2:B:1631:GLN:HA | 2.03 | 0.41 |
| 2:B:940:GLY:O | 2:B:1052:ASN:N | 2.53 | 0.41 |
| 2:B:2299:VAL:O | 2:B:2303:ALA:N | 2.50 | 0.41 |
| 2:E:877:ASN:HD22 | 2:E:1045:THR:HG23 | 1.85 | 0.41 |
| 2:E:989:ALA:O | 2:E:1035:ASN:ND2 | 2.52 | 0.41 |
| 2:E:1641:ILE:HA | 2:E:1642:PRO:HD3 | 1.93 | 0.41 |
| 2:E:2004:GLU:HA | 2:E:2007:ASN:HD22 | 1.86 | 0.41 |
| 2:E:2674:UNK:O | 2:E:2676:UNK:N | 2.54 | 0.41 |
| 2:I:786:GLY:HA2 | 2:I:1631:GLN:HA | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:983:THR:O | 2:G:987:ARG:N | 2.48 | 0.41 |
| 2:E:103:TYR:HB3 | 2:E:152:PRO:HD3 | 2.01 | 0.41 |
| 2:E:750:LEU:HD21 | 2:E:777:PHE:HE2 | 1.86 | 0.41 |
| 2:E:940:GLY:O | 2:E:1052:ASN:N | 2.53 | 0.41 |
| 2:I:113:HIS:CE1 | 2:I:402:ARG:HB3 | 2.55 | 0.41 |
| 2:I:1725:ARG:HA | 2:I:1728:ARG:HG2 | 2.01 | 0.41 |
| 2:I:2810:LYS:O | 2:I:2814:LYS:N | 2.45 | 0.41 |
| 2:I:2823:ILE:HG12 | 2:I:2937:VAL:HG22 | 2.03 | 0.41 |
| 2:G:4697:VAL:O | 2:G:4701:TRP:N | 2.52 | 0.41 |
| 1:F:2:VAL:HG21 | 1:F:61:GLU:HB2 | 2.02 | 0.41 |
| 1:A:7:ILE:N | 1:A:71:ARG:O | 2.50 | 0.41 |
| 1:J:7:ILE:N | 1:J:71:ARG:O | 2.50 | 0.41 |
| 2:B:767:VAL:HG12 | 2:B:769:GLU:HG3 | 2.03 | 0.41 |
| 2:B:877:ASN:HD22 | 2:B:1045:THR:HG23 | 1.85 | 0.41 |
| 2:B:2674:UNK:O | 2:B:2676:UNK:N | 2.54 | 0.41 |
| 2:B:2823:ILE:HG12 | 2:B:2937:VAL:HG22 | 2.03 | 0.41 |
| 2:B:3647:HIS:O | 2:B:3651:ASN:ND2 | 2.53 | 0.41 |
| 2:B:4084:PRO:HD2 | 2:B:4085:ARG:NH1 | 2.36 | 0.41 |
| 2:B:4960:ILE:HD11 | 2:B:4985:LEU:CD2 | 2.51 | 0.41 |
| 2:E:1141:ARG:H | 2:E:1141:ARG:HD2 | 1.86 | 0.41 |
| 2:E:1154:ASP:O | 2:E:1158:ASN:N | 2.53 | 0.41 |
| 2:E:1863:LEU:HB3 | 2:E:1870:VAL:HG21 | 2.03 | 0.41 |
| 2:I:2243:SER:HB3 | 2:I:2246:ASN:H | 1.86 | 0.41 |
| 2:I:3971:GLY:N | 2:I:4032:GLU:OE2 | 2.47 | 0.41 |
| 2:I:4833:ASN:ND2 | 2:I:4935:LEU:O | 2.52 | 0.41 |
| 2:G:647:ASN:ND2 | 2:G:820:ARG:O | 2.50 | 0.41 |
| 2:G:2004:GLU:HA | 2:G:2007:ASN:HD22 | 1.86 | 0.41 |
| 1:H:2:VAL:HG21 | 1:H:61:GLU:HB2 | 2.02 | 0.41 |
| 1:J:2:VAL:HG21 | 1:J:61:GLU:HB2 | 2.02 | 0.41 |
| 2:B:1863:LEU:HB3 | 2:B:1870:VAL:HG21 | 2.03 | 0.41 |
| 2:B:2024:PRO:HB2 | 2:B:2027:ILE:HG12 | 2.02 | 0.41 |
| 2:E:767:VAL:HG12 | 2:E:769:GLU:HG3 | 2.03 | 0.41 |
| 2:E:790:ARG:HG2 | 2:E:1627:ALA:HA | 2.03 | 0.41 |
| 2:E:4957:LYS:HG2 | 2:E:4964:GLY:CA | 2.51 | 0.41 |
| 2:I:2517:UNK:O | 2:I:2521:UNK:N | 2.53 | 0.41 |
| 2:I:3971:GLY:H | 2:I:5005:GLY:HA3 | 1.86 | 0.41 |
| 2:G:877:ASN:HD22 | 2:G:1045:THR:HG23 | 1.85 | 0.41 |
| 2:G:2823:ILE:HG12 | 2:G:2937:VAL:HG22 | 2.03 | 0.41 |
| 2:B:4886:HIS:O | 2:B:4890:GLY:N | 2.52 | 0.40 |
| 2:E:4976:GLU:HA | 2:E:4979:THR:CG2 | 2.52 | 0.40 |
| 2:I:864:PRO:HD2 | 2:I:867:LEU:HD12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1237:TRP:HH2 | 2:I:1652:GLU:HA | 1.85 | 0.40 |
| 2:I:2466:LEU:HD23 | 2:I:2469:ILE:HD12 | 2.03 | 0.40 |
| 2:I:4148:THR:HG21 | 2:I:4178:LEU:HD21 | 2.02 | 0.40 |
| 2:G:37:LEU:HD11 | 2:G:47:CYS:HB3 | 2.04 | 0.40 |
| 2:G:2095:GLN:HA | 2:G:2127:GLN:NE2 | 2.37 | 0.40 |
| 2:G:4763:GLY:O | 2:G:4766:THR:OG1 | 2.32 | 0.40 |
| 2:E:1103:GLY:HA3 | 2:E:1123:VAL:HA | 2.02 | 0.40 |
| 2:I:1802:ILE:HG21 | 2:I:1807:LEU:HD22 | 2.04 | 0.40 |
| 2:I:4960:ILE:HD11 | 2:I:4985:LEU:CD2 | 2.51 | 0.40 |
| 2:G:767:VAL:HG12 | 2:G:769:GLU:HG3 | 2.03 | 0.40 |
| 2:G:1653:LEU:HB3 | 2:G:1660:GLN:HB2 | 2.04 | 0.40 |
| 2:B:358:THR:HG21 | 2:B:382:GLY:HA2 | 2.04 | 0.40 |
| 2:B:1078:GLU:HB3 | 2:B:1081:TYR:HD2 | 1.86 | 0.40 |
| 2:B:1808:ARG:HD3 | 2:B:1853:ILE:HG22 | 2.04 | 0.40 |
| 2:B:2004:GLU:HA | 2:B:2007:ASN:HD22 | 1.86 | 0.40 |
| 2:B:4080:TYR:CZ | 2:B:4096:ALA:HB3 | 2.56 | 0.40 |
| 2:E:2034:PHE:O | 2:E:2038:LEU:N | 2.55 | 0.40 |
| 2:I:37:LEU:HD11 | 2:I:47:CYS:HB3 | 2.03 | 0.40 |
| 2:G:4976:GLU:HA | 2:G:4979:THR:CG2 | 2.52 | 0.40 |
| 2:B:750:LEU:HD21 | 2:B:777:PHE:HE2 | 1.86 | 0.40 |
| 2:B:1154:ASP:O | 2:B:1158:ASN:N | 2.53 | 0.40 |
| 2:E:786:GLY:HA2 | 2:E:1631:GLN:HA | 2.03 | 0.40 |
| 2:E:2095:GLN:HA | 2:E:2127:GLN:NE2 | 2.36 | 0.40 |
| 2:E:2466:LEU:HA | 2:E:2469:ILE:HD12 | 2.03 | 0.40 |
| 2:E:4156:HIS:CE1 | 2:E:5036:LEU:HD11 | 2.56 | 0.40 |
| 2:I:280:LEU:HD21 | 2:I:316:PHE:HE2 | 1.86 | 0.40 |
| 2:I:2034:PHE:O | 2:I:2038:LEU:N | 2.55 | 0.40 |
| 2:I:4987:ASN:HA | 2:I:4990:PHE:HD2 | 1.87 | 0.40 |
| 2:G:786:GLY:HA2 | 2:G:1631:GLN:HA | 2.03 | 0.40 |
| 2:G:1078:GLU:HG3 | 2:G:1237:TRP:HE1 | 1.87 | 0.40 |
| 2:G:2243:SER:HB3 | 2:G:2246:ASN:H | 1.86 | 0.40 |
| 2:G:4987:ASN:HA | 2:G:4990:PHE:HD2 | 1.87 | 0.40 |
| 2:B:2095:GLN:HA | 2:B:2127:GLN:NE2 | 2.37 | 0.40 |
| 2:B:2214:VAL:HG23 | 2:B:2215:LEU:HD12 | 2.03 | 0.40 |
| 2:B:4984:ASN:C | 2:B:4986:ALA:N | 2.75 | 0.40 |
| 2:I:750:LEU:HD21 | 2:I:777:PHE:HE2 | 1.86 | 0.40 |
| 2:I:1653:LEU:HB3 | 2:I:1660:GLN:HB2 | 2.04 | 0.40 |
| 2:I:1863:LEU:HB3 | 2:I:1870:VAL:HG21 | 2.03 | 0.40 |
| 2:I:2095:GLN:HA | 2:I:2127:GLN:NE2 | 2.36 | 0.40 |
| 2:G:794:GLY:H | 2:G:798:GLY:HA3 | 1.87 | 0.40 |
| 2:G:2466:LEU:HA | 2:G:2469:ILE:HD12 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:3971:GLY:H | 2:G:5005:GLY:HA3 | 1.86 | 0.40 |
| 2:G:4148:THR:HG21 | 2:G:4178:LEU:HD21 | 2.02 | 0.40 |
| 2:G:4156:HIS:CE1 | 2:G:5036:LEU:HD11 | 2.56 | 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%) | 98 (93%) | 7 (7%) | 0 | 100 | 100 |
| 1 | F | 105/108 (97%) | 98 (93%) | 7 (7%) | 0 | 100 | 100 |
| 1 | H | 105/108 (97%) | 98 (93%) | 7 (7%) | 0 | 100 | 100 |
| 1 | J | 105/108 (97%) | 98 (93%) | 7 (7%) | 0 | 100 | 100 |
| 2 | B | 3235/4416 (73%) | 2891 (89%) | 338 (10%) | 6 (0%) | 47 | 81 |
| 2 | E | 3235/4416 (73%) | 2892 (89%) | 338 (10%) | 5 (0%) | 47 | 81 |
| 2 | G | 3235/4416 (73%) | 2890 (89%) | 340 (10%) | 5 (0%) | 47 | 81 |
| 2 | I | 3235/4416 (73%) | 2889 (89%) | 340 (10%) | 6 (0%) | 47 | 81 |
| All | All | 13360/18096 (74%) | 11954 (90%) | 1384 (10%) | 22 (0%) | 50 | 81 |

All (22) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 5028 | PHE |
| 2 | E | 5028 | PHE |
| 2 | I | 5028 | PHE |
| 2 | G | 5028 | PHE |
| 2 | B | 1932 | PRO |
| 2 | E | 1932 | PRO |
| 2 | I | 1932 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 1932 | PRO |
| 2 | B | 1708 | ARG |
| 2 | E | 1708 | ARG |
| 2 | I | 1708 | ARG |
| 2 | G | 1708 | ARG |
| 2 | B | 1840 | PRO |
| 2 | B | 4641 | PRO |
| 2 | E | 1840 | PRO |
| 2 | E | 4641 | PRO |
| 2 | I | 1840 | PRO |
| 2 | I | 4641 | PRO |
| 2 | G | 1840 | PRO |
| 2 | G | 4641 | PRO |
| 2 | B | 4985 | LEU |
| 2 | I | 4985 | LEU |

### 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%) | 2474 (99%) | 19 (1%) | 81 | 89 |
| 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%) | 10251 (99%) | 73 (1%) | 84 | 90 |

All (73) 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 | 1076 | ARG |
| 2 | B | 1141 | ARG |
| 2 | B | 1600 | LEU |
| 2 | B | 1676 | LEU |
| 2 | B | 1964 | ARG |
| 2 | B | 3787 | LYS |
| 2 | B | 3896 | ASN |
| 2 | B | 4034 | ASN |
| 2 | B | 4085 | ARG |
| 2 | B | 4120 | ASN |
| 2 | B | 4131 | ARG |
| 2 | B | 4137 | ARG |
| 2 | B | 4913 | ARG |
| 2 | B | 4944 | ARG |
| 2 | B | 4961 | CYS |
| 2 | E | 131 | LEU |
| 2 | E | 534 | ARG |
| 2 | E | 553 | ARG |
| 2 | E | 1076 | ARG |
| 2 | E | 1141 | ARG |
| 2 | E | 1600 | LEU |
| 2 | E | 1676 | LEU |
| 2 | E | 1964 | ARG |
| 2 | E | 3787 | LYS |
| 2 | E | 3805 | LEU |
| 2 | E | 3896 | ASN |
| 2 | E | 4034 | ASN |
| 2 | E | 4085 | ARG |
| 2 | E | 4120 | ASN |
| 2 | E | 4131 | ARG |
| 2 | E | 4137 | ARG |
| 2 | E | 4913 | ARG |
| 2 | E | 4944 | ARG |
| 2 | E | 4961 | CYS |
| 2 | I | 131 | LEU |
| 2 | I | 534 | ARG |
| 2 | I | 553 | ARG |
| 2 | I | 1076 | ARG |
| 2 | I | 1141 | ARG |
| 2 | I | 1600 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 1676 | LEU |
| 2 | I | 1964 | ARG |
| 2 | I | 3787 | LYS |
| 2 | I | 3896 | ASN |
| 2 | I | 4034 | ASN |
| 2 | I | 4085 | ARG |
| 2 | I | 4120 | ASN |
| 2 | I | 4131 | ARG |
| 2 | I | 4137 | ARG |
| 2 | I | 4913 | ARG |
| 2 | I | 4944 | ARG |
| 2 | I | 4961 | CYS |
| 2 | G | 131 | LEU |
| 2 | G | 534 | ARG |
| 2 | G | 553 | ARG |
| 2 | G | 1076 | ARG |
| 2 | G | 1141 | ARG |
| 2 | G | 1600 | LEU |
| 2 | G | 1676 | LEU |
| 2 | G | 1964 | ARG |
| 2 | G | 3787 | LYS |
| 2 | G | 3896 | ASN |
| 2 | G | 4034 | ASN |
| 2 | G | 4085 | ARG |
| 2 | G | 4120 | ASN |
| 2 | G | 4131 | ARG |
| 2 | G | 4137 | ARG |
| 2 | G | 4913 | ARG |
| 2 | G | 4944 | ARG |
| 2 | G | 4961 | CYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) 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 | 113 | HIS |
| 2 | B | 224 | HIS |
| 2 | B | 273 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 379 | HIS |
| 2 | B | 383 | HIS |
| 2 | B | 395 | GLN |
| 2 | B | 413 | GLN |
| 2 | B | 479 | GLN |
| 2 | B | 520 | ASN |
| 2 | B | 582 | HIS |
| 2 | B | 725 | HIS |
| 2 | B | 1598 | GLN |
| 2 | B | 1679 | ASN |
| 2 | B | 1688 | HIS |
| 2 | B | 1691 | GLN |
| 2 | B | 1693 | GLN |
| 2 | B | 1719 | HIS |
| 2 | B | 1775 | HIS |
| 2 | B | 1972 | ASN |
| 2 | B | 2005 | GLN |
| 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 | 3976 | ASN |
| 2 | B | 4034 | ASN |
| 2 | B | 4054 | ASN |
| 2 | B | 4120 | ASN |
| 2 | B | 4142 | ASN |
| 2 | B | 4209 | GLN |
| 2 | B | 4806 | ASN |
| 2 | B | 4983 | HIS |
| 2 | B | 5003 | HIS |
| 2 | E | 57 | ASN |
| 2 | E | 111 | HIS |
| 2 | E | 113 | HIS |
| 2 | E | 224 | HIS |
| 2 | E | 273 | HIS |
| 2 | E | 379 | HIS |
| 2 | E | 383 | HIS |
| 2 | E | 395 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 413 | GLN |
| 2 | E | 479 | GLN |
| 2 | E | 520 | ASN |
| 2 | E | 582 | HIS |
| 2 | E | 725 | HIS |
| 2 | E | 1598 | GLN |
| 2 | E | 1679 | ASN |
| 2 | E | 1688 | HIS |
| 2 | E | 1691 | GLN |
| 2 | E | 1693 | GLN |
| 2 | E | 1719 | HIS |
| 2 | E | 1775 | HIS |
| 2 | E | 1972 | ASN |
| 2 | E | 2005 | GLN |
| 2 | E | 2127 | GLN |
| 2 | E | 3766 | GLN |
| 2 | E | 3809 | ASN |
| 2 | E | 3889 | GLN |
| 2 | E | 3896 | ASN |
| 2 | E | 3946 | GLN |
| 2 | E | 3950 | ASN |
| 2 | E | 3960 | GLN |
| 2 | E | 3976 | ASN |
| 2 | E | 4034 | ASN |
| 2 | E | 4054 | ASN |
| 2 | E | 4120 | ASN |
| 2 | E | 4209 | GLN |
| 2 | E | 4806 | ASN |
| 2 | E | 4983 | HIS |
| 2 | E | 5003 | HIS |
| 2 | I | 57 | ASN |
| 2 | I | 111 | HIS |
| 2 | I | 113 | HIS |
| 2 | I | 224 | HIS |
| 2 | I | 273 | HIS |
| 2 | I | 379 | HIS |
| 2 | I | 383 | HIS |
| 2 | I | 395 | GLN |
| 2 | I | 413 | GLN |
| 2 | I | 479 | GLN |
| 2 | I | 520 | ASN |
| 2 | I | 582 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 725 | HIS |
| 2 | I | 1598 | GLN |
| 2 | I | 1679 | ASN |
| 2 | I | 1688 | HIS |
| 2 | I | 1691 | GLN |
| 2 | I | 1693 | GLN |
| 2 | I | 1719 | HIS |
| 2 | I | 1775 | HIS |
| 2 | I | 1972 | ASN |
| 2 | I | 2005 | GLN |
| 2 | I | 2127 | GLN |
| 2 | I | 3766 | GLN |
| 2 | I | 3809 | ASN |
| 2 | I | 3889 | GLN |
| 2 | I | 3896 | ASN |
| 2 | I | 3946 | GLN |
| 2 | I | 3950 | ASN |
| 2 | I | 3960 | GLN |
| 2 | I | 3976 | ASN |
| 2 | I | 4034 | ASN |
| 2 | I | 4054 | ASN |
| 2 | I | 4120 | ASN |
| 2 | I | 4142 | ASN |
| 2 | I | 4209 | GLN |
| 2 | I | 4806 | ASN |
| 2 | I | 4983 | HIS |
| 2 | I | 5003 | HIS |
| 2 | G | 57 | ASN |
| 2 | G | 111 | HIS |
| 2 | G | 113 | HIS |
| 2 | G | 224 | HIS |
| 2 | G | 273 | HIS |
| 2 | G | 379 | HIS |
| 2 | G | 383 | HIS |
| 2 | G | 395 | GLN |
| 2 | G | 413 | GLN |
| 2 | G | 479 | GLN |
| 2 | G | 582 | HIS |
| 2 | G | 725 | HIS |
| 2 | G | 1598 | GLN |
| 2 | G | 1679 | ASN |
| 2 | G | 1688 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 1691 | GLN |
| 2 | G | 1693 | GLN |
| 2 | G | 1719 | HIS |
| 2 | G | 1775 | HIS |
| 2 | G | 1972 | ASN |
| 2 | G | 2005 | GLN |
| 2 | G | 2127 | GLN |
| 2 | G | 3766 | GLN |
| 2 | G | 3809 | ASN |
| 2 | G | 3889 | GLN |
| 2 | G | 3896 | ASN |
| 2 | G | 3946 | GLN |
| 2 | G | 3950 | ASN |
| 2 | G | 3960 | GLN |
| 2 | G | 3976 | ASN |
| 2 | G | 4034 | ASN |
| 2 | G | 4054 | ASN |
| 2 | G | 4120 | ASN |
| 2 | G | 4209 | GLN |
| 2 | G | 4806 | ASN |
| 2 | G | 4983 | HIS |
| 2 | G | 5003 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 4 | CFF | I | 5102 | - | 8,15,15 | 2.51 | 3 (37%) | 8,23,23 | 1.24 | 1 (12%) |
| 4 | CFF | G | 5102 | - | 8,15,15 | 2.51 | 3 (37%) | 8,23,23 | 1.24 | 1 (12%) |
| 4 | CFF | E | 5102 | - | 8,15,15 | 2.51 | 3 (37%) | 8,23,23 | 1.24 | 1 (12%) |
| 3 | ATP | I | 5101 | - | 26,33,33 | 0.88 | 1 (3%) | 31,52,52 | 1.51 | 5 (16%) |
| 3 | ATP | G | 5101 | - | 26,33,33 | 0.88 | 1 (3%) | 31,52,52 | 1.51 | 5 (16%) |
| 4 | CFF | B | 5102 | - | 8,15,15 | 2.51 | 3 (37%) | 8,23,23 | 1.24 | 1 (12%) |
| 3 | ATP | B | 5101 | - | 26,33,33 | 0.88 | 1 (3%) | 31,52,52 | 1.52 | 5 (16%) |
| 3 | ATP | E | 5101 | - | 26,33,33 | 0.88 | 1 (3%) | 31,52,52 | 1.51 | 5 (16%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | CFF | I | 5102 | - | - | - | 0/2/2/2 |
| 4 | CFF | G | 5102 | - | - | - | 0/2/2/2 |
| 4 | CFF | E | 5102 | - | - | - | 0/2/2/2 |
| 3 | ATP | I | 5101 | - | - | 6/18/38/38 | 0/3/3/3 |
| 3 | ATP | G | 5101 | - | - | 6/18/38/38 | 0/3/3/3 |
| 4 | CFF | B | 5102 | - | - | - | 0/2/2/2 |
| 3 | ATP | B | 5101 | - | - | 6/18/38/38 | 0/3/3/3 |
| 3 | ATP | E | 5101 | - | - | 6/18/38/38 | 0/3/3/3 |

All (16) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | B | 5102 | CFF | C5-C4 | -4.59 | 1.33 | 1.39 |
| 4 | E | 5102 | CFF | C5-C4 | -4.59 | 1.33 | 1.39 |
| 4 | I | 5102 | CFF | C5-C4 | -4.59 | 1.33 | 1.39 |
| 4 | G | 5102 | CFF | C5-C4 | -4.59 | 1.33 | 1.39 |
| 4 | G | 5102 | CFF | C6-N1 | -4.05 | 1.32 | 1.38 |
| 4 | I | 5102 | CFF | C6-N1 | -4.05 | 1.32 | 1.38 |
| 4 | B | 5102 | CFF | C6-N1 | -4.03 | 1.32 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | E | 5102 | CFF | C6-N1 | -4.03 | 1.32 | 1.38 |
| 4 | B | 5102 | CFF | O13-C6 | -2.38 | 1.18 | 1.24 |
| 4 | E | 5102 | CFF | O13-C6 | -2.38 | 1.18 | 1.24 |
| 4 | I | 5102 | CFF | O13-C6 | -2.38 | 1.18 | 1.24 |
| 4 | G | 5102 | CFF | O13-C6 | -2.38 | 1.18 | 1.24 |
| 3 | B | 5101 | ATP | C5-C4 | 2.31 | 1.47 | 1.40 |
| 3 | I | 5101 | ATP | C5-C4 | 2.31 | 1.47 | 1.40 |
| 3 | G | 5101 | ATP | C5-C4 | 2.29 | 1.47 | 1.40 |
| 3 | E | 5101 | ATP | C5-C4 | 2.27 | 1.46 | 1.40 |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | B | 5101 | ATP | PB-O3B-PG | -3.40 | 121.16 | 132.83 |
| 3 | I | 5101 | ATP | PB-O3B-PG | -3.40 | 121.16 | 132.83 |
| 3 | E | 5101 | ATP | PB-O3B-PG | -3.40 | 121.17 | 132.83 |
| 3 | G | 5101 | ATP | PB-O3B-PG | -3.39 | 121.18 | 132.83 |
| 3 | G | 5101 | ATP | PA-O3A-PB | -3.28 | 121.58 | 132.83 |
| 3 | B | 5101 | ATP | PA-O3A-PB | -3.27 | 121.61 | 132.83 |
| 3 | I | 5101 | ATP | PA-O3A-PB | -3.27 | 121.61 | 132.83 |
| 3 | E | 5101 | ATP | PA-O3A-PB | -3.26 | 121.63 | 132.83 |
| 3 | E | 5101 | ATP | C3'-C2'-C1' | 3.10 | 105.64 | 100.98 |
| 3 | G | 5101 | ATP | C3'-C2'-C1' | 3.09 | 105.64 | 100.98 |
| 3 | B | 5101 | ATP | C3'-C2'-C1' | 3.09 | 105.64 | 100.98 |
| 3 | G | 5101 | ATP | N3-C2-N1 | -3.07 | 123.88 | 128.68 |
| 3 | I | 5101 | ATP | C3'-C2'-C1' | 3.06 | 105.59 | 100.98 |
| 3 | B | 5101 | ATP | N3-C2-N1 | -3.06 | 123.90 | 128.68 |
| 3 | I | 5101 | ATP | N3-C2-N1 | -3.04 | 123.92 | 128.68 |
| 3 | E | 5101 | ATP | N3-C2-N1 | -3.04 | 123.93 | 128.68 |
| 4 | I | 5102 | CFF | C14-N7-C8 | -2.85 | 111.73 | 125.43 |
| 4 | B | 5102 | CFF | C14-N7-C8 | -2.84 | 111.76 | 125.43 |
| 4 | E | 5102 | CFF | C14-N7-C8 | -2.84 | 111.76 | 125.43 |
| 4 | G | 5102 | CFF | C14-N7-C8 | -2.84 | 111.77 | 125.43 |
| 3 | I | 5101 | ATP | C4-C5-N7 | -2.38 | 106.92 | 109.40 |
| 3 | B | 5101 | ATP | C4-C5-N7 | -2.35 | 106.95 | 109.40 |
| 3 | G | 5101 | ATP | C4-C5-N7 | -2.34 | 106.96 | 109.40 |
| 3 | E | 5101 | ATP | C4-C5-N7 | -2.33 | 106.97 | 109.40 |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | B | 5101 | ATP | C5'-O5'-PA-O1A |
| 3 | B | 5101 | ATP | C5'-O5'-PA-O2A |
| 3 | E | 5101 | ATP | C5'-O5'-PA-O1A |
| 3 | E | 5101 | ATP | C5'-O5'-PA-O2A |
| 3 | I | 5101 | ATP | C5'-O5'-PA-O1A |
| 3 | I | 5101 | ATP | C5'-O5'-PA-O2A |
| 3 | G | 5101 | ATP | C5'-O5'-PA-O1A |
| 3 | G | 5101 | ATP | C5'-O5'-PA-O2A |
| 3 | B | 5101 | ATP | O4'-C4'-C5'-O5' |
| 3 | E | 5101 | ATP | O4'-C4'-C5'-O5' |
| 3 | I | 5101 | ATP | O4'-C4'-C5'-O5' |
| 3 | G | 5101 | ATP | O4'-C4'-C5'-O5' |
| 3 | B | 5101 | ATP | C4'-C5'-O5'-PA |
| 3 | E | 5101 | ATP | C4'-C5'-O5'-PA |
| 3 | I | 5101 | ATP | C4'-C5'-O5'-PA |
| 3 | G | 5101 | ATP | C4'-C5'-O5'-PA |
| 3 | B | 5101 | ATP | C3'-C4'-C5'-O5' |
| 3 | E | 5101 | ATP | C3'-C4'-C5'-O5' |
| 3 | I | 5101 | ATP | C3'-C4'-C5'-O5' |
| 3 | G | 5101 | ATP | C3'-C4'-C5'-O5' |
| 3 | B | 5101 | ATP | C5'-O5'-PA-O3A |
| 3 | E | 5101 | ATP | C5'-O5'-PA-O3A |
| 3 | I | 5101 | ATP | C5'-O5'-PA-O3A |
| 3 | G | 5101 | ATP | C5'-O5'-PA-O3A |

There are no ring outliers.

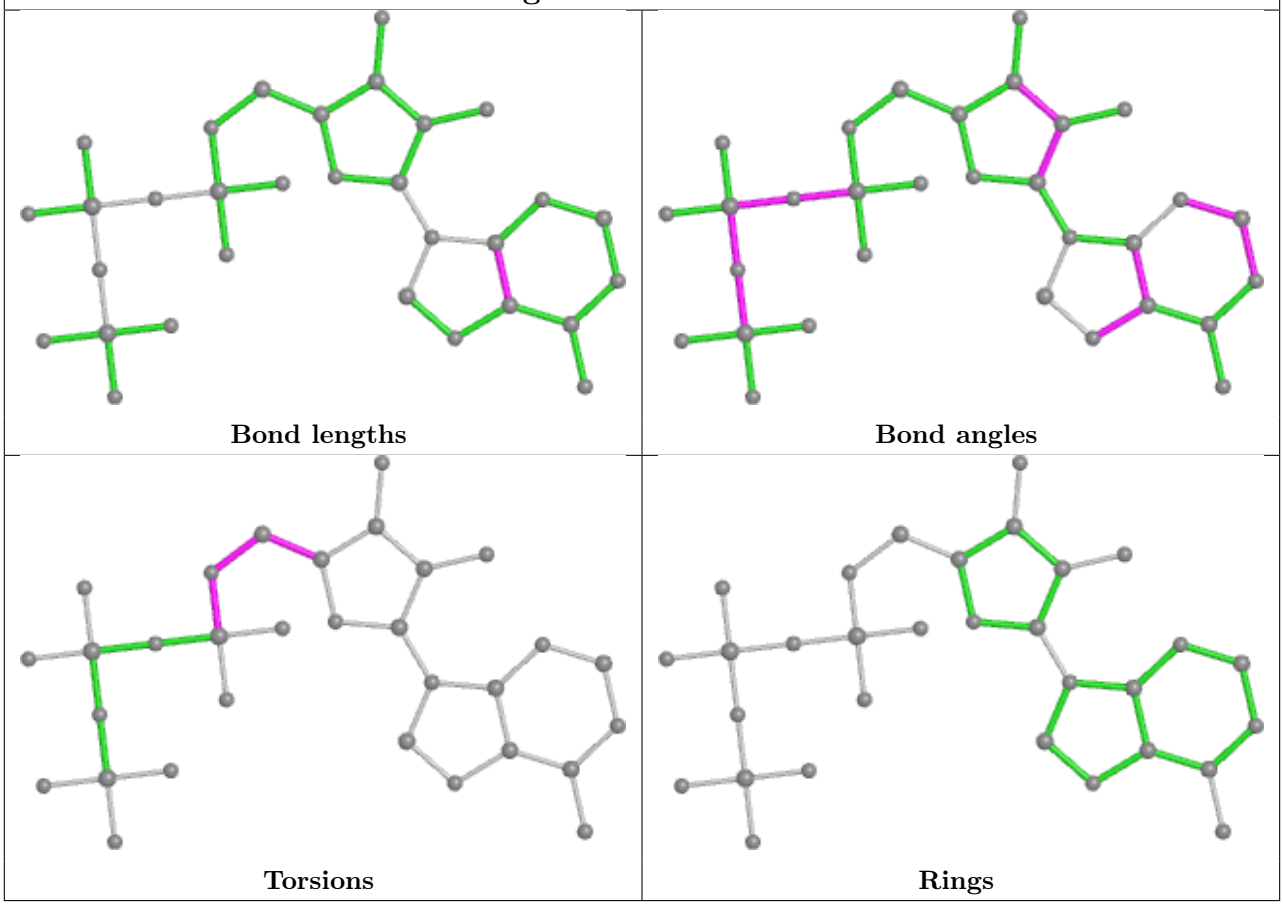
8 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | I | 5102 | CFF | 1 | 0 |
| 4 | G | 5102 | CFF | 1 | 0 |
| 4 | E | 5102 | CFF | 1 | 0 |
| 3 | I | 5101 | ATP | 2 | 0 |
| 3 | G | 5101 | ATP | 2 | 0 |
| 4 | B | 5102 | CFF | 1 | 0 |
| 3 | B | 5101 | ATP | 2 | 0 |
| 3 | E | 5101 | ATP | 2 | 0 |

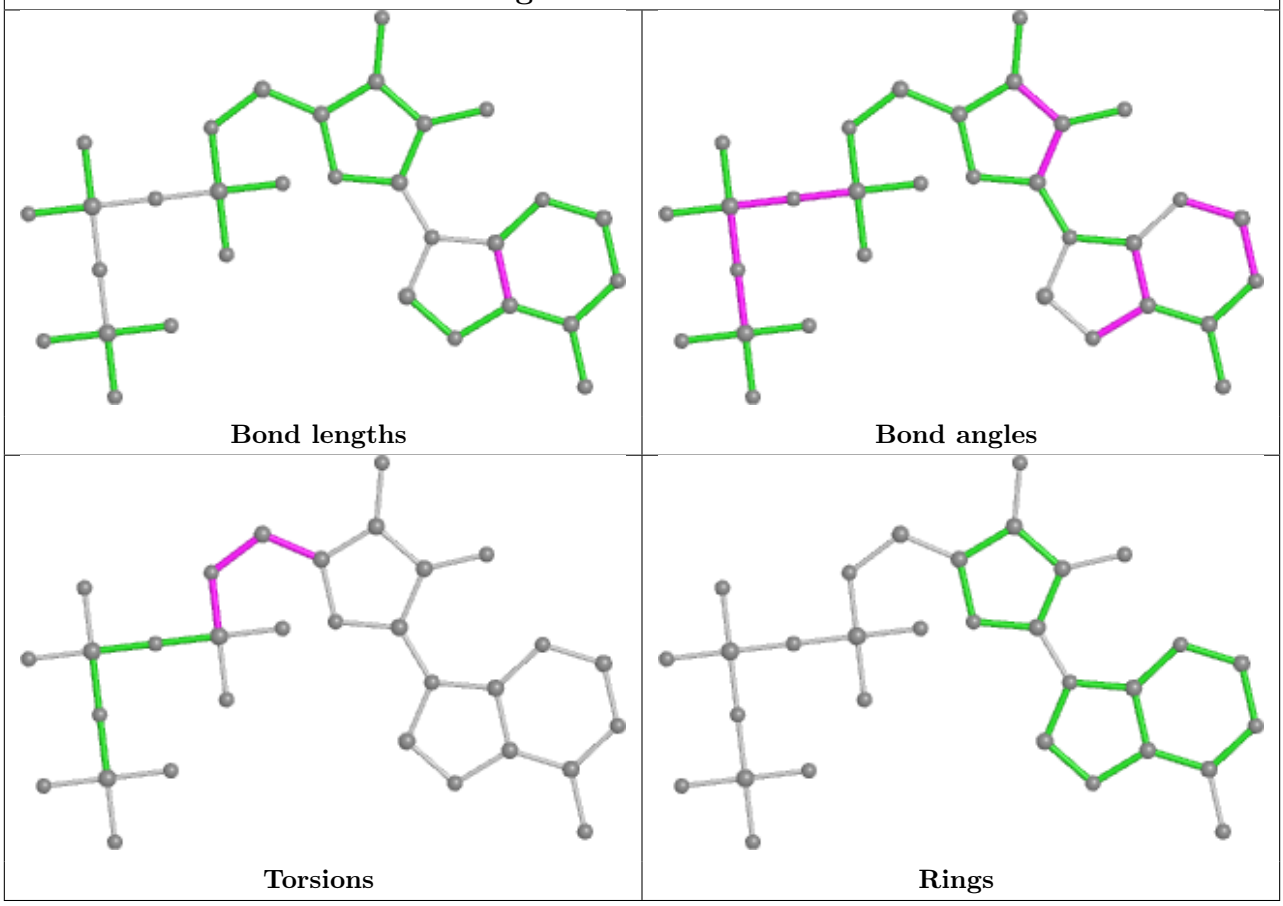
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

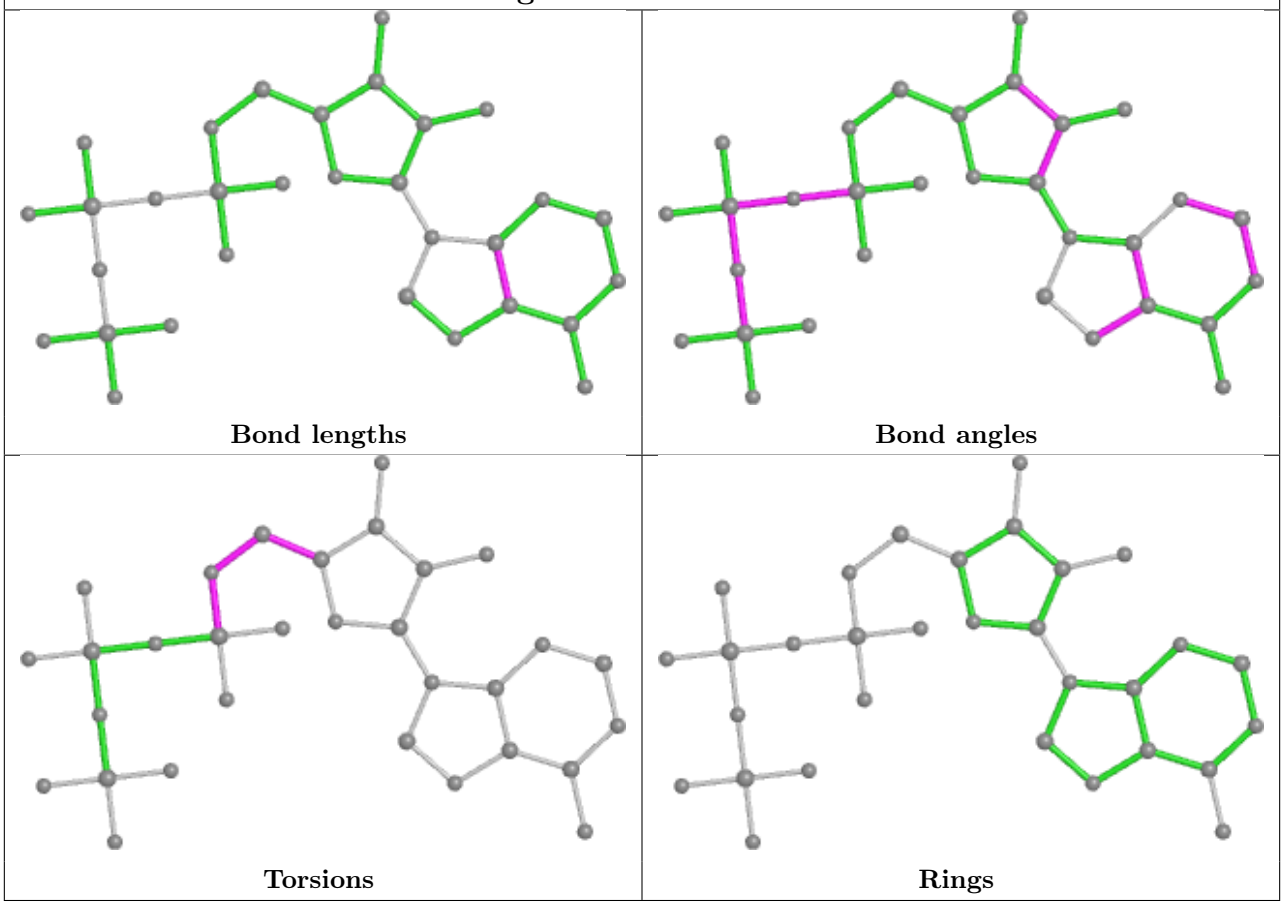
**Ligand ATP I 5101**



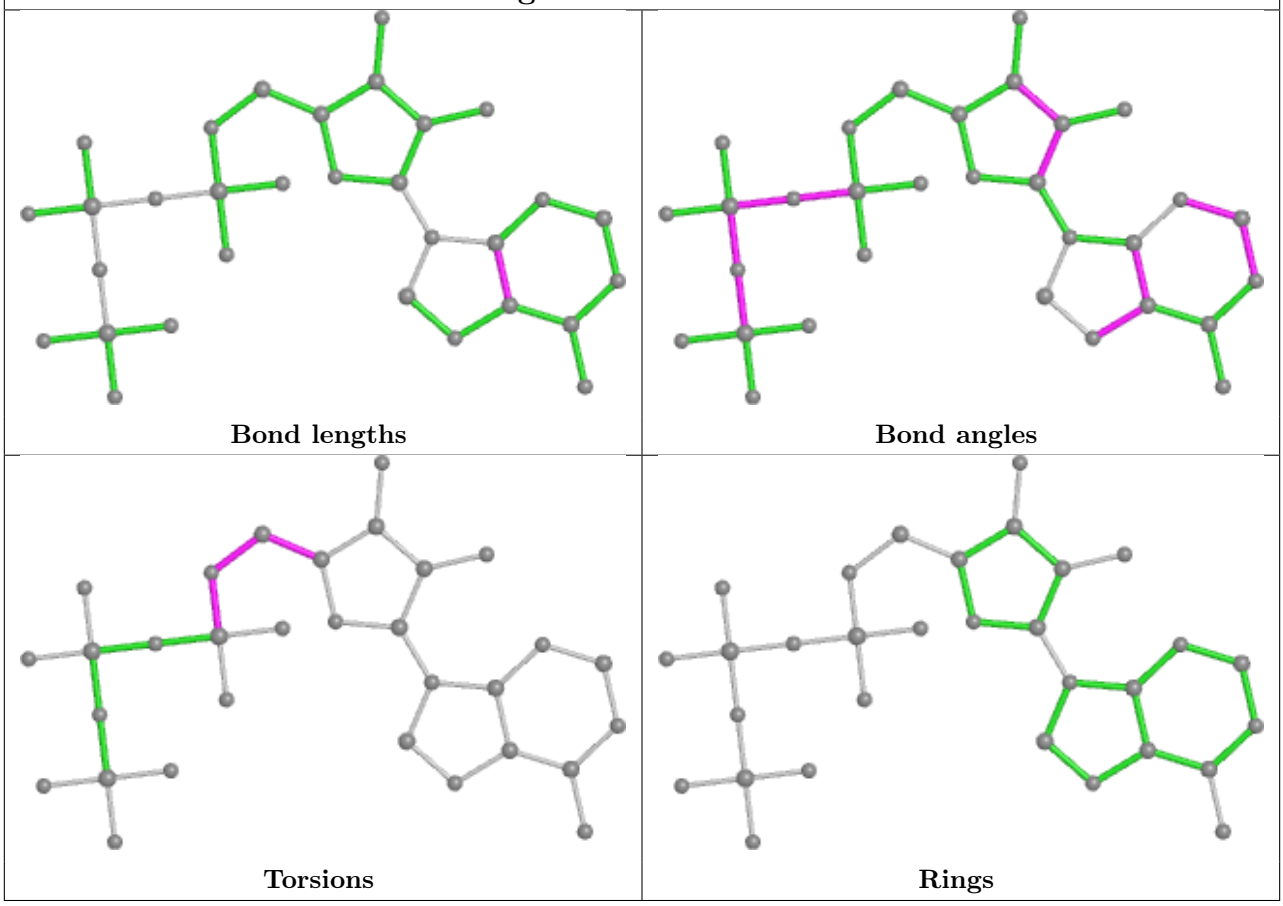
**Ligand ATP G 5101**



**Ligand ATP B 5101**



**Ligand ATP E 5101**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 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 | 72.88 |
| 1 | E | 4345:UNK | C | 4540:PHE | N | 72.88 |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | I | 4345:UNK | C | 4540:PHE | N | 72.88 |
| 1 | G | 4345:UNK | C | 4540:PHE | N | 72.88 |
| 1 | B | 3613:UNK | C | 3639:THR | N | 43.44 |
| 1 | E | 3613:UNK | C | 3639:THR | N | 43.44 |
| 1 | I | 3613:UNK | C | 3639:THR | N | 43.44 |
| 1 | G | 3613:UNK | C | 3639:THR | N | 43.44 |
| 1 | B | 4253:GLU | C | 4320:UNK | N | 27.19 |
| 1 | E | 4253:GLU | C | 4320:UNK | N | 27.19 |
| 1 | I | 4253:GLU | C | 4320:UNK | N | 27.19 |
| 1 | G | 4253:GLU | C | 4320:UNK | N | 27.19 |
| 1 | B | 3163:UNK | C | 3170:UNK | N | 15.93 |
| 1 | E | 3163:UNK | C | 3170:UNK | N | 15.93 |
| 1 | I | 3163:UNK | C | 3170:UNK | N | 15.93 |
| 1 | G | 3163:UNK | C | 3170:UNK | N | 15.93 |
| 1 | E | 3063:UNK | C | 3134:UNK | N | 15.07 |
| 1 | G | 3063:UNK | C | 3134:UNK | N | 15.07 |
| 1 | B | 3063:UNK | C | 3134:UNK | N | 15.06 |
| 1 | I | 3063:UNK | C | 3134:UNK | N | 15.06 |
| 1 | B | 3468:UNK | C | 3511:UNK | N | 14.28 |
| 1 | E | 3468:UNK | C | 3511:UNK | N | 14.28 |
| 1 | I | 3468:UNK | C | 3511:UNK | N | 14.28 |
| 1 | G | 3468:UNK | C | 3511:UNK | N | 14.28 |
| 1 | B | 2703:UNK | C | 2734:ASN | N | 14.09 |
| 1 | E | 2703:UNK | C | 2734:ASN | N | 14.09 |
| 1 | I | 2703:UNK | C | 2734:ASN | N | 14.09 |
| 1 | G | 2703:UNK | C | 2734:ASN | N | 14.09 |
| 1 | B | 3236:UNK | C | 3241:UNK | N | 13.30 |
| 1 | E | 3236:UNK | C | 3241:UNK | N | 13.30 |
| 1 | I | 3236:UNK | C | 3241:UNK | N | 13.30 |
| 1 | G | 3236:UNK | C | 3241:UNK | N | 13.30 |
| 1 | B | 1564:UNK | C | 1573:MET | N | 12.36 |
| 1 | E | 1564:UNK | C | 1573:MET | N | 12.36 |
| 1 | I | 1564:UNK | C | 1573:MET | N | 12.36 |
| 1 | G | 1564:UNK | C | 1573:MET | N | 12.36 |
| 1 | B | 2976:UNK | C | 2995:UNK | N | 12.29 |
| 1 | E | 2976:UNK | C | 2995:UNK | N | 12.29 |
| 1 | I | 2976:UNK | C | 2995:UNK | N | 12.29 |
| 1 | G | 2976:UNK | C | 2995:UNK | N | 12.29 |
| 1 | B | 3254:UNK | C | 3261:UNK | N | 8.12 |
| 1 | E | 3254:UNK | C | 3261:UNK | N | 8.12 |
| 1 | I | 3254:UNK | C | 3261:UNK | N | 8.12 |
| 1 | G | 3254:UNK | C | 3261:UNK | N | 8.12 |

*Continued on next page...*

*Continued from previous page...*

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | B | 1297:UNK | C | 1430:UNK | N | 6.33 |
| 1 | E | 1297:UNK | C | 1430:UNK | N | 6.33 |
| 1 | I | 1297:UNK | C | 1430:UNK | N | 6.33 |
| 1 | G | 1297:UNK | C | 1430:UNK | N | 6.33 |
| 1 | B | 2939:ARG | C | 2942:UNK | N | 3.27 |
| 1 | E | 2939:ARG | C | 2942:UNK | N | 3.27 |
| 1 | I | 2939:ARG | C | 2942:UNK | N | 3.27 |
| 1 | G | 2939:ARG | C | 2942:UNK | N | 3.27 |
| 1 | B | 2479:LEU | C | 2487:UNK | N | 3.24 |
| 1 | E | 2479:LEU | C | 2487:UNK | N | 3.24 |
| 1 | I | 2479:LEU | C | 2487:UNK | N | 3.24 |
| 1 | G | 2479:LEU | C | 2487:UNK | N | 3.24 |

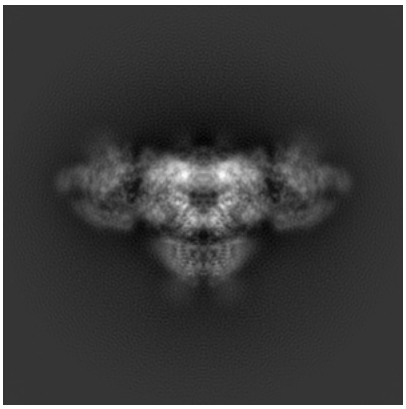
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8379. These allow visual inspection of the internal detail of the map and identification of artifacts.

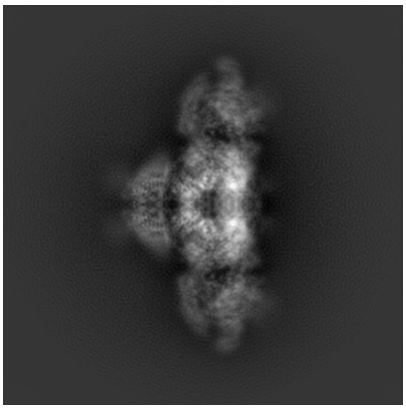
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

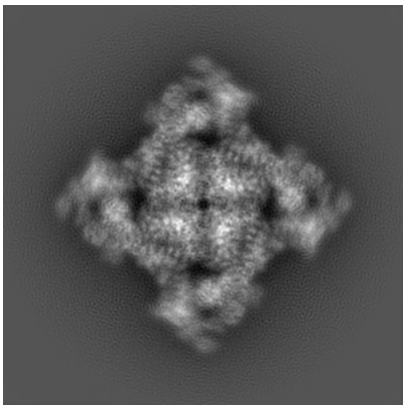
### 6.1.1 Primary map



X

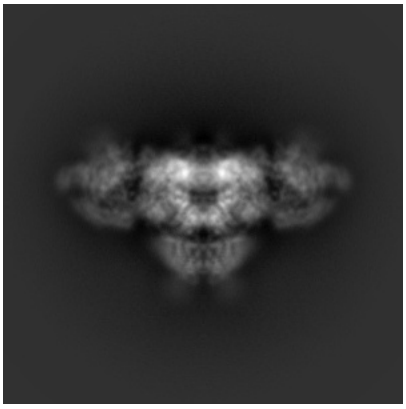


Y

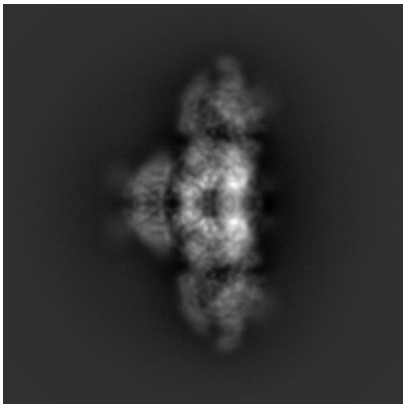


Z

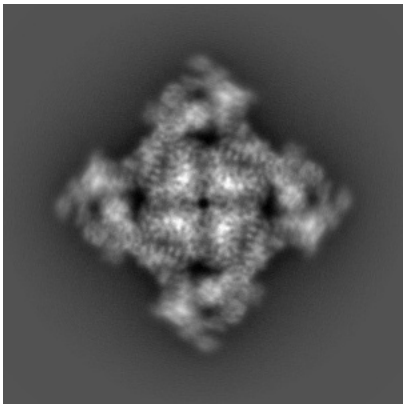
### 6.1.2 Raw map



X



Y

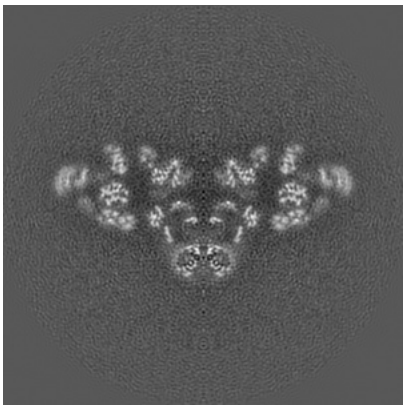


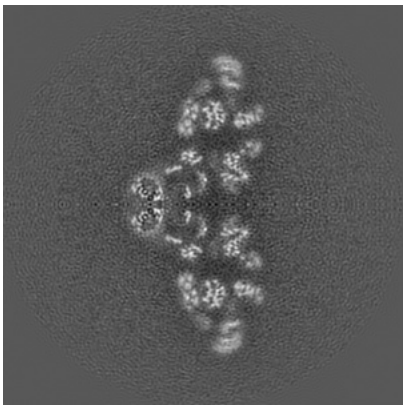
Z

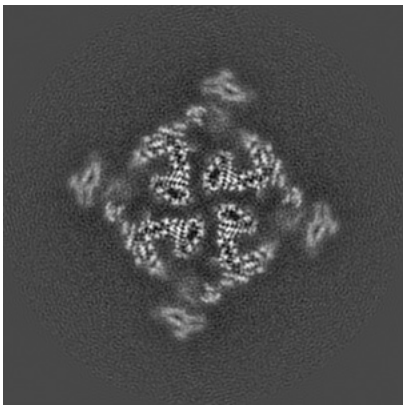
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

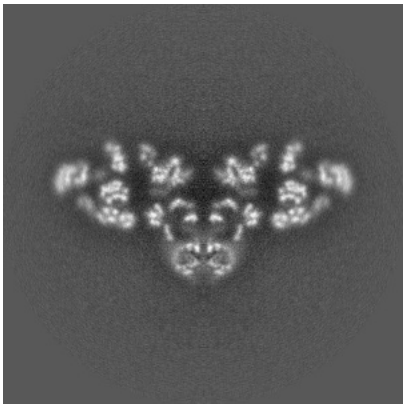
### 6.2.1 Primary map

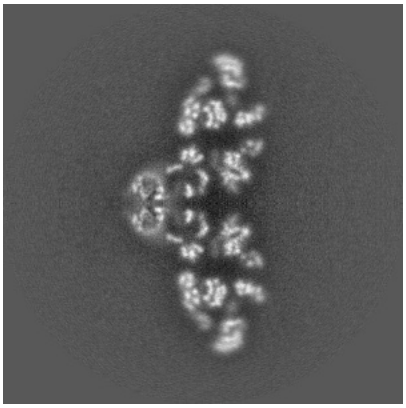

X Index: 200

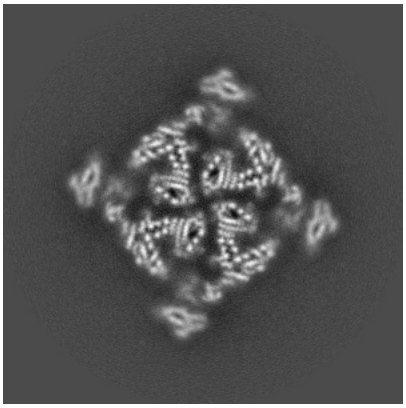

Y Index: 200


Z Index: 200

### 6.2.2 Raw map


X Index: 200

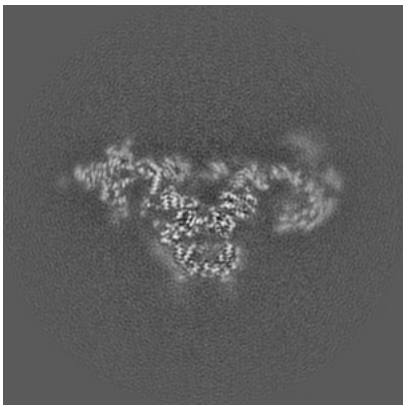

Y Index: 200

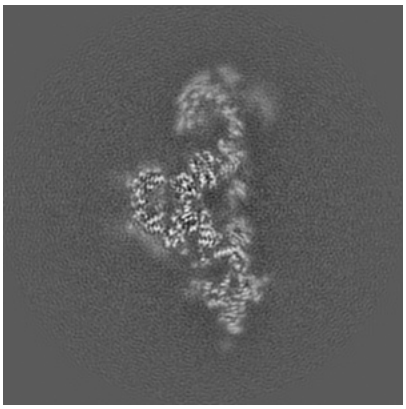

Z Index: 200

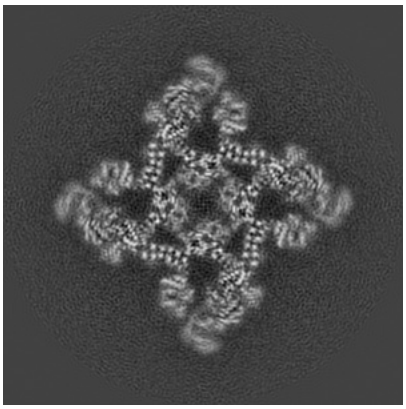
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

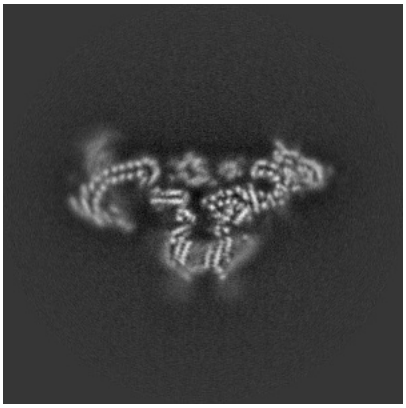
### 6.3.1 Primary map

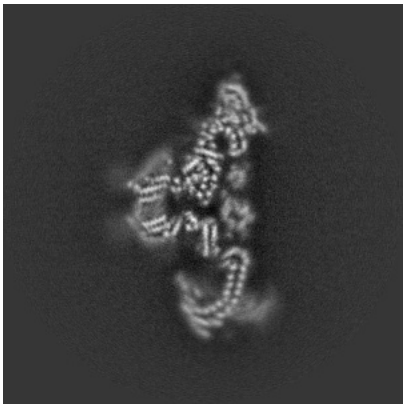

X Index: 217

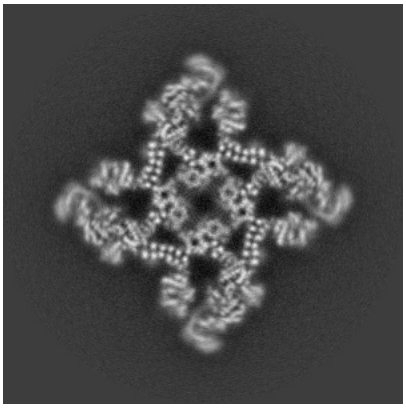

Y Index: 183


Z Index: 226

### 6.3.2 Raw map


X Index: 176


Y Index: 224


Z Index: 227

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.

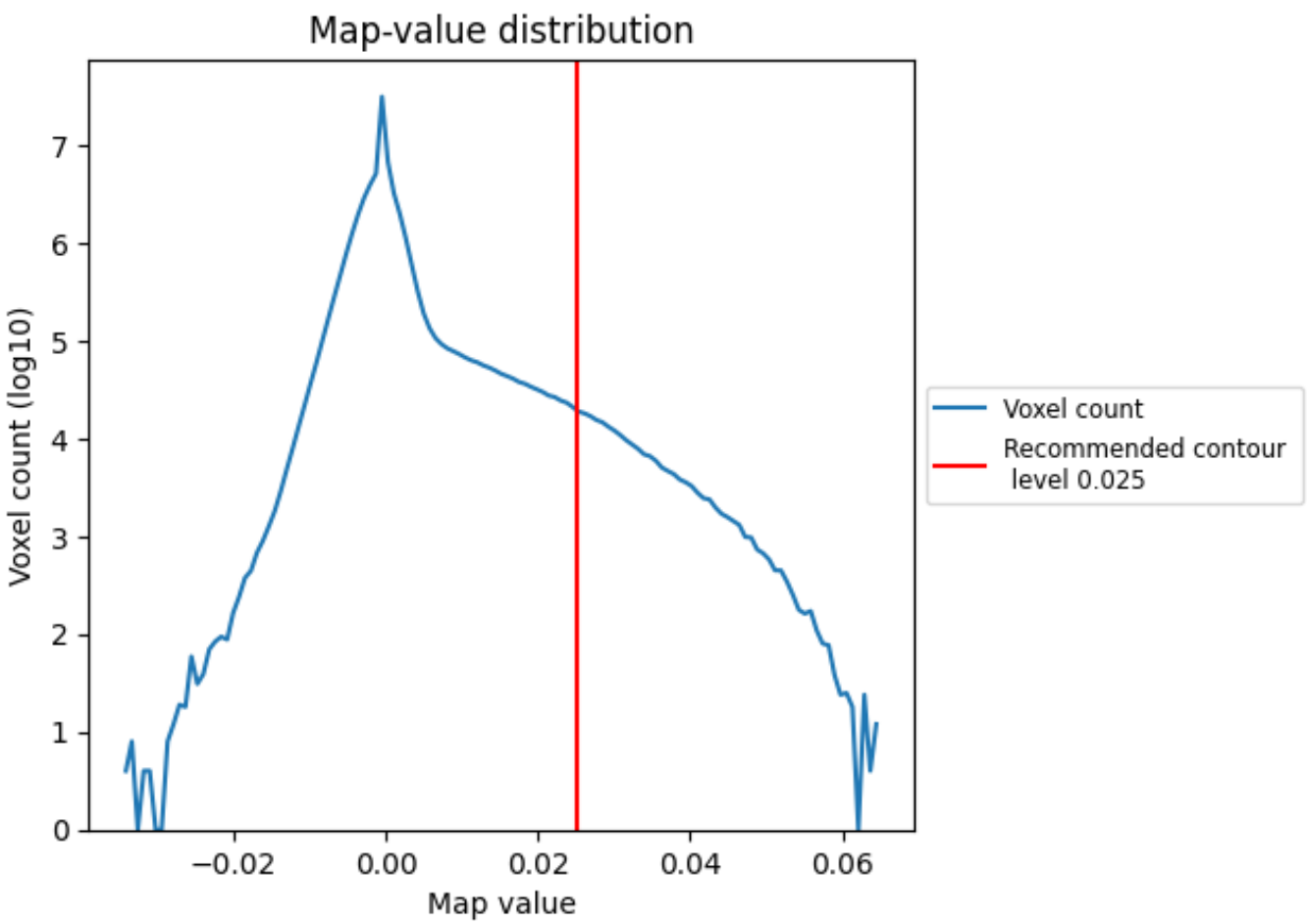
## 6.5 Mask visualisation (i)

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

# 7 Map analysis (i)

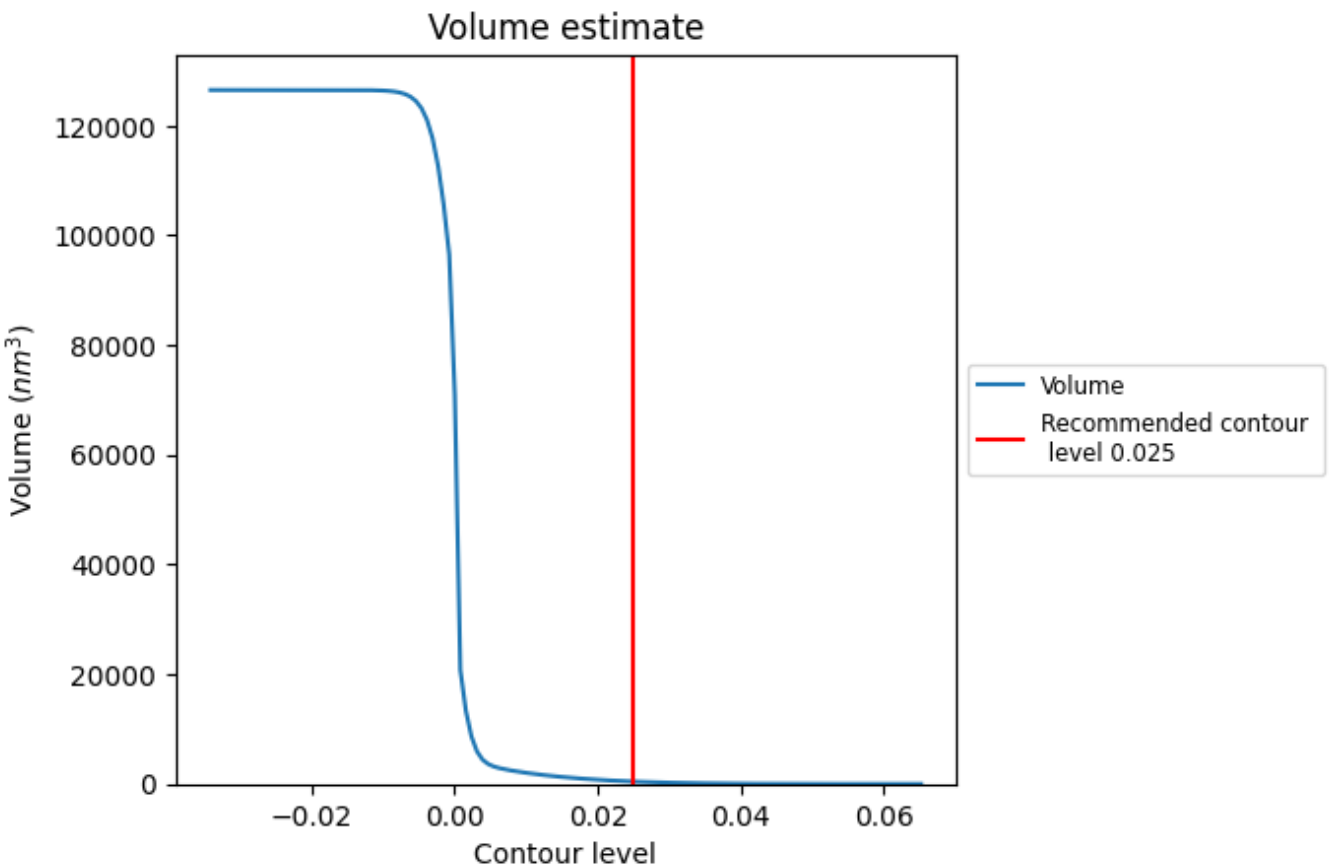
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

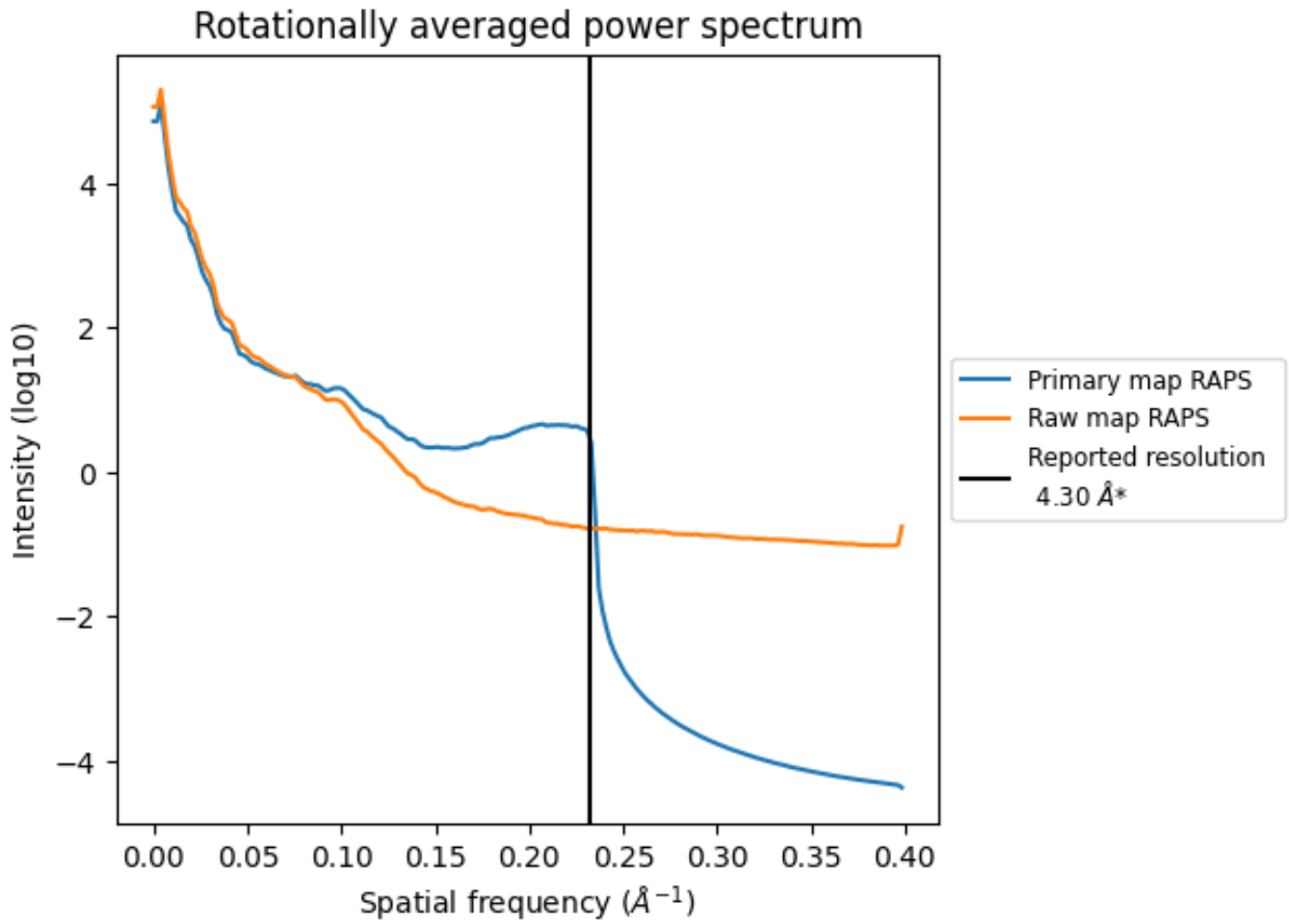
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 437 $nm^3$; this corresponds to an approximate mass of 395 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)

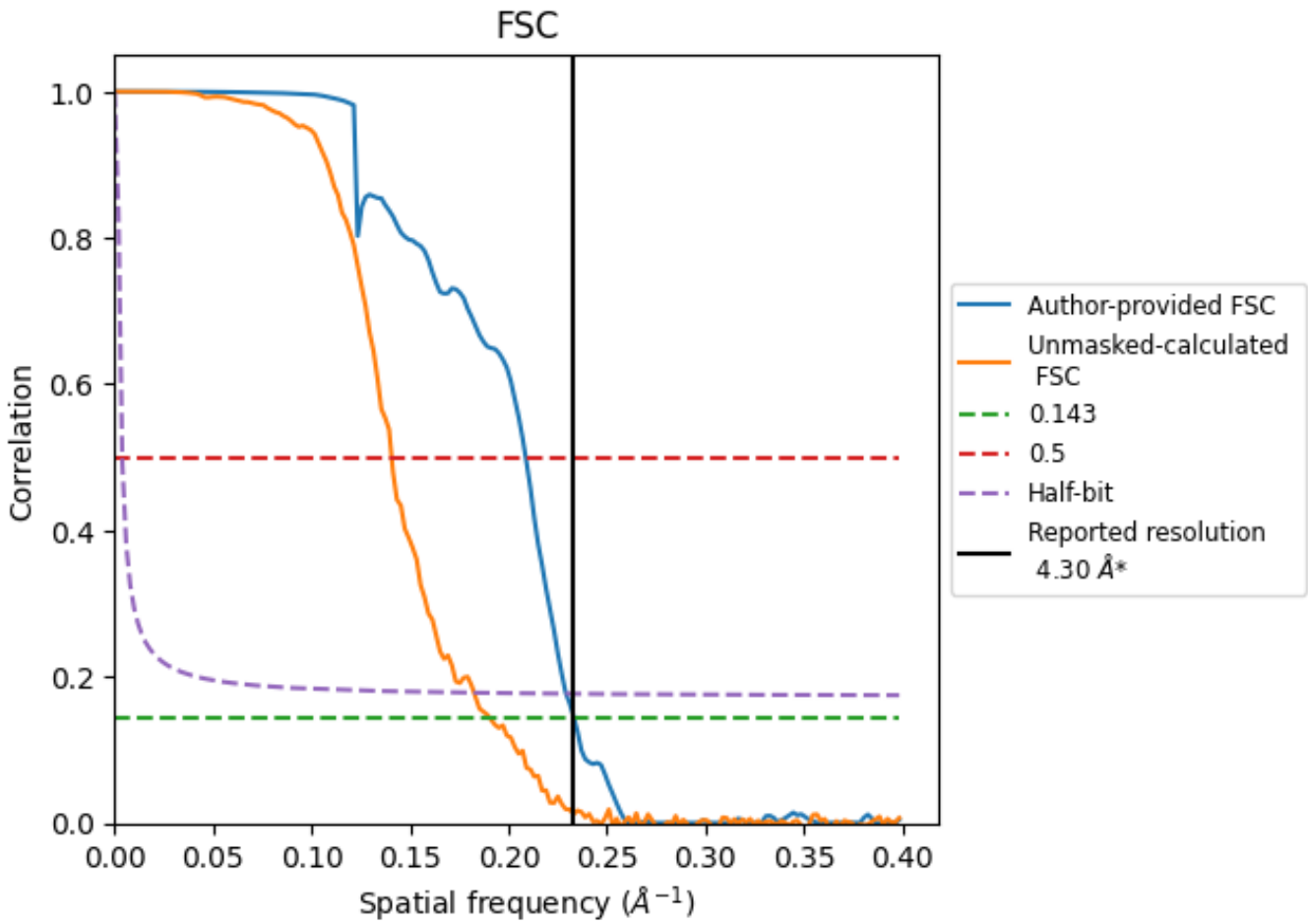



*Reported resolution corresponds to spatial frequency of 0.233 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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 (i)




*Reported resolution corresponds to spatial frequency of 0.233 Å$^{-1}$

## 8.2 Resolution estimates (i)

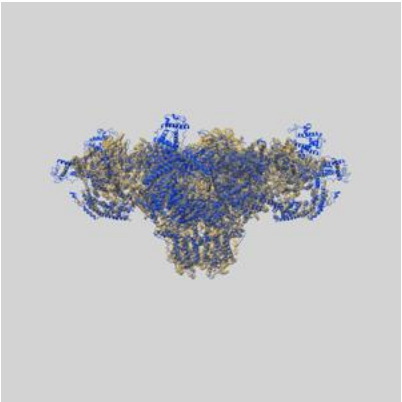
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.30 | - | - |
| Author-provided FSC curve | 4.29 | 4.79 | 4.36 |
| Unmasked-calculated* | 5.25 | 7.11 | 5.48 |

*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 5.25 differs from the reported value 4.3 by more than 10 %

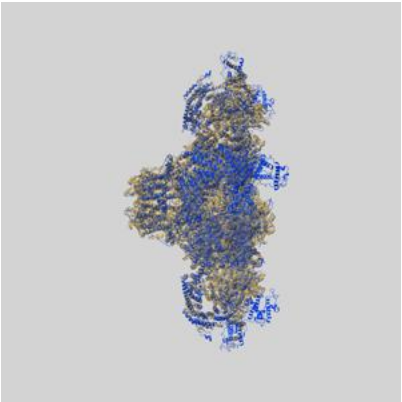
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8379 and PDB model 5TAM. Per-residue inclusion information can be found in section 3 on page 6.

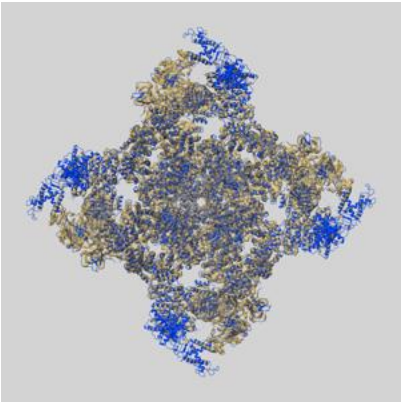
## 9.1 Map-model overlay (i)



X



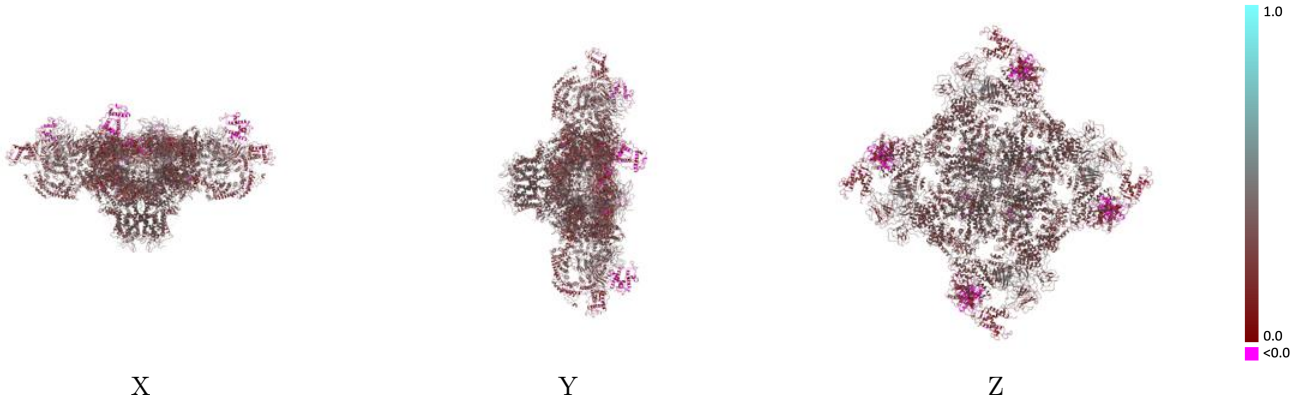
Y



Z

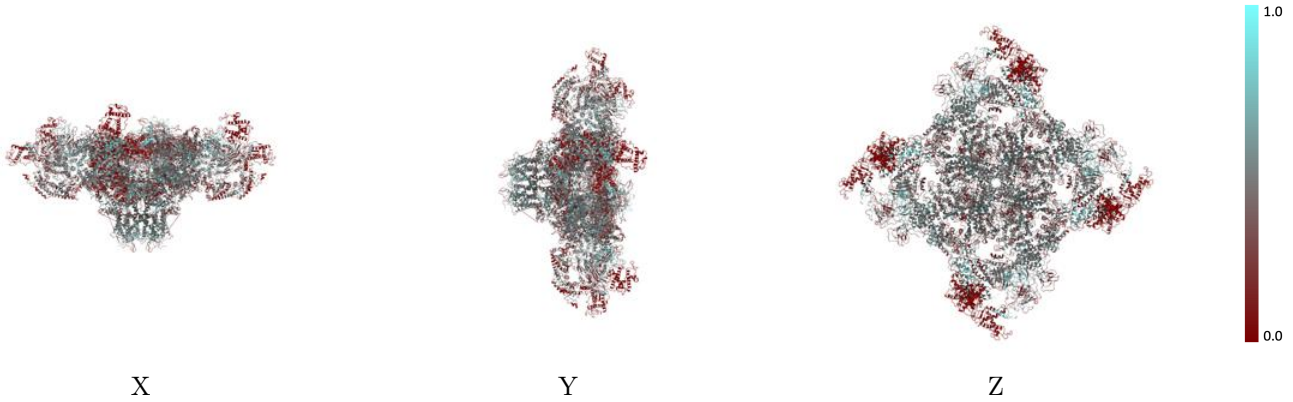
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model (i)



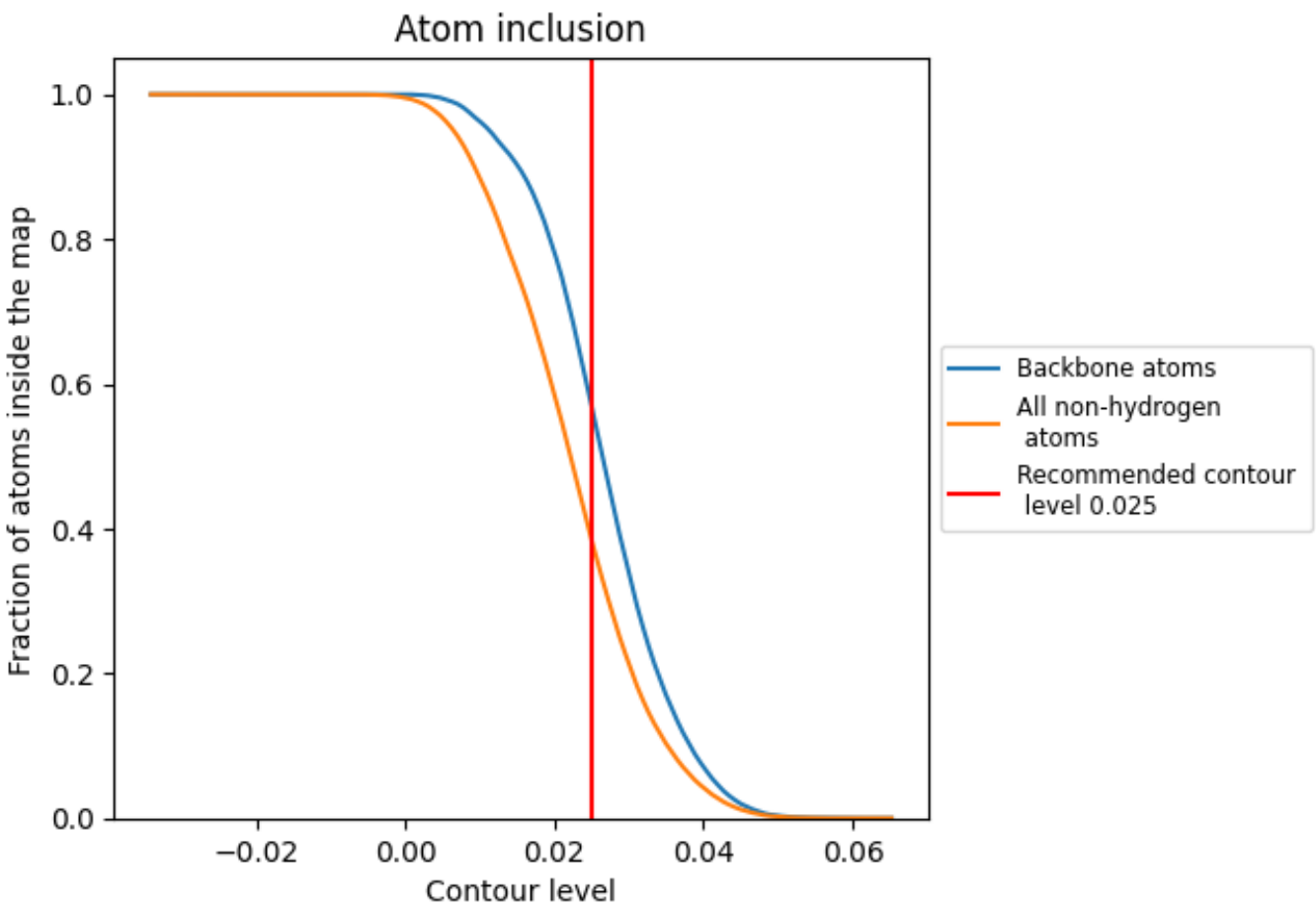

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model (i)




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, 57% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

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 | 0.3837 | 0.3030 |
| A | 0.3524 | 0.3310 |
| B | 0.3847 | 0.3020 |
| E | 0.3846 | 0.3020 |
| F | 0.3573 | 0.3360 |
| G | 0.3845 | 0.3020 |
| H | 0.3536 | 0.3360 |
| I | 0.3842 | 0.3020 |
| J | 0.3561 | 0.3340 |