Full wwPDB EM Validation Report (i)

Mar 2, 2024 – 09:49 AM EST

PDB ID	:	5TAN
EMDB ID	:	EMD-8380
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/Ca2+ dataset, class 3)
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:

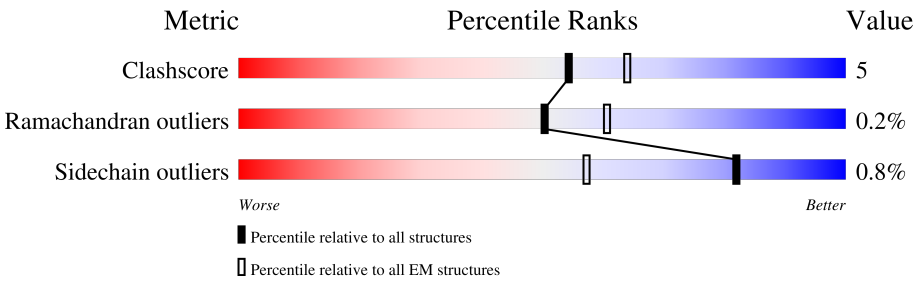
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	58% / 81% / 19% / •
1	F	108	59% / 81% / 19% / •
1	H	108	60% / 81% / 19% / •
1	J	108	58% / 81% / 19% / •
2	B	4416	46% / 84% / 11% / 5%
2	E	4416	46% / 83% / 11% / 5%
2	G	4416	46% / 83% / 11% / 5%
2	I	4416	46% / 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.

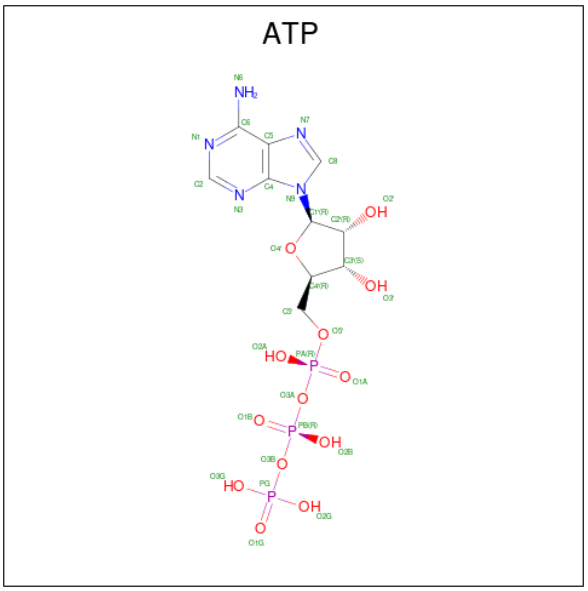
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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.

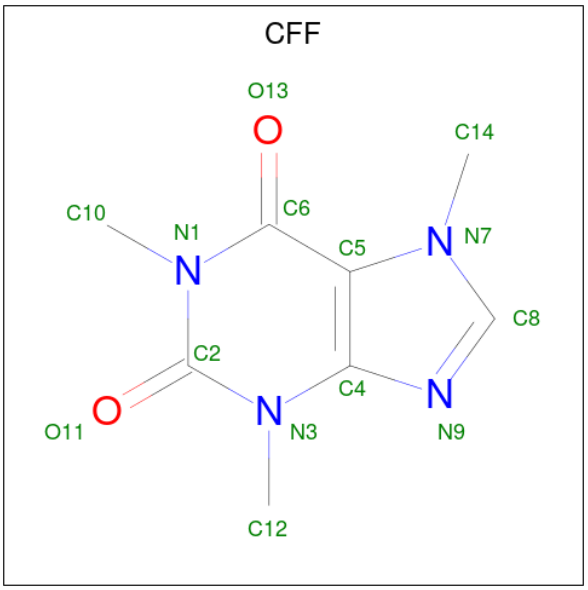
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4194	29499	18686	5228	5428	157	0	0
2	E	4194	29499	18686	5228	5428	157	0	0
2	I	4194	29499	18686	5228	5428	157	0	0
2	G	4194	29499	18686	5228	5428	157	0	0

- 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
			Total	C	N	O	P	
3	B	1	31	10	5	13	3	0
			Total	C	N	O	P	
3	E	1	31	10	5	13	3	0
			Total	C	N	O	P	
3	I	1	31	10	5	13	3	0
			Total	C	N	O	P	
3	G	1	31	10	5	13	3	0

- 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).

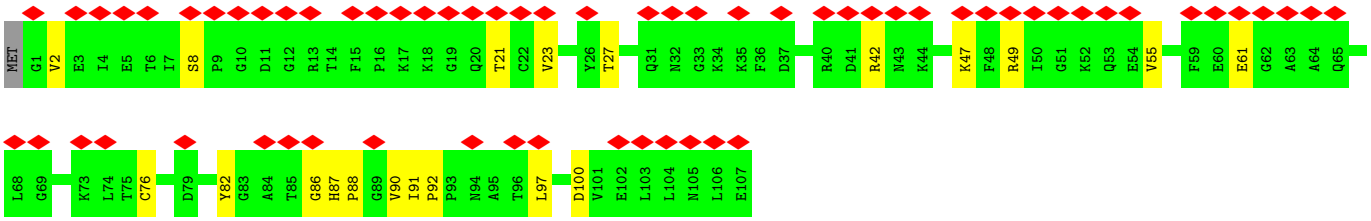
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
6	B	1	1	1	0
6	E	1	1	1	0
6	I	1	1	1	0
6	G	1	1	1	0

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.

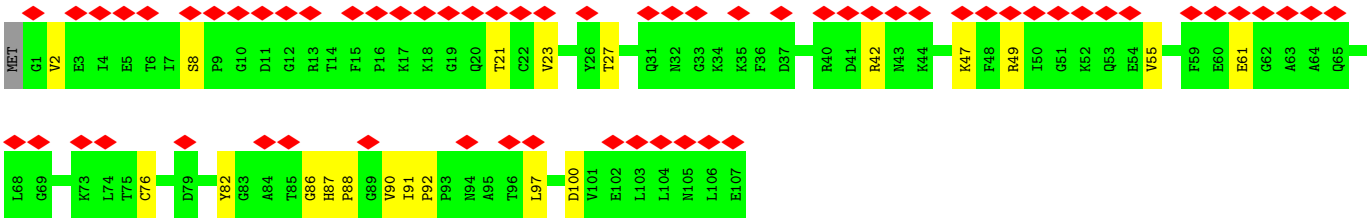
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



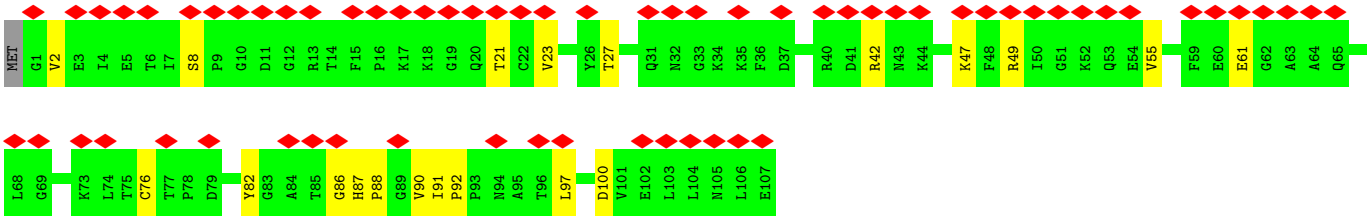
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



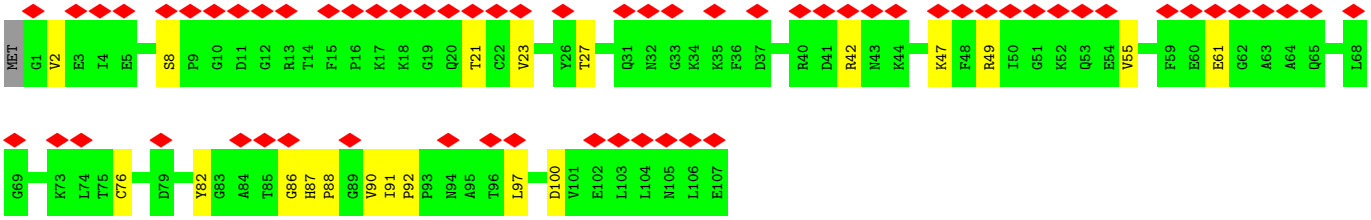
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



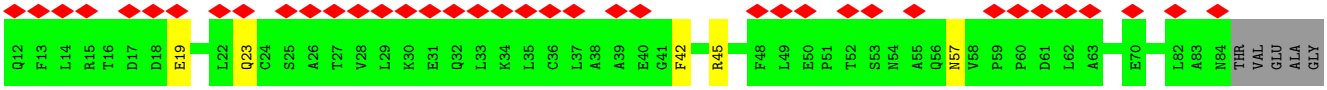
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

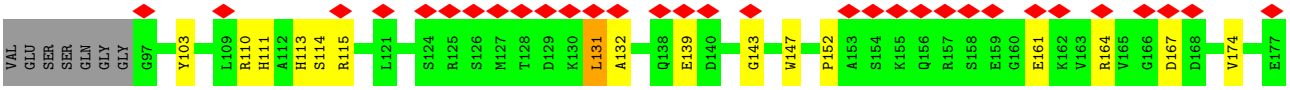
Chain J:

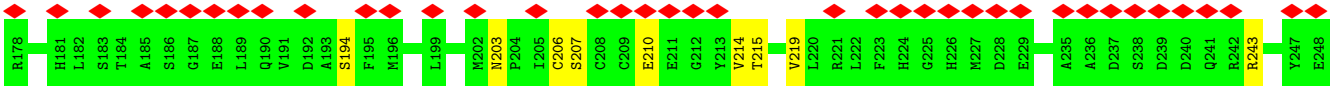


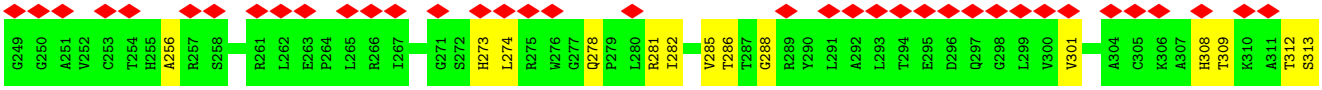
- Molecule 2: Ryanodine receptor 1

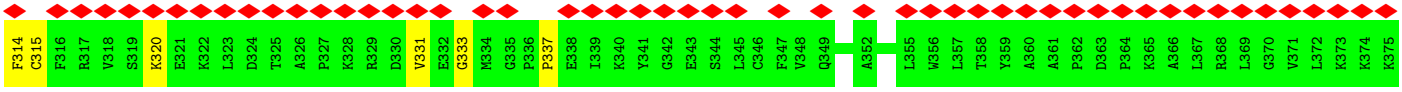
Chain B:

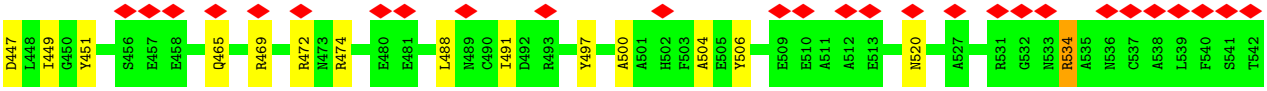


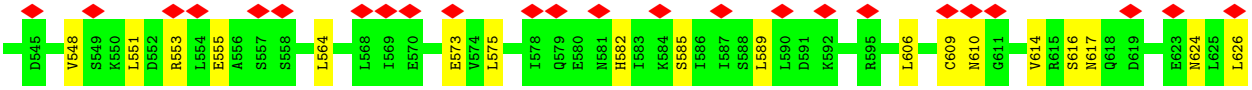


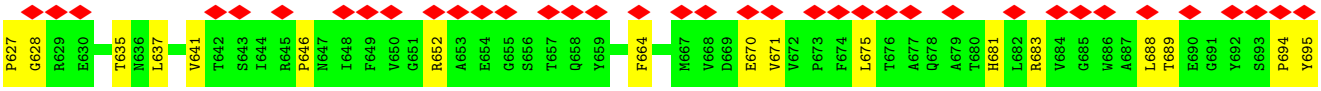


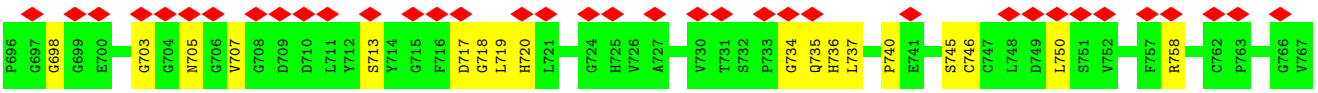


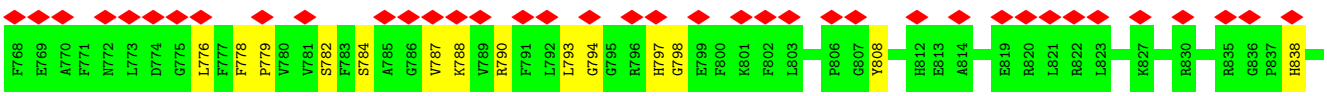












G841 P842 S843 R844 C845 L846 S847 H848 T849 D850 F851 V852 P853 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900

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 A997 R998 D999 Q1003 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 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 R1076 A1077 E1078 K1079 S1080 Y1081 S1085 G1086 R1087 W1088 Y1089 E1093 A1094 V1095 T1096 T1097 G1098

E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 L1115 D1118 E1119 L1120 V1123 F1124 R1128 G1129 Q1130 R1131 L1134 G1135 S1136 F1139 G1140 R1141 S1145 G1146 D1147 V1148 M1152 I1153 D1154 L1155 T1156 E1157 N1158 I1161 F1162 T1163 D1172 S1173 G1174 S1175 E1176 T1177

A1178 F1179 R1180 E1181 I1184 G1185 D1186 G1187 F1188 L1189 V1199 G1200 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 A1215 I1216 C1217 G1218 L1219 Q1220 E1221 G1222 F1223 Q1231 R1232 T1236 W1237 E1251 H1254 Y1255 E1256 R1259 M1260 D1261 G1262 T1263 V1264 D1265 T1266 C1269 L1270

R1271 L1272 A1273 H1274 R1275 X1276 X1277 X1278 X1279 X1280 X1281 X1282 X1283 X1284 X1285 X1291 X1430 X1441 X1442 X1446 X1447 X1450 X1475 X1476 X1477 X1478 X1479 X1480 X1481 X1482 X1486 X1504 X1505 X1516 X1517 X1518 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1536

X1537 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 M1573 P1574 L1575 S1576 M1579 F1580 E1583 P1589 Q1590 P1593 R1594 L1595 L1600 W1605 S1606 R1607 M1608 H1611 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 M1637 A1638 L1639

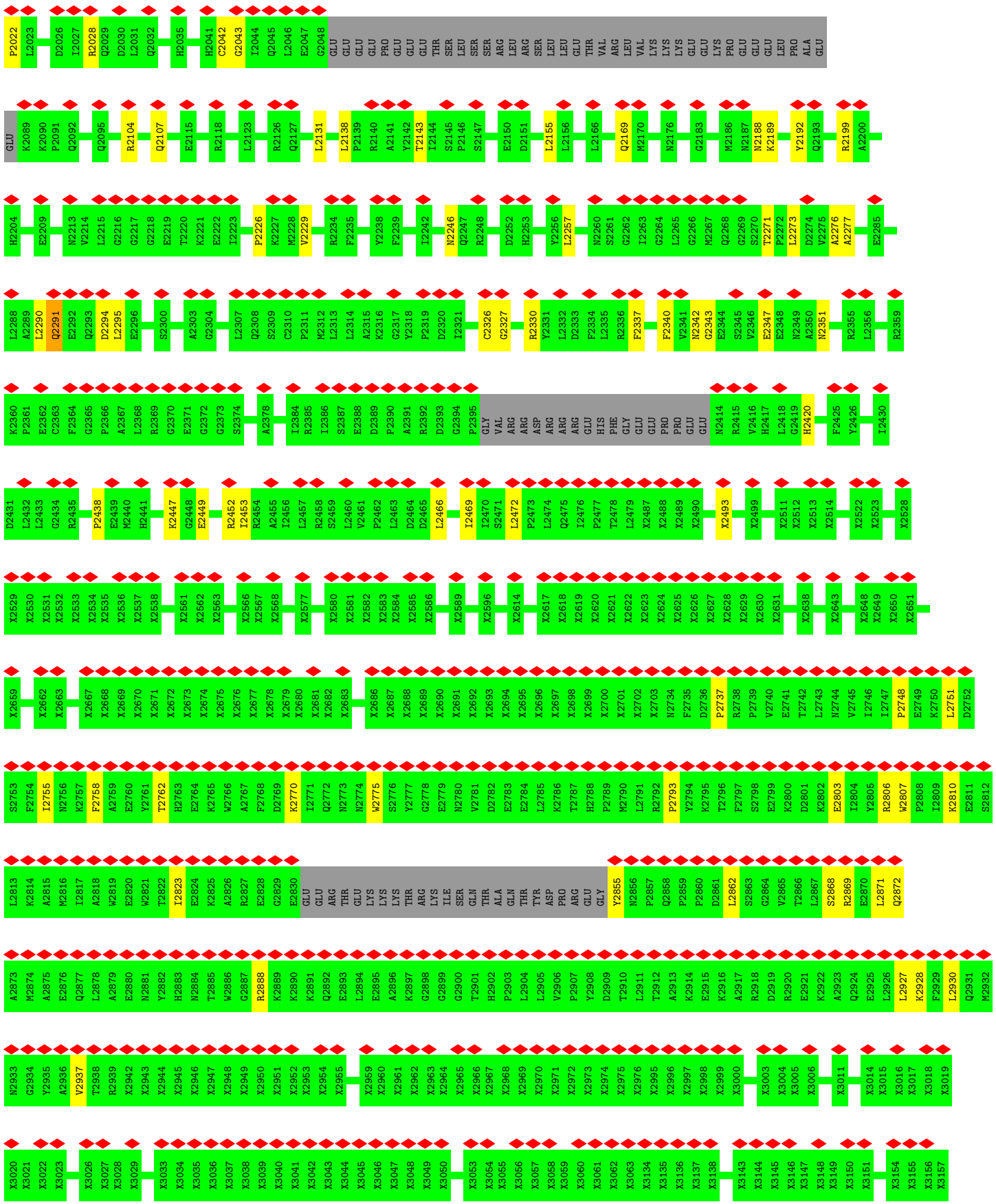
E1644 N1645 E1655 R1656 L1657 D1658 H1663 S1664 H1665 T1666 L1667 R1668 L1669 Y1670 R1671 L1676 N1679 R1680 L1685 H1688 V1689 D1690 Q1691 L1694 L1695 H1696 A1697 L1698 E1699 D1700 A1701 H1702 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 S1729 M1730 L1731

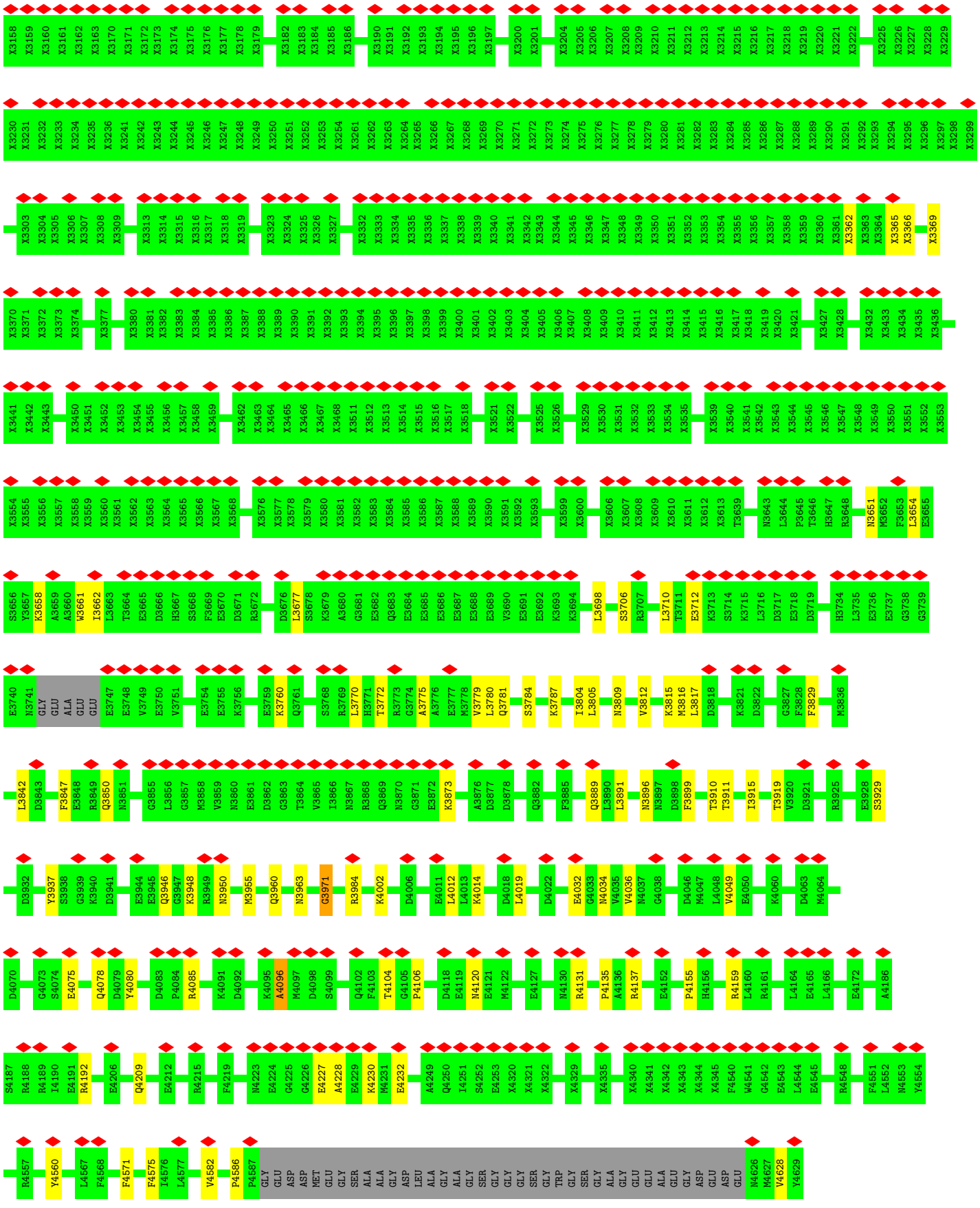
S1732 E1733 Y1734 I1735 P1740 E1741 T1742 R1743 A1744 I1745 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 L1771 R1772 P1773 P1774 H1775 H1776 F1777 F1782 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798

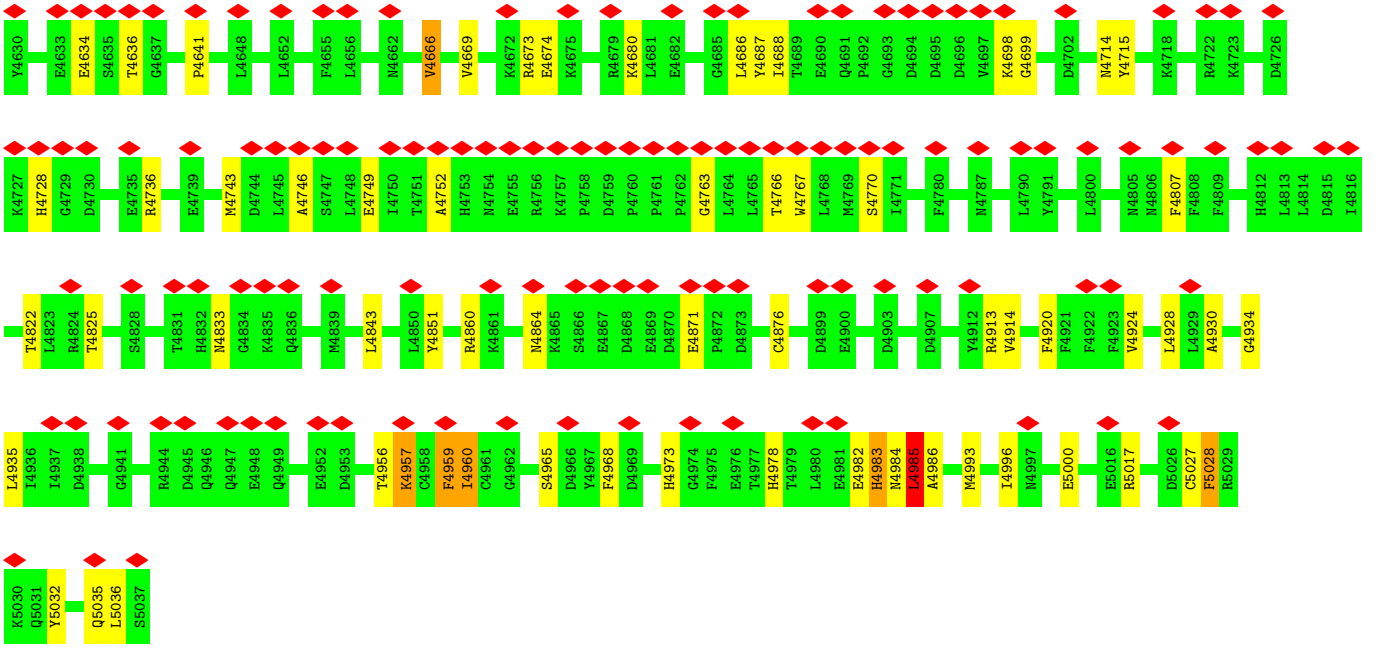
I1802 E1805 A1806 L1807 R1808 R1813 M1814 L1815 G1816 E1817 R1820 D1821 Q1824 H1825 A1826 R1827 D1828 G1831 Q1837 F1838 V1839 P1840 V1845 L1848 I1853 F1854 G1855 D1856 V1859 K1860 Q1861 I1862 L1863 K1864 M1865 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU

GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 L1931 P1932 K1936 L1937 Q1938 M1939 C1940 Q1949 L1958 A1959 A1960

F1961 A1962 E1963 R1964 Y1965 K1968 L1969 Q1970 A1971 N1972 Q1973 R1974 S1975 R1976 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006 N2007 M2008 L2009 L2010 H2011 F2012 K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021

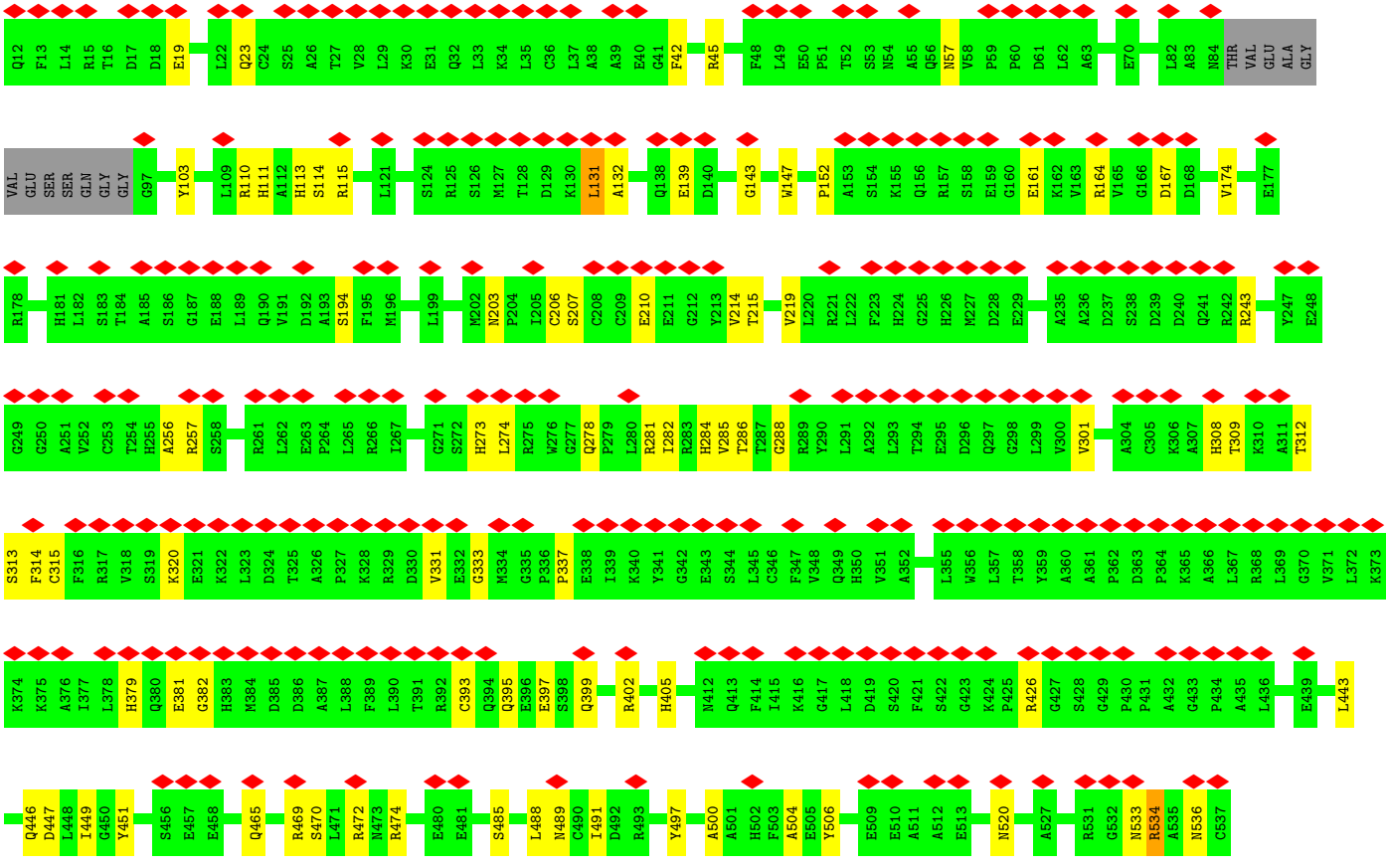

P2022 L2023 D2026 I2027 R2028 Q2029 D2030 L2031 Q2032 H2035 H2041 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU
GLU K2089 K2090 P2091 Q2092 Q2095 R2104 Q2107 E2115 R2118 L2123 R2126 Q2127 L2131 L2138 P2139 R2140 A2141 Y2142 T2143 I2144 S2145 P2146 S2147 E2150 D2151 L2155 L2156 L2166 Q2169 M2170 N2176 G2183 M2186 N2187 N2188 K2189 Y2192 Q2193 R2199 A2200
H2204 E2209 N2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 P2226 K2227 M2228 V2229 R2234 F2235 Y2238 F2239 I2242 N2246 Q2247 R2248 D2252 H2253 Y2256 L2257 N2260 S2261 G2262 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 S2270 T2271 P2272 L2273 D2274 V2275 A2276 A2277 E2285
L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295 E2296 S2300 A2303 G2304 L2307 Q2308 S2309 C2310 P2311 M2312 L2313 L2314 A2315 K2316 G2317 Y2318 P2319 D2320 I2321 C2326 G2327 R2330 Y2331 L2332 D2333 F2334 L2335 R2336 F2337 F2340 V2341 N2342 G2343 E2344 S2345 V2346 E2347 E2348 N2349 A2350 N2351 R2355 L2356 R2359
K2360 P2361 E2362 C2363 F2364 G2365 P2366 A2367 L2368 R2369 G2370 E2371 G2372 G2373 S2374 A2378 I2384 R2385 I2386 S2387 E2388 D2389 P2390 A2391 R2392 D2393 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 H2417 L2418 G2419 H2420 F2425 Y2426 I2430
D2431 L2432 L2433 G2434 R2435 P2438 E2439 M2440 H2441 K2447 G2448 E2449 R2452 I2453 R2454 A2455 I2456 L2457 R2458 S2459 L2460 V2461 P2462 L2463 D2464 D2465 L2466 I2469 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479 X2487 X2488 X2489 X2490 X2493 X2499 X2511 X2512 X2513 X2514 X2522 X2523 X2528
X2529 X2530 X2531 X2532 X2533 X2534 X2535 X2536 X2537 X2538 X2561 X2562 X2563 X2566 X2567 X2568 X2577 X2580 X2581 X2582 X2583 X2584 X2585 X2586 X2589 X2596 X2614 X2617 X2618 X2619 X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2630 X2631 X2638 X2643 X2648 X2649 X2650 X2651
X2659 X2662 X2663 X2667 X2668 X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678 X2679 X2680 X2681 X2682 X2683 X2686 X2687 X2688 X2689 X2690 X2691 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 Y2745 I2746 I2747 P2748 E2749 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 S2799 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 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932
N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2955 X2959 X2960 X2961 X2962 X2963 X2964 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2995 X2996 X2997 X2998 X2999 X3000 X3003 X3004 X3005 X3006 X3011 X3014 X3015 X3016 X3017 X3018 X3019
X3020 X3021 X3022 X3023 X3026 X3027 X3028 X3029 X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040 X3041 X3042 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3053 X3054 X3055 X3056 X3057 X3058 X3059 X3060 X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3143 X3144 X3145 X3146 X3147 X3148 X3149 X3150 X3151 X3154 X3155 X3156 X3157


X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3182 X3183 X3184 X3185 X3186 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3201 X3204 X3205 X3206 X3207 X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3225 X3226 X3227 X3228 X3229
X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299
X3303 X3304 X3305 X3306 X3307 X3308 X3309 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3323 X3324 X3325 X3326 X3327 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344 X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3369
X3370 X3371 X3372 X3373 X3374 X3377 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412 X3413 X3414 X3415 X3416 X3417 X3418 X3419 X3420 X3421 X3427 X3428 X3432 X3433 X3434 X3435 X3436
X3441 X3442 X3443 X3450 X3451 X3452 X3453 X3454 X3455 X3456 X3457 X3458 X3459 X3462 X3463 X3464 X3465 X3466 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3521 X3522 X3525 X3526 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553
X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3576 X3577 X3578 X3579 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3592 X3593 X3599 X3600 X3606 X3607 X3608 X3609 X3610 X3611 X3612 X3613 T3639 N3643 L3644 P3645 T3646 H3647 R3648 N3651 M3652 F3653 L3654 E3655
S3656 Y3657 K3658 A3659 A3660 W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 F3669 E3670 D3671 R3672 D3676 L3677 S3678 K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 L3698 S3706 R3707 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 H3734 L3735 E3736 E3737 G3738 G3739
E3740 N3741 GLY GLU ALA GLU E3747 E3748 V3749 E3750 V3751 E3754 E3755 K3756 E3759 K3760 Q3761 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 A3776 E3777 M3778 V3779 L3780 Q3781 S3784 K3787 I3804 L3805 N3809 V3812 K3815 M3816 L3817 D3818 K3821 D3822 G3827 F3828 F3829 M3836
L3842 D3843 F3847 E3848 R3849 Q3850 N3851 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 T3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 A3876 D3877 D3878 Q3882 F3885 Q3889 L3890 L3891 N3896 N3897 D3898 F3899 T3910 T3911 I3915 T3919 V3920 D3921 R3925 E3928 S3929
D3932 Y3937 S3938 G3939 K3940 D3941 E3944 E3945 Q3946 G3947 K3948 R3949 N3950 M3955 Q3960 N3963 G3971 R3984 K4002 D4006 E4011 L4012 L4013 K4014 D4018 L4019 D4022 E4032 G4033 N4034 V4035 V4036 N4037 G4038 D4046 M4047 L4048 V4049 E4050 K4060 D4063 M4064
D4070 G4073 S4074 E4075 Q4078 D4079 Y4080 D4083 P4084 R4085 K4091 D4092 K4095 A4096 M4097 D4098 S4099 Q4102 F4103 T4104 G4105 P4106 D4118 E4119 N4120 E4121 M4122 E4127 N4130 R4131 P4135 A4136 R4137 E4152 P4155 H4156 R4159 L4160 R4161 L4164 E4165 L4166 E4172 A4186
S4187 R4188 R4189 I4190 E4191 R4192 E4206 Q4209 E4212 R4215 F4219 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4232 A4249 Q4250 I4251 S4252 E4253 X4320 X4321 X4322 X4329 X4335 X4340 X4341 X4342 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 N4548 F4551 L4552 N4553 Y4554
R4557 Y4560 L4567 F4568 F4571 F4575 I4576 L4577 V4582 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 M4627 V4628 Y4629



- Molecule 2: Ryanodine receptor 1

Chain E:



A538 L539 F540 S541 T542 D545 V548 S549 K550 L551 D552 R553 L554 E555 A556 S557 S558 L564 L568 I569 E570 E573 V574 L575 I578 Q579 E580 N581 H582 I583 K584 S585 I586 I587 S588 L589 L590 D591 K592 R595 L606 C609 N610 G611 V614 R615 S616 N617 Q618 D619

E623 N624 L625 L626 P627 G628 R629 E630 Q634 T635 N636 L637 V641 T642 S643 I644 R645 P646 N647 I648 F649 V650 G651 R652 A653 E554 G655 S656 T657 Q658 Y659 W662 Y663 F664 M667 V668 D669 E670 V671 V672 P673 F674 L675 T676 A677 Q678 A679 T680 H681 L682 R683 V684 G685 W686 A687

L688 T689 E690 G691 Y692 S693 P694 Y695 P696 G697 G698 G699 E700 G703 G704 N705 G706 V707 G708 D709 D710 L711 Y712 S713 Y714 G715 F716 D717 G718 L719 H720 L721 G724 H725 V726 A727 V730 T731 S732 P733 G734 Q735 H736 L737 P740 E741 S745 C746 C747 L748 D749 L750 S751 V752

F757 R758 C762 P763 G766 V767 F768 E769 A770 F771 N772 L773 D774 G775 L776 F777 F778 P779 V780 V781 S782 F783 S784 A785 G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 H797 G798 E799 F800 K801 F802 L803 P806 G807 Y808 C811 H812 E813 A814 E819 R820 L821 R822 L823

K827 R830 R835 G836 P837 H838 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 A997 R998 D999 Q1003 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022

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 R1076 A1077 E1078 K1079 S1080 Y1081 S1085 G1086 R1087

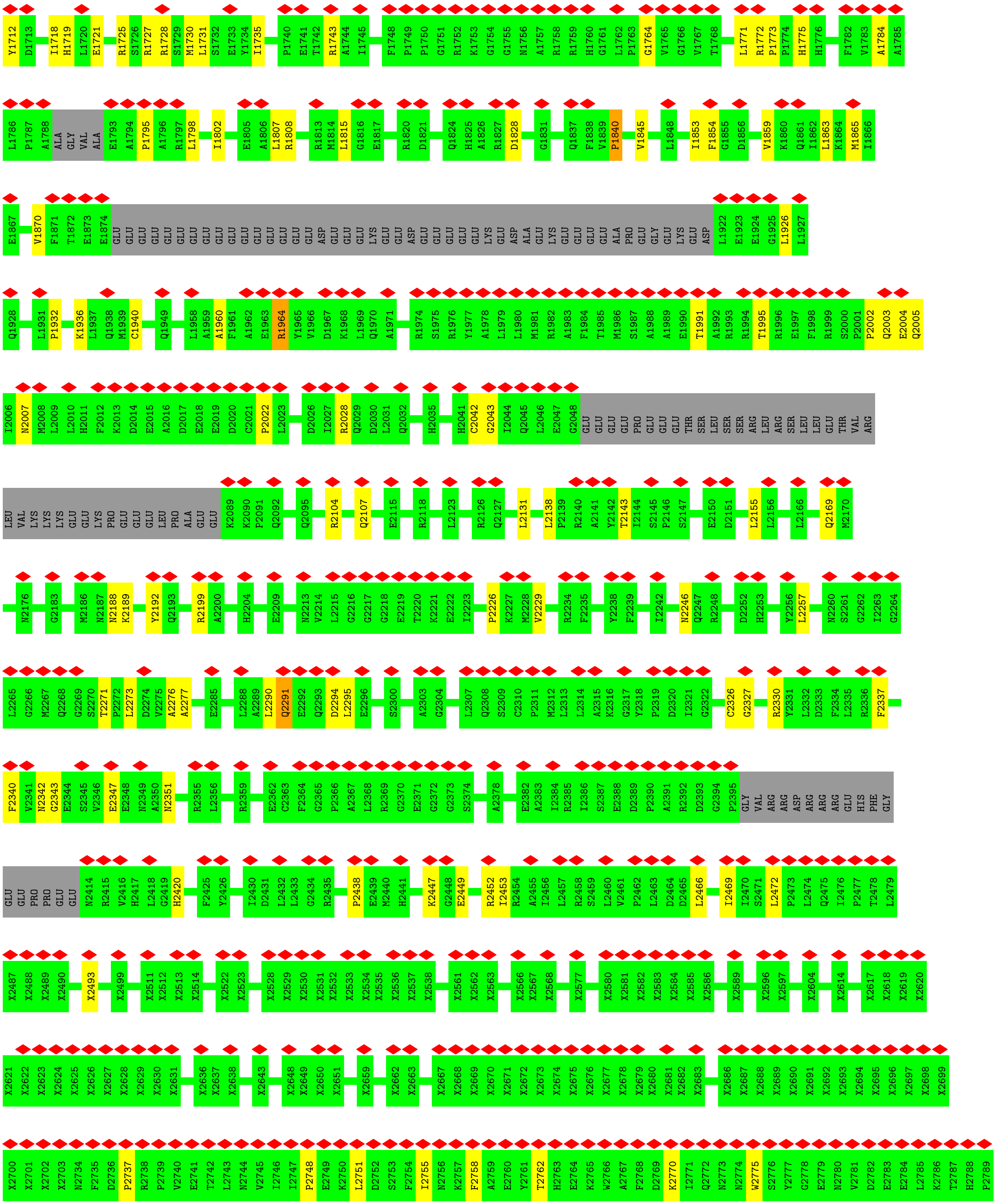
W1088 Y1089 E1093 A1094 V1095 T1096 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 V1113 E1114 L1115 D1118 E1119 L1120 V1123 F1124 R1128 G1129 Q1130 R1131 L1134 G1135 S1136 F1139 G1140 R1141 S1145 G1146 D1147 V1148 M1152 I1153 D1154 L1155 T1156 E1157 N1158 I1161

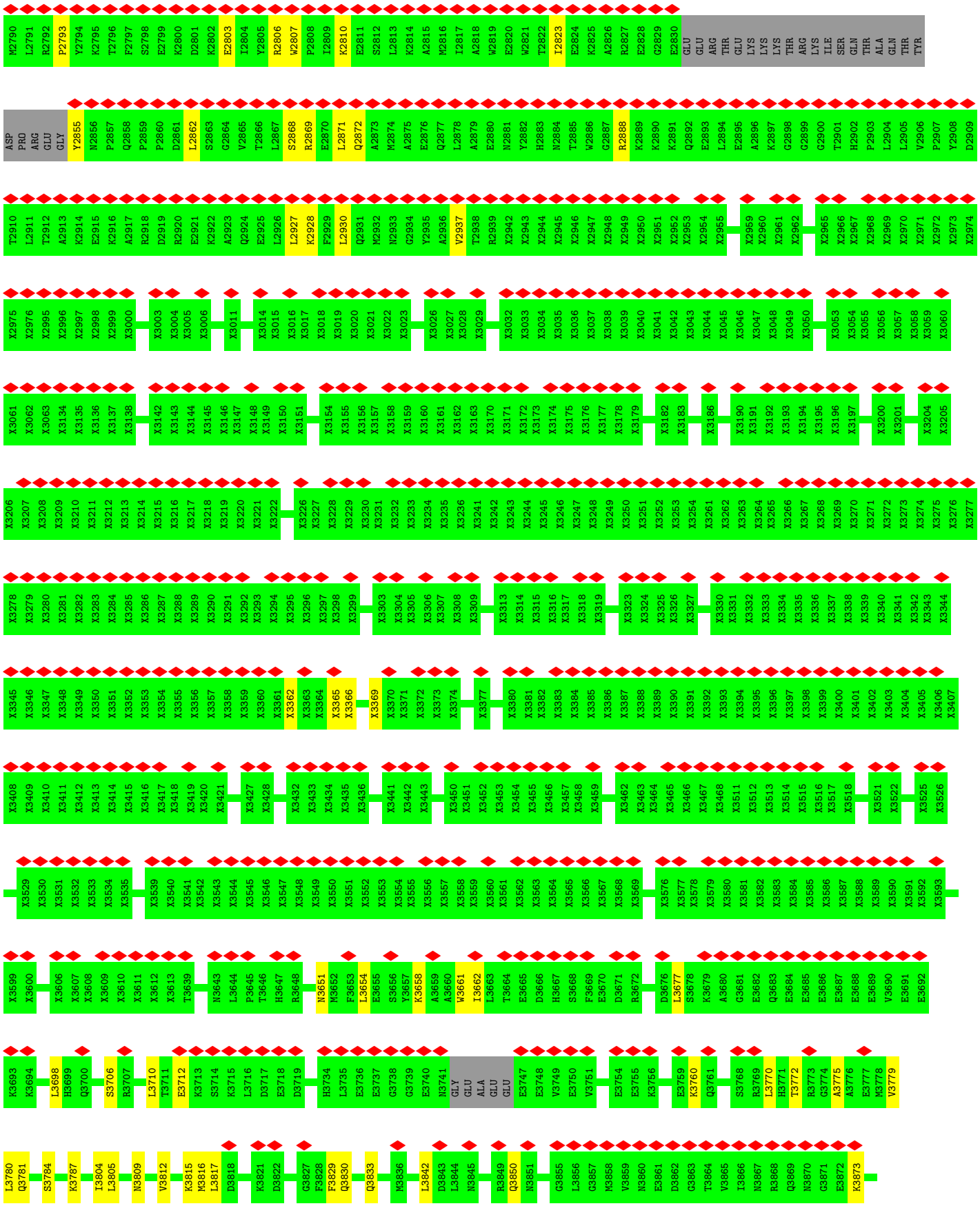
F1162 T1163 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1184 G1185 D1186 G1187 F1188 L1189 V1199 G1200 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 A1215 T1216 C1217 G1218 L1219 Q1220 E1221 G1222 F1223 Q1231 R1232 W1237 P1247 E1251 H1254 Y1255 E1256 R1259

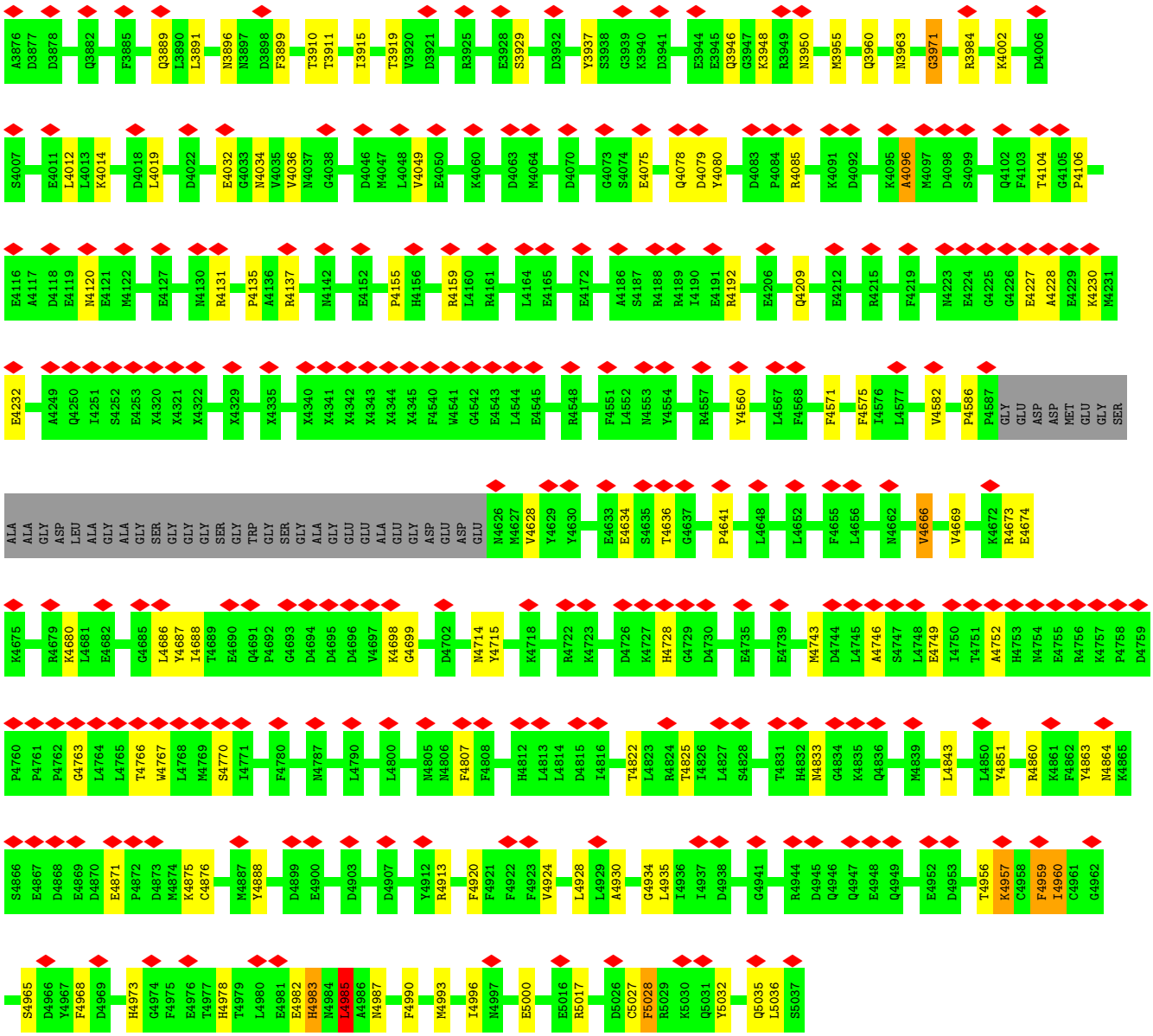
M1260 D1261 G1262 T1263 V1264 D1265 T1266 C1269 L1270 R1271 L1272 A1273 H1274 R1275 X1276 X1277 X1278 X1279 X1280 X1281 X1282 X1283 X1284 X1285 X1291 X1430 X1441 X1442 X1446 X1447 X1448 X1449 X1450 X1475 X1476 X1477 X1478 X1479 X1480 X1481 X1482 X1486 X1504 X1505 X1516 X1517 X1518 X1519 X1520 X1521 X1522

X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1536 X1537 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 M1573 P1574 L1575 M1579 F1580 E1583 P1589 Q1590 P1593 R1594 L1595 Q1598 M1599 L1600 W1605 S1606 R1607 H1611 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624

A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 M1637 A1638 L1639 E1644 N1645 E1655 R1656 L1657 D1658 H1663 S1664 H1665 T1666 L1667 R1668 L1669 Y1670 R1671 L1676 N1679 R1680 V1681 A1682 L1685 H1688 V1689 D1690 Q1691 L1694 L1695 H1696 A1697 L1698 E1699 D1700 A1701 G1705 R1708 A1709 G1710 Y1711

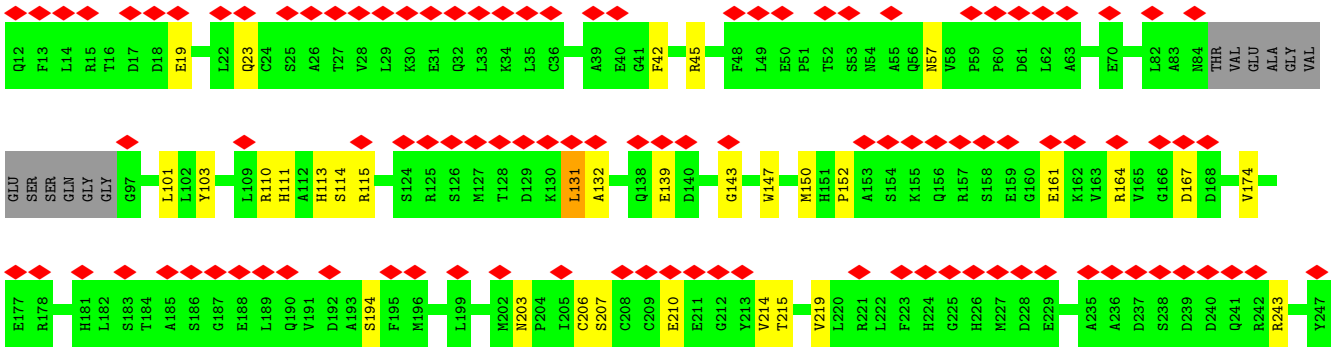

Y1712 D1713 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 S1729 M1730 L1731 S1732 E1733 Y1734 I1735 P1740 E1741 T1742 R1743 A1744 I1745 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1761 L1762 P1763 G1764 V1765 G1766 V1767 T1768 L1771 R1772 P1773 P1774 H1775 H1776 F1782 V1783 A1784 A1785
L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798 I1802 E1805 A1806 L1807 R1808 R1813 M1814 L1815 G1816 E1817 R1820 D1821 Q1824 H1825 A1826 R1827 D1828 G1831 Q1837 F1838 V1839 P1840 V1845 L1848 I1853 F1854 G1855 D1856 V1859 K1860 Q1861 I1862 L1863 K1864 M1865 I1866
E1867 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927
Q1928 L1931 P1932 K1936 L1937 Q1938 M1939 C1940 Q1949 L1958 A1959 A1960 F1961 A1962 E1963 R1964 Y1965 V1966 D1967 K1968 L1969 Q1970 A1971 R1974 S1975 R1976 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005
I2006 N2007 M2008 L2009 L2010 H2011 F2012 K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 P2022 L2023 D2026 I2027 R2028 Q2029 D2030 L2031 Q2032 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 E2115 R2118 L2123 R2126 Q2127 L2131 L2138 P2139 R2140 A2141 Y2142 T2143 I2144 S2145 P2146 S2147 E2150 D2151 L2155 L2156 L2166 Q2169 M2170
N2176 G2183 M2186 N2187 N2188 K2189 Y2192 Q2193 R2199 A2200 H2204 E2209 N2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 P2226 K2227 M2228 V2229 R2234 F2235 Y2238 F2239 I2242 N2246 Q2247 R2248 D2252 H2253 Y2256 L2257 N2260 S2261 G2262 I2263 G2264
L2265 G2266 M2267 Q2268 G2269 S2270 T2271 P2272 L2273 D2274 V2275 A2276 A2277 E2285 L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295 E2296 S2300 A2303 G2304 L2307 Q2308 S2309 C2310 P2311 M2312 L2313 L2314 A2315 K2316 G2317 Y2318 P2319 D2320 I2321 G2322 C2326 G2327 R2330 Y2331 L2332 D2333 F2334 L2335 R2336 F2337
F2340 V2341 N2342 G2343 E2344 S2345 V2346 E2347 E2348 N2349 A2350 N2351 R2355 L2356 R2359 E2362 C2363 F2364 G2365 P2366 A2367 L2368 R2369 G2370 E2371 G2372 G2373 S2374 A2378 E2382 A2383 I2384 R2385 I2386 S2387 E2388 D2389 P2390 A2391 R2392 D2393 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY
GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 H2417 L2418 G2419 H2420 F2425 Y2426 I2430 D2431 L2432 L2433 G2434 R2435 P2438 E2439 M2440 H2441 K2447 G2448 E2449 R2452 I2453 R2454 A2455 I2456 L2457 R2458 S2459 L2460 V2461 P2462 L2463 D2464 D2465 L2466 I2469 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479
X2487 X2488 X2489 X2490 X2493 X2499 X2511 X2512 X2513 X2514 X2522 X2523 X2528 X2529 X2530 X2531 X2532 X2533 X2534 X2535 X2536 X2537 X2538 X2561 X2562 X2563 X2566 X2567 X2568 X2577 X2580 X2581 X2582 X2583 X2584 X2585 X2586 X2589 X2596 X2597 X2604 X2614 X2617 X2618 X2619 X2620
X2621 X2622 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2630 X2631 X2636 X2637 X2638 X2643 X2648 X2649 X2650 X2651 X2659 X2662 X2663 X2667 X2668 X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678 X2679 X2680 X2681 X2682 X2683 X2686 X2687 X2688 X2689 X2690 X2691 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699
X2700 X2701 X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 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

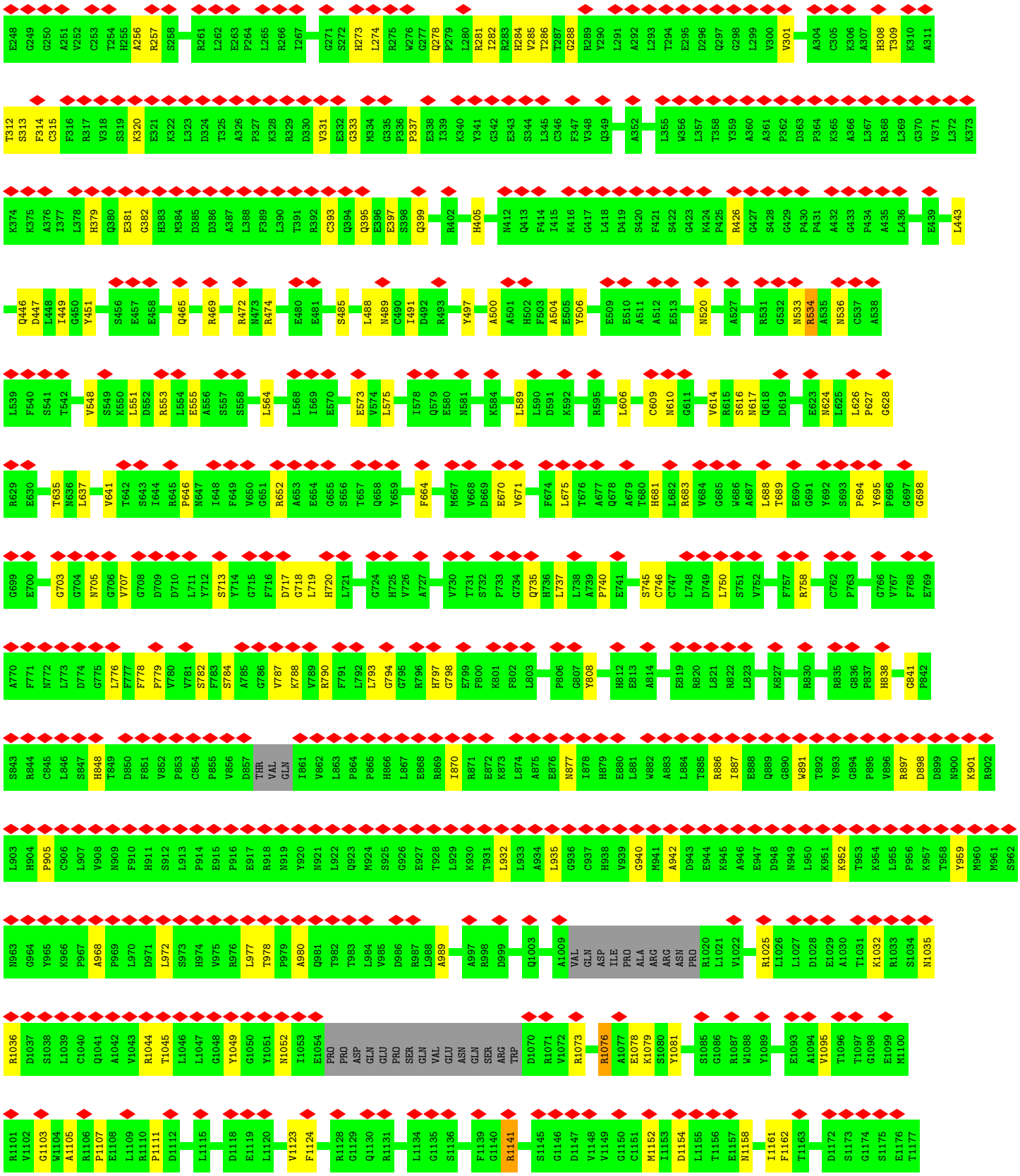

M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN 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 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2955 X2959 X2960 X2961 X2962 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974
X2975 X2976 X2995 X2996 X2997 X2998 X2999 X3000 X3003 X3004 X3005 X3006 X3011 X3014 X3015 X3016 X3017 X3018 X3019 X3020 X3021 X3022 X3023 X3026 X3027 X3028 X3029 X3032 X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040 X3041 X3042 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3053 X3054 X3055 X3056 X3057 X3058 X3059 X3060
X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3142 X3143 X3144 X3145 X3146 X3147 X3148 X3149 X3150 X3151 X3154 X3155 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3182 X3183 X3186 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3201 X3204 X3205
X3206 X3207 X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3226 X3227 X3228 X3229 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277
X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299 X3303 X3304 X3305 X3306 X3307 X3308 X3309 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3323 X3324 X3325 X3326 X3327 X3330 X3331 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344
X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3369 X3370 X3371 X3372 X3373 X3374 X3377 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407
X3408 X3409 X3410 X3411 X3412 X3413 X3414 X3415 X3416 X3417 X3418 X3419 X3420 X3421 X3427 X3428 X3432 X3433 X3434 X3435 X3436 X3441 X3442 X3443 X3450 X3451 X3452 X3453 X3454 X3455 X3456 X3457 X3458 X3459 X3462 X3463 X3464 X3465 X3466 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3521 X3522 X3525 X3526
X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3576 X3577 X3578 X3579 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3592 X3593
X3599 X3600 X3606 X3607 X3608 X3609 X3610 X3611 X3612 X3613 T3639 N3643 L3644 P3645 T3646 H3647 R3648 N3651 M3652 F3653 L3654 E3655 S3656 Y3657 K3658 A3659 A3660 W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 F3669 E3670 D3671 R3672 D3676 L3677 S3678 K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692
K3693 K3694 L3698 H3699 Q3700 S3706 R3707 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 E3754 E3755 K3756 E3759 K3760 Q3761 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 A3776 E3777 M3778 V3779
L3780 Q3781 S3784 K3787 I3804 L3805 N3809 V3812 K3815 M3816 L3817 D3818 K3821 D3822 G3827 F3828 F3829 Q3830 Q3833 M3836 L3842 D3843 L3844 N3845 R3849 Q3850 N3851 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873



- Molecule 2: Ryanodine receptor 1

Chain I:




E248 G249 G250 A251 V252 C253 T254 H255 A256 R257 S258 R261 L262 E263 P264 L265 R266 I267 G271 S272 H273 L274 R275 W276 G277 Q278 P279 L280 R281 I282 R283 H284 V285 T286 T287 G288 R289 Y290 L291 A292 L293 T294 E295 D296 Q297 G298 L299 V300 V301 A304 C305 K306 A307 H308 T309 K310 A311
T312 S313 F314 C315 F316 R317 V318 S319 K320 E321 K322 L323 D324 T325 A326 P327 K328 R329 D330 V331 E332 G333 M334 G335 P336 P337 E338 I339 K340 Y341 G342 E343 S344 L345 C346 F347 V348 Q349 A352 L355 W356 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 K373
K374 K375 A376 I377 L378 H379 Q380 E381 G382 H383 M384 D385 D386 A387 L388 F389 L390 T391 R392 C393 Q394 Q395 E396 E397 S398 Q399 R402 H405 N412 Q413 F414 I415 K416 G417 L418 D419 S420 F421 S422 G423 K424 P425 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 L436 E439 L443
Q446 D447 L448 I449 G450 Y451 S456 E457 E458 Q465 R469 R472 N473 R474 E480 E481 S485 L488 N489 C490 I491 D492 R493 Y497 A500 A501 H502 F503 A504 E505 Y506 E509 E510 A511 A512 E513 N520 A527 R531 G532 N533 R534 A535 N536 C537 A538
L539 F540 S541 T542 V548 S549 K550 L551 D552 R553 L554 E555 A556 S557 S558 L564 L568 I569 E570 E573 V574 L575 I578 Q579 E580 N581 K584 L589 L590 D591 K592 R595 L606 C609 N610 G611 V614 R615 S616 N617 Q618 D619 E623 N624 L625 L626 P627 G628
R629 E630 T635 N636 L637 V641 T642 S643 I644 R645 P646 N647 I648 F649 V650 G651 R652 A653 E654 G655 S656 T657 Q658 Y659 F664 M667 V668 D669 E670 V671 F674 L675 T676 A677 Q678 A679 T680 H681 L682 R683 V684 G685 W686 A687 L688 T689 E690 G691 Y692 S693 P694 Y695 P696 G697 G698
G699 E700 G703 G704 N705 G706 V707 G708 D709 D710 L711 Y712 S713 Y714 G715 F716 D717 G718 L719 H720 L721 G724 H725 V726 A727 V730 T731 S732 P733 G734 Q735 H736 L737 L738 A739 P740 E741 S745 C746 C747 L748 D749 L750 S751 V752 F757 R758 C762 P763 G766 V767 F768 E769
A770 F771 N772 L773 D774 G775 L776 F777 F778 P779 V780 V781 S782 F783 S784 A785 G786 V787 K788 V789 R790 F791 L792 L793 G794 G795 R796 H797 G798 E799 F800 K801 F802 L803 P806 G807 Y808 H812 E813 A814 E819 R820 L821 R822 L823 K827 R830 R835 G836 P837 H838 G841 F842
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 A997 R998 D999 Q1003 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 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 R1076 A1077 E1078 K1079 S1080 Y1081 S1085 G1086 R1087 W1088 Y1089 E1093 A1094 V1095 T1096 T1097 G1098 E1099 M1100
R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 L1115 D1118 E1119 L1120 V1123 F1124 R1128 G1129 Q1130 R1131 L1134 G1135 S1136 F1139 G1140 R1141 S1145 G1146 D1147 V1148 V1149 G1150 C1151 M1152 I1153 D1154 L1155 T1156 E1157 N1158 I1161 F1162 T1163 D1172 S1173 G1174 S1175 E1176 T1177

A1178 F1179 R1180 E1181 I1184 G1185 D1186 G1187 F1188 L1189 V1199 G1200 H1201 L1202 N1203 L1204 G1205 Q1206 S1210 L1211 R1212 F1213 F1214 A1215 I1216 C1217 G1218 L1219 Q1220 E1221 G1222 F1223 Q1231 R1232 T1236 W1237 E1251 H1254 Y1255 E1256 R1259 M1260 D1261 G1262 T1263 V1264 D1265 T1266 C1269 L1270 R1271

L1272 A1273 H1274 R1275 X1276 X1277 X1278 X1279 X1280 X1281 X1282 X1283 X1284 X1285 X1430 X1441 X1442 X1446 X1447 X1450 X1475 X1476 X1477 X1478 X1479 X1480 X1481 X1482 X1486 X1504 X1505 X1516 X1517 X1518 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527 X1528 X1529 X1530 X1531 X1536 X1537 X1543

X1544 X1545 X1546 X1547 X1548 X1549 X1550 M1573 P1574 L1575 S1576 M1579 F1580 E1583 P1589 Q1590 P1593 R1594 L1595 L1600 W1605 S1606 R1607 M1608 H1611 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 M1637 A1638 L1639 E1644 N1645

D1649 E1655 R1656 L1657 D1658 H1663 S1664 H1665 T1666 L1667 R1668 L1669 Y1670 R1671 L1676 N1679 R1680 L1685 H1688 V1689 D1690 Q1691 L1694 L1695 H1696 A1697 L1698 E1699 D1700 A1701 H1702 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 R1725 S1726 R1727 R1728 S1729 M1730 L1731 S1732

E1733 Y1734 I1735 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 T1768 L1771 R1772 P1773 P1774 H1775 H1776 F1777 F1782 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 L1798 I1802

E1805 A1806 L1807 R1808 R1813 M1814 L1815 G1816 E1817 R1820 D1821 Q1824 H1825 A1826 R1827 D1828 G1831 Q1837 F1838 V1839 P1840 V1845 L1848 I1853 F1854 G1855 D1856 V1859 K1860 Q1861 I1862 L1863 K1864 M1865 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU

GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU 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 L1931 P1932 K1936 L1937 Q1938 M1939 C1940 Q1949 L1968 A1959 A1960 F1961

A1962 E1963 R1964 Y1965 K1968 L1969 Q1970 A1971 N1972 Q1973 R1974 S1975 R1976 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006 N2007 M2008 L2009 L2010 H2011 F2012 K2013 D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 P2022

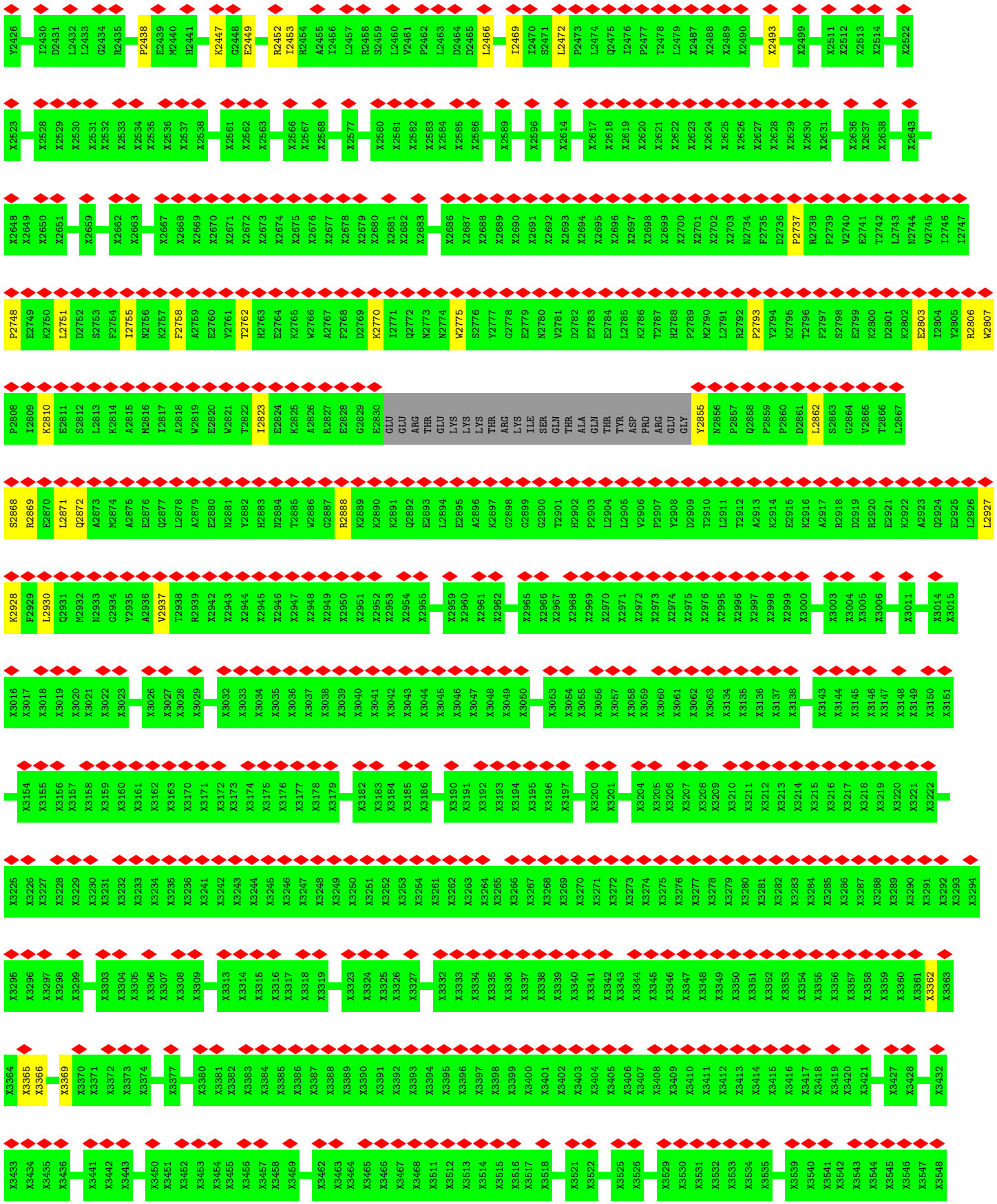
L2023 D2026 I2027 R2028 Q2029 D2030 L2031 Q2032 D2033 F2034 H2035 H2041 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU GLU PRO GLU GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU

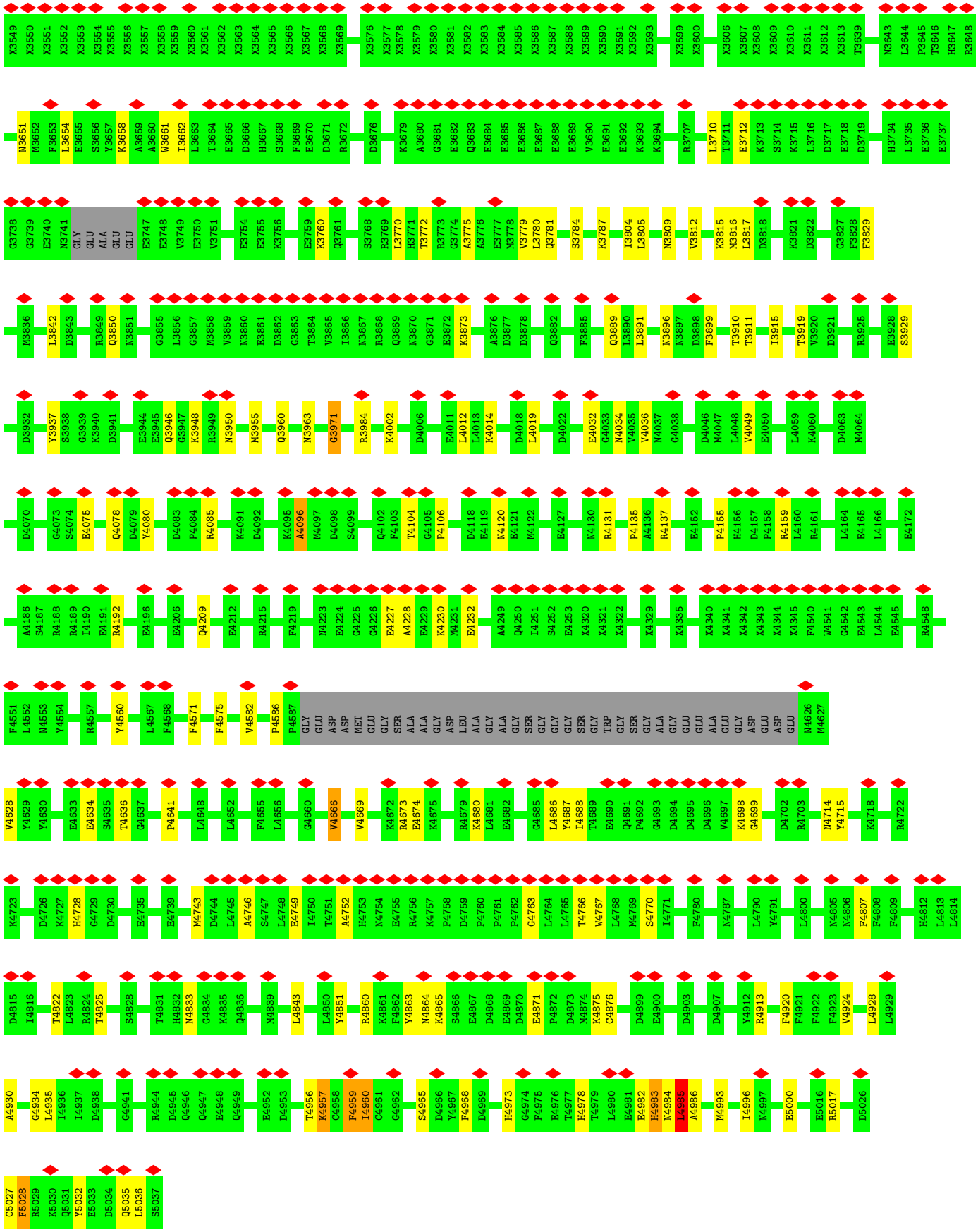
GLU K2089 K2090 P2091 Q2092 Q2095 R2104 Q2107 E2115 R2118 L2123 R2126 Q2127 L2131 L2138 P2139 R2140 A2141 Y2142 T2143 I2144 S2145 P2146 S2147 E2150 D2151 L2155 L2156 L2166 Q2169 M2170 N2176 G2183 M2186 N2187 N2188 K2189 Y2192 Q2193 R2199 A2200

H2204 E2209 N2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 P2226 K2227 M2228 V2229 R2234 F2235 Y2238 F2239 I2242 N2246 Q2247 R2248 D2252 H2253 Y2256 L2257 N2260 S2261 G2262 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 S2270 T2271 P2272 L2273 D2274 V2275 A2276 A2277 E2285

L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295 E2296 K2297 V2298 V2299 S2300 Y2301 L2302 A2303 G2304 L2307 Q2308 S2309 C2310 P2311 M2312 L2313 L2314 A2315 K2316 G2317 Y2318 P2319 D2320 I2321 C2326 G2327 R2330 Y2331 L2332 D2333 F2334 L2335 R2336 F2337 F2340 V2341 N2342 G2343 E2344 S2345 V2346 E2347 E2348 N2349 A2350 N2351 R2355

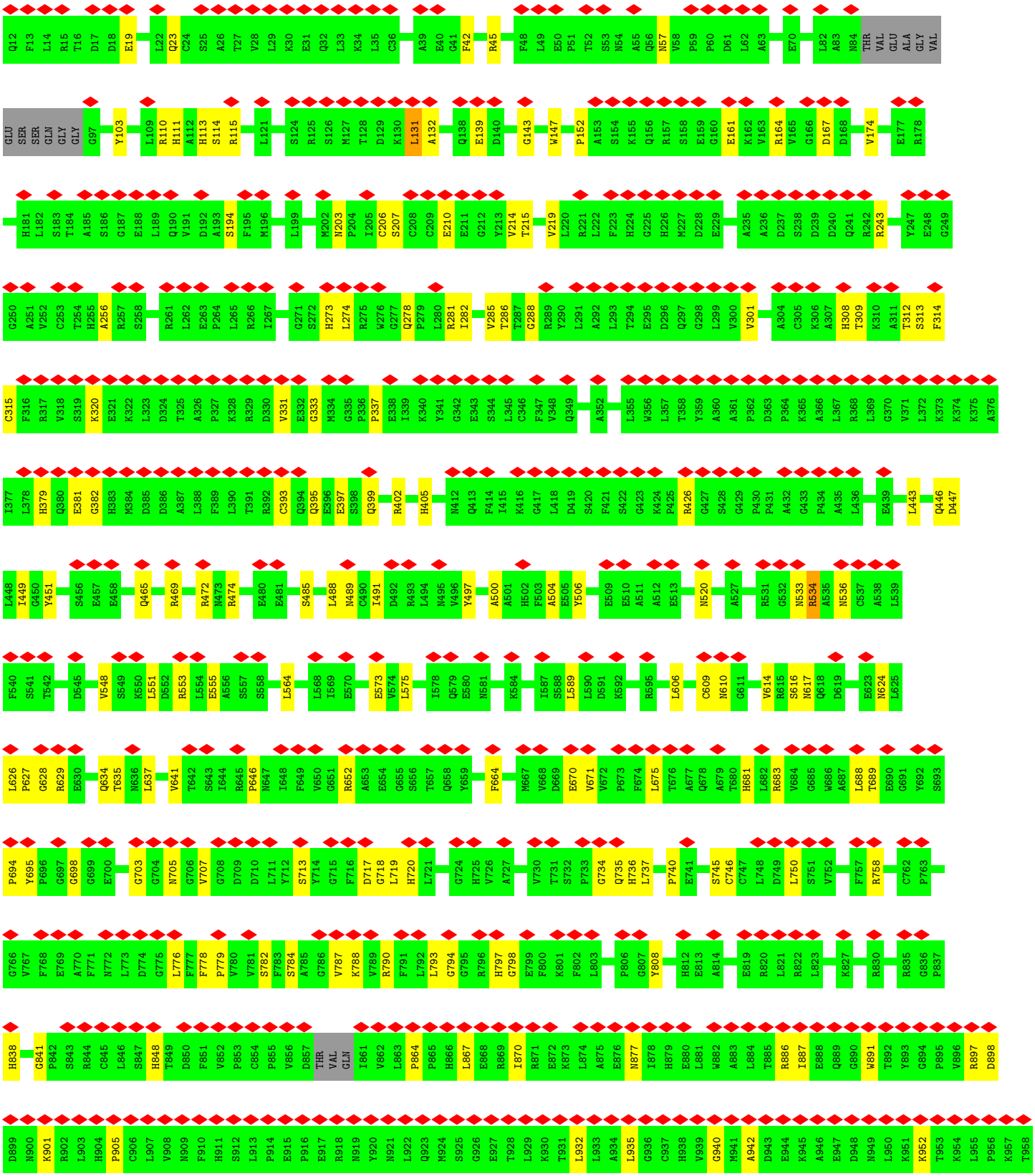
L2356 R2359 K2360 P2361 E2362 C2363 F2364 G2365 P2366 A2367 L2368 R2369 G2370 E2371 G2372 G2373 S2374 A2378 I2384 R2385 I2386 S2387 E2388 D2389 P2390 A2391 R2392 D2393 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 V2416 H2417 L2418 G2419 H2420 F2425


Y2426 I2430 D2431 L2432 L2433 G2434 R2435 P2438 E2439 M2440 H2441 K2447 G2448 E2449 R2452 I2453 R2454 A2455 I2456 L2457 R2458 S2459 L2460 V2461 P2462 L2463 D2464 D2465 L2466 I2469 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479 X2487 X2488 X2489 X2490 X2493 X2499 X2511 X2512 X2513 X2514 X2522
X2523 X2528 X2529 X2530 X2531 X2532 X2533 X2534 X2535 X2536 X2537 X2538 X2561 X2562 X2563 X2566 X2567 X2568 X2577 X2580 X2581 X2582 X2583 X2584 X2585 X2586 X2589 X2596 X2614 X2617 X2618 X2619 X2620 X2621 X2622 X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2630 X2631 X2636 X2637 X2638 X2643
X2648 X2649 X2650 X2651 X2659 X2662 X2663 X2667 X2668 X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678 X2679 X2680 X2681 X2682 X2683 X2686 X2687 X2688 X2689 X2690 X2691 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702 X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 T2747
P2748 E2749 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 V2777 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 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927
K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2955 X2959 X2960 X2961 X2962 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2995 X2996 X2997 X2998 X2999 X3000 X3003 X3004 X3005 X3006 X3011 X3014 X3015
X3016 X3017 X3018 X3019 X3020 X3021 X3022 X3023 X3026 X3027 X3028 X3029 X3032 X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040 X3041 X3042 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3053 X3054 X3055 X3056 X3057 X3058 X3059 X3060 X3061 X3062 X3063 X3134 X3135 X3136 X3137 X3138 X3143 X3144 X3145 X3146 X3147 X3148 X3149 X3150 X3151
X3154 X3155 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3182 X3183 X3184 X3185 X3186 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3201 X3204 X3205 X3206 X3207 X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222
X3225 X3226 X3227 X3228 X3229 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294
X3295 X3296 X3297 X3298 X3299 X3303 X3304 X3305 X3306 X3307 X3308 X3309 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3323 X3324 X3325 X3326 X3327 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344 X3345 X3346 X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363
X3364 X3365 X3366 X3369 X3370 X3371 X3372 X3373 X3374 X3377 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409 X3410 X3411 X3412 X3413 X3414 X3415 X3416 X3417 X3418 X3419 X3420 X3421 X3427 X3428 X3432
X3433 X3434 X3435 X3436 X3441 X3442 X3443 X3450 X3451 X3452 X3453 X3454 X3455 X3456 X3457 X3458 X3459 X3462 X3463 X3464 X3465 X3466 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3521 X3522 X3525 X3526 X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548

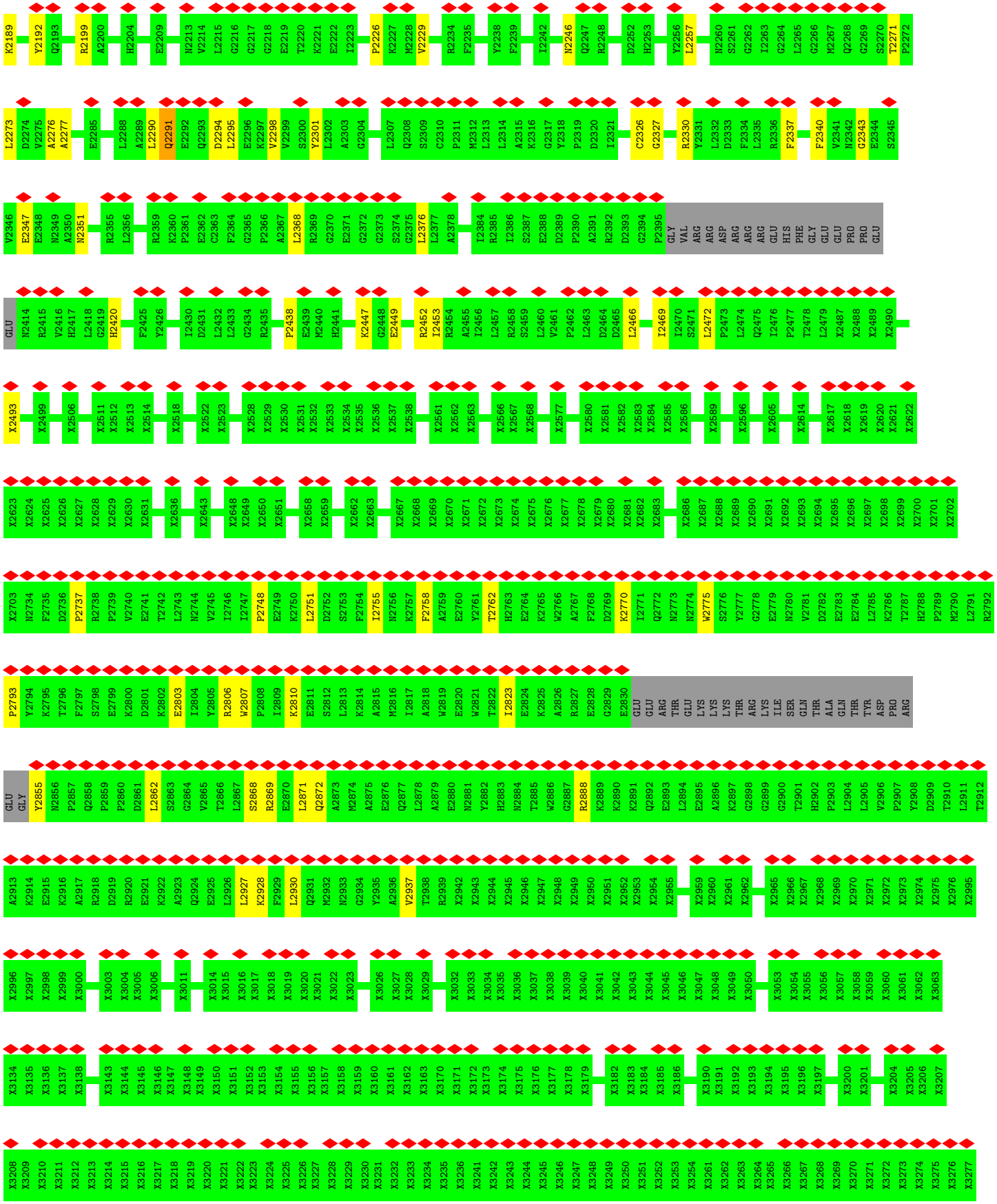

X3549 X3550 X3551 X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3569 X3576 X3577 X3578 X3579 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3592 X3593 X3599 X3600 X3606 X3607 X3608 X3609 X3610 X3611 X3612 X3613 T3639 M3643 L3644 P3645 T3646 H3647 R3648
N3651 H3652 F3653 L3654 E3655 S3656 Y3657 K3658 A3659 A3660 W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 F3669 E3670 D3671 R3672 D3676 K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 R3707 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 H3734 L3735 E3736 E3737
G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 E3754 E3755 K3756 E3759 K3760 Q3761 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 A3776 E3777 H3778 V3779 L3780 Q3781 S3784 K3787 T3804 L3805 N3809 V3812 K3815 M3816 L3817 D3818 K3821 D3822 G3827 F3828 F3829
M3836 L3842 D3843 R3849 Q3850 N3851 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 A3876 D3877 D3878 Q3882 F3885 Q3889 L3890 L3891 N3896 N3897 D3898 F3899 T3910 T3911 I3915 T3919 V3920 D3921 R3925 E3928 S3929
D3932 Y3937 S3938 G3939 K3940 D3941 E3944 E3945 Q3946 G3947 K3948 R3949 N3950 M3955 Q3960 N3963 G3971 R3984 K4002 D4006 E4011 L4012 L4013 K4014 D4018 L4019 D4022 E4032 G4033 N4034 V4035 V4036 N4037 G4038 D4046 M4047 L4048 V4049 E4050 L4059 K4060 D4063 M4064
D4070 G4073 S4074 E4075 Q4078 D4079 Y4080 D4083 P4084 R4085 K4091 D4092 K4095 A4096 M4097 D4098 S4099 Q4102 F4103 T4104 G4105 P4106 D4118 E4119 N4120 E4121 M4122 E4127 N4130 R4131 P4135 A4136 R4137 E4152 P4155 H4156 D4157 P4158 R4159 L4160 R4161 L4164 E4165 L4166 E4172
A4186 S4187 R4188 R4189 I4190 E4191 R4192 E4196 E4206 Q4209 E4212 R4215 F4219 N4223 E4224 G4225 G4226 E4227 A4228 E4229 K4230 M4231 E4232 A4249 Q4250 I4251 S4252 E4253 X4320 X4321 X4322 X4329 X4335 X4340 X4341 X4342 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 R4548
F4551 L4552 N4553 Y4554 R4557 Y4560 L4567 F4568 F4571 F4575 V4582 P4586 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 M4627
V4628 Y4629 Y4630 E4633 E4634 S4635 T4636 G4637 P4641 L4648 L4652 F4655 L4656 G4660 V4666 V4669 K4672 R4673 E4674 K4675 R4679 K4680 L4681 E4682 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 D4696 V4697 K4698 G4699 D4702 R4703 N4714 Y4715 K4718 R4722
K4723 D4726 K4727 H4728 G4729 D4730 E4735 E4739 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 F4780 N4787 L4790 Y4791 L4800 N4805 N4806 F4807 F4808 F4809 H4812 L4813 L4814
D4815 I4816 T4822 L4823 R4824 T4825 S4828 T4831 H4832 N4833 G4834 K4835 Q4836 M4839 L4843 L4850 Y4851 R4860 K4861 F4862 Y4863 N4864 K4865 S4866 E4867 D4868 E4869 P4870 E4871 P4872 D4873 M4874 K4875 C4876 D4899 E4900 D4903 D4907 Y4912 R4913 F4920 F4921 F4922 F4923 V4924 L4928 L4929
A4930 G4934 L4935 I4936 I4937 D4938 G4941 R4944 D4945 Q4946 Q4947 E4948 Q4949 E4952 D4953 T4956 K4957 C4958 F4959 I4960 C4961 G4962 S4965 D4966 Y4967 F4968 D4969 H4973 G4974 F4975 E4976 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986 M4993 I4996 N4997 E5000 E5016 R5017 D5026
C5027 F5028 R5029 K5030 Q5031 Y5032 E5033 D5034 Q5035 L5036 S5037

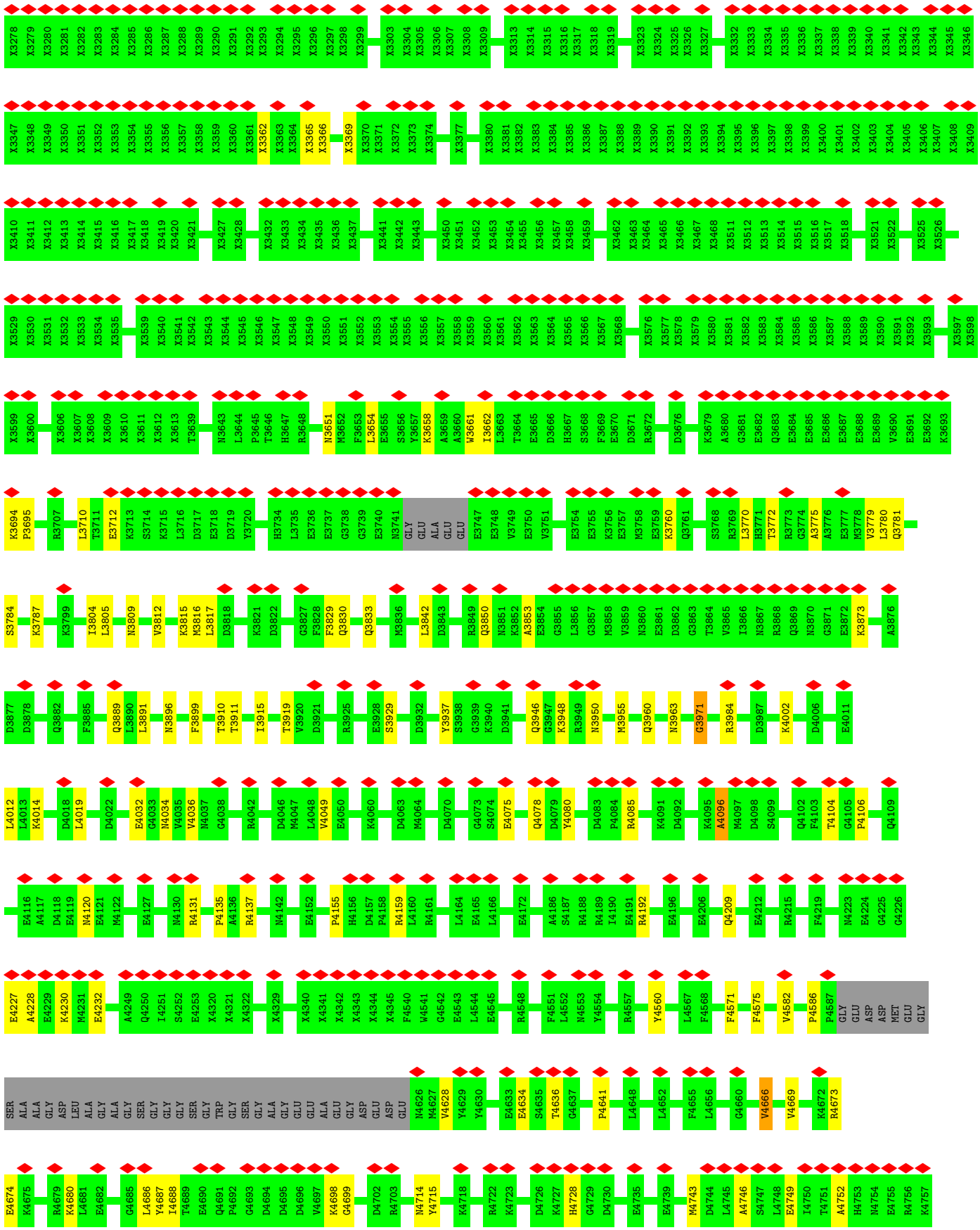
- Molecule 2: Ryanodine receptor 1

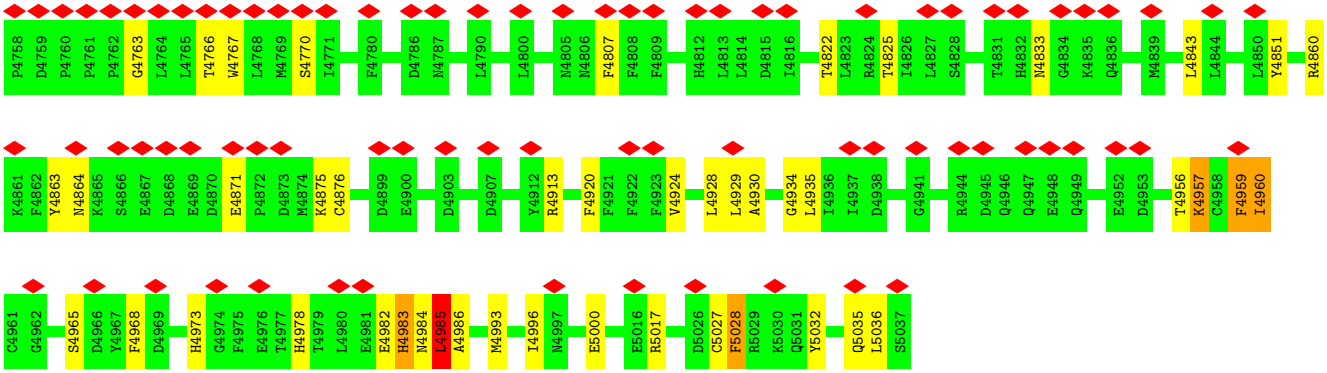
Chain G:



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 A997 R998 D999 Q1003 A1009 VAL GLN ASP ILE PRO ALA ARG ASN PRO R1020 L1021 V1022 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 R1076 A1077 E1078 K1079 S1080 Y1081 S1085 G1086 R1087 W1088 Y1089 E1093 A1094 V1095 T1096
T1097 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 L1115 D1118 E1119 L1120 V1123 F1124 R1128 G1129 Q1130 R1131 L1134 G1135 S1136 F1139 G1140 R1141 S1145 G1146 D1147 V1148 M1152 I1153 D1154 L1155 T1156 E1157 M1158 I1161 F1162 T1163 D1172 S1173 G1174 S1175
E1176 T1177 A1178 F1179 R1180 E1181 I1184 G1185 D1186 G1187 F1188 L1189 V1199 G1200 H1201 L1202 N1203 L1204 G1205 Q1206 D1207 S1210 L1211 R1212 F1213 F1214 A1215 I1216 C1217 G1218 L1219 Q1220 E1221 G1222 F1223 Q1231 R1232 T1236 W1237 P1247 E1251 H1254 Y1255 E1256 R1259 M1260 D1261 G1262 T1263 V1264 D1265
T1266 C1269 L1270 R1271 L1272 A1273 H1274 R1275 X1276 X1277 X1278 X1279 X1280 X1281 X1282 X1283 X1284 X1285 X1291 X1292 X1430 X1441 X1442 X1446 X1447 X1448 X1449 X1450 X1475 X1476 X1477 X1478 X1479 X1480 X1481 X1482 X1486 X1504 X1505 X1516 X1517 X1518 X1519 X1520 X1521 X1522 X1523 X1524 X1525 X1526 X1527
X1528 X1529 X1530 X1531 X1536 X1537 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 M1573 P1574 L1575 M1579 F1580 E1583 P1589 Q1590 P1593 R1594 L1595 Q1598 M1599 L1600 W1605 S1606 R1607 M1608 H1611 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624 A1627 V1628 Q1629 C1630
Q1631 D1632 P1633 L1634 M1637 A1638 L1639 E1644 N1645 E1655 R1656 L1657 D1658 H1663 S1664 H1665 T1666 L1667 R1668 L1669 Y1670 R1671 L1676 N1679 R1680 L1685 H1688 V1689 D1690 Q1691 L1694 L1695 H1696 A1697 L1698 E1699 D1700 A1701 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721
R1725 S1726 R1727 R1728 S1729 M1730 L1731 S1732 E1733 Y1734 I1735 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 L1771 R1772 P1773 P1774 H1775 H1776 F1782 V1783 A1784 A1785 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794
P1795 A1796 R1797 L1798 I1802 E1805 A1806 L1807 R1808 R1813 M1814 L1815 G1816 E1817 R1820 D1821 Q1824 H1825 A1826 R1827 D1828 G1831 Q1837 F1838 V1839 P1840 V1845 L1848 I1853 F1854 G1855 D1856 V1859 K1860 Q1861 I1862 L1863 K1864 M1865 I1866 E1867 V1870 F1871 T1872 E1873 E1874 GLU GLU
GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 G1925 L1926 L1927 Q1928 L1931 P1932 K1936 L1937 Q1938 M1939
C1940 Q1949 L1958 A1959 A1960 F1961 A1962 E1963 R1964 Y1965 V1966 D1967 K1968 L1969 Q1970 A1971 N1972 Q1973 R1974 S1975 R1976 Y1977 A1978 L1979 L1980 M1981 R1982 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 P2002 Q2003 E2004 Q2005 I2006 N2007 M2008 L2009 L2010 H2011 F2012 K2013
D2014 E2015 A2016 D2017 E2018 E2019 D2020 C2021 P2022 L2023 D2026 I2027 R2028 Q2029 D2030 L2031 Q2032 H2035 H2041 C2042 G2043 I2044 Q2045 L2046 E2047 C2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU 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 E2115 R2118 L2123 R2126 Q2127 L2131 L2138 P2139 R2140 A2141 Y2142 T2143 I2144 S2145 P2146 S2147 E2150 D2151 L2155 L2156 L2166 Q2169 M2170 N2176 G2183 M2186 N2187 N2188


K2189 Y2192 Q2193 R2199 A2200 H2204 E2209 N2213 V2214 L2215 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 P2226 K2227 M2228 V2229 R2234 F2235 Y2238 F2239 I2242 N2246 Q2247 R2248 D2252 H2253 Y2256 L2257 N2260 S2261 G2262 I2263 G2264 L2265 G2266 M2267 Q2268 G2269 S2270 T2271 P2272
L2273 D2274 V2275 A2276 A2277 E2285 L2288 A2289 L2290 Q2291 E2292 Q2293 D2294 L2295 E2296 K2297 V2298 V2299 S2300 Y2301 L2302 A2303 G2304 L2307 Q2308 S2309 C2310 P2311 M2312 L2313 L2314 A2315 K2316 G2317 Y2318 P2319 D2320 I2321 C2326 G2327 R2330 Y2331 L2332 D2333 F2334 L2335 R2336 F2337 F2340 V2341 N2342 G2343 E2344 S2345
V2346 E2347 E2348 N2349 A2350 N2351 R2355 L2356 R2359 K2360 P2361 E2362 C2363 F2364 G2365 P2366 A2367 L2368 R2369 G2370 E2371 G2372 G2373 S2374 G2375 L2376 L2377 A2378 I2384 R2385 I2386 S2387 E2388 D2389 P2390 A2391 R2392 D2393 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU
GLU N2414 R2415 V2416 H2417 L2418 G2419 H2420 F2425 Y2426 I2430 D2431 L2432 L2433 G2434 R2435 P2438 E2439 M2440 H2441 K2447 G2448 E2449 R2452 I2453 R2454 A2455 I2456 L2457 R2458 S2459 L2460 V2461 P2462 L2463 D2464 D2465 L2466 I2469 I2470 S2471 L2472 P2473 L2474 Q2475 I2476 P2477 T2478 L2479 X2487 X2488 X2489 X2490
X2493 X2499 X2506 X2511 X2512 X2513 X2514 X2518 X2522 X2523 X2528 X2529 X2530 X2531 X2532 X2533 X2534 X2535 X2536 X2537 X2538 X2561 X2562 X2563 X2566 X2567 X2568 X2577 X2580 X2581 X2582 X2583 X2584 X2585 X2586 X2589 X2596 X2605 X2614 X2617 X2618 X2619 X2620 X2621 X2622
X2623 X2624 X2625 X2626 X2627 X2628 X2629 X2630 X2631 X2636 X2643 X2648 X2649 X2650 X2651 X2658 X2659 X2662 X2663 X2667 X2668 X2669 X2670 X2671 X2672 X2673 X2674 X2675 X2676 X2677 X2678 X2679 X2680 X2681 X2682 X2683 X2686 X2687 X2688 X2689 X2690 X2691 X2692 X2693 X2694 X2695 X2696 X2697 X2698 X2699 X2700 X2701 X2702
X2703 N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 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 T2912
A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2955 X2959 X2960 X2961 X2962 X2965 X2966 X2967 X2968 X2969 X2970 X2971 X2972 X2973 X2974 X2975 X2976 X2995
X2996 X2997 X2998 X2999 X3000 X3003 X3004 X3005 X3006 X3011 X3014 X3015 X3016 X3017 X3018 X3019 X3020 X3021 X3022 X3023 X3026 X3027 X3028 X3029 X3032 X3033 X3034 X3035 X3036 X3037 X3038 X3039 X3040 X3041 X3042 X3043 X3044 X3045 X3046 X3047 X3048 X3049 X3050 X3053 X3054 X3055 X3056 X3057 X3058 X3059 X3060 X3061 X3062 X3063
X3134 X3135 X3136 X3137 X3138 X3143 X3144 X3145 X3146 X3147 X3148 X3149 X3150 X3151 X3152 X3153 X3154 X3155 X3156 X3157 X3158 X3159 X3160 X3161 X3162 X3163 X3170 X3171 X3172 X3173 X3174 X3175 X3176 X3177 X3178 X3179 X3182 X3183 X3184 X3185 X3186 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3200 X3201 X3204 X3205 X3206 X3207
X3208 X3209 X3210 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223 X3224 X3225 X3226 X3227 X3228 X3229 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277


X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3292 X3293 X3294 X3295 X3296 X3297 X3298 X3299 X3303 X3304 X3305 X3306 X3307 X3308 X3309 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3323 X3324 X3325 X3326 X3327 X3332 X3333 X3334 X3335 X3336 X3337 X3338 X3339 X3340 X3341 X3342 X3343 X3344 X3345 X3346
X3347 X3348 X3349 X3350 X3351 X3352 X3353 X3354 X3355 X3356 X3357 X3358 X3359 X3360 X3361 X3362 X3363 X3364 X3365 X3366 X3369 X3370 X3371 X3372 X3373 X3374 X3377 X3380 X3381 X3382 X3383 X3384 X3385 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3401 X3402 X3403 X3404 X3405 X3406 X3407 X3408 X3409
X3410 X3411 X3412 X3413 X3414 X3415 X3416 X3417 X3418 X3419 X3420 X3421 X3427 X3428 X3432 X3433 X3434 X3435 X3436 X3437 X3441 X3442 X3443 X3450 X3451 X3452 X3453 X3454 X3455 X3456 X3457 X3458 X3459 X3462 X3463 X3464 X3465 X3466 X3467 X3468 X3511 X3512 X3513 X3514 X3515 X3516 X3517 X3518 X3521 X3522 X3525 X3526
X3529 X3530 X3531 X3532 X3533 X3534 X3535 X3539 X3540 X3541 X3542 X3543 X3544 X3545 X3546 X3547 X3548 X3549 X3550 X3551 X3552 X3553 X3554 X3555 X3556 X3557 X3558 X3559 X3560 X3561 X3562 X3563 X3564 X3565 X3566 X3567 X3568 X3576 X3577 X3578 X3579 X3580 X3581 X3582 X3583 X3584 X3585 X3586 X3587 X3588 X3589 X3590 X3591 X3592 X3593 X3597 X3598
X3599 X3600 X3606 X3607 X3608 X3609 X3610 X3611 X3612 X3613 T3639 N3643 L3644 P3645 T3646 H3647 R3648 N3651 M3652 F3653 L3654 E3655 S3656 Y3657 K3658 A3659 A3660 W3661 I3662 L3663 T3664 E3665 D3666 H3667 S3668 F3669 E3670 D3671 R3672 D3676 K3679 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693
K3694 P3695 R3707 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 H3734 L3735 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 E3754 E3755 K3756 E3757 M3758 E3759 K3760 Q3761 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 A3776 E3777 M3778 V3779 L3780 Q3781
S3784 K3787 K3799 I3804 L3805 N3809 V3812 K3815 M3816 L3817 D3818 K3821 D3822 G3827 F3828 F3829 Q3830 Q3833 M3836 L3842 D3843 R3849 Q3850 N3851 K3852 A3853 E3854 G3855 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 A3876
D3877 D3878 Q3882 F3885 Q3889 L3890 L3891 N3896 F3899 T3910 T3911 I3915 T3919 V3920 D3921 R3925 E3928 S3929 D3932 Y3937 S3938 G3939 K3940 D3941 Q3946 K3947 K3948 R3949 N3950 M3955 Q3960 N3963 G3971 R3984 D3987 K4002 D4006 E4011
L4012 L4013 K4014 D4018 L4019 D4022 E4032 G4033 N4034 V4035 V4036 N4037 G4038 R4042 D4046 M4047 L4048 V4049 E4050 K4060 D4063 M4064 D4070 G4073 S4074 E4075 Q4078 D4079 Y4080 D4083 P4084 R4085 K4091 D4092 K4095 A4096 M4097 D4098 S4099 Q4102 F4103 T4104 G4105 P4106 Q4109
E4116 A4117 D4118 E4119 N4120 E4121 M4122 E4127 N4130 R4131 P4135 A4136 R4137 N4142 E4152 P4155 H4156 D4157 P4158 R4159 L4160 R4161 L4164 E4165 L4166 E4172 A4186 S4187 R4188 R4189 I4190 E4191 R4192 E4196 E4206 Q4209 E4212 R4215 F4219 N4223 E4224 G4225 G4226
E4227 A4228 E4229 K4230 M4231 E4232 A4249 Q4250 I4251 S4252 E4253 X4320 X4321 X4322 X4329 X4340 X4341 X4342 X4343 X4344 X4345 F4540 W4541 G4542 E4543 L4544 E4545 R4548 F4551 L4552 N4553 Y4554 R4557 Y4560 L4567 F4568 F4571 F4575 V4582 P4586 P4587 GLY GLU ASP ASP MET GLU GLY
SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 M4627 V4628 Y4629 Y4630 E4633 E4634 S4635 T4636 G4637 P4641 L4648 L4652 F4655 L4656 G4660 V4666 V4669 K4672 R4673
E4674 K4675 R4679 K4680 L4681 E4682 G4685 L4686 Y4687 I4688 T4689 E4690 Q4691 P4692 G4693 D4694 D4695 D4696 V4697 K4698 G4699 D4702 R4703 N4714 Y4715 K4718 R4722 K4723 D4726 K4727 H4728 G4729 D4730 E4735 E4739 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
F4780
D4786 N4787
L4790
L4800
M4805 M4806 F4807 F4808 F4809
H4812 L4813 L4814 D4815 I4816
T4822 L4823 R4824 T4825 I4826 L4827 S4828
T4831 H4832 N4833 G4834 K4835 Q4836
M4839
L4843 L4844
L4850 Y4851
R4860
K4861 F4862 Y4863 N4864 K4865 S4866 E4867 D4868 E4869 D4870 E4871 P4872 D4873 M4874 K4875 C4876
D4899 E4900
D4903
D4907
Y4912 R4913
F4920 F4921 F4922 F4923 V4924
L4928 L4929 A4930
G4934 L4935 I4936 I4937 D4938
G4941
R4944 D4945 Q4946 Q4947 E4948 Q4949
E4952 D4953
T4956 K4957 C4958 F4959 I4960
C4961 G4962
S4965
D4966 Y4967 F4968 D4969
H4973 G4974 F4975 E4976 T4977 H4978 T4979 L4980 E4981 E4982 H4983 N4984 L4985 A4986
M4993
I4996 N4997
E5000
E5016 R5017
D5026 C5027 F5028 R5029 K5030 Q5031 Y5032
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	0.070	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: ATP, ZN, CFF, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.32	0/834	0.53	0/1123
1	F	0.32	0/834	0.53	0/1123
1	H	0.32	0/834	0.53	0/1123
1	J	0.32	0/834	0.53	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (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	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	131	LEU	CA-CB-CG	8.10	133.92	115.30
2	B	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	E	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	G	131	LEU	CA-CB-CG	8.09	133.90	115.30
2	I	4985	LEU	CA-CB-CG	6.89	131.16	115.30
2	B	1600	LEU	CA-CB-CG	6.89	131.15	115.30
2	G	1600	LEU	CA-CB-CG	6.88	131.14	115.30
2	E	1600	LEU	CA-CB-CG	6.88	131.12	115.30
2	G	4985	LEU	CA-CB-CG	6.88	131.12	115.30
2	B	4985	LEU	CA-CB-CG	6.88	131.11	115.30
2	I	1600	LEU	CA-CB-CG	6.87	131.11	115.30
2	E	4985	LEU	CA-CB-CG	6.86	131.08	115.30
2	B	1676	LEU	CA-CB-CG	6.77	130.87	115.30
2	I	1676	LEU	CA-CB-CG	6.77	130.87	115.30
2	E	1676	LEU	CA-CB-CG	6.76	130.85	115.30
2	G	1676	LEU	CA-CB-CG	6.76	130.85	115.30
2	G	977	LEU	CA-CB-CG	6.08	129.29	115.30
2	E	977	LEU	CA-CB-CG	6.07	129.27	115.30
2	B	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	I	977	LEU	CA-CB-CG	6.06	129.24	115.30
2	E	2290	LEU	CA-CB-CG	5.73	128.48	115.30
2	G	2290	LEU	CA-CB-CG	5.72	128.47	115.30
2	B	2290	LEU	CA-CB-CG	5.72	128.46	115.30
2	I	2290	LEU	CA-CB-CG	5.71	128.44	115.30
2	I	688	LEU	CA-CB-CG	5.41	127.73	115.30
2	B	688	LEU	CA-CB-CG	5.40	127.71	115.30
2	E	688	LEU	CA-CB-CG	5.39	127.69	115.30
2	G	688	LEU	CA-CB-CG	5.38	127.68	115.30
2	B	1667	LEU	CA-CB-CG	5.20	127.25	115.30
2	E	1667	LEU	CA-CB-CG	5.20	127.26	115.30
2	G	1667	LEU	CA-CB-CG	5.20	127.25	115.30
2	I	1667	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

All (76) 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
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	4096	ALA	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	624	ASN	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	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	4096	ALA	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	624	ASN	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	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
2	G	2807	TRP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4096	ALA	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	624	ASN	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	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	4096	ALA	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	624	ASN	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	12	0
1	F	818	0	824	12	0
1	H	818	0	824	12	0
1	J	818	0	824	12	0
2	B	29499	0	24753	296	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	29499	0	24753	305	0
2	G	29499	0	24753	299	0
2	I	29499	0	24753	295	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	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	102396	1213	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 (1213) 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:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.32	1.18
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.32	1.17
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.32	1.17
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.32	1.16
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.64	1.16
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.64	1.15
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.64	1.14
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.64	1.14
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.67	1.12
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.67	1.11
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.67	1.10
2:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.67	1.09
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.54	0.94
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	1.81	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	1.81	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	1.81	0.92
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.54	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.54	0.91
2:B:4230:LYS:HD2	2:B:4959:PHE:CD1	2.05	0.90
2:I:4230:LYS:HD2	2:I:4959:PHE:CD1	2.05	0.90
2:G:4230:LYS:HD2	2:G:4959:PHE:CD1	2.05	0.90
2:E:4230:LYS:HD2	2:E:4959:PHE:CD1	2.05	0.90
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	1.81	0.89
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.16	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.16	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.16	0.80
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.16	0.80
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	1.96	0.78
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	1.96	0.78
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	1.96	0.78
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	1.96	0.78
2:E:4192:ARG:HH11	2:E:5028:PHE:HD2	1.36	0.74
2:B:4192:ARG:HH11	2:B:5028:PHE:HD2	1.36	0.73
2:G:4192:ARG:HH11	2:G:5028:PHE:HD2	1.36	0.73
2:I:4192:ARG:HH11	2:I:5028:PHE:HD2	1.36	0.72
2:B:111:HIS:HD2	2:B:114:SER:H	1.41	0.69
2:G:111:HIS:HD2	2:G:114:SER:H	1.41	0.68
2:E:111:HIS:HD2	2:E:114:SER:H	1.41	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.42	0.68
2:E:4957:LYS:NZ	2:E:4957:LYS:HB2	2.08	0.68
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.58	0.68
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.58	0.68
2:G:4957:LYS:HB2	2:G:4957:LYS:NZ	2.08	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.42	0.68
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.58	0.68
2:I:111:HIS:HD2	2:I:114:SER:H	1.41	0.68
2:B:4957:LYS:HB2	2:B:4957:LYS:NZ	2.08	0.67
2:E:5028:PHE:HE1	2:E:5032:TYR:HE2	1.39	0.67
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.58	0.67
2:I:4957:LYS:HB2	2:I:4957:LYS:NZ	2.08	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.42	0.66
2:E:4230:LYS:HG2	2:E:4959:PHE:HE1	1.60	0.66
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.78	0.66
2:E:379:HIS:HD2	2:E:382:GLY:H	1.42	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.78	0.65
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.15	0.65
2:B:4230:LYS:HG2	2:B:4959:PHE:HE1	1.60	0.65
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.78	0.65
2:I:4230:LYS:HG2	2:I:4959:PHE:HE1	1.60	0.65
2:G:4230:LYS:HD2	2:G:4959:PHE:HD1	1.62	0.65
2:E:161:GLU:HA	2:G:3984:ARG:HH22	1.62	0.64
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.15	0.64
2:I:4230:LYS:CD	2:I:4959:PHE:CE1	2.81	0.64
2:G:4230:LYS:HG2	2:G:4959:PHE:HE1	1.61	0.64
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.31	0.64
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.80	0.64
2:B:3984:ARG:HH22	2:I:161:GLU:HA	1.63	0.64
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.31	0.64
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.78	0.63
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.80	0.63
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.81	0.63
2:I:4230:LYS:HD2	2:I:4959:PHE:HD1	1.62	0.63
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.15	0.63
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.80	0.63
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.81	0.63
2:E:4230:LYS:CD	2:E:4959:PHE:CE1	2.81	0.63
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.80	0.63
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.80	0.63
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.80	0.63
2:G:4230:LYS:CD	2:G:4959:PHE:CE1	2.81	0.63
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.15	0.62
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.32	0.62
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.32	0.62
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.33	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.31	0.62
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.31	0.62
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.32	0.62
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.32	0.62
2:B:331:VAL:HG12	2:B:333:GLY:H	1.65	0.62
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.62
2:B:4228:ALA:HB2	2:E:4973:HIS:HE1	1.64	0.62
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.62
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.82	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.81	0.61
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3984:ARG:HH22	2:G:161:GLU:HA	1.65	0.61
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.61
2:E:331:VAL:HG12	2:E:333:GLY:H	1.65	0.61
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.33	0.61
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.61
2:I:331:VAL:HG12	2:I:333:GLY:H	1.65	0.61
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.33	0.61
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.80	0.61
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.83	0.61
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.82	0.61
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.33	0.61
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.82	0.61
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.82	0.61
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.83	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.61
2:B:5028:PHE:HE1	2:B:5032:TYR:HE2	1.39	0.61
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.61
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.83	0.61
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.81	0.61
2:G:5028:PHE:HE1	2:G:5032:TYR:HE2	1.39	0.61
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.61
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.33	0.61
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.83	0.60
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.83	0.60
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.60
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.33	0.60
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.84	0.60
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.82	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.66	0.60
2:G:331:VAL:HG12	2:G:333:GLY:H	1.65	0.60
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.81	0.60
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.66	0.60
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.84	0.60
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.90	0.60
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.84	0.60
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.84	0.60
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.84	0.60
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.84	0.60
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.84	0.60
2:I:5028:PHE:HE1	2:I:5032:TYR:HE2	1.39	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.84	0.60
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.84	0.60
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.60
2:B:161:GLU:HA	2:E:3984:ARG:HH22	1.66	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.84	0.59
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.84	0.59
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.84	0.59
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.36	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.75	0.59
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.84	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.75	0.59
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.90	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.75	0.59
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.85	0.59
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.90	0.59
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.84	0.59
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.66	0.59
2:B:4230:LYS:HD2	2:B:4959:PHE:HD1	1.62	0.59
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.84	0.59
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.66	0.59
2:B:4973:HIS:HE1	2:I:4228:ALA:HB2	1.67	0.59
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.85	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.75	0.58
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.37	0.58
2:E:4228:ALA:HB2	2:G:4973:HIS:HE1	1.68	0.58
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.37	0.58
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.85	0.58
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.35	0.58
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.90	0.58
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.84	0.58
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.36	0.58
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.37	0.58
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.37	0.58
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.86	0.58
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.83	0.58
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.85	0.58
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.69	0.58
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.37	0.58
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.86	0.58
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.85	0.58
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.77	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.36	0.58
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.85	0.58
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.86	0.58
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.36	0.58
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.77	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.86	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.69	0.57
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.37	0.57
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.87	0.57
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.86	0.57
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.86	0.57
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.77	0.57
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.86	0.57
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.86	0.57
2:I:4973:HIS:HE1	2:G:4228:ALA:HB2	1.68	0.57
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.68	0.57
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.86	0.57
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.57
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.87	0.57
2:B:614:VAL:HG22	2:B:616:SER:H	1.70	0.57
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.82	0.57
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.77	0.57
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.73	0.57
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.70	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.86	0.56
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.87	0.56
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.87	0.56
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.87	0.56
2:E:614:VAL:HG22	2:E:616:SER:H	1.70	0.56
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.87	0.56
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.87	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.56
1:F:55:VAL:HA	2:E:1784:ALA:HA	1.87	0.56
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.87	0.56
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.39	0.56
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.87	0.56
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.87	0.56
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.86	0.56
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.70	0.56
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.39	0.56
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.73	0.56
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.39	0.56
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.36	0.56
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.87	0.56
2:I:614:VAL:HG22	2:I:616:SER:H	1.70	0.56
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.39	0.56
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.87	0.55
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.89	0.55
2:B:3770:LEU:HD21	2:B:3775:ALA:HB3	1.88	0.55
2:E:4230:LYS:HD2	2:E:4959:PHE:HD1	1.62	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.87	0.55
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.89	0.55
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.70	0.55
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.88	0.55
2:G:626:LEU:HG	2:G:628:GLY:H	1.71	0.55
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.87	0.55
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.86	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.72	0.55
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.40	0.55
2:B:626:LEU:HG	2:B:628:GLY:H	1.71	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.40	0.55
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.87	0.55
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.38	0.55
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.87	0.55
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.88	0.55
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.36	0.55
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.89	0.55
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.40	0.55
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.89	0.55
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.88	0.55
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.40	0.55
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.89	0.55
2:E:626:LEU:HG	2:E:628:GLY:H	1.72	0.55
2:I:3770:LEU:HD21	2:I:3775:ALA:HB3	1.88	0.54
2:G:3770:LEU:HD21	2:G:3775:ALA:HB3	1.88	0.54
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.88	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.90	0.54
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.81	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.81	0.54
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.90	0.54
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.40	0.54
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.72	0.54
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.73	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.54
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.23	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.90	0.54
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.40	0.54
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.73	0.54
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.38	0.54
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.88	0.54
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.72	0.54
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.73	0.54
2:G:614:VAL:HG22	2:G:616:SER:H	1.70	0.54
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.90	0.54
2:E:520:ASN:ND2	2:E:555:GLU:OE2	2.41	0.54
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.89	0.54
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.81	0.54
2:B:309:THR:O	2:B:313:SER:OG	2.26	0.54
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.73	0.54
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.90	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	2.20	0.54
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.41	0.54
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.73	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.23	0.54
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.73	0.54
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.41	0.54
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.90	0.54
2:G:520:ASN:ND2	2:G:555:GLU:OE2	2.41	0.54
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.54
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.90	0.54
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.89	0.53
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.73	0.53
2:E:309:THR:O	2:E:313:SER:OG	2.26	0.53
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.81	0.53
2:E:3770:LEU:HD21	2:E:3775:ALA:HB3	1.88	0.53
2:E:5028:PHE:CD1	2:E:5032:TYR:CD2	2.96	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:309:THR:O	2:G:313:SER:OG	2.26	0.53
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.90	0.53
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.42	0.53
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.91	0.53
2:B:520:ASN:ND2	2:B:555:GLU:OE2	2.41	0.53
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.90	0.53
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.53
2:I:520:ASN:ND2	2:I:555:GLU:OE2	2.41	0.53
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.90	0.53
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.90	0.53
1:F:76:CYS:HB2	1:F:97:LEU:HB2	1.90	0.53
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.91	0.53
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.90	0.53
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.73	0.53
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.41	0.53
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.40	0.53
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.73	0.53
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.91	0.53
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.22	0.53
2:I:652:ARG:HD2	2:I:750:LEU:HB3	1.91	0.53
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.91	0.53
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.53
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.38	0.53
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.53
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	1.91	0.53
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.91	0.53
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	2.20	0.53
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.90	0.53
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.91	0.53
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	1.91	0.53
2:G:978:THR:HB	2:G:980:ALA:H	1.74	0.53
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.91	0.52
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.73	0.52
2:E:978:THR:HB	2:E:980:ALA:H	1.74	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.73	0.52
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.91	0.52
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	1.91	0.52
2:B:4960:ILE:N	2:B:4960:ILE:HD13	2.23	0.52
1:A:76:CYS:HB2	1:A:97:LEU:HB2	1.90	0.52
1:J:76:CYS:HB2	1:J:97:LEU:HB2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.36	0.52
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.40	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.43	0.52
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.43	0.52
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.43	0.52
2:B:5028:PHE:CD1	2:B:5032:TYR:CD2	2.96	0.52
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.38	0.52
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.52
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.52
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.52
2:B:111:HIS:CD2	2:B:114:SER:H	2.26	0.52
2:B:652:ARG:HD2	2:B:750:LEU:HB3	1.91	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.91	0.52
2:I:309:THR:O	2:I:313:SER:OG	2.26	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.43	0.52
2:B:3760:LYS:NZ	2:B:5000:GLU:OE1	2.41	0.52
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.43	0.52
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.91	0.52
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.43	0.52
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.91	0.52
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.43	0.52
2:G:652:ARG:HD2	2:G:750:LEU:HB3	1.91	0.52
1:H:55:VAL:HA	2:G:1784:ALA:HA	1.91	0.52
1:H:76:CYS:HB2	1:H:97:LEU:HB2	1.90	0.52
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.43	0.52
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.52
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.40	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.43	0.52
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.40	0.52
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.92	0.52
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.36	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.91	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.40	0.52
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.92	0.52
2:E:652:ARG:HD2	2:E:750:LEU:HB3	1.91	0.51
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.91	0.51
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:ALA:HA	2:I:194:SER:HB2	1.91	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.93	0.51
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.51
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.92	0.51
2:E:3891:LEU:HB3	2:E:3899:PHE:HE2	1.76	0.51
2:E:4860:ARG:HG3	2:E:4876:CYS:HB3	1.91	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.92	0.51
2:G:3891:LEU:HB3	2:G:3899:PHE:HE2	1.76	0.51
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.91	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.92	0.51
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.91	0.51
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.44	0.51
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.51
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.92	0.51
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.92	0.51
2:G:5028:PHE:CD1	2:G:5032:TYR:CD2	2.95	0.51
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.93	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.74	0.51
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.91	0.51
2:G:132:ALA:HA	2:G:194:SER:HB2	1.91	0.51
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.51
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.93	0.51
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.93	0.51
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.36	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.91	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.91	0.51
2:B:132:ALA:HA	2:B:194:SER:HB2	1.91	0.51
2:E:132:ALA:HA	2:E:194:SER:HB2	1.91	0.51
2:E:4985:LEU:HB2	3:E:5101:ATP:HN61	1.76	0.51
2:I:1637:MET:SD	2:I:1708:ARG:NH1	2.84	0.51
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.44	0.51
2:I:3891:LEU:HB3	2:I:3899:PHE:HE2	1.76	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.51
2:B:4985:LEU:HB2	3:B:5101:ATP:HN61	1.76	0.51
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.43	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.51
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.44	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.51
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.44	0.51
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:111:HIS:CD2	2:I:114:SER:H	2.26	0.51
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.77	0.51
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.43	0.51
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.77	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.44	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.26	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.93	0.50
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.44	0.50
2:I:4985:LEU:HB2	3:I:5101:ATP:HN61	1.76	0.50
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.92	0.50
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.92	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.44	0.50
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.77	0.50
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.92	0.50
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.77	0.50
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.93	0.50
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.92	0.50
2:G:1637:MET:SD	2:G:1708:ARG:NH1	2.84	0.50
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.44	0.50
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.44	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.94	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.76	0.50
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.77	0.50
2:B:3891:LEU:HB3	2:B:3899:PHE:HE2	1.76	0.50
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.77	0.50
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.93	0.50
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.92	0.50
2:B:1637:MET:SD	2:B:1708:ARG:NH1	2.84	0.50
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.94	0.50
2:I:4956:THR:O	2:I:4965:SER:N	2.42	0.50
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.94	0.50
2:I:5028:PHE:CD1	2:I:5032:TYR:CD2	2.96	0.50
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.77	0.50
2:B:2868:SER:O	2:B:2872:GLN:N	2.44	0.50
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.77	0.50
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.44	0.50
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.94	0.50
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.40	0.50
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.45	0.49
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.77	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.76	0.49
2:G:4985:LEU:HB2	3:G:5101:ATP:HN61	1.76	0.49
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.94	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.93	0.49
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.49
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.95	0.49
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.49
2:E:3760:LYS:NZ	2:E:5000:GLU:OE1	2.41	0.49
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.93	0.49
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.95	0.49
1:A:21:THR:HA	1:A:49:ARG:HA	1.95	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.94	0.49
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.94	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.93	0.49
2:E:1637:MET:SD	2:E:1708:ARG:NH1	2.84	0.49
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.45	0.49
2:B:320:LYS:NZ	2:B:381:GLU:O	2.42	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.76	0.49
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.94	0.49
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.94	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.84	0.49
2:E:548:VAL:HG12	2:E:564:LEU:HD22	1.95	0.49
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.95	0.49
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.94	0.49
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.49
1:F:21:THR:HA	1:F:49:ARG:HA	1.95	0.49
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.95	0.49
1:J:21:THR:HA	1:J:49:ARG:HA	1.95	0.49
2:B:794:GLY:H	2:B:798:GLY:HA3	1.78	0.49
2:G:548:VAL:HG12	2:G:564:LEU:HD22	1.95	0.49
2:G:794:GLY:H	2:G:798:GLY:HA3	1.78	0.49
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.46	0.49
2:E:794:GLY:H	2:E:798:GLY:HA3	1.78	0.49
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.95	0.49
2:B:1259:ARG:HH12	2:B:1593:PRO:HA	1.78	0.49
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.77	0.49
2:I:794:GLY:H	2:I:798:GLY:HA3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.94	0.49
2:I:3760:LYS:NZ	2:I:5000:GLU:OE1	2.41	0.49
2:G:1259:ARG:HH12	2:G:1593:PRO:HA	1.78	0.49
2:B:548:VAL:HG12	2:B:564:LEU:HD22	1.95	0.49
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.95	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.95	0.49
2:I:548:VAL:HG12	2:I:564:LEU:HD22	1.95	0.49
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.95	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.49
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.77	0.49
1:H:21:THR:HA	1:H:49:ARG:HA	1.95	0.48
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.95	0.48
2:E:1259:ARG:HH12	2:E:1593:PRO:HA	1.78	0.48
2:I:1259:ARG:HH12	2:I:1593:PRO:HA	1.78	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.95	0.48
2:G:4956:THR:O	2:G:4965:SER:N	2.42	0.48
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.94	0.48
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.95	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.95	0.48
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.77	0.48
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.43	0.48
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	1.96	0.48
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.95	0.48
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.39	0.48
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.46	0.48
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.95	0.48
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.95	0.48
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.95	0.48
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.84	0.48
2:I:776:LEU:HG	2:I:848:HIS:HA	1.95	0.48
2:G:776:LEU:HG	2:G:848:HIS:HA	1.95	0.48
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.96	0.48
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.45	0.48
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.48
2:E:4957:LYS:NZ	2:E:4957:LYS:CB	2.77	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.46	0.48
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.95	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.45	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.95	0.48
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.46	0.48
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.95	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.26	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.46	0.48
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.48
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.48
2:I:2758:PHE:O	2:I:2762:THR:N	2.46	0.48
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.46	0.48
2:B:776:LEU:HG	2:B:848:HIS:HA	1.95	0.48
2:E:776:LEU:HG	2:E:848:HIS:HA	1.95	0.48
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.48
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.96	0.48
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	1.96	0.48
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.96	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.32	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.95	0.48
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.48
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.31	0.48
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.48
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.47	0.48
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.96	0.48
2:I:4571:PHE:O	2:I:4575:PHE:N	2.47	0.48
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.47	0.48
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.96	0.47
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	1.96	0.47
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.96	0.47
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.95	0.47
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.32	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.47	0.47
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.96	0.47
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.96	0.47
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.95	0.47
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.44	0.47
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.95	0.47
2:I:4957:LYS:HB2	2:I:4957:LYS:HZ1	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.95	0.47
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.32	0.47
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.80	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.47
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.47	0.47
2:E:4763:GLY:O	2:E:4766:THR:OG1	2.31	0.47
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.79	0.47
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	2.20	0.47
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.95	0.47
1:F:27:THR:HB	1:F:100:ASP:HB3	1.97	0.47
1:A:27:THR:HB	1:A:100:ASP:HB3	1.97	0.47
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.96	0.47
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.96	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.95	0.47
2:G:2758:PHE:O	2:G:2762:THR:N	2.46	0.47
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	2.20	0.47
2:G:4957:LYS:NZ	2:G:4957:LYS:CB	2.77	0.47
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.47
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.32	0.47
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.47
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.39	0.47
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.79	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.95	0.47
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.96	0.47
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.39	0.47
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.96	0.47
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.95	0.47
2:I:164:ARG:N	2:I:167:ASP:OD2	2.46	0.47
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.84	0.47
2:B:164:ARG:N	2:B:167:ASP:OD2	2.46	0.47
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.47
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.47
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.95	0.47
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.80	0.47
2:G:320:LYS:NZ	2:G:381:GLU:O	2.42	0.47
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.96	0.47
2:G:3760:LYS:NZ	2:G:5000:GLU:OE1	2.41	0.47
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.95	0.47
2:E:243:ARG:NH1	2:E:301:VAL:O	2.43	0.47
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.48	0.47
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.80	0.47
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	1.97	0.47
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.48	0.47
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.48	0.47
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.50	0.47
2:I:215:THR:HG22	2:I:273:HIS:HA	1.97	0.47
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.47	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.80	0.47
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.47	0.47
2:B:3915:ILE:O	2:B:3919:THR:N	2.47	0.47
2:I:320:LYS:NZ	2:I:381:GLU:O	2.42	0.47
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.47
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.96	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.50	0.47
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.95	0.46
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.38	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.98	0.46
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.97	0.46
2:G:379:HIS:CD2	2:G:381:GLU:H	2.33	0.46
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.48	0.46
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.98	0.46
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	1.97	0.46
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.31	0.46
2:I:4822:THR:O	2:I:4825:THR:OG1	2.29	0.46
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.43	0.46
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.48	0.46
2:B:215:THR:HG22	2:B:273:HIS:HA	1.97	0.46
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.97	0.46
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	1.96	0.46
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.48	0.46
2:I:379:HIS:CD2	2:I:381:GLU:H	2.33	0.46
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:I:4957:LYS:NZ	2:I:4957:LYS:CB	2.77	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.80	0.46
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.98	0.46
2:E:215:THR:HG22	2:E:273:HIS:HA	1.97	0.46
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.98	0.46
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.48	0.46
2:E:4930:ALA:O	2:E:4934:GLY:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.84	0.46
1:A:55:VAL:HA	2:B:1784:ALA:HA	1.96	0.46
1:J:27:THR:HB	1:J:100:ASP:HB3	1.97	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.46	0.46
2:G:215:THR:HG22	2:G:273:HIS:HA	1.97	0.46
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.46
1:H:27:THR:HB	1:H:100:ASP:HB3	1.97	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.43	0.46
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.97	0.46
2:E:1991:THR:O	2:E:1995:THR:OG1	2.34	0.46
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	1.98	0.46
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.98	0.46
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.97	0.46
2:G:4930:ALA:O	2:G:4934:GLY:N	2.49	0.46
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.97	0.46
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.98	0.46
2:B:4957:LYS:NZ	2:B:4957:LYS:CB	2.77	0.46
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.96	0.46
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.98	0.46
2:I:4930:ALA:O	2:I:4934:GLY:N	2.49	0.46
1:H:87:HIS:H	1:H:91:ILE:HB	1.81	0.46
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	1.98	0.46
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.98	0.46
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.98	0.46
2:G:1991:THR:O	2:G:1995:THR:OG1	2.34	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.98	0.46
2:G:3915:ILE:O	2:G:3919:THR:N	2.47	0.46
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.98	0.46
1:F:87:HIS:H	1:F:91:ILE:HB	1.81	0.46
1:J:55:VAL:HA	2:I:1784:ALA:HA	1.97	0.46
1:J:87:HIS:H	1:J:91:ILE:HB	1.81	0.46
2:B:793:LEU:HB2	2:B:797:HIS:H	1.81	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.98	0.46
2:B:4822:THR:O	2:B:4825:THR:OG1	2.29	0.46
2:B:4930:ALA:O	2:B:4934:GLY:N	2.49	0.46
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.46
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.98	0.46
2:G:243:ARG:NH1	2:G:301:VAL:O	2.43	0.46
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	1.98	0.46
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	1.97	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.33	0.45
2:E:451:TYR:O	2:E:474:ARG:NH1	2.47	0.45
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	1.98	0.45
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	1.97	0.45
2:I:243:ARG:NH1	2:I:301:VAL:O	2.43	0.45
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.98	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.50	0.45
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.48	0.45
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.98	0.45
2:B:1936:LYS:O	2:B:1940:CYS:N	2.46	0.45
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.43	0.45
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.98	0.45
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	1.99	0.45
2:G:451:TYR:O	2:G:474:ARG:NH1	2.47	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.50	0.45
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.45
2:E:3842:LEU:O	2:E:3929:SER:OG	2.33	0.45
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.32	0.45
2:E:4822:THR:O	2:E:4825:THR:OG1	2.29	0.45
2:I:451:TYR:O	2:I:474:ARG:NH1	2.47	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:4209:GLN:HE22	2:I:4560:TYR:HE2	1.64	0.45
2:G:793:LEU:HB2	2:G:797:HIS:H	1.81	0.45
1:A:87:HIS:H	1:A:91:ILE:HB	1.81	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.33	0.45
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.98	0.45
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.98	0.45
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.98	0.45
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.98	0.45
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.97	0.45
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.98	0.45
2:G:4978:HIS:CD2	2:G:4982:GLU:HB2	2.52	0.45
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.80	0.45
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.45
2:I:793:LEU:HB2	2:I:797:HIS:H	1.81	0.45
2:G:206:CYS:SG	2:G:207:SER:N	2.89	0.45
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.31	0.45
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	1.99	0.45
2:I:206:CYS:SG	2:I:207:SER:N	2.89	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.97	0.45
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	1.99	0.45
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.98	0.45
2:B:940:GLY:O	2:B:1052:ASN:N	2.49	0.45
2:B:2758:PHE:O	2:B:2762:THR:N	2.46	0.45
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.82	0.45
2:E:379:HIS:CD2	2:E:381:GLU:H	2.33	0.45
2:E:793:LEU:HB2	2:E:797:HIS:H	1.81	0.45
2:I:4978:HIS:CD2	2:I:4982:GLU:HB2	2.52	0.45
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.98	0.45
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.32	0.45
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.98	0.45
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.50	0.45
2:B:4209:GLN:HE22	2:B:4560:TYR:HE2	1.64	0.45
2:B:4851:TYR:HD2	2:B:4920:PHE:HD1	1.65	0.45
2:I:1991:THR:O	2:I:1995:THR:OG1	2.34	0.45
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.82	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	1.99	0.45
2:B:1991:THR:O	2:B:1995:THR:OG1	2.34	0.45
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.82	0.45
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	1.99	0.45
2:E:206:CYS:SG	2:E:207:SER:N	2.89	0.45
2:E:4209:GLN:HE22	2:E:4560:TYR:HE2	1.64	0.45
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.98	0.45
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	1.99	0.45
2:B:451:TYR:O	2:B:474:ARG:NH1	2.47	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.33	0.45
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.98	0.45
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.98	0.44
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.98	0.44
2:B:3971:GLY:N	2:B:4032:GLU:OE2	2.50	0.44
2:E:1105:ALA:N	2:E:1189:LEU:O	2.51	0.44
2:E:1731:LEU:HA	2:E:1772:ARG:HH12	1.82	0.44
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.99	0.44
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.82	0.44
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.98	0.44
2:I:4851:TYR:HD2	2:I:4920:PHE:HD1	1.65	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.82	0.44
2:B:379:HIS:NE2	2:B:381:GLU:OE1	2.50	0.44
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.38	0.44
2:B:1731:LEU:HA	2:B:1772:ARG:HH12	1.82	0.44
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.44
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.82	0.44
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.00	0.44
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.44
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.32	0.44
2:E:257:ARG:O	2:E:284:HIS:NE2	2.48	0.44
2:E:4571:PHE:O	2:E:4575:PHE:N	2.47	0.44
2:I:1078:GLU:HB3	2:I:1081:TYR:HD2	1.82	0.44
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.39	0.44
2:G:4209:GLN:HE22	2:G:4560:TYR:HE2	1.64	0.44
2:B:1105:ALA:N	2:B:1189:LEU:O	2.51	0.44
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.00	0.44
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.00	0.44
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.99	0.44
2:B:4978:HIS:CD2	2:B:4982:GLU:HB2	2.52	0.44
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.44
2:G:1731:LEU:HA	2:G:1772:ARG:HH12	1.83	0.44
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.98	0.44
2:B:206:CYS:SG	2:B:207:SER:N	2.89	0.44
2:B:1663:HIS:O	2:B:1667:LEU:N	2.51	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.44
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.99	0.44
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	1.99	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.99	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.33	0.44
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.98	0.44
2:B:2452:ARG:NH1	2:I:174:VAL:O	2.50	0.44
2:E:379:HIS:NE2	2:E:381:GLU:OE1	2.50	0.44
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.00	0.44
2:I:379:HIS:NE2	2:I:381:GLU:OE1	2.50	0.44
2:G:379:HIS:NE2	2:G:381:GLU:OE1	2.50	0.44
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	1.99	0.44
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.00	0.44
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.53	0.44
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	2.00	0.44
2:E:4851:TYR:HD2	2:E:4920:PHE:HD1	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.44
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.98	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.83	0.44
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.00	0.44
2:G:1105:ALA:N	2:G:1189:LEU:O	2.51	0.44
2:B:282:ILE:HD12	2:B:314:PHE:HD2	1.83	0.44
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	2.00	0.44
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.00	0.44
2:B:4571:PHE:O	2:B:4575:PHE:N	2.47	0.44
2:E:1802:ILE:HG21	2:E:1807:LEU:HD22	2.00	0.44
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.53	0.44
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	2.00	0.44
2:G:4851:TYR:HD2	2:G:4920:PHE:HD1	1.65	0.44
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.43
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.99	0.43
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.83	0.43
2:E:4978:HIS:CD2	2:E:4982:GLU:HB2	2.52	0.43
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.83	0.43
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.43
2:I:4673:ARG:HH12	2:I:4698:LYS:HE3	1.83	0.43
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	2.00	0.43
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.00	0.43
2:G:4673:ARG:HH12	2:G:4698:LYS:HE3	1.83	0.43
2:G:4822:THR:O	2:G:4825:THR:OG1	2.29	0.43
1:F:87:HIS:HA	1:F:88:PRO:HD3	1.90	0.43
1:A:82:TYR:O	1:A:86:GLY:N	2.51	0.43
2:B:1078:GLU:HB3	2:B:1081:TYR:HD2	1.82	0.43
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.42	0.43
2:B:4956:THR:O	2:B:4965:SER:N	2.42	0.43
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.51	0.43
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	2.00	0.43
2:I:606:LEU:O	2:I:617:ASN:ND2	2.51	0.43
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.00	0.43
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.00	0.43
2:G:606:LEU:O	2:G:617:ASN:ND2	2.51	0.43
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.43
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	2.00	0.43
2:B:606:LEU:O	2:B:617:ASN:ND2	2.51	0.43
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.43
2:B:4996:ILE:HG12	4:B:5102:CFF:H123	2.00	0.43
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.38	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.00	0.43
2:G:282:ILE:HD12	2:G:314:PHE:HD2	1.83	0.43
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.00	0.43
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.82	0.43
2:G:5028:PHE:CG	2:G:5028:PHE:O	2.70	0.43
1:F:82:TYR:O	1:F:86:GLY:N	2.51	0.43
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.83	0.43
2:E:282:ILE:HD12	2:E:314:PHE:HD2	1.83	0.43
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
2:I:446:GLN:HA	2:I:449:ILE:HD12	2.01	0.43
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.00	0.43
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	2.00	0.43
2:G:1663:HIS:O	2:G:1667:LEU:N	2.51	0.43
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.99	0.43
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.99	0.43
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.49	0.43
2:E:606:LEU:O	2:E:617:ASN:ND2	2.51	0.43
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.00	0.43
2:I:1731:LEU:HA	2:I:1772:ARG:HH12	1.82	0.43
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.53	0.43
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.99	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.52	0.43
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.52	0.43
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.99	0.43
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	2.00	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.82	0.43
2:E:4673:ARG:HH12	2:E:4698:LYS:HE3	1.83	0.43
2:I:534:ARG:NH2	2:I:573:GLU:OE2	2.52	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.52	0.43
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.52	0.43
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	2.00	0.43
2:G:446:GLN:HA	2:G:449:ILE:HD12	2.01	0.43
2:G:1078:GLU:HB3	2:G:1081:TYR:HD2	1.82	0.43
2:B:4673:ARG:HH12	2:B:4698:LYS:HE3	1.83	0.43
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.43
2:G:1936:LYS:O	2:G:1940:CYS:N	2.46	0.43
2:E:278:GLN:N	2:E:315:CYS:SG	2.92	0.43
2:E:446:GLN:HA	2:E:449:ILE:HD12	2.01	0.43
2:E:1078:GLU:HB3	2:E:1081:TYR:HD2	1.82	0.43
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	2.00	0.43
2:I:101:LEU:HB3	2:I:150:MET:HE1	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2823:ILE:HG12	2:I:2937:VAL:HG22	2.01	0.43
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.40	0.43
2:E:689:THR:H	2:E:778:PHE:HE2	1.67	0.43
2:E:1032:LYS:O	2:E:1036:ARG:N	2.47	0.43
2:E:2823:ILE:HG12	2:E:2937:VAL:HG22	2.01	0.43
2:E:4957:LYS:HB2	2:E:4957:LYS:HZ1	1.83	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:3915:ILE:O	2:I:3919:THR:N	2.47	0.43
2:B:446:GLN:HA	2:B:449:ILE:HD12	2.01	0.43
2:B:1973:GLN:O	2:B:1977:TYR:N	2.44	0.43
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	2.00	0.43
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	2.01	0.43
2:E:4996:ILE:HG12	4:E:5102:CFF:H123	2.00	0.43
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.54	0.42
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.49	0.42
2:E:1936:LYS:O	2:E:1940:CYS:N	2.46	0.42
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.53	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.42
2:I:689:THR:H	2:I:778:PHE:HE2	1.66	0.42
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.84	0.42
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.83	0.42
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.54	0.42
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.53	0.42
2:G:2823:ILE:HG12	2:G:2937:VAL:HG22	2.01	0.42
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.00	0.42
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.84	0.42
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.54	0.42
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.83	0.42
2:I:1973:GLN:O	2:I:1977:TYR:N	2.44	0.42
2:G:534:ARG:NH2	2:G:573:GLU:OE2	2.52	0.42
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.42
1:J:82:TYR:O	1:J:86:GLY:N	2.51	0.42
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.83	0.42
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.52	0.42
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	2.01	0.42
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.85	0.42
2:I:1105:ALA:N	2:I:1189:LEU:O	2.51	0.42
2:I:2138:LEU:HD11	2:I:3654:LEU:HD11	2.01	0.42
2:I:4996:ILE:HG12	4:I:5102:CFF:H123	2.00	0.42
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	2.01	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:HIS:HA	1:H:88:PRO:HD3	1.90	0.42
2:B:113:HIS:O	2:B:399:GLN:NE2	2.53	0.42
2:B:465:GLN:HG3	2:B:3710:LEU:HB3	2.02	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	2.01	0.42
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.52	0.42
2:E:2138:LEU:HD11	2:E:3654:LEU:HD11	2.01	0.42
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.84	0.42
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	2.00	0.42
2:G:4996:ILE:HG12	4:G:5102:CFF:H123	2.00	0.42
1:H:82:TYR:O	1:H:86:GLY:N	2.51	0.42
2:B:2823:ILE:HG12	2:B:2937:VAL:HG22	2.01	0.42
2:E:113:HIS:O	2:E:399:GLN:NE2	2.53	0.42
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.40	0.42
2:E:3365:UNK:O	2:E:3369:UNK:N	2.53	0.42
2:I:681:HIS:HB3	2:I:784:SER:HB3	2.02	0.42
2:I:1663:HIS:O	2:I:1667:LEU:N	2.51	0.42
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.01	0.42
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	2.02	0.42
2:I:3365:UNK:O	2:I:3369:UNK:N	2.53	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.84	0.42
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.01	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:B:4984:ASN:C	2:B:4986:ALA:H	2.23	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.02	0.42
2:E:1154:ASP:O	2:E:1158:ASN:N	2.52	0.42
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.85	0.42
2:I:1236:THR:OG1	2:I:1608:MET:SD	2.77	0.42
2:I:1936:LYS:O	2:I:1940:CYS:N	2.46	0.42
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	2.01	0.42
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.53	0.42
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.02	0.42
2:B:1154:ASP:O	2:B:1158:ASN:N	2.52	0.42
2:B:3365:UNK:O	2:B:3369:UNK:N	2.53	0.42
2:B:4736:ARG:NH1	2:E:4079:ASP:OD1	2.53	0.42
2:E:670:GLU:HG3	2:E:787:VAL:HG13	2.01	0.42
2:E:1124:PHE:HB2	2:E:1162:PHE:CE2	2.55	0.42
2:I:282:ILE:HD12	2:I:314:PHE:HD2	1.83	0.42
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.02	0.42
2:B:2138:LEU:HD11	2:B:3654:LEU:HD11	2.01	0.42
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3677:LEU:O	2:B:3698:LEU:N	2.52	0.42
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.53	0.42
2:I:465:GLN:HG3	2:I:3710:LEU:HB3	2.02	0.42
2:I:1124:PHE:HB2	2:I:1162:PHE:CE2	2.55	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.01	0.42
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	2.02	0.42
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.32	0.42
2:G:3365:UNK:O	2:G:3369:UNK:N	2.53	0.42
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.53	0.42
2:B:681:HIS:HB3	2:B:784:SER:HB3	2.02	0.42
2:B:689:THR:H	2:B:778:PHE:HE2	1.67	0.42
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.53	0.42
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.84	0.42
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.02	0.42
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.83	0.42
2:I:3971:GLY:N	2:I:4032:GLU:OE2	2.50	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	2.02	0.42
2:G:278:GLN:N	2:G:315:CYS:SG	2.92	0.42
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.77	0.42
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	2.02	0.42
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.84	0.42
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.90	0.42
2:B:551:LEU:HD21	2:B:589:LEU:HB2	2.02	0.42
2:B:1124:PHE:HB2	2:B:1162:PHE:CE2	2.55	0.42
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.85	0.42
2:I:1032:LYS:O	2:I:1036:ARG:N	2.47	0.42
2:G:614:VAL:HA	2:G:2169:GLN:HB3	2.02	0.42
2:G:1124:PHE:HB2	2:G:1162:PHE:CE2	2.55	0.42
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	2.01	0.42
2:G:3971:GLY:N	2:G:4032:GLU:OE2	2.50	0.42
2:B:670:GLU:HG3	2:B:787:VAL:HG13	2.01	0.41
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	2.02	0.41
2:E:465:GLN:HG3	2:E:3710:LEU:HB3	2.02	0.41
2:E:681:HIS:HB3	2:E:784:SER:HB3	2.02	0.41
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	2.01	0.41
2:E:3915:ILE:O	2:E:3919:THR:N	2.47	0.41
2:E:4228:ALA:O	2:E:4232:GLU:N	2.52	0.41
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.85	0.41
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.53	0.41
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.85	0.41
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.41
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.84	0.41
2:E:614:VAL:HA	2:E:2169:GLN:HB3	2.02	0.41
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.01	0.41
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.01	0.41
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.84	0.41
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	2.02	0.41
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.01	0.41
2:G:2138:LEU:HD11	2:G:3654:LEU:HD11	2.01	0.41
2:G:4080:TYR:CZ	2:G:4096:ALA:HB3	2.55	0.41
2:B:614:VAL:HA	2:B:2169:GLN:HB3	2.02	0.41
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.01	0.41
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.41
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.01	0.41
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.01	0.41
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.53	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.01	0.41
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.01	0.41
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	2.01	0.41
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.38	0.41
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.85	0.41
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.86	0.41
2:G:113:HIS:O	2:G:399:GLN:NE2	2.53	0.41
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.56	0.41
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.86	0.41
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.77	0.41
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.86	0.41
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.53	0.41
2:E:3971:GLY:N	2:E:4032:GLU:OE2	2.50	0.41
2:E:4586:PRO:HA	2:E:4628:VAL:HG11	2.02	0.41
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.86	0.41
2:I:614:VAL:HA	2:I:2169:GLN:HB3	2.02	0.41
2:I:1708:ARG:HG2	2:I:1711:TYR:CE2	2.54	0.41
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	2.01	0.41
2:I:4865:LYS:HG3	2:I:4875:LYS:HZ3	1.84	0.41
2:G:681:HIS:HB3	2:G:784:SER:HB3	2.02	0.41
2:G:689:THR:H	2:G:778:PHE:HE2	1.66	0.41
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	2.02	0.41
2:G:4984:ASN:C	2:G:4986:ALA:H	2.23	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.40	0.41
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.52	0.41
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.53	0.41
2:I:4863:TYR:HD2	2:I:4875:LYS:HB2	1.86	0.41
2:I:4984:ASN:C	2:I:4986:ALA:H	2.23	0.41
2:I:5027:CYS:SG	2:I:5027:CYS:O	2.79	0.41
2:G:1032:LYS:O	2:G:1036:ARG:N	2.47	0.41
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.90	0.41
2:B:1032:LYS:O	2:B:1036:ARG:N	2.47	0.41
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.03	0.41
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.56	0.41
2:E:320:LYS:NZ	2:E:381:GLU:O	2.42	0.41
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.41
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	2.02	0.41
2:I:113:HIS:O	2:I:399:GLN:NE2	2.53	0.41
2:I:670:GLU:HG3	2:I:787:VAL:HG13	2.02	0.41
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.01	0.41
2:I:4014:LYS:HE2	2:I:4135:PRO:HG3	2.03	0.41
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.95	0.41
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.41
2:G:5027:CYS:SG	2:G:5027:CYS:O	2.79	0.41
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.53	0.41
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	2.02	0.41
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.53	0.41
2:E:698:GLY:HA2	2:E:703:GLY:HA2	2.03	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.03	0.41
2:E:2871:LEU:HD22	2:E:2927:LEU:HD22	2.02	0.41
2:E:4014:LYS:HE2	2:E:4135:PRO:HG3	2.03	0.41
2:E:4080:TYR:CZ	2:E:4096:ALA:HB3	2.55	0.41
2:G:465:GLN:HG3	2:G:3710:LEU:HB3	2.02	0.41
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.02	0.41
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.03	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.01	0.41
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.86	0.41
2:B:4914:VAL:HG23	2:E:4888:TYR:CD1	2.56	0.41
2:E:1663:HIS:O	2:E:1667:LEU:N	2.51	0.41
2:E:3706:SER:OG	2:E:3781:GLN:NE2	2.54	0.41
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.02	0.41
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.49	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.41
2:I:2871:LEU:HD22	2:I:2927:LEU:HD22	2.02	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.01	0.41
2:G:4863:TYR:HD2	2:G:4875:LYS:HB2	1.86	0.41
2:B:698:GLY:HA2	2:B:703:GLY:HA2	2.03	0.41
2:B:4014:LYS:HE2	2:B:4135:PRO:HG3	2.03	0.41
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.86	0.41
2:E:534:ARG:NH2	2:E:573:GLU:OE2	2.52	0.41
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.85	0.41
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	2.02	0.41
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.84	0.41
2:I:257:ARG:O	2:I:284:HIS:NE2	2.48	0.41
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.03	0.41
2:I:4586:PRO:HA	2:I:4628:VAL:HG11	2.02	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.02	0.41
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.85	0.41
2:G:4586:PRO:HA	2:G:4628:VAL:HG11	2.02	0.41
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.56	0.41
2:B:2871:LEU:HD22	2:B:2927:LEU:HD22	2.02	0.41
2:E:470:SER:O	2:E:474:ARG:NE	2.50	0.41
2:E:4956:THR:O	2:E:4965:SER:N	2.42	0.41
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.56	0.41
2:I:4080:TYR:CZ	2:I:4096:ALA:HB3	2.55	0.41
2:G:42:PHE:HD1	2:G:447:ASP:HB3	1.86	0.41
2:G:113:HIS:CE1	2:G:402:ARG:HB3	2.56	0.41
2:G:551:LEU:HD21	2:G:589:LEU:HB2	2.02	0.41
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	2.03	0.41
2:B:4957:LYS:HB2	2:B:4957:LYS:HZ1	1.82	0.40
2:E:113:HIS:CE1	2:E:402:ARG:HB3	2.56	0.40
2:E:551:LEU:HD21	2:E:589:LEU:HB2	2.02	0.40
2:E:582:HIS:O	2:E:585:SER:OG	2.30	0.40
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.56	0.40
2:I:551:LEU:HD21	2:I:589:LEU:HB2	2.02	0.40
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.56	0.40
2:G:1973:GLN:O	2:G:1977:TYR:N	2.44	0.40
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	2.02	0.40
2:G:2871:LEU:HD22	2:G:2927:LEU:HD22	2.02	0.40
2:G:4929:LEU:HD13	2:G:4929:LEU:HA	1.92	0.40
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.40
2:B:113:HIS:CE1	2:B:402:ARG:HB3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:HIS:O	2:B:585:SER:OG	2.30	0.40
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.87	0.40
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.02	0.40
2:B:3706:SER:OG	2:B:3781:GLN:NE2	2.54	0.40
2:B:4080:TYR:CZ	2:B:4096:ALA:HB3	2.55	0.40
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.87	0.40
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.87	0.40
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.84	0.40
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.40
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	2.02	0.40
2:B:3847:PHE:HE1	2:B:3950:ASN:HD22	1.70	0.40
2:B:5027:CYS:SG	2:B:5027:CYS:O	2.79	0.40
2:B:5028:PHE:CD1	2:B:5028:PHE:O	2.75	0.40
2:E:42:PHE:HD1	2:E:447:ASP:HB3	1.86	0.40
2:E:662:TRP:HZ3	2:E:811:CYS:HA	1.87	0.40
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.03	0.40
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	2.03	0.40
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	2.04	0.40
2:E:4987:ASN:HA	2:E:4990:PHE:HD2	1.87	0.40
2:E:5028:PHE:CD1	2:E:5028:PHE:O	2.75	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.87	0.40
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.03	0.40
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.40
2:B:870:ILE:HD12	2:B:870:ILE:HA	1.92	0.40
2:B:4586:PRO:HA	2:B:4628:VAL:HG11	2.02	0.40
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.04	0.40
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	2.02	0.40
2:E:1705:GLY:HA2	2:E:1709:ALA:HB3	2.04	0.40
2:E:3677:LEU:O	2:E:3698:LEU:N	2.52	0.40
2:E:5027:CYS:O	2:E:5027:CYS:SG	2.79	0.40
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.86	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.01	0.40
2:I:2029:GLN:O	2:I:2033:ASP:N	2.48	0.40
2:I:2298:VAL:HA	2:I:2301:TYR:HB2	2.03	0.40
2:I:3805:LEU:H	2:I:3805:LEU:HG	1.77	0.40
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.49	0.40
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.04	0.40
2:G:4014:LYS:HE2	2:G:4135:PRO:HG3	2.03	0.40
2:B:534:ARG:NH2	2:B:573:GLU:OE2	2.52	0.40
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.40
2:E:864:PRO:HA	2:E:865:PRO:HD3	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4863:TYR:HD2	2:E:4875:LYS:HB2	1.86	0.40
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.40
2:I:278:GLN:N	2:I:315:CYS:SG	2.92	0.40
2:I:698:GLY:HA2	2:I:703:GLY:HA2	2.03	0.40
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.86	0.40
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.04	0.40
2:G:698:GLY:HA2	2:G:703:GLY:HA2	2.03	0.40
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.56	0.40
2:G:2298:VAL:HA	2:G:2301:TYR:HB2	2.03	0.40
2:G:2368:LEU:HD13	2:G:2376:LEU:HD23	2.04	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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	47	81
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	47	81
2	G	3235/4416 (73%)	2890 (89%)	339 (10%)	6 (0%)	47	81
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	11941 (89%)	1395 (10%)	24 (0%)	50	81

All (24) 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	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	B	4641	PRO
2	B	4985	LEU
2	E	1932	PRO
2	E	4641	PRO
2	E	4985	LEU
2	I	1932	PRO
2	I	4641	PRO
2	I	4985	LEU
2	G	1932	PRO
2	G	4641	PRO
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/89 (99%)	88 (100%)	0	100 100
1	F	88/89 (99%)	88 (100%)	0	100 100
1	H	88/89 (99%)	88 (100%)	0	100 100
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3022 (82%)	2473 (99%)	20 (1%)	81 89
2	E	2493/3022 (82%)	2473 (99%)	20 (1%)	81 89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	2493/3022 (82%)	2473 (99%)	20 (1%)	81 89
2	I	2493/3022 (82%)	2473 (99%)	20 (1%)	81 89
All	All	10324/12444 (83%)	10244 (99%)	80 (1%)	82 89

All (80) 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	4957	LYS
2	B	4959	PHE
2	B	4960	ILE
2	B	4983	HIS
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	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	4137	ARG
2	E	4913	ARG
2	E	4957	LYS
2	E	4959	PHE
2	E	4960	ILE
2	E	4983	HIS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
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	4957	LYS
2	I	4959	PHE
2	I	4960	ILE
2	I	4983	HIS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	4957	LYS
2	G	4959	PHE
2	G	4960	ILE
2	G	4983	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (149) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	25	HIS
1	F	87	HIS
1	A	25	HIS
1	A	87	HIS
1	H	25	HIS
1	H	87	HIS
1	J	25	HIS
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	413	GLN
2	B	520	ASN
2	B	797	HIS
2	B	838	HIS
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2007	ASN
2	B	2127	GLN
2	B	2291	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	4933	GLN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	413	GLN
2	E	520	ASN
2	E	797	HIS
2	E	838	HIS
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2127	GLN
2	E	2291	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	4142	ASN
2	E	4201	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	4209	GLN
2	E	4806	ASN
2	E	4933	GLN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	413	GLN
2	I	520	ASN
2	I	797	HIS
2	I	838	HIS
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2127	GLN
2	I	2291	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	4201	ASN
2	I	4209	GLN
2	I	4806	ASN
2	I	4933	GLN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	413	GLN
2	G	520	ASN
2	G	797	HIS
2	G	838	HIS
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2127	GLN
2	G	2291	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	4142	ASN
2	G	4201	ASN
2	G	4209	GLN
2	G	4806	ASN
2	G	4933	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
3	ATP	G	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.56	6 (19%)
3	ATP	E	5101	-	26,33,33	0.85	1 (3%)	31,52,52	1.55	6 (19%)
4	CFF	I	5102	-	8,15,15	2.48	3 (37%)	8,23,23	1.23	1 (12%)
4	CFF	G	5102	-	8,15,15	2.49	3 (37%)	8,23,23	1.24	1 (12%)
3	ATP	I	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.55	6 (19%)
4	CFF	B	5102	-	8,15,15	2.49	3 (37%)	8,23,23	1.24	1 (12%)
4	CFF	E	5102	-	8,15,15	2.50	3 (37%)	8,23,23	1.23	1 (12%)
3	ATP	B	5101	-	26,33,33	0.84	1 (3%)	31,52,52	1.55	6 (19%)

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
3	ATP	G	5101	-	-	4/18/38/38	0/3/3/3
3	ATP	E	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	-	0/2/2/2
4	CFF	G	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	4/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	-	0/2/2/2
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	4/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-4.67	1.33	1.39
4	B	5102	CFF	C5-C4	-4.60	1.33	1.39
4	I	5102	CFF	C5-C4	-4.60	1.33	1.39
4	G	5102	CFF	C5-C4	-4.60	1.33	1.39
4	E	5102	CFF	C6-N1	-3.99	1.32	1.38
4	B	5102	CFF	C6-N1	-3.98	1.32	1.38
4	G	5102	CFF	C6-N1	-3.95	1.32	1.38
4	I	5102	CFF	C6-N1	-3.92	1.32	1.38
4	E	5102	CFF	O13-C6	-2.32	1.18	1.24
4	B	5102	CFF	O13-C6	-2.32	1.18	1.24
4	I	5102	CFF	O13-C6	-2.32	1.18	1.24
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24
3	E	5101	ATP	C5-C4	2.17	1.46	1.40
3	B	5101	ATP	C5-C4	2.15	1.46	1.40
3	G	5101	ATP	C5-C4	2.15	1.46	1.40
3	I	5101	ATP	C5-C4	2.14	1.46	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	5101	ATP	PB-O3B-PG	-3.60	120.46	132.83
3	E	5101	ATP	PB-O3B-PG	-3.60	120.47	132.83
3	G	5101	ATP	PB-O3B-PG	-3.60	120.48	132.83
3	B	5101	ATP	PB-O3B-PG	-3.60	120.48	132.83
3	G	5101	ATP	N3-C2-N1	-3.48	123.24	128.68
3	B	5101	ATP	N3-C2-N1	-3.47	123.26	128.68
3	I	5101	ATP	N3-C2-N1	-3.47	123.26	128.68
3	E	5101	ATP	N3-C2-N1	-3.47	123.26	128.68
3	B	5101	ATP	PA-O3A-PB	-3.18	121.91	132.83
3	G	5101	ATP	PA-O3A-PB	-3.18	121.91	132.83
3	I	5101	ATP	PA-O3A-PB	-3.18	121.92	132.83
3	E	5101	ATP	PA-O3A-PB	-3.18	121.93	132.83
4	E	5102	CFF	C14-N7-C8	-2.82	111.86	125.43
4	B	5102	CFF	C14-N7-C8	-2.82	111.88	125.43
4	I	5102	CFF	C14-N7-C8	-2.81	111.91	125.43
4	G	5102	CFF	C14-N7-C8	-2.81	111.91	125.43
3	G	5101	ATP	C3'-C2'-C1'	2.57	104.84	100.98
3	E	5101	ATP	C3'-C2'-C1'	2.55	104.81	100.98
3	B	5101	ATP	C3'-C2'-C1'	2.54	104.80	100.98
3	I	5101	ATP	C3'-C2'-C1'	2.51	104.76	100.98
3	B	5101	ATP	C4-C5-N7	-2.09	107.22	109.40
3	E	5101	ATP	C4-C5-N7	-2.07	107.24	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	5101	ATP	C4-C5-N7	-2.07	107.24	109.40
3	G	5101	ATP	C4-C5-N7	-2.07	107.25	109.40
3	G	5101	ATP	C2-N1-C6	2.05	122.26	118.75
3	E	5101	ATP	C2-N1-C6	2.04	122.24	118.75
3	B	5101	ATP	C2-N1-C6	2.03	122.23	118.75
3	I	5101	ATP	C2-N1-C6	2.03	122.23	118.75

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A
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
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	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'

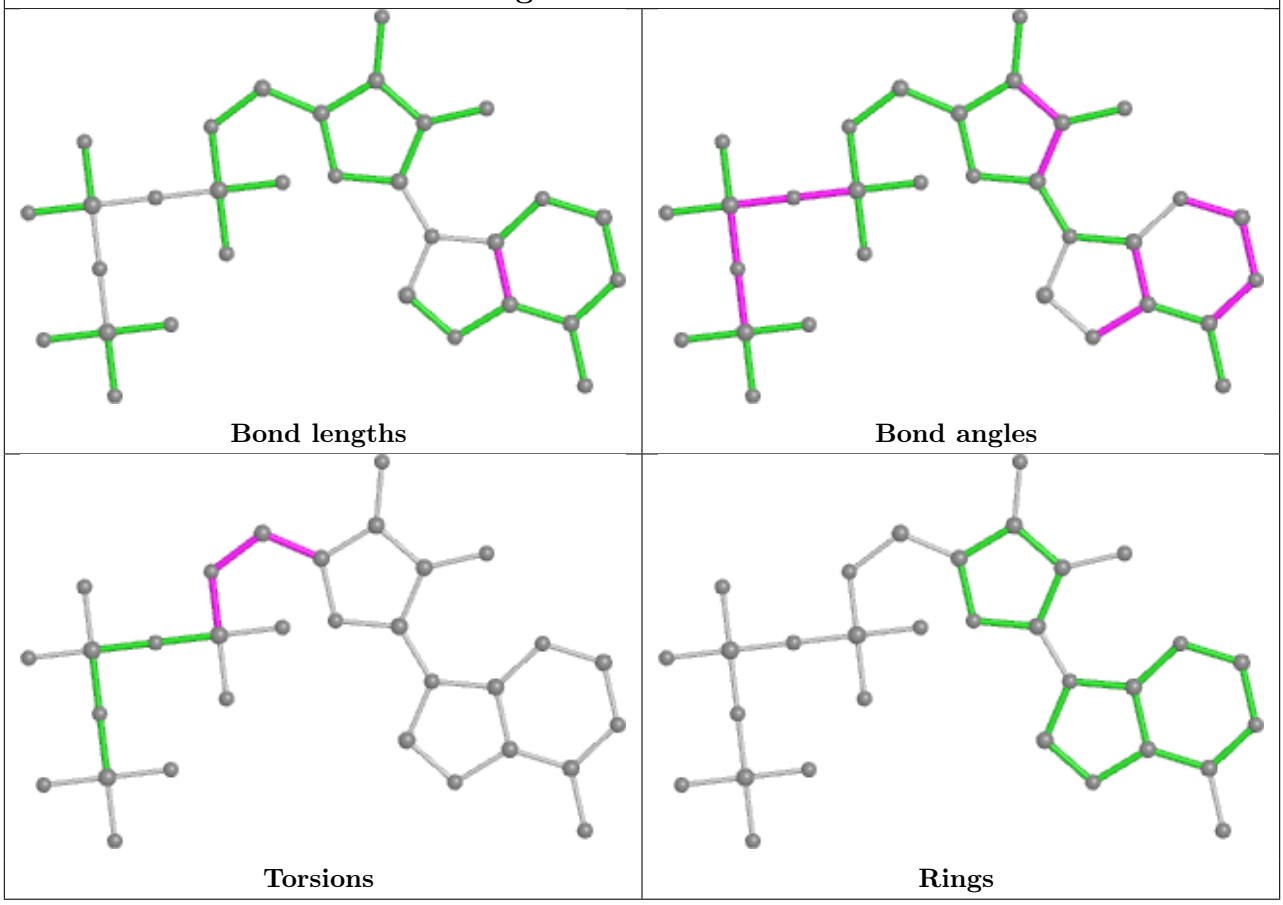
There are no ring outliers.

8 monomers are involved in 8 short contacts:

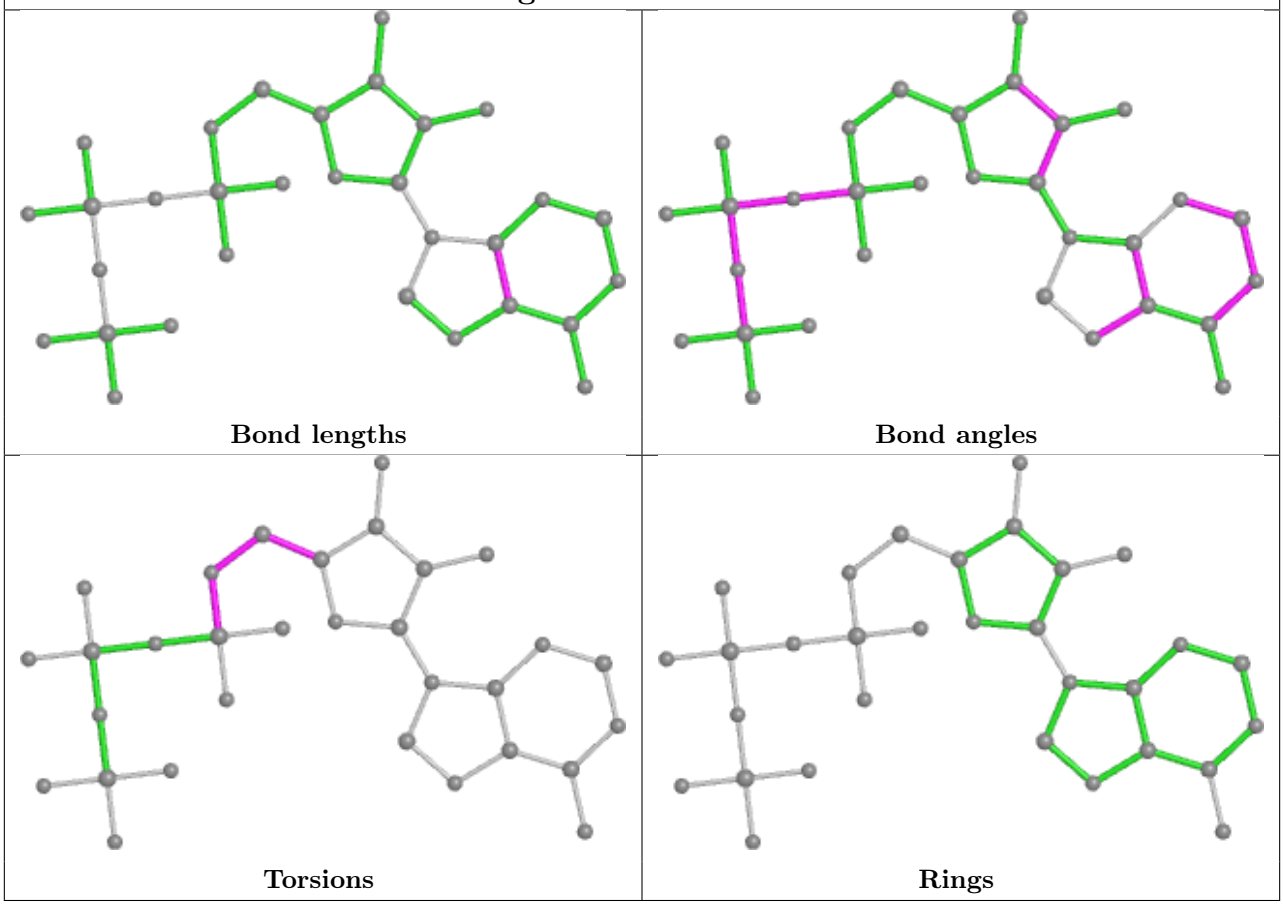
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5101	ATP	1	0
3	E	5101	ATP	1	0
4	I	5102	CFF	1	0
4	G	5102	CFF	1	0
3	I	5101	ATP	1	0
4	B	5102	CFF	1	0
4	E	5102	CFF	1	0
3	B	5101	ATP	1	0

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.

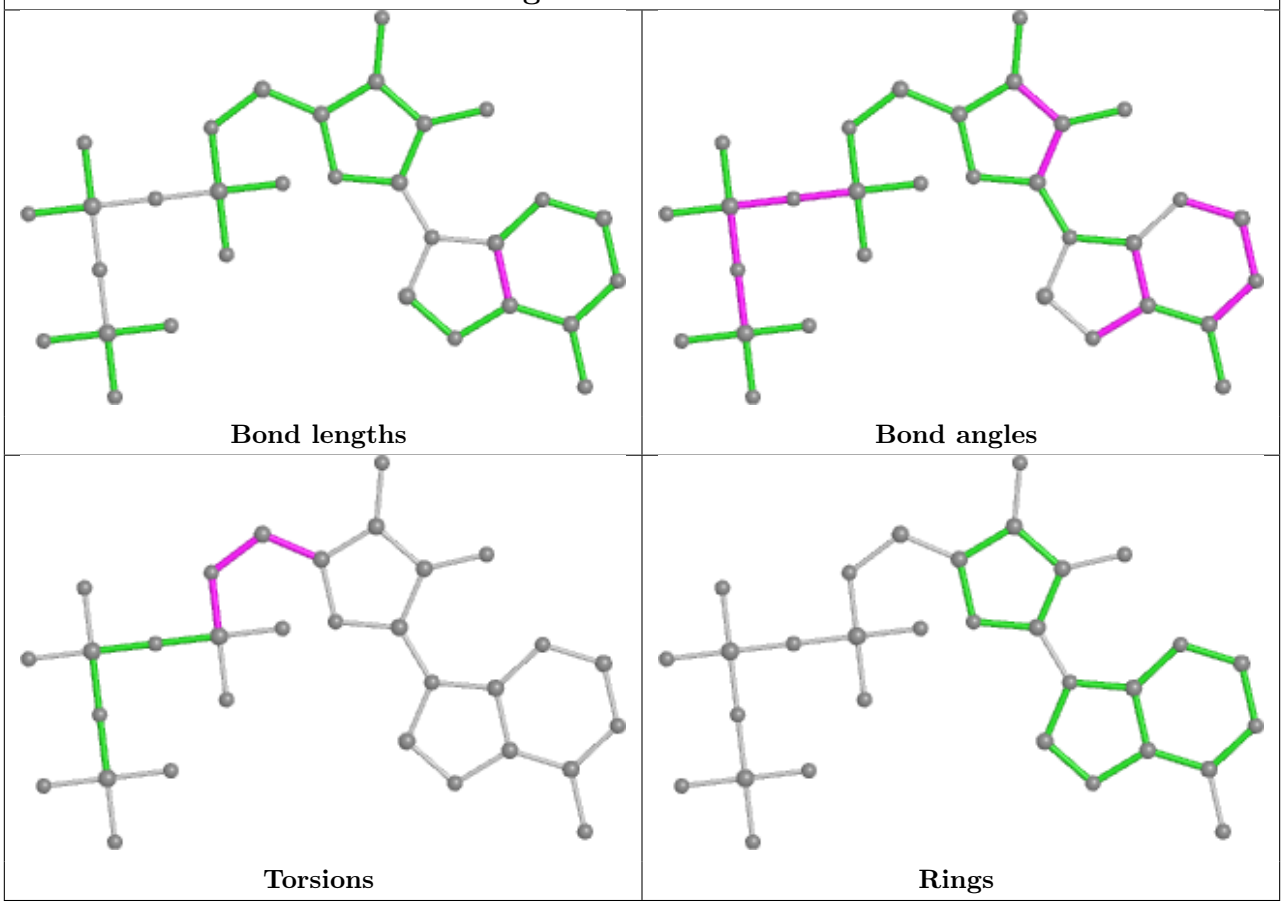
Ligand ATP G 5101



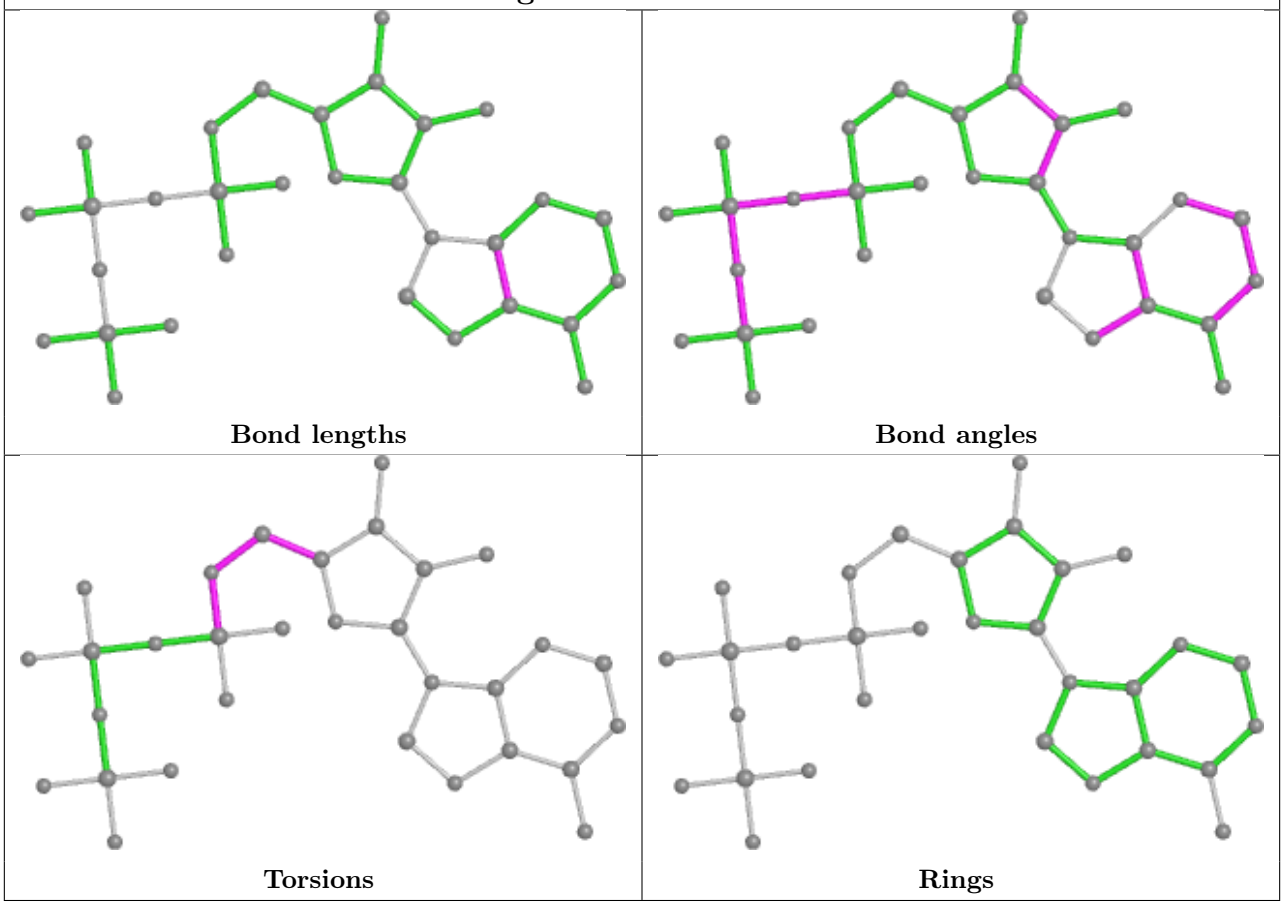
Ligand ATP E 5101



Ligand ATP I 5101



Ligand ATP B 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	72.44
1	E	4345:UNK	C	4540:PHE	N	72.44

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.44
1	G	4345:UNK	C	4540:PHE	N	72.44
1	B	3613:UNK	C	3639:THR	N	42.93
1	E	3613:UNK	C	3639:THR	N	42.93
1	I	3613:UNK	C	3639:THR	N	42.93
1	G	3613:UNK	C	3639:THR	N	42.93
1	B	4253:GLU	C	4320:UNK	N	27.35
1	E	4253:GLU	C	4320:UNK	N	27.35
1	I	4253:GLU	C	4320:UNK	N	27.35
1	G	4253:GLU	C	4320:UNK	N	27.35
1	B	3163:UNK	C	3170:UNK	N	16.17
1	E	3163:UNK	C	3170:UNK	N	16.17
1	I	3163:UNK	C	3170:UNK	N	16.17
1	G	3163:UNK	C	3170:UNK	N	16.17
1	B	3063:UNK	C	3134:UNK	N	14.81
1	E	3063:UNK	C	3134:UNK	N	14.81
1	I	3063:UNK	C	3134:UNK	N	14.81
1	G	3063:UNK	C	3134:UNK	N	14.81
1	B	2703:UNK	C	2734:ASN	N	14.74
1	E	2703:UNK	C	2734:ASN	N	14.74
1	I	2703:UNK	C	2734:ASN	N	14.74
1	G	2703:UNK	C	2734:ASN	N	14.74
1	B	3468:UNK	C	3511:UNK	N	14.16
1	E	3468:UNK	C	3511:UNK	N	14.16
1	I	3468:UNK	C	3511:UNK	N	14.16
1	G	3468:UNK	C	3511:UNK	N	14.16
1	B	3236:UNK	C	3241:UNK	N	13.24
1	E	3236:UNK	C	3241:UNK	N	13.24
1	I	3236:UNK	C	3241:UNK	N	13.24
1	G	3236:UNK	C	3241:UNK	N	13.24
1	B	2976:UNK	C	2995:UNK	N	12.70
1	E	2976:UNK	C	2995:UNK	N	12.70
1	I	2976:UNK	C	2995:UNK	N	12.70
1	G	2976:UNK	C	2995:UNK	N	12.70
1	B	1564:UNK	C	1573:MET	N	12.34
1	E	1564:UNK	C	1573:MET	N	12.34
1	I	1564:UNK	C	1573:MET	N	12.34
1	G	1564:UNK	C	1573:MET	N	12.34
1	B	3254:UNK	C	3261:UNK	N	8.53
1	E	3254:UNK	C	3261:UNK	N	8.53
1	I	3254:UNK	C	3261:UNK	N	8.53
1	G	3254:UNK	C	3261:UNK	N	8.53

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	6.12
1	E	1297:UNK	C	1430:UNK	N	6.12
1	I	1297:UNK	C	1430:UNK	N	6.12
1	G	1297:UNK	C	1430:UNK	N	6.12
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
1	B	2939:ARG	C	2942:UNK	N	3.23
1	E	2939:ARG	C	2942:UNK	N	3.23
1	G	2939:ARG	C	2942:UNK	N	3.23
1	I	2939:ARG	C	2942:UNK	N	3.22

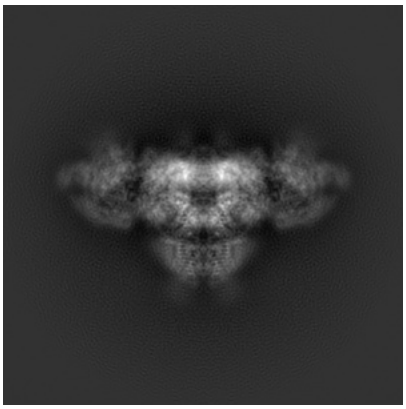
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8380. These allow visual inspection of the internal detail of the map and identification of artifacts.

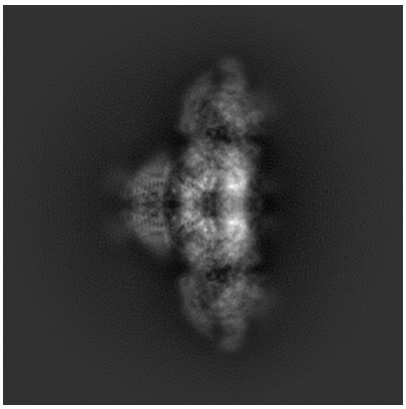
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

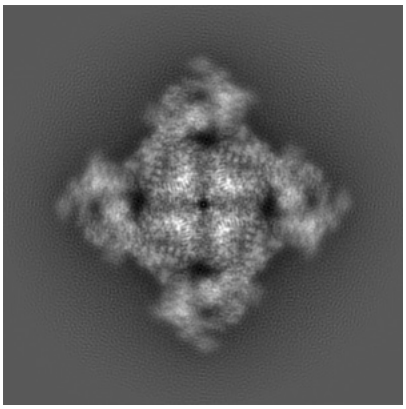
6.1.1 Primary map



X

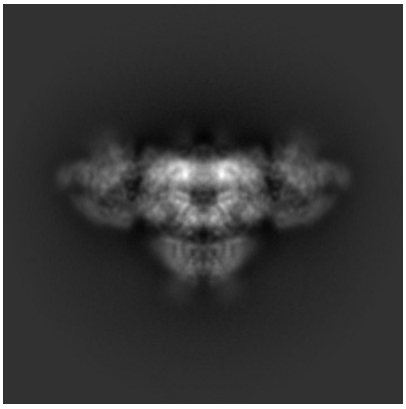


Y

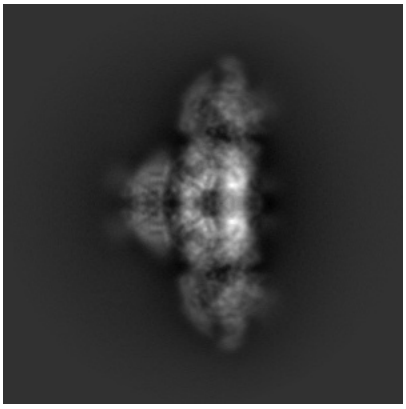


Z

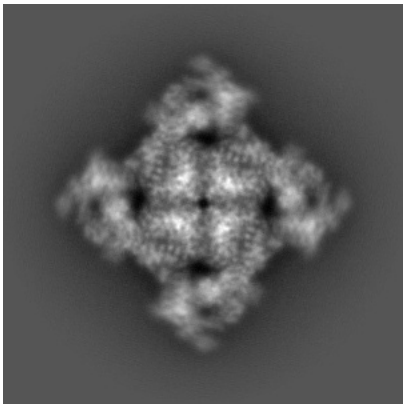
6.1.2 Raw map



X



Y

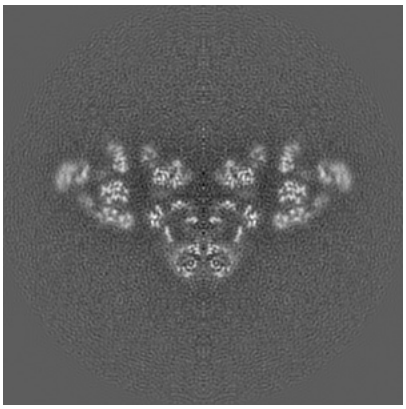


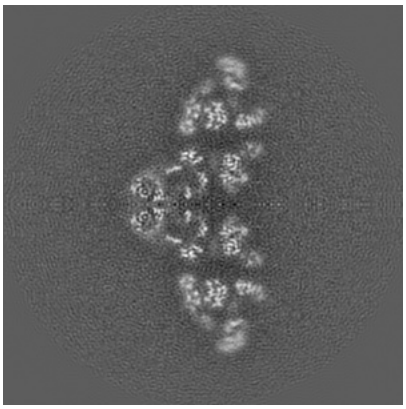
Z

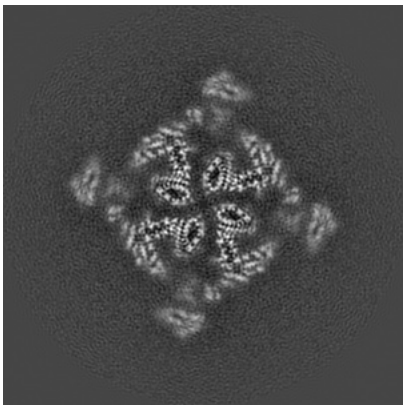
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

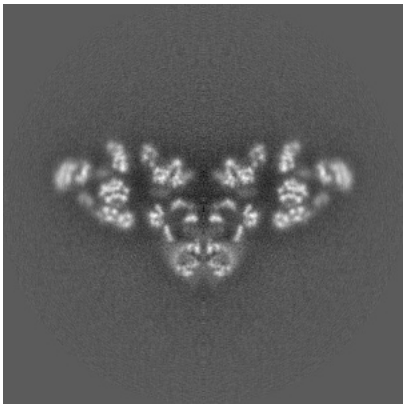
6.2.1 Primary map

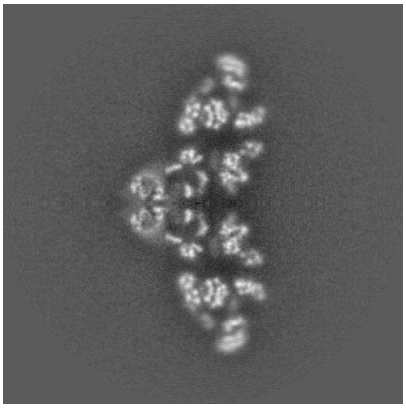

X Index: 200

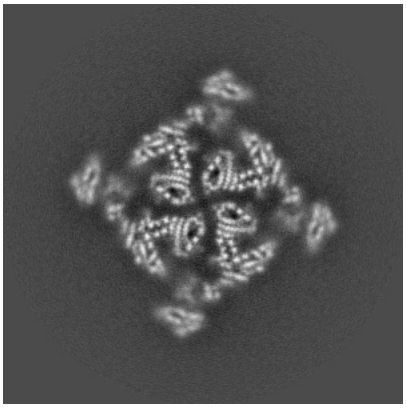

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

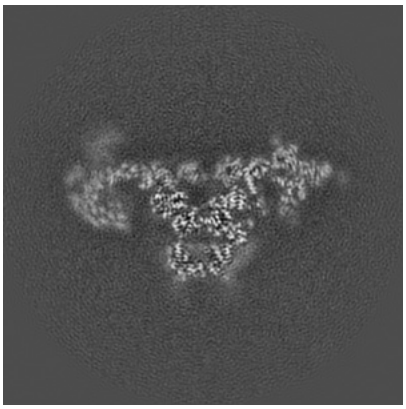

Y Index: 200


Z Index: 200

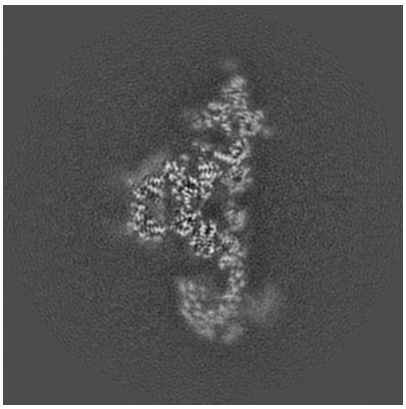
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

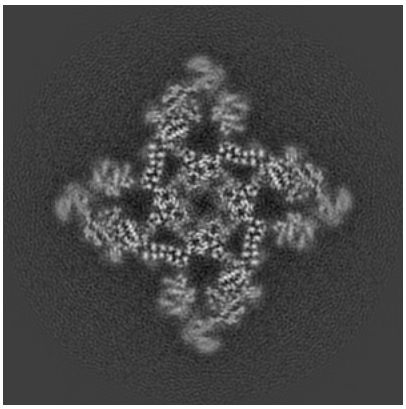
6.3.1 Primary map



X Index: 183

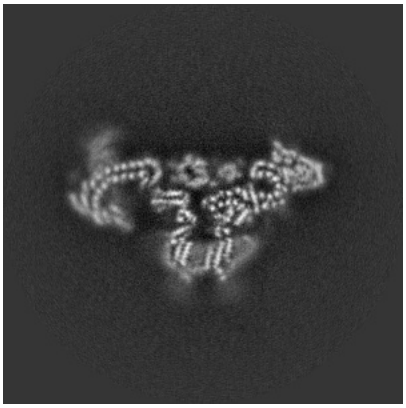


Y Index: 217

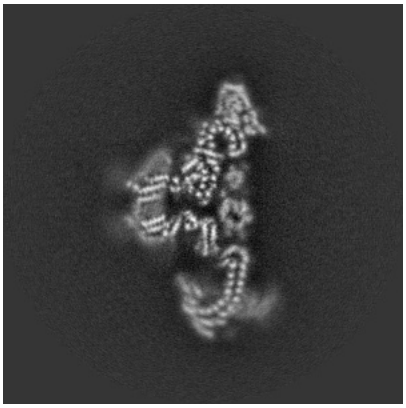


Z Index: 226

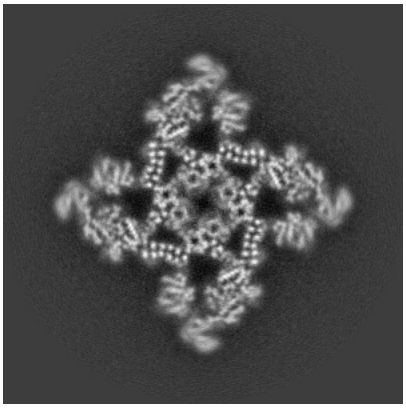
6.3.2 Raw map



X Index: 176



Y Index: 224

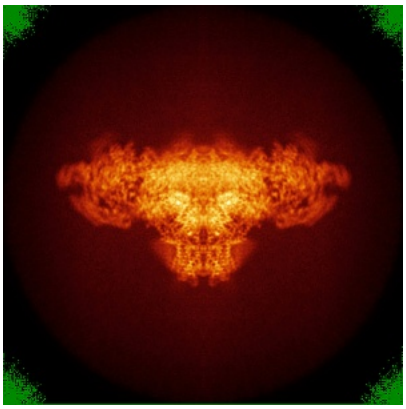


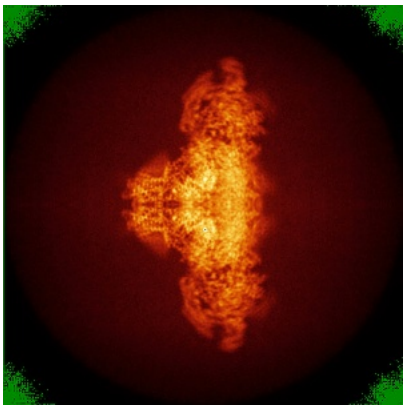
Z Index: 226

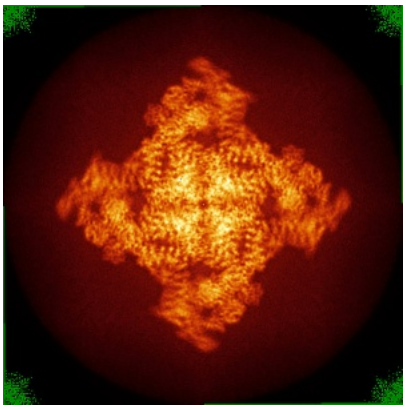
The images above show the largest variance slices of the map in three orthogonal directions.

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

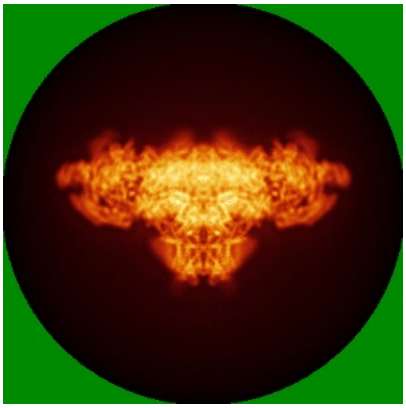
6.4.1 Primary map

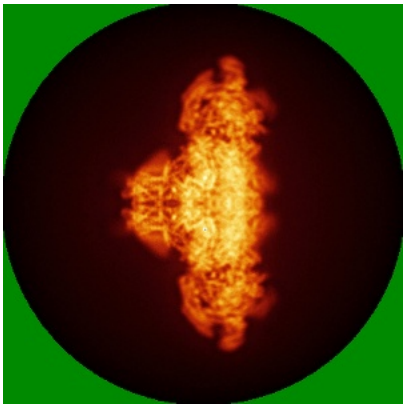

X

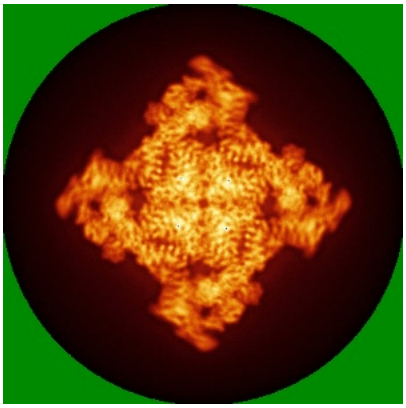

Y


Z

6.4.2 Raw map


X

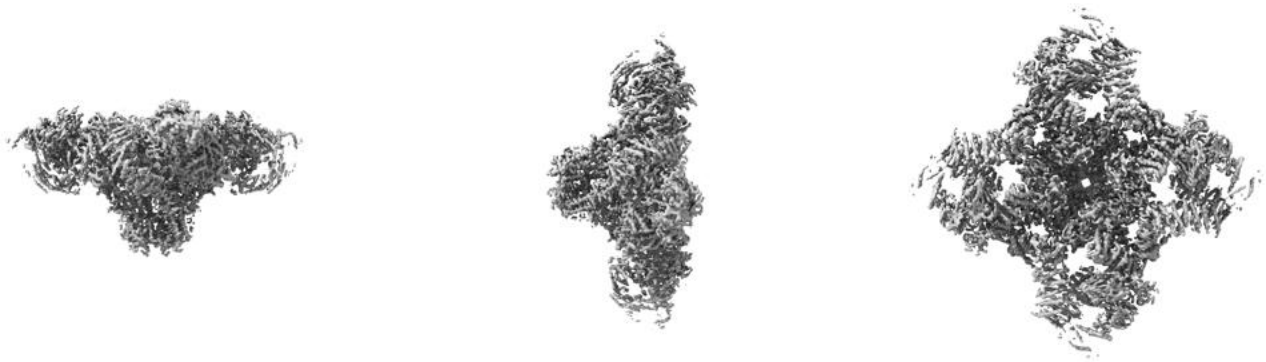

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

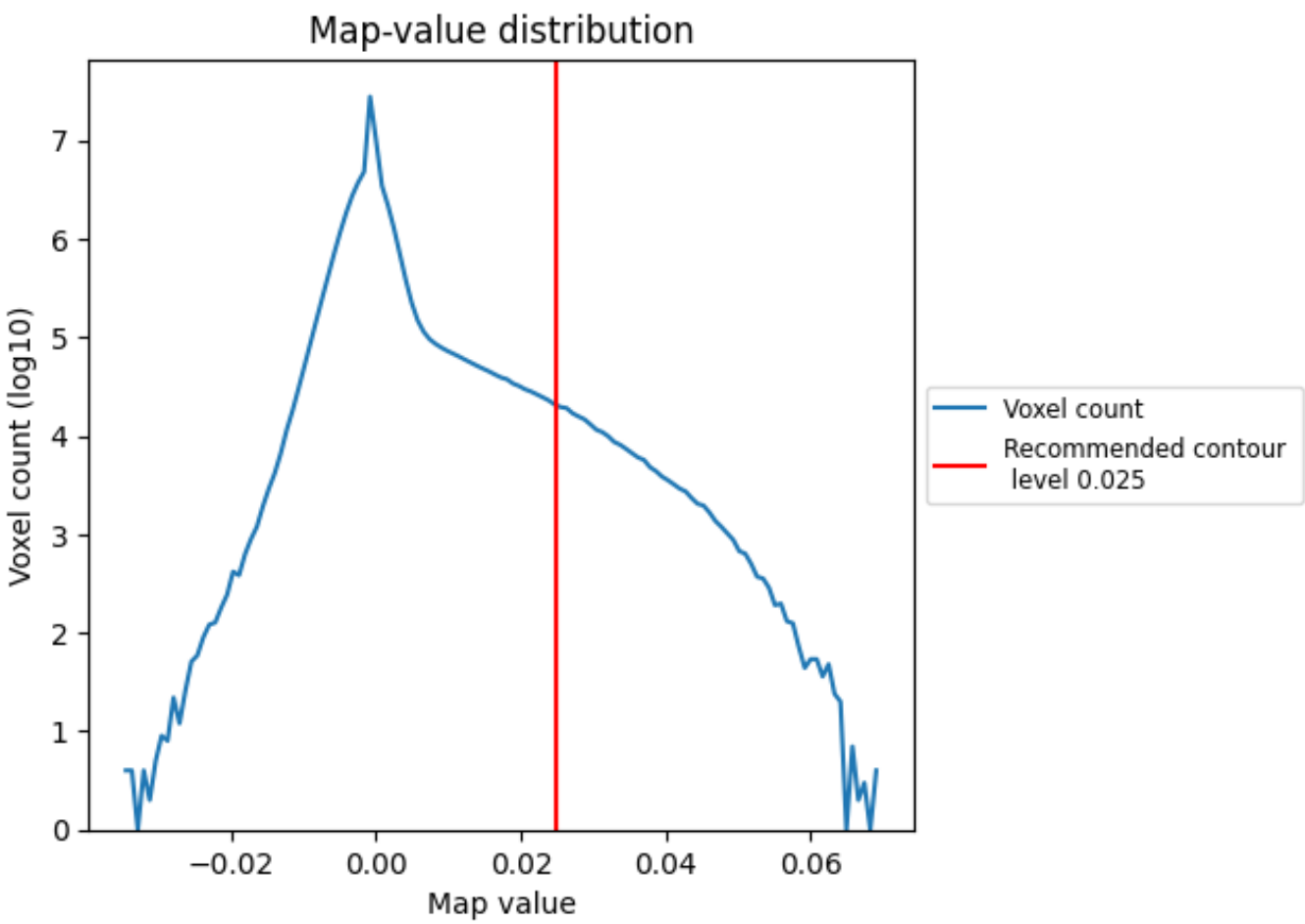
6.6 Mask visualisation (i)

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

7 Map analysis (i)

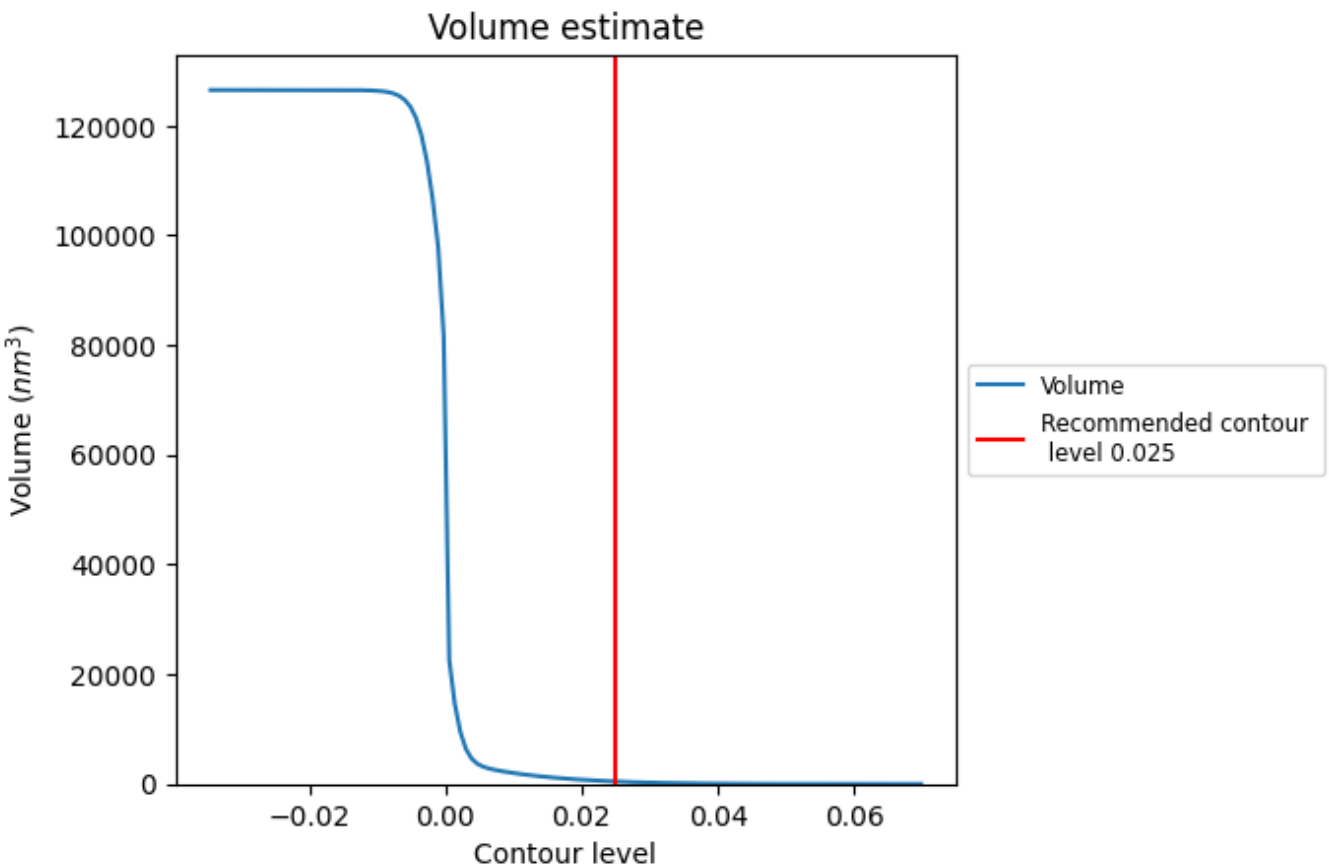
This section contains the results of statistical analysis of the map.

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.

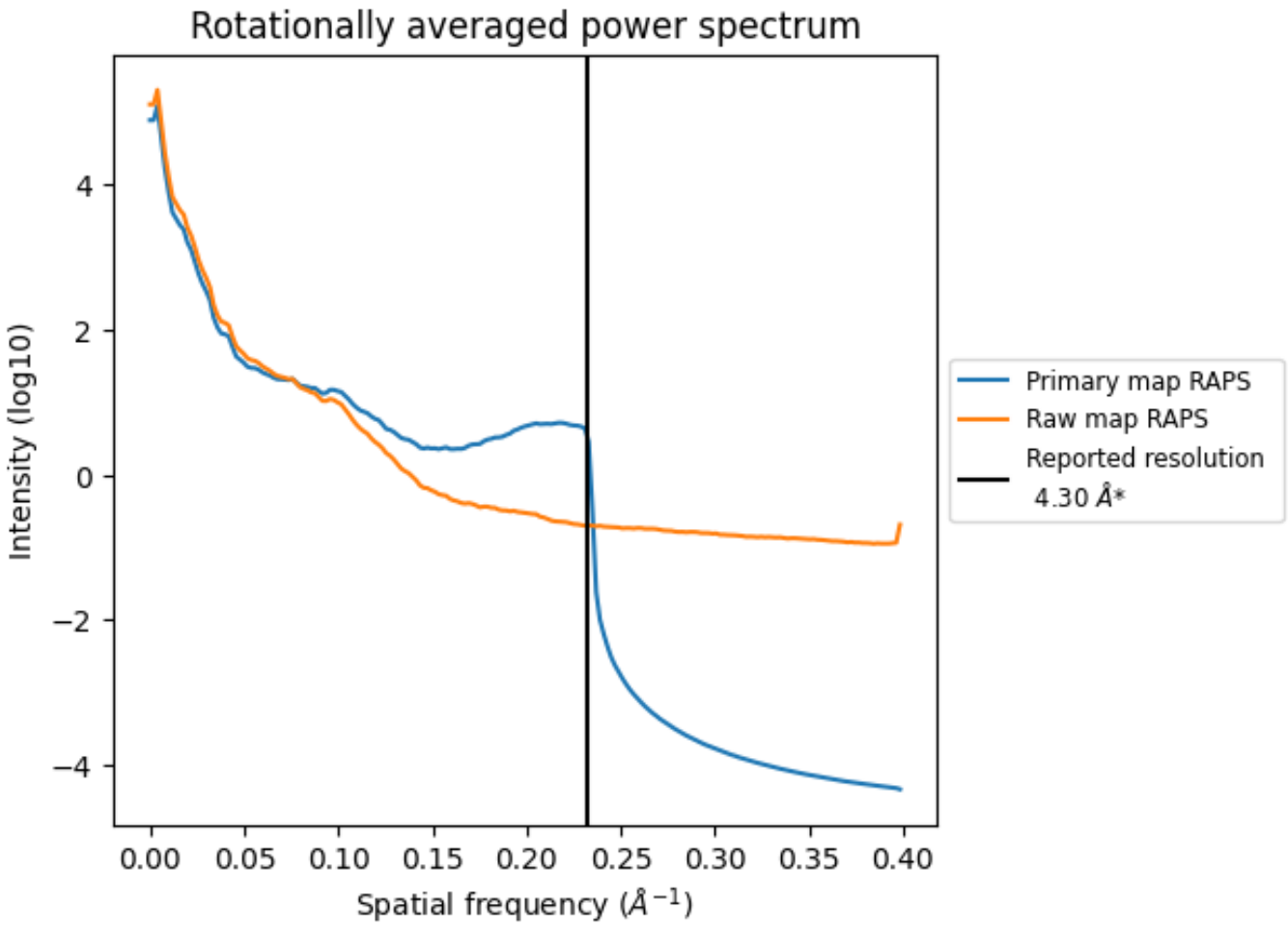
7.2 Volume estimate (i)



The volume at the recommended contour level is 452 nm^3; this corresponds to an approximate mass of 408 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)

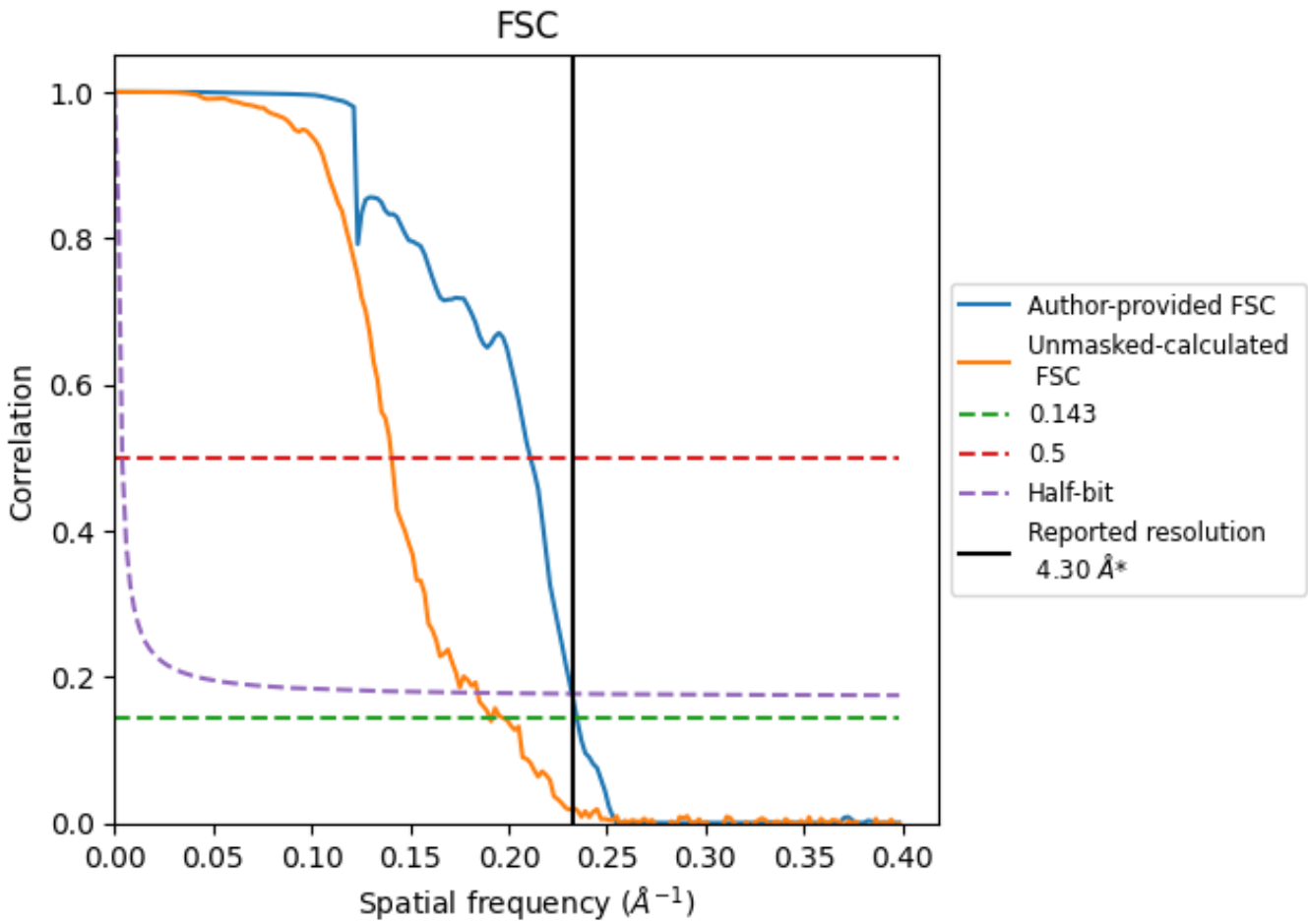


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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)

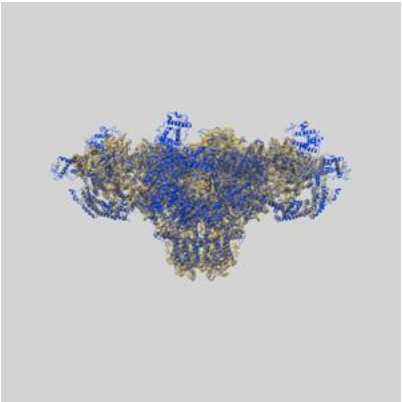
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.26	4.74	4.31
Unmasked-calculated*	5.24	7.11	5.43

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

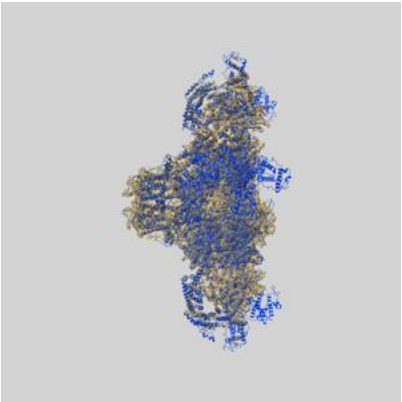
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8380 and PDB model 5TAN. Per-residue inclusion information can be found in section 3 on page 6.

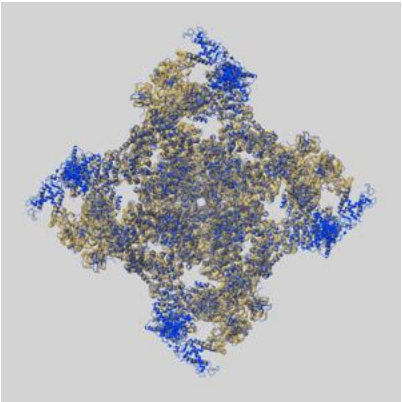
9.1 Map-model overlay (i)



X



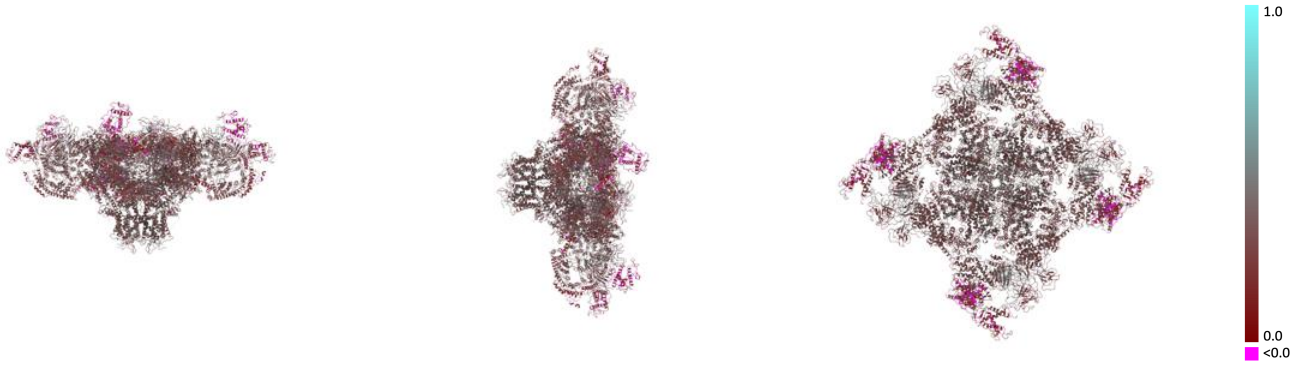
Y



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.

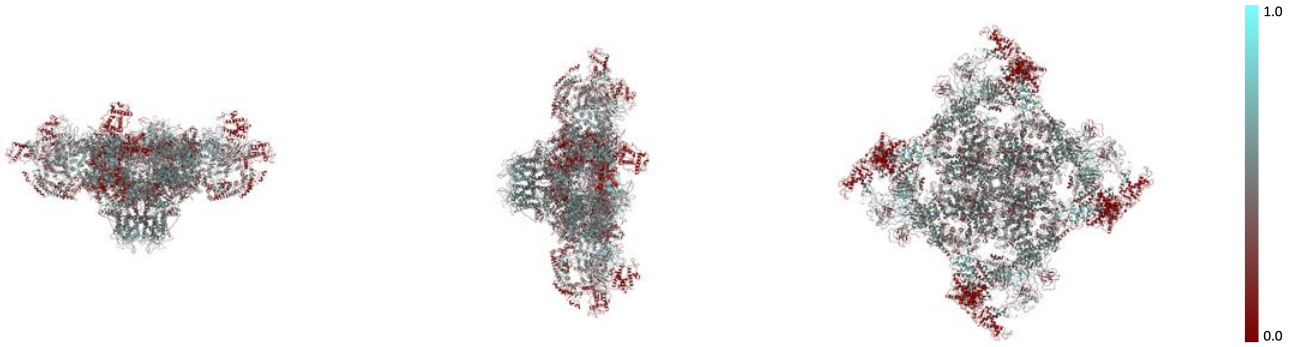
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

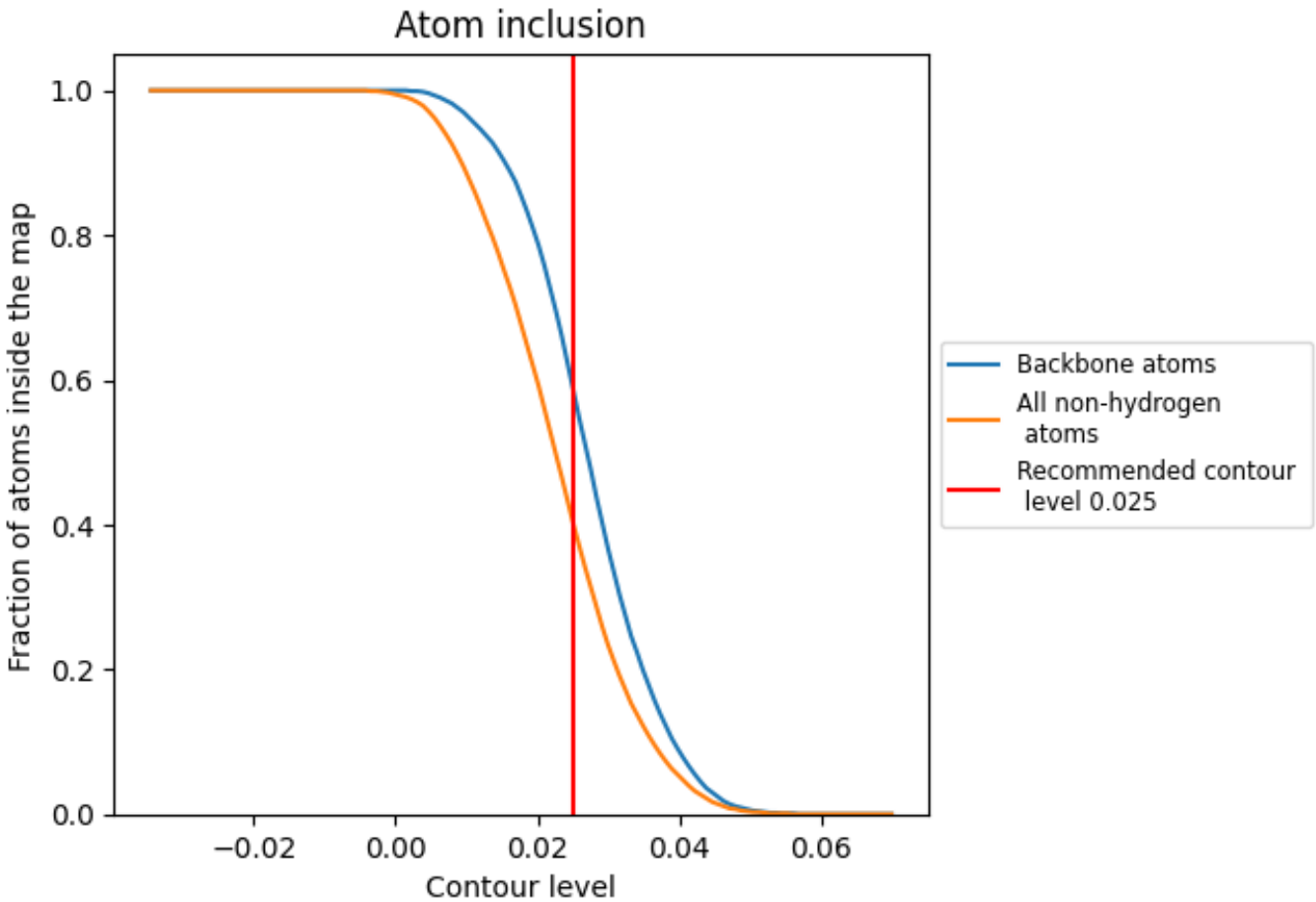
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 40% 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	0.4020	0.3150
A	0.3500	0.3180
B	0.4040	0.3140
E	0.4030	0.3140
F	0.3450	0.3230
G	0.4030	0.3140
H	0.3470	0.3230
I	0.4040	0.3140
J	0.3500	0.3190