Full wwPDB EM Validation Report ⓘ

Jun 7, 2023 – 03:21 PM EDT

PDB ID	:	8EZ9
EMDB ID	:	EMD-28731
Title	:	Dimeric complex of DNA-PKcs
Authors	:	Chen, S.; He, Y.
Deposited on	:	2022-10-31
Resolution	:	5.67 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

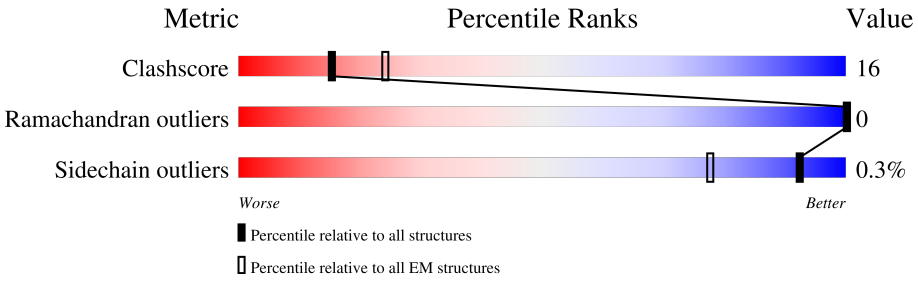
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 5.67 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	Q	20	25% 90% 10%
1	R	20	25% 90% 10%
2	C	4128	30% 58% 30% 11%
2	L	4128	31% 59% 30% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 58770 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 unknown region of DNA-PKcs.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	R	20	Total	C	N	O	0	0
			101	60	20	21		
1	Q	20	Total	C	N	O	0	0
			101	60	20	21		

- Molecule 2 is a protein called DNA-dependent protein kinase catalytic subunit.

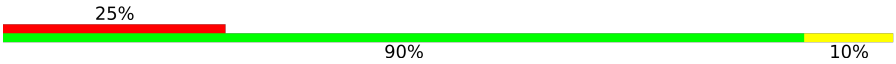
Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	3662	Total	C	N	O	S	0	0
			29284	18776	4946	5370	192		
2	C	3662	Total	C	N	O	S	0	0
			29284	18776	4946	5370	192		

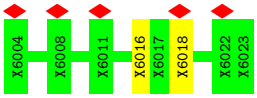
3 Residue-property plots (i)

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: unknown region of DNA-PKcs

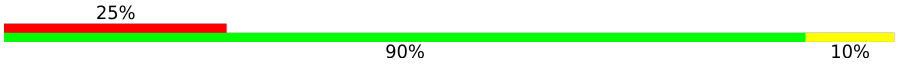
Chain R:

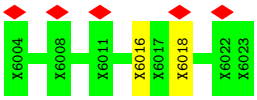




• Molecule 1: unknown region of DNA-PKcs

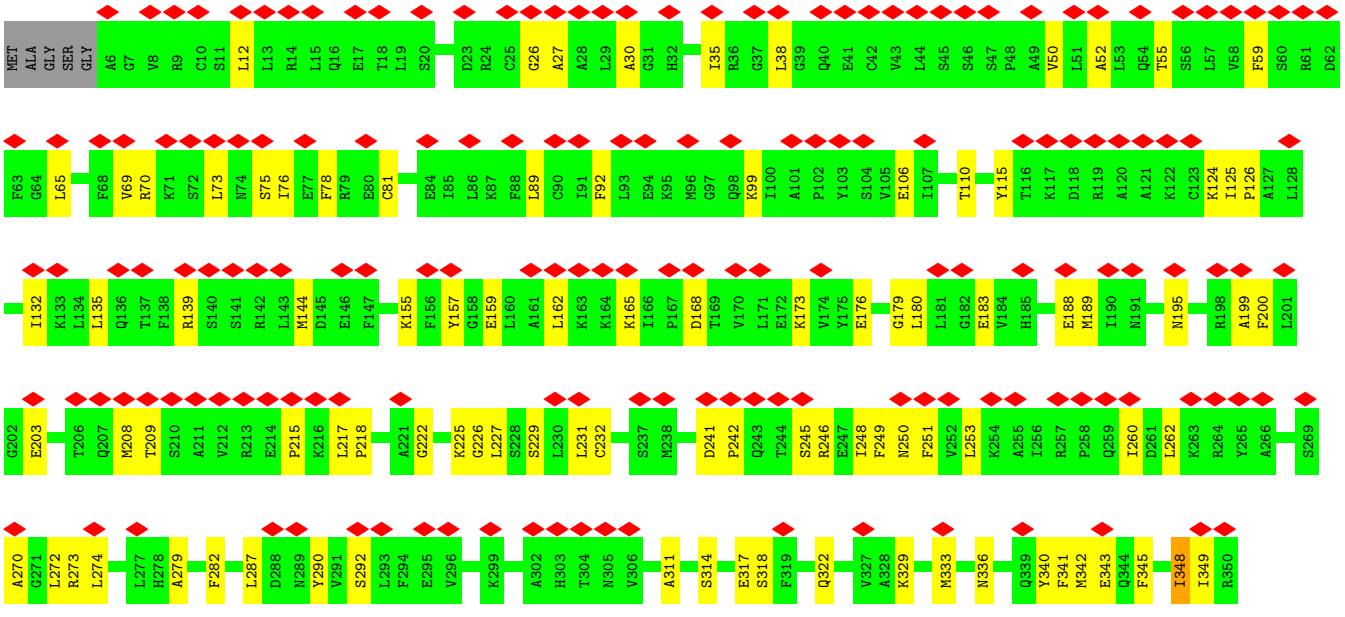
Chain Q:

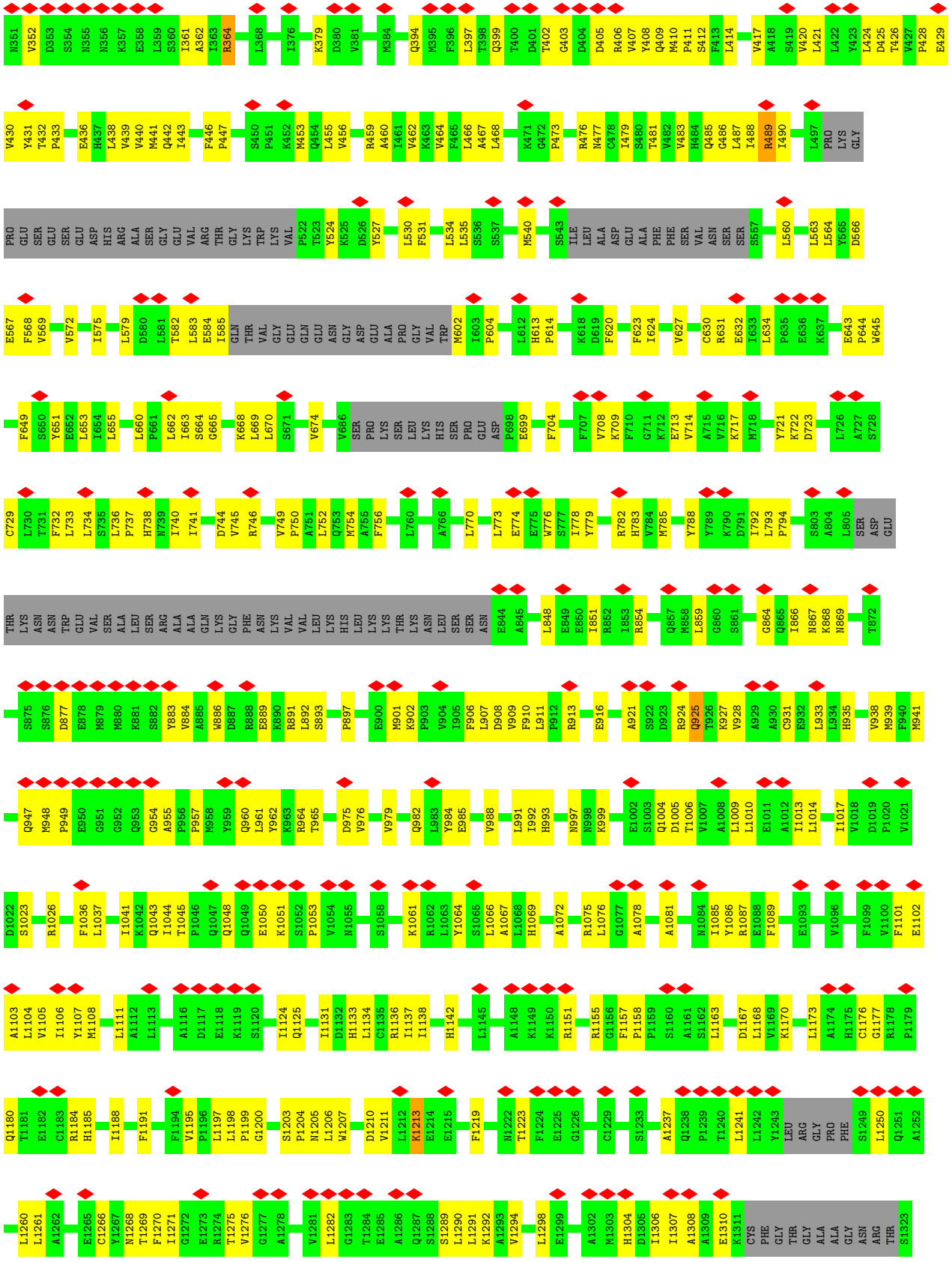


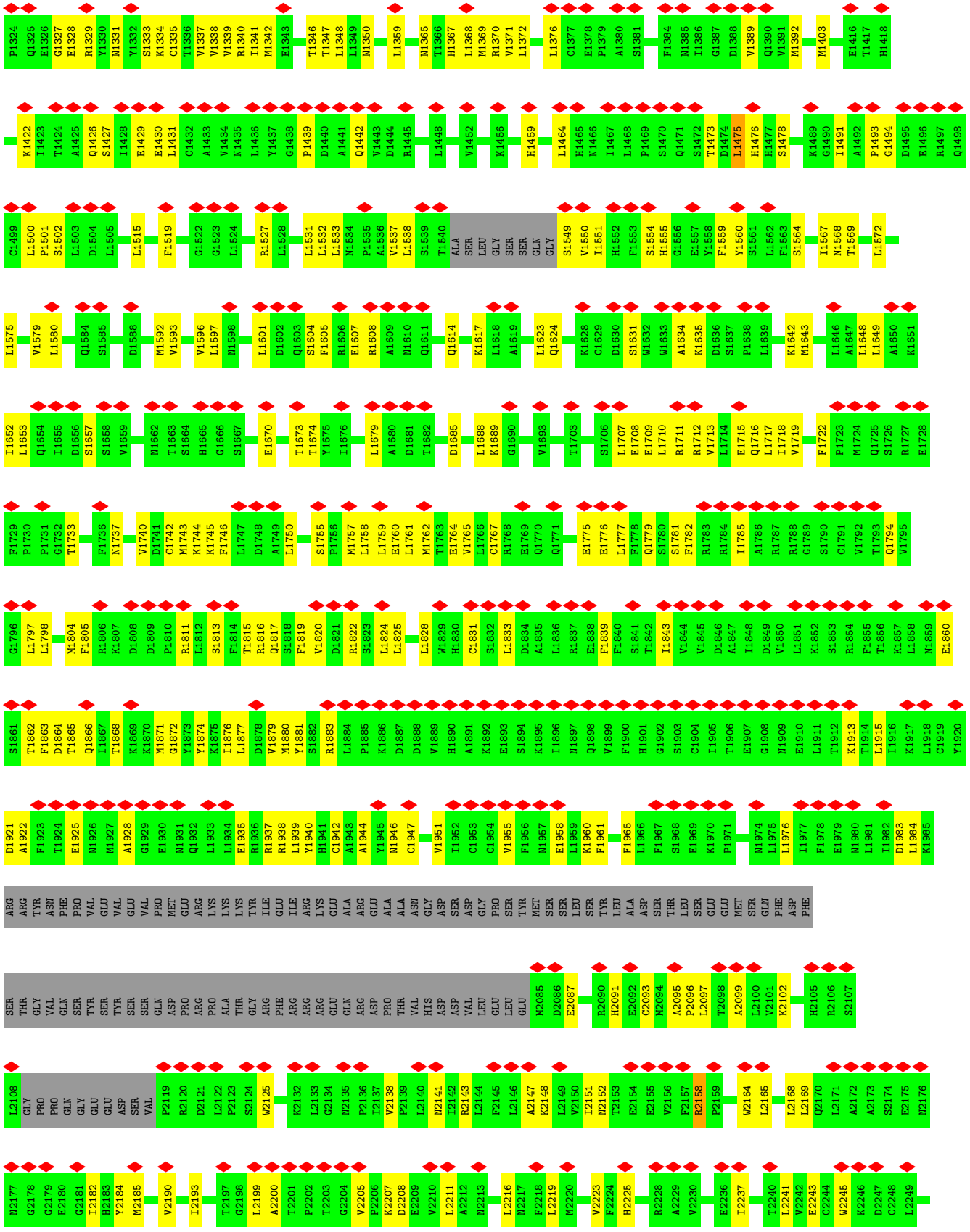


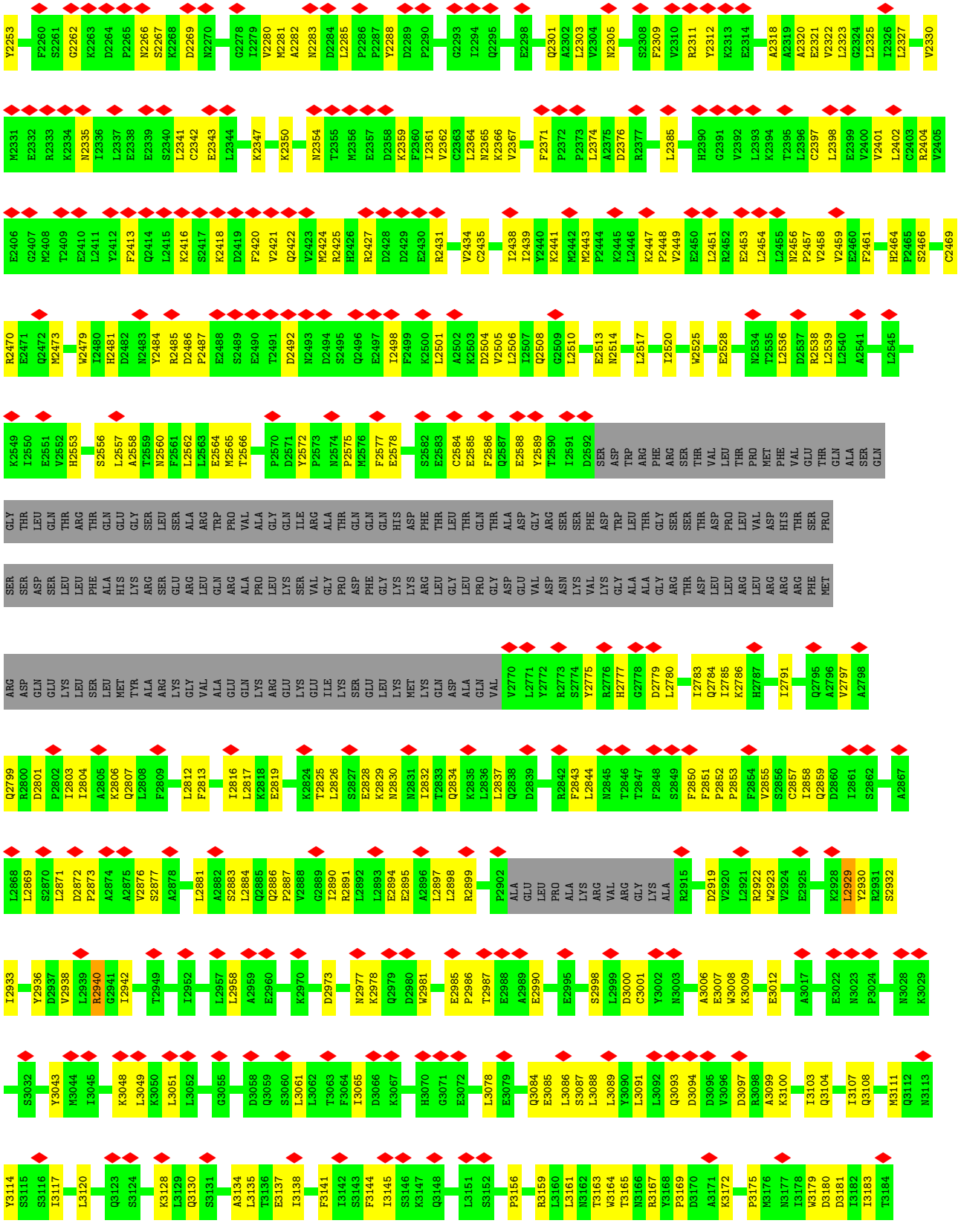
• Molecule 2: DNA-dependent protein kinase catalytic subunit

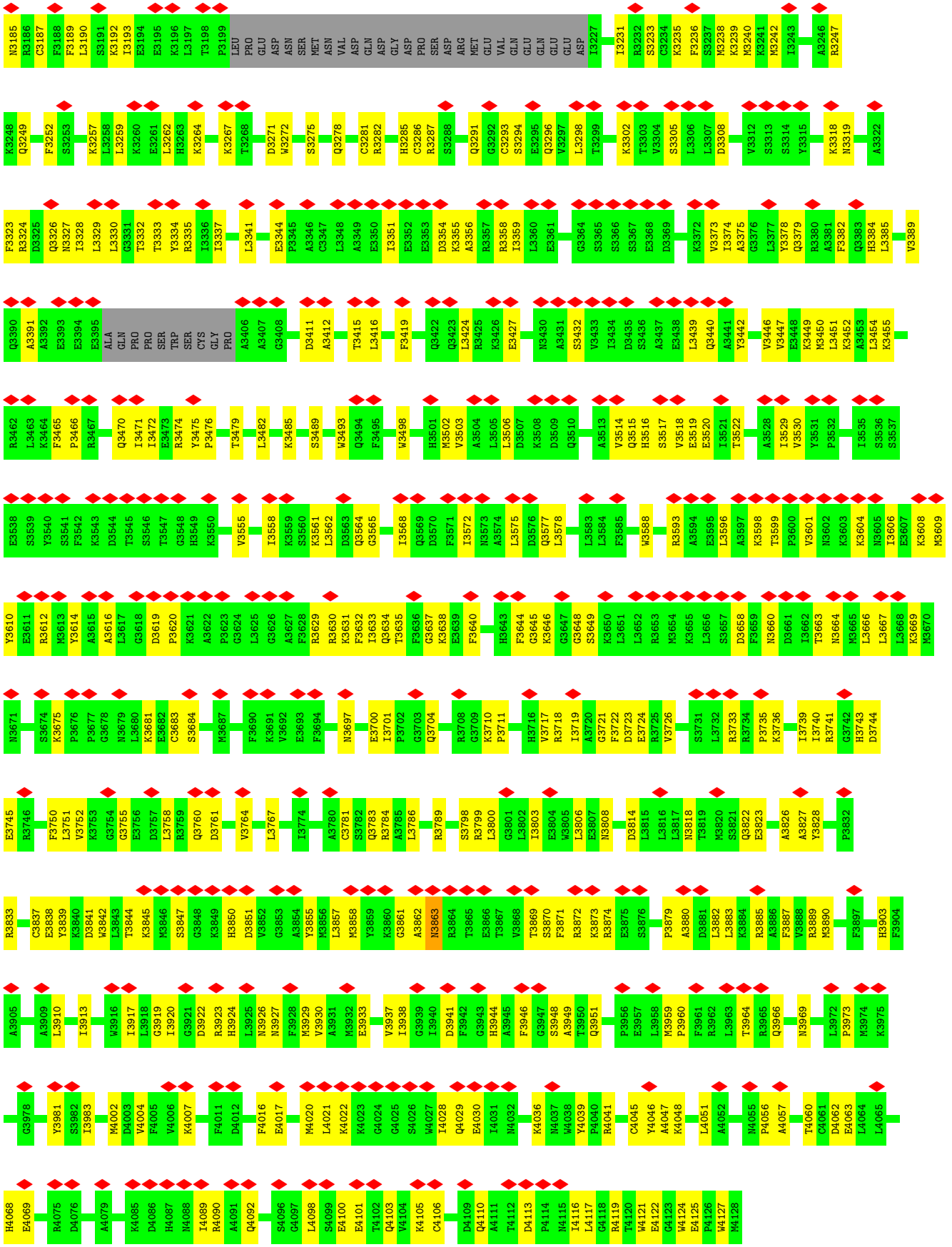
Chain L:




N351 V352 D353 S354 N355 N356 K357 E358 L359 S360 I361 A362 I363 R364 L368 I376 K379 D380 V381 M384 Q394 M395 F396 L397 T398 Q399 T400 D401 T402 G403 D404 D405 R406 V407 Y408 Q409 M410 P411 S412 F413 L414 V417 A418 S419 V420 L421 L422 Y423 L424 D425 T426 V427 P428 E429
V430 Y431 T432 P433 E436 H437 L438 V439 V440 M441 Q442 I443 F446 P447 S450 P451 K452 M453 Q454 L455 V456 R459 A460 I461 V462 K463 V464 F465 L466 A467 L468 K471 G472 P473 R476 N477 C478 I479 S480 T481 V482 V483 H484 Q485 G486 L487 I488 R489 I490 L497 PRO LYS GLY
PRO GLU SER GLU SER GLU ASP HIS ARG ALA SER GLY GLU VAL ARG THR GLY LYS TRP LYS VAL P522 T523 Y524 K525 D526 Y527 L530 F531 L534 L535 S536 S537 M540 S543 ILE LEU ALA ASP GLU ALA PHE PHE SER VAL ASN SER SER S557 L560 L563 L564 Y565 D566
E567 F568 V569 V572 I575 L579 D580 L581 T582 L583 E584 I585 GLN THR VAL GLY GLU GLN GLU ASN GLY ASP GLU ALA PRO GLY VAL TRP M602 I603 P604 L612 H613 P614 K618 D619 F620 F623 I624 V627 C630 R631 E632 I633 L634 P635 E636 K637 E643 P644 W645
F649 S650 Y651 E652 L653 I654 L655 L660 P661 L662 I663 S664 G665 K668 L669 L670 S671 V674 V686 SER PRO LYS SER LEU LYS HIS SER PRO GLU ASP P698 E699 F704 F707 V708 K709 F710 G711 K712 E713 V714 A715 V716 K717 M718 Y721 K722 D723 L726 A727 S728
C729 L730 T731 F732 L733 L734 S735 L736 P737 H738 N739 I740 I741 D744 V745 R746 V749 P750 A751 L752 Q753 M754 A755 F756 L760 A766 L770 L773 E774 E775 W776 S777 I778 Y779 R782 H783 V784 M785 Y788 Y789 K790 D791 I792 L793 P794 S803 A804 L805 SER ASP GLU
THR LYS ASN ASN TRP GLU VAL SER ALA LEU LEU SER ARG ALA ALA GLN LYS GLY PHE ASN LYS VAL VAL LEU LEU LYS HIS LEU LEU LYS LYS THR LYS ASN LEU SER SER ASN E844 A845 L848 E849 E850 I851 R852 I853 R854 Q857 M858 L859 G860 S861 G864 G865 I866 N867 K868 N869 T872
S875 S876 D877 E878 M879 M880 K881 S882 Y883 V884 A885 W886 D887 R888 E889 K890 R891 L892 S893 P897 E900 M901 K902 P903 V904 I905 F906 L907 D908 V909 F910 L911 P912 R913 E916 A921 S922 D923 R924 Q925 T926 K927 V928 A929 A930 C931 E932 L933 L934 H935 V938 M939 F940 M941
Q947 N948 P949 E950 G951 G952 Q953 G954 A955 P956 P957 M958 Y959 Q960 L961 Y962 K963 R964 T965 D975 V976 V979 Q982 L983 Y984 E985 V988 L991 I992 H993 N997 N998 K999 E1002 S1003 Q1004 D1005 T1006 V1007 A1008 L1009 L1010 E1011 A1012 I1013 L1014 I1017 Y1018 D1019 P1020 V1021
D1022 S1023 R1026 F1036 L1037 I1041 K1042 Q1043 I1044 T1045 P1046 Q1047 Q1048 Q1049 E1050 K1051 S1052 P1053 V1054 N1055 S1058 K1061 R1062 L1063 Y1064 S1065 L1066 A1067 L1068 H1069 A1072 R1075 L1076 G1077 A1078 A1081 N1084 I1085 Y1086 R1087 E1088 F1089 E1093 Y1096 F1099 V1100 F1101 E1102
A1103 L1104 V1105 I1106 Y1107 M1108 L1111 A1112 L1113 A1116 D1117 E1118 K1119 S1120 I1124 Q1125 I1131 D1132 H1133 L1134 C1135 R1136 I1137 I1138 H1142 L1145 A1148 K1149 K1150 R1151 R1155 G1156 F1157 P1158 P1159 S1160 A1161 S1162 L1163 D1167 L1168 V1169 K1170 L1173 A1174 H1175 C1176 G1177 R1178 P1179
Q1180 T1181 E1182 C1183 R1184 H1185 I1188 F1191 F1194 V1195 P1196 L1197 L1198 P1199 G1200 S1203 P1204 N1205 L1206 W1207 D1210 V1211 L1212 K1213 E1214 E1215 F1219 N1222 T1223 F1224 E1225 G1226 C1229 S1233 A1237 Q1238 P1239 T1240 L1241 L1242 Y1243 LEU ARG GLY PRO PHE S1249 L1250 Q1251 A1252
L1260 L1261 A1262 E1265 C1266 Y1267 N1268 T1269 F1270 I1271 G1272 E1273 R1274 T1275 V1276 G1277 A1278 V1281 L1282 G1283 T1284 E1285 A1286 Q1287 S1288 S1289 L1290 L1291 K1292 A1293 V1294 L1298 E1299 A1302 M1303 H1304 D1305 I1306 I1307 A1308 A1309 E1310 K1311 CYS PHE GLY THR GLY ALA ALA GLY ASN ARG THR S1323

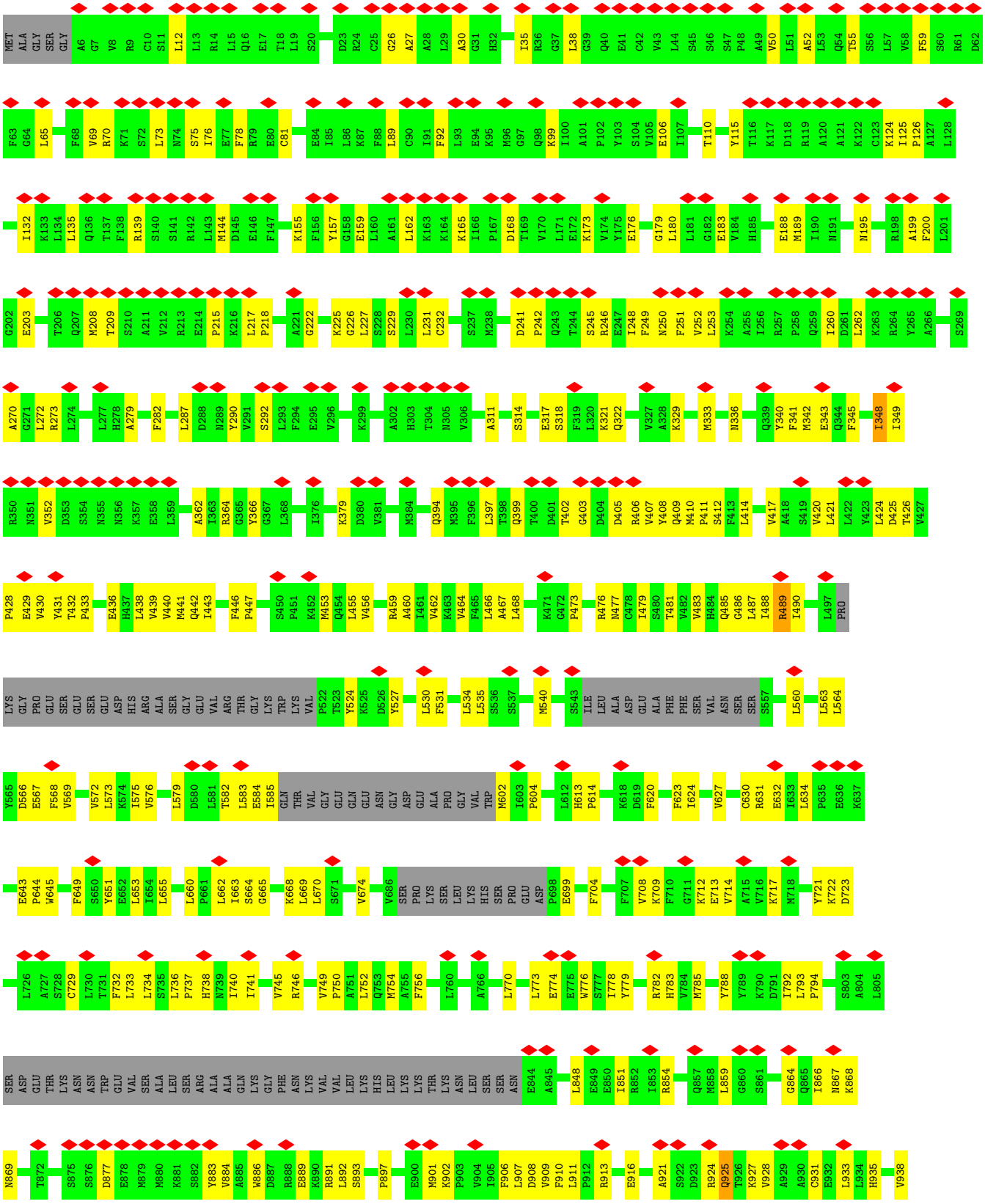

P1324 Q1325 E1326 G1327 E1328 R1329 Y1330 N1331 Y1332 S1333 K1334 C1335 T1336 V1337 V1338 V1339 R1340 I1341 M1342 E1343 T1346 T1347 L1348 L1349 N1350 L1359 N1365 T1366 H1367 L1368 M1369 R1370 V1371 L1372 L1376 C1377 E1378 P1379 A1380 S1381 F1384 N1385 I1386 G1387 D1388 V1389 Q1390 V1391 M1392 M1403 E1416 T1417 H1418
K1422 I1423 T1424 A1425 Q1426 S1427 I1428 E1429 E1430 L1431 C1432 A1433 V1434 N1435 L1436 Y1437 G1438 P1439 D1440 A1441 Q1442 V1443 D1444 R1445 L1448 V1452 K1456 H1459 L1464 H1466 N1466 I1467 L1468 P1469 S1470 Q1471 S1472 T1473 D1474 L1475 H1476 H1477 S1478 K1489 G1490 I1491 A1492 P1493 G1494 D1495 E1496 R1497 Q1498
C1499 L1500 P1501 S1502 L1503 D1504 L1505 L1515 F1519 G1522 G1523 L1524 R1527 L1528 L1531 L1532 L1533 N1534 P1535 A1536 V1537 L1538 S1539 T1540 ALA SER LEU GLY SER SER GLN GLY S1549 V1550 I1551 H1552 F1553 S1554 H1555 G1556 E1557 Y1558 F1559 Y1560 S1561 L1562 F1563 S1564 I1567 N1568 T1569 L1572
L1575 V1579 L1580 Q1584 S1585 D1588 M1592 V1593 V1596 L1597 N1598 L1601 D1602 Q1603 S1604 F1605 R1606 E1607 R1608 A1609 N1610 Q1611 Q1614 K1617 L1618 A1619 L1623 Q1624 K1628 C1629 D1630 S1631 W1632 W1633 A1634 K1635 D1636 S1637 P1638 L1639 K1642 M1643 L1646 A1647 L1648 L1649 A1650 K1651
I1652 L1653 Q1654 I1655 D1656 S1657 S1658 V1659 N1662 T1663 S1664 H1665 G1666 S1667 E1670 T1673 T1674 Y1675 I1676 L1679 A1680 D1681 T1682 D1685 L1688 K1689 G1690 V1693 T1703 S1706 L1707 E1708 E1709 L1710 R1711 R1712 V1713 L1714 E1715 Q1716 L1717 I1718 V1719 F1722 P1723 M1724 Q1725 S1726 R1727 E1728
F1729 P1730 P1731 G1732 T1733 F1736 N1737 V1740 D1741 C1742 M1743 K1744 K1745 F1746 L1747 D1748 A1749 L1750 S1755 P1756 M1757 L1758 L1759 E1760 L1761 M1762 T1763 E1764 V1765 L1766 C1767 R1768 E1769 Q1770 Q1771 E1775 E1776 L1777 F1778 Q1779 S1780 S1781 F1782 R1783 R1784 I1785 A1786 R1787 R1788 G1789 S1790 C1791 V1792 T1793 Q1794 V1795
G1796 L1797 L1798 M1804 F1805 R1806 K1807 D1808 D1809 P1810 R1811 E1812 S1813 F1814 T1815 R1816 Q1817 S1818 F1819 V1820 D1821 R1822 S1823 L1824 L1825 L1828 W1829 H1830 C1831 S1832 L1833 D1834 A1835 L1836 R1837 E1838 F1839 F1840 S1841 T1842 I1843 V1844 V1845 D1846 A1847 I1848 D1849 V1850 L1851 K1852 S1853 R1854 F1855 T1856 K1857 L1858 N1859 E1860
S1861 T1862 F1863 D1864 T1865 Q1866 I1867 T1868 K1869 K1870 M1871 G1872 Y1873 Y1874 K1875 I1876 L1877 D1878 V1879 M1880 Y1881 S1882 R1883 L1884 P1885 K1886 D1887 D1888 V1889 H1890 A1891 K1892 E1893 S1894 K1895 I1896 N1897 Q1898 V1899 F1900 H1901 G1902 S1903 C1904 I1905 T1906 E1907 G1908 N1909 E1910 L1911 T1912 K1913 T1914 L1915 I1916 K1917 L1918 C1919 Y1920
D1921 A1922 F1923 T1924 E1925 N1926 M1927 A1928 G1929 E1930 N1931 Q1932 L1933 L1934 E1935 R1936 R1937 R1938 L1939 Y1940 H1941 C1942 A1943 A1944 Y1945 N1946 C1947 V1951 I1952 C1953 C1954 V1955 F1956 N1957 E1958 L1959 K1960 F1961 F1965 L1966 F1967 S1968 E1969 K1970 P1971 N1974 L1975 L1976 I1977 F1978 E1979 N1980 L1981 I1982 D1983 L1984 K1985
ARG ARG TYR ASN PHE PRO VAL GLU VAL GLU VAL PRO MET GLU ARG LYS LYS LYS TYR ILE GLU ILE ARG LYS GLU ALA ARG GLU ALA ALA ASN GLY ASP SER ASP GLY PRO SER TYR MET SER SER LEU SER TYR LEU ALA ASP SER THR LEU SER GLU GLU MET SER GLN PHE ASP PHE
SER THR GLY VAL GLN SER TYR SER TYR SER SER GLN ASP PRO ARG PRO ALA THR GLY ARG PHE ARG ARG ARG GLU GLN ARG ASP PRO THR VAL HIS ASP ASP VAL LEU GLU LEU GLU M2086 D2086 E2087 R2090 H2091 E2092 C2093 M2094 A2095 P2096 L2097 T2098 A2099 L2100 V2101 K2102 H2105 R2106 S2107
L2108 GLY PRO PRO GLN GLY GLU GLU ASP SER VAL P2119 R2120 D2121 L2122 P2123 S2124 W2125 K2132 L2133 G2134 N2135 P2136 I2137 V2138 P2139 L2140 N2141 I2142 R2143 L2144 F2145 L2146 A2147 K2148 L2149 V2150 I2151 N2152 T2153 E2154 E2155 V2156 F2157 R2158 P2159 W2164 L2165 L2168 L2169 Q2170 L2171 A2172 A2173 S2174 E2175 N2176
N2177 G2178 G2179 E2180 G2181 I2182 H2183 Y2184 M2185 V2190 I2193 T2197 G2198 L2199 A2200 T2201 P2202 T2203 G2204 V2205 P2206 K2207 D2208 E2209 V2210 L2211 A2212 N2213 L2216 N2217 F2218 L2219 M2220 V2223 F2224 H2225 R2228 A2229 V2230 E2236 I2237 T2240 L2241 V2242 E2243 C2244 W2245 K2246 D2247 C2248 L2249

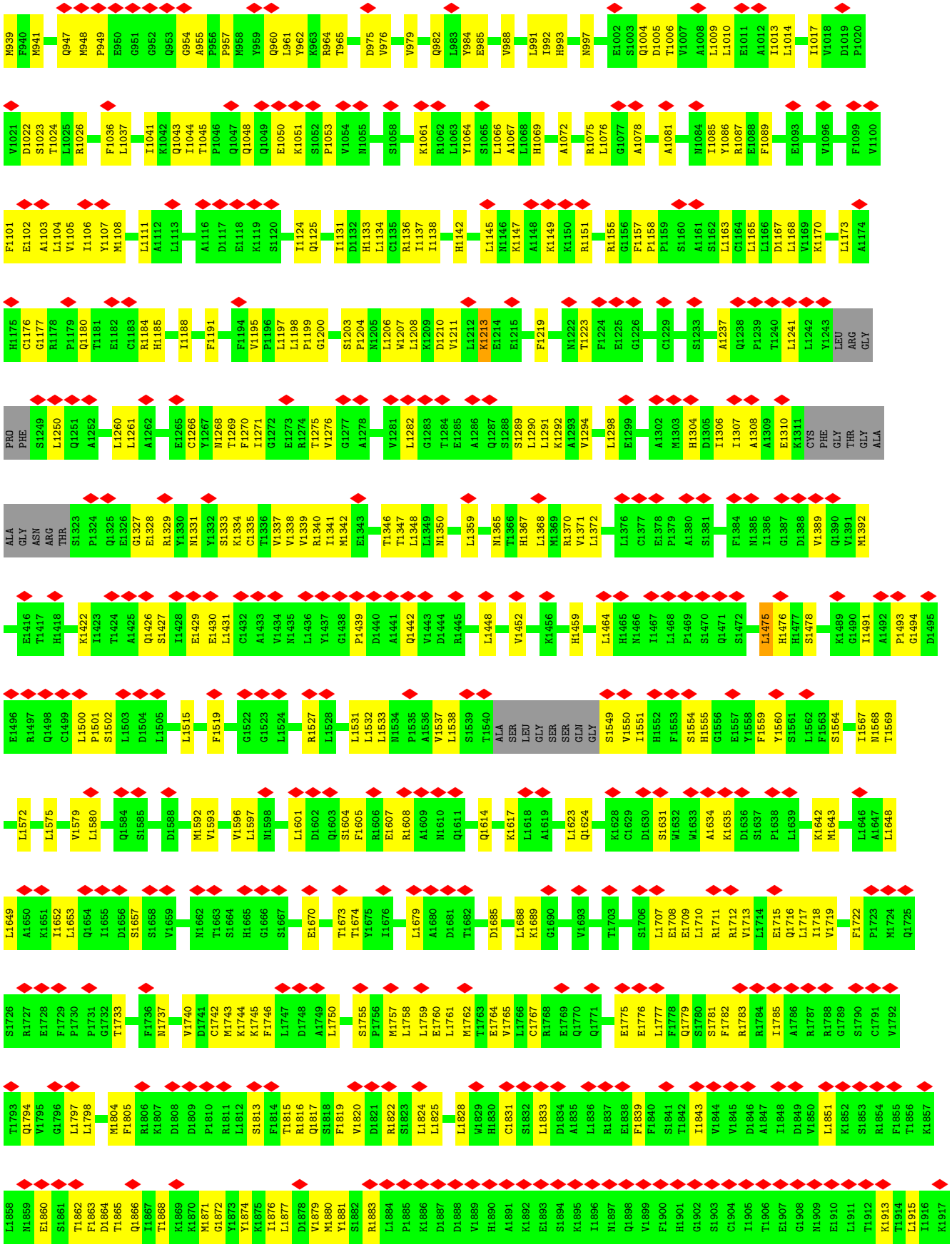

Y2253 F2260 S2261 G2262 K2263 D2264 P2265 N2266 S2267 K2268 D2269 N2270 G2278 I2279 V2280 M2281 A2282 N2283 D2284 L2285 P2286 P2287 Y2288 D2289 P2290 G2293 I2294 Q2295 E2298 Q2301 A2302 L2303 V2304 N2305 S2308 F2309 V2310 R2311 Y2312 K2313 E2314 A2318 A2319 A2320 E2321 V2322 L2323 G2324 L2325 I2326 L2327 V2330
M2331 E2332 R2333 K2334 N2335 I2336 L2337 E2338 E2339 S2340 L2341 C2342 E2343 L2344 K2347 K2350 N2354 T2355 M2356 E2357 D2358 K2359 F2360 I2361 V2362 C2363 L2364 N2365 K2366 V2367 F2371 P2372 P2373 L2374 A2375 D2376 R2377 L2385 H2390 G2391 V2392 L2393 K2394 T2395 L2396 C2397 L2398 E2399 V2400 V2401 L2402 C2403 R2404 V2405
E2406 G2407 M2408 T2409 E2410 L2411 Y2412 F2413 Q2414 L2415 K2416 S2417 K2418 D2419 F2420 V2421 Q2422 V2423 M2424 R2425 H2426 R2427 D2428 D2429 E2430 R2431 V2434 C2435 I2438 I2439 Y2440 K2441 M2442 M2443 P2444 K2445 L2446 K2447 P2448 V2449 E2450 L2451 R2452 E2453 L2454 L2455 N2456 P2457 V2458 V2459 E2460 F2461 H2464 P2465 S2466 C2469
R2470 E2471 Q2472 M2473 W2479 I2480 H2481 D2482 N2483 Y2484 R2485 D2486 P2487 E2488 S2489 E2490 T2491 D2492 N2493 D2494 S2495 Q2496 E2497 I2498 F2499 K2500 L2501 A2502 K2503 D2504 V2505 L2506 I2507 Q2508 G2509 L2510 E2513 N2514 L2517 I2520 W2525 E2528 N2534 T2535 L2536 D2537 R2538 L2539 L2540 A2541 L2545
K2549 I2550 E2551 V2552 H2553 S2556 L2557 A2558 T2559 N2560 F2561 L2562 L2563 E2564 M2565 T2566 P2570 D2571 Y2572 P2573 N2574 P2575 M2576 F2577 E2578 S2582 E2583 C2584 E2585 F2586 Q2587 E2588 Y2589 T2590 I2591 D2592 SER ASP TRP ARG PHE ARG SER THR VAL LEU THR PRO MET PHE VAL GLU THR GLN ALA SER GLN
GLY THR LEU GLN THR ARG THR GLN GLU GLY SER LEU SER ALA ARG TRP PRO VAL ALA ALA GLY GLN ILE ARG ALA THR GLN GLN HIS ASP PHE THR LEU THR GLN THR ALA ASP GLY ARG SER SER PHE ASP TRP LEU THR GLY SER SER THR ASP PRO LEU VAL ASP HIS THR SER PRO
SER SER ASP SER LEU LEU PHE ALA HIS LYS ARG SER GLU ARG LEU GLN ARG ALA PRO LEU LYS SER VAL GLY PRO ASP PHE GLY LYS LYS ARG LEU GLY LEU PRO GLY ASP GLU VAL ASP ASN LYS VAL LYS GLY ALA ALA GLY ARG THR ASP LEU LEU ARG LEU ARG ARG ARG PHE MET
ARG ASP GLN GLU LYS LEU SER LEU MET TYR ALA ALA ARG LYS GLY VAL ALA GLU GLN LYS ARG GLU LYS GLU ILE LYS SER GLU LEU LYS MET LYS GLN ASP ALA GLN VAL V2770 L2771 Y2772 R2773 S2774 Y2775 R2776 H2777 G2778 D2779 L2780 I2783 Q2784 I2785 K2786 H2787 I2791 Q2795 A2796 V2797 A2798
Q2799 R2800 D2801 P2802 I2803 I2804 A2805 K2806 Q2807 L2808 F2809 L2812 F2813 I2816 L2817 K2818 E2819 K2824 T2825 L2826 S2827 E2828 K2829 N2830 N2831 I2832 T2833 Q2834 K2835 L2836 L2837 Q2838 D2839 R2842 F2843 L2844 N2845 T2846 T2847 F2848 S2849 F2850 F2851 P2852 P2853 F2854 V2855 S2856 C2857 I2858 Q2859 D2860 I2861 S2862 A2867
L2868 L2869 S2870 L2871 D2872 P2873 A2874 A2875 V2876 S2877 A2878 L2881 A2882 S2883 L2884 Q2885 Q2886 P2887 V2888 G2889 I2890 R2891 L2892 L2893 E2894 E2895 A2896 L2897 L2898 R2899 P2902 ALA GLU LEU PRO ALA LYS ARG VAL ARG GLY LYS ALA R2915 D2919 V2920 L2921 R2922 W2923 V2924 E2925 K2928 L2929 Y2930 R2931 S2932
I2933 Y2936 D2937 V2938 L2939 R2940 G2941 I2942 T2949 I2952 L2957 L2958 A2959 E2960 K2970 D2973 N2977 K2978 Q2979 D2980 W2981 E2985 P2986 T2987 E2988 A2989 E2990 E2995 S2998 L2999 D3000 C3001 Y3002 N3003 A3006 E3007 W3008 K3009 E3012 A3017 E3022 N3023 P3024 N3028 K3029
S3032 Y3043 M3044 I3045 K3048 L3049 K3050 L3051 L3052 G3055 D3058 Q3059 S3060 L3061 L3062 T3063 F3064 I3065 D3066 K3067 H3070 G3071 E3072 L3078 E3079 Q3084 E3085 L3086 S3087 L3088 L3089 Y3090 L3091 L3092 Q3093 D3094 D3095 V3096 D3097 R3098 A3099 K3100 I3103 Q3104 I3107 Q3108 M3111 Q3112 N3113
Y3114 S3115 S3116 I3117 L3120 Q3123 S3124 K3128 L3129 Q3130 S3131 A3134 L3135 T3136 E3137 I3138 F3141 I3142 S3143 F3144 I3145 S3146 K3147 Q3148 L3151 S3152 P3156 R3159 L3160 L3161 N3162 T3163 W3164 T3165 N3166 R3167 Y3168 P3169 D3170 A3171 K3172 P3175 M3176 N3177 I3178 W3179 D3180 D3181 I3182 I3183 T3184

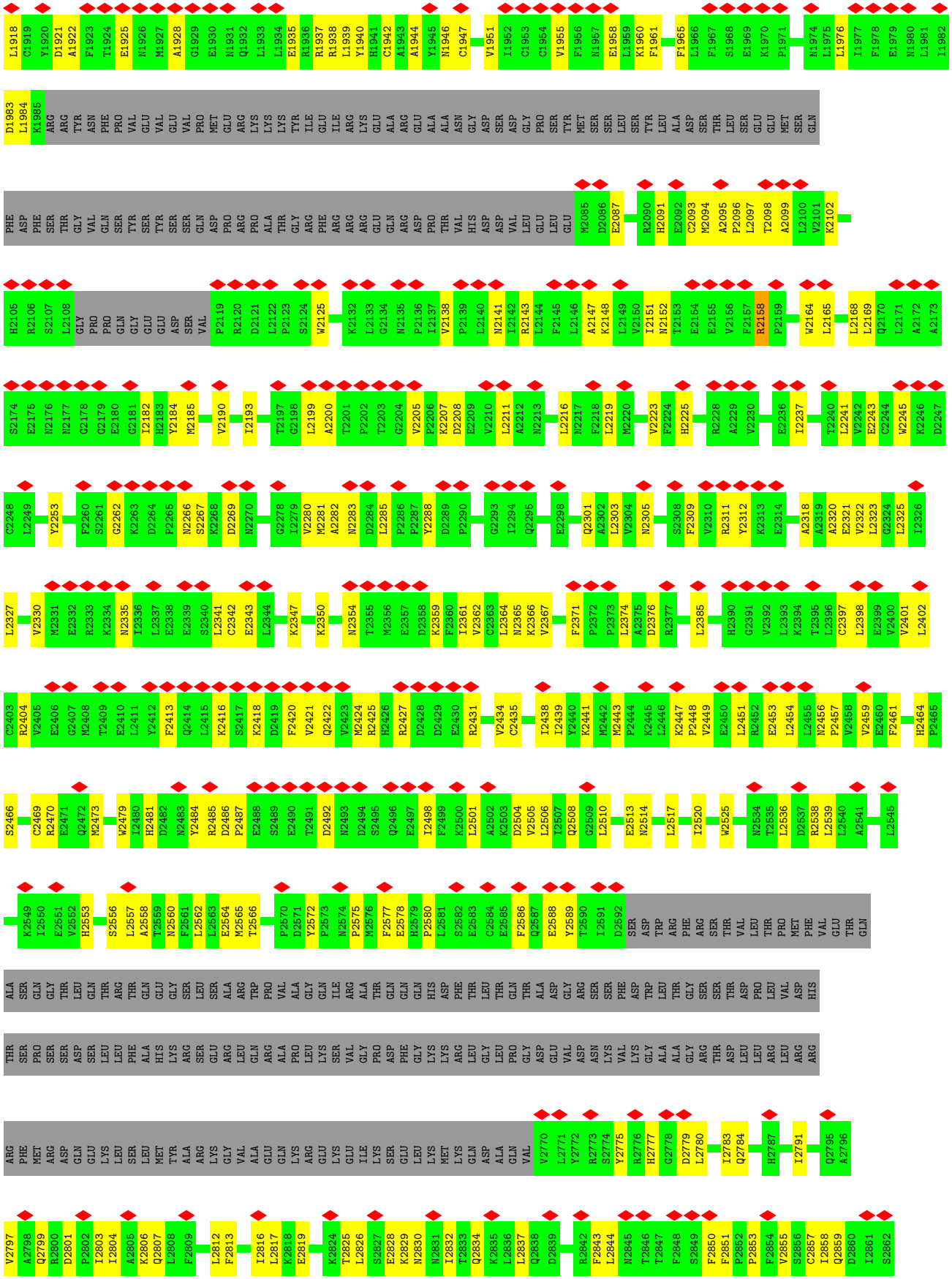

N3185 R3186 C3187 F3188 F3189 L3190 S3191 K3192 I3193 E3194 E3195 K3196 L3197 T3198 P3199 LEU PRO GLU ASP ASN SER MET ASN VAL ASP GLN ASP GLY ASP PRO SER ASP ARG MET GLU VAL GLN GLU GLN GLU GLU ASP I3227 I3231 R3232 S3233 C3234 K3235 F3236 S3237 M3238 K3239 M3240 K3241 M3242 I3243 A3246 R3247
K3248 Q3249 F3252 S3253 K3257 L3258 L3259 K3260 E3261 L3262 H3263 K3264 K3267 T3268 D3271 W3272 S3275 Q3278 C3281 R3282 H3285 C3286 R3287 S3288 Q3291 G3292 C3293 S3294 E3295 Q3296 V3297 L3298 T3299 K3302 T3303 V3304 S3305 L3306 L3307 D3308 V3312 S3313 S3314 Y3315 K3318 N3319 A3322
F3323 R3324 D3325 Q3326 N3327 I3328 L3329 L3330 G3331 T3332 T3333 Y3334 R3335 I3336 I3337 L3341 E3344 P3345 A3346 C3347 L3348 A3349 E3350 I3351 E3352 E3353 D3354 K3355 A3356 R3357 R3358 I3359 L3360 E3361 G3364 S3365 S3366 S3367 E3368 D3369 K3372 V3373 I3374 A3375 G3376 L3377 Y3378 Q3379 R3380 A3381 F3382 Q3383 H3384 L3385 V3389
Q3390 A3391 A3392 E3393 E3394 E3395 ALA GLN PRO PRO SER TRP SER CYS GLY PRO A3406 A3407 G3408 D3411 A3412 T3415 L3416 F3419 Q3422 Q3423 L3424 R3425 K3426 E3427 N3430 A3431 S3432 V3433 I3434 D3435 S3436 A3437 E3438 L3439 Q3440 A3441 Y3442 V3446 V3447 E3448 K3449 M3450 L3451 K3452 A3453 L3454 K3455
R3462 L3463 K3464 F3465 P3466 R3467 Q3470 I3471 I3472 E3473 R3474 Y3475 P3476 T3479 L3482 K3485 S3489 W3493 Q3494 F3495 W3498 H3501 M3502 V3503 A3504 L3505 L3506 D3507 K3508 D3509 Q3510 A3513 V3514 Q3515 H3516 S3517 V3518 E3519 E3520 I3521 T3522 A3528 I3529 V3530 Y3531 P3532 I3535 S3536 S3537
E3538 S3539 Y3540 S3541 F3542 K3543 D3544 T3545 S3546 T3547 G3548 H3549 K3550 V3555 I3558 K3559 S3560 K3561 L3562 D3563 Q3564 G3565 I3568 Q3569 D3570 F3571 I3572 N3573 A3574 L3575 D3576 Q3577 L3578 L3583 L3584 F3585 W3588 R3593 A3594 E3595 L3596 A3597 K3598 T3599 P3600 V3601 N3602 K3603 K3604 N3605 I3606 E3607 K3608 M3609
Y3610 E3611 R3612 M3613 Y3614 A3615 A3616 L3617 G3618 D3619 P3620 K3621 A3622 P3623 G3624 L3625 G3626 A3627 F3628 R3629 R3630 K3631 F3632 I3633 Q3634 T3635 F3636 G3637 K3638 E3639 F3640 H3643 F3644 G3645 K3646 G3647 G3648 S3649 K3650 L3651 L3652 R3653 M3654 K3655 L3656 S3657 D3658 F3659 N3660 D3661 I3662 T3663 N3664 M3665 L3666 L3667 L3668 K3669 M3670
N3671 S3674 K3675 P3676 P3677 G3678 N3679 L3680 K3681 E3682 C3683 S3684 M3687 F3690 K3691 V3692 E3693 F3694 N3697 E3700 I3701 P3702 G3703 Q3704 R3708 G3709 K3710 P3711 H3716 V3717 R3718 I3719 A3720 G3721 F3722 D3723 E3724 R3725 V3726 S3731 L3732 R3733 R3734 P3735 K3736 I3739 I3740 R3741 G3742 H3743 D3744
E3745 R3746 F3750 L3751 V3752 K3753 G3754 G3755 E3756 D3757 L3758 R3759 Q3760 D3761 V3764 L3767 I3774 A3780 C3781 S3782 Q3783 R3784 A3785 L3786 R3789 S3798 R3799 L3800 G3801 L3802 I3803 E3804 W3805 L3806 E3807 N3808 D3814 L3815 L3816 L3817 N3818 T3819 M3820 S3821 Q3822 E3823 A3826 A3827 Y3828 P3832
R3833 C3837 E3838 Y3839 K3840 D3841 W3842 L3843 T3844 K3845 M3846 S3847 G3848 K3849 H3850 D3851 V3852 G3853 A3854 Y3855 M3856 L3857 M3858 Y3859 K3860 G3861 A3862 N3863 R3864 T3865 E3866 T3867 V3868 T3869 S3870 F3871 R3872 K3873 R3874 E3875 S3876 P3879 A3880 D3881 L3882 L3883 K3884 R3885 A3886 F3887 V3888 R3889 M3890 F3897 H3903 F3904
A3905 A3909 L3910 I3913 W3916 I3917 L3918 G3919 I3920 G3921 D3922 R3923 H3924 L3925 N3926 N3927 F3928 M3929 V3930 A3931 M3932 E3933 V3937 I3938 G3939 I3940 D3941 F3942 G3943 H3944 A3945 F3946 G3947 S3948 A3949 T3950 Q3951 P3956 E3957 L3958 M3959 P3960 F3961 R3962 L3963 T3964 R3965 Q3966 N3969 L3972 P3973 M3974 K3975
G3978 Y3981 S3982 I3983 M4002 D4003 V4004 F4005 V4006 K4007 F4011 D4012 F4016 E4017 M4020 L4021 K4022 K4023 G4024 G4025 S4026 W4027 I4028 Q4029 E4030 I4031 N4032 K4036 N4037 W4038 Y4039 P4040 R4041 C4045 Y4046 A4047 K4048 L4051 A4052 N4055 P4056 A4057 T4060 C4061 D4062 E4063 L4064 L4065
H4068 E4069 R4075 D4076 A4079 K4085 D4086 H4087 W4088 I4089 R4090 A4091 Q4092 S4096 C4097 L4098 S4099 E4100 E4101 T4102 Q4103 V4104 K4105 C4106 D4109 Q4110 A4111 T4112 D4113 P4114 N4115 I4116 L4117 G4118 R4119 T4120 W4121 E4122 G4123 W4124 E4125 P4126 W4127 W4128

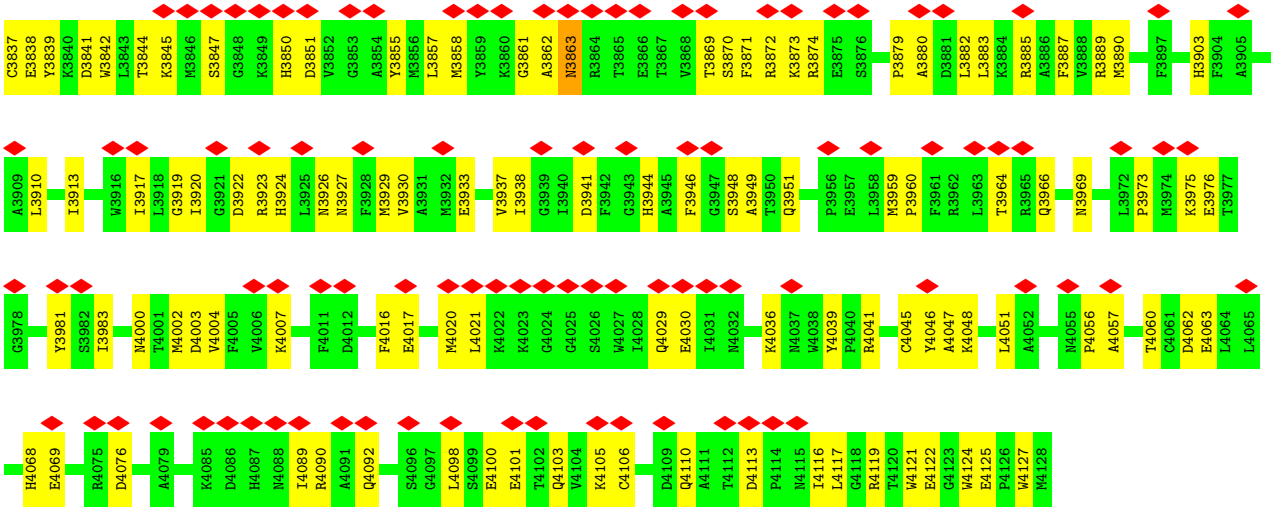
• Molecule 2: DNA-dependent protein kinase catalytic subunit

Chain C:




M939 F940 M941 Q947 M948 P949 E950 G951 Q952 Q953 G954 A955 P956 P957 M958 Y959 Q960 L961 Y962 K963 R964 T965 D975 V976 V979 Q982 L983 Y984 E985 V988 L991 I992 H993 N997 E1002 S1003 Q1004 D1005 T1006 V1007 A1008 L1009 L1010 E1011 A1012 I1013 L1014 I1017 V1018 D1019 P1020
V1021 D1022 S1023 T1024 L1025 R1026 F1036 L1037 I1041 K1042 Q1043 I1044 T1045 P1046 Q1047 Q1048 Q1049 E1050 K1051 S1052 P1053 V1054 N1055 S1058 K1061 R1062 L1063 Y1064 S1065 L1066 A1067 L1068 H1069 A1072 R1075 L1076 G1077 A1078 A1081 N1084 I1085 Y1086 R1087 E1088 F1089 E1093 V1096 F1099 V1100
F1101 E1102 A1103 L1104 V1105 I1106 Y1107 M1108 L1111 A1112 L1113 A1116 D1117 E1118 K1119 S1120 I1124 Q1125 I1131 D1132 H1133 L1134 C1135 R1136 I1137 I1138 H1142 L1145 N1146 K1147 A1148 K1149 K1150 R1151 R1155 C1156 F1157 P1158 P1159 S1160 A1161 S1162 L1163 C1164 L1165 L1166 D1167 L1168 V1169 K1170 L1173 A1174
H1175 C1176 G1177 R1178 P1179 Q1180 T1181 E1182 C1183 R1184 H1185 I1188 F1191 F1194 V1195 P1196 L1197 L1198 P1199 G1200 S1203 P1204 N1205 L1206 W1207 L1208 K1209 D1210 V1211 L1212 K1213 E1214 E1215 F1219 N1222 T1223 F1224 E1225 G1226 C1229 S1233 A1237 Q1238 P1239 T1240 L1241 L1242 Y1243 LEU ARG GLY
PRO PHE S1249 L1250 Q1251 A1252 L1260 L1261 A1262 E1265 C1266 Y1267 N1268 T1269 F1270 I1271 G1272 E1273 R1274 T1275 V1276 G1277 A1278 V1281 L1282 G1283 T1284 E1285 A1286 Q1287 S1288 S1289 L1290 L1291 K1292 A1293 V1294 L1298 E1299 A1302 M1303 H1304 D1305 I1306 I1307 A1308 A1309 E1310 K1311 CYS PHE GLY THR GLY ALA
ALA GLY ASN ARG THR S1323 P1324 Q1325 E1326 G1327 E1328 R1329 Y1330 N1331 Y1332 S1333 K1334 C1335 T1336 V1337 V1338 V1339 R1340 I1341 M1342 E1343 T1346 T1347 L1348 L1349 N1350 L1359 N1365 T1366 H1367 L1368 M1369 R1370 V1371 L1372 L1376 C1377 E1378 P1379 A1380 S1381 F1384 N1385 I1386 G1387 D1388 V1389 Q1390 V1391 M1392
E1416 T1417 H1418 K1422 I1423 T1424 A1425 Q1426 S1427 I1428 E1429 E1430 L1431 C1432 A1433 V1434 N1435 L1436 Y1437 G1438 P1439 D1440 A1441 Q1442 V1443 D1444 R1445 L1448 V1452 K1456 H1459 L1464 H1465 N1466 I1467 L1468 P1469 S1470 Q1471 S1472 L1475 H1476 H1477 S1478 K1489 G1490 I1491 A1492 P1493 G1494 D1495
E1496 R1497 Q1498 C1499 L1500 P1501 S1502 L1503 D1504 L1505 L1515 F1519 G1522 G1523 L1524 R1527 L1528 L1531 L1532 L1533 W1534 P1535 A1536 V1537 L1538 S1539 T1540 ALA SER LEU GLY SER SER GLN GLY S1549 V1550 I1551 H1552 F1553 S1554 H1555 G1556 E1557 Y1558 F1559 Y1560 S1561 L1562 F1563 S1564 I1567 N1568 T1569
L1572 L1575 V1579 L1580 Q1584 S1585 D1588 M1592 V1593 V1596 L1597 N1598 L1601 D1602 Q1603 S1604 F1605 R1606 E1607 R1608 A1609 N1610 Q1611 Q1614 K1617 L1618 A1619 L1623 Q1624 K1628 C1629 D1630 S1631 W1632 W1633 A1634 K1635 D1636 S1637 P1638 L1639 K1642 M1643 L1646 A1647 L1648
L1649 A1650 K1651 I1652 L1653 Q1654 I1655 D1656 S1657 S1658 V1659 N1662 T1663 S1664 H1665 G1666 S1667 E1670 T1673 T1674 Y1675 I1676 L1679 A1680 D1681 T1682 D1685 L1688 K1689 G1690 V1693 T1703 S1706 L1707 E1708 E1709 L1710 R1711 R1712 V1713 L1714 E1715 Q1716 L1717 I1718 V1719 F1722 P1723 M1724 Q1725
S1726 R1727 E1728 F1729 P1730 P1731 G1732 T1733 F1736 N1737 V1740 D1741 C1742 M1743 K1744 K1745 F1746 L1747 D1748 A1749 L1750 S1755 P1756 M1757 L1758 L1759 E1760 L1761 M1762 T1763 E1764 V1765 L1766 C1767 R1768 E1769 Q1770 Q1771 E1775 E1776 L1777 F1778 Q1779 S1780 S1781 F1782 R1783 R1784 I1785 A1786 R1787 R1788 G1789 S1790 C1791 V1792
T1793 Q1794 V1795 G1796 L1797 L1798 M1804 F1805 R1806 K1807 D1808 D1809 P1810 R1811 L1812 S1813 F1814 T1815 R1816 D1817 S1818 F1819 V1820 D1821 R1822 S1823 L1824 L1825 L1828 W1829 H1830 C1831 S1832 L1833 D1834 A1835 L1836 R1837 E1838 F1839 F1840 S1841 T1842 I1843 V1844 V1845 D1846 A1847 I1848 D1849 V1850 L1851 K1852 S1853 R1854 F1855 T1856 K1857
L1858 N1859 E1860 S1861 T1862 F1863 D1864 T1865 Q1866 I1867 T1868 K1869 K1870 M1871 G1872 Y1873 Y1874 K1875 I1876 L1877 D1878 V1879 M1880 Y1881 S1882 R1883 L1884 P1885 K1886 D1887 D1888 V1889 H1890 A1891 K1892 E1893 S1894 K1895 L1896 N1897 Q1898 V1899 F1900 H1901 G1902 S1903 C1904 I1905 T1906 E1907 G1908 N1909 E1910 L1911 T1912 K1913 T1914 L1915 I1916 K1917


L1918 C1919 Y1920 D1921 A1922 F1923 T1924 E1925 N1926 M1927 A1928 G1929 E1930 N1931 Q1932 L1933 L1934 E1935 R1936 R1937 R1938 L1939 Y1940 H1941 C1942 A1943 A1944 Y1945 N1946 C1947 V1951 I1952 C1953 C1964 V1955 F1956 N1957 E1958 L1959 K1960 F1961 F1965 L1966 F1967 S1968 E1969 K1970 P1971 N1974 L1975 L1976 I1977 F1978 E1979 N1980 L1981 I1982
D1983 L1984 K1985 ARG ARG TYR ASN PHE PRO VAL GLU VAL GLU VAL PRO MET GLU ARG LYS LYS LYS TYR ILE GLU ILE ARG LYS GLU ALA ALA ARG GLU ALA ALA ASN GLY ASP SER ASP GLY PRO SER TYR MET SER SER LEU SER TYR LEU ALA ASP SER THR LEU SER GLU GLU MET SER GLN
PHE ASP PHE SER THR GLY VAL GLN SER TYR SER TYR SER SER GLN ASP PRO ARG PRO ALA THR GLY ARG PHE ARG ARG ARG GLU GLN ARG ASP PRO THR VAL HIS ASP ASP VAL LEU GLU LEU GLU M2085 D2086 E2087 R2090 H2091 E2092 C2093 M2094 A2095 P2096 L2097 T2098 A2099 L2100 V2101 K2102
H2105 R2106 S2107 L2108 GLY PRO PRO GLN GLY GLU GLU ASP SER VAL P2119 R2120 D2121 L2122 P2123 S2124 W2125 K2132 L2133 G2134 N2135 P2136 I2137 V2138 P2139 L2140 N2141 I2142 R2143 L2144 F2145 L2146 A2147 K2148 L2149 V2150 I2151 N2152 T2153 E2154 E2155 V2156 F2157 R2158 P2159 W2164 L2165 L2168 L2169 Q2170 L2171 A2172 A2173
S2174 E2175 N2176 N2177 G2178 G2179 E2180 G2181 I2182 H2183 Y2184 M2185 V2190 I2193 T2197 G2198 L2199 A2200 T2201 P2202 T2203 G2204 V2205 P2206 K2207 D2208 E2209 V2210 L2211 A2212 N2213 L2216 N2217 F2218 L2219 M2220 V2223 F2224 H2225 R2228 A2229 V2230 E2236 I2237 T2240 L2241 V2242 E2243 C2244 W2245 K2246 D2247
C2248 L2249 Y2253 F2260 S2261 G2262 K2263 D2264 P2265 N2266 S2267 K2268 D2269 N2270 G2278 T2279 V2280 M2281 A2282 N2283 D2284 L2285 P2286 P2287 Y2288 D2289 P2290 G2293 I2294 Q2295 E2298 Q2301 A2302 L2303 V2304 N2305 S2308 F2309 V2310 R2311 Y2312 K2313 E2314 A2318 A2319 A2320 E2321 V2322 L2323 G2324 L2325 T2326
L2327 V2330 M2331 E2332 R2333 K2334 N2335 I2336 L2337 E2338 E2339 S2340 L2341 C2342 E2343 L2344 K2347 K2350 N2354 T2355 M2356 E2357 D2358 K2359 F2360 I2361 V2362 C2363 L2364 N2365 K2366 V2367 F2371 P2372 P2373 L2374 A2375 D2376 R2377 L2385 H2390 G2391 V2392 L2393 K2394 T2395 L2396 C2397 L2398 E2399 V2400 V2401 L2402
C2403 R2404 V2405 E2406 G2407 M2408 T2409 E2410 L2411 Y2412 F2413 Q2414 L2415 K2416 S2417 K2418 D2419 F2420 V2421 Q2422 V2423 M2424 R2425 H2426 R2427 D2428 D2429 E2430 R2431 V2434 C2435 I2438 I2439 Y2440 K2441 M2442 M2443 P2444 K2445 L2446 K2447 P2448 V2449 E2450 L2451 R2452 E2453 L2454 L2455 N2456 P2457 V2458 V2459 E2460 F2461 H2464 P2465
S2466 C2469 R2470 E2471 Q2472 M2473 W2479 I2480 H2481 D2482 N2483 Y2484 R2485 D2486 P2487 E2488 S2489 E2490 T2491 D2492 N2493 D2494 S2495 Q2496 E2497 I2498 P2499 K2500 L2501 A2502 K2503 D2504 V2505 L2506 I2507 Q2508 G2509 L2510 E2513 N2514 L2517 I2520 W2525 N2534 T2535 L2536 D2537 R2538 L2539 L2540 A2541 L2545
K2549 I2550 E2551 V2552 H2553 S2556 L2557 A2558 T2559 N2560 F2561 L2562 L2563 E2564 M2565 T2566 P2570 D2571 Y2572 P2573 N2574 P2575 M2576 F2577 E2578 H2579 P2580 L2581 S2582 E2583 C2584 E2585 F2586 Q2587 E2588 Y2589 T2590 I2591 D2592 SER ASP TRP TRP ARG PHE ARG SER THR VAL LEU THR PRO MET PHE VAL GLU THR GLN
ALA SER GLN GLY THR LEU GLN THR ARG THR GLN GLU GLY SER LEU SER ALA ARG TRP PRO VAL ALA GLY GLN ILE ARG ALA THR GLN GLN HIS ASP PHE THR LEU THR GLN THR ALA ASP GLY ARG SER SER PHE ASP TRP LEU THR GLY SER SER THR ASP PRO LEU VAL ASP HIS
THR SER PRO SER SER ASP SER LEU LEU PHE ALA HIS LYS ARG SER GLU ARG LEU GLN ARG ALA PRO LEU LYS SER VAL GLY PRO ASP PHE GLY LYS LYS ARG LEU GLY LEU PRO GLY ASP GLU VAL ASP ASN LYS VAL LYS GLY ALA ALA GLY ARG THR ASP LEU LEU ARG LEU ARG ARG
ARG PHE MET ARG ASP GLN GLU LYS LEU LYS SER GLU LEU MET TYR ALA ARG LYS GLY VAL ALA GLU GLN LYS ARG GLU LYS GLU ILE LYS SER GLU LEU LYS MET LYS GLN ASP ALA GLN VAL V2770 L2771 Y2772 R2773 S2774 Y2775 R2776 H2777 G2778 D2779 L2780 I2783 Q2784 H2787 I2791 Q2795 A2796
V2797 A2798 Q2799 R2800 D2801 P2802 I2803 I2804 A2805 K2806 Q2807 L2808 F2809 L2812 F2813 I2816 L2817 K2818 E2819 K2824 T2825 L2826 S2827 E2828 K2829 N2830 N2831 I2832 T2833 Q2834 K2835 L2836 L2837 Q2838 D2839 R2842 F2843 L2844 N2845 T2846 T2847 F2848 S2849 F2850 F2851 P2852 P2853 F2854 V2855 S2856 C2857 I2858 Q2859 D2860 I2861 S2862


C3837 E3838 Y3839 K3840 D3841 W3842 L3843 T3844 K3845 M3846 S3847 G3848 K3849 H3850 D3851 V3852 G3853 A3854 Y3855 M3856 L3857 M3858 Y3859 K3860 G3861 A3862 M3863 R3864 T3865 E3866 T3867 V3868 T3869 S3870 F3871 R3872 K3873 R3874 E3875 S3876 P3879 A3880 D3881 L3882 L3883 K3884 R3885 A3886 F3887 V3888 R3889 M3890 F3897 H3903 F3904 A3905
A3909 L3910 I3913 W3916 I3917 L3918 G3919 I3920 G3921 D3922 R3923 H3924 L3925 N3926 N3927 F3928 M3929 V3930 A3931 M3932 E3933 V3937 I3938 G3939 I3940 D3941 F3942 G3943 H3944 A3945 F3946 G3947 S3948 A3949 T3950 Q3951 P3956 E3957 L3958 M3959 P3960 F3961 R3962 L3963 T3964 R3965 Q3966 N3969 L3972 P3973 M3974 K3975 E3976 T3977
G3978 Y3981 S3982 I3983 N4000 T4001 M4002 D4003 V4004 F4005 V4006 K4007 F4011 D4012 F4016 E4017 M4020 L4021 K4022 K4023 G4024 G4025 S4026 W4027 I4028 Q4029 E4030 I4031 N4032 K4036 N4037 W4038 Y4039 P4040 R4041 C4045 Y4046 A4047 K4048 L4051 A4052 N4055 P4056 A4057 T4060 C4061 D4062 E4063 L4064 L4065
H4068 E4069 R4075 D4076 A4079 K4085 D4086 H4087 N4088 I4089 R4090 A4091 Q4092 S4096 G4097 L4098 S4099 E4100 E4101 T4102 Q4103 V4104 K4105 C4106 D4109 Q4110 A4111 T4112 D4113 P4114 N4115 I4116 L4117 G4118 R4119 T4120 W4121 E4122 G4123 W4124 E4125 P4126 W4127 M4128

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	356.6592, 356.6592, 356.6592	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8256, 0.8256, 0.8256	Depositor

5 Model quality

5.1 Standard geometry

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	$\#\|Z\| > 5$
2	C	0.30	0/29884	0.61	9/40387 (0.0%)
2	L	0.30	0/29884	0.61	8/40387 (0.0%)
All	All	0.30	0/59768	0.61	17/80774 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
2	L	0	2
All	All	0	5

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2929	LEU	CB-CG-CD2	-7.05	99.01	111.00
2	L	139	ARG	NE-CZ-NH2	7.04	123.82	120.30
2	L	2929	LEU	CB-CG-CD2	-7.04	99.03	111.00
2	C	139	ARG	NE-CZ-NH2	7.02	123.81	120.30
2	C	746	ARG	CA-CB-CG	5.94	126.47	113.40
2	L	746	ARG	CA-CB-CG	5.93	126.44	113.40
2	C	348	ILE	C-N-CA	5.46	135.36	121.70
2	L	348	ILE	C-N-CA	5.45	135.33	121.70
2	L	1475	LEU	CA-CB-CG	5.18	127.21	115.30
2	C	1475	LEU	CA-CB-CG	5.18	127.21	115.30
2	L	333	MET	CG-SD-CE	5.17	108.47	100.20
2	C	333	MET	CG-SD-CE	5.17	108.47	100.20
2	C	333	MET	CA-CB-CG	5.15	122.05	113.30
2	L	333	MET	CA-CB-CG	5.13	122.03	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3462	ARG	NE-CZ-NH2	5.11	122.86	120.30
2	L	2341	LEU	CA-CB-CG	5.09	127.00	115.30
2	C	2341	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	364	ARG	Sidechain
2	C	366	TYR	Sidechain
2	C	489	ARG	Sidechain
2	L	364	ARG	Sidechain
2	L	489	ARG	Sidechain

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	Q	101	0	25	3	0
1	R	101	0	25	3	0
2	C	29284	0	29680	975	0
2	L	29284	0	29680	981	0
All	All	58770	0	59410	1928	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 16.

All (1928) 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:L:3606:ILE:O	2:L:3610:TYR:HB2	1.53	1.08
2:C:3606:ILE:O	2:C:3610:TYR:HB2	1.53	1.07
2:L:26:GLY:C	2:C:76:ILE:HD12	1.84	0.97
2:L:76:ILE:HD12	2:C:26:GLY:C	1.86	0.96
2:C:2890:ILE:HG12	2:C:2929:LEU:HD21	1.47	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2890:ILE:HG12	2:L:2929:LEU:HD21	1.47	0.95
2:L:1750:LEU:HD23	2:L:1759:LEU:HD12	1.53	0.90
2:C:1750:LEU:HD23	2:C:1759:LEU:HD12	1.53	0.90
2:L:1184:ARG:NH2	2:L:1266:CYS:SG	2.45	0.89
2:L:414:LEU:HD22	2:L:442:GLN:HG2	1.55	0.88
2:C:1184:ARG:NH2	2:C:1266:CYS:SG	2.45	0.88
2:C:414:LEU:HD22	2:C:442:GLN:HG2	1.55	0.88
2:C:3789:ARG:HH12	2:C:3806:LEU:HD11	1.42	0.85
2:L:1198:LEU:HD12	2:L:1199:PRO:HD2	1.59	0.85
2:L:1713:VAL:HG23	2:L:1716:GLN:HE21	1.42	0.84
2:C:1713:VAL:HG23	2:C:1716:GLN:HE21	1.42	0.84
2:C:1198:LEU:HD12	2:C:1199:PRO:HD2	1.59	0.83
2:L:3789:ARG:HH12	2:L:3806:LEU:HD11	1.42	0.82
2:L:411:PRO:HA	2:L:414:LEU:HG	1.61	0.82
2:C:411:PRO:HA	2:C:414:LEU:HG	1.61	0.81
2:L:76:ILE:CD1	2:C:26:GLY:C	2.49	0.81
2:L:26:GLY:C	2:C:76:ILE:CD1	2.48	0.80
2:L:3786:LEU:HD23	2:L:3910:LEU:HD13	1.64	0.80
2:C:3786:LEU:HD23	2:C:3910:LEU:HD13	1.63	0.80
2:C:1494:GLY:HA3	2:C:1538:LEU:HB2	1.62	0.79
2:L:352:VAL:HG11	2:L:1733:THR:CG2	2.12	0.79
2:C:352:VAL:HG11	2:C:1733:THR:CG2	2.12	0.79
2:L:1494:GLY:HA3	2:L:1538:LEU:HB2	1.62	0.79
2:L:3847:SER:HB2	2:L:3857:LEU:HD13	1.64	0.79
2:L:26:GLY:O	2:C:76:ILE:HG13	1.82	0.79
2:L:76:ILE:HG13	2:C:26:GLY:O	1.83	0.79
2:L:3078:LEU:HD12	2:L:3086:LEU:HD11	1.65	0.78
2:C:3078:LEU:HD12	2:C:3086:LEU:HD11	1.65	0.78
2:L:962:TYR:HA	2:L:965:THR:HG22	1.66	0.78
2:C:3847:SER:HB2	2:C:3857:LEU:HD13	1.64	0.77
2:C:962:TYR:HA	2:C:965:THR:HG22	1.66	0.77
2:L:3100:LYS:O	2:L:3104:GLN:NE2	2.18	0.76
2:C:3100:LYS:O	2:C:3104:GLN:NE2	2.18	0.76
2:C:3424:LEU:HD21	2:C:3446:VAL:HG21	1.68	0.76
2:L:27:ALA:HA	2:C:76:ILE:HD11	1.67	0.76
2:L:397:LEU:HB3	2:L:1744:LYS:HE2	1.67	0.76
2:L:3424:LEU:HD21	2:L:3446:VAL:HG21	1.68	0.76
2:C:397:LEU:HB3	2:C:1744:LYS:HE2	1.67	0.75
2:C:2498:ILE:HA	2:C:2501:LEU:HG	1.69	0.75
2:C:935:HIS:O	2:C:939:MET:HG2	1.87	0.75
2:L:2404:ARG:HE	2:L:2441:LYS:HE3	1.51	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2498:ILE:HA	2:L:2501:LEU:HG	1.68	0.74
2:L:76:ILE:HD11	2:C:27:ALA:HA	1.68	0.73
2:C:2404:ARG:HE	2:C:2441:LYS:HE3	1.51	0.73
2:C:3588:TRP:HD1	2:C:3610:TYR:HH	1.36	0.73
2:L:935:HIS:O	2:L:939:MET:HG2	1.87	0.73
2:C:1306:ILE:HG23	2:C:1307:ILE:HG12	1.70	0.73
2:L:3298:LEU:HD22	2:L:3351:ILE:HD13	1.71	0.73
2:L:1306:ILE:HG23	2:L:1307:ILE:HG12	1.70	0.73
2:C:2243:GLU:OE1	2:C:2283:ASN:ND2	2.22	0.73
2:L:242:PRO:HA	2:L:246:ARG:HD3	1.70	0.72
2:C:997:ASN:HD22	2:C:1043:GLN:HG3	1.54	0.72
2:C:3760:GLN:NE2	2:C:3761:ASP:OD2	2.22	0.72
2:L:1176:CYS:O	2:L:1184:ARG:NH2	2.23	0.72
2:L:1816:ARG:HA	2:L:1819:PHE:HD2	1.55	0.72
2:L:2243:GLU:OE1	2:L:2283:ASN:ND2	2.22	0.72
2:L:3760:GLN:NE2	2:L:3761:ASP:OD2	2.22	0.72
2:C:242:PRO:HA	2:C:246:ARG:HD3	1.70	0.72
2:L:27:ALA:N	2:C:76:ILE:HD12	2.05	0.72
2:C:157:TYR:OH	2:C:195:ASN:ND2	2.22	0.72
2:L:208:MET:HG3	2:L:209:THR:HG23	1.70	0.72
2:L:157:TYR:OH	2:L:195:ASN:ND2	2.22	0.72
2:C:992:ILE:HD11	2:C:1036:PHE:HD1	1.55	0.72
2:C:208:MET:HG3	2:C:209:THR:HG23	1.70	0.72
2:C:3137:GLU:OE1	2:C:3164:TRP:NE1	2.23	0.71
2:C:3169:PRO:HG2	2:C:3179:TRP:HE3	1.56	0.71
2:C:1816:ARG:HA	2:C:1819:PHE:HD2	1.55	0.71
2:L:3169:PRO:HG2	2:L:3179:TRP:HE3	1.56	0.71
2:C:1176:CYS:O	2:C:1184:ARG:NH2	2.23	0.71
2:L:76:ILE:HD12	2:C:27:ALA:N	2.06	0.71
2:L:997:ASN:HD22	2:L:1043:GLN:HG3	1.54	0.71
2:C:485:GLN:HA	2:C:488:ILE:HD12	1.73	0.71
2:C:3298:LEU:HD22	2:C:3351:ILE:HD13	1.71	0.71
2:C:3726:VAL:HB	2:C:3736:LYS:HZ1	1.56	0.71
2:L:485:GLN:HB3	2:L:489:ARG:HH22	1.56	0.70
2:L:3606:ILE:O	2:L:3610:TYR:CB	2.37	0.70
2:L:3808:ASN:ND2	2:L:3933:GLU:OE1	2.22	0.70
2:C:3718:ARG:H	2:C:3743:HIS:CE1	2.09	0.70
2:L:992:ILE:HD11	2:L:1036:PHE:HD1	1.55	0.70
2:L:2303:LEU:HD21	2:L:2320:ALA:H	1.56	0.70
2:L:3455:LYS:HE3	2:L:3489:SER:HB3	1.73	0.70
2:L:1831:CYS:O	2:L:1883:ARG:NH1	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2303:LEU:HD21	2:C:2320:ALA:H	1.56	0.70
2:C:3455:LYS:HE3	2:C:3489:SER:HB3	1.73	0.70
2:L:1268:ASN:OD1	2:L:1347:THR:OG1	2.07	0.70
2:C:1051:LYS:HB2	2:C:1053:PRO:HD2	1.72	0.70
2:L:4007:LYS:HE2	2:L:4041:ARG:HA	1.74	0.70
2:L:1051:LYS:HB2	2:L:1053:PRO:HD2	1.72	0.70
2:L:3450:MET:SD	2:L:3475:TYR:OH	2.49	0.69
2:L:3137:GLU:OE1	2:L:3164:TRP:NE1	2.23	0.69
2:C:2887:PRO:HA	2:C:2890:ILE:HD12	1.75	0.69
2:C:3922:ASP:O	2:C:3927:ASN:ND2	2.24	0.69
2:L:485:GLN:HA	2:L:488:ILE:HD12	1.73	0.69
2:C:3838:GLU:HB3	2:C:3874:ARG:HD3	1.74	0.69
2:C:4007:LYS:HE2	2:C:4041:ARG:HA	1.74	0.69
2:L:3838:GLU:HB3	2:L:3874:ARG:HD3	1.74	0.69
2:L:3718:ARG:H	2:L:3743:HIS:CE1	2.09	0.69
2:C:1779:GLN:OE1	2:C:1822:ARG:NH1	2.26	0.69
2:L:1134:LEU:HD23	2:L:1137:ILE:HD13	1.75	0.69
2:L:3922:ASP:O	2:L:3927:ASN:ND2	2.24	0.69
2:C:960:GLN:N	2:C:960:GLN:OE1	2.26	0.69
2:L:2887:PRO:HA	2:L:2890:ILE:HD12	1.74	0.69
2:L:2350:LYS:NZ	2:C:162:LEU:HD13	2.07	0.69
2:L:2536:LEU:HA	2:L:2539:LEU:HD12	1.75	0.69
2:C:1134:LEU:HD23	2:C:1137:ILE:HD13	1.75	0.69
2:L:939:MET:HB3	2:L:2783:ILE:HA	1.75	0.68
2:C:1268:ASN:OD1	2:C:1347:THR:OG1	2.07	0.68
2:L:975:ASP:OD1	2:L:976:VAL:N	2.27	0.68
2:L:3522:THR:HG22	2:L:3529:ILE:HG21	1.75	0.68
2:C:485:GLN:HB3	2:C:489:ARG:HH22	1.56	0.68
2:C:2536:LEU:HA	2:C:2539:LEU:HD12	1.75	0.68
2:C:2825:THR:OG1	2:C:2828:GLU:OE2	2.12	0.68
2:L:180:LEU:HD21	2:L:225:LYS:HE3	1.76	0.68
2:C:438:LEU:HD12	2:C:441:MET:HB3	1.76	0.68
2:C:3281:CYS:O	2:C:3285:HIS:ND1	2.27	0.68
2:C:3808:ASN:ND2	2:C:3933:GLU:OE1	2.22	0.68
2:L:428:PRO:HA	2:L:1551:ILE:HG21	1.76	0.67
2:L:438:LEU:HD12	2:L:441:MET:HB3	1.76	0.67
2:C:439:VAL:O	2:C:442:GLN:HB3	1.95	0.67
2:C:975:ASP:OD1	2:C:976:VAL:N	2.27	0.67
2:L:440:VAL:HG11	2:L:489:ARG:NH1	2.09	0.67
2:L:1045:THR:O	2:L:1048:GLN:NE2	2.28	0.67
2:C:440:VAL:HG11	2:C:489:ARG:NH1	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1045:THR:O	2:C:1048:GLN:NE2	2.28	0.67
2:C:1831:CYS:O	2:C:1883:ARG:NH1	2.24	0.67
2:C:2890:ILE:CG1	2:C:2929:LEU:HD21	2.22	0.67
2:C:3179:TRP:HE1	2:C:3242:MET:HA	1.60	0.67
2:L:3281:CYS:O	2:L:3285:HIS:ND1	2.27	0.67
2:C:125:ILE:O	2:C:173:LYS:NZ	2.28	0.67
2:L:439:VAL:O	2:L:442:GLN:HB3	1.95	0.67
2:L:960:GLN:OE1	2:L:960:GLN:N	2.26	0.67
2:C:939:MET:HB3	2:C:2783:ILE:HA	1.75	0.67
2:L:1779:GLN:OE1	2:L:1822:ARG:NH1	2.26	0.67
2:C:180:LEU:HD21	2:C:225:LYS:HE3	1.76	0.67
2:L:4090:ARG:NH2	2:L:4106:CYS:O	2.29	0.67
2:C:3522:THR:HG22	2:C:3529:ILE:HG21	1.75	0.67
2:L:162:LEU:HD13	2:C:2350:LYS:NZ	2.09	0.66
2:C:486:GLY:O	2:C:490:ILE:HG12	1.95	0.66
2:L:125:ILE:O	2:L:173:LYS:NZ	2.28	0.66
2:C:892:LEU:HD12	2:C:961:LEU:HD13	1.78	0.66
2:C:3606:ILE:O	2:C:3610:TYR:CB	2.37	0.66
2:C:3726:VAL:HB	2:C:3736:LYS:NZ	2.10	0.66
2:L:745:VAL:HB	2:L:788:TYR:CZ	2.31	0.66
2:L:2936:TYR:HB3	2:L:2940:ARG:HH22	1.60	0.66
2:C:3259:LEU:HA	2:C:3262:LEU:HD12	1.77	0.66
2:L:486:GLY:O	2:L:490:ILE:HG12	1.95	0.66
2:L:2825:THR:OG1	2:L:2828:GLU:OE2	2.12	0.66
2:L:2890:ILE:CG1	2:L:2929:LEU:HD21	2.22	0.66
2:L:3179:TRP:HE1	2:L:3242:MET:HA	1.60	0.66
2:L:3190:LEU:HD12	2:L:3231:ILE:HG23	1.78	0.66
2:L:2850:PHE:HB3	2:L:2883:SER:HB3	1.78	0.66
2:C:2566:THR:O	2:C:2572:TYR:OH	2.14	0.66
2:L:3259:LEU:HA	2:L:3262:LEU:HD12	1.77	0.66
2:L:3726:VAL:HB	2:L:3736:LYS:NZ	2.10	0.66
2:C:745:VAL:HB	2:C:788:TYR:CZ	2.31	0.66
2:C:3450:MET:SD	2:C:3475:TYR:OH	2.49	0.66
2:L:1718:ILE:O	2:L:1722:PHE:N	2.18	0.65
2:C:3324:ARG:HH21	2:C:3391:ALA:HB3	1.61	0.65
2:L:643:GLU:HG2	2:L:644:PRO:HD3	1.79	0.65
2:L:2539:LEU:HD11	2:L:2816:ILE:HG21	1.78	0.65
2:C:632:GLU:OE1	2:C:632:GLU:N	2.26	0.65
2:C:2850:PHE:HB3	2:C:2883:SER:HB3	1.78	0.65
2:C:428:PRO:HA	2:C:1551:ILE:HG21	1.76	0.65
2:L:1304:HIS:HB2	2:L:1308:ALA:HB2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1327:GLY:O	2:L:1331:ASN:ND2	2.29	0.65
2:L:2492:ASP:HB2	2:C:3093:GLN:HE21	1.61	0.65
2:C:1304:HIS:HB2	2:C:1308:ALA:HB2	1.78	0.65
2:C:4090:ARG:NH2	2:C:4106:CYS:O	2.29	0.65
2:L:897:PRO:HA	2:L:902:LYS:HG3	1.78	0.65
2:L:3883:LEU:HD23	2:L:3966:GLN:HB3	1.78	0.65
2:C:1327:GLY:O	2:C:1331:ASN:ND2	2.29	0.65
2:C:2539:LEU:HD11	2:C:2816:ILE:HG21	1.78	0.65
2:C:3721:GLY:N	2:C:3741:ARG:O	2.29	0.65
2:L:3093:GLN:HE21	2:C:2492:ASP:HB2	1.60	0.65
2:C:2301:GLN:NE2	2:C:2305:ASN:OD1	2.30	0.65
2:C:3190:LEU:HD12	2:C:3231:ILE:HG23	1.78	0.65
2:L:2566:THR:O	2:L:2572:TYR:OH	2.14	0.65
2:C:2978:LYS:HE2	2:C:2981:TRP:HA	1.79	0.65
2:C:2987:THR:OG1	2:C:2990:GLU:OE1	2.11	0.65
2:C:3883:LEU:HD23	2:C:3966:GLN:HB3	1.78	0.65
2:L:2987:THR:OG1	2:L:2990:GLU:OE1	2.11	0.65
2:C:2936:TYR:HB3	2:C:2940:ARG:HH22	1.60	0.65
2:C:3723:ASP:OD1	2:C:3724:GLU:N	2.28	0.65
2:L:2421:VAL:HG13	2:L:2457:PRO:HG3	1.79	0.65
2:C:3470:GLN:HG3	2:C:4004:VAL:HB	1.79	0.65
2:L:3723:ASP:OD1	2:L:3724:GLU:N	2.28	0.64
2:C:2280:VAL:HA	2:C:2285:LEU:HD12	1.78	0.64
2:C:3634:GLN:NE2	2:C:3635:THR:OG1	2.31	0.64
2:L:892:LEU:HD12	2:L:961:LEU:HD13	1.78	0.64
2:L:2280:VAL:HA	2:L:2285:LEU:HD12	1.78	0.64
2:C:2138:VAL:O	2:C:2143:ARG:NH1	2.27	0.64
2:L:1426:GLN:NE2	2:L:1429:GLU:OE1	2.30	0.64
2:L:3324:ARG:HH21	2:L:3391:ALA:HB3	1.61	0.64
2:C:643:GLU:HG2	2:C:644:PRO:HD3	1.79	0.64
2:C:3302:LYS:HE2	2:C:3355:LYS:HE2	1.79	0.64
2:C:1426:GLN:NE2	2:C:1429:GLU:OE1	2.30	0.64
2:L:921:ALA:HB3	2:L:927:LYS:HE2	1.80	0.64
2:L:1023:SER:HA	2:L:1026:ARG:HE	1.63	0.64
2:L:1737:ASN:HA	2:L:1740:VAL:HG22	1.80	0.64
2:C:75:SER:HB2	2:C:78:PHE:HB3	1.79	0.64
2:C:3048:LYS:HE3	2:C:3061:LEU:HB2	1.80	0.64
2:L:2973:ASP:OD1	2:L:2977:ASN:ND2	2.30	0.64
2:L:3634:GLN:NE2	2:L:3635:THR:OG1	2.31	0.64
2:C:2973:ASP:OD1	2:C:2977:ASN:ND2	2.30	0.64
2:L:75:SER:HB2	2:L:78:PHE:HB3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1537:VAL:HA	2:L:1554:SER:HA	1.80	0.64
2:L:2301:GLN:NE2	2:L:2305:ASN:OD1	2.30	0.64
2:L:3470:GLN:HG3	2:L:4004:VAL:HB	1.79	0.64
2:C:485:GLN:HB3	2:C:489:ARG:HH12	1.63	0.64
2:C:921:ALA:HB3	2:C:927:LYS:HE2	1.80	0.64
2:C:1023:SER:HA	2:C:1026:ARG:HE	1.63	0.64
2:C:2421:VAL:HG13	2:C:2457:PRO:HG3	1.79	0.64
2:L:485:GLN:HB3	2:L:489:ARG:HH12	1.63	0.64
2:L:3721:GLY:N	2:L:3741:ARG:O	2.29	0.64
2:L:3871:PHE:HA	2:L:3874:ARG:HH22	1.62	0.64
2:L:2978:LYS:HE2	2:L:2981:TRP:HA	1.79	0.63
2:C:1737:ASN:HA	2:C:1740:VAL:HG22	1.80	0.63
2:C:3871:PHE:HA	2:C:3874:ARG:HH22	1.62	0.63
2:C:897:PRO:HA	2:C:902:LYS:HG3	1.78	0.63
2:C:1767:CYS:HB2	2:C:1815:THR:HB	1.80	0.63
2:C:2448:PRO:HB3	2:C:2451:LEU:HD12	1.79	0.63
2:L:1864:ASP:O	2:L:1868:THR:HG23	1.98	0.63
2:C:176:GLU:HG2	2:C:225:LYS:HB3	1.80	0.63
2:C:1742:CYS:O	2:C:1745:LYS:HG2	1.99	0.63
2:C:2359:LYS:HG2	2:C:2361:ILE:H	1.63	0.63
2:C:2578:GLU:N	2:C:2784:GLN:HE22	1.97	0.63
2:C:3278:GLN:HG3	2:C:3282:ARG:HH12	1.64	0.63
2:L:1742:CYS:O	2:L:1745:LYS:HG2	1.99	0.63
2:L:3588:TRP:HD1	2:L:3610:TYR:HH	1.46	0.63
2:L:3842:TRP:HA	2:L:3845:LYS:HB2	1.81	0.63
2:C:3871:PHE:HA	2:C:3874:ARG:NH2	2.14	0.63
2:L:3169:PRO:HG2	2:L:3179:TRP:CE3	2.33	0.63
2:C:1537:VAL:HA	2:C:1554:SER:HA	1.80	0.63
2:L:485:GLN:HB3	2:L:489:ARG:NH2	2.14	0.63
2:L:2343:GLU:O	2:L:2347:LYS:HG2	1.99	0.63
2:L:2826:LEU:O	2:L:2829:LYS:NZ	2.32	0.63
2:L:3302:LYS:HE2	2:L:3355:LYS:HE2	1.79	0.63
2:C:3842:TRP:HA	2:C:3845:LYS:HB2	1.81	0.63
2:L:1767:CYS:HB2	2:L:1815:THR:HB	1.81	0.63
2:L:2844:LEU:HD21	2:L:2858:ILE:HG21	1.80	0.63
2:L:3828:TYR:OH	2:L:4127:TRP:NE1	2.32	0.63
2:C:1177:GLY:HA2	2:C:1184:ARG:HH22	1.63	0.63
2:L:2359:LYS:HG2	2:L:2361:ILE:H	1.63	0.62
2:L:2448:PRO:HB3	2:L:2451:LEU:HD12	1.80	0.62
2:L:3084:GLN:HE21	2:L:3135:LEU:HD12	1.64	0.62
2:C:889:GLU:OE1	2:C:891:ARG:HB2	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1061:LYS:HA	2:C:1064:TYR:HD2	1.64	0.62
2:C:2826:LEU:O	2:C:2829:LYS:NZ	2.32	0.62
2:L:1061:LYS:HA	2:L:1064:TYR:HD2	1.64	0.62
2:C:1532:LEU:HD22	2:C:1559:PHE:HD2	1.64	0.62
2:L:3871:PHE:HA	2:L:3874:ARG:NH2	2.14	0.62
2:C:2343:GLU:O	2:C:2347:LYS:HG2	1.99	0.62
2:C:3137:GLU:OE2	2:C:3167:ARG:NH1	2.32	0.62
2:L:3726:VAL:HB	2:L:3736:LYS:HZ1	1.64	0.62
2:C:714:VAL:HA	2:C:717:LYS:HG2	1.82	0.62
2:C:3169:PRO:HG2	2:C:3179:TRP:CE3	2.33	0.62
2:L:889:GLU:OE1	2:L:891:ARG:HB2	1.99	0.62
2:L:2575:PRO:HB2	2:L:2784:GLN:HE21	1.64	0.62
2:L:1177:GLY:HA2	2:L:1184:ARG:HH22	1.63	0.62
2:C:1864:ASP:O	2:C:1868:THR:HG23	1.98	0.62
2:L:770:LEU:HD13	2:L:773:LEU:HD12	1.82	0.62
2:C:1776:GLU:HG3	2:C:1777:LEU:HD12	1.81	0.62
2:C:3612:ARG:NE	2:C:3799:ARG:HH22	1.97	0.62
2:L:3048:LYS:HE3	2:L:3061:LEU:HB2	1.80	0.62
2:L:1776:GLU:HG3	2:L:1777:LEU:HD12	1.81	0.62
2:L:3137:GLU:OE2	2:L:3167:ARG:NH1	2.32	0.62
2:L:3612:ARG:NE	2:L:3799:ARG:HH22	1.97	0.62
2:C:485:GLN:HB3	2:C:489:ARG:NH2	2.14	0.62
2:C:2844:LEU:HD21	2:C:2858:ILE:HG21	1.80	0.62
2:L:2578:GLU:H	2:L:2784:GLN:HE22	1.47	0.61
2:C:770:LEU:HD13	2:C:773:LEU:HD12	1.82	0.61
2:L:1532:LEU:HD22	2:L:1559:PHE:HD2	1.64	0.61
2:C:2575:PRO:HB2	2:C:2784:GLN:HE21	1.64	0.61
2:L:2138:VAL:O	2:L:2143:ARG:NH1	2.27	0.61
2:C:464:VAL:O	2:C:468:LEU:HG	2.00	0.61
2:C:2322:VAL:HG13	2:C:2325:LEU:HD12	1.83	0.61
2:L:176:GLU:HG2	2:L:225:LYS:HB3	1.80	0.61
2:L:464:VAL:O	2:L:468:LEU:HG	2.00	0.61
2:L:1715:GLU:OE1	2:L:1715:GLU:N	2.30	0.61
2:L:3264:LYS:HA	2:L:3267:LYS:HD3	1.82	0.61
2:L:3278:GLN:HG3	2:L:3282:ARG:HH12	1.64	0.61
2:C:3828:TYR:OH	2:C:4127:TRP:NE1	2.32	0.61
2:L:2322:VAL:HG13	2:L:2325:LEU:HD12	1.83	0.61
2:L:3923:ARG:HA	2:L:3927:ASN:HD22	1.66	0.61
2:C:3183:ILE:HG23	2:C:3238:MET:SD	2.40	0.61
2:C:2588:GLU:OE2	2:C:2775:TYR:OH	2.15	0.61
2:L:2588:GLU:OE2	2:L:2775:TYR:OH	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3633:ILE:HG23	2:C:3637:GLY:HA3	1.83	0.61
2:C:4036:LYS:HE2	2:C:4068:HIS:CD2	2.36	0.61
2:L:714:VAL:HA	2:L:717:LYS:HG2	1.82	0.61
2:C:3084:GLN:HE21	2:C:3135:LEU:HD12	1.64	0.61
2:L:1167:ASP:OD1	2:L:1168:LEU:N	2.34	0.61
2:L:1593:VAL:HA	2:L:1596:VAL:HG22	1.82	0.61
2:L:2578:GLU:N	2:L:2784:GLN:HE22	1.97	0.61
2:C:2578:GLU:H	2:C:2784:GLN:HE22	1.47	0.61
2:C:3719:ILE:HD11	2:C:3740:ILE:HB	1.83	0.61
2:L:585:ILE:HA	2:L:613:HIS:H	1.66	0.60
2:L:2267:SER:HB3	2:L:2309:PHE:CE1	2.36	0.60
2:L:3183:ILE:HG23	2:L:3238:MET:SD	2.40	0.60
2:C:848:LEU:HD13	2:C:851:ILE:HD11	1.82	0.60
2:C:3923:ARG:HA	2:C:3927:ASN:HD22	1.66	0.60
2:L:27:ALA:N	2:C:76:ILE:CD1	2.64	0.60
2:L:2504:ASP:O	2:L:2508:GLN:NE2	2.34	0.60
2:L:2873:PRO:HD3	2:L:2922:ARG:HH22	1.66	0.60
2:C:866:ILE:O	2:C:869:ASN:ND2	2.32	0.60
2:C:1185:HIS:O	2:C:1188:ILE:HG12	2.02	0.60
2:C:2267:SER:HB3	2:C:2309:PHE:CE1	2.36	0.60
2:L:3007:GLU:HB3	2:L:3257:LYS:HZ2	1.67	0.60
2:C:1104:LEU:HD11	2:C:1131:ILE:HA	1.83	0.60
2:C:1167:ASP:OD1	2:C:1168:LEU:N	2.34	0.60
2:C:3264:LYS:HA	2:C:3267:LYS:HD3	1.82	0.60
2:L:1064:TYR:CD1	2:L:1106:ILE:HD11	2.37	0.60
2:L:2427:ARG:HG2	2:L:2431:ARG:HD2	1.83	0.60
2:C:394:GLN:HG3	2:C:397:LEU:HD12	1.83	0.60
2:C:585:ILE:HA	2:C:613:HIS:H	1.66	0.60
2:C:1960:LYS:HG3	2:C:1965:PHE:HB3	1.84	0.60
2:L:2894:GLU:HG3	2:L:3973:PRO:HG2	1.84	0.60
2:L:3719:ILE:HD11	2:L:3740:ILE:HB	1.83	0.60
2:L:4036:LYS:HE2	2:L:4068:HIS:CD2	2.36	0.60
2:C:1427:SER:O	2:C:1431:LEU:N	2.21	0.60
2:L:632:GLU:OE1	2:L:632:GLU:N	2.25	0.60
2:L:892:LEU:HD13	2:L:941:MET:HG3	1.84	0.60
2:L:1013:ILE:O	2:L:1017:ILE:HG13	2.02	0.60
2:L:2517:LEU:HD23	2:L:2520:ILE:HD12	1.84	0.60
2:L:2936:TYR:HB3	2:L:2940:ARG:NH2	2.17	0.60
2:L:3964:THR:HG22	2:L:4117:LEU:HD22	1.84	0.60
2:C:1592:MET:O	2:C:1596:VAL:HG13	2.02	0.60
2:C:1593:VAL:HA	2:C:1596:VAL:HG22	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2958:LEU:HD11	2:C:4101:GLU:HG3	1.83	0.60
2:C:3447:VAL:O	2:C:3451:LEU:HG	2.02	0.60
2:L:27:ALA:CA	2:C:76:ILE:HD11	2.31	0.60
2:L:399:GLN:HB2	2:L:402:THR:HB	1.84	0.60
2:L:2350:LYS:HZ1	2:C:162:LEU:HD13	1.65	0.60
2:L:2958:LEU:HD11	2:L:4101:GLU:HG3	1.83	0.60
2:C:399:GLN:HB2	2:C:402:THR:HB	1.84	0.60
2:C:2091:HIS:CE1	2:C:2093:CYS:HG	2.19	0.60
2:C:3814:ASP:OD1	2:C:3818:ASN:ND2	2.35	0.60
2:C:3964:THR:HG22	2:C:4117:LEU:HD22	1.84	0.60
2:L:1564:SER:OG	2:L:1567:ILE:HD12	2.02	0.59
2:L:2575:PRO:HB2	2:L:2784:GLN:NE2	2.18	0.59
2:L:2855:VAL:O	2:L:2858:ILE:HG22	2.02	0.59
2:L:3633:ILE:HG23	2:L:3637:GLY:HA3	1.83	0.59
2:L:3814:ASP:OD1	2:L:3818:ASN:ND2	2.35	0.59
2:C:1013:ILE:O	2:C:1017:ILE:HG13	2.02	0.59
2:C:1064:TYR:CD1	2:C:1106:ILE:HD11	2.37	0.59
2:C:1715:GLU:OE1	2:C:1715:GLU:N	2.30	0.59
2:L:1820:VAL:O	2:L:1825:LEU:HD23	2.02	0.59
2:C:417:VAL:HA	2:C:420:VAL:HG12	1.85	0.59
2:C:1346:THR:O	2:C:1350:ASN:ND2	2.35	0.59
2:C:1718:ILE:O	2:C:1722:PHE:N	2.18	0.59
2:C:3183:ILE:HG13	2:C:3242:MET:SD	2.42	0.59
2:L:1185:HIS:O	2:L:1188:ILE:HG12	2.02	0.59
2:C:1750:LEU:HD22	2:C:1762:MET:HE3	1.84	0.59
2:C:2575:PRO:HB2	2:C:2784:GLN:NE2	2.18	0.59
2:L:2877:SER:O	2:L:2881:LEU:HD12	2.03	0.59
2:C:938:VAL:HA	2:C:941:MET:HE1	1.84	0.59
2:C:2855:VAL:O	2:C:2858:ILE:HG22	2.02	0.59
2:C:892:LEU:HD13	2:C:941:MET:HG3	1.84	0.59
2:C:1564:SER:OG	2:C:1567:ILE:HD12	2.02	0.59
2:C:1820:VAL:O	2:C:1825:LEU:HD23	2.02	0.59
2:L:1104:LEU:HD11	2:L:1131:ILE:HA	1.83	0.59
2:C:2427:ARG:HG2	2:C:2431:ARG:HD2	1.83	0.59
2:L:848:LEU:HD13	2:L:851:ILE:HD11	1.82	0.59
2:C:241:ASP:HA	2:C:245:SER:HB2	1.85	0.59
2:C:3094:ASP:OD1	2:C:3192:LYS:NZ	2.31	0.59
1:R:6016:UNK:O	1:R:6018:UNK:N	2.32	0.59
2:L:417:VAL:HA	2:L:420:VAL:HG12	1.85	0.59
2:L:2897:LEU:HD23	2:L:3973:PRO:HB3	1.85	0.59
2:C:2873:PRO:HD3	2:C:2922:ARG:HH22	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2894:GLU:HG3	2:C:3973:PRO:HG2	1.84	0.59
2:L:394:GLN:HG3	2:L:397:LEU:HD12	1.83	0.59
2:L:3183:ILE:HG13	2:L:3242:MET:SD	2.42	0.59
2:L:3620:PRO:HD3	2:L:3638:LYS:HD3	1.84	0.59
2:C:1805:PHE:CE2	2:C:1820:VAL:HG13	2.38	0.59
2:C:2091:HIS:ND1	2:C:2093:CYS:SG	2.75	0.59
2:L:1592:MET:O	2:L:1596:VAL:HG13	2.02	0.59
2:L:1805:PHE:CE2	2:L:1820:VAL:HG13	2.38	0.59
2:C:2897:LEU:HD23	2:C:3973:PRO:HB3	1.85	0.59
2:L:1198:LEU:HG	2:L:1200:GLY:H	1.68	0.58
2:L:1960:LYS:HG3	2:L:1965:PHE:HB3	1.84	0.58
2:L:3447:VAL:O	2:L:3451:LEU:HG	2.02	0.58
2:L:3503:VAL:HA	2:L:3506:LEU:HD13	1.85	0.58
2:C:2517:LEU:HD23	2:C:2520:ILE:HD12	1.84	0.58
2:C:3293:CYS:O	2:C:3296:GLN:HG3	2.03	0.58
2:L:4060:THR:HA	2:L:4063:GLU:OE1	2.03	0.58
2:C:1076:LEU:HD13	2:C:1124:ILE:HD13	1.84	0.58
2:L:1076:LEU:HD13	2:L:1124:ILE:HD13	1.84	0.58
2:L:2806:LYS:HG2	2:L:2857:CYS:HB2	1.85	0.58
2:C:272:LEU:HD13	2:C:311:ALA:HB1	1.86	0.58
2:C:2806:LYS:HG2	2:C:2857:CYS:HB2	1.85	0.58
2:C:4060:THR:HA	2:C:4063:GLU:OE1	2.03	0.58
2:L:272:LEU:HD13	2:L:311:ALA:HB1	1.86	0.58
2:C:3130:GLN:HE22	2:C:3175:PRO:HD2	1.69	0.58
2:L:2266:ASN:OD1	2:L:2267:SER:N	2.37	0.58
2:C:2877:SER:O	2:C:2881:LEU:HD12	2.03	0.58
2:L:76:ILE:CD1	2:C:27:ALA:N	2.66	0.58
2:L:1937:ARG:HA	2:L:1940:TYR:CZ	2.38	0.58
2:C:2936:TYR:HB3	2:C:2940:ARG:NH2	2.17	0.58
2:C:3446:VAL:O	2:C:3450:MET:HG3	2.04	0.58
2:L:485:GLN:HB3	2:L:489:ARG:NH1	2.19	0.58
2:C:1937:ARG:HA	2:C:1940:TYR:CZ	2.38	0.58
2:C:2504:ASP:O	2:C:2508:GLN:NE2	2.35	0.58
2:C:3007:GLU:HB3	2:C:3257:LYS:HZ2	1.68	0.58
2:C:3646:LYS:HE2	2:C:3663:THR:HG22	1.85	0.58
2:L:76:ILE:HD11	2:C:27:ALA:CA	2.32	0.58
2:L:997:ASN:HA	2:L:1043:GLN:HG3	1.86	0.58
2:C:3929:MET:HB2	2:C:3938:ILE:HG23	1.85	0.58
2:L:3130:GLN:HE22	2:L:3175:PRO:HD2	1.69	0.58
2:C:663:ILE:HG13	2:C:664:SER:H	1.69	0.58
1:Q:6016:UNK:O	1:Q:6018:UNK:N	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2303:LEU:HD23	2:L:2323:LEU:HD22	1.86	0.57
2:C:1198:LEU:HG	2:C:1200:GLY:H	1.68	0.57
2:L:1268:ASN:HD22	2:L:1340:ARG:NH1	2.02	0.57
2:L:1298:LEU:HD22	2:L:1371:VAL:HG11	1.87	0.57
2:C:485:GLN:HB3	2:C:489:ARG:NH1	2.19	0.57
2:C:3503:VAL:HA	2:C:3506:LEU:HD13	1.85	0.57
2:L:663:ILE:HG13	2:L:664:SER:H	1.69	0.57
2:L:3293:CYS:O	2:L:3296:GLN:HG3	2.03	0.57
2:C:3577:GLN:HB2	2:C:3630:ARG:HD3	1.86	0.57
2:L:241:ASP:HA	2:L:245:SER:HB2	1.85	0.57
2:C:1134:LEU:HA	2:C:1137:ILE:HD13	1.87	0.57
2:C:1268:ASN:HD22	2:C:1340:ARG:NH1	2.02	0.57
2:C:2266:ASN:OD1	2:C:2267:SER:N	2.37	0.57
2:C:3159:ARG:O	2:C:3163:THR:HG23	2.04	0.57
2:C:3620:PRO:HD3	2:C:3638:LYS:HD3	1.84	0.57
2:L:179:GLY:HA3	2:L:226:GLY:HA2	1.85	0.57
2:L:3929:MET:HB2	2:L:3938:ILE:HG23	1.85	0.57
2:L:928:VAL:HA	2:L:931:CYS:SG	2.45	0.57
2:L:3341:LEU:HD22	2:L:3373:VAL:HG21	1.86	0.57
2:L:3446:VAL:O	2:L:3450:MET:HG3	2.04	0.57
2:C:736:LEU:HD12	2:C:740:ILE:HG13	1.86	0.57
2:C:1298:LEU:HD22	2:C:1371:VAL:HG11	1.86	0.57
2:C:1338:VAL:O	2:C:1342:MET:HG2	2.04	0.57
2:C:2303:LEU:HD23	2:C:2323:LEU:HD22	1.86	0.57
2:C:3341:LEU:HD22	2:C:3373:VAL:HG21	1.86	0.57
2:L:1155:ARG:HD2	2:L:1157:PHE:H	1.70	0.57
2:L:3646:LYS:HE2	2:L:3663:THR:HG22	1.85	0.57
2:L:3887:PHE:HA	2:L:3890:MET:HE3	1.87	0.57
2:C:183:GLU:OE1	2:C:273:ARG:NH1	2.38	0.57
2:C:997:ASN:HA	2:C:1043:GLN:HG3	1.86	0.57
2:C:1685:ASP:HB3	2:C:1688:LEU:HD13	1.87	0.57
2:L:3159:ARG:O	2:L:3163:THR:HG23	2.04	0.57
2:L:3577:GLN:HB2	2:L:3630:ARG:HD3	1.86	0.57
2:L:3924:HIS:HD2	2:L:3926:ASN:HB2	1.70	0.57
2:C:928:VAL:HA	2:C:931:CYS:SG	2.45	0.57
2:L:1685:ASP:HB3	2:L:1688:LEU:HD13	1.87	0.56
2:C:447:PRO:HG2	2:C:527:TYR:CE1	2.40	0.56
2:L:2577:PHE:H	2:L:2784:GLN:NE2	2.04	0.56
2:L:1338:VAL:O	2:L:1342:MET:HG2	2.04	0.56
2:L:1915:LEU:HD13	2:L:1951:VAL:HG21	1.88	0.56
2:L:2425:ARG:HB2	2:L:2464:HIS:CE1	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:179:GLY:HA3	2:C:226:GLY:HA2	1.85	0.56
2:C:859:LEU:O	2:C:867:ASN:ND2	2.38	0.56
2:C:3887:PHE:HA	2:C:3890:MET:HE3	1.87	0.56
2:L:1750:LEU:HD22	2:L:1762:MET:CE	2.35	0.56
2:L:3701:ILE:HD11	2:L:3750:PHE:HE2	1.70	0.56
2:L:859:LEU:O	2:L:867:ASN:ND2	2.38	0.56
2:C:1750:LEU:HD22	2:C:1762:MET:CE	2.35	0.56
2:C:4039:TYR:CE2	2:C:4041:ARG:HB2	2.40	0.56
2:L:4098:LEU:HB2	2:L:4103:GLN:OE1	2.06	0.56
2:C:1794:GLN:HE22	2:C:1833:LEU:HD13	1.70	0.56
2:C:3610:TYR:HE1	2:C:3612:ARG:CZ	2.19	0.56
2:C:3632:PHE:HZ	2:C:3675:LYS:HB2	1.70	0.56
2:C:4098:LEU:HB2	2:C:4103:GLN:OE1	2.06	0.56
2:L:183:GLU:OE1	2:L:273:ARG:NH1	2.38	0.56
2:L:1794:GLN:HE22	2:L:1833:LEU:HD13	1.70	0.56
2:L:3094:ASP:OD1	2:L:3192:LYS:NZ	2.31	0.56
2:L:4039:TYR:CE2	2:L:4041:ARG:HB2	2.40	0.56
2:C:913:ARG:NH2	2:C:916:GLU:OE1	2.39	0.56
2:C:4125:GLU:HG3	2:C:4127:TRP:CE2	2.41	0.56
2:L:52:ALA:HB2	2:L:99:LYS:HE3	1.88	0.56
2:L:1743:MET:HA	2:L:1746:PHE:HD1	1.70	0.56
2:L:3610:TYR:HE1	2:L:3612:ARG:CZ	2.19	0.56
2:C:1915:LEU:HD13	2:C:1951:VAL:HG21	1.88	0.56
2:C:3447:VAL:HB	2:C:3485:LYS:NZ	2.21	0.56
2:L:260:ILE:HG23	2:L:262:LEU:H	1.71	0.56
2:L:1348:LEU:HD21	2:L:1359:LEU:HD21	1.87	0.56
2:L:1928:ALA:O	2:L:1937:ARG:NH2	2.33	0.56
2:L:3629:ARG:NH2	2:L:3630:ARG:O	2.38	0.56
2:C:1191:PHE:O	2:C:1195:VAL:HG13	2.06	0.56
2:C:2425:ARG:HB2	2:C:2464:HIS:CE1	2.41	0.56
2:C:3949:ALA:HA	2:C:4020:MET:HE3	1.88	0.56
2:L:399:GLN:OE1	2:L:406:ARG:NH1	2.39	0.56
2:L:447:PRO:HG2	2:L:527:TYR:CE1	2.40	0.56
2:L:630:CYS:HB2	2:L:634:LEU:HD23	1.88	0.56
2:L:913:ARG:HH11	2:L:2803:ILE:HD13	1.71	0.56
2:L:3424:LEU:O	2:L:3427:GLU:N	2.39	0.56
2:C:52:ALA:HB2	2:C:99:LYS:HE3	1.88	0.56
2:C:399:GLN:OE1	2:C:406:ARG:NH1	2.39	0.56
2:C:2402:LEU:O	2:C:2404:ARG:NH2	2.39	0.56
2:C:2577:PHE:H	2:C:2784:GLN:NE2	2.04	0.56
2:C:3629:ARG:NH2	2:C:3630:ARG:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3701:ILE:HD11	2:C:3750:PHE:HE2	1.70	0.56
2:L:736:LEU:HD12	2:L:740:ILE:HG13	1.86	0.55
2:L:913:ARG:NH2	2:L:916:GLU:OE1	2.39	0.55
2:C:1348:LEU:HD21	2:C:1359:LEU:HD21	1.87	0.55
2:C:3085:GLU:OE1	2:C:3085:GLU:N	2.32	0.55
2:L:3093:GLN:NE2	2:C:2492:ASP:HB2	2.21	0.55
2:L:3632:PHE:HZ	2:L:3675:LYS:HB2	1.70	0.55
2:C:260:ILE:HG23	2:C:262:LEU:H	1.71	0.55
2:L:1134:LEU:HA	2:L:1137:ILE:HD13	1.87	0.55
2:L:2402:LEU:O	2:L:2404:ARG:NH2	2.39	0.55
2:L:3447:VAL:HB	2:L:3485:LYS:NZ	2.21	0.55
2:C:1188:ILE:HD12	2:C:1269:THR:HG21	1.89	0.55
2:L:776:TRP:HB3	2:L:785:MET:HE1	1.88	0.55
2:L:1188:ILE:HD12	2:L:1269:THR:HG21	1.89	0.55
2:L:3271:ASP:OD1	2:L:3271:ASP:N	2.38	0.55
2:C:630:CYS:HB2	2:C:634:LEU:HD23	1.88	0.55
2:C:913:ARG:HH11	2:C:2803:ILE:HD13	1.71	0.55
2:C:1743:MET:HA	2:C:1746:PHE:HD1	1.71	0.55
2:C:1928:ALA:O	2:C:1937:ARG:NH2	2.33	0.55
2:C:3187:CYS:SG	2:C:3235:LYS:NZ	2.66	0.55
2:C:3334:TYR:HA	2:C:3337:ILE:HD12	1.88	0.55
2:C:3924:HIS:HD2	2:C:3926:ASN:HB2	1.70	0.55
2:C:3758:LEU:HD22	2:C:3803:ILE:HD11	1.89	0.55
2:L:938:VAL:HA	2:L:941:MET:HE1	1.88	0.55
2:L:1004:GLN:OE1	2:L:1004:GLN:N	2.26	0.55
2:L:2205:VAL:HG13	2:L:2208:ASP:HB2	1.89	0.55
2:C:439:VAL:O	2:C:443:ILE:HD12	2.07	0.55
2:C:752:LEU:HG	2:C:756:PHE:HE1	1.71	0.55
2:C:3424:LEU:O	2:C:3427:GLU:N	2.39	0.55
2:C:3761:ASP:HA	2:C:3764:VAL:HG12	1.88	0.55
2:C:3837:CYS:SG	2:C:3838:GLU:N	2.80	0.55
2:C:3885:ARG:O	2:C:3889:ARG:HG3	2.07	0.55
2:L:866:ILE:O	2:L:869:ASN:ND2	2.32	0.55
2:L:1191:PHE:O	2:L:1195:VAL:HG13	2.06	0.55
2:L:2929:LEU:O	2:L:2932:SER:OG	2.18	0.55
2:L:3179:TRP:O	2:L:3183:ILE:HG12	2.07	0.55
2:L:3949:ALA:HA	2:L:4020:MET:HE3	1.89	0.55
2:C:1155:ARG:HD2	2:C:1157:PHE:H	1.70	0.55
2:C:1515:LEU:HB2	2:C:1519:PHE:CE2	2.42	0.55
2:C:1839:PHE:O	2:C:1843:ILE:HG12	2.07	0.55
2:C:2930:TYR:HA	2:C:2933:ILE:HG22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3334:TYR:HA	2:L:3337:ILE:HD12	1.88	0.55
2:L:3758:LEU:HD22	2:L:3803:ILE:HD11	1.89	0.55
2:L:4125:GLU:HG3	2:L:4127:TRP:CE2	2.41	0.55
2:C:931:CYS:HB2	2:C:984:TYR:HE2	1.72	0.55
2:C:3612:ARG:HG3	2:C:3799:ARG:HH12	1.72	0.55
2:C:3858:MET:SD	2:C:4119:ARG:HB2	2.47	0.55
2:L:1346:THR:O	2:L:1350:ASN:ND2	2.35	0.54
2:L:2091:HIS:ND1	2:L:2093:CYS:SG	2.75	0.54
2:L:2930:TYR:HA	2:L:2933:ILE:HG22	1.88	0.54
2:L:3885:ARG:O	2:L:3889:ARG:HG3	2.07	0.54
2:L:4089:ILE:HA	2:L:4092:GLN:HG3	1.89	0.54
2:C:132:ILE:HA	2:C:135:LEU:HD12	1.89	0.54
2:C:1775:GLU:O	2:C:1779:GLN:HG2	2.07	0.54
2:C:1951:VAL:HG13	2:C:1955:VAL:HG11	1.89	0.54
2:C:2929:LEU:O	2:C:2932:SER:OG	2.18	0.54
2:L:644:PRO:HG2	2:L:645:TRP:CD1	2.42	0.54
2:L:1515:LEU:HB2	2:L:1519:PHE:CE2	2.42	0.54
2:L:4056:PRO:HB2	2:L:4090:ARG:HH12	1.72	0.54
2:C:27:ALA:HB3	2:C:30:ALA:HB2	1.89	0.54
2:L:931:CYS:HB2	2:L:984:TYR:HE2	1.72	0.54
2:C:933:LEU:HD22	2:C:2797:VAL:HG21	1.89	0.54
2:L:1775:GLU:O	2:L:1779:GLN:HG2	2.07	0.54
2:C:1820:VAL:HG12	2:C:1824:LEU:HD12	1.89	0.54
2:C:2205:VAL:HG13	2:C:2208:ASP:HB2	1.89	0.54
2:L:1579:VAL:HG23	2:L:1580:LEU:HD23	1.89	0.54
2:L:1935:GLU:O	2:L:1938:ARG:HG2	2.08	0.54
2:L:3612:ARG:CZ	2:L:3799:ARG:HH22	2.21	0.54
2:C:3172:LYS:O	2:C:3783:GLN:NE2	2.40	0.54
2:L:877:ASP:OD1	2:L:3903:HIS:NE2	2.40	0.54
2:L:1491:ILE:HG23	2:L:1493:PRO:HD3	1.89	0.54
2:C:644:PRO:HG2	2:C:645:TRP:CD1	2.42	0.54
2:L:2216:LEU:HD21	2:L:2241:LEU:HD22	1.90	0.54
2:L:2513:GLU:OE2	2:L:2514:ASN:ND2	2.41	0.54
2:L:3612:ARG:HG3	2:L:3799:ARG:HH12	1.72	0.54
2:C:1261:LEU:HD11	2:C:1340:ARG:HB2	1.90	0.54
2:C:3179:TRP:O	2:C:3183:ILE:HG12	2.07	0.54
2:L:439:VAL:O	2:L:443:ILE:HD12	2.07	0.54
2:L:3156:PRO:HA	2:L:3159:ARG:HE	1.73	0.54
2:L:3416:LEU:HD12	2:L:3419:PHE:HE1	1.73	0.54
2:L:3837:CYS:SG	2:L:3838:GLU:N	2.80	0.54
2:L:3858:MET:SD	2:L:4119:ARG:HB2	2.47	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3471:ILE:HG12	2:C:3474:ARG:HH22	1.73	0.54
2:L:132:ILE:HA	2:L:135:LEU:HD12	1.89	0.54
2:L:162:LEU:HD13	2:C:2350:LYS:HZ1	1.72	0.54
2:L:1605:PHE:O	2:L:1608:ARG:NH2	2.41	0.54
2:L:1781:SER:O	2:L:1785:ILE:HG13	2.07	0.54
2:L:1839:PHE:O	2:L:1843:ILE:HG12	2.07	0.54
2:L:2492:ASP:HB2	2:C:3093:GLN:NE2	2.23	0.54
2:L:3065:ILE:HD13	2:L:3089:LEU:HD23	1.90	0.54
2:L:3172:LYS:O	2:L:3783:GLN:NE2	2.40	0.54
2:L:3761:ASP:HA	2:L:3764:VAL:HG12	1.88	0.54
2:C:1605:PHE:O	2:C:1608:ARG:NH2	2.41	0.54
2:C:3416:LEU:HD12	2:C:3419:PHE:HE1	1.73	0.54
2:C:4089:ILE:HA	2:C:4092:GLN:HG3	1.89	0.54
2:L:76:ILE:CG1	2:C:26:GLY:O	2.55	0.54
2:C:877:ASP:OD1	2:C:3903:HIS:NE2	2.40	0.54
2:C:897:PRO:HD2	2:C:2566:THR:HG23	1.90	0.54
2:C:1069:HIS:HD2	2:C:3741:ARG:CZ	2.21	0.54
2:C:1935:GLU:O	2:C:1938:ARG:HG2	2.08	0.54
2:C:3666:LEU:HA	2:C:3669:LYS:HB2	1.90	0.54
2:L:1951:VAL:HG13	2:L:1955:VAL:HG11	1.89	0.53
2:L:752:LEU:HG	2:L:756:PHE:HE1	1.71	0.53
2:L:3700:GLU:HA	2:L:3718:ARG:HA	1.90	0.53
2:C:453:MET:HA	2:C:456:VAL:HG12	1.91	0.53
2:C:575:ILE:O	2:C:579:LEU:HG	2.09	0.53
2:C:1014:LEU:HD23	2:C:1017:ILE:HD12	1.90	0.53
2:C:4056:PRO:HB2	2:C:4090:ARG:HH12	1.72	0.53
2:L:27:ALA:HB3	2:L:30:ALA:HB2	1.89	0.53
2:L:699:GLU:OE1	2:L:699:GLU:N	2.42	0.53
2:L:1014:LEU:HD23	2:L:1017:ILE:HD12	1.90	0.53
2:C:3271:ASP:N	2:C:3271:ASP:OD1	2.38	0.53
2:L:26:GLY:CA	2:C:76:ILE:HD12	2.39	0.53
2:L:714:VAL:HG11	2:L:732:PHE:HE2	1.72	0.53
2:L:3471:ILE:HA	2:L:3474:ARG:NH2	2.23	0.53
2:L:3471:ILE:HG12	2:L:3474:ARG:HH22	1.73	0.53
2:L:4068:HIS:O	2:L:4069:GLU:HG3	2.09	0.53
2:C:714:VAL:HG11	2:C:732:PHE:HE2	1.72	0.53
2:C:1579:VAL:HG23	2:C:1580:LEU:HD23	1.89	0.53
2:C:3471:ILE:HA	2:C:3474:ARG:NH2	2.23	0.53
2:L:575:ILE:O	2:L:579:LEU:HG	2.09	0.53
2:C:651:TYR:O	2:C:655:LEU:HG	2.09	0.53
2:C:1037:LEU:HD23	2:C:1085:ILE:HG23	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1781:SER:O	2:C:1785:ILE:HG13	2.07	0.53
2:C:4068:HIS:O	2:C:4069:GLU:HG3	2.09	0.53
2:L:342:MET:HG3	2:L:343:GLU:OE1	2.09	0.53
2:L:752:LEU:HD23	2:L:792:ILE:HD12	1.91	0.53
2:L:889:GLU:HA	2:L:3889:ARG:HH11	1.74	0.53
2:L:1679:LEU:HG	2:L:1717:LEU:HD11	1.91	0.53
2:L:1874:TYR:CD2	2:L:1944:ALA:HA	2.44	0.53
2:L:2461:PHE:HA	2:L:2464:HIS:HB3	1.91	0.53
2:L:3666:LEU:HA	2:L:3669:LYS:HB2	1.90	0.53
2:C:3612:ARG:CZ	2:C:3799:ARG:HH22	2.20	0.53
2:C:3700:GLU:HA	2:C:3718:ARG:HA	1.90	0.53
2:L:651:TYR:O	2:L:655:LEU:HG	2.09	0.53
2:L:933:LEU:HD22	2:L:2797:VAL:HG21	1.89	0.53
2:L:2435:CYS:HA	2:L:2438:ILE:HD12	1.90	0.53
2:L:4045:CYS:HA	2:L:4048:LYS:NZ	2.24	0.53
2:C:3744:ASP:OD1	2:C:3745:GLU:N	2.42	0.53
2:L:453:MET:HA	2:L:456:VAL:HG12	1.91	0.53
2:C:752:LEU:HD23	2:C:792:ILE:HD12	1.90	0.53
2:C:1491:ILE:HG23	2:C:1493:PRO:HD3	1.89	0.53
2:C:2513:GLU:OE2	2:C:2514:ASN:ND2	2.41	0.53
2:L:26:GLY:O	2:C:76:ILE:CG1	2.54	0.53
2:L:1069:HIS:HD2	2:L:3741:ARG:CZ	2.21	0.53
2:L:2327:LEU:HD23	2:L:2371:PHE:HB3	1.91	0.53
2:C:1004:GLN:OE1	2:C:1004:GLN:N	2.26	0.53
2:L:1037:LEU:HD23	2:L:1085:ILE:HG23	1.91	0.52
2:L:1261:LEU:HD11	2:L:1340:ARG:HB2	1.90	0.52
2:L:1266:CYS:O	2:L:1269:THR:HG22	2.10	0.52
2:L:1874:TYR:HD2	2:L:1944:ALA:HA	1.74	0.52
2:L:2321:GLU:HG3	2:L:2366:LYS:HD2	1.91	0.52
2:L:3374:ILE:HB	2:L:3378:TYR:CE2	2.44	0.52
2:C:466:LEU:HB2	2:C:560:LEU:HD12	1.91	0.52
2:C:889:GLU:HA	2:C:3889:ARG:HH11	1.74	0.52
2:C:3156:PRO:HA	2:C:3159:ARG:HE	1.73	0.52
2:C:3374:ILE:HB	2:C:3378:TYR:CE2	2.44	0.52
2:L:770:LEU:O	2:L:854:ARG:NH1	2.43	0.52
2:L:2376:ASP:OD1	2:L:2376:ASP:N	2.42	0.52
2:L:3141:PHE:O	2:L:3145:ILE:HG12	2.10	0.52
2:C:1679:LEU:HG	2:C:1717:LEU:HD11	1.91	0.52
2:C:3558:ILE:O	2:C:3562:LEU:N	2.42	0.52
2:C:3798:SER:C	2:C:3799:ARG:HD3	2.30	0.52
2:C:4045:CYS:HA	2:C:4048:LYS:NZ	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3275:SER:O	2:L:3278:GLN:HG2	2.10	0.52
2:C:183:GLU:HA	2:C:232:CYS:SG	2.49	0.52
2:C:2216:LEU:HD21	2:C:2241:LEU:HD22	1.90	0.52
2:C:2327:LEU:HD23	2:C:2371:PHE:HB3	1.90	0.52
2:C:2376:ASP:N	2:C:2376:ASP:OD1	2.42	0.52
2:C:3236:PHE:O	2:C:3240:MET:HG2	2.10	0.52
2:C:3919:GLY:O	2:C:3946:PHE:N	2.42	0.52
2:C:3948:SER:HB2	2:C:4016:PHE:CZ	2.45	0.52
2:L:421:LEU:HG	2:L:464:VAL:HG13	1.92	0.52
2:L:1820:VAL:HG12	2:L:1824:LEU:HD12	1.89	0.52
2:L:2895:GLU:HA	2:L:2898:LEU:HD13	1.92	0.52
2:L:3558:ILE:O	2:L:3562:LEU:N	2.42	0.52
2:C:38:LEU:HD22	2:C:65:LEU:HD21	1.90	0.52
2:C:352:VAL:HG11	2:C:1733:THR:HG23	1.91	0.52
2:C:770:LEU:O	2:C:854:ARG:NH1	2.42	0.52
2:C:2553:HIS:HB3	2:C:2557:LEU:HD23	1.92	0.52
2:L:774:GLU:O	2:L:778:ILE:HG12	2.09	0.52
2:L:3128:LYS:HE2	2:L:3128:LYS:HA	1.92	0.52
2:C:1874:TYR:CD2	2:C:1944:ALA:HA	2.43	0.52
2:L:3294:SER:OG	2:L:3344:GLU:OE1	2.27	0.52
2:L:3744:ASP:OD1	2:L:3745:GLU:N	2.42	0.52
2:C:2586:PHE:HA	2:C:2777:HIS:CD2	2.45	0.52
2:L:897:PRO:HD2	2:L:2566:THR:HG23	1.90	0.52
2:C:774:GLU:O	2:C:778:ILE:HG12	2.09	0.52
2:C:2435:CYS:HA	2:C:2438:ILE:HD12	1.90	0.52
2:C:2461:PHE:HA	2:C:2464:HIS:HB3	1.91	0.52
2:C:2895:GLU:HA	2:C:2898:LEU:HD13	1.91	0.52
2:C:2938:VAL:O	2:C:2942:ILE:HG13	2.10	0.52
2:C:3065:ILE:HD13	2:C:3089:LEU:HD23	1.90	0.52
2:L:3239:LYS:O	2:L:3242:MET:HB3	2.10	0.52
2:C:447:PRO:HG2	2:C:527:TYR:HE1	1.75	0.52
2:C:3141:PHE:O	2:C:3145:ILE:HG12	2.10	0.52
2:C:3275:SER:O	2:C:3278:GLN:HG2	2.10	0.52
2:C:3294:SER:OG	2:C:3344:GLU:OE1	2.27	0.52
2:C:3951:GLN:HB2	2:C:4036:LYS:HZ2	1.75	0.52
2:L:466:LEU:HB2	2:L:560:LEU:HD12	1.91	0.52
2:L:908:ASP:O	2:L:911:LEU:HG	2.10	0.52
2:L:1500:LEU:HD12	2:L:1501:PRO:HD2	1.91	0.52
2:L:1782:PHE:HA	2:L:1785:ILE:HD12	1.91	0.52
2:L:3107:ILE:HD13	2:L:3135:LEU:HD23	1.91	0.52
2:L:3960:PRO:HD2	2:L:4110:GLN:CD	2.30	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:MET:HG3	2:C:343:GLU:OE1	2.09	0.52
2:C:699:GLU:OE1	2:C:699:GLU:N	2.42	0.52
2:C:1009:LEU:O	2:C:1013:ILE:HG12	2.10	0.52
2:C:3128:LYS:HA	2:C:3128:LYS:HE2	1.92	0.52
2:L:3798:SER:C	2:L:3799:ARG:HD3	2.30	0.52
2:C:490:ILE:HG23	2:C:527:TYR:HD2	1.75	0.52
2:C:1500:LEU:HD12	2:C:1501:PRO:HD2	1.91	0.52
2:C:1782:PHE:HA	2:C:1785:ILE:HD12	1.91	0.52
2:L:447:PRO:HG2	2:L:527:TYR:HE1	1.75	0.51
2:L:3919:GLY:O	2:L:3946:PHE:N	2.42	0.51
2:C:1266:CYS:O	2:C:1269:THR:HG22	2.10	0.51
2:C:1439:PRO:O	2:C:1442:GLN:NE2	2.40	0.51
2:C:3239:LYS:O	2:C:3242:MET:HB3	2.10	0.51
2:L:183:GLU:HA	2:L:232:CYS:SG	2.49	0.51
2:L:524:TYR:HA	2:L:527:TYR:CG	2.45	0.51
2:L:2586:PHE:HA	2:L:2777:HIS:CD2	2.45	0.51
2:C:908:ASP:O	2:C:911:LEU:HG	2.10	0.51
2:C:1022:ASP:OD2	2:C:1024:THR:OG1	2.21	0.51
2:C:1874:TYR:HD2	2:C:1944:ALA:HA	1.74	0.51
2:C:2321:GLU:HG3	2:C:2366:LYS:HD2	1.91	0.51
2:C:2813:PHE:CD1	2:C:2817:LEU:HD23	2.46	0.51
2:L:446:PHE:CD1	2:L:530:LEU:HD12	2.46	0.51
2:L:582:THR:HB	2:L:584:GLU:OE1	2.10	0.51
2:L:1427:SER:O	2:L:1431:LEU:N	2.21	0.51
2:L:1757:MET:O	2:L:1760:GLU:HG3	2.11	0.51
2:L:3889:ARG:HH21	2:L:3889:ARG:HG2	1.76	0.51
2:C:440:VAL:HG11	2:C:489:ARG:HH11	1.75	0.51
2:C:446:PHE:CD1	2:C:530:LEU:HD12	2.46	0.51
2:L:287:LEU:HD12	2:L:329:LYS:HE2	1.92	0.51
2:L:440:VAL:CG1	2:L:489:ARG:HH11	2.24	0.51
2:L:3328:ILE:HD11	2:L:3412:ALA:HB2	1.93	0.51
2:L:3681:LYS:HE3	2:L:3724:GLU:HA	1.92	0.51
2:C:287:LEU:HD12	2:C:329:LYS:HE2	1.92	0.51
2:C:414:LEU:HD13	2:C:442:GLN:NE2	2.26	0.51
2:C:1757:MET:O	2:C:1760:GLU:HG3	2.10	0.51
2:C:3681:LYS:HE3	2:C:3724:GLU:HA	1.92	0.51
2:C:3913:ILE:O	2:C:3917:ILE:HG12	2.10	0.51
2:L:38:LEU:HD22	2:L:65:LEU:HD21	1.91	0.51
2:L:414:LEU:HD13	2:L:442:GLN:HE21	1.75	0.51
2:C:3948:SER:HA	2:C:3951:GLN:OE1	2.11	0.51
2:L:352:VAL:HG11	2:L:1733:THR:HG23	1.90	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1009:LEU:O	2:L:1013:ILE:HG12	2.10	0.51
2:L:2553:HIS:HB3	2:L:2557:LEU:HD23	1.92	0.51
2:L:2938:VAL:O	2:L:2942:ILE:HG13	2.10	0.51
2:L:3236:PHE:O	2:L:3240:MET:HG2	2.10	0.51
2:L:3913:ILE:O	2:L:3917:ILE:HG12	2.10	0.51
2:C:405:ASP:O	2:C:408:TYR:N	2.27	0.51
2:C:3475:TYR:N	2:C:3476:PRO:HD2	2.26	0.51
2:C:3880:ALA:HB1	2:C:3969:ASN:HD21	1.76	0.51
2:L:1134:LEU:O	2:L:1138:ILE:HG12	2.11	0.51
2:L:2834:GLN:O	2:L:2837:LEU:HG	2.11	0.51
2:L:3358:ARG:O	2:L:3358:ARG:HD3	2.11	0.51
2:L:3735:PRO:HB2	2:L:3751:LEU:HD11	1.93	0.51
2:L:3948:SER:HB2	2:L:4016:PHE:CZ	2.45	0.51
2:C:414:LEU:HD13	2:C:442:GLN:HE21	1.75	0.51
2:C:440:VAL:CG1	2:C:489:ARG:HH11	2.24	0.51
2:C:2364:LEU:HA	2:C:2367:VAL:HG12	1.93	0.51
2:C:2834:GLN:O	2:C:2837:LEU:HG	2.11	0.51
2:C:3000:ASP:OD1	2:C:3043:TYR:OH	2.20	0.51
2:C:3328:ILE:HD11	2:C:3412:ALA:HB2	1.93	0.51
2:C:3842:TRP:O	2:C:3842:TRP:HD1	1.94	0.51
2:C:3869:THR:HA	2:C:3872:ARG:HG2	1.93	0.51
2:L:3842:TRP:O	2:L:3842:TRP:HD1	1.94	0.51
2:C:1134:LEU:O	2:C:1138:ILE:HG12	2.11	0.51
2:C:1922:ALA:HA	2:C:1925:GLU:HB2	1.93	0.51
2:C:3568:ILE:O	2:C:3572:ILE:HG12	2.10	0.51
2:C:3960:PRO:HD2	2:C:4110:GLN:CD	2.30	0.51
2:L:2813:PHE:CD1	2:L:2817:LEU:HD23	2.46	0.51
2:L:3326:GLN:HA	2:L:3329:LEU:HG	1.93	0.51
2:L:3578:LEU:HD23	2:L:3752:VAL:HG21	1.92	0.51
2:C:421:LEU:HG	2:C:464:VAL:HG13	1.92	0.51
2:C:1270:PHE:HB3	2:C:1276:VAL:HB	1.93	0.51
2:C:1670:GLU:HA	2:C:1673:THR:HG22	1.92	0.51
2:L:490:ILE:HG23	2:L:527:TYR:HD2	1.75	0.51
2:L:1568:ASN:O	2:L:1572:LEU:HG	2.11	0.51
2:L:2418:LYS:O	2:L:2420:PHE:N	2.38	0.51
2:L:3568:ILE:O	2:L:3572:ILE:HG12	2.10	0.51
2:L:3841:ASP:O	2:L:3844:THR:OG1	2.21	0.51
2:L:3880:ALA:HB1	2:L:3969:ASN:HD21	1.76	0.51
2:C:3107:ILE:HD13	2:C:3135:LEU:HD23	1.91	0.51
2:C:3141:PHE:CE1	2:C:3145:ILE:HD11	2.46	0.51
2:L:162:LEU:HD13	2:C:2350:LYS:HZ2	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1270:PHE:HB3	2:L:1276:VAL:HB	1.93	0.50
2:L:1670:GLU:HA	2:L:1673:THR:HG22	1.92	0.50
2:L:3000:ASP:OD1	2:L:3043:TYR:OH	2.20	0.50
2:L:3619:ASP:HB2	2:L:3620:PRO:HD2	1.93	0.50
2:C:1708:GLU:O	2:C:1712:ARG:HG2	2.10	0.50
2:C:3601:VAL:HA	2:C:3604:LYS:HG2	1.93	0.50
2:C:3619:ASP:HB2	2:C:3620:PRO:HD2	1.93	0.50
2:L:115:TYR:O	2:C:2354:ASN:CG	2.50	0.50
2:L:176:GLU:HG3	2:L:222:GLY:HA2	1.93	0.50
2:L:1708:GLU:O	2:L:1712:ARG:HG2	2.10	0.50
2:L:1757:MET:O	2:L:1761:LEU:HG	2.11	0.50
2:L:2364:LEU:HA	2:L:2367:VAL:HG12	1.93	0.50
2:C:524:TYR:HA	2:C:527:TYR:CG	2.45	0.50
2:C:3578:LEU:HD23	2:C:3752:VAL:HG21	1.92	0.50
2:C:3841:ASP:O	2:C:3844:THR:OG1	2.21	0.50
2:L:414:LEU:HD13	2:L:442:GLN:NE2	2.26	0.50
2:L:649:PHE:O	2:L:653:LEU:HD23	2.12	0.50
2:L:734:LEU:HD11	2:L:752:LEU:HD13	1.93	0.50
2:C:3130:GLN:NE2	2:C:3175:PRO:HD2	2.27	0.50
2:C:3822:GLN:O	2:C:3826:ALA:N	2.37	0.50
2:C:3839:TYR:HB3	2:C:4122:GLU:HG3	1.93	0.50
2:L:2359:LYS:HD2	2:L:2361:ILE:HB	1.94	0.50
2:C:582:THR:HB	2:C:584:GLU:OE1	2.10	0.50
2:C:1335:CYS:O	2:C:1339:VAL:HG22	2.12	0.50
2:L:992:ILE:HD11	2:L:1036:PHE:CD1	2.42	0.50
2:L:1005:ASP:OD1	2:L:1006:THR:N	2.45	0.50
2:L:3601:VAL:HA	2:L:3604:LYS:HG2	1.93	0.50
2:C:3944:HIS:HB3	2:C:4016:PHE:HE1	1.76	0.50
2:L:2354:ASN:CG	2:C:115:TYR:O	2.50	0.50
2:L:3951:GLN:HB2	2:L:4036:LYS:HZ2	1.76	0.50
2:C:460:ALA:O	2:C:464:VAL:HG23	2.12	0.50
2:C:3889:ARG:HG2	2:C:3889:ARG:HH21	1.76	0.50
2:L:35:ILE:HG12	2:L:81:CYS:SG	2.52	0.50
2:L:460:ALA:O	2:L:464:VAL:HG23	2.12	0.50
2:L:2828:GLU:O	2:L:2832:ILE:HG12	2.12	0.50
2:L:3141:PHE:CE1	2:L:3145:ILE:HD11	2.46	0.50
2:L:3475:TYR:N	2:L:3476:PRO:HD2	2.26	0.50
2:L:3851:ASP:O	2:L:3855:TYR:N	2.44	0.50
2:C:734:LEU:HD11	2:C:752:LEU:HD13	1.93	0.50
2:C:3446:VAL:HA	2:C:3449:LYS:HE2	1.93	0.50
2:L:1560:TYR:HD1	2:L:1564:SER:HG	1.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2190:VAL:HG13	2:L:2237:ILE:HG12	1.94	0.50
2:L:3869:THR:HA	2:L:3872:ARG:HG2	1.93	0.50
2:C:176:GLU:HG3	2:C:222:GLY:HA2	1.93	0.50
2:C:217:LEU:HD11	2:C:260:ILE:HG22	1.93	0.50
2:C:1976:LEU:HD22	2:C:2141:ASN:HB3	1.94	0.50
2:C:2424:MET:SD	2:C:2435:CYS:HB3	2.52	0.50
2:L:3948:SER:HA	2:L:3951:GLN:OE1	2.11	0.50
2:C:992:ILE:HD11	2:C:1036:PHE:CD1	2.42	0.50
2:C:3735:PRO:HB2	2:C:3751:LEU:HD11	1.93	0.50
2:L:982:GLN:NE2	2:L:2589:TYR:HB3	2.27	0.49
2:L:1750:LEU:HD22	2:L:1762:MET:HE3	1.93	0.49
2:L:1976:LEU:HD22	2:L:2141:ASN:HB3	1.94	0.49
2:L:3130:GLN:NE2	2:L:3175:PRO:HD2	2.27	0.49
2:C:2586:PHE:HA	2:C:2777:HIS:HD2	1.77	0.49
2:C:3358:ARG:O	2:C:3358:ARG:HD3	2.11	0.49
2:L:462:VAL:HG13	2:L:560:LEU:HD11	1.93	0.49
2:L:1334:LYS:O	2:L:1338:VAL:HG13	2.11	0.49
2:L:2514:ASN:HB2	2:L:2517:LEU:HB2	1.94	0.49
2:L:3701:ILE:HG23	2:L:3704:GLN:HE22	1.77	0.49
2:C:982:GLN:NE2	2:C:2589:TYR:HB3	2.27	0.49
2:C:1271:ILE:HA	2:C:1276:VAL:O	2.12	0.49
2:C:1757:MET:O	2:C:1761:LEU:HG	2.12	0.49
2:C:1805:PHE:HE2	2:C:1816:ARG:O	1.95	0.49
2:C:2469:CYS:O	2:C:2473:MET:HG3	2.12	0.49
2:C:3326:GLN:HA	2:C:3329:LEU:HG	1.93	0.49
2:C:3851:ASP:O	2:C:3855:TYR:N	2.44	0.49
2:L:336:ASN:OD1	2:L:340:TYR:OH	2.23	0.49
2:L:704:PHE:O	2:L:708:VAL:HG23	2.12	0.49
2:L:1335:CYS:O	2:L:1339:VAL:HG22	2.12	0.49
2:L:3107:ILE:O	2:L:3111:MET:HG3	2.12	0.49
2:L:3247:ARG:HD2	2:L:3286:CYS:SG	2.53	0.49
2:L:3944:HIS:HB3	2:L:4016:PHE:HE1	1.76	0.49
2:L:993:HIS:ND1	2:L:997:ASN:OD1	2.46	0.49
2:L:1960:LYS:HD2	2:L:2125:TRP:HB3	1.95	0.49
2:L:2779:ASP:OD1	2:L:2780:LEU:N	2.43	0.49
2:L:3233:SER:HB2	2:L:3272:TRP:HZ2	1.78	0.49
2:L:3596:LEU:HD11	2:L:3604:LYS:HA	1.95	0.49
2:C:1334:LYS:O	2:C:1338:VAL:HG13	2.11	0.49
2:C:3291:GLN:O	2:C:3296:GLN:HG2	2.13	0.49
2:C:3374:ILE:HG13	2:C:3375:ALA:H	1.78	0.49
2:L:540:MET:N	2:L:540:MET:SD	2.85	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1813:SER:OG	2:L:1868:THR:HG21	2.13	0.49
2:L:1922:ALA:HA	2:L:1925:GLU:HB2	1.93	0.49
2:L:3374:ILE:HG13	2:L:3375:ALA:H	1.78	0.49
2:L:3379:GLN:HA	2:L:3382:PHE:CZ	2.48	0.49
2:L:3640:PHE:CG	2:L:3640:PHE:O	2.65	0.49
2:L:3842:TRP:CD1	2:L:3845:LYS:HB3	2.48	0.49
2:C:208:MET:HA	2:C:215:PRO:HB3	1.94	0.49
2:C:349:ILE:HG22	2:C:362:ALA:HA	1.94	0.49
2:C:462:VAL:HG13	2:C:560:LEU:HD11	1.93	0.49
2:C:540:MET:N	2:C:540:MET:SD	2.85	0.49
2:C:649:PHE:O	2:C:653:LEU:HD23	2.12	0.49
2:C:1568:ASN:O	2:C:1572:LEU:HG	2.11	0.49
2:C:2828:GLU:O	2:C:2832:ILE:HG12	2.12	0.49
2:C:3107:ILE:O	2:C:3111:MET:HG3	2.13	0.49
2:L:455:LEU:HD12	2:L:459:ARG:HH11	1.77	0.49
2:L:2424:MET:SD	2:L:2435:CYS:HB3	2.52	0.49
2:L:2448:PRO:HB3	2:L:2451:LEU:HB2	1.95	0.49
2:L:2586:PHE:HA	2:L:2777:HIS:HD2	1.77	0.49
2:L:3291:GLN:O	2:L:3296:GLN:HG2	2.13	0.49
2:C:70:ARG:NH1	2:C:106:GLU:O	2.46	0.49
2:C:2190:VAL:HG13	2:C:2237:ILE:HG12	1.94	0.49
2:C:3471:ILE:O	2:C:3474:ARG:HG2	2.13	0.49
2:C:4045:CYS:HA	2:C:4048:LYS:HZ2	1.78	0.49
2:L:774:GLU:OE2	2:L:854:ARG:NH1	2.34	0.49
2:L:1051:LYS:NZ	2:L:1053:PRO:O	2.45	0.49
2:L:1335:CYS:HA	2:L:1338:VAL:HG22	1.94	0.49
2:L:2182:ILE:HD11	2:L:2219:LEU:HG	1.95	0.49
2:L:2443:MET:SD	2:L:2479:TRP:CE2	3.05	0.49
2:L:3446:VAL:HA	2:L:3449:LYS:HE2	1.93	0.49
2:L:3951:GLN:HB2	2:L:4036:LYS:NZ	2.28	0.49
2:C:421:LEU:HD13	2:C:424:LEU:HD12	1.94	0.49
2:C:2801:ASP:HB3	2:C:2804:ILE:HG22	1.94	0.49
2:C:3233:SER:HB2	2:C:3272:TRP:HZ2	1.78	0.49
2:C:3640:PHE:CG	2:C:3640:PHE:O	2.65	0.49
2:L:76:ILE:HD12	2:C:26:GLY:CA	2.40	0.49
2:L:1439:PRO:O	2:L:1442:GLN:NE2	2.40	0.49
2:L:1958:GLU:O	2:L:1961:PHE:HB2	2.12	0.49
2:L:2320:ALA:HB3	2:L:2323:LEU:HB2	1.94	0.49
2:L:2469:CYS:O	2:L:2473:MET:HG3	2.13	0.49
2:L:3114:TYR:O	2:L:3117:ILE:HG22	2.13	0.49
2:C:2514:ASN:HB2	2:C:2517:LEU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:651:TYR:CE1	2:L:655:LEU:HD21	2.48	0.49
2:L:1271:ILE:HA	2:L:1276:VAL:O	2.12	0.49
2:C:1335:CYS:HA	2:C:1338:VAL:HG22	1.94	0.49
2:C:2165:LEU:O	2:C:2168:LEU:HG	2.13	0.49
2:C:2320:ALA:HB3	2:C:2323:LEU:HB2	1.94	0.49
2:C:2779:ASP:OD1	2:C:2780:LEU:N	2.43	0.49
2:C:3104:GLN:O	2:C:3108:GLN:HG2	2.13	0.49
2:C:3575:LEU:HB2	2:C:3800:LEU:HD21	1.95	0.49
2:C:3596:LEU:HD11	2:C:3604:LYS:HA	1.95	0.49
2:C:3842:TRP:CD1	2:C:3845:LYS:HB3	2.48	0.49
2:L:217:LEU:HD11	2:L:260:ILE:HG22	1.93	0.49
2:L:524:TYR:HA	2:L:527:TYR:HB2	1.95	0.49
2:L:1538:LEU:HB3	2:L:1555:HIS:CD2	2.48	0.49
2:L:2481:HIS:HA	2:L:2484:TYR:CE1	2.48	0.49
2:L:3442:TYR:O	2:L:3446:VAL:HG13	2.12	0.49
2:L:3471:ILE:O	2:L:3474:ARG:HG2	2.13	0.49
2:L:4057:ALA:HB2	2:L:4090:ARG:HH11	1.78	0.49
2:C:455:LEU:HD12	2:C:459:ARG:HH11	1.77	0.49
2:C:1958:GLU:O	2:C:1961:PHE:HB2	2.12	0.49
2:C:2359:LYS:HD2	2:C:2361:ILE:HB	1.94	0.49
2:C:2443:MET:SD	2:C:2479:TRP:CE2	3.05	0.49
2:C:2566:THR:HG21	2:C:2791:ILE:HG12	1.95	0.49
2:C:3379:GLN:HA	2:C:3382:PHE:CZ	2.47	0.49
2:C:3701:ILE:HG23	2:C:3704:GLN:HE22	1.77	0.49
2:C:3828:TYR:OH	2:C:4127:TRP:CD1	2.66	0.49
2:L:421:LEU:HD13	2:L:424:LEU:HD12	1.93	0.48
2:L:1743:MET:HA	2:L:1746:PHE:CD1	2.48	0.48
2:L:1805:PHE:HE2	2:L:1816:ARG:O	1.95	0.48
2:L:2566:THR:HG21	2:L:2791:ILE:HG12	1.95	0.48
2:L:2843:PHE:HD2	2:L:2858:ILE:HD11	1.78	0.48
2:C:1282:LEU:HD21	2:C:1289:SER:HB3	1.95	0.48
2:C:1711:ARG:HD2	2:C:1761:LEU:HD11	1.95	0.48
2:C:1813:SER:OG	2:C:1868:THR:HG21	2.13	0.48
2:C:1960:LYS:HD2	2:C:2125:TRP:HB3	1.95	0.48
2:C:2418:LYS:O	2:C:2420:PHE:N	2.38	0.48
2:C:3442:TYR:O	2:C:3446:VAL:HG13	2.12	0.48
2:C:3828:TYR:HH	2:C:4127:TRP:HE1	1.59	0.48
2:L:341:PHE:O	2:L:345:PHE:N	2.47	0.48
2:L:430:VAL:HG23	2:L:431:TYR:CD2	2.48	0.48
2:L:3183:ILE:HD12	2:L:3238:MET:SD	2.53	0.48
2:L:3608:LYS:O	2:L:3609:MET:HB2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3839:TYR:HB3	2:L:4122:GLU:HG3	1.94	0.48
2:L:3844:THR:HG22	2:L:3850:HIS:HB3	1.94	0.48
2:C:348:ILE:HG23	2:C:349:ILE:HG23	1.95	0.48
2:C:2481:HIS:HA	2:C:2484:TYR:CE1	2.48	0.48
2:C:3156:PRO:HB3	2:C:3159:ARG:HH11	1.78	0.48
2:C:3183:ILE:HD12	2:C:3238:MET:SD	2.53	0.48
2:C:3252:PHE:HB3	2:C:3287:ARG:HD3	1.96	0.48
2:C:3844:THR:HG22	2:C:3850:HIS:HB3	1.94	0.48
2:L:26:GLY:O	2:C:76:ILE:CD1	2.62	0.48
2:L:348:ILE:HG23	2:L:349:ILE:HG23	1.95	0.48
2:L:440:VAL:HG11	2:L:489:ARG:HH11	1.75	0.48
2:L:644:PRO:HG2	2:L:645:TRP:HD1	1.79	0.48
2:L:745:VAL:O	2:L:749:VAL:HG23	2.13	0.48
2:L:782:ARG:NH2	2:L:783:HIS:HB2	2.28	0.48
2:L:3104:GLN:O	2:L:3108:GLN:HG2	2.13	0.48
2:L:3633:ILE:O	2:L:3638:LYS:N	2.47	0.48
2:L:3920:ILE:HG22	2:L:3923:ARG:HH22	1.78	0.48
2:C:524:TYR:HA	2:C:527:TYR:HB2	1.95	0.48
2:C:1804:MET:O	2:C:1816:ARG:NH2	2.46	0.48
2:C:2843:PHE:HD2	2:C:2858:ILE:HD11	1.78	0.48
2:C:3100:LYS:CG	2:C:3104:GLN:HE22	2.26	0.48
2:C:3247:ARG:HD2	2:C:3286:CYS:SG	2.53	0.48
2:C:3518:VAL:O	2:C:3522:THR:HG23	2.13	0.48
2:C:3920:ILE:HG22	2:C:3923:ARG:HH22	1.78	0.48
2:L:349:ILE:HG22	2:L:362:ALA:HA	1.94	0.48
2:L:1067:ALA:HB2	2:L:1107:TYR:HE1	1.78	0.48
2:L:1804:MET:O	2:L:1816:ARG:NH2	2.46	0.48
2:L:1983:ASP:N	2:L:1983:ASP:OD1	2.46	0.48
2:L:2451:LEU:HD23	2:L:2454:LEU:HD12	1.94	0.48
2:L:3085:GLU:OE1	2:L:3085:GLU:N	2.32	0.48
2:L:3100:LYS:CG	2:L:3104:GLN:HE22	2.26	0.48
2:L:3518:VAL:O	2:L:3522:THR:HG23	2.13	0.48
2:C:1005:ASP:OD1	2:C:1006:THR:N	2.45	0.48
2:C:1983:ASP:OD1	2:C:1983:ASP:N	2.46	0.48
2:L:1750:LEU:HD21	2:L:1758:LEU:HG	1.95	0.48
2:L:2404:ARG:NE	2:L:2441:LYS:HE3	2.26	0.48
2:L:3471:ILE:HG22	2:L:3475:TYR:HE2	1.79	0.48
2:C:430:VAL:HG23	2:C:431:TYR:CD2	2.48	0.48
2:C:569:VAL:HA	2:C:572:VAL:HG22	1.95	0.48
2:C:745:VAL:O	2:C:749:VAL:HG23	2.13	0.48
2:C:2182:ILE:HD11	2:C:2219:LEU:HG	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3100:LYS:HG2	2:C:3104:GLN:HE22	1.79	0.48
2:C:3134:ALA:O	2:C:3138:ILE:HG12	2.13	0.48
2:C:3596:LEU:HD11	2:C:3604:LYS:HD2	1.95	0.48
2:L:70:ARG:NH1	2:L:106:GLU:O	2.46	0.48
2:L:2165:LEU:O	2:L:2168:LEU:HG	2.13	0.48
2:L:2801:ASP:HB3	2:L:2804:ILE:HG22	1.94	0.48
2:L:3134:ALA:O	2:L:3138:ILE:HG12	2.13	0.48
2:C:35:ILE:HG12	2:C:81:CYS:SG	2.52	0.48
2:C:402:THR:HA	2:C:405:ASP:HB2	1.95	0.48
2:C:665:GLY:O	2:C:669:LEU:HG	2.13	0.48
2:C:1051:LYS:NZ	2:C:1053:PRO:O	2.45	0.48
2:C:2158:ARG:HD3	2:C:2158:ARG:H	1.79	0.48
2:C:2448:PRO:HB3	2:C:2451:LEU:HB2	1.95	0.48
2:L:476:ARG:HA	2:L:479:ILE:HG12	1.96	0.48
2:L:3575:LEU:HB2	2:L:3800:LEU:HD21	1.95	0.48
2:C:534:LEU:HB3	2:C:564:LEU:HD13	1.96	0.48
2:C:782:ARG:NH2	2:C:783:HIS:HB2	2.28	0.48
2:C:993:HIS:ND1	2:C:997:ASN:OD1	2.46	0.48
2:C:1067:ALA:HB2	2:C:1107:TYR:HE1	1.78	0.48
2:C:3329:LEU:O	2:C:3333:THR:HG23	2.13	0.48
2:C:3841:ASP:OD1	2:C:3842:TRP:N	2.47	0.48
2:L:208:MET:HA	2:L:215:PRO:HB3	1.94	0.48
2:L:566:ASP:OD2	2:L:1502:SER:HB3	2.14	0.48
2:L:3156:PRO:HB3	2:L:3159:ARG:HH11	1.78	0.48
2:L:3862:ALA:O	2:L:3863:ASN:ND2	2.42	0.48
2:C:2447:LYS:O	2:C:2449:VAL:N	2.46	0.48
2:C:2451:LEU:HD23	2:C:2454:LEU:HD12	1.95	0.48
2:L:665:GLY:O	2:L:669:LEU:HG	2.13	0.48
2:L:1282:LEU:HD21	2:L:1289:SER:HB3	1.96	0.48
2:L:3100:LYS:HG2	2:L:3104:GLN:HE22	1.79	0.48
2:L:3596:LEU:HD11	2:L:3604:LYS:HD2	1.95	0.48
2:L:4045:CYS:HA	2:L:4048:LYS:HZ2	1.79	0.48
2:C:89:LEU:HA	2:C:92:PHE:HB3	1.96	0.48
2:C:188:GLU:HB3	2:C:189:MET:HG2	1.95	0.48
2:C:704:PHE:O	2:C:708:VAL:HG23	2.12	0.48
2:C:1072:ALA:HA	2:C:1075:ARG:NH2	2.28	0.48
2:C:1635:LYS:HA	2:C:1642:LYS:HE2	1.96	0.48
2:C:3114:TYR:O	2:C:3117:ILE:HG22	2.13	0.48
2:L:1260:LEU:HD21	2:L:1290:LEU:HD13	1.96	0.48
2:L:1711:ARG:HD2	2:L:1761:LEU:HD11	1.95	0.48
2:L:3329:LEU:O	2:L:3333:THR:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3723:ASP:HB3	2:L:3739:ILE:HB	1.96	0.48
2:L:3828:TYR:OH	2:L:4127:TRP:CD1	2.66	0.48
2:C:403:GLY:HA2	2:C:407:VAL:HG23	1.95	0.48
2:C:1086:TYR:HA	2:C:1089:PHE:HB3	1.95	0.48
2:C:1260:LEU:HD21	2:C:1290:LEU:HD13	1.96	0.48
2:C:1560:TYR:CE2	2:C:1596:VAL:HG12	2.49	0.48
2:C:2262:GLY:HA3	2:C:2269:ASP:HB3	1.96	0.48
2:C:3951:GLN:HB2	2:C:4036:LYS:NZ	2.28	0.48
2:L:432:THR:N	2:L:433:PRO:HD2	2.29	0.47
2:L:1072:ALA:HA	2:L:1075:ARG:NH2	2.28	0.47
2:L:2262:GLY:HA3	2:L:2269:ASP:HB3	1.96	0.47
2:L:2464:HIS:O	2:L:2470:ARG:NH1	2.47	0.47
2:L:3465:PHE:CG	2:L:3466:PRO:HD3	2.49	0.47
2:C:336:ASN:OD1	2:C:340:TYR:OH	2.23	0.47
2:C:1538:LEU:HB3	2:C:1555:HIS:CD2	2.48	0.47
2:L:35:ILE:HA	2:L:38:LEU:HD12	1.96	0.47
2:L:52:ALA:HA	2:L:99:LYS:HG2	1.97	0.47
2:L:1086:TYR:HA	2:L:1089:PHE:HB3	1.95	0.47
2:L:1180:GLN:OE1	2:L:1180:GLN:HA	2.14	0.47
2:L:1597:LEU:O	2:L:1601:LEU:HG	2.14	0.47
2:L:3479:THR:OG1	2:L:3482:LEU:HB3	2.14	0.47
2:C:341:PHE:O	2:C:345:PHE:N	2.47	0.47
2:C:651:TYR:CE1	2:C:655:LEU:HD21	2.48	0.47
2:C:1597:LEU:O	2:C:1601:LEU:HG	2.14	0.47
2:C:1863:PHE:HA	2:C:1866:GLN:HG2	1.97	0.47
2:C:2464:HIS:O	2:C:2470:ARG:NH1	2.47	0.47
2:C:3181:ASP:O	2:C:3185:ASN:ND2	2.48	0.47
2:L:1828:LEU:HD12	2:L:1880:MET:HB3	1.96	0.47
2:L:2398:LEU:O	2:L:2434:VAL:HG11	2.14	0.47
2:L:3822:GLN:O	2:L:3826:ALA:N	2.38	0.47
2:L:3946:PHE:HZ	2:L:4002:MET:HG2	1.79	0.47
2:C:1679:LEU:HD12	2:C:1689:LYS:HD2	1.96	0.47
2:C:1743:MET:HA	2:C:1746:PHE:CD1	2.48	0.47
2:C:2398:LEU:O	2:C:2434:VAL:HG11	2.14	0.47
2:C:3470:GLN:CG	2:C:4004:VAL:HB	2.43	0.47
2:C:3479:THR:OG1	2:C:3482:LEU:HB3	2.15	0.47
2:C:3946:PHE:HZ	2:C:4002:MET:HG2	1.79	0.47
2:L:752:LEU:HD21	2:L:773:LEU:HD21	1.96	0.47
2:L:3252:PHE:HB3	2:L:3287:ARG:HD3	1.96	0.47
2:C:432:THR:N	2:C:433:PRO:HD2	2.29	0.47
2:C:620:PHE:CZ	2:C:624:ILE:HD11	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2099:ALA:HA	2:C:2102:LYS:HB3	1.97	0.47
2:L:188:GLU:HB3	2:L:189:MET:HG2	1.95	0.47
2:L:1365:ASN:O	2:L:1368:LEU:HB3	2.14	0.47
2:L:1679:LEU:HD12	2:L:1689:LYS:HD2	1.96	0.47
2:L:3470:GLN:CG	2:L:4004:VAL:HB	2.43	0.47
2:L:3515:GLN:OE1	2:L:3515:GLN:N	2.48	0.47
2:C:35:ILE:HA	2:C:38:LEU:HD12	1.96	0.47
2:C:1365:ASN:O	2:C:1368:LEU:HB3	2.14	0.47
2:C:1828:LEU:HD12	2:C:1880:MET:HB3	1.96	0.47
2:C:2466:SER:O	2:C:2470:ARG:NH2	2.48	0.47
2:C:3633:ILE:O	2:C:3638:LYS:N	2.47	0.47
2:C:4057:ALA:HB2	2:C:4090:ARG:HH11	1.78	0.47
2:L:89:LEU:HA	2:L:92:PHE:HB3	1.96	0.47
2:L:402:THR:HA	2:L:405:ASP:HB2	1.95	0.47
2:L:405:ASP:O	2:L:408:TYR:N	2.27	0.47
2:L:1863:PHE:HA	2:L:1866:GLN:HG2	1.97	0.47
2:L:2350:LYS:HZ2	2:C:162:LEU:HD13	1.78	0.47
2:L:3841:ASP:OD1	2:L:3842:TRP:N	2.47	0.47
2:C:925:GLN:HE21	2:C:925:GLN:HB3	1.57	0.47
2:L:314:SER:O	2:L:317:GLU:HG2	2.15	0.47
2:L:403:GLY:HA2	2:L:407:VAL:HG23	1.95	0.47
2:L:534:LEU:HB3	2:L:564:LEU:HD13	1.96	0.47
2:L:566:ASP:HA	2:L:569:VAL:HG12	1.97	0.47
2:L:569:VAL:HA	2:L:572:VAL:HG22	1.95	0.47
2:L:1338:VAL:HA	2:L:1341:ILE:HG12	1.97	0.47
2:L:1710:LEU:HA	2:L:1713:VAL:HG12	1.97	0.47
2:L:2169:LEU:HB3	2:L:2211:LEU:HD13	1.97	0.47
2:L:2466:SER:O	2:L:2470:ARG:NH2	2.48	0.47
2:L:3784:ARG:HB2	2:L:3786:LEU:CD1	2.45	0.47
2:C:52:ALA:HA	2:C:99:LYS:HG2	1.97	0.47
2:C:225:LYS:HD2	2:C:270:ALA:HB2	1.97	0.47
2:C:476:ARG:HA	2:C:479:ILE:HG12	1.96	0.47
2:C:729:CYS:O	2:C:733:LEU:HD23	2.15	0.47
2:C:745:VAL:HB	2:C:788:TYR:CE2	2.50	0.47
2:C:1631:SER:HB3	2:C:1634:ALA:HB3	1.97	0.47
2:C:1713:VAL:HA	2:C:1716:GLN:HG2	1.96	0.47
2:C:1750:LEU:HD21	2:C:1758:LEU:HG	1.95	0.47
2:C:2087:GLU:OE2	2:C:2091:HIS:HD2	1.98	0.47
2:C:2095:ALA:HB3	2:C:2096:PRO:HD3	1.97	0.47
2:C:3723:ASP:HB3	2:C:3739:ILE:HB	1.96	0.47
2:L:162:LEU:O	2:L:165:LYS:HG3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2891:ARG:HH22	2:L:2895:GLU:HB2	1.80	0.47
2:C:752:LEU:HD21	2:C:773:LEU:HD21	1.95	0.47
2:C:776:TRP:HB3	2:C:785:MET:HE1	1.96	0.47
2:C:883:TYR:CE1	2:C:3120:LEU:HD11	2.49	0.47
2:C:1045:THR:HB	2:C:1048:GLN:HE22	1.80	0.47
2:C:1761:LEU:O	2:C:1765:VAL:HG23	2.15	0.47
2:L:135:LEU:HD23	2:L:144:MET:HE1	1.97	0.47
2:L:2470:ARG:HA	2:L:2473:MET:SD	2.55	0.47
2:L:3181:ASP:O	2:L:3185:ASN:ND2	2.48	0.47
2:C:1180:GLN:OE1	2:C:1180:GLN:HA	2.14	0.47
2:C:3608:LYS:O	2:C:3609:MET:HB2	2.13	0.47
2:C:3784:ARG:HB2	2:C:3786:LEU:CD1	2.45	0.47
2:C:3862:ALA:O	2:C:3863:ASN:ND2	2.42	0.47
2:C:3889:ARG:HG2	2:C:3889:ARG:NH2	2.30	0.47
2:L:2158:ARG:H	2:L:2158:ARG:HD3	1.79	0.47
2:L:3187:CYS:SG	2:L:3235:LYS:NZ	2.66	0.47
2:L:3446:VAL:HA	2:L:3449:LYS:HG2	1.97	0.47
2:C:709:LYS:O	2:C:713:GLU:OE1	2.33	0.47
2:C:997:ASN:HD22	2:C:1043:GLN:CG	2.23	0.47
2:C:1839:PHE:CE2	2:C:1843:ILE:HD13	2.50	0.47
2:C:2404:ARG:NE	2:C:2441:LYS:HE3	2.26	0.47
2:C:3099:ALA:O	2:C:3103:ILE:HG12	2.15	0.47
2:C:3354:ASP:N	2:C:3354:ASP:OD1	2.48	0.47
2:L:883:TYR:CE1	2:L:3120:LEU:HD11	2.49	0.46
2:L:1839:PHE:CE2	2:L:1843:ILE:HD13	2.50	0.46
2:C:1338:VAL:HA	2:C:1341:ILE:HG12	1.97	0.46
2:C:3471:ILE:HG22	2:C:3475:TYR:HE2	1.79	0.46
2:L:1631:SER:HB3	2:L:1634:ALA:HB3	1.97	0.46
2:L:1713:VAL:HA	2:L:1716:GLN:HG2	1.96	0.46
2:L:2099:ALA:HA	2:L:2102:LYS:HB3	1.97	0.46
2:C:162:LEU:O	2:C:165:LYS:HG3	2.15	0.46
2:C:566:ASP:HA	2:C:569:VAL:HG12	1.97	0.46
2:C:3465:PHE:CG	2:C:3466:PRO:HD3	2.50	0.46
2:L:745:VAL:HB	2:L:788:TYR:CE2	2.50	0.46
2:L:1560:TYR:CE2	2:L:1596:VAL:HG12	2.49	0.46
2:L:2451:LEU:HA	2:L:2454:LEU:HB2	1.97	0.46
2:C:70:ARG:HE	2:C:110:THR:HA	1.80	0.46
2:C:644:PRO:HG2	2:C:645:TRP:HD1	1.78	0.46
2:C:955:ALA:O	2:C:957:PRO:HD3	2.15	0.46
2:C:2470:ARG:HA	2:C:2473:MET:SD	2.55	0.46
2:C:2891:ARG:HH22	2:C:2895:GLU:HB2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3493:TRP:CZ2	2:C:3710:LYS:HB3	2.50	0.46
2:L:168:ASP:OD1	2:L:218:PRO:HB2	2.15	0.46
2:L:620:PHE:CZ	2:L:624:ILE:HD11	2.50	0.46
2:L:750:PRO:O	2:L:754:MET:HG2	2.16	0.46
2:L:1761:LEU:O	2:L:1765:VAL:HG23	2.15	0.46
2:L:1764:GLU:HA	2:L:1767:CYS:SG	2.55	0.46
2:C:752:LEU:HG	2:C:756:PHE:CE1	2.50	0.46
2:C:2451:LEU:HA	2:C:2454:LEU:HB2	1.97	0.46
2:C:2813:PHE:HD1	2:C:2817:LEU:HD23	1.80	0.46
2:C:3515:GLN:OE1	2:C:3515:GLN:N	2.48	0.46
2:L:729:CYS:O	2:L:733:LEU:HD23	2.15	0.46
2:L:1476:HIS:CD2	2:L:1478:SER:HB2	2.50	0.46
2:L:1817:GLN:HE22	2:L:1871:MET:CE	2.28	0.46
2:L:2165:LEU:HD23	2:L:2168:LEU:HD11	1.96	0.46
2:C:1219:PHE:O	2:C:1223:THR:OG1	2.29	0.46
2:C:1290:LEU:HG	2:C:1294:VAL:HB	1.96	0.46
2:L:988:VAL:HA	2:L:991:LEU:HG	1.98	0.46
2:L:2095:ALA:HB3	2:L:2096:PRO:HD3	1.97	0.46
2:L:2813:PHE:HD1	2:L:2817:LEU:HD23	1.79	0.46
2:C:55:THR:HA	2:C:59:PHE:HD1	1.81	0.46
2:C:566:ASP:OD2	2:C:1502:SER:HB3	2.14	0.46
2:C:1151:ARG:O	2:C:1163:LEU:HG	2.16	0.46
2:C:1331:ASN:HA	2:C:1334:LYS:NZ	2.31	0.46
2:L:76:ILE:CD1	2:C:26:GLY:O	2.63	0.46
2:L:955:ALA:O	2:L:957:PRO:HD3	2.15	0.46
2:L:1203:SER:HB3	2:L:1206:LEU:HB2	1.97	0.46
2:L:2309:PHE:CE2	2:L:2318:ALA:N	2.84	0.46
2:L:2985:GLU:HG3	2:L:2986:PRO:HD2	1.97	0.46
2:L:3099:ALA:O	2:L:3103:ILE:HG12	2.15	0.46
2:C:379:LYS:NZ	2:C:1551:ILE:HD11	2.30	0.46
2:C:426:THR:HB	2:C:1550:VAL:HG22	1.98	0.46
2:C:1476:HIS:CD2	2:C:1478:SER:HB2	2.50	0.46
2:C:1942:CYS:O	2:C:1946:ASN:ND2	2.48	0.46
2:C:2158:ARG:O	2:C:2158:ARG:HG2	2.15	0.46
2:L:55:THR:HA	2:L:59:PHE:HD1	1.81	0.46
2:L:752:LEU:HG	2:L:756:PHE:CE1	2.50	0.46
2:L:901:MET:HG3	2:L:2819:GLU:OE1	2.16	0.46
2:L:1290:LEU:HG	2:L:1294:VAL:HB	1.96	0.46
2:L:1635:LYS:HA	2:L:1642:LYS:HE2	1.96	0.46
2:L:3558:ILE:HA	2:L:3561:LYS:HG2	1.98	0.46
2:C:2165:LEU:HD23	2:C:2168:LEU:HD11	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:483:VAL:HG11	2:L:567:GLU:OE2	2.15	0.46
2:L:906:PHE:O	2:L:909:VAL:HG12	2.16	0.46
2:L:2184:TYR:CD1	2:L:2185:MET:HG2	2.51	0.46
2:L:2447:LYS:O	2:L:2449:VAL:N	2.46	0.46
2:L:3493:TRP:CZ2	2:L:3710:LYS:HB3	2.50	0.46
2:L:3889:ARG:HG2	2:L:3889:ARG:NH2	2.30	0.46
2:C:314:SER:O	2:C:317:GLU:HG2	2.15	0.46
2:C:410:MET:HB2	2:C:411:PRO:HD3	1.98	0.46
2:C:446:PHE:CG	2:C:530:LEU:HD12	2.51	0.46
2:C:750:PRO:O	2:C:754:MET:HG2	2.16	0.46
2:C:1710:LEU:HA	2:C:1713:VAL:HG12	1.97	0.46
2:C:2169:LEU:HB3	2:C:2211:LEU:HD13	1.97	0.46
2:C:3823:GLU:O	2:C:3827:ALA:N	2.49	0.46
2:L:997:ASN:HD22	2:L:1043:GLN:CG	2.23	0.46
2:L:1942:CYS:O	2:L:1946:ASN:ND2	2.48	0.46
2:L:2309:PHE:HE2	2:L:2318:ALA:N	2.14	0.46
2:C:483:VAL:HG11	2:C:567:GLU:OE2	2.16	0.46
2:L:1331:ASN:HA	2:L:1334:LYS:NZ	2.31	0.45
2:L:2362:VAL:HA	2:L:2365:ASN:HB3	1.97	0.45
2:C:225:LYS:HZ1	2:C:229:SER:HB2	1.80	0.45
2:C:722:LYS:HG2	2:C:723:ASP:OD2	2.16	0.45
2:C:901:MET:HG3	2:C:2819:GLU:OE1	2.16	0.45
2:C:1569:THR:HA	2:C:1572:LEU:HD12	1.99	0.45
2:C:1764:GLU:HA	2:C:1767:CYS:SG	2.55	0.45
2:C:1817:GLN:HE22	2:C:1871:MET:CE	2.28	0.45
2:C:2985:GLU:HG3	2:C:2986:PRO:HD2	1.97	0.45
2:C:3009:LYS:HG3	2:C:3051:LEU:HD11	1.97	0.45
2:C:3558:ILE:HA	2:C:3561:LYS:HG2	1.98	0.45
2:L:410:MET:HB2	2:L:411:PRO:HD3	1.98	0.45
2:L:709:LYS:O	2:L:713:GLU:OE1	2.33	0.45
2:L:1476:HIS:HD2	2:L:1478:SER:HB2	1.81	0.45
2:L:2577:PHE:H	2:L:2784:GLN:HE22	1.63	0.45
2:L:3427:GLU:O	2:L:3432:SER:HB3	2.17	0.45
2:L:3823:GLU:O	2:L:3827:ALA:N	2.49	0.45
2:C:249:PHE:CE1	2:C:253:LEU:HD21	2.52	0.45
2:C:2184:TYR:CD1	2:C:2185:MET:HG2	2.51	0.45
2:C:2812:LEU:O	2:C:2816:ILE:HG12	2.16	0.45
2:C:3516:HIS:O	2:C:3519:GLU:HG3	2.17	0.45
2:C:3719:ILE:HG12	2:C:3722:PHE:HE1	1.81	0.45
2:L:155:LYS:O	2:L:159:GLU:HG2	2.16	0.45
2:L:225:LYS:HD2	2:L:270:ALA:HB2	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:426:THR:HB	2:L:1550:VAL:HG22	1.98	0.45
2:L:938:VAL:HA	2:L:941:MET:CE	2.46	0.45
2:L:1045:THR:HB	2:L:1048:GLN:HE22	1.80	0.45
2:L:2506:LEU:HG	2:L:2525:TRP:CZ2	2.52	0.45
2:L:3719:ILE:HG12	2:L:3722:PHE:HE1	1.81	0.45
2:C:168:ASP:OD1	2:C:218:PRO:HB2	2.15	0.45
2:C:776:TRP:HB3	2:C:785:MET:CE	2.47	0.45
2:C:1195:VAL:HG21	2:C:1204:PRO:HB3	1.99	0.45
2:C:3427:GLU:O	2:C:3432:SER:HB3	2.17	0.45
2:L:70:ARG:HE	2:L:110:THR:HA	1.80	0.45
2:L:1759:LEU:O	2:L:1762:MET:HG2	2.16	0.45
2:L:2087:GLU:OE2	2:L:2091:HIS:HD2	1.98	0.45
2:L:2158:ARG:HG2	2:L:2158:ARG:O	2.15	0.45
2:L:2578:GLU:H	2:L:2784:GLN:NE2	2.13	0.45
2:C:155:LYS:O	2:C:159:GLU:HG2	2.17	0.45
2:C:583:LEU:HD13	2:C:614:PRO:HA	1.99	0.45
2:C:910:PHE:HE1	2:C:2807:GLN:HG2	1.82	0.45
2:C:976:VAL:O	2:C:976:VAL:HG13	2.16	0.45
2:C:1560:TYR:HD1	2:C:1564:SER:HG	1.64	0.45
2:C:1759:LEU:O	2:C:1762:MET:HG2	2.16	0.45
2:C:2347:LYS:O	2:C:2350:LYS:HG2	2.17	0.45
2:L:379:LYS:NZ	2:L:1551:ILE:HD11	2.30	0.45
2:L:1195:VAL:HG21	2:L:1204:PRO:HB3	1.99	0.45
2:L:3354:ASP:N	2:L:3354:ASP:OD1	2.48	0.45
2:L:3439:LEU:O	2:L:3440:GLN:HG3	2.16	0.45
2:L:3704:GLN:OE1	2:L:3704:GLN:N	2.50	0.45
2:L:3786:LEU:HD11	2:L:3983:ILE:HD11	1.99	0.45
2:C:426:THR:HA	2:C:1549:SER:HA	1.99	0.45
2:C:487:LEU:HD11	2:C:568:PHE:CE1	2.51	0.45
2:C:906:PHE:O	2:C:909:VAL:HG12	2.16	0.45
2:C:1203:SER:HB3	2:C:1206:LEU:HB2	1.97	0.45
2:C:3048:LYS:CE	2:C:3061:LEU:HB2	2.47	0.45
2:L:2253:TYR:OH	2:L:2288:TYR:N	2.42	0.45
2:C:988:VAL:HA	2:C:991:LEU:HG	1.98	0.45
2:C:1104:LEU:HD12	2:C:1104:LEU:HA	1.86	0.45
2:C:3704:GLN:OE1	2:C:3704:GLN:N	2.50	0.45
2:C:4017:GLU:O	2:C:4021:LEU:HG	2.16	0.45
2:L:115:TYR:CG	2:L:124:LYS:HE3	2.52	0.45
2:L:249:PHE:CE1	2:L:253:LEU:HD21	2.52	0.45
2:L:446:PHE:CG	2:L:530:LEU:HD12	2.51	0.45
2:L:3009:LYS:HG3	2:L:3051:LEU:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3144:PHE:CE1	2:L:3193:ILE:HD11	2.52	0.45
2:L:3179:TRP:CD1	2:L:3242:MET:SD	3.10	0.45
2:L:3318:LYS:HG3	2:L:3319:ASN:N	2.32	0.45
2:L:3472:ILE:H	2:L:3472:ILE:HD12	1.81	0.45
2:C:793:LEU:N	2:C:794:PRO:HD2	2.32	0.45
2:C:1210:ASP:O	2:C:1213:LYS:HG3	2.17	0.45
2:C:1531:LEU:HB3	2:C:1559:PHE:HE2	1.82	0.45
2:C:1707:LEU:HD23	2:C:1709:GLU:OE2	2.17	0.45
2:C:2193:ILE:HD12	2:C:2245:TRP:HH2	1.82	0.45
2:C:2577:PHE:H	2:C:2784:GLN:HE22	1.63	0.45
2:C:3318:LYS:HG3	2:C:3319:ASN:N	2.31	0.45
2:C:4047:ALA:O	2:C:4051:LEU:HD23	2.16	0.45
2:L:487:LEU:HD11	2:L:568:PHE:CE1	2.51	0.45
2:L:1648:LEU:O	2:L:1652:ILE:HG12	2.17	0.45
2:L:2897:LEU:HD21	2:L:2923:TRP:CZ2	2.52	0.45
2:L:3516:HIS:O	2:L:3519:GLU:HG3	2.17	0.45
2:C:473:PRO:O	2:C:476:ARG:HB2	2.17	0.45
2:C:531:PHE:O	2:C:535:LEU:HG	2.17	0.45
2:C:2309:PHE:HE2	2:C:2318:ALA:N	2.14	0.45
2:C:3446:VAL:HA	2:C:3449:LYS:HG2	1.98	0.45
2:C:3755:GLY:N	2:C:3799:ARG:O	2.50	0.45
2:L:864:GLY:HA2	2:L:867:ASN:OD1	2.17	0.45
2:L:1010:LEU:HD21	2:L:1036:PHE:CE1	2.52	0.45
2:L:1111:LEU:HD12	2:L:1131:ILE:HD11	1.99	0.45
2:L:1151:ARG:O	2:L:1163:LEU:HG	2.16	0.45
2:L:1707:LEU:HD23	2:L:1709:GLU:OE2	2.17	0.45
2:L:2199:LEU:HD23	2:L:2200:ALA:N	2.32	0.45
2:L:2528:GLU:OE1	2:L:2528:GLU:N	2.48	0.45
2:L:3755:GLY:N	2:L:3799:ARG:O	2.50	0.45
2:C:2311:ARG:HE	2:C:2312:TYR:H	1.64	0.45
2:C:3138:ILE:HD13	2:C:3189:PHE:HZ	1.82	0.45
2:C:3439:LEU:O	2:C:3440:GLN:HG3	2.16	0.45
2:C:3786:LEU:HD11	2:C:3983:ILE:HD11	1.99	0.45
2:L:1569:THR:HA	2:L:1572:LEU:HD12	1.99	0.45
2:L:2311:ARG:HE	2:L:2312:TYR:H	1.64	0.45
2:C:485:GLN:HB3	2:C:489:ARG:CZ	2.46	0.45
2:C:485:GLN:CB	2:C:489:ARG:HH12	2.29	0.45
2:C:3144:PHE:CE1	2:C:3193:ILE:HD11	2.52	0.45
2:L:426:THR:HA	2:L:1549:SER:HA	1.99	0.44
2:L:485:GLN:HB3	2:L:489:ARG:CZ	2.46	0.44
2:L:909:VAL:HG22	2:L:2807:GLN:NE2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:976:VAL:HG13	2:L:976:VAL:O	2.16	0.44
2:L:2347:LYS:O	2:L:2350:LYS:HG2	2.17	0.44
2:L:2439:ILE:HD12	2:L:2451:LEU:HD21	1.98	0.44
2:L:3870:SER:O	2:L:3873:LYS:HG2	2.17	0.44
2:L:4047:ALA:O	2:L:4051:LEU:HD23	2.16	0.44
2:C:290:TYR:HD1	2:C:292:SER:H	1.65	0.44
2:C:2199:LEU:HD23	2:C:2200:ALA:N	2.32	0.44
2:C:3472:ILE:H	2:C:3472:ILE:HD12	1.81	0.44
2:L:290:TYR:HD1	2:L:292:SER:H	1.65	0.44
2:L:722:LYS:HG2	2:L:723:ASP:OD2	2.16	0.44
2:L:2855:VAL:O	2:L:2859:GLN:OE1	2.35	0.44
2:L:3760:GLN:OE1	2:L:3760:GLN:N	2.48	0.44
2:L:3833:ARG:NH2	2:L:3838:GLU:HB2	2.33	0.44
2:C:712:LYS:HE2	2:C:712:LYS:HB3	1.86	0.44
2:C:1476:HIS:HD2	2:C:1478:SER:HB2	1.82	0.44
2:C:2147:ALA:O	2:C:2151:ILE:HG13	2.17	0.44
2:C:2362:VAL:HA	2:C:2365:ASN:HB3	1.97	0.44
2:C:2453:GLU:OE1	2:C:2453:GLU:N	2.45	0.44
2:C:3097:ASP:N	2:C:3097:ASP:OD1	2.48	0.44
2:C:3577:GLN:NE2	2:C:3684:SER:OG	2.50	0.44
2:L:793:LEU:N	2:L:794:PRO:HD2	2.32	0.44
2:L:1210:ASP:O	2:L:1213:LYS:HG3	2.17	0.44
2:L:1653:LEU:HA	2:L:1657:SER:OG	2.17	0.44
2:L:2397:CYS:O	2:L:2401:VAL:HG23	2.17	0.44
2:L:3097:ASP:N	2:L:3097:ASP:OD1	2.49	0.44
2:C:115:TYR:CG	2:C:124:LYS:HE3	2.52	0.44
2:C:1742:CYS:HG	2:C:1746:PHE:HE1	1.65	0.44
2:C:3326:GLN:O	2:C:3330:LEU:HD23	2.17	0.44
2:C:3870:SER:O	2:C:3873:LYS:HG2	2.17	0.44
2:L:352:VAL:HG11	2:L:1733:THR:HG22	1.98	0.44
2:L:910:PHE:HE1	2:L:2807:GLN:HG2	1.82	0.44
2:L:1531:LEU:HB3	2:L:1559:PHE:HE2	1.82	0.44
2:L:2884:LEU:HG	2:L:2886:GLN:HE22	1.82	0.44
2:L:3577:GLN:NE2	2:L:3684:SER:OG	2.50	0.44
2:C:250:ASN:OD1	2:C:251:PHE:N	2.50	0.44
2:C:563:LEU:O	2:C:567:GLU:HG2	2.18	0.44
2:C:1010:LEU:HD21	2:C:1036:PHE:CE1	2.52	0.44
2:C:1102:GLU:OE1	2:C:1155:ARG:HB2	2.18	0.44
2:C:2439:ILE:HD12	2:C:2451:LEU:HD21	1.98	0.44
2:C:2855:VAL:O	2:C:2859:GLN:OE1	2.35	0.44
2:C:3630:ARG:N	2:C:3633:ILE:HD12	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:208:MET:HG3	2:L:209:THR:N	2.32	0.44
2:L:250:ASN:OD1	2:L:251:PHE:N	2.50	0.44
2:L:737:PRO:O	2:L:741:ILE:HG12	2.18	0.44
2:L:1102:GLU:OE1	2:L:1155:ARG:HB2	2.18	0.44
2:L:3981:TYR:HE2	2:L:4105:LYS:HG3	1.83	0.44
2:L:4017:GLU:O	2:L:4021:LEU:HG	2.16	0.44
2:C:225:LYS:NZ	2:C:229:SER:HB2	2.33	0.44
2:C:249:PHE:O	2:C:253:LEU:HG	2.18	0.44
2:C:2397:CYS:O	2:C:2401:VAL:HG23	2.17	0.44
2:C:3179:TRP:CD1	2:C:3242:MET:SD	3.10	0.44
2:C:3465:PHE:CD1	2:C:3466:PRO:HD3	2.52	0.44
2:L:1010:LEU:HD23	2:L:1010:LEU:HA	1.84	0.44
2:L:1711:ARG:HE	2:L:1761:LEU:HD21	1.82	0.44
2:L:3138:ILE:HD13	2:L:3189:PHE:HZ	1.82	0.44
2:C:737:PRO:O	2:C:741:ILE:HG12	2.18	0.44
2:C:1653:LEU:HA	2:C:1657:SER:OG	2.17	0.44
2:C:1937:ARG:HA	2:C:1940:TYR:CE2	2.53	0.44
2:C:3736:LYS:O	2:C:3751:LEU:HD12	2.18	0.44
2:C:3833:ARG:NH2	2:C:3838:GLU:HB2	2.33	0.44
2:L:473:PRO:O	2:L:476:ARG:HB2	2.17	0.44
2:L:583:LEU:HD13	2:L:614:PRO:HA	1.99	0.44
2:L:776:TRP:HB3	2:L:785:MET:CE	2.47	0.44
2:L:1572:LEU:O	2:L:1575:LEU:HD22	2.17	0.44
2:L:2385:LEU:HA	2:C:73:LEU:HD22	2.00	0.44
2:C:477:ASN:O	2:C:481:THR:HG23	2.18	0.44
2:C:909:VAL:HG22	2:C:2807:GLN:NE2	2.33	0.44
2:C:1427:SER:HA	2:C:1430:GLU:HB2	2.00	0.44
2:C:2897:LEU:HD21	2:C:2923:TRP:CZ2	2.52	0.44
2:L:531:PHE:O	2:L:535:LEU:HG	2.17	0.44
2:L:1389:VAL:HA	2:L:1392:MET:HB3	1.99	0.44
2:L:2280:VAL:HG13	2:L:2285:LEU:HB2	2.00	0.44
2:L:2851:PHE:CE2	2:L:2853:PRO:HG2	2.53	0.44
2:L:3658:ASP:OD2	2:L:3660:ASN:ND2	2.49	0.44
2:C:1368:LEU:O	2:C:1372:LEU:HG	2.18	0.44
2:C:1572:LEU:O	2:C:1575:LEU:HD22	2.17	0.44
2:C:2219:LEU:O	2:C:2223:VAL:HG23	2.18	0.44
2:C:3308:ASP:HB3	2:C:3330:LEU:HD21	1.99	0.44
2:L:2371:PHE:HE2	2:L:2374:LEU:HB3	1.83	0.44
2:L:2812:LEU:O	2:L:2816:ILE:HG12	2.16	0.44
2:L:3736:LYS:O	2:L:3751:LEU:HD12	2.18	0.44
2:C:741:ILE:HG21	2:C:776:TRP:CE2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:864:GLY:HA2	2:C:867:ASN:OD1	2.17	0.44
2:C:1782:PHE:HD1	2:C:1785:ILE:HD12	1.83	0.44
2:C:2470:ARG:O	2:C:2473:MET:HB2	2.18	0.44
2:C:2506:LEU:HG	2:C:2525:TRP:CZ2	2.52	0.44
2:C:3789:ARG:HB2	2:C:3938:ILE:HD13	2.00	0.44
2:L:73:LEU:HD22	2:C:2385:LEU:HA	1.99	0.43
2:L:948:MET:N	2:L:949:PRO:HD3	2.33	0.43
2:L:1648:LEU:HD12	2:L:1649:LEU:HD12	2.00	0.43
2:L:1712:ARG:HA	2:L:1715:GLU:OE2	2.18	0.43
2:L:2330:VAL:HG22	2:L:2335:ASN:H	1.83	0.43
2:L:2470:ARG:O	2:L:2473:MET:HB2	2.18	0.43
2:L:3530:VAL:HG11	2:L:3568:ILE:HG21	1.99	0.43
2:L:3630:ARG:N	2:L:3633:ILE:HD12	2.32	0.43
2:L:3920:ILE:CG2	2:L:3923:ARG:HH22	2.31	0.43
2:C:352:VAL:HG11	2:C:1733:THR:HG22	1.97	0.43
2:C:397:LEU:HB3	2:C:1744:LYS:CE	2.43	0.43
2:C:1389:VAL:HA	2:C:1392:MET:HB3	1.98	0.43
2:C:1648:LEU:O	2:C:1652:ILE:HG12	2.17	0.43
2:C:1983:ASP:O	2:C:1984:LEU:HB2	2.18	0.43
2:C:2556:SER:HB2	2:C:2799:GLN:HA	2.00	0.43
2:C:2884:LEU:HG	2:C:2886:GLN:HE22	1.82	0.43
2:L:741:ILE:HG21	2:L:776:TRP:CE2	2.52	0.43
2:L:2812:LEU:HD12	2:L:2813:PHE:N	2.34	0.43
2:L:3012:GLU:OE2	2:L:3048:LYS:HG2	2.18	0.43
2:C:208:MET:HG3	2:C:209:THR:N	2.32	0.43
2:C:948:MET:N	2:C:949:PRO:HD3	2.33	0.43
2:C:1111:LEU:HD12	2:C:1131:ILE:HD11	1.99	0.43
2:C:1877:LEU:O	2:C:1881:TYR:HB2	2.18	0.43
2:C:2253:TYR:OH	2:C:2288:TYR:N	2.42	0.43
2:C:3006:ALA:HB3	2:C:3257:LYS:HZ1	1.83	0.43
2:C:3012:GLU:OE2	2:C:3048:LYS:HG2	2.18	0.43
2:L:429:GLU:HA	2:L:432:THR:HG23	2.01	0.43
2:L:560:LEU:O	2:L:564:LEU:HG	2.18	0.43
2:L:893:SER:HA	2:L:907:LEU:H	1.83	0.43
2:L:1376:LEU:HD12	2:L:1403:MET:HE3	2.01	0.43
2:L:1760:GLU:HB2	2:L:1804:MET:SD	2.58	0.43
2:L:2147:ALA:O	2:L:2151:ILE:HG13	2.17	0.43
2:L:3308:ASP:HB3	2:L:3330:LEU:HD21	1.99	0.43
2:C:938:VAL:HA	2:C:941:MET:CE	2.46	0.43
2:C:1760:GLU:HB2	2:C:1804:MET:SD	2.58	0.43
2:C:2182:ILE:HD12	2:C:2225:HIS:NE2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2421:VAL:HG12	2:C:2422:GLN:OE1	2.17	0.43
2:C:2851:PHE:CE2	2:C:2853:PRO:HG2	2.53	0.43
2:L:1368:LEU:O	2:L:1372:LEU:HG	2.18	0.43
2:L:1459:HIS:HB2	2:L:1464:LEU:HD22	2.00	0.43
2:L:2219:LEU:O	2:L:2223:VAL:HG23	2.18	0.43
2:L:2556:SER:HB2	2:L:2799:GLN:HA	2.00	0.43
2:L:3190:LEU:HD12	2:L:3231:ILE:CG2	2.48	0.43
2:L:3411:ASP:O	2:L:3415:THR:HG23	2.19	0.43
2:L:3498:TRP:O	2:L:3502:MET:HG2	2.18	0.43
2:C:3839:TYR:CE2	2:C:4121:TRP:HA	2.54	0.43
2:L:713:GLU:HG2	2:L:717:LYS:NZ	2.33	0.43
2:L:1877:LEU:O	2:L:1881:TYR:HB2	2.18	0.43
2:L:2164:TRP:O	2:L:2164:TRP:CD1	2.71	0.43
2:L:2421:VAL:HG12	2:L:2422:GLN:OE1	2.18	0.43
2:L:3326:GLN:O	2:L:3330:LEU:HD23	2.17	0.43
2:L:3959:MET:HA	2:L:4110:GLN:HE22	1.82	0.43
2:C:135:LEU:HD23	2:C:144:MET:HE1	2.01	0.43
2:C:1921:ASP:N	2:C:1921:ASP:OD1	2.51	0.43
2:C:2164:TRP:CD1	2:C:2164:TRP:O	2.71	0.43
2:C:2280:VAL:HG13	2:C:2285:LEU:HB2	2.00	0.43
2:C:2578:GLU:H	2:C:2784:GLN:NE2	2.13	0.43
2:L:1593:VAL:O	2:L:1596:VAL:HG22	2.18	0.43
2:L:2148:LYS:HD2	2:L:2148:LYS:HA	1.73	0.43
2:L:3465:PHE:CD1	2:L:3466:PRO:HD3	2.52	0.43
2:C:199:ALA:O	2:C:203:GLU:HG2	2.19	0.43
2:C:420:VAL:O	2:C:424:LEU:HG	2.19	0.43
2:C:1711:ARG:HE	2:C:1761:LEU:HD21	1.82	0.43
2:C:1712:ARG:HA	2:C:1715:GLU:OE2	2.18	0.43
2:C:2560:ASN:O	2:C:2564:GLU:HG2	2.19	0.43
2:C:3530:VAL:HG11	2:C:3568:ILE:HG21	1.99	0.43
2:L:12:LEU:HG	2:L:50:VAL:HG21	2.00	0.43
2:L:125:ILE:HB	2:L:126:PRO:HD3	2.01	0.43
2:L:3049:LEU:HD11	2:L:3085:GLU:HB3	2.00	0.43
2:L:3144:PHE:HE2	2:L:3156:PRO:HB2	1.84	0.43
2:L:3324:ARG:HD2	2:L:3391:ALA:HB3	2.00	0.43
2:L:3839:TYR:CE2	2:L:4121:TRP:HA	2.54	0.43
2:L:3981:TYR:OH	2:L:4101:GLU:HB2	2.19	0.43
2:C:231:LEU:HD11	2:C:248:ILE:HD11	2.01	0.43
2:C:713:GLU:HG2	2:C:717:LYS:NZ	2.33	0.43
2:C:1017:ILE:HD13	2:C:1081:ALA:HB2	2.01	0.43
2:C:1593:VAL:O	2:C:1596:VAL:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1643:MET:N	2:C:1643:MET:SD	2.92	0.43
2:C:3144:PHE:HE2	2:C:3156:PRO:HB2	1.84	0.43
2:C:3354:ASP:OD1	2:C:3355:LYS:HD2	2.19	0.43
2:L:249:PHE:O	2:L:253:LEU:HG	2.18	0.43
2:L:420:VAL:O	2:L:424:LEU:HG	2.19	0.43
2:L:1017:ILE:HD13	2:L:1081:ALA:HB2	2.01	0.43
2:L:1983:ASP:O	2:L:1984:LEU:HB2	2.18	0.43
2:L:2182:ILE:HD12	2:L:2225:HIS:NE2	2.33	0.43
2:L:2871:LEU:HD23	2:L:2872:ASP:N	2.34	0.43
2:L:3305:SER:HB2	2:L:3358:ARG:HH21	1.84	0.43
2:L:3701:ILE:HD11	2:L:3750:PHE:CE2	2.52	0.43
2:C:279:ALA:HA	2:C:282:PHE:CE1	2.54	0.43
2:C:1614:GLN:OE1	2:C:1617:LYS:HB2	2.19	0.43
2:C:1623:LEU:HG	2:C:1624:GLN:OE1	2.18	0.43
2:C:2812:LEU:HD12	2:C:2813:PHE:N	2.33	0.43
2:C:3498:TRP:O	2:C:3502:MET:HG2	2.18	0.43
2:C:3823:GLU:HA	2:C:3826:ALA:HB3	2.01	0.43
2:L:563:LEU:O	2:L:567:GLU:HG2	2.18	0.43
2:L:1010:LEU:HD21	2:L:1036:PHE:CZ	2.54	0.43
2:L:1367:HIS:HA	2:L:1370:ARG:HB2	2.01	0.43
2:L:1623:LEU:HG	2:L:1624:GLN:OE1	2.18	0.43
2:L:3565:GLY:HA3	2:L:3697:ASN:HB2	2.01	0.43
2:C:560:LEU:O	2:C:564:LEU:HG	2.18	0.43
2:C:1270:PHE:HA	2:C:1275:THR:HB	2.01	0.43
2:C:1367:HIS:HA	2:C:1370:ARG:HB2	2.01	0.43
2:C:1459:HIS:HB2	2:C:1464:LEU:HD22	2.00	0.43
2:C:2371:PHE:HE2	2:C:2374:LEU:HB3	1.83	0.43
2:C:3842:TRP:HZ3	2:C:3870:SER:CB	2.32	0.43
2:L:225:LYS:NZ	2:L:229:SER:HB2	2.33	0.43
2:L:774:GLU:CD	2:L:854:ARG:HH12	2.20	0.43
2:L:788:TYR:O	2:L:792:ILE:HG12	2.19	0.43
2:L:1427:SER:HA	2:L:1430:GLU:HB2	2.00	0.43
2:L:1874:TYR:HB3	2:L:1947:CYS:HB2	2.01	0.43
2:L:2193:ILE:HD12	2:L:2245:TRP:HH2	1.82	0.43
2:L:3789:ARG:HB2	2:L:3938:ILE:HD13	2.00	0.43
2:C:1066:LEU:HB3	2:C:1078:ALA:HB2	2.01	0.43
2:C:1142:HIS:CG	2:C:1197:LEU:HD12	2.54	0.43
2:C:2094:MET:O	2:C:2098:THR:OG1	2.19	0.43
2:C:2510:LEU:HD13	2:C:2557:LEU:HG	2.01	0.43
2:C:2538:ARG:NH1	2:C:2565:MET:SD	2.92	0.43
2:C:3305:SER:HB2	2:C:3358:ARG:HH21	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3411:ASP:O	2:C:3415:THR:HG23	2.19	0.43
2:C:3629:ARG:HH12	2:C:3634:GLN:HB3	1.84	0.43
2:L:886:TRP:CE2	2:L:964:ARG:HD3	2.54	0.42
2:L:1270:PHE:HA	2:L:1275:THR:HB	2.01	0.42
2:L:1291:LEU:HD12	2:L:1292:LYS:N	2.34	0.42
2:L:1643:MET:N	2:L:1643:MET:SD	2.91	0.42
2:L:1782:PHE:HD1	2:L:1785:ILE:HD12	1.83	0.42
2:L:1937:ARG:HA	2:L:1940:TYR:CE2	2.53	0.42
2:L:2560:ASN:O	2:L:2564:GLU:HG2	2.19	0.42
2:L:2869:LEU:HD21	2:L:2899:ARG:HG3	2.01	0.42
2:L:3088:LEU:HA	2:L:3091:LEU:HD12	2.00	0.42
2:L:3354:ASP:OD1	2:L:3355:LYS:HD2	2.19	0.42
2:L:3951:GLN:O	2:L:4036:LYS:HE3	2.19	0.42
2:C:886:TRP:CE2	2:C:964:ARG:HD3	2.54	0.42
2:C:2330:VAL:HG22	2:C:2335:ASN:H	1.83	0.42
2:C:2871:LEU:HD23	2:C:2872:ASP:N	2.34	0.42
2:C:3447:VAL:HG12	2:C:3475:TYR:CE1	2.54	0.42
2:C:3760:GLN:OE1	2:C:3760:GLN:N	2.48	0.42
2:C:3920:ILE:CG2	2:C:3923:ARG:HH22	2.31	0.42
2:C:3923:ARG:HB2	2:C:4124:TRP:CH2	2.54	0.42
2:C:3959:MET:HA	2:C:4110:GLN:HE22	1.83	0.42
2:C:3981:TYR:HE2	2:C:4105:LYS:HG3	1.83	0.42
2:L:1237:ALA:O	2:L:1241:LEU:HG	2.20	0.42
2:L:1921:ASP:OD1	2:L:1921:ASP:N	2.51	0.42
2:L:2148:LYS:NZ	2:L:2152:ASN:OD1	2.45	0.42
2:L:2413:PHE:CD1	2:L:2416:LYS:HD2	2.54	0.42
2:L:2510:LEU:HD13	2:L:2557:LEU:HG	2.01	0.42
2:L:2919:ASP:OD1	2:L:2919:ASP:N	2.52	0.42
2:L:3008:TRP:HB2	2:L:3051:LEU:CD2	2.49	0.42
2:L:3103:ILE:O	2:L:3107:ILE:HG12	2.19	0.42
2:L:3629:ARG:HH12	2:L:3634:GLN:HB3	1.84	0.42
2:C:1101:PHE:CZ	2:C:1168:LEU:HD12	2.54	0.42
2:C:1125:GLN:OE1	2:C:1125:GLN:N	2.44	0.42
2:C:1794:GLN:O	2:C:1797:LEU:HG	2.19	0.42
2:C:3008:TRP:HB2	2:C:3051:LEU:CD2	2.49	0.42
2:C:3332:THR:O	2:C:3335:ARG:HG2	2.19	0.42
2:C:3614:TYR:C	2:C:3616:ALA:H	2.22	0.42
2:L:485:GLN:CB	2:L:489:ARG:HH12	2.29	0.42
2:L:1935:GLU:O	2:L:1939:LEU:HD23	2.19	0.42
2:L:3701:ILE:HG22	2:L:3717:VAL:O	2.19	0.42
2:C:1188:ILE:CD1	2:C:1269:THR:HG21	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1291:LEU:HD12	2:C:1292:LYS:N	2.34	0.42
2:C:1648:LEU:HD12	2:C:1649:LEU:HD12	2.00	0.42
2:C:3842:TRP:HZ3	2:C:3870:SER:HB3	1.84	0.42
2:L:199:ALA:O	2:L:203:GLU:HG2	2.19	0.42
2:L:2281:MET:SD	2:L:2282:ALA:N	2.92	0.42
2:L:3048:LYS:CE	2:L:3061:LEU:HB2	2.47	0.42
2:L:3781:CYS:SG	2:L:3786:LEU:HD22	2.59	0.42
2:L:3923:ARG:HB2	2:L:4124:TRP:CH2	2.54	0.42
2:C:569:VAL:HG13	2:C:645:TRP:CZ3	2.54	0.42
2:C:884:VAL:HA	2:C:3890:MET:O	2.19	0.42
2:C:1872:GLY:O	2:C:1876:ILE:HG12	2.19	0.42
2:C:2281:MET:SD	2:C:2282:ALA:N	2.92	0.42
2:C:2829:LYS:HG3	2:C:2830:ASN:N	2.35	0.42
2:C:3179:TRP:NE1	2:C:3242:MET:SD	2.93	0.42
2:C:3565:GLY:HA3	2:C:3697:ASN:HB2	2.01	0.42
2:C:3781:CYS:SG	2:C:3786:LEU:HD22	2.59	0.42
2:L:279:ALA:HA	2:L:282:PHE:CE1	2.54	0.42
2:L:477:ASN:O	2:L:481:THR:HG23	2.18	0.42
2:L:569:VAL:HG13	2:L:645:TRP:CZ3	2.54	0.42
2:L:1041:ILE:O	2:L:1044:ILE:HG12	2.20	0.42
2:L:1825:LEU:HD12	2:L:1879:VAL:HG21	2.01	0.42
2:L:3179:TRP:NE1	2:L:3242:MET:SD	2.93	0.42
2:L:3332:THR:O	2:L:3335:ARG:HG2	2.19	0.42
2:L:3450:MET:SD	2:L:3451:LEU:N	2.92	0.42
2:L:3598:LYS:HG3	2:L:3599:THR:H	1.84	0.42
2:L:3681:LYS:HZ3	2:L:3724:GLU:HG3	1.85	0.42
2:L:3838:GLU:HB3	2:L:3874:ARG:CD	2.45	0.42
2:L:3842:TRP:HZ3	2:L:3870:SER:HB3	1.84	0.42
2:C:893:SER:HA	2:C:907:LEU:H	1.83	0.42
2:C:2413:PHE:CD1	2:C:2416:LYS:HD2	2.54	0.42
2:C:3088:LEU:HA	2:C:3091:LEU:HD12	2.00	0.42
2:C:3103:ILE:O	2:C:3107:ILE:HG12	2.19	0.42
2:C:3447:VAL:HB	2:C:3485:LYS:HZ3	1.83	0.42
2:C:3879:PRO:HG2	2:C:3882:LEU:HD21	2.02	0.42
2:C:3951:GLN:O	2:C:4036:LYS:HE3	2.19	0.42
2:L:979:VAL:HA	2:L:982:GLN:HE21	1.85	0.42
2:L:1066:LEU:HB3	2:L:1078:ALA:HB2	2.01	0.42
2:L:1422:LYS:N	2:L:1422:LYS:HD2	2.35	0.42
2:L:1648:LEU:CD1	2:L:1649:LEU:HD12	2.50	0.42
2:L:1872:GLY:O	2:L:1876:ILE:HG12	2.19	0.42
2:L:2538:ARG:NH1	2:L:2565:MET:SD	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2998:SER:HA	2:L:3001:CYS:SG	2.60	0.42
2:L:3842:TRP:HZ3	2:L:3870:SER:CB	2.32	0.42
2:L:4100:GLU:H	2:L:4100:GLU:CD	2.23	0.42
2:C:318:SER:O	2:C:322:GLN:HG2	2.20	0.42
2:C:602:MET:O	2:C:604:PRO:HD3	2.20	0.42
2:C:909:VAL:HG22	2:C:2807:GLN:HE21	1.84	0.42
2:C:1708:GLU:OE1	2:C:1712:ARG:HB3	2.19	0.42
2:C:1860:GLU:HB3	2:C:1862:THR:HG22	2.02	0.42
2:C:2931:ARG:NH2	2:C:3000:ASP:OD2	2.52	0.42
2:C:3450:MET:SD	2:C:3451:LEU:N	2.93	0.42
2:C:3701:ILE:HG22	2:C:3717:VAL:O	2.19	0.42
2:C:3981:TYR:OH	2:C:4101:GLU:HB2	2.19	0.42
2:L:602:MET:O	2:L:604:PRO:HD3	2.19	0.42
2:L:741:ILE:O	2:L:745:VAL:HG22	2.20	0.42
2:L:884:VAL:HA	2:L:3890:MET:O	2.19	0.42
2:L:1604:SER:HA	2:L:1607:GLU:HG3	2.02	0.42
2:L:2327:LEU:HD11	2:L:2342:CYS:SG	2.60	0.42
2:L:3502:MET:SD	2:L:3514:VAL:HG11	2.60	0.42
2:L:3645:GLY:HA2	2:L:3649:SER:N	2.34	0.42
2:C:979:VAL:HA	2:C:982:GLN:NE2	2.34	0.42
2:C:2327:LEU:HD11	2:C:2342:CYS:SG	2.60	0.42
2:C:3305:SER:HB2	2:C:3358:ARG:NH2	2.34	0.42
2:C:3681:LYS:HZ3	2:C:3724:GLU:HG3	1.84	0.42
2:L:1101:PHE:CZ	2:L:1168:LEU:HD12	2.54	0.42
2:L:1328:GLU:OE1	2:L:1329:ARG:HD2	2.20	0.42
2:L:3305:SER:HB2	2:L:3358:ARG:NH2	2.34	0.42
2:C:429:GLU:HA	2:C:432:THR:HG23	2.01	0.42
2:C:788:TYR:O	2:C:792:ILE:HG12	2.19	0.42
2:C:2486:ASP:HB3	2:C:2487:PRO:HD3	2.02	0.42
2:C:4046:TYR:OH	2:C:4062:ASP:HB3	2.19	0.42
2:L:69:VAL:HA	2:L:78:PHE:CZ	2.55	0.42
2:L:421:LEU:HD12	2:L:467:ALA:HB3	2.02	0.42
2:L:891:ARG:HD3	2:L:955:ALA:HB1	2.02	0.42
2:L:947:GLN:HE21	2:L:954:GLY:HA2	1.85	0.42
2:L:1125:GLN:OE1	2:L:1125:GLN:N	2.44	0.42
2:L:1170:LYS:HA	2:L:1173:LEU:HD12	2.02	0.42
2:L:1670:GLU:O	2:L:1674:THR:HG23	2.20	0.42
2:L:2834:GLN:HA	2:L:2837:LEU:HG	2.02	0.42
2:L:3385:LEU:O	2:L:3389:VAL:HG13	2.19	0.42
2:L:3823:GLU:HA	2:L:3826:ALA:HB3	2.01	0.42
2:L:3930:VAL:HG13	2:L:3937:VAL:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:ILE:HB	2:C:126:PRO:HD3	2.01	0.42
2:C:1328:GLU:OE1	2:C:1329:ARG:NH2	2.53	0.42
2:C:1825:LEU:HD12	2:C:1879:VAL:HG21	2.01	0.42
2:C:1935:GLU:O	2:C:1939:LEU:HD23	2.19	0.42
2:C:2309:PHE:CE2	2:C:2318:ALA:N	2.84	0.42
2:C:3049:LEU:HD11	2:C:3085:GLU:HB3	2.00	0.42
2:C:3324:ARG:HD2	2:C:3391:ALA:HB3	2.01	0.42
2:L:225:LYS:HZ1	2:L:229:SER:HB2	1.85	0.42
2:L:397:LEU:HB3	2:L:1744:LYS:CE	2.44	0.42
2:L:414:LEU:CD2	2:L:442:GLN:HG2	2.39	0.42
2:L:999:LYS:HB2	2:L:999:LYS:HE3	1.94	0.42
2:L:1188:ILE:CD1	2:L:1269:THR:HG21	2.49	0.42
2:L:1614:GLN:OE1	2:L:1617:LYS:HB2	2.19	0.42
2:L:3561:LYS:HB2	2:L:3561:LYS:HE3	1.85	0.42
2:C:741:ILE:O	2:C:745:VAL:HG22	2.20	0.42
2:C:774:GLU:OE2	2:C:854:ARG:NH1	2.33	0.42
2:C:1237:ALA:O	2:C:1241:LEU:HG	2.20	0.42
2:C:1648:LEU:CD1	2:C:1649:LEU:HD12	2.49	0.42
2:C:3190:LEU:O	2:C:3193:ILE:HG22	2.20	0.42
2:C:3593:ARG:NH2	2:C:3598:LYS:HA	2.35	0.42
2:C:3645:GLY:HA2	2:C:3649:SER:N	2.34	0.42
2:C:3658:ASP:OD2	2:C:3660:ASN:ND2	2.49	0.42
2:C:3857:LEU:O	2:C:3861:GLY:N	2.52	0.42
2:L:631:ARG:NH1	2:L:668:LYS:HD2	2.35	0.41
2:L:924:ARG:O	2:L:927:LYS:HB3	2.20	0.41
2:L:1533:LEU:O	2:L:1533:LEU:HD23	2.20	0.41
2:L:1708:GLU:OE1	2:L:1712:ARG:HB3	2.19	0.41
2:L:1876:ILE:HG13	2:L:1877:LEU:N	2.35	0.41
2:L:3327:ASN:HB3	2:L:3384:HIS:HB3	2.02	0.41
2:L:3517:SER:O	2:L:3520:GLU:HG3	2.20	0.41
2:C:200:PHE:HB3	2:C:227:LEU:HD13	2.01	0.41
2:C:425:ASP:O	2:C:1549:SER:HA	2.20	0.41
2:C:436:GLU:O	2:C:440:VAL:HG23	2.20	0.41
2:C:732:PHE:HD2	2:C:733:LEU:HD22	1.85	0.41
2:C:947:GLN:HE21	2:C:954:GLY:HA2	1.85	0.41
2:C:979:VAL:HA	2:C:982:GLN:HE21	1.85	0.41
2:C:1067:ALA:HB2	2:C:1107:TYR:CE1	2.54	0.41
2:C:1103:ALA:HB1	2:C:1107:TYR:CE2	2.55	0.41
2:C:2148:LYS:HA	2:C:2148:LYS:HD2	1.73	0.41
2:C:3356:ALA:HA	2:C:3359:ILE:HD12	2.02	0.41
2:L:200:PHE:HB3	2:L:227:LEU:HD13	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:409:GLN:HB3	2:L:412:SER:OG	2.20	0.41
2:L:425:ASP:O	2:L:1549:SER:HA	2.20	0.41
2:L:1041:ILE:HA	2:L:1044:ILE:HG23	2.03	0.41
2:L:1067:ALA:HB2	2:L:1107:TYR:CE1	2.54	0.41
2:L:1102:GLU:O	2:L:1106:ILE:HG12	2.20	0.41
2:L:3664:ASN:HA	2:L:3667:LEU:HB2	2.02	0.41
2:L:3857:LEU:O	2:L:3861:GLY:N	2.52	0.41
2:L:4046:TYR:OH	2:L:4062:ASP:HB3	2.19	0.41
2:C:12:LEU:HG	2:C:50:VAL:HG21	2.00	0.41
2:C:924:ARG:O	2:C:927:LYS:HB3	2.20	0.41
2:C:1709:GLU:H	2:C:1709:GLU:CD	2.23	0.41
2:C:2834:GLN:HA	2:C:2837:LEU:HG	2.02	0.41
2:C:2998:SER:HA	2:C:3001:CYS:SG	2.60	0.41
2:C:3087:SER:O	2:C:3091:LEU:HG	2.20	0.41
2:C:3327:ASN:HB3	2:C:3384:HIS:HB3	2.02	0.41
2:C:3555:VAL:HA	2:C:3558:ILE:HG22	2.03	0.41
2:C:3858:MET:SD	2:C:4119:ARG:HD3	2.60	0.41
2:C:4100:GLU:H	2:C:4100:GLU:CD	2.23	0.41
1:Q:6016:UNK:C	1:Q:6018:UNK:H	2.28	0.41
2:L:231:LEU:HD11	2:L:248:ILE:HD11	2.01	0.41
2:L:670:LEU:O	2:L:674:VAL:HG22	2.20	0.41
2:L:979:VAL:HA	2:L:982:GLN:NE2	2.34	0.41
2:L:1105:VAL:HA	2:L:1108:MET:CE	2.51	0.41
2:L:1219:PHE:O	2:L:1223:THR:OG1	2.29	0.41
2:L:1473:THR:OG1	2:L:1475:LEU:O	2.30	0.41
2:L:1876:ILE:O	2:L:1880:MET:HG3	2.20	0.41
2:L:2148:LYS:HA	2:L:2151:ILE:HD12	2.02	0.41
2:L:2413:PHE:HA	2:L:2416:LYS:HG3	2.02	0.41
2:L:2453:GLU:HA	2:L:2456:ASN:ND2	2.35	0.41
2:L:2829:LYS:HG3	2:L:2830:ASN:N	2.35	0.41
2:L:3447:VAL:HG12	2:L:3475:TYR:CE1	2.55	0.41
2:C:176:GLU:O	2:C:180:LEU:HD23	2.21	0.41
2:C:572:VAL:HA	2:C:575:ILE:HG12	2.02	0.41
2:C:623:PHE:O	2:C:627:VAL:HG23	2.21	0.41
2:C:1010:LEU:HD21	2:C:1036:PHE:CZ	2.54	0.41
2:C:1050:GLU:HA	2:C:1050:GLU:OE1	2.21	0.41
2:C:1147:LYS:HZ2	2:C:1149:LYS:HD3	1.86	0.41
2:C:1333:SER:O	2:C:1337:VAL:HG23	2.20	0.41
2:C:2148:LYS:NZ	2:C:2152:ASN:OD1	2.45	0.41
2:C:2459:VAL:HG22	2:C:2505:VAL:HG11	2.03	0.41
2:C:3074:GLN:O	2:C:3078:LEU:HD23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3517:SER:O	2:C:3520:GLU:HG3	2.20	0.41
2:L:155:LYS:HB3	2:L:155:LYS:HE3	1.93	0.41
2:L:229:SER:HA	2:L:273:ARG:HH22	1.85	0.41
2:L:1133:HIS:O	2:L:1136:ARG:HB2	2.20	0.41
2:L:1142:HIS:CG	2:L:1197:LEU:HD12	2.54	0.41
2:L:1168:LEU:O	2:L:1168:LEU:HD23	2.21	0.41
2:L:1862:THR:O	2:L:1865:THR:HG22	2.21	0.41
2:L:3454:LEU:HD11	2:L:3471:ILE:HG21	2.02	0.41
2:C:631:ARG:NH1	2:C:668:LYS:HD2	2.35	0.41
2:C:1168:LEU:HD23	2:C:1168:LEU:O	2.21	0.41
2:C:1207:TRP:O	2:C:1211:VAL:HG23	2.20	0.41
2:C:1422:LYS:HD2	2:C:1422:LYS:N	2.35	0.41
2:C:1862:THR:O	2:C:1865:THR:HG22	2.21	0.41
2:C:1874:TYR:HB3	2:C:1947:CYS:HB2	2.01	0.41
2:C:2148:LYS:HA	2:C:2151:ILE:HD12	2.02	0.41
2:C:3161:LEU:O	2:C:3165:THR:HG23	2.20	0.41
2:L:909:VAL:HG22	2:L:2807:GLN:HE21	1.84	0.41
2:L:1794:GLN:O	2:L:1797:LEU:HG	2.19	0.41
2:L:3006:ALA:HB3	2:L:3257:LYS:NZ	2.36	0.41
2:L:3612:ARG:CG	2:L:3799:ARG:HH12	2.34	0.41
2:L:3644:PHE:CD2	2:L:3648:GLY:HA3	2.56	0.41
2:C:939:MET:HE3	2:C:2783:ILE:HG13	2.03	0.41
2:C:1137:ILE:H	2:C:1137:ILE:HD12	1.86	0.41
2:C:1604:SER:HA	2:C:1607:GLU:HG3	2.02	0.41
2:C:1851:LEU:HB3	2:C:1918:LEU:HD13	2.03	0.41
2:C:3598:LYS:HG3	2:C:3599:THR:H	1.84	0.41
2:C:3628:PHE:CD2	2:C:3685:PRO:HG2	2.56	0.41
2:L:653:LEU:HD11	2:L:669:LEU:HD12	2.02	0.41
2:L:660:LEU:O	2:L:662:LEU:N	2.49	0.41
2:L:721:TYR:HD2	2:L:729:CYS:SG	2.44	0.41
2:L:738:HIS:CD2	2:L:779:TYR:HB3	2.56	0.41
2:L:1050:GLU:HA	2:L:1050:GLU:OE1	2.21	0.41
2:L:1328:GLU:OE1	2:L:1329:ARG:NH2	2.53	0.41
2:L:2205:VAL:HG22	2:L:2207:LYS:H	1.86	0.41
2:L:3593:ARG:NH2	2:L:3598:LYS:HA	2.35	0.41
2:C:1041:ILE:O	2:C:1044:ILE:HG12	2.20	0.41
2:C:2205:VAL:HG22	2:C:2207:LYS:H	1.86	0.41
2:C:2371:PHE:CE2	2:C:2374:LEU:HB3	2.55	0.41
2:C:3930:VAL:HG13	2:C:3937:VAL:HG12	2.01	0.41
2:C:4036:LYS:O	2:C:4036:LYS:HG3	2.21	0.41
2:L:176:GLU:O	2:L:180:LEU:HD23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2453:GLU:OE1	2:L:2453:GLU:N	2.45	0.41
2:L:3087:SER:O	2:L:3091:LEU:HG	2.20	0.41
2:L:3447:VAL:HB	2:L:3485:LYS:HZ3	1.85	0.41
2:C:738:HIS:CD2	2:C:779:TYR:HB3	2.56	0.41
2:C:1250:LEU:HB2	2:C:1310:GLU:OE2	2.21	0.41
2:C:1475:LEU:HD12	2:C:1475:LEU:O	2.20	0.41
2:C:1707:LEU:HG	2:C:1709:GLU:HG3	2.03	0.41
2:C:1715:GLU:O	2:C:1719:VAL:HG22	2.21	0.41
2:C:2456:ASN:O	2:C:2459:VAL:HB	2.21	0.41
2:C:3385:LEU:O	2:C:3389:VAL:HG13	2.19	0.41
2:C:3701:ILE:HD11	2:C:3750:PHE:CE2	2.52	0.41
2:L:414:LEU:HA	2:L:417:VAL:HG22	2.03	0.41
2:L:602:MET:HA	2:L:1087:ARG:NH1	2.36	0.41
2:L:732:PHE:HD2	2:L:733:LEU:HD22	1.85	0.41
2:L:1104:LEU:HD12	2:L:1104:LEU:HA	1.86	0.41
2:L:1137:ILE:H	2:L:1137:ILE:HD12	1.85	0.41
2:L:2168:LEU:HD13	2:L:2193:ILE:HG22	2.02	0.41
2:L:2435:CYS:O	2:L:2438:ILE:HB	2.21	0.41
2:L:2458:VAL:HG12	2:L:2473:MET:HE3	2.02	0.41
2:L:3323:PHE:O	2:L:3326:GLN:HG3	2.20	0.41
2:L:3374:ILE:HG13	2:L:3375:ALA:N	2.35	0.41
2:L:3561:LYS:O	2:L:3564:GLN:NE2	2.54	0.41
2:L:3879:PRO:HG2	2:L:3882:LEU:HD21	2.02	0.41
2:C:1041:ILE:HA	2:C:1044:ILE:HG23	2.02	0.41
2:C:1105:VAL:HA	2:C:1108:MET:CE	2.51	0.41
2:C:1170:LYS:HA	2:C:1173:LEU:HD12	2.02	0.41
2:C:1261:LEU:HD22	2:C:1337:VAL:HG22	2.03	0.41
2:C:2168:LEU:HD13	2:C:2193:ILE:HG22	2.02	0.41
2:C:3323:PHE:O	2:C:3326:GLN:HG3	2.20	0.41
2:C:3502:MET:SD	2:C:3514:VAL:HG11	2.60	0.41
2:C:3644:PHE:CD2	2:C:3648:GLY:HA3	2.56	0.41
1:R:6016:UNK:C	1:R:6018:UNK:N	2.84	0.41
2:L:274:LEU:HA	2:L:274:LEU:HD12	1.87	0.41
2:L:361:ILE:HD12	2:L:364:ARG:HB2	2.03	0.41
2:L:436:GLU:O	2:L:440:VAL:HG23	2.20	0.41
2:L:744:ASP:OD1	2:L:745:VAL:N	2.54	0.41
2:L:1205:ASN:OD1	2:L:1275:THR:HA	2.21	0.41
2:L:1207:TRP:O	2:L:1211:VAL:HG23	2.20	0.41
2:L:1333:SER:O	2:L:1337:VAL:HG23	2.20	0.41
2:L:1475:LEU:O	2:L:1475:LEU:HD12	2.20	0.41
2:L:1709:GLU:H	2:L:1709:GLU:CD	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1794:GLN:O	2:L:1798:LEU:HG	2.21	0.41
2:L:1860:GLU:HB3	2:L:1862:THR:HG22	2.02	0.41
2:L:1976:LEU:HD21	2:L:2087:GLU:HG2	2.03	0.41
2:L:2456:ASN:O	2:L:2459:VAL:HB	2.21	0.41
2:L:2459:VAL:HG22	2:L:2505:VAL:HG11	2.03	0.41
2:L:2558:ALA:O	2:L:2562:LEU:HG	2.21	0.41
2:L:2851:PHE:HA	2:L:2852:PRO:HD3	1.95	0.41
2:L:3180:ASP:OD1	2:L:3180:ASP:N	2.54	0.41
2:L:3249:GLN:HE22	2:L:3783:GLN:NE2	2.19	0.41
2:L:3356:ALA:HA	2:L:3359:ILE:HD12	2.02	0.41
2:L:3588:TRP:HD1	2:L:3610:TYR:OH	2.01	0.41
2:L:3614:TYR:C	2:L:3616:ALA:H	2.22	0.41
2:L:4022:LYS:HA	2:L:4028:ILE:HD11	2.03	0.41
2:C:248:ILE:O	2:C:252:VAL:HG23	2.21	0.41
2:C:602:MET:HA	2:C:1087:ARG:NH1	2.36	0.41
2:C:891:ARG:HD3	2:C:955:ALA:HB1	2.02	0.41
2:C:1328:GLU:OE1	2:C:1329:ARG:HD2	2.20	0.41
2:C:1448:LEU:O	2:C:1452:VAL:HG12	2.21	0.41
2:C:1533:LEU:HD23	2:C:1533:LEU:O	2.20	0.41
2:C:1670:GLU:O	2:C:1674:THR:HG23	2.20	0.41
2:C:1876:ILE:HG13	2:C:1877:LEU:N	2.35	0.41
2:C:2093:CYS:SG	2:C:2097:LEU:HD12	2.61	0.41
2:C:2558:ALA:O	2:C:2562:LEU:HG	2.21	0.41
2:C:2869:LEU:HD21	2:C:2899:ARG:HG3	2.01	0.41
2:C:3764:VAL:HG11	2:C:3941:ASP:OD2	2.21	0.41
2:C:3975:LYS:HD2	2:C:3976:GLU:H	1.86	0.41
2:C:4113:ASP:HB3	2:C:4116:ILE:HG12	2.03	0.41
2:L:623:PHE:O	2:L:627:VAL:HG23	2.21	0.41
2:L:643:GLU:HG2	2:L:644:PRO:CD	2.49	0.41
2:L:2371:PHE:CE2	2:L:2374:LEU:HB3	2.55	0.41
2:L:3161:LEU:O	2:L:3165:THR:HG23	2.20	0.41
2:L:3190:LEU:O	2:L:3193:ILE:HG22	2.20	0.41
2:L:3598:LYS:HG3	2:L:3599:THR:N	2.36	0.41
2:L:4113:ASP:HB3	2:L:4116:ILE:HG12	2.03	0.41
2:C:35:ILE:H	2:C:35:ILE:HD12	1.86	0.41
2:C:69:VAL:HA	2:C:78:PHE:CZ	2.55	0.41
2:C:670:LEU:O	2:C:674:VAL:HG22	2.20	0.41
2:C:985:GLU:HA	2:C:988:VAL:HG12	2.02	0.41
2:C:1145:LEU:HD23	2:C:1165:LEU:HD13	2.03	0.41
2:C:1755:SER:O	2:C:1759:LEU:HD13	2.21	0.41
2:C:2266:ASN:O	2:C:2309:PHE:HE1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2580:PRO:HA	2:C:2780:LEU:HD11	2.03	0.41
2:C:3180:ASP:OD1	2:C:3180:ASP:N	2.54	0.41
2:C:3374:ILE:HG13	2:C:3375:ALA:N	2.36	0.41
2:C:3598:LYS:HG3	2:C:3599:THR:N	2.36	0.41
2:C:4000:ASN:HA	2:C:4003:ASP:OD2	2.21	0.41
2:L:318:SER:O	2:L:322:GLN:HG2	2.20	0.40
2:L:379:LYS:HZ3	2:L:1551:ILE:HD11	1.86	0.40
2:L:572:VAL:HA	2:L:575:ILE:HG12	2.02	0.40
2:L:1250:LEU:HB2	2:L:1310:GLU:OE2	2.21	0.40
2:L:3764:VAL:HG11	2:L:3941:ASP:OD2	2.21	0.40
2:L:4029:GLN:HG2	2:L:4030:GLU:N	2.36	0.40
2:C:421:LEU:HD12	2:C:467:ALA:HB3	2.02	0.40
2:C:1102:GLU:O	2:C:1106:ILE:HG12	2.20	0.40
2:C:1794:GLN:O	2:C:1798:LEU:HG	2.21	0.40
2:C:2453:GLU:HA	2:C:2456:ASN:ND2	2.35	0.40
2:C:3475:TYR:HB3	2:C:3479:THR:CG2	2.51	0.40
2:C:3789:ARG:CB	2:C:3938:ILE:HD13	2.51	0.40
2:C:4029:GLN:HG2	2:C:4030:GLU:N	2.36	0.40
1:Q:6016:UNK:C	1:Q:6018:UNK:N	2.84	0.40
2:L:1715:GLU:O	2:L:1719:VAL:HG22	2.21	0.40
2:L:1755:SER:O	2:L:1759:LEU:HD13	2.21	0.40
2:L:2266:ASN:O	2:L:2309:PHE:HE1	2.03	0.40
2:L:2486:ASP:HB3	2:L:2487:PRO:HD3	2.02	0.40
2:L:2859:GLN:HE21	2:L:2876:VAL:HG23	1.86	0.40
2:L:3645:GLY:HA2	2:L:3649:SER:H	1.86	0.40
2:L:3764:VAL:HA	2:L:3767:LEU:HG	2.03	0.40
2:C:631:ARG:HH11	2:C:668:LYS:HD2	1.87	0.40
2:C:1131:ILE:H	2:C:1131:ILE:HD12	1.86	0.40
2:C:1750:LEU:HD11	2:C:1758:LEU:CD2	2.52	0.40
2:C:3561:LYS:O	2:C:3564:GLN:NE2	2.54	0.40
2:C:3664:ASN:HA	2:C:3667:LEU:HB2	2.02	0.40
2:L:985:GLU:HA	2:L:988:VAL:HG12	2.03	0.40
2:L:1131:ILE:HD12	2:L:1131:ILE:H	1.86	0.40
2:L:2093:CYS:SG	2:L:2097:LEU:HD12	2.61	0.40
2:L:2584:CYS:SG	2:L:2585:GLU:N	2.94	0.40
2:C:409:GLN:HB3	2:C:412:SER:OG	2.20	0.40
2:C:573:LEU:HA	2:C:576:VAL:HG12	2.03	0.40
2:C:660:LEU:O	2:C:662:LEU:N	2.49	0.40
2:C:732:PHE:CD2	2:C:733:LEU:HD22	2.57	0.40
2:C:1133:HIS:O	2:C:1136:ARG:HB2	2.20	0.40
2:C:1560:TYR:HE2	2:C:1596:VAL:HB	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1876:ILE:O	2:C:1880:MET:HG3	2.20	0.40
2:C:3454:LEU:HD11	2:C:3471:ILE:HG21	2.02	0.40
2:C:3471:ILE:HA	2:C:3474:ARG:HH21	1.85	0.40
2:L:585:ILE:C	2:L:613:HIS:HB2	2.42	0.40
2:L:732:PHE:CD2	2:L:733:LEU:HD22	2.57	0.40
2:L:889:GLU:HA	2:L:3889:ARG:NH1	2.36	0.40
2:L:925:GLN:HE21	2:L:925:GLN:HB3	1.57	0.40
2:L:1155:ARG:NE	2:L:1158:PRO:HD2	2.36	0.40
2:L:1758:LEU:HA	2:L:1761:LEU:HD12	2.03	0.40
2:L:2785:ILE:HG22	2:L:2786:LYS:N	2.37	0.40
2:L:3555:VAL:HA	2:L:3558:ILE:HG22	2.02	0.40
2:L:3710:LYS:HA	2:L:3711:PRO:HD3	1.95	0.40
2:L:3858:MET:SD	2:L:4119:ARG:HD3	2.60	0.40
2:C:1208:LEU:HD23	2:C:1208:LEU:HA	1.92	0.40
2:C:1779:GLN:O	2:C:1783:ARG:HG3	2.22	0.40
2:C:2413:PHE:HA	2:C:2416:LYS:HG3	2.03	0.40
2:C:2435:CYS:O	2:C:2438:ILE:HB	2.21	0.40
2:C:4076:ASP:OD1	2:C:4076:ASP:N	2.54	0.40
1:R:6016:UNK:C	1:R:6018:UNK:H	2.28	0.40
2:L:1103:ALA:HB1	2:L:1107:TYR:CE2	2.55	0.40
2:L:1261:LEU:HD22	2:L:1337:VAL:HG22	2.03	0.40
2:L:1369:MET:HA	2:L:1372:LEU:HD12	2.04	0.40
2:L:1750:LEU:HD11	2:L:1758:LEU:CD2	2.52	0.40
2:L:1811:ARG:HD2	2:L:1816:ARG:NH1	2.37	0.40
2:L:3577:GLN:HE22	2:L:3684:SER:CB	2.34	0.40
2:L:3631:LYS:HG3	2:L:3683:CYS:HA	2.04	0.40
2:L:3842:TRP:HA	2:L:3845:LYS:CB	2.50	0.40
2:L:4036:LYS:HG3	2:L:4036:LYS:O	2.21	0.40
2:C:321:LYS:O	2:C:321:LYS:HD2	2.21	0.40
2:C:414:LEU:HA	2:C:417:VAL:HG22	2.03	0.40
2:C:627:VAL:HG13	2:C:669:LEU:HD21	2.04	0.40
2:C:721:TYR:HD2	2:C:729:CYS:SG	2.44	0.40
2:C:1155:ARG:NE	2:C:1158:PRO:HD2	2.36	0.40
2:C:2859:GLN:HE21	2:C:2876:VAL:HG23	1.87	0.40
2:C:3006:ALA:HB3	2:C:3257:LYS:NZ	2.36	0.40
2:C:3041:LEU:N	2:C:3042:PRO:HD2	2.36	0.40
2:C:3367:SER:OG	2:C:3368:GLU:N	2.55	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	
2	C	3632/4128 (88%)	3344 (92%)	288 (8%)	0	100	100
2	L	3632/4128 (88%)	3343 (92%)	289 (8%)	0	100	100
All	All	7264/8256 (88%)	6687 (92%)	577 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	C	3266/3671 (89%)	3255 (100%)	11 (0%)	92	94
2	L	3266/3671 (89%)	3255 (100%)	11 (0%)	92	94
All	All	6532/7342 (89%)	6510 (100%)	22 (0%)	92	94

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	868	LYS
2	L	925	GLN
2	L	1213	LYS
2	L	1527	ARG
2	L	1913	LYS
2	L	2158	ARG
2	L	2485	ARG
2	L	2940	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	3452	LYS
2	L	3733	ARG
2	L	3863	ASN
2	C	868	LYS
2	C	925	GLN
2	C	1213	LYS
2	C	1527	ARG
2	C	1913	LYS
2	C	2158	ARG
2	C	2485	ARG
2	C	2940	ARG
2	C	3452	LYS
2	C	3733	ARG
2	C	3863	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	982	GLN
2	L	997	ASN
2	L	1115	HIS
2	L	1325	GLN
2	L	1418	HIS
2	L	1555	HIS
2	L	1716	GLN
2	L	1721	HIS
2	L	1772	HIS
2	L	2301	GLN
2	L	2305	ASN
2	L	2784	GLN
2	L	3084	GLN
2	L	3104	GLN
2	L	3130	GLN
2	L	3249	GLN
2	L	3577	GLN
2	L	3634	GLN
2	L	3743	HIS
2	L	3927	ASN
2	C	982	GLN
2	C	997	ASN
2	C	1115	HIS
2	C	1325	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1418	HIS
2	C	1555	HIS
2	C	1716	GLN
2	C	1772	HIS
2	C	2301	GLN
2	C	2305	ASN
2	C	2784	GLN
2	C	3084	GLN
2	C	3104	GLN
2	C	3130	GLN
2	C	3185	ASN
2	C	3249	GLN
2	C	3577	GLN
2	C	3634	GLN
2	C	3743	HIS
2	C	3927	ASN
2	C	4110	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

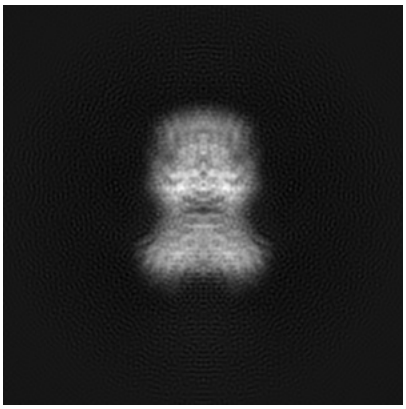
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28731. These allow visual inspection of the internal detail of the map and identification of artifacts.

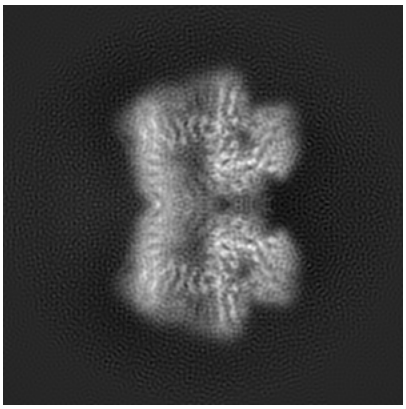
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

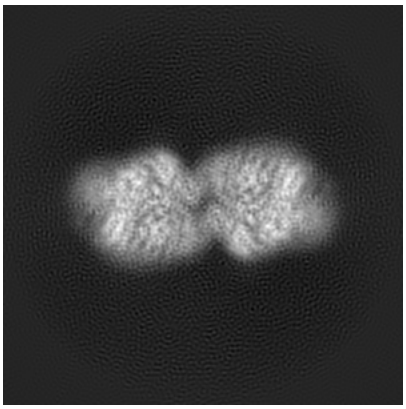
6.1.1 Primary map



X

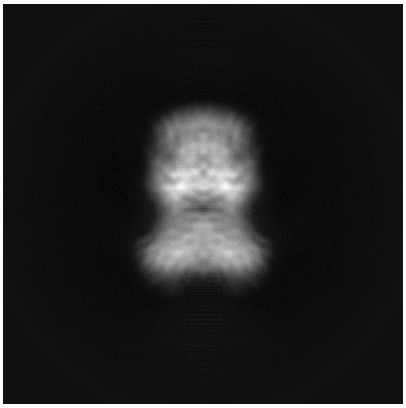


Y

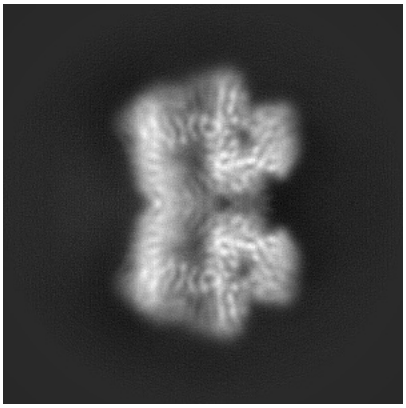


Z

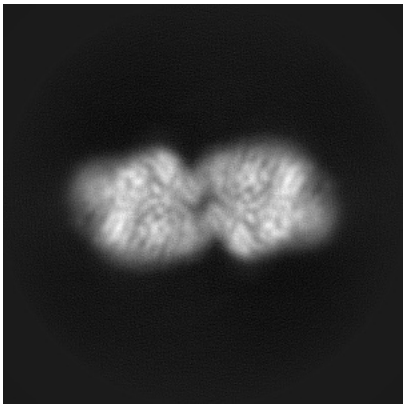
6.1.2 Raw map



X



Y

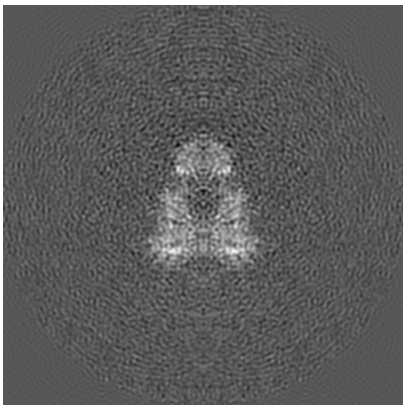


Z

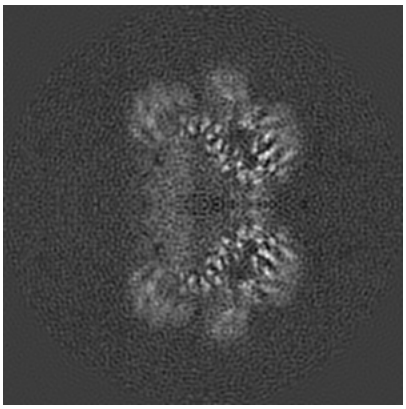
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

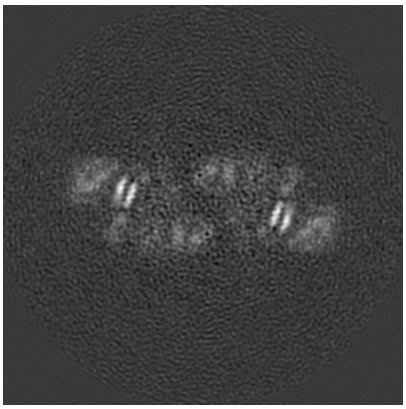
6.2.1 Primary map



X Index: 216

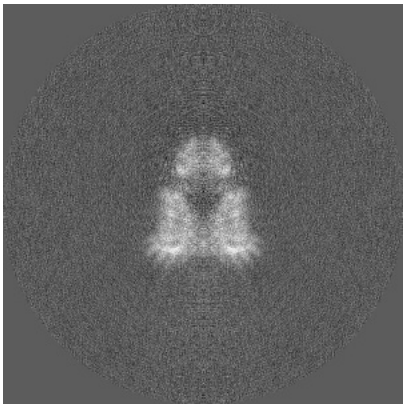


Y Index: 216

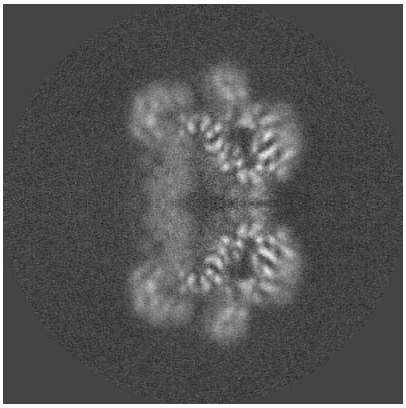


Z Index: 216

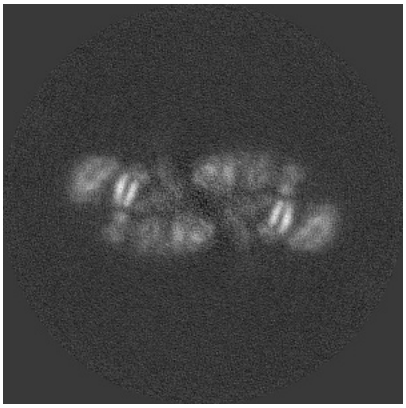
6.2.2 Raw map



X Index: 216



Y Index: 216

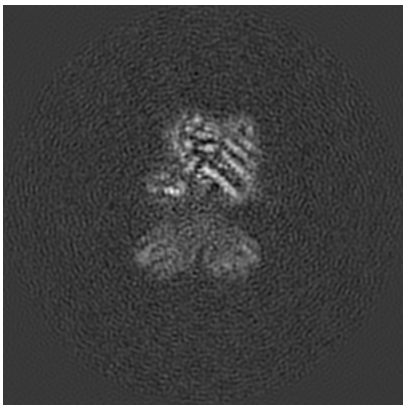


Z Index: 216

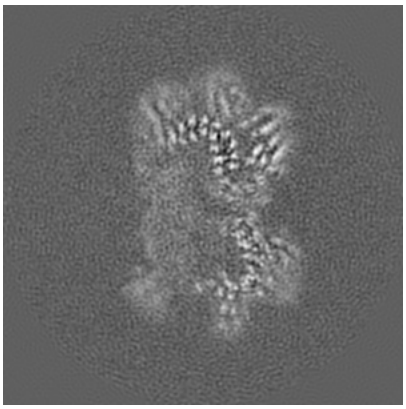
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

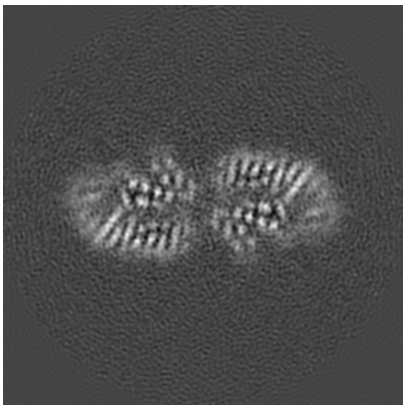
6.3.1 Primary map



X Index: 174

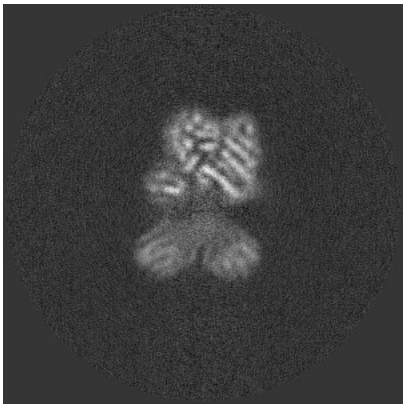


Y Index: 204

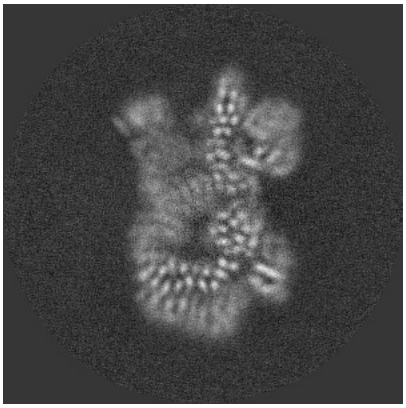


Z Index: 234

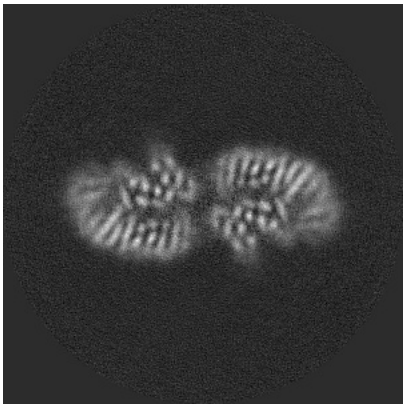
6.3.2 Raw map



X Index: 174



Y Index: 239

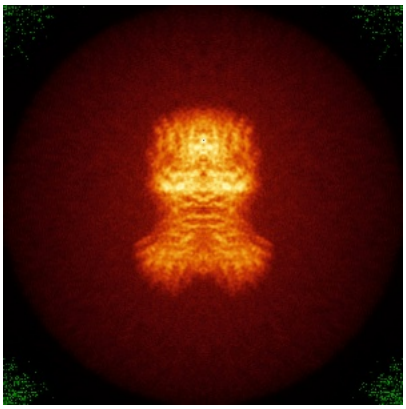


Z Index: 234

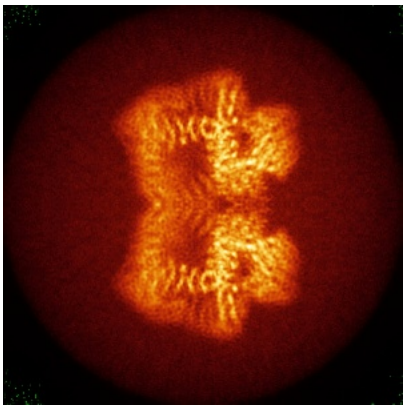
The images above show the largest variance slices of the map in three orthogonal directions.

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

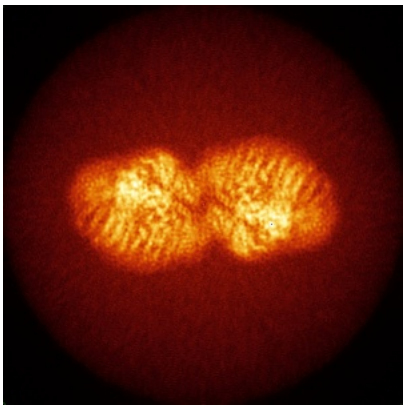
6.4.1 Primary map



X

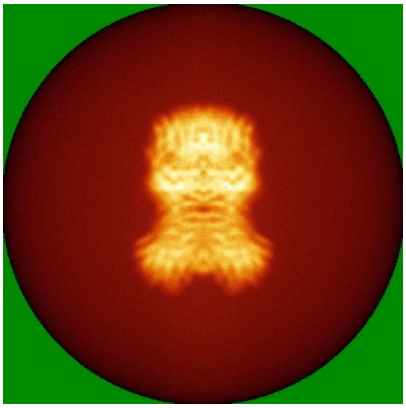


Y

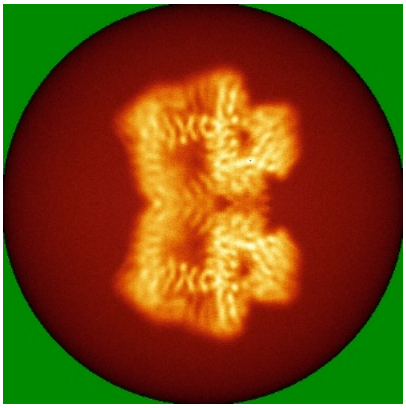


Z

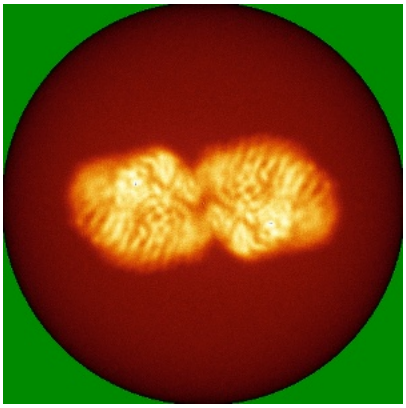
6.4.2 Raw map



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.

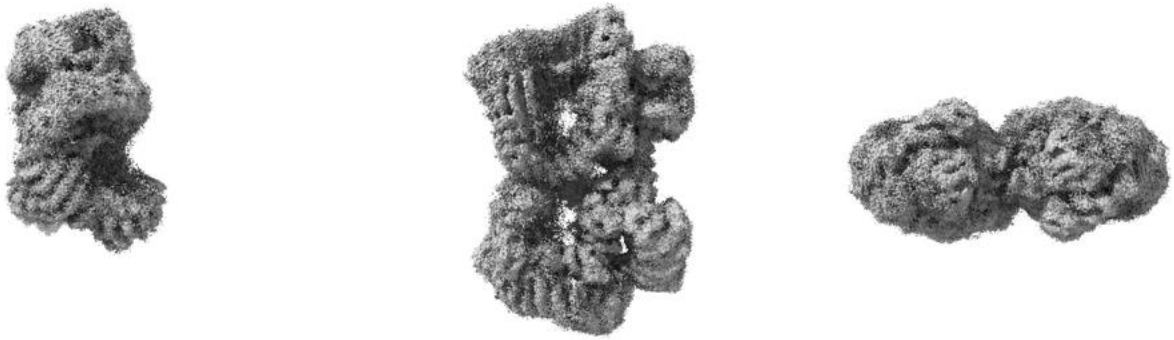
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

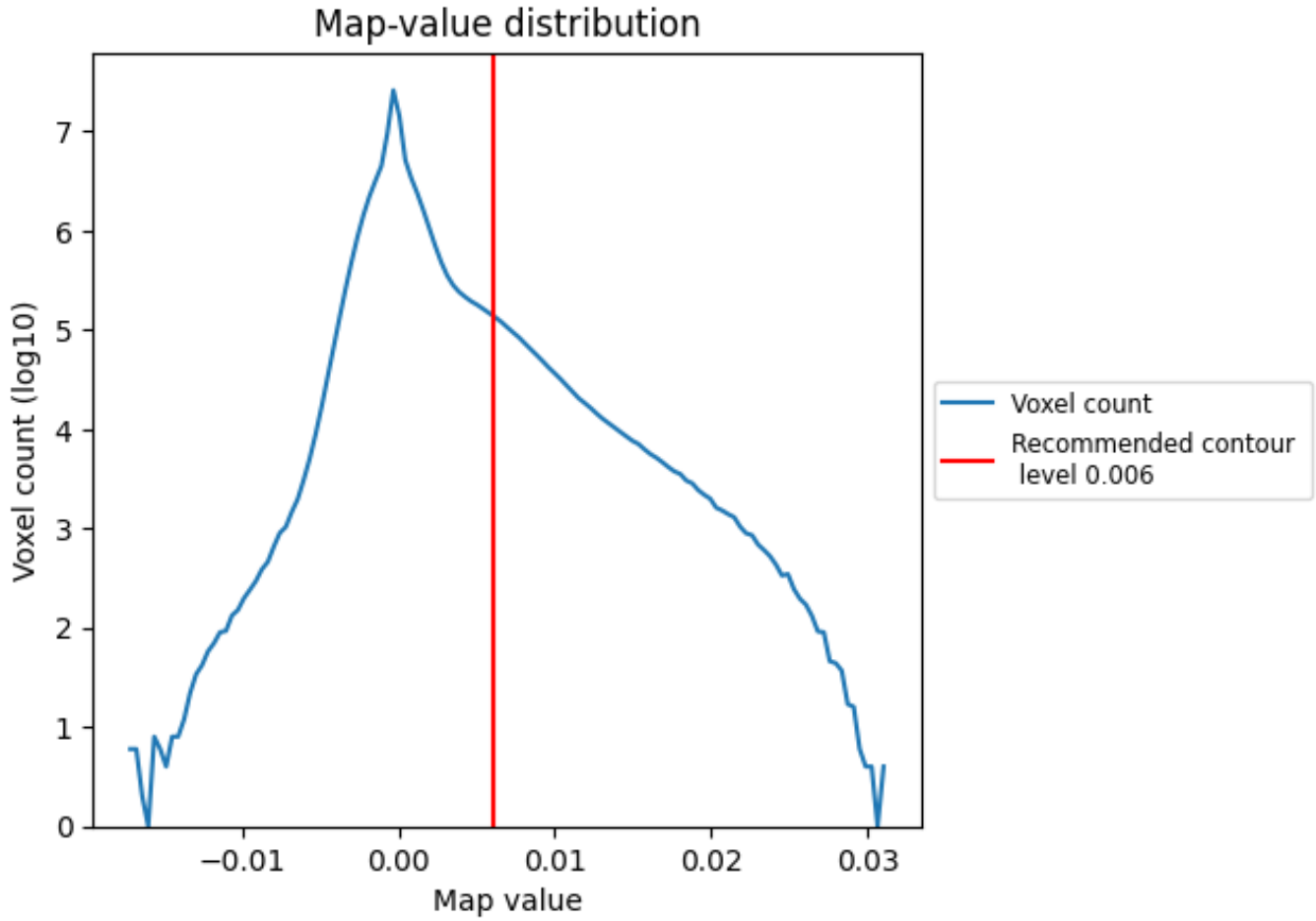
6.6 Mask visualisation (i)

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

7 Map analysis

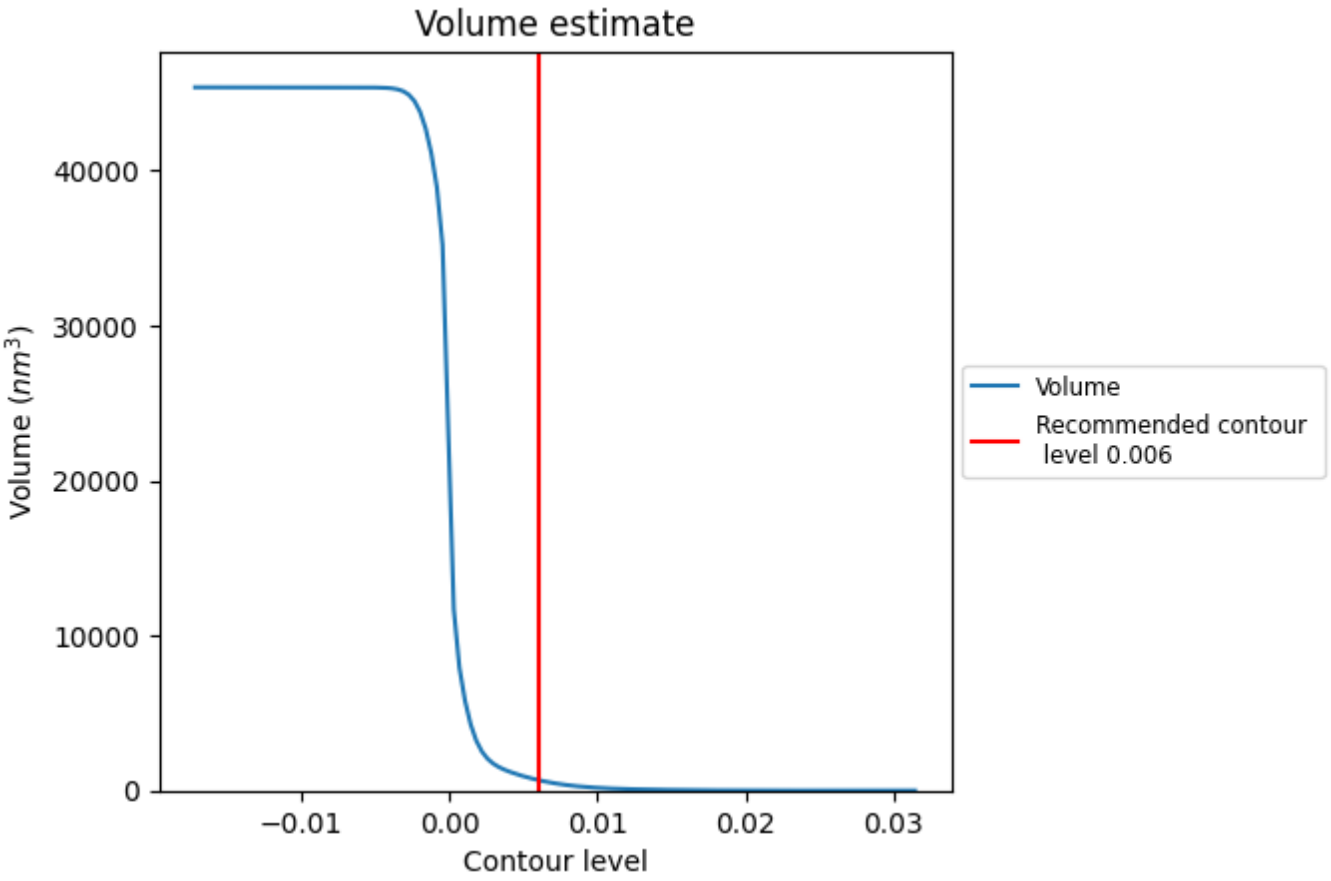
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

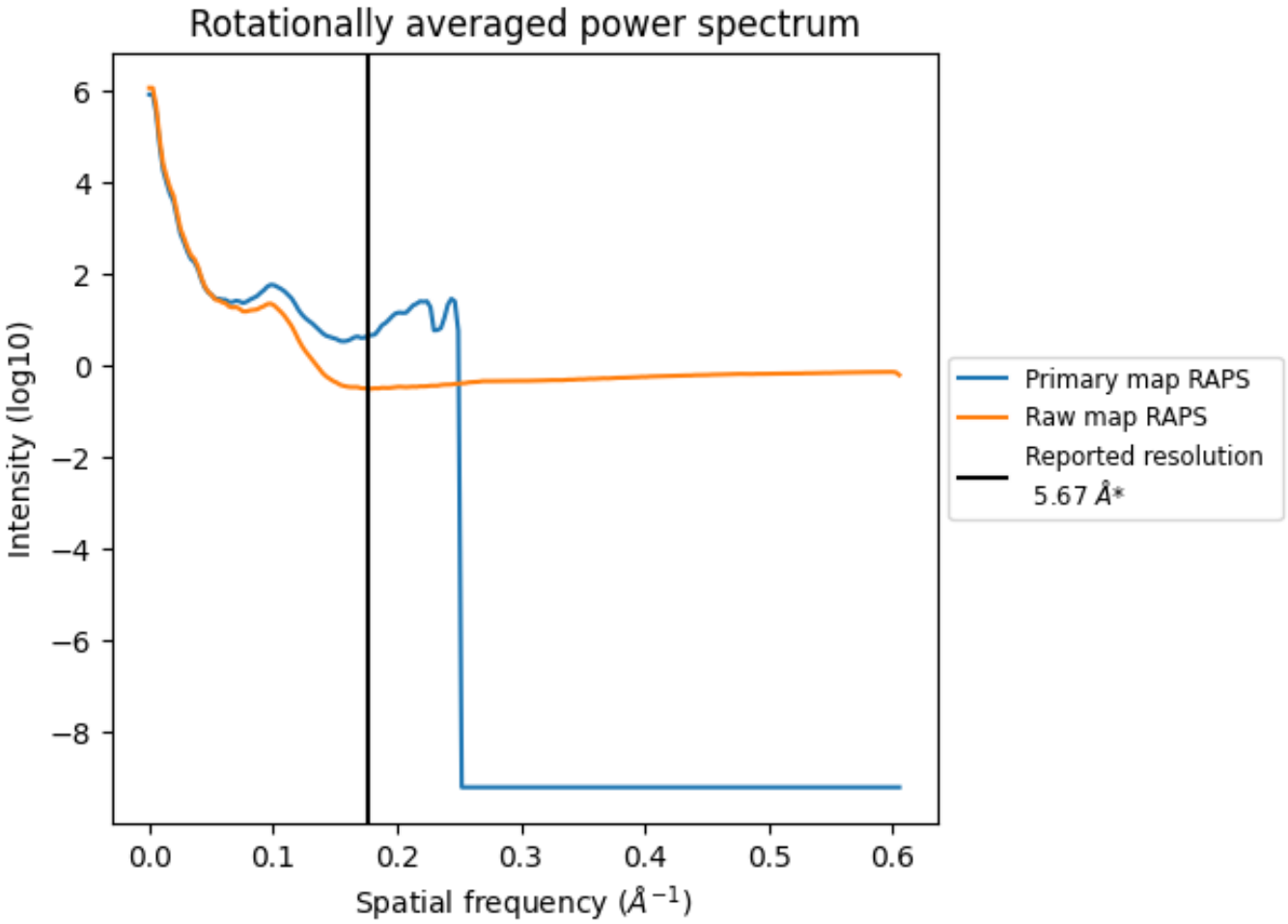
7.2 Volume estimate



The volume at the recommended contour level is 677 nm^3; this corresponds to an approximate mass of 612 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)

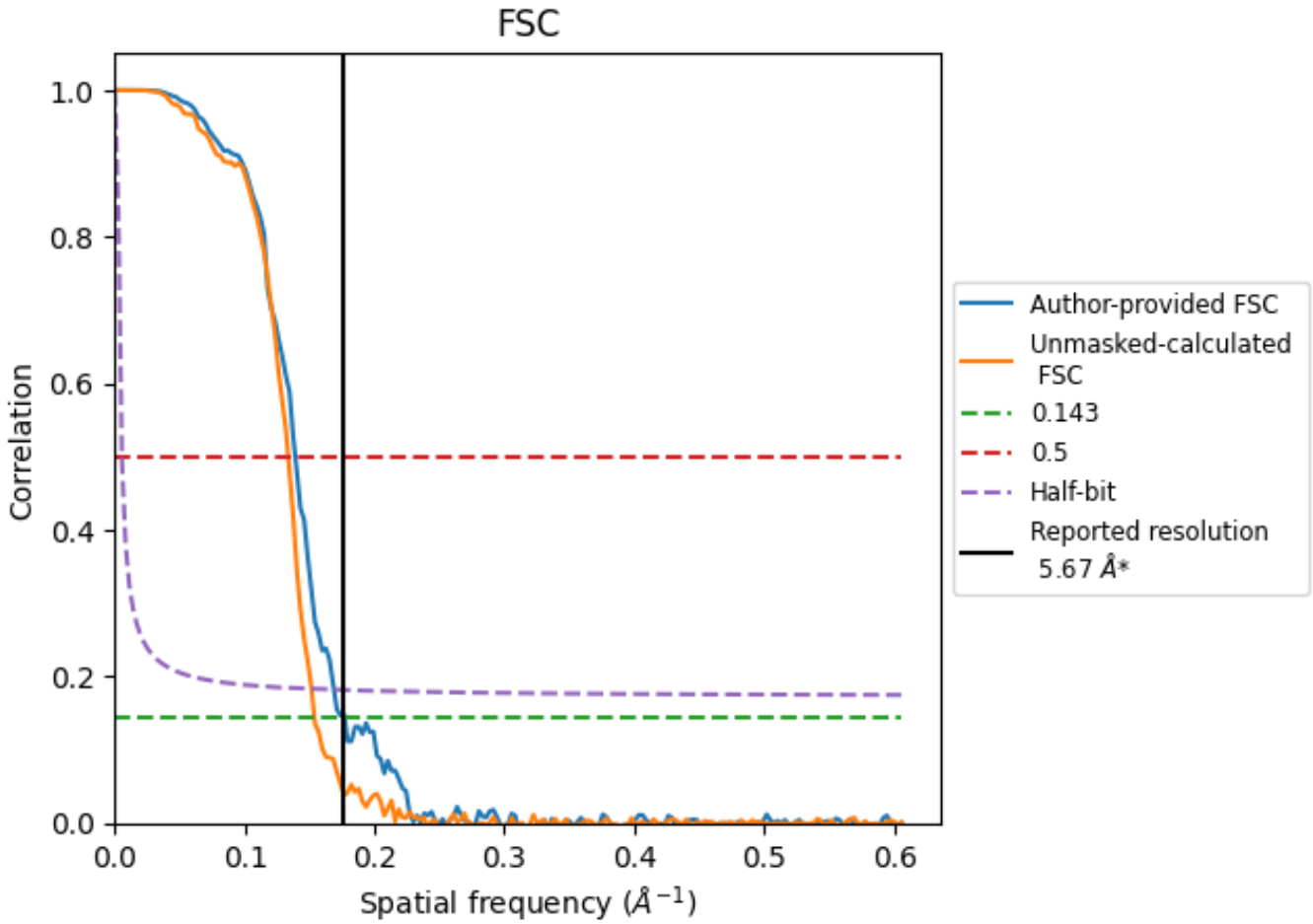


*Reported resolution corresponds to spatial frequency of 0.176 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.176 Å^{-1}

8.2 Resolution estimates (i)

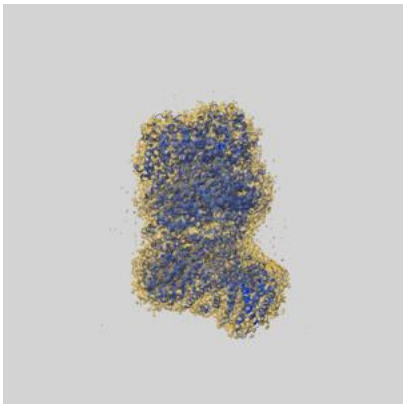
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.67	-	-
Author-provided FSC curve	5.65	7.19	5.92
Unmasked-calculated*	6.50	7.49	6.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.50 differs from the reported value 5.67 by more than 10 %

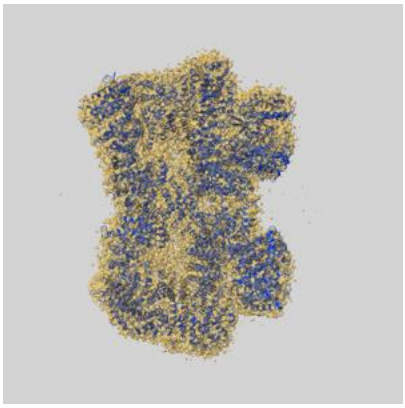
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28731 and PDB model 8EZ9. Per-residue inclusion information can be found in section 3 on page 4.

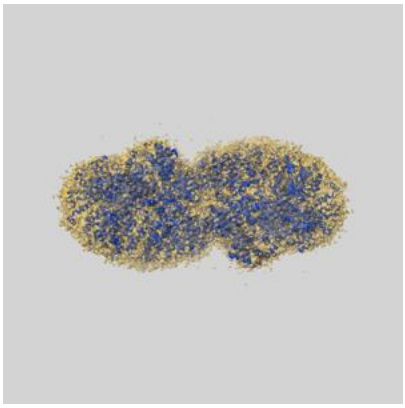
9.1 Map-model overlay



X



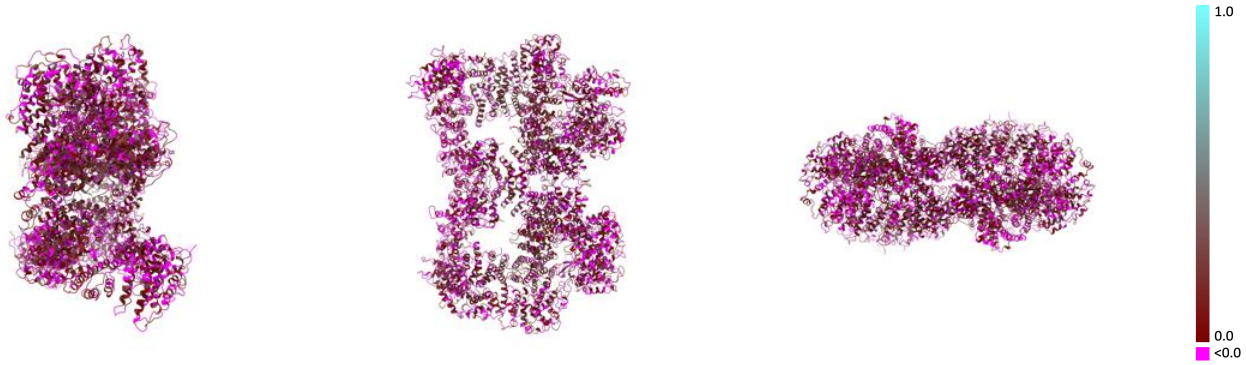
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

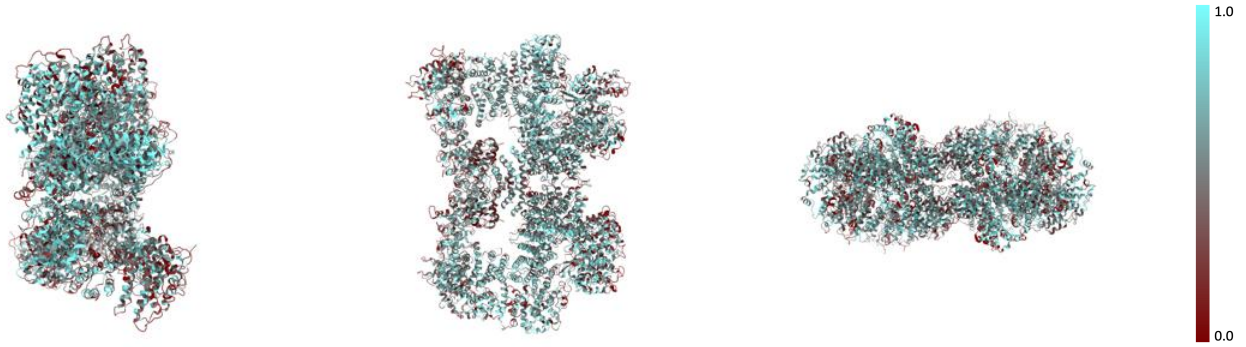
9.2 Q-score mapped to coordinate model (i)



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.

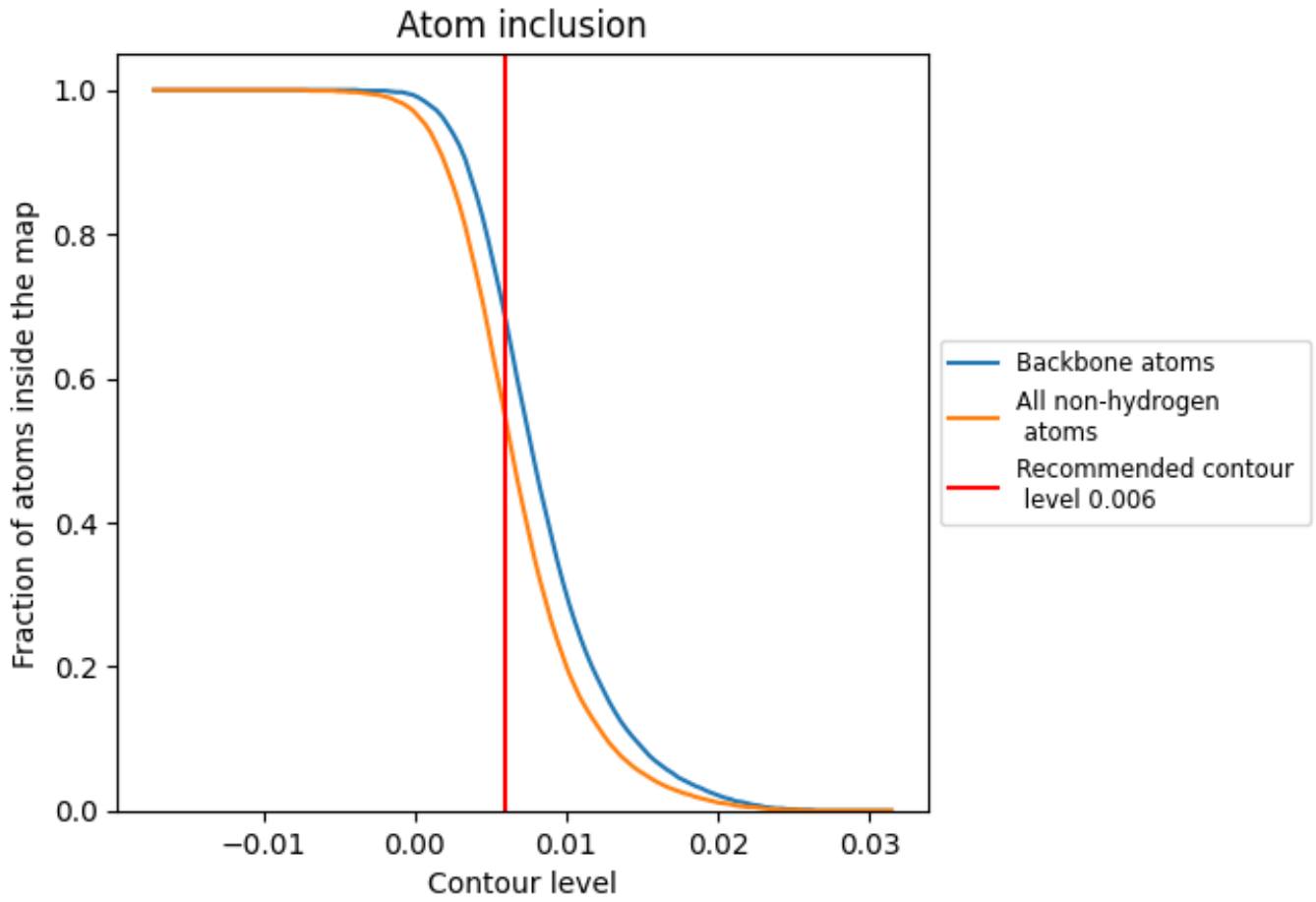
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5420	0.0740
C	0.5420	0.0740
L	0.5420	0.0720
Q	0.6040	0.2000
R	0.6240	0.1960