



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:25 pm BST

PDB ID : 5LUQ
Title : Crystal Structure of Human DNA-dependent Protein Kinase Catalytic Subunit (DNA-PKcs)
Authors : Sibanda, B.L.; Chirgadze, D.Y.; Ascher, D.B.; Blundell, T.L.
Deposited on : 2016-09-09
Resolution : 4.30 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

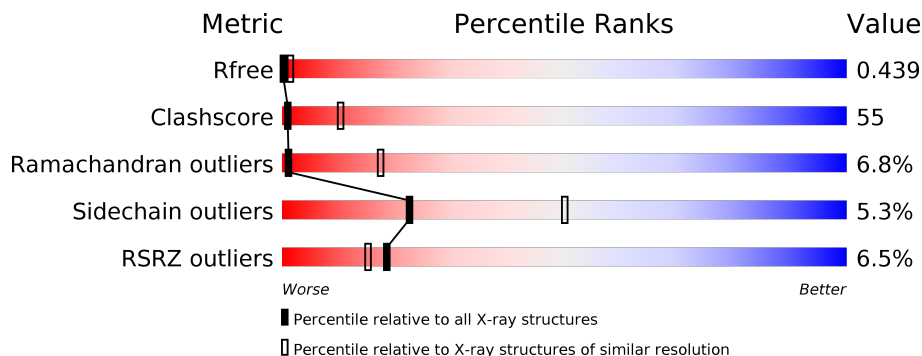
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R_{free} | 130704 | 1014 (4.80-3.80) |
| Clashscore | 141614 | 1077 (4.80-3.80) |
| Ramachandran outliers | 138981 | 1029 (4.80-3.80) |
| Sidechain outliers | 138945 | 1012 (4.80-3.80) |
| RSRZ outliers | 127900 | 1075 (4.90-3.70) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 4128 | |
| 1 | B | 4128 | |
| 2 | K | 194 | |
| 2 | S | 194 | |

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 59694 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-dependent protein kinase catalytic subunit,DNA-dependent Protein Kinase Catalytic Subunit,DNA-dependent protein kinase catalytic subunit.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|----|-----|---------|---------|-------|
| | | | Total | C | N | O | S | Se | | | |
| 1 | A | 3725 | 29574 | 18907 | 5016 | 5460 | 81 | 110 | 0 | 0 | 0 |
| 1 | B | 3725 | 29574 | 18907 | 5016 | 5460 | 81 | 110 | 0 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 1 | MSE | - | expression tag | UNP P78527 |
| A | 4128 | MSE | - | expression tag | UNP P78527 |
| B | 1 | MSE | - | expression tag | UNP P78527 |
| B | 4128 | MSE | - | expression tag | UNP P78527 |

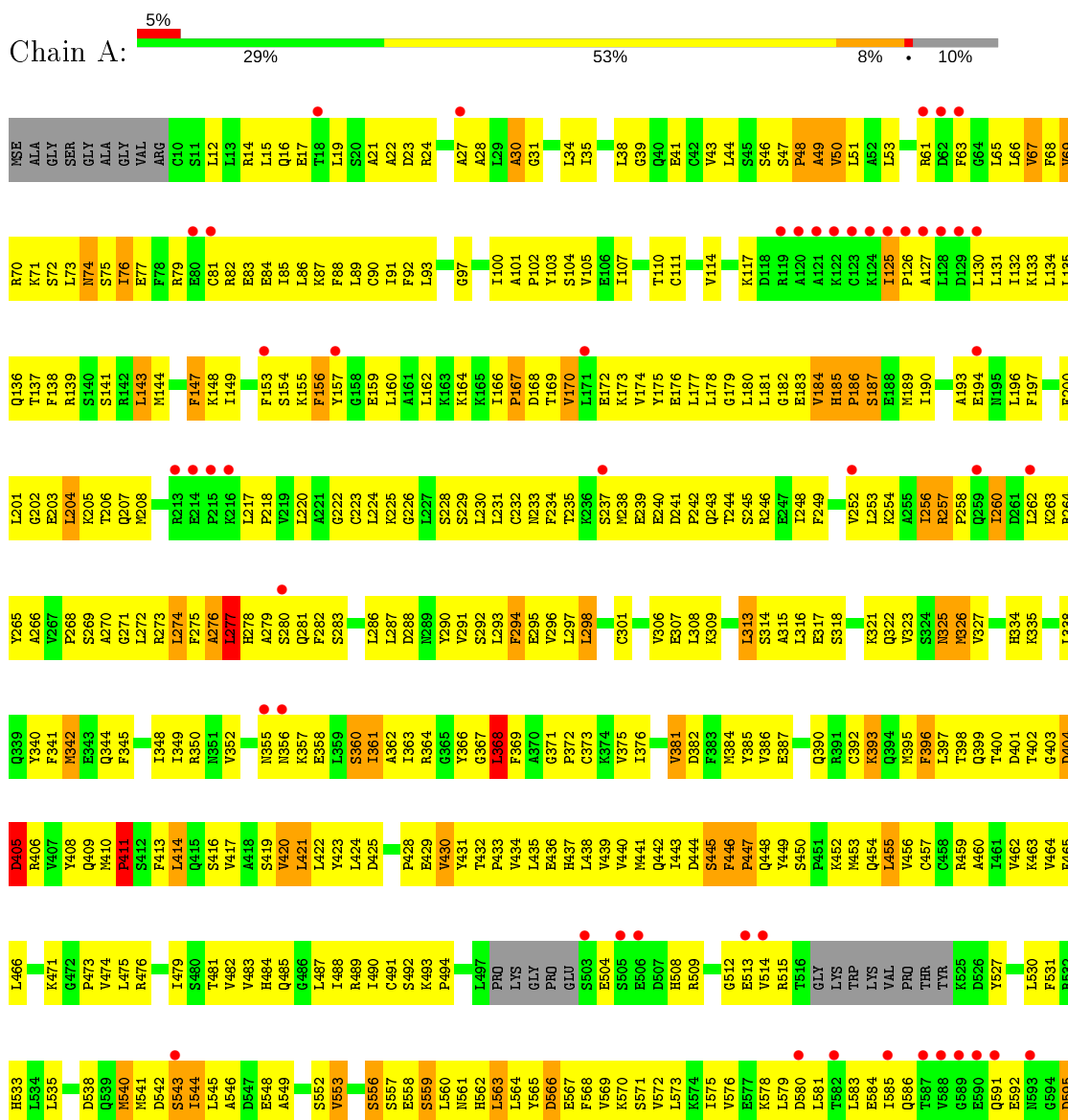
- Molecule 2 is a protein called C-terminal fragment of KU80 (KU80ct194).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| | | | Total | C | N | O | Se | | | |
| 2 | K | 54 | 273 | 164 | 54 | 54 | 1 | 0 | 0 | 0 |
| 2 | S | 54 | 273 | 164 | 54 | 54 | 1 | 0 | 0 | 0 |

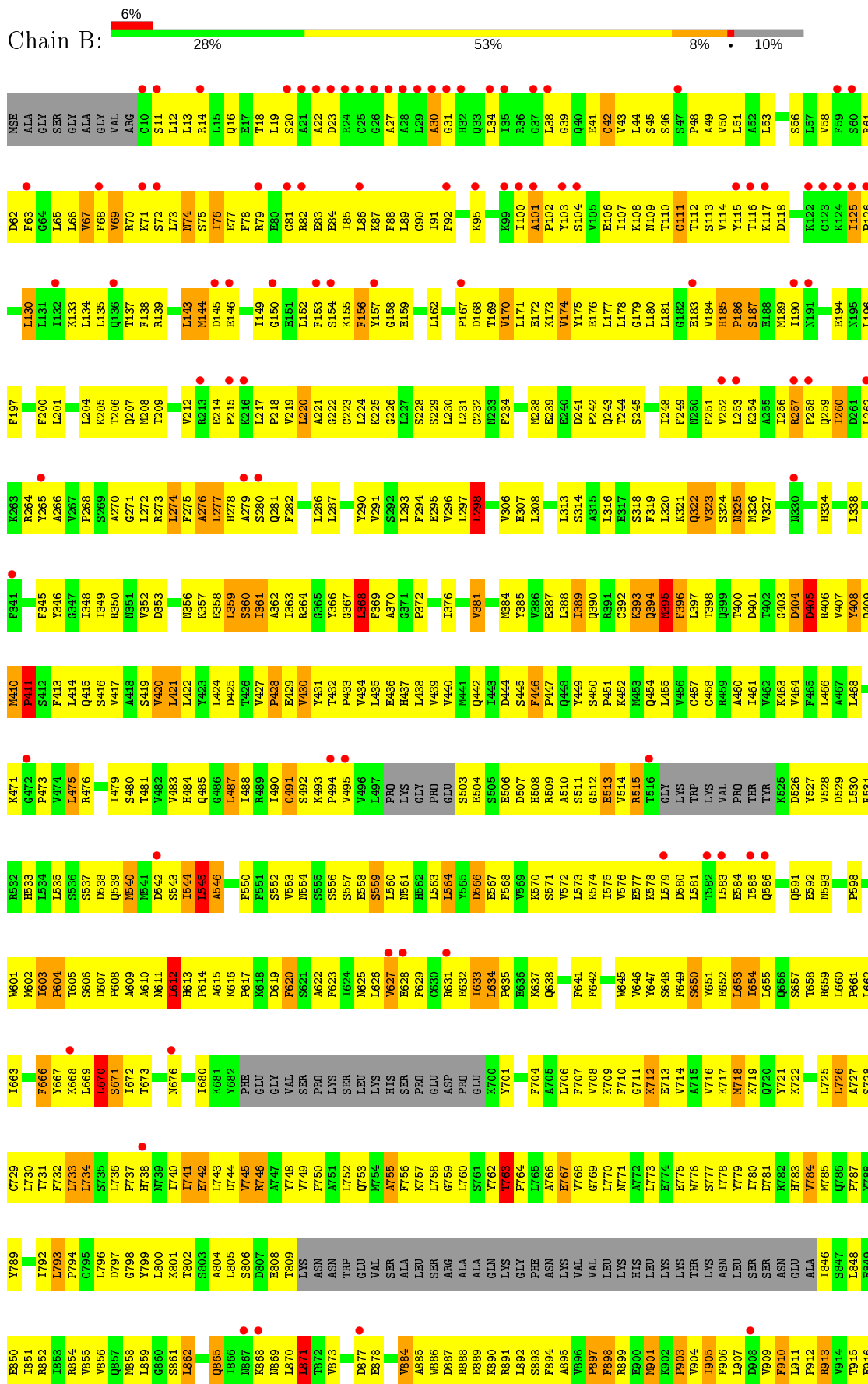
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: DNA-dependent protein kinase catalytic subunit, DNA-dependent Protein Kinase Catalytic Subunit, DNA-dependent protein kinase catalytic subunit



| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| V2272 | E2209 | L2140 | Q2071 | I2007 | Y1945 | V1879 | S1818 | Q1754 | Q1691 | D1630 | I1567 | D1504 |
| G2273 | V2210 | N2141 | R2072 | R2008 | M1946 | M1880 | F1819 | S1755 | A1692 | S1631 | M1568 | L1505 |
| L2274 | L2211 | L2142 | P2073 | K2009 | N1946 | M1881 | V1820 | P1756 | V1693 | W1633 | T1569 | C1507 |
| Q2275 | A2212 | R2143 | D2074 | E2010 | C1947 | S1882 | D1821 | M1758 | T1694 | W1632 | E1570 | K1503 |
| L2276 | N2213 | L2144 | T2075 | A2011 | A1948 | R1883 | R1822 | L1758 | L1695 | K1634 | L1571 | K1503 |
| G2276 | R2214 | F2145 | V2076 | R2012 | I1949 | L1884 | SER | L1758 | L1696 | K1635 | L1572 | Q1509 |
| L2279 | L2215 | L2146 | H2077 | E2013 | S1950 | P1885 | LEU | E1760 | P1697 | D1636 | K1573 | L1510 |
| L2280 | L2216 | A2147 | D2078 | A2014 | V1951 | K1886 | LEU | M1762 | F1698 | S1637 | L1574 | A1511 |
| N2281 | L2219 | K2148 | D2079 | A2015 | I1952 | K1887 | THR | T1763 | F1699 | P1638 | S1572 | G1513 |
| A2282 | M2220 | I2151 | V2080 | N2016 | C1953 | D1888 | LEU | GLU | T1700 | L1639 | D1576 | L1517 |
| N2283 | K2221 | N2152 | E2082 | G2017 | C1954 | S1701 | LEU | A1640 | S1701 | L1639 | D1576 | L1517 |
| H2284 | H2222 | T2153 | L2083 | D2018 | V1955 | H1890 | TRP | L1702 | L1702 | T1641 | D1577 | L1577 |
| L2285 | V2223 | E2154 | E2084 | G2021 | M1956 | A1891 | HIS | T1703 | T1703 | K1642 | A1578 | L1516 |
| F2286 | F2224 | E2155 | M2085 | P2022 | E1958 | S1894 | SER | S1706 | S1706 | M1643 | L1582 | L1516 |
| F2287 | H2225 | V2156 | D2086 | P2023 | L1959 | L1895 | LEU | ARG | A1644 | A1644 | M1583 | A1518 |
| Y2288 | P2226 | F2157 | K2087 | Y2024 | K1960 | M1896 | ASP | GLN | V1645 | V1645 | A1520 | Q1584 |
| D2289 | K2227 | L2088 | F1961 | Y2024 | F1961 | I1896 | ASP | GLN | L1646 | L1646 | S1585 | F1521 |
| P2290 | N2089 | A2161 | Y1962 | S2037 | Y1962 | T1906 | LEU | HIS | A1647 | A1647 | G1522 | G1523 |
| Q2291 | R2090 | K2162 | R2090 | L2028 | Q1963 | G1908 | ARG | VAL | L1648 | L1648 | V1587 | L1524 |
| C2292 | H2091 | R2163 | H2091 | L2028 | Q1964 | H1901 | ARG | MSE | A1650 | A1650 | C1525 | C1526 |
| G2293 | E2092 | L2164 | E2092 | Y2030 | F1965 | I1905 | VAL | GLU | K1651 | K1651 | T1590 | ARG |
| R2294 | R2232 | L2165 | C2093 | L2031 | F1966 | L1895 | PHE | GLU | E1714 | E1714 | K1591 | LEU |
| H2295 | H2233 | S2166 | M2094 | A2032 | F1967 | T1907 | SER | LEU | E1745 | E1745 | M1592 | VAL |
| S2296 | N2234 | F2167 | A2095 | D2033 | S1968 | E1907 | THR | PHE | Q1746 | Q1746 | V1593 | VAL |
| S2297 | L2235 | L2168 | P2096 | S2034 | E1969 | G1908 | ILE | GLN | L1747 | L1747 | C1525 | SER |
| E2298 | E2236 | L2169 | L2097 | T2035 | K1970 | M1909 | VAL | SER | I1718 | I1718 | A1526 | ARG |
| Y2299 | I2237 | Q2170 | Q2170 | L2036 | P1971 | E1910 | VAL | SER | V1719 | V1719 | LEU | LEU |
| Q2300 | I2238 | L2171 | A2099 | S2037 | P1971 | L1911 | ASP | PHE | A1720 | A1720 | L1597 | LEU |
| Q2301 | K2239 | L2171 | L2100 | S2037 | L1975 | T1912 | ALA | ARG | F1722 | F1722 | M1598 | LEU |
| A2302 | T2240 | N2176 | L2100 | E2039 | L1976 | K1913 | ILE | ARG | P1723 | P1723 | G1599 | ASN |
| L2303 | R2241 | N2177 | H2103 | E2039 | I1977 | T1914 | ASP | ILE | M1724 | M1724 | L1601 | PRO |
| V2304 | V2242 | E2182 | M2104 | S2041 | F1978 | L1915 | VAL | ALA | Q1725 | Q1725 | D1602 | ALA |
| N2305 | E2243 | R2183 | R2106 | Q2042 | E1979 | K1917 | LEU | R1787 | R1787 | R1787 | Q1603 | VAL |
| N2306 | C2244 | Y2184 | R2106 | D2044 | M1980 | L1918 | LYS | R1788 | R1788 | R1788 | S1604 | LEU |
| N2307 | W2245 | V2185 | P2110 | F2045 | I1982 | G1919 | SER | G1789 | G1789 | G1789 | F1605 | THR |
| S2308 | K2246 | V2186 | P2111 | S2046 | L1983 | Y1920 | ARG | T1793 | T1793 | T1793 | R1606 | ALA |
| E2309 | C2247 | V2187 | Q2112 | T2047 | L1984 | D1921 | PHE | L1793 | L1793 | L1793 | E1607 | SER |
| C2248 | L2249 | E2188 | G2113 | G2048 | K1985 | A1922 | THR | T1733 | T1733 | T1733 | R1608 | LEU |
| S2250 | S2250 | I2189 | E2114 | V2049 | R1986 | F1923 | L1858 | P1734 | P1734 | P1734 | A1609 | GLY |
| I2251 | P2252 | V2190 | E2115 | Q2050 | R1987 | T1924 | M1859 | R1735 | R1735 | R1735 | ASN | SER |
| E2314 | P2253 | A2191 | D2116 | S2051 | Y1988 | E1925 | E1860 | F1736 | F1736 | F1736 | LYS | GLN |
| V2315 | Y2253 | T2192 | T2116 | Y2052 | M1989 | M1926 | S1861 | M1737 | M1737 | M1737 | HIS | GLN |
| Y2316 | R2264 | L2193 | R2120 | S2053 | F1990 | M1927 | LEU | Y1802 | Y1802 | Y1802 | GLN | G1543 |
| A2317 | L2255 | L2194 | D2121 | Y2054 | P1991 | A1928 | D1864 | E1803 | E1803 | E1803 | GLY | S1549 |
| A2318 | I2256 | S2195 | L2122 | S2055 | V1992 | G1929 | T1865 | M1804 | M1804 | M1804 | GLY | I1550 |
| A2319 | F2257 | W2196 | L2122 | S2056 | E1999 | E1930 | Q1866 | F1805 | F1805 | F1805 | LEU | I1551 |
| A2320 | E2258 | T2197 | Q2057 | Q2057 | E1993 | M1931 | I1867 | R1806 | R1806 | R1806 | LYS | H1552 |
| E2321 | K2259 | G2198 | D2058 | D2058 | V1996 | Q1932 | T1868 | K1807 | K1807 | K1807 | ALA | S1554 |
| V2322 | F2260 | L2199 | P2059 | P2059 | P1997 | L1933 | K1869 | D1808 | D1808 | D1808 | THR | H1555 |
| L2323 | S2261 | A2200 | R2060 | R2060 | M1998 | L1934 | K1744 | K1744 | K1744 | K1744 | THR | H1555 |
| G2324 | G2262 | T2201 | P2061 | P2061 | E1999 | E1935 | K1870 | D1809 | D1809 | D1809 | ILE | Y1558 |
| L2325 | K2263 | T2202 | G2134 | R2065 | R2000 | R1936 | M1871 | P1810 | P1810 | P1810 | ILE | F1559 |
| L2326 | D2264 | T2203 | G2134 | R2066 | R2001 | R1937 | G1872 | R1811 | R1811 | R1811 | LEU | F1559 |
| L2327 | G2204 | V2205 | P2136 | R2067 | K2002 | K1938 | Y1874 | L1812 | L1812 | L1812 | GLN | Y1560 |
| R2328 | V2205 | P2206 | L2137 | R2068 | K2003 | L1939 | K1875 | F1814 | F1814 | F1814 | HIS | Y1563 |
| Y2329 | G2267 | R2207 | L2138 | R2069 | Y2004 | H1940 | I1876 | E1751 | E1751 | E1751 | TRP | S1564 |
| V2330 | N2270 | K2207 | V2138 | R2069 | I2005 | H1941 | L1877 | L1815 | L1815 | L1815 | LYS | E1565 |
| N2331 | S2271 | D2208 | P2139 | E2070 | E2006 | C1942 | D1878 | Q1817 | Q1817 | Q1817 | CYS | T1566 |



| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| L917 | R981 | K1042 | V1105 | V1169 | P1232 | E1299 | C1364 | E1430 | L1500 | S1564 | GLN | H1687 |
| S922 | Q982 | Q1043 | I1106 | K1170 | A1237 | S1300 | N1366 | L1431 | L1501 | E1566 | HIS | L1688 |
| D923 | L983 | I1044 | V1107 | W1171 | A1238 | I1301 | H1367 | V1434 | P1502 | T1566 | THR | K1689 |
| R924 | Y984 | T1045 | M1108 | A1174 | Q1239 | A1302 | H1368 | L1436 | S1503 | I1567 | LVS | G1690 |
| Q925 | E985 | P1046 | E1109 | H1175 | P1240 | M1303 | M1369 | L1456 | D1504 | T1569 | CYS | A1691 |
| T926 | P986 | S1110 | S1110 | R1178 | L1241 | D1305 | R1370 | Y1437 | L1505 | E1570 | D1630 | V1693 |
| K927 | L987 | Q1049 | L1111 | R1179 | L1242 | I1306 | V1371 | G1438 | S1506 | L1571 | S1631 | T1694 |
| V928 | W988 | E1050 | A1112 | P1179 | L1244 | I1307 | L1372 | P1439 | C1507 | L1572 | W1632 | L1695 |
| A929 | M989 | K1051 | L1113 | Q1180 | P1247 | ALA | V1373 | D1440 | K1508 | K1582 | A1633 | L1696 |
| A930 | Q990 | S1052 | A1114 | GLU | F1248 | LYS | Q1374 | A1441 | Q1509 | N1583 | A1634 | P1697 |
| C931 | L991 | P1053 | H1115 | CYS | S1249 | GLY | L1376 | Q1442 | L1510 | L1574 | K1635 | F1698 |
| E932 | I992 | V1054 | E1118 | ARG | L1250 | CYS | C1377 | R1445 | A1511 | L1575 | D1636 | F1699 |
| L933 | W994 | M1055 | K1119 | THR | Q1251 | PHE | E1378 | R1447 | S1512 | L1577 | S1637 | T1700 |
| L934 | F995 | L1059 | L1120 | HIS | A1252 | GLY | P1379 | R1448 | G1513 | A1578 | P1638 | S1701 |
| H935 | T996 | F1060 | L1121 | LVS | L1253 | THR | L1448 | L1449 | L1517 | V1579 | L1639 | L1702 |
| S936 | M997 | G1122 | G1122 | SER | T1254 | ARG | C1455 | A1454 | A1520 | E1580 | E1640 | |
| M937 | N998 | K1061 | R1062 | ILE | C1255 | ALA | I1382 | A1455 | A1521 | E1581 | E1641 | |
| V938 | Q999 | L1063 | E1129 | GLU | W1256 | ALA | N1385 | A1450 | A1522 | L1582 | M1643 | G1705 |
| M939 | K1000 | Y1064 | C1127 | LEU | L1257 | GLY | I1386 | V1451 | L1524 | L1583 | A1644 | S1706 |
| F940 | F1001 | S1065 | C1128 | PHE | L1258 | ALA | G1387 | V1452 | L1525 | R1584 | A1645 | L1707 |
| M941 | E1002 | L1066 | D1129 | TYR | A1259 | ASN | G1388 | S1453 | C1526 | S1585 | L1646 | V1645 |
| L942 | S1003 | A1067 | A1130 | LVS | L1260 | ARG | D1388 | A1454 | ARG | S1586 | A1647 | E1709 |
| G943 | Q1004 | L1068 | I1131 | PHE | L1261 | THR | V1389 | C1455 | LEU | V1587 | L1648 | L1710 |
| K944 | D1005 | H1069 | D1132 | VAL | A1263 | S1323 | Q1390 | L1458 | VAL | D1588 | L1649 | R1711 |
| A945 | T1006 | P1070 | H1133 | PRO | L1264 | P1324 | Y1391 | H1459 | SER | N1589 | A1650 | R1712 |
| Q946 | Y1007 | M1071 | L1134 | LEU | E1265 | Y1330 | M1392 | R1460 | LEU | K1591 | K1651 | E1715 |
| M948 | A1008 | A1072 | C1135 | LEU | C1266 | L1265 | A1393 | H1461 | LEU | M1592 | L1652 | Q1716 |
| P949 | R1009 | F1073 | R1136 | PRO | Y1267 | G1333 | D1397 | L1463 | LEU | V1593 | L1653 | L1717 |
| R950 | L1010 | K1074 | I1137 | GLY | M1268 | C1334 | N1398 | L1464 | ASN | S1594 | Q1654 | I1718 |
| G951 | E1011 | R1075 | I1138 | ASN | T1269 | K1335 | C1399 | H1465 | PRO | A1596 | I1655 | |
| Q952 | A1012 | L1076 | E1139 | ARG | F1270 | F1336 | V1400 | H1466 | ALA | V1596 | S1658 | |
| G953 | I1013 | G1077 | K1140 | SER | L1271 | V1337 | N1401 | L1467 | VAL | L1597 | VAL | S1658 |
| G954 | D1014 | A1078 | H1141 | PRO | G1272 | L1402 | M1402 | L1468 | LEU | M1598 | SER | M1724 |
| A955 | L1016 | L1080 | V1143 | LEU | E1273 | V1338 | M1403 | P1469 | SER | G1599 | PHE | Q1725 |
| P956 | G1017 | A1081 | S1144 | TRP | R1274 | R1340 | K1404 | S1470 | THR | M1600 | ASN | S1726 |
| R957 | V1018 | F1082 | L1145 | LEU | L1275 | I1341 | A1405 | Q1471 | ALA | L1601 | THR | R1727 |
| M958 | D1019 | M1083 | M1146 | LVS | V1276 | M1342 | L1406 | S1472 | SER | L1602 | SER | E1728 |
| Q959 | P1020 | M1084 | K1147 | ASP | L1279 | E1343 | K1407 | T1473 | LEU | D1603 | HIS | F1729 |
| L961 | D1022 | I1085 | K1149 | VAL | Q1280 | F1344 | M1408 | D1474 | GLY | F1604 | GLY | P1731 |
| Y962 | S1023 | R1087 | K1150 | LEU | L1282 | T1345 | S1409 | H1476 | SER | R1605 | PHE | G1732 |
| K963 | L1024 | E1088 | R1151 | E1214 | G1283 | L1347 | P1410 | V1479 | GLN | E1607 | GLU | I1733 |
| R964 | L1025 | F1089 | R1152 | E1215 | T1284 | L1348 | K1412 | | G1548 | R1608 | | A1734 |
| T965 | R1026 | R1090 | L1153 | G1216 | E1285 | L1349 | D1413 | L1483 | S1549 | A1609 | ASN | F1735 |
| F966 | D1027 | E1091 | P1154 | V1217 | A1286 | N1350 | I1414 | L1484 | V1550 | GLN | ASN | F1736 |
| P967 | F1028 | E1092 | R1155 | S1218 | A1287 | K1351 | L1415 | S1485 | H1551 | GLN | GLN | M1737 |
| V968 | C1029 | E1093 | G1156 | F1219 | Q1287 | T1352 | E1416 | L1486 | H1552 | LVS | LVS | M1738 |
| L969 | G1030 | S1094 | L1157 | L1220 | S1288 | P1353 | T1417 | Y1488 | F1553 | HIS | HIS | Y1739 |
| L970 | R1031 | L1095 | F1158 | I1221 | S1289 | E1354 | H1418 | K1489 | S1554 | GLN | GLN | V1740 |
| R971 | C1032 | W1096 | P1159 | M1222 | L1290 | E1356 | L1419 | K1490 | H1555 | GLY | GLY | D1741 |
| L972 | I1033 | E1097 | T1223 | T1223 | K1292 | K1356 | R1420 | G1490 | L1556 | LEU | LEU | C1742 |
| A973 | R1034 | F1099 | F1224 | F1224 | K1293 | K1357 | E1421 | L1492 | E1557 | LVS | LVS | M1743 |
| C974 | E1035 | F1099 | E1225 | V1294 | A1295 | L1358 | I1423 | A1493 | F1558 | ALA | ALA | K1744 |
| D977 | L1036 | V1100 | C1164 | G1228 | F1296 | L1359 | T1424 | G1494 | Y1560 | THR | THR | K1745 |
| Q978 | L1037 | F1101 | L1165 | C1229 | F1297 | K1360 | T1425 | L1495 | S1561 | THR | THR | L1746 |
| W1039 | K1038 | A1102 | L1166 | G1230 | L1298 | K1361 | Q1426 | E1496 | L1562 | ILE | ILE | L1747 |
| T980 | W1039 | A1103 | D1167 | G1231 | L1298 | L1363 | | | F1563 | LEU | LEU | L1750 |
| | | | | | | | | | | | | E1751 |

4 Data and refinement statistics

| Property | Value | Source |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 169.12Å 132.64Å 296.59Å 90.00° 105.53° 90.00° | Depositor |
| Resolution (Å) | 49.92 – 4.30 49.92 – 4.30 | Depositor EDS |
| % Data completeness (in resolution range) | 97.8 (49.92-4.30) 97.6 (49.92-4.30) | Depositor EDS |
| R_{merge} | 0.16 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.33 (at 4.29Å) | Xtrriage |
| Refinement program | PHENIX (1.10_2155: ???) | Depositor |
| R, R_{free} | 0.386 , 0.437 0.388 , 0.439 | Depositor DCC |
| R_{free} test set | 2009 reflections (2.32%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 184.6 | Xtrriage |
| Anisotropy | 0.337 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.29 , 188.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$ | Xtrriage |
| Estimated twinning fraction | 0.019 for h,-k,-h-l | Xtrriage |
| F_o, F_c correlation | 0.83 | EDS |
| Total number of atoms | 59694 | wwPDB-VP |
| Average B, all atoms (Å ²) | 253.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | A | 0.45 | 3/29743 (0.0%) | 0.77 | 47/40014 (0.1%) |
| 1 | B | 0.46 | 6/29743 (0.0%) | 0.77 | 49/40014 (0.1%) |
| 2 | K | 0.22 | 0/7 | 0.50 | 0/7 |
| 2 | S | 0.45 | 0/7 | 0.34 | 0/7 |
| All | All | 0.46 | 9/59500 (0.0%) | 0.77 | 96/80042 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 8 |
| 1 | B | 0 | 6 |
| All | All | 0 | 14 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1 | A | 1069 | HIS | C-N | -9.65 | 1.16 | 1.34 |
| 1 | B | 3794 | VAL | C-N | -8.26 | 1.18 | 1.34 |
| 1 | B | 1069 | HIS | C-N | 7.70 | 1.48 | 1.34 |
| 1 | B | 4124 | TRP | CB-CG | -6.16 | 1.39 | 1.50 |
| 1 | A | 601 | TRP | CB-CG | -5.75 | 1.40 | 1.50 |
| 1 | B | 3981 | TYR | CD1-CE1 | -5.53 | 1.31 | 1.39 |
| 1 | B | 2546 | TYR | CB-CG | -5.38 | 1.43 | 1.51 |
| 1 | B | 2546 | TYR | CD2-CE2 | -5.37 | 1.31 | 1.39 |
| 1 | A | 2362 | VAL | CB-CG1 | -5.04 | 1.42 | 1.52 |

All (96) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 1 | A | 726 | LEU | CA-CB-CG | -10.22 | 91.80 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | B | 3456 | LEU | CA-CB-CG | 9.67 | 137.54 | 115.30 |
| 1 | B | 1009 | LEU | CB-CG-CD1 | -9.35 | 95.11 | 111.00 |
| 1 | A | 3456 | LEU | CA-CB-CG | 9.33 | 136.75 | 115.30 |
| 1 | B | 726 | LEU | CA-CB-CG | -9.12 | 94.32 | 115.30 |
| 1 | B | 1010 | LEU | CA-CB-CG | 9.01 | 136.02 | 115.30 |
| 1 | A | 2926 | LEU | CA-CB-CG | 8.88 | 135.71 | 115.30 |
| 1 | A | 1010 | LEU | CA-CB-CG | 8.37 | 134.55 | 115.30 |
| 1 | A | 3882 | LEU | CA-CB-CG | -8.14 | 96.57 | 115.30 |
| 1 | B | 2542 | LEU | CA-CB-CG | 7.94 | 133.56 | 115.30 |
| 1 | A | 3575 | LEU | CA-CB-CG | 7.75 | 133.12 | 115.30 |
| 1 | A | 1165 | LEU | CA-CB-CG | 7.67 | 132.95 | 115.30 |
| 1 | A | 2542 | LEU | CA-CB-CG | 7.53 | 132.63 | 115.30 |
| 1 | B | 1165 | LEU | CA-CB-CG | 7.50 | 132.54 | 115.30 |
| 1 | A | 1976 | LEU | CB-CG-CD1 | -7.38 | 98.45 | 111.00 |
| 1 | B | 1695 | LEU | CA-CB-CG | 7.22 | 131.91 | 115.30 |
| 1 | B | 4051 | LEU | CA-CB-CG | 6.89 | 131.15 | 115.30 |
| 1 | A | 3321 | LEU | CB-CG-CD2 | -6.88 | 99.31 | 111.00 |
| 1 | A | 3788 | LEU | CA-CB-CG | -6.87 | 99.49 | 115.30 |
| 1 | B | 1717 | LEU | CA-CB-CG | -6.85 | 99.53 | 115.30 |
| 1 | A | 1025 | LEU | CA-CB-CG | -6.81 | 99.63 | 115.30 |
| 1 | B | 3397 | GLN | CA-CB-CG | 6.52 | 127.75 | 113.40 |
| 1 | B | 220 | LEU | CA-CB-CG | 6.52 | 130.29 | 115.30 |
| 1 | B | 515 | ARG | NE-CZ-NH1 | -6.47 | 117.07 | 120.30 |
| 1 | A | 3480 | LEU | CA-CB-CG | 6.27 | 129.73 | 115.30 |
| 1 | A | 455 | LEU | CA-CB-CG | 6.26 | 129.70 | 115.30 |
| 1 | B | 862 | LEU | CB-CG-CD2 | -6.26 | 100.36 | 111.00 |
| 1 | A | 3665 | MSE | CB-CG-SE | 6.25 | 131.43 | 112.70 |
| 1 | B | 1580 | LEU | CA-CB-CG | 6.24 | 129.65 | 115.30 |
| 1 | A | 1111 | LEU | CA-CB-CG | -6.24 | 100.95 | 115.30 |
| 1 | A | 2241 | LEU | CA-CB-CG | -6.19 | 101.07 | 115.30 |
| 1 | B | 1984 | LEU | CA-CB-CG | 6.17 | 129.49 | 115.30 |
| 1 | B | 2892 | LEU | CA-CB-CG | 6.14 | 129.43 | 115.30 |
| 1 | B | 1812 | LEU | CA-CB-CG | 6.14 | 129.43 | 115.30 |
| 1 | A | 1524 | LEU | CA-CB-CG | 6.13 | 129.41 | 115.30 |
| 1 | A | 1145 | LEU | CA-CB-CG | 6.13 | 129.40 | 115.30 |
| 1 | B | 2921 | LEU | CA-CB-CG | 6.09 | 129.30 | 115.30 |
| 1 | B | 3667 | LEU | CA-CB-CG | 6.07 | 129.26 | 115.30 |
| 1 | B | 3416 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 1 | A | 718 | MSE | CB-CG-SE | -6.02 | 94.64 | 112.70 |
| 1 | B | 942 | LEU | CB-CG-CD1 | -6.02 | 100.77 | 111.00 |
| 1 | A | 1648 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 1 | A | 901 | MSE | CA-CB-CG | -5.94 | 103.20 | 113.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | B | 1025 | LEU | CA-CB-CG | -5.93 | 101.66 | 115.30 |
| 1 | B | 3988 | LEU | CA-CB-CG | -5.87 | 101.80 | 115.30 |
| 1 | A | 204 | LEU | CA-CB-CG | -5.84 | 101.87 | 115.30 |
| 1 | B | 913 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 1 | B | 3230 | LEU | CA-CB-CG | 5.79 | 128.61 | 115.30 |
| 1 | A | 1984 | LEU | CA-CB-CG | 5.75 | 128.52 | 115.30 |
| 1 | A | 3963 | LEU | CA-CB-CG | 5.75 | 128.52 | 115.30 |
| 1 | B | 942 | LEU | CA-CB-CG | 5.73 | 128.47 | 115.30 |
| 1 | B | 734 | LEU | CA-CB-CG | -5.71 | 102.17 | 115.30 |
| 1 | B | 130 | LEU | CB-CG-CD1 | -5.69 | 101.33 | 111.00 |
| 1 | B | 545 | LEU | CA-CB-CG | 5.68 | 128.37 | 115.30 |
| 1 | B | 1686 | LEU | CA-CB-CG | -5.66 | 102.29 | 115.30 |
| 1 | B | 3734 | ARG | NE-CZ-NH2 | -5.64 | 117.48 | 120.30 |
| 1 | B | 2097 | LEU | CB-CG-CD2 | -5.62 | 101.44 | 111.00 |
| 1 | A | 1752 | LEU | CA-CB-CG | -5.56 | 102.50 | 115.30 |
| 1 | B | 612 | LEU | CA-CB-CG | 5.56 | 128.08 | 115.30 |
| 1 | A | 1812 | LEU | CA-CB-CG | 5.54 | 128.05 | 115.30 |
| 1 | B | 1643 | MSE | CB-CG-SE | -5.52 | 96.14 | 112.70 |
| 1 | B | 583 | LEU | CA-CB-CG | 5.51 | 127.97 | 115.30 |
| 1 | B | 2539 | LEU | CA-CB-CG | 5.50 | 127.95 | 115.30 |
| 1 | A | 2921 | LEU | CA-CB-CG | 5.49 | 127.92 | 115.30 |
| 1 | A | 414 | LEU | CA-CB-CG | -5.43 | 102.81 | 115.30 |
| 1 | B | 3788 | LEU | CA-CB-CG | -5.38 | 102.94 | 115.30 |
| 1 | A | 2235 | LEU | CA-CB-CG | 5.37 | 127.65 | 115.30 |
| 1 | A | 1415 | LEU | CA-CB-CG | -5.37 | 102.96 | 115.30 |
| 1 | A | 1976 | LEU | CA-CB-CG | 5.35 | 127.61 | 115.30 |
| 1 | A | 1915 | LEU | CA-CB-CG | 5.33 | 127.55 | 115.30 |
| 1 | A | 3667 | LEU | CA-CB-CG | 5.33 | 127.56 | 115.30 |
| 1 | B | 1572 | LEU | CA-CB-CG | 5.28 | 127.44 | 115.30 |
| 1 | B | 359 | LEU | CA-CB-CG | 5.25 | 127.39 | 115.30 |
| 1 | A | 313 | LEU | CA-CB-CG | 5.25 | 127.37 | 115.30 |
| 1 | A | 421 | LEU | CA-CB-CG | 5.24 | 127.35 | 115.30 |
| 1 | B | 1930 | GLU | CA-CB-CG | 5.22 | 124.89 | 113.40 |
| 1 | B | 421 | LEU | CA-CB-CG | 5.21 | 127.28 | 115.30 |
| 1 | A | 933 | LEU | CA-CB-CG | -5.21 | 103.32 | 115.30 |
| 1 | A | 2808 | LEU | CB-CG-CD1 | -5.20 | 102.16 | 111.00 |
| 1 | A | 563 | LEU | CB-CG-CD1 | -5.17 | 102.20 | 111.00 |
| 1 | A | 3152 | SER | C-N-CA | 5.17 | 134.63 | 121.70 |
| 1 | A | 1095 | LEU | CA-CB-CG | 5.16 | 127.17 | 115.30 |
| 1 | B | 2926 | LEU | CB-CG-CD2 | -5.16 | 102.23 | 111.00 |
| 1 | B | 3575 | LEU | CA-CB-CG | 5.14 | 127.13 | 115.30 |
| 1 | A | 892 | LEU | CA-CB-CG | -5.13 | 103.51 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1 | A | 2398 | LEU | CA-CB-CG | 5.12 | 127.09 | 115.30 |
| 1 | A | 1762 | MSE | CB-CG-SE | 5.12 | 128.06 | 112.70 |
| 1 | B | 2122 | LEU | CA-CB-CG | 5.12 | 127.07 | 115.30 |
| 1 | A | 2396 | LEU | CB-CG-CD2 | -5.11 | 102.31 | 111.00 |
| 1 | A | 758 | LEU | CA-CB-CG | -5.07 | 103.65 | 115.30 |
| 1 | B | 564 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 |
| 1 | B | 475 | LEU | CA-CB-CG | 5.04 | 126.89 | 115.30 |
| 1 | B | 871 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |
| 1 | A | 1582 | LEU | CA-CB-CG | -5.01 | 103.77 | 115.30 |
| 1 | B | 670 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |
| 1 | B | 3159 | ARG | NE-CZ-NH2 | -5.01 | 117.80 | 120.30 |

There are no chirality outliers.

All (14) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | A | 1323 | SER | Peptide |
| 1 | A | 2283 | ASN | Peptide |
| 1 | A | 2372 | PRO | Peptide |
| 1 | A | 3547 | THR | Peptide |
| 1 | A | 3980 | MSE | Peptide |
| 1 | A | 411 | PRO | Peptide |
| 1 | A | 4119 | ARG | Peptide |
| 1 | A | 634 | LEU | Peptide |
| 1 | B | 1323 | SER | Peptide |
| 1 | B | 2372 | PRO | Peptide |
| 1 | B | 3547 | THR | Peptide |
| 1 | B | 411 | PRO | Peptide |
| 1 | B | 4119 | ARG | Peptide |
| 1 | B | 634 | LEU | Peptide |

5.2 Too-close contacts [\(i\)](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 29574 | 0 | 29642 | 3223 | 0 |
| 1 | B | 29574 | 0 | 29642 | 3283 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | K | 273 | 0 | 70 | 9 | 0 |
| 2 | S | 273 | 0 | 73 | 8 | 0 |
| All | All | 59694 | 0 | 59427 | 6514 | 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 55.

All (6514) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2183:HIS:O | 1:B:2187:VAL:HB | 1.30 | 1.31 |
| 1:B:662:LEU:O | 1:B:666:PHE:HB2 | 1.28 | 1.30 |
| 1:A:3521:ILE:O | 1:A:3525:TYR:HB2 | 1.32 | 1.28 |
| 1:B:3683:CYS:SG | 1:B:3736:LYS:NZ | 2.12 | 1.23 |
| 1:B:2167:PRO:O | 1:B:2171:LEU:HB2 | 1.39 | 1.18 |
| 1:B:1344:PHE:O | 1:B:1348:LEU:HB2 | 1.41 | 1.18 |
| 1:A:3923:ARG:HG2 | 1:A:3962:ARG:HH22 | 1.07 | 1.17 |
| 1:B:1407:LYS:NZ | 1:B:1460:ARG:O | 1.77 | 1.16 |
| 1:B:3521:ILE:O | 1:B:3525:TYR:HB2 | 1.43 | 1.16 |
| 1:A:2183:HIS:O | 1:A:2187:VAL:HB | 1.39 | 1.16 |
| 1:A:368:LEU:HD21 | 1:A:384:MSE:HB2 | 1.25 | 1.15 |
| 1:B:3868:VAL:O | 1:B:3872:ARG:HB3 | 1.44 | 1.15 |
| 1:B:2872:ASP:O | 1:B:2913:LYS:NZ | 1.80 | 1.15 |
| 1:B:2477:LEU:O | 1:B:2481:HIS:HB3 | 1.44 | 1.14 |
| 1:B:3467:ARG:O | 1:B:3471:ILE:HB | 1.46 | 1.14 |
| 1:B:1931:ASN:O | 1:B:1938:ARG:NH2 | 1.80 | 1.13 |
| 1:B:974:CYS:HA | 1:B:981:ARG:HD2 | 1.17 | 1.13 |
| 1:A:3167:ARG:HD3 | 1:A:3186:ARG:HG2 | 1.29 | 1.12 |
| 1:B:67:VAL:O | 1:B:71:LYS:HB2 | 1.50 | 1.12 |
| 1:B:2100:LEU:HD21 | 1:B:2104:MSE:HE3 | 1.31 | 1.11 |
| 1:B:3099:ALA:O | 1:B:3103:ILE:HB | 1.47 | 1.11 |
| 1:A:3812:LEU:O | 1:A:3816:LEU:HB2 | 1.49 | 1.11 |
| 1:A:560:LEU:HB3 | 1:A:616:LYS:HZ3 | 1.12 | 1.11 |
| 1:B:2960:GLU:OE2 | 1:B:3289:ARG:NH1 | 1.83 | 1.10 |
| 1:B:19:LEU:O | 1:B:23:ASP:HB2 | 1.51 | 1.10 |
| 1:B:2891:ARG:HH22 | 1:B:3884:LYS:HD3 | 0.97 | 1.10 |
| 1:B:3581:PRO:HG2 | 1:B:3674:SER:HB2 | 1.34 | 1.09 |
| 1:A:3467:ARG:O | 1:A:3471:ILE:HB | 1.49 | 1.09 |
| 1:B:909:VAL:HG13 | 1:B:913:ARG:HH11 | 1.16 | 1.08 |
| 1:B:899:ARG:HH12 | 1:B:2570:PRO:HB2 | 1.17 | 1.08 |
| 1:B:3772:ASN:HB2 | 1:B:3787:GLN:HG3 | 1.36 | 1.07 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3868:VAL:O | 1:A:3872:ARG:HB3 | 1.54 | 1.07 |
| 1:B:3117:ILE:HD12 | 1:B:3125:ARG:HH11 | 1.15 | 1.07 |
| 1:A:887:ASP:HB3 | 1:A:3889:ARG:HB3 | 1.35 | 1.04 |
| 1:B:2304:VAL:HG11 | 1:B:2344:LEU:HB3 | 1.40 | 1.04 |
| 1:B:3534:ILE:HG12 | 1:B:3704:GLN:HE22 | 1.22 | 1.03 |
| 1:B:2991:LYS:NZ | 1:B:2995:GLU:OE2 | 1.91 | 1.03 |
| 1:A:2227:LYS:HD2 | 1:A:2235:LEU:HG | 1.37 | 1.03 |
| 1:A:4082:ARG:HG3 | 1:A:4091:ALA:HB2 | 1.40 | 1.03 |
| 1:A:963:LYS:NZ | 1:A:1006:THR:OG1 | 1.92 | 1.02 |
| 1:B:90:CYS:HB3 | 1:B:137:THR:HG22 | 1.40 | 1.02 |
| 1:A:327:VAL:HG22 | 1:A:338:LEU:HD13 | 1.38 | 1.02 |
| 1:B:2887:PRO:HB3 | 1:B:2922:ARG:HH11 | 1.24 | 1.02 |
| 1:B:4071:ALA:O | 1:B:4075:ARG:HB3 | 1.58 | 1.01 |
| 1:B:3917:ILE:O | 1:B:4048:LYS:NZ | 1.92 | 1.01 |
| 1:A:1491:ILE:O | 1:A:1497:ARG:NH1 | 1.93 | 1.00 |
| 1:B:3284:SER:HB2 | 1:B:3287:ARG:HH21 | 1.23 | 1.00 |
| 1:A:974:CYS:HA | 1:A:981:ARG:HD2 | 1.41 | 1.00 |
| 1:A:1808:ASP:HB2 | 1:A:1814:PHE:HB3 | 1.41 | 0.99 |
| 1:B:2216:LEU:HD22 | 1:B:2249:LEU:HD11 | 1.43 | 0.99 |
| 1:B:2166:SER:O | 1:B:2170:GLN:HB3 | 1.60 | 0.99 |
| 1:A:1471:GLN:O | 1:A:1475:LEU:HB3 | 1.63 | 0.98 |
| 1:B:985:GLU:HG3 | 1:B:1031:ARG:HH22 | 1.25 | 0.98 |
| 1:B:2879:GLY:HA2 | 1:B:2886:GLN:HG2 | 1.42 | 0.98 |
| 1:B:3284:SER:HA | 1:B:3287:ARG:HE | 1.24 | 0.98 |
| 1:B:3699:LEU:O | 1:B:3718:ARG:NH1 | 1.97 | 0.98 |
| 1:A:4103:GLN:O | 1:A:4107:LEU:HB2 | 1.64 | 0.98 |
| 1:B:963:LYS:NZ | 1:B:1006:THR:OG1 | 1.96 | 0.98 |
| 1:A:3819:THR:OG1 | 1:A:3889:ARG:NH1 | 1.96 | 0.97 |
| 1:B:1959:LEU:HD13 | 1:B:1998:MSE:HE3 | 1.44 | 0.97 |
| 1:A:357:LYS:HB3 | 1:A:360:SER:HB2 | 1.46 | 0.97 |
| 1:B:366:TYR:O | 1:B:369:PHE:HB3 | 1.62 | 0.97 |
| 1:A:366:TYR:O | 1:A:369:PHE:HB3 | 1.63 | 0.97 |
| 1:B:357:LYS:HB3 | 1:B:360:SER:HB2 | 1.44 | 0.97 |
| 1:B:2424:MSE:HG2 | 1:B:2433:LYS:HD2 | 1.47 | 0.96 |
| 1:B:3923:ARG:HG2 | 1:B:3962:ARG:HH22 | 1.30 | 0.96 |
| 1:A:2943:PHE:HD1 | 1:A:2944:THR:H | 1.13 | 0.96 |
| 1:B:1093:GLU:N | 1:B:1097:GLU:OE2 | 1.98 | 0.96 |
| 1:A:2070:GLU:HG3 | 1:A:2072:ARG:HG3 | 1.47 | 0.96 |
| 1:B:2243:GLU:HA | 1:B:2246:LYS:HD2 | 1.46 | 0.96 |
| 1:A:2375:ALA:O | 1:A:2379:MSE:HB3 | 1.66 | 0.96 |
| 1:B:1249:SER:O | 1:B:1253:THR:HB | 1.64 | 0.96 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1435:ASN:OD1 | 1:B:1489:LYS:NZ | 1.99 | 0.96 |
| 1:B:3931:ALA:O | 1:B:3935:GLY:HA2 | 1.63 | 0.96 |
| 1:A:3182:ILE:HB | 1:A:3186:ARG:NH1 | 1.80 | 0.95 |
| 1:A:3923:ARG:O | 1:A:3962:ARG:NH1 | 1.98 | 0.95 |
| 1:A:385:TYR:HD1 | 1:A:420:VAL:HG13 | 1.30 | 0.95 |
| 1:B:3819:THR:OG1 | 1:B:3889:ARG:NH1 | 2.00 | 0.95 |
| 1:B:2228:ARG:NH1 | 1:B:2269:ASP:OD1 | 1.98 | 0.95 |
| 1:A:560:LEU:HB3 | 1:A:616:LYS:NZ | 1.81 | 0.95 |
| 1:A:2962:ARG:HB2 | 1:A:3253:SER:HB3 | 1.47 | 0.95 |
| 1:B:440:VAL:HB | 1:B:483:VAL:HG12 | 1.46 | 0.95 |
| 1:B:2308:SER:HB3 | 1:B:2348:GLN:HG2 | 1.49 | 0.95 |
| 1:B:2538:ARG:HH11 | 1:B:2565:MSE:HB3 | 1.32 | 0.95 |
| 1:B:801:LYS:NZ | 1:B:877:ASP:OD2 | 2.00 | 0.95 |
| 1:A:1685:ASP:HB2 | 1:A:1727:ARG:HH22 | 1.28 | 0.94 |
| 1:B:3887:PHE:HB3 | 1:B:3897:PHE:HE1 | 1.31 | 0.94 |
| 1:A:1010:LEU:HB2 | 1:A:1028:PHE:CD1 | 2.02 | 0.94 |
| 1:A:1733:THR:HG21 | 1:A:1877:LEU:HB3 | 1.47 | 0.94 |
| 1:A:3885:ARG:HE | 1:A:3889:ARG:HD2 | 1.32 | 0.94 |
| 1:A:1883:ARG:HB2 | 1:A:1927:MSE:HE1 | 1.48 | 0.94 |
| 1:B:3923:ARG:HG2 | 1:B:3962:ARG:NH2 | 1.82 | 0.94 |
| 1:B:2416:LYS:O | 1:B:2420:PHE:HB3 | 1.68 | 0.94 |
| 1:B:3772:ASN:HD22 | 1:B:3788:LEU:H | 1.16 | 0.94 |
| 1:B:3722:PHE:HE1 | 1:B:3740:ILE:HG12 | 1.31 | 0.93 |
| 1:B:753:GLN:O | 1:B:757:LYS:HB2 | 1.68 | 0.93 |
| 1:A:3923:ARG:HG2 | 1:A:3962:ARG:NH2 | 1.83 | 0.93 |
| 1:B:3920:ILE:HG13 | 1:B:3923:ARG:HD2 | 1.50 | 0.93 |
| 1:B:977:ASP:HB2 | 1:B:981:ARG:HB3 | 1.50 | 0.93 |
| 1:B:2891:ARG:NH2 | 1:B:3884:LYS:HD3 | 1.81 | 0.93 |
| 1:B:61:ARG:O | 1:B:65:LEU:HB2 | 1.68 | 0.93 |
| 1:A:2443:MSE:HE3 | 1:A:2476:ILE:HB | 1.48 | 0.93 |
| 1:A:3789:ARG:NH2 | 1:A:3806:LEU:HD22 | 1.83 | 0.93 |
| 1:B:1966:LEU:HD22 | 1:B:1991:PRO:HB3 | 1.50 | 0.93 |
| 1:A:964:ARG:HB2 | 1:A:1009:LEU:HD22 | 1.49 | 0.93 |
| 1:A:3521:ILE:O | 1:A:3525:TYR:CB | 2.16 | 0.93 |
| 1:A:473:PRO:HA | 1:A:476:ARG:HH22 | 1.33 | 0.93 |
| 1:B:760:LEU:HD11 | 1:B:799:TYR:HB2 | 1.48 | 0.93 |
| 1:A:2549:LYS:HZ1 | 1:A:2557:LEU:HD22 | 1.30 | 0.92 |
| 1:B:659:ARG:HH22 | 1:B:662:LEU:HG | 1.33 | 0.92 |
| 1:B:3462:ARG:HB2 | 1:B:3498:TRP:HB3 | 1.47 | 0.92 |
| 1:A:2330:VAL:HG21 | 1:A:2338:GLU:HB3 | 1.52 | 0.92 |
| 1:A:2457:PRO:HA | 1:A:2460:GLU:HB2 | 1.52 | 0.92 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3872:ARG:HH11 | 1:A:3965:ARG:NH1 | 1.67 | 0.92 |
| 1:B:1949:ILE:HD12 | 1:B:1952:ILE:HG21 | 1.51 | 0.92 |
| 1:B:2330:VAL:HG22 | 1:B:2335:ASN:HA | 1.51 | 0.92 |
| 1:B:756:PHE:HA | 1:B:773:LEU:HD13 | 1.50 | 0.92 |
| 1:B:1343:GLU:O | 1:B:1347:THR:OG1 | 1.88 | 0.92 |
| 1:B:1729:PHE:HE2 | 1:B:1870:LYS:HA | 1.32 | 0.91 |
| 1:B:2390:HIS:HA | 1:B:2397:CYS:HB2 | 1.52 | 0.91 |
| 1:A:3462:ARG:HB2 | 1:A:3498:TRP:HB3 | 1.49 | 0.91 |
| 1:B:970:LEU:HD22 | 1:B:1031:ARG:HH21 | 1.34 | 0.91 |
| 1:B:2330:VAL:HG21 | 1:B:2338:GLU:HB3 | 1.52 | 0.91 |
| 1:B:2011:ALA:HB3 | 1:B:2014:ALA:HB2 | 1.50 | 0.91 |
| 1:A:363:ILE:O | 1:A:367:GLY:N | 2.03 | 0.91 |
| 1:A:2375:ALA:O | 1:A:2379:MSE:CB | 2.19 | 0.91 |
| 1:A:616:LYS:O | 1:A:620:PHE:HB2 | 1.71 | 0.91 |
| 1:B:808:GLU:HG2 | 1:B:852:ARG:HH21 | 1.31 | 0.91 |
| 1:B:1107:TYR:O | 1:B:1110:SER:HB2 | 1.71 | 0.91 |
| 1:B:2361:ILE:HD12 | 1:B:2364:LEU:HD12 | 1.49 | 0.91 |
| 1:B:2559:THR:HG21 | 1:B:2808:LEU:HD13 | 1.53 | 0.91 |
| 1:B:1743:MSE:SE | 1:B:1880:MSE:SE | 2.90 | 0.90 |
| 1:A:3498:TRP:CD1 | 1:A:3502:MSE:HB2 | 2.05 | 0.90 |
| 1:B:1010:LEU:HD13 | 1:B:1028:PHE:HE1 | 1.36 | 0.90 |
| 1:B:3839:TYR:HE1 | 1:B:3867:THR:HB | 1.36 | 0.90 |
| 1:B:429:GLU:O | 1:B:431:TYR:N | 2.04 | 0.90 |
| 1:A:1905:ILE:HG12 | 1:A:1951:VAL:HG11 | 1.51 | 0.90 |
| 1:A:1987:ARG:O | 1:A:1991:PRO:HD3 | 1.71 | 0.90 |
| 1:A:2837:LEU:HD22 | 1:A:2868:LEU:HG | 1.51 | 0.90 |
| 1:A:1106:ILE:O | 1:A:1110:SER:N | 2.05 | 0.89 |
| 1:A:1155:ARG:NH1 | 1:A:1155:ARG:O | 2.04 | 0.89 |
| 1:B:4082:ARG:HG3 | 1:B:4091:ALA:HB2 | 1.54 | 0.89 |
| 1:B:2562:LEU:HD12 | 1:B:2812:LEU:HD21 | 1.53 | 0.89 |
| 1:A:1090:ARG:HH21 | 1:A:1100:VAL:HG11 | 1.35 | 0.89 |
| 1:A:2467:THR:HB | 1:A:2518:GLN:HE22 | 1.35 | 0.89 |
| 1:A:2552:VAL:HG23 | 1:A:2852:PRO:HG2 | 1.54 | 0.89 |
| 1:B:1552:HIS:O | 1:B:1555:HIS:ND1 | 2.05 | 0.89 |
| 1:B:2142:ILE:HA | 1:B:2145:PHE:CD2 | 2.07 | 0.89 |
| 1:A:429:GLU:O | 1:A:431:TYR:N | 2.06 | 0.89 |
| 1:B:2352:HIS:HB3 | 1:B:2360:PHE:HB3 | 1.54 | 0.89 |
| 1:B:1651:LYS:HB2 | 1:B:1684:LEU:HD11 | 1.53 | 0.89 |
| 1:B:3887:PHE:HB3 | 1:B:3897:PHE:CE1 | 2.08 | 0.89 |
| 1:A:1931:ASN:O | 1:A:1938:ARG:NH2 | 2.06 | 0.89 |
| 1:A:3816:LEU:HD13 | 1:A:3966:GLN:HE22 | 1.36 | 0.89 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3696:ARG:NH1 | 1:A:3720:ALA:O | 2.05 | 0.88 |
| 1:B:3259:LEU:O | 1:B:3263:HIS:HB2 | 1.73 | 0.88 |
| 1:B:2891:ARG:HD3 | 1:B:3972:LEU:HD22 | 1.55 | 0.88 |
| 1:A:1729:PHE:HE2 | 1:A:1870:LYS:HA | 1.39 | 0.88 |
| 1:A:2957:LEU:HB3 | 1:A:3989:ARG:NH1 | 1.87 | 0.88 |
| 1:B:993:HIS:HB2 | 1:B:1038:LYS:HG2 | 1.55 | 0.88 |
| 1:B:3048:LYS:HD3 | 1:B:3061:LEU:HD23 | 1.55 | 0.88 |
| 1:B:3762:GLN:HA | 1:B:3793:VAL:HG21 | 1.54 | 0.88 |
| 1:B:473:PRO:HA | 1:B:476:ARG:HH22 | 1.36 | 0.88 |
| 1:A:2390:HIS:HA | 1:A:2397:CYS:HB2 | 1.54 | 0.88 |
| 1:B:1241:LEU:HD11 | 1:B:1253:THR:HG21 | 1.54 | 0.88 |
| 1:B:2326:ILE:O | 1:B:2330:VAL:HB | 1.74 | 0.88 |
| 1:A:1010:LEU:HB2 | 1:A:1028:PHE:HD1 | 1.36 | 0.88 |
| 1:B:3923:ARG:O | 1:B:3962:ARG:NH1 | 2.07 | 0.88 |
| 1:A:3589:SER:O | 1:A:3593:ARG:HB2 | 1.74 | 0.88 |
| 1:A:3772:ASN:HB2 | 1:A:3787:GLN:HG3 | 1.55 | 0.88 |
| 1:A:801:LYS:HB2 | 1:A:805:LEU:HD12 | 1.56 | 0.88 |
| 1:B:1582:LEU:HD22 | 1:B:1600:MSE:HE1 | 1.52 | 0.88 |
| 1:A:90:CYS:HB3 | 1:A:137:THR:HG22 | 1.56 | 0.88 |
| 1:A:3772:ASN:ND2 | 1:A:3788:LEU:O | 2.06 | 0.88 |
| 1:A:185:HIS:H | 1:A:186:PRO:HD2 | 1.38 | 0.88 |
| 1:A:2022:PRO:HB2 | 1:A:2072:ARG:HH21 | 1.36 | 0.88 |
| 1:A:658:THR:HA | 1:A:733:LEU:HD22 | 1.55 | 0.88 |
| 1:B:1018:VAL:HB | 1:B:1074:LYS:HB2 | 1.54 | 0.88 |
| 1:B:741:ILE:O | 1:B:744:ASP:N | 2.05 | 0.88 |
| 1:B:662:LEU:O | 1:B:666:PHE:CB | 2.20 | 0.87 |
| 1:B:658:THR:HA | 1:B:733:LEU:HD22 | 1.55 | 0.87 |
| 1:A:473:PRO:HA | 1:A:476:ARG:NH2 | 1.88 | 0.87 |
| 1:A:535:LEU:HD21 | 1:A:623:PHE:HA | 1.55 | 0.87 |
| 1:B:1808:ASP:HB2 | 1:B:1814:PHE:HB3 | 1.54 | 0.87 |
| 1:B:2546:TYR:CE1 | 1:B:2558:ALA:HB2 | 2.09 | 0.87 |
| 1:A:105:VAL:HG21 | 1:A:149:ILE:HD13 | 1.53 | 0.87 |
| 1:B:252:VAL:HG11 | 1:B:265:TYR:HB2 | 1.56 | 0.87 |
| 1:A:3003:ASN:ND2 | 1:A:3014:CYS:SG | 2.47 | 0.87 |
| 1:A:2378:PHE:HE1 | 1:A:2408:MSE:HE1 | 1.40 | 0.87 |
| 1:B:2307:MSE:HB3 | 1:B:2348:GLN:HE22 | 1.39 | 0.87 |
| 1:A:2477:LEU:O | 1:A:2481:HIS:HB3 | 1.74 | 0.87 |
| 1:B:591:GLN:OE1 | 1:B:1026:ARG:NH1 | 2.08 | 0.87 |
| 1:B:2253:TYR:HD1 | 1:B:2256:ILE:HD12 | 1.37 | 0.86 |
| 1:A:866:ILE:HD13 | 1:A:3129:LEU:HB3 | 1.57 | 0.86 |
| 1:B:3530:VAL:HG11 | 1:B:3702:PRO:HD3 | 1.55 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1107:TYR:O | 1:A:1110:SER:HB2 | 1.74 | 0.86 |
| 1:A:3492:CYS:O | 1:A:3495:PHE:HB3 | 1.74 | 0.86 |
| 1:B:2286:PRO:HB2 | 1:B:2289:ASP:HA | 1.57 | 0.86 |
| 1:A:1407:LYS:O | 1:A:1409:SER:N | 2.08 | 0.86 |
| 1:A:1919:CYS:O | 1:A:1923:PHE:HB2 | 1.76 | 0.86 |
| 1:A:793:LEU:HA | 1:A:796:LEU:HG | 1.58 | 0.86 |
| 1:A:2563:LEU:O | 1:A:2567:SER:OG | 1.93 | 0.86 |
| 1:B:2837:LEU:HA | 1:B:2840:PHE:HD2 | 1.40 | 0.86 |
| 1:A:1603:GLN:OE1 | 1:A:1606:ARG:NH2 | 2.08 | 0.86 |
| 1:A:4071:ALA:O | 1:A:4075:ARG:HB3 | 1.76 | 0.86 |
| 1:B:2253:TYR:HB2 | 1:B:2291:GLN:HG2 | 1.56 | 0.86 |
| 1:B:2443:MSE:SE | 1:B:2476:ILE:HB | 2.25 | 0.86 |
| 1:A:1749:ALA:HA | 1:A:1752:LEU:HD12 | 1.55 | 0.86 |
| 1:B:3167:ARG:HH11 | 1:B:3167:ARG:HG3 | 1.40 | 0.86 |
| 1:B:658:THR:HG22 | 1:B:659:ARG:NH1 | 1.89 | 0.86 |
| 1:A:3326:GLN:HB2 | 1:A:3393:GLU:HG2 | 1.56 | 0.86 |
| 1:A:659:ARG:HH22 | 1:A:662:LEU:HG | 1.41 | 0.86 |
| 1:A:1762:MSE:SE | 1:A:1896:ILE:HG23 | 2.26 | 0.85 |
| 1:A:3581:PRO:HG2 | 1:A:3674:SER:HB2 | 1.58 | 0.85 |
| 1:B:1733:THR:HG21 | 1:B:1877:LEU:HB3 | 1.55 | 0.85 |
| 1:A:2142:ILE:HA | 1:A:2145:PHE:CD2 | 2.11 | 0.85 |
| 1:B:745:VAL:HG11 | 1:B:776:TRP:HZ2 | 1.39 | 0.85 |
| 1:A:527:TYR:OH | 1:A:615:ALA:O | 1.93 | 0.85 |
| 1:A:1010:LEU:HA | 1:A:1013:ILE:HG12 | 1.56 | 0.85 |
| 1:B:2358:ASP:HB2 | 1:B:2396:LEU:HD21 | 1.57 | 0.85 |
| 1:B:3326:GLN:HB2 | 1:B:3393:GLU:HG2 | 1.57 | 0.85 |
| 1:B:3868:VAL:O | 1:B:3872:ARG:CB | 2.24 | 0.85 |
| 1:A:3613:MSE:HE1 | 1:A:3617:LEU:HD12 | 1.56 | 0.85 |
| 1:A:4007:LYS:HG3 | 1:A:4041:ARG:HD2 | 1.55 | 0.85 |
| 1:B:3632:PHE:O | 1:B:3637:GLY:N | 2.08 | 0.85 |
| 1:A:2330:VAL:HG22 | 1:A:2335:ASN:HA | 1.57 | 0.85 |
| 1:B:3487:ILE:HG21 | 1:B:3495:PHE:HB2 | 1.58 | 0.85 |
| 1:B:725:LEU:O | 1:B:728:SER:OG | 1.94 | 0.85 |
| 1:A:2043:PHE:O | 1:A:2047:THR:OG1 | 1.93 | 0.85 |
| 1:B:2227:LYS:HD2 | 1:B:2235:LEU:HG | 1.58 | 0.85 |
| 1:B:2375:ALA:O | 1:B:2379:MSE:HB3 | 1.76 | 0.85 |
| 1:B:2478:MSE:O | 1:B:2482:ASP:HB3 | 1.76 | 0.85 |
| 1:A:971:ARG:HG3 | 1:A:972:LEU:N | 1.90 | 0.85 |
| 1:A:2007:ILE:HG22 | 1:A:2009:LYS:HB2 | 1.57 | 0.85 |
| 1:B:2070:GLU:HG3 | 1:B:2072:ARG:HG3 | 1.57 | 0.85 |
| 1:B:3589:SER:O | 1:B:3593:ARG:HB2 | 1.77 | 0.85 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:974:CYS:HA | 1:A:981:ARG:CD | 2.07 | 0.84 |
| 1:B:1010:LEU:HB2 | 1:B:1028:PHE:HD1 | 1.40 | 0.84 |
| 1:B:2481:HIS:HE1 | 1:B:2485:ARG:NH1 | 1.75 | 0.84 |
| 1:B:3583:LEU:HD11 | 1:B:3733:ARG:HB3 | 1.57 | 0.84 |
| 1:A:2161:ALA:HA | 1:A:2164:TRP:HD1 | 1.42 | 0.84 |
| 1:B:2300:PHE:CZ | 1:B:2341:LEU:HB2 | 2.12 | 0.84 |
| 1:B:3811:THR:OG1 | 1:B:3813:LYS:NZ | 2.09 | 0.84 |
| 1:A:2292:CYS:HB3 | 1:A:2300:PHE:HB2 | 1.57 | 0.84 |
| 1:A:2837:LEU:HA | 1:A:2840:PHE:HD2 | 1.41 | 0.84 |
| 1:B:2196:TRP:CD2 | 1:B:2199:LEU:HD11 | 2.12 | 0.84 |
| 1:B:3182:ILE:HB | 1:B:3186:ARG:NH1 | 1.91 | 0.84 |
| 1:A:286:LEU:HB2 | 1:A:290:TYR:HB2 | 1.59 | 0.84 |
| 1:B:978:GLN:HA | 1:B:981:ARG:HE | 1.42 | 0.84 |
| 1:B:3243:ILE:HG12 | 1:B:3258:LEU:HD11 | 1.58 | 0.84 |
| 1:B:3725:ARG:HH12 | 1:B:3737:ARG:NH2 | 1.74 | 0.84 |
| 1:B:3879:PRO:HA | 1:B:3882:LEU:HB2 | 1.58 | 0.84 |
| 1:A:3174:ASP:H | 1:A:3175:PRO:HD2 | 1.42 | 0.84 |
| 1:A:3868:VAL:HG11 | 1:A:4114:PRO:HB3 | 1.60 | 0.84 |
| 1:B:3117:ILE:HD12 | 1:B:3125:ARG:NH1 | 1.91 | 0.84 |
| 1:A:3092:LEU:HA | 1:A:3192:LYS:HE3 | 1.58 | 0.84 |
| 1:A:361:ILE:HB | 1:A:364:ARG:NH2 | 1.92 | 0.84 |
| 1:B:1162:SER:H | 1:B:1165:LEU:HD12 | 1.42 | 0.84 |
| 1:B:2552:VAL:HG23 | 1:B:2852:PRO:HG2 | 1.57 | 0.84 |
| 1:B:3486:GLU:HG3 | 1:B:3487:ILE:H | 1.43 | 0.84 |
| 1:B:3858:MSE:HE3 | 1:B:4119:ARG:HA | 1.60 | 0.84 |
| 1:B:2161:ALA:HA | 1:B:2164:TRP:HD1 | 1.43 | 0.84 |
| 1:B:2329:TYR:O | 1:B:2333:ARG:N | 2.11 | 0.84 |
| 1:A:1410:PRO:HB2 | 1:A:1414:ILE:HD12 | 1.58 | 0.84 |
| 1:A:1743:MSE:O | 1:A:1747:LEU:HB2 | 1.78 | 0.83 |
| 1:A:1992:VAL:O | 1:A:1996:VAL:HG22 | 1.78 | 0.83 |
| 1:A:2542:LEU:HB2 | 1:A:2546:TYR:HE2 | 1.42 | 0.83 |
| 1:B:3687:MSE:O | 1:B:3689:ASP:N | 2.11 | 0.83 |
| 1:B:2152:ASN:HB3 | 1:B:2153:THR:HA | 1.60 | 0.83 |
| 1:B:3900:LEU:HD21 | 1:B:3935:GLY:HA3 | 1.59 | 0.83 |
| 1:B:4103:GLN:O | 1:B:4107:LEU:HB2 | 1.77 | 0.83 |
| 1:A:2415:LEU:O | 1:A:2419:ASP:HB2 | 1.78 | 0.83 |
| 1:A:968:VAL:HG23 | 1:A:971:ARG:HD3 | 1.60 | 0.83 |
| 1:B:2813:PHE:HD2 | 1:B:2859:GLN:HG3 | 1.43 | 0.83 |
| 1:B:3499:ILE:HG23 | 1:B:3535:ILE:HD13 | 1.60 | 0.83 |
| 1:B:971:ARG:HG3 | 1:B:972:LEU:N | 1.93 | 0.83 |
| 1:A:352:VAL:HG23 | 1:A:357:LYS:H | 1.43 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3521:ILE:O | 1:B:3525:TYR:CB | 2.27 | 0.83 |
| 1:B:2274:ILE:HD13 | 1:B:2318:ALA:HB2 | 1.60 | 0.83 |
| 1:A:4090:ARG:HH11 | 1:A:4106:CYS:HA | 1.41 | 0.83 |
| 1:A:61:ARG:O | 1:A:65:LEU:HB2 | 1.77 | 0.83 |
| 1:B:1073:PHE:HD1 | 1:B:1074:LYS:H | 1.27 | 0.83 |
| 1:B:609:ALA:H | 1:B:1798:LEU:HD12 | 1.43 | 0.83 |
| 1:B:3725:ARG:NH1 | 1:B:3737:ARG:HH22 | 1.76 | 0.83 |
| 2:K:106:UNK:O | 2:K:110:UNK:N | 2.11 | 0.83 |
| 1:A:2361:ILE:HD12 | 1:A:2364:LEU:HD12 | 1.61 | 0.83 |
| 1:A:2478:MSE:O | 1:A:2482:ASP:HB3 | 1.78 | 0.83 |
| 1:B:658:THR:HG22 | 1:B:659:ARG:HH11 | 1.41 | 0.83 |
| 1:A:1886:LYS:HZ2 | 1:A:1924:THR:HB | 1.44 | 0.83 |
| 1:B:215:PRO:HG3 | 1:B:251:PHE:HB3 | 1.59 | 0.83 |
| 1:B:2435:CYS:O | 1:B:2439:ILE:HB | 1.77 | 0.83 |
| 1:B:245:SER:HA | 1:B:248:ILE:HD12 | 1.58 | 0.83 |
| 1:B:1087:ARG:HD3 | 1:B:1134:LEU:HB3 | 1.60 | 0.83 |
| 1:B:3012:GLU:HB2 | 1:B:3050:LYS:NZ | 1.94 | 0.83 |
| 1:A:575:ILE:HA | 1:A:578:LYS:HB2 | 1.61 | 0.83 |
| 1:B:3034:PRO:HG2 | 1:B:3037:GLN:HB2 | 1.61 | 0.83 |
| 1:A:1138:ILE:HD13 | 1:A:1150:LYS:HE2 | 1.60 | 0.82 |
| 1:A:3961:PHE:CE1 | 1:A:3963:LEU:HB2 | 2.14 | 0.82 |
| 1:A:3972:LEU:O | 1:A:3974:MSE:N | 2.10 | 0.82 |
| 1:B:2957:LEU:HD22 | 1:B:4100:GLU:HG3 | 1.61 | 0.82 |
| 1:B:598:PRO:HB3 | 1:B:1022:ASP:HB2 | 1.59 | 0.82 |
| 1:B:1010:LEU:HB2 | 1:B:1028:PHE:CD1 | 2.14 | 0.82 |
| 1:A:1751:GLU:O | 1:A:1755:SER:N | 2.11 | 0.82 |
| 1:B:3737:ARG:HH11 | 1:B:3739:ILE:HD11 | 1.43 | 0.82 |
| 1:B:3816:LEU:HD21 | 1:B:3883:LEU:HD13 | 1.59 | 0.82 |
| 1:A:1651:LYS:HB3 | 1:A:1680:ALA:HB1 | 1.59 | 0.82 |
| 1:A:2196:TRP:CD2 | 1:A:2199:LEU:HD11 | 2.14 | 0.82 |
| 1:A:1007:VAL:O | 1:A:1011:GLU:HB2 | 1.79 | 0.82 |
| 1:A:2002:LYS:O | 1:A:2004:TYR:N | 2.12 | 0.82 |
| 1:A:1070:PRO:HB2 | 1:A:1073:PHE:CZ | 2.14 | 0.82 |
| 1:A:2049:VAL:HA | 1:A:2052:TYR:HD2 | 1.42 | 0.82 |
| 1:A:203:GLU:O | 1:A:207:GLN:HB2 | 1.78 | 0.82 |
| 1:A:3722:PHE:HE1 | 1:A:3740:ILE:HG12 | 1.44 | 0.82 |
| 1:A:4057:ALA:HB3 | 1:A:4059:ILE:HB | 1.60 | 0.82 |
| 1:B:3751:LEU:O | 1:B:3802:LEU:HG | 1.80 | 0.82 |
| 1:A:3789:ARG:HH22 | 1:A:3806:LEU:HD22 | 1.42 | 0.82 |
| 1:A:70:ARG:HD3 | 1:A:82:ARG:HD3 | 1.59 | 0.82 |
| 1:A:959:TYR:O | 1:A:963:LYS:HB2 | 1.80 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2375:ALA:O | 1:B:2379:MSE:CB | 2.28 | 0.82 |
| 1:B:488:ILE:HG21 | 1:B:616:LYS:HD2 | 1.60 | 0.82 |
| 1:A:3152:SER:HB3 | 1:A:3153:SER:HB3 | 1.61 | 0.82 |
| 1:B:1346:THR:HG21 | 1:B:1401:ASN:HB3 | 1.62 | 0.82 |
| 1:B:1729:PHE:CE2 | 1:B:1870:LYS:HA | 2.15 | 0.82 |
| 1:A:3820:MSE:HA | 1:A:3882:LEU:HD22 | 1.62 | 0.81 |
| 1:A:978:GLN:HA | 1:A:981:ARG:HE | 1.44 | 0.81 |
| 1:B:2126:MSE:HG3 | 1:B:2129:LEU:HD12 | 1.61 | 0.81 |
| 1:B:2531:LEU:HG | 1:B:2538:ARG:HB2 | 1.62 | 0.81 |
| 1:B:974:CYS:HA | 1:B:981:ARG:CD | 2.07 | 0.81 |
| 1:A:3872:ARG:O | 1:A:3876:SER:OG | 1.98 | 0.81 |
| 1:B:3449:LYS:HA | 1:B:3452:LYS:HD2 | 1.62 | 0.81 |
| 1:B:956:PRO:HB2 | 1:B:957:PRO:HD3 | 1.62 | 0.81 |
| 1:A:1155:ARG:HH12 | 1:A:1159:PRO:HD3 | 1.45 | 0.81 |
| 1:A:1696:LEU:HA | 1:A:1700:THR:HG21 | 1.61 | 0.81 |
| 1:A:3762:GLN:HA | 1:A:3793:VAL:HG21 | 1.62 | 0.81 |
| 1:B:1729:PHE:CZ | 1:B:1870:LYS:HG3 | 2.15 | 0.81 |
| 1:B:1744:LYS:HG3 | 1:B:1880:MSE:HE3 | 1.60 | 0.81 |
| 1:B:1930:GLU:N | 1:B:1930:GLU:OE2 | 2.13 | 0.81 |
| 1:B:3044:MSE:O | 1:B:3047:SER:OG | 1.96 | 0.81 |
| 1:A:2167:PRO:O | 1:A:2171:LEU:CB | 2.28 | 0.81 |
| 1:B:1987:ARG:O | 1:B:1991:PRO:HD3 | 1.80 | 0.81 |
| 1:A:2167:PRO:O | 1:A:2171:LEU:HB2 | 1.79 | 0.81 |
| 1:B:3498:TRP:CD1 | 1:B:3502:MSE:HB2 | 2.14 | 0.81 |
| 1:B:3572:ILE:HA | 1:B:3575:LEU:HD22 | 1.62 | 0.81 |
| 1:A:2538:ARG:NH1 | 1:A:2562:LEU:O | 2.13 | 0.81 |
| 1:A:3269:ARG:NH1 | 1:A:3312:VAL:HA | 1.96 | 0.81 |
| 1:B:1877:LEU:O | 1:B:1920:TYR:OH | 1.98 | 0.81 |
| 1:B:3238:MSE:SE | 1:B:3242:MSE:SE | 2.99 | 0.81 |
| 1:B:431:TYR:HA | 1:B:434:VAL:HG12 | 1.63 | 0.81 |
| 1:A:1080:LEU:HD12 | 1:A:1081:ALA:H | 1.46 | 0.81 |
| 1:B:2260:PHE:HD1 | 1:B:2274:ILE:HG22 | 1.46 | 0.81 |
| 1:B:916:GLU:HB3 | 1:B:930:ALA:HB1 | 1.63 | 0.81 |
| 1:A:741:ILE:O | 1:A:744:ASP:N | 2.09 | 0.81 |
| 1:B:2031:LEU:HB2 | 1:B:2033:ASP:HB2 | 1.61 | 0.81 |
| 1:A:1729:PHE:CZ | 1:A:1870:LYS:HG3 | 2.16 | 0.81 |
| 1:A:2239:LYS:HG3 | 1:A:2279:ILE:HG23 | 1.62 | 0.81 |
| 1:A:3319:ASN:HD22 | 1:A:3407:ALA:HB1 | 1.45 | 0.81 |
| 1:A:382:ASP:O | 1:A:386:VAL:HB | 1.79 | 0.81 |
| 1:B:1017:ILE:HG21 | 1:B:1025:LEU:HD22 | 1.63 | 0.81 |
| 1:A:1594:SER:O | 1:A:1598:ASN:HB2 | 1.81 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1090:ARG:HH21 | 1:B:1100:VAL:HG11 | 1.45 | 0.81 |
| 1:A:977:ASP:HB3 | 1:A:981:ARG:H | 1.46 | 0.81 |
| 1:B:2379:MSE:HE1 | 1:B:2404:ARG:HD3 | 1.61 | 0.81 |
| 1:B:2446:LEU:O | 1:B:2451:LEU:HB2 | 1.81 | 0.81 |
| 1:B:891:ARG:HE | 1:B:894:PHE:HB3 | 1.46 | 0.81 |
| 1:A:1552:HIS:O | 1:A:1555:HIS:ND1 | 2.14 | 0.80 |
| 1:A:970:LEU:CD2 | 1:A:1031:ARG:HH21 | 1.94 | 0.80 |
| 1:B:959:TYR:O | 1:B:963:LYS:HB2 | 1.81 | 0.80 |
| 1:A:3872:ARG:HH11 | 1:A:3965:ARG:HH12 | 1.27 | 0.80 |
| 1:A:459:ARG:HG2 | 1:A:540:MSE:HE1 | 1.60 | 0.80 |
| 1:B:1729:PHE:HZ | 1:B:1870:LYS:HG3 | 1.45 | 0.80 |
| 1:B:3530:VAL:HG21 | 1:B:3701:ILE:HA | 1.63 | 0.80 |
| 1:A:2559:THR:HG21 | 1:A:2808:LEU:HD13 | 1.61 | 0.80 |
| 1:A:805:LEU:HD22 | 1:A:3125:ARG:HH11 | 1.45 | 0.80 |
| 1:B:1090:ARG:HH12 | 1:B:1096:VAL:HG13 | 1.45 | 0.80 |
| 1:B:893:SER:HB3 | 1:B:906:PHE:HB2 | 1.63 | 0.80 |
| 1:B:931:CYS:SG | 1:B:984:TYR:OH | 2.39 | 0.80 |
| 1:A:2243:GLU:HA | 1:A:2246:LYS:HD2 | 1.63 | 0.80 |
| 1:B:266:ALA:HB2 | 1:B:308:LEU:HG | 1.63 | 0.80 |
| 1:A:3638:LYS:HA | 1:A:3641:ASP:HB2 | 1.63 | 0.80 |
| 1:A:369:PHE:CD1 | 1:A:416:SER:HA | 2.17 | 0.80 |
| 1:A:619:ASP:O | 1:A:622:ALA:N | 2.14 | 0.80 |
| 1:B:2253:TYR:CD1 | 1:B:2256:ILE:HD12 | 2.16 | 0.80 |
| 1:A:725:LEU:O | 1:A:728:SER:OG | 1.99 | 0.80 |
| 1:B:1996:VAL:HG11 | 1:B:2048:GLY:HA2 | 1.63 | 0.80 |
| 1:A:939:MSE:SE | 1:A:2783:ILE:HG12 | 2.30 | 0.80 |
| 1:A:3046:ARG:NH2 | 1:A:3181:ASP:OD2 | 2.14 | 0.80 |
| 1:A:627:VAL:HG12 | 1:A:628:GLU:H | 1.46 | 0.80 |
| 1:B:295:GLU:HA | 1:B:298:LEU:HD22 | 1.63 | 0.80 |
| 1:A:1429:GLU:O | 1:A:1433:ALA:HB2 | 1.81 | 0.79 |
| 1:A:705:ALA:HB1 | 1:A:1385:ASN:HD21 | 1.46 | 0.79 |
| 1:B:16:GLN:O | 1:B:20:SER:HB3 | 1.81 | 0.79 |
| 1:B:3255:ALA:O | 1:B:3282:ARG:NH2 | 2.15 | 0.79 |
| 1:B:1112:ALA:HA | 1:B:1115:HIS:CE1 | 2.17 | 0.79 |
| 1:B:2546:TYR:HE1 | 1:B:2558:ALA:HB2 | 1.43 | 0.79 |
| 1:A:2861:ILE:HG21 | 1:A:2889:GLY:HA2 | 1.61 | 0.79 |
| 1:B:286:LEU:HB2 | 1:B:290:TYR:HB2 | 1.65 | 0.79 |
| 1:B:3252:PHE:HA | 1:B:3282:ARG:HD2 | 1.65 | 0.79 |
| 1:B:1918:LEU:HD11 | 1:B:1957:ASN:HB3 | 1.63 | 0.79 |
| 1:B:2423:VAL:O | 1:B:2425:ARG:N | 2.15 | 0.79 |
| 1:B:2837:LEU:HD22 | 1:B:2868:LEU:HG | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2987:THR:HB | 1:B:2991:LYS:H | 1.46 | 0.79 |
| 1:B:726:LEU:HA | 1:B:729:CYS:SG | 2.22 | 0.79 |
| 1:A:1886:LYS:HG3 | 1:A:1890:HIS:HE1 | 1.46 | 0.79 |
| 1:A:770:LEU:HD12 | 1:A:851:ILE:HD13 | 1.61 | 0.79 |
| 1:B:1410:PRO:HB2 | 1:B:1414:ILE:HD12 | 1.64 | 0.79 |
| 1:A:2474:TYR:HB3 | 1:A:2478:MSE:HE3 | 1.64 | 0.79 |
| 1:A:3989:ARG:HH21 | 1:A:4100:GLU:CB | 1.95 | 0.79 |
| 1:B:12:LEU:HD22 | 1:B:38:LEU:HA | 1.65 | 0.79 |
| 1:A:3450:MSE:SE | 1:A:3464:LYS:HG2 | 2.33 | 0.79 |
| 1:B:637:LYS:O | 1:B:641:PHE:HB3 | 1.81 | 0.79 |
| 1:A:2351:GLN:O | 1:A:2355:THR:OG1 | 2.00 | 0.79 |
| 1:B:1718:ILE:HG23 | 1:B:1750:LEU:HD11 | 1.62 | 0.79 |
| 1:B:298:LEU:HD23 | 1:B:316:LEU:HD13 | 1.62 | 0.79 |
| 1:A:1000:LYS:O | 1:A:1002:GLU:N | 2.15 | 0.79 |
| 1:A:796:LEU:HA | 1:A:799:TYR:CE2 | 2.18 | 0.79 |
| 1:A:767:GLU:HG3 | 1:A:851:ILE:HD11 | 1.65 | 0.79 |
| 1:B:1655:ILE:HG23 | 1:B:1677:SER:HB3 | 1.65 | 0.79 |
| 1:B:2121:ASP:HA | 1:B:2126:MSE:HB3 | 1.63 | 0.79 |
| 1:B:2443:MSE:HB3 | 1:B:2480:ILE:HG12 | 1.65 | 0.79 |
| 1:A:162:LEU:HD21 | 1:A:196:LEU:HD13 | 1.65 | 0.79 |
| 1:A:3955:VAL:HG12 | 1:A:4027:TRP:HE1 | 1.47 | 0.79 |
| 1:B:527:TYR:OH | 1:B:619:ASP:N | 2.16 | 0.79 |
| 1:B:627:VAL:HG12 | 1:B:628:GLU:H | 1.46 | 0.79 |
| 1:A:3314:SER:HA | 1:A:3315:TYR:HB3 | 1.64 | 0.78 |
| 1:A:3397:GLN:HE22 | 1:A:3449:LYS:HD3 | 1.49 | 0.78 |
| 1:A:714:VAL:HG13 | 1:A:734:LEU:HD13 | 1.65 | 0.78 |
| 1:B:1011:GLU:OE2 | 1:B:1062:ARG:NE | 2.17 | 0.78 |
| 1:B:1029:CYS:HB3 | 1:B:1085:ILE:HG13 | 1.63 | 0.78 |
| 1:A:2890:ILE:HG21 | 1:A:2922:ARG:HH12 | 1.49 | 0.78 |
| 1:B:1762:MSE:SE | 1:B:1896:ILE:HG23 | 2.33 | 0.78 |
| 1:B:2100:LEU:O | 1:B:2104:MSE:HB2 | 1.82 | 0.78 |
| 1:B:2153:THR:OG1 | 1:B:2154:GLU:N | 2.14 | 0.78 |
| 1:A:3736:LYS:HB3 | 1:A:3752:VAL:HB | 1.64 | 0.78 |
| 1:A:3868:VAL:O | 1:A:3872:ARG:CB | 2.29 | 0.78 |
| 1:B:1986:ARG:HH12 | 1:B:2036:LEU:HD22 | 1.46 | 0.78 |
| 1:A:15:LEU:HD23 | 1:A:2359:LYS:HZ3 | 1.48 | 0.78 |
| 1:A:2379:MSE:HE1 | 1:A:2404:ARG:HH11 | 1.49 | 0.78 |
| 1:A:903:PRO:HB2 | 1:A:2811:SER:HB2 | 1.65 | 0.78 |
| 1:B:1802:TYR:HA | 1:B:1805:PHE:HD2 | 1.47 | 0.78 |
| 1:B:2911:ARG:HG2 | 1:B:2914:ALA:HB3 | 1.66 | 0.78 |
| 1:B:538:ASP:HB3 | 1:B:627:VAL:HG13 | 1.66 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3499:ILE:HG23 | 1:A:3535:ILE:HD13 | 1.63 | 0.78 |
| 1:A:3904:PHE:O | 1:A:3907:SER:OG | 2.01 | 0.78 |
| 1:B:3529:ILE:HG23 | 1:B:3532:PRO:HD2 | 1.63 | 0.78 |
| 1:B:439:VAL:HG11 | 1:B:479:ILE:HD13 | 1.65 | 0.78 |
| 1:A:2467:THR:HA | 1:A:2470:ARG:HG3 | 1.64 | 0.78 |
| 1:A:376:ILE:HG13 | 1:A:381:VAL:HG21 | 1.65 | 0.78 |
| 1:B:808:GLU:CG | 1:B:852:ARG:HH21 | 1.96 | 0.78 |
| 1:A:960:GLN:HG3 | 1:A:1009:LEU:HD21 | 1.65 | 0.78 |
| 1:B:3575:LEU:HG | 1:B:3687:MSE:HG2 | 1.65 | 0.78 |
| 1:B:3923:ARG:NH2 | 1:B:3941:ASP:O | 2.17 | 0.78 |
| 1:A:980:THR:HG23 | 1:A:984:TYR:HE1 | 1.49 | 0.78 |
| 1:B:281:GLN:HA | 1:B:326:MSE:SE | 2.34 | 0.78 |
| 1:A:1582:LEU:HD22 | 1:A:1600:MSE:HE1 | 1.66 | 0.77 |
| 1:A:3922:ASP:O | 1:A:3927:ASN:ND2 | 2.17 | 0.77 |
| 1:B:2538:ARG:NH1 | 1:B:2565:MSE:HB3 | 1.98 | 0.77 |
| 1:B:3421:ASP:OD2 | 1:B:3464:LYS:NZ | 2.16 | 0.77 |
| 1:A:87:LYS:HG2 | 1:A:133:LYS:HG3 | 1.66 | 0.77 |
| 1:A:1886:LYS:HG3 | 1:A:1890:HIS:CE1 | 2.19 | 0.77 |
| 1:A:2190:VAL:HG21 | 1:A:2241:LEU:HD13 | 1.66 | 0.77 |
| 1:A:3479:THR:O | 1:A:3483:MSE:HB2 | 1.83 | 0.77 |
| 1:B:1407:LYS:O | 1:B:1409:SER:N | 2.14 | 0.77 |
| 1:B:2193:ILE:HA | 1:B:2196:TRP:CZ2 | 2.20 | 0.77 |
| 1:B:909:VAL:HG13 | 1:B:913:ARG:NH1 | 1.96 | 0.77 |
| 1:A:1640:GLU:O | 1:A:1644:ALA:HB2 | 1.85 | 0.77 |
| 1:A:1890:HIS:HB3 | 1:A:1937:ARG:HA | 1.65 | 0.77 |
| 1:A:2253:TYR:CD1 | 1:A:2256:ILE:HD12 | 2.18 | 0.77 |
| 1:A:2879:GLY:HA2 | 1:A:2886:GLN:HG2 | 1.65 | 0.77 |
| 1:B:3684:SER:O | 1:B:3688:SER:OG | 2.01 | 0.77 |
| 1:B:3732:LEU:HD21 | 1:B:3926:ASN:HD21 | 1.48 | 0.77 |
| 1:A:1073:PHE:HD1 | 1:A:1074:LYS:H | 1.30 | 0.77 |
| 1:A:1374:GLN:HB3 | 1:A:1377:CYS:HB3 | 1.64 | 0.77 |
| 1:A:1590:THR:O | 1:A:1592:MSE:N | 2.16 | 0.77 |
| 1:A:1718:ILE:HA | 1:A:1725:GLN:HE21 | 1.50 | 0.77 |
| 1:A:1946:ASN:ND2 | 1:A:1993:GLU:OE2 | 2.17 | 0.77 |
| 1:B:2235:LEU:O | 1:B:2239:LYS:N | 2.16 | 0.77 |
| 1:B:2457:PRO:HA | 1:B:2460:GLU:HB2 | 1.66 | 0.77 |
| 1:B:979:VAL:HG21 | 1:B:2656:UNK:HA | 1.66 | 0.77 |
| 1:B:3137:GLU:OE1 | 1:B:3167:ARG:NH1 | 2.18 | 0.77 |
| 1:B:805:LEU:HD22 | 1:B:3125:ARG:NH1 | 2.00 | 0.77 |
| 1:A:2412:TYR:HE1 | 1:A:2415:LEU:HD23 | 1.48 | 0.77 |
| 1:A:2467:THR:HG22 | 1:A:2470:ARG:NH1 | 2.00 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:552:SER:O | 1:A:556:SER:OG | 2.02 | 0.77 |
| 1:A:977:ASP:HB2 | 1:A:981:ARG:HB3 | 1.64 | 0.77 |
| 1:B:1080:LEU:HD13 | 1:B:1127:CYS:HB3 | 1.66 | 0.77 |
| 1:A:2083:LEU:O | 1:A:2087:GLU:N | 2.17 | 0.77 |
| 1:A:2161:ALA:HA | 1:A:2164:TRP:CD1 | 2.19 | 0.77 |
| 1:A:2847:THR:HB | 1:A:2850:PHE:CD2 | 2.20 | 0.77 |
| 1:A:2891:ARG:NH2 | 1:A:3884:LYS:HD3 | 2.00 | 0.77 |
| 1:B:2300:PHE:HZ | 1:B:2341:LEU:HB2 | 1.46 | 0.77 |
| 1:B:3148:GLN:HB2 | 1:B:3156:PRO:HB3 | 1.67 | 0.77 |
| 1:B:852:ARG:NH1 | 1:B:3111:MSE:SE | 2.68 | 0.77 |
| 1:A:2049:VAL:HG11 | 1:A:2100:LEU:HD12 | 1.66 | 0.77 |
| 1:A:2890:ILE:HG21 | 1:A:2922:ARG:NH1 | 2.00 | 0.77 |
| 1:B:2459:VAL:HG21 | 1:B:2501:LEU:HD21 | 1.67 | 0.77 |
| 1:B:4057:ALA:HB3 | 1:B:4059:ILE:HB | 1.65 | 0.77 |
| 1:A:2462:VAL:HB | 1:A:2473:MSE:SE | 2.35 | 0.77 |
| 1:A:3704:GLN:HB2 | 1:A:3796:MSE:HE2 | 1.66 | 0.77 |
| 1:A:3813:LYS:HE2 | 1:A:3926:ASN:HB2 | 1.67 | 0.77 |
| 1:A:67:VAL:O | 1:A:71:LYS:HB2 | 1.83 | 0.77 |
| 1:B:2236:GLU:HA | 1:B:2239:LYS:HB3 | 1.67 | 0.77 |
| 1:B:3152:SER:HB3 | 1:B:3153:SER:HB3 | 1.65 | 0.77 |
| 1:B:3923:ARG:CG | 1:B:3962:ARG:HH22 | 1.97 | 0.77 |
| 1:B:385:TYR:HD1 | 1:B:420:VAL:HG13 | 1.49 | 0.77 |
| 1:B:446:PHE:HA | 1:B:449:TYR:CE2 | 2.20 | 0.77 |
| 1:B:936:SER:HB3 | 1:B:2791:ILE:HG12 | 1.66 | 0.77 |
| 1:A:1343:GLU:O | 1:A:1347:THR:HB | 1.85 | 0.77 |
| 1:A:753:GLN:O | 1:A:757:LYS:HB2 | 1.84 | 0.77 |
| 1:B:1350:ASN:HD21 | 1:B:1404:LYS:HG2 | 1.47 | 0.77 |
| 1:B:1919:CYS:O | 1:B:1923:PHE:HB2 | 1.85 | 0.77 |
| 1:B:323:VAL:O | 1:B:327:VAL:HB | 1.84 | 0.77 |
| 1:B:1469:PRO:HA | 1:B:1472:SER:HB3 | 1.67 | 0.77 |
| 1:A:1356:TRP:CZ2 | 1:A:1409:SER:HB3 | 2.20 | 0.76 |
| 1:A:2239:LYS:O | 1:A:2242:VAL:HB | 1.85 | 0.76 |
| 1:A:2220:MSE:SE | 1:A:2256:ILE:HD11 | 2.34 | 0.76 |
| 1:A:2560:ASN:HB2 | 1:A:2800:ARG:HD3 | 1.66 | 0.76 |
| 1:B:2382:VAL:HG21 | 1:B:2404:ARG:HG3 | 1.64 | 0.76 |
| 1:B:3590:ASN:OD1 | 1:B:3593:ARG:NH2 | 2.18 | 0.76 |
| 1:A:1086:TYR:HE2 | 1:A:1090:ARG:HE | 1.33 | 0.76 |
| 1:A:1930:GLU:OE1 | 1:A:1987:ARG:NH1 | 2.18 | 0.76 |
| 1:A:2809:PHE:HB3 | 1:A:2859:GLN:NE2 | 1.99 | 0.76 |
| 1:A:46:SER:H | 1:A:51:LEU:HD13 | 1.49 | 0.76 |
| 1:B:16:GLN:O | 1:B:20:SER:CB | 2.32 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:942:LEU:HD22 | 1:B:2783:ILE:HG21 | 1.67 | 0.76 |
| 1:A:1081:ALA:O | 1:A:1085:ILE:HG12 | 1.86 | 0.76 |
| 1:A:3057:ALA:HB1 | 1:A:3062:LEU:HD11 | 1.67 | 0.76 |
| 1:A:805:LEU:CD2 | 1:A:3125:ARG:HH11 | 1.99 | 0.76 |
| 1:B:1987:ARG:O | 1:B:1990:PHE:N | 2.18 | 0.76 |
| 1:A:2253:TYR:CE2 | 1:A:2287:PRO:HB3 | 2.19 | 0.76 |
| 1:A:890:LYS:HG3 | 1:A:891:ARG:HD3 | 1.66 | 0.76 |
| 1:B:2473:MSE:O | 1:B:2476:ILE:HG12 | 1.85 | 0.76 |
| 1:B:3019:ILE:HG23 | 1:B:3021:SER:H | 1.51 | 0.76 |
| 1:A:1966:LEU:HD22 | 1:A:1991:PRO:HB3 | 1.66 | 0.76 |
| 1:B:1594:SER:O | 1:B:1598:ASN:HB2 | 1.85 | 0.76 |
| 1:B:2147:ALA:HB1 | 1:B:2151:ILE:HD12 | 1.67 | 0.76 |
| 1:B:2281:MSE:HE2 | 1:B:2322:VAL:HA | 1.66 | 0.76 |
| 1:B:2883:SER:O | 1:B:2886:GLN:HG3 | 1.84 | 0.76 |
| 1:A:2397:CYS:O | 1:A:2401:VAL:HB | 1.86 | 0.76 |
| 1:A:971:ARG:HG3 | 1:A:972:LEU:H | 1.50 | 0.76 |
| 1:B:3479:THR:O | 1:B:3483:MSE:HB2 | 1.86 | 0.76 |
| 1:B:891:ARG:HE | 1:B:894:PHE:CB | 1.99 | 0.76 |
| 1:A:3243:ILE:HD13 | 1:A:3262:LEU:HD22 | 1.65 | 0.76 |
| 1:A:385:TYR:CD1 | 1:A:420:VAL:HG13 | 2.18 | 0.76 |
| 1:A:638:GLN:HE22 | 1:A:669:LEU:HB2 | 1.51 | 0.76 |
| 1:B:1178:ARG:HB3 | 1:B:1179:PRO:HD3 | 1.68 | 0.76 |
| 1:B:185:HIS:H | 1:B:186:PRO:HD2 | 1.49 | 0.76 |
| 1:B:2453:GLU:O | 1:B:2457:PRO:HD3 | 1.85 | 0.76 |
| 1:A:1655:ILE:HD13 | 1:A:1681:ASP:HB3 | 1.68 | 0.76 |
| 1:A:2364:LEU:O | 1:A:2368:THR:OG1 | 2.03 | 0.76 |
| 1:B:1138:ILE:HG21 | 1:B:1150:LYS:HE2 | 1.68 | 0.76 |
| 1:B:2891:ARG:HH22 | 1:B:3884:LYS:CD | 1.88 | 0.76 |
| 1:B:3629:ARG:HH22 | 1:B:3638:LYS:NZ | 1.84 | 0.76 |
| 1:B:576:VAL:HG13 | 1:B:601:TRP:HE3 | 1.51 | 0.76 |
| 1:A:3019:ILE:HG23 | 1:A:3021:SER:H | 1.49 | 0.76 |
| 1:B:1091:GLU:HG2 | 1:B:1137:ILE:HG21 | 1.68 | 0.76 |
| 1:B:138:PHE:HD2 | 1:B:173:LYS:HE3 | 1.51 | 0.76 |
| 1:B:904:VAL:O | 1:B:906:PHE:N | 2.18 | 0.76 |
| 1:A:1700:THR:HA | 1:A:1703:THR:HB | 1.67 | 0.76 |
| 1:A:2313:LYS:HA | 1:A:2316:TYR:CE2 | 2.21 | 0.76 |
| 1:B:1036:PHE:HA | 1:B:1055:ASN:HD21 | 1.50 | 0.76 |
| 1:B:1070:PRO:HD3 | 1:B:1075:ARG:HD2 | 1.67 | 0.76 |
| 1:B:3534:ILE:HG12 | 1:B:3704:GLN:NE2 | 1.99 | 0.76 |
| 1:A:1007:VAL:O | 1:A:1011:GLU:CB | 2.33 | 0.75 |
| 1:A:1060:PHE:HA | 1:A:1063:LEU:HD12 | 1.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:143:LEU:H | 1:A:143:LEU:HD12 | 1.51 | 0.75 |
| 1:A:3176:MSE:HE2 | 1:A:3251:ASN:ND2 | 2.01 | 0.75 |
| 1:A:891:ARG:HG3 | 1:A:894:PHE:HB2 | 1.68 | 0.75 |
| 1:A:926:THR:O | 1:A:930:ALA:HB3 | 1.85 | 0.75 |
| 1:A:3487:ILE:HG21 | 1:A:3495:PHE:HB2 | 1.67 | 0.75 |
| 1:A:661:PRO:HG2 | 1:A:733:LEU:HA | 1.67 | 0.75 |
| 1:B:2062:ALA:HB1 | 1:B:2066:PHE:HE2 | 1.52 | 0.75 |
| 1:B:2542:LEU:HB2 | 1:B:2546:TYR:HE2 | 1.51 | 0.75 |
| 1:B:3520:GLU:OE1 | 1:B:3524:ASN:ND2 | 2.19 | 0.75 |
| 1:B:3872:ARG:O | 1:B:3876:SER:OG | 2.00 | 0.75 |
| 1:B:3989:ARG:HH21 | 1:B:4100:GLU:CG | 1.99 | 0.75 |
| 1:A:2183:HIS:CE1 | 1:A:2237:ILE:HG21 | 2.21 | 0.75 |
| 1:A:3487:ILE:HD11 | 1:A:3498:TRP:HH2 | 1.51 | 0.75 |
| 1:B:608:PRO:HG2 | 1:B:1798:LEU:HG | 1.68 | 0.75 |
| 1:B:19:LEU:O | 1:B:23:ASP:CB | 2.33 | 0.75 |
| 1:B:3284:SER:CB | 1:B:3287:ARG:HH21 | 1.99 | 0.75 |
| 1:A:1637:SER:O | 1:A:1640:GLU:N | 2.19 | 0.75 |
| 1:A:1751:GLU:HG2 | 1:A:1870:LYS:HE2 | 1.68 | 0.75 |
| 1:A:3305:SER:HA | 1:A:3308:ASP:HB3 | 1.68 | 0.75 |
| 1:A:1118:GLU:HG3 | 1:A:3743:HIS:HE1 | 1.51 | 0.75 |
| 1:A:1587:VAL:HB | 1:A:1643:MSE:HE2 | 1.68 | 0.75 |
| 1:A:2449:VAL:HA | 1:A:2452:ARG:HD2 | 1.67 | 0.75 |
| 1:A:3979:LEU:HA | 1:A:3981:TYR:HB3 | 1.67 | 0.75 |
| 1:B:1039:TRP:HZ2 | 1:B:1049:GLN:HA | 1.52 | 0.75 |
| 1:B:1356:TRP:CZ2 | 1:B:1409:SER:HB3 | 2.22 | 0.75 |
| 1:B:153:PHE:HB2 | 1:B:157:TYR:HE2 | 1.52 | 0.75 |
| 1:B:1992:VAL:O | 1:B:1996:VAL:HG22 | 1.85 | 0.75 |
| 1:B:3414:MSE:SE | 1:B:3450:MSE:SE | 3.04 | 0.75 |
| 1:A:3269:ARG:NH1 | 1:A:3312:VAL:HG12 | 2.02 | 0.75 |
| 1:B:2458:VAL:HA | 1:B:2461:PHE:CE2 | 2.22 | 0.75 |
| 1:B:2887:PRO:HG3 | 1:B:2921:LEU:HD13 | 1.68 | 0.75 |
| 1:B:3243:ILE:HG21 | 1:B:3262:LEU:HD22 | 1.68 | 0.75 |
| 1:A:2363:CYS:O | 1:A:2367:VAL:HG12 | 1.87 | 0.75 |
| 1:B:1086:TYR:CD2 | 1:B:1090:ARG:HG2 | 2.22 | 0.75 |
| 1:B:3144:PHE:CD1 | 1:B:3160:LEU:HD11 | 2.21 | 0.75 |
| 1:B:3491:PRO:HB3 | 1:B:3711:PRO:HB3 | 1.69 | 0.75 |
| 1:A:2300:PHE:CZ | 1:A:2341:LEU:HB2 | 2.22 | 0.74 |
| 1:A:2372:PRO:HB2 | 1:A:2374:LEU:HD13 | 1.68 | 0.74 |
| 1:B:353:ASP:O | 1:B:1859:ASN:ND2 | 2.19 | 0.74 |
| 1:B:2806:LYS:HD3 | 1:B:2855:VAL:HG13 | 1.67 | 0.74 |
| 1:B:253:LEU:HD21 | 1:B:297:LEU:HA | 1.68 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3583:LEU:HD11 | 1:A:3733:ARG:HB3 | 1.66 | 0.74 |
| 1:B:3012:GLU:HB2 | 1:B:3050:LYS:HZ1 | 1.51 | 0.74 |
| 1:B:385:TYR:HE1 | 1:B:421:LEU:HD23 | 1.52 | 0.74 |
| 1:B:1217:VAL:HG13 | 1:B:1274:ARG:HH12 | 1.50 | 0.74 |
| 1:B:1977:ILE:O | 1:B:1979:GLU:N | 2.17 | 0.74 |
| 1:B:2253:TYR:CZ | 1:B:2287:PRO:HB3 | 2.22 | 0.74 |
| 1:B:2311:ARG:HG3 | 1:B:2363:CYS:HB2 | 1.70 | 0.74 |
| 1:B:971:ARG:HG3 | 1:B:972:LEU:H | 1.52 | 0.74 |
| 1:A:1010:LEU:HD13 | 1:A:1028:PHE:HE1 | 1.51 | 0.74 |
| 1:A:3974:MSE:HB3 | 1:A:3976:GLU:H | 1.52 | 0.74 |
| 1:A:766:ALA:O | 1:A:768:VAL:N | 2.17 | 0.74 |
| 1:B:4021:LEU:HD22 | 1:B:4028:ILE:HD12 | 1.68 | 0.74 |
| 1:B:714:VAL:HG12 | 1:B:734:LEU:HD11 | 1.69 | 0.74 |
| 1:B:978:GLN:O | 1:B:981:ARG:HG2 | 1.88 | 0.74 |
| 1:A:2960:GLU:OE2 | 1:A:3289:ARG:NH1 | 2.19 | 0.74 |
| 1:B:1221:ILE:HG13 | 1:B:1274:ARG:HH11 | 1.53 | 0.74 |
| 1:B:3314:SER:HA | 1:B:3315:TYR:HB3 | 1.68 | 0.74 |
| 1:B:3447:VAL:HG12 | 1:B:3468:LEU:HD22 | 1.69 | 0.74 |
| 1:B:616:LYS:HB3 | 1:B:617:PRO:HD2 | 1.68 | 0.74 |
| 1:A:1976:LEU:HD11 | 1:A:2031:LEU:HB3 | 1.69 | 0.74 |
| 1:B:2810:SER:HA | 1:B:2813:PHE:CE2 | 2.23 | 0.74 |
| 1:B:3503:VAL:HG11 | 1:B:3535:ILE:HB | 1.70 | 0.74 |
| 1:A:242:PRO:HB3 | 1:A:282:PHE:CD1 | 2.22 | 0.74 |
| 1:A:3323:PHE:O | 1:A:3326:GLN:N | 2.19 | 0.74 |
| 1:A:2549:LYS:NZ | 1:A:2554:PHE:HA | 2.02 | 0.74 |
| 1:B:1012:ALA:O | 1:B:1015:ASP:HB3 | 1.87 | 0.74 |
| 1:B:3397:GLN:N | 1:B:3397:GLN:OE1 | 2.19 | 0.74 |
| 1:B:3459:ASN:O | 1:B:3462:ARG:HG2 | 1.87 | 0.74 |
| 1:B:4071:ALA:O | 1:B:4075:ARG:CB | 2.35 | 0.74 |
| 1:B:4084:SER:O | 1:B:4088:ASN:N | 2.21 | 0.74 |
| 1:B:793:LEU:HG | 1:B:796:LEU:HD12 | 1.68 | 0.74 |
| 1:A:3575:LEU:O | 1:A:3577:GLN:N | 2.21 | 0.74 |
| 1:A:3762:GLN:NE2 | 1:A:3763:ARG:HH11 | 1.85 | 0.74 |
| 1:B:2260:PHE:CD1 | 1:B:2274:ILE:HG22 | 2.23 | 0.74 |
| 1:B:4089:ILE:HB | 1:B:4090:ARG:NH2 | 2.02 | 0.74 |
| 1:A:2274:ILE:O | 1:A:2277:LEU:N | 2.21 | 0.74 |
| 1:A:2404:ARG:HG2 | 1:A:2408:MSE:HE3 | 1.68 | 0.74 |
| 1:A:940:PHE:CE2 | 1:A:2576:MSE:SE | 2.91 | 0.74 |
| 1:A:2877:SER:O | 1:A:2879:GLY:N | 2.21 | 0.74 |
| 1:A:273:ARG:HD2 | 1:A:314:SER:HB3 | 1.69 | 0.74 |
| 1:A:726:LEU:HA | 1:A:729:CYS:SG | 2.28 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:1871:MSE:HA | 1:B:1874:TYR:HB2 | 1.70 | 0.74 |
| 1:B:2379:MSE:HE1 | 1:B:2404:ARG:NH1 | 2.03 | 0.74 |
| 1:B:3110:PHE:O | 1:B:3114:TYR:HD1 | 1.69 | 0.74 |
| 1:B:968:VAL:HG23 | 1:B:971:ARG:HD3 | 1.70 | 0.74 |
| 1:A:3034:PRO:HG2 | 1:A:3037:GLN:HB2 | 1.69 | 0.73 |
| 1:A:432:THR:HG23 | 1:A:475:LEU:HD13 | 1.70 | 0.73 |
| 1:B:2068:ARG:O | 1:B:2070:GLU:N | 2.20 | 0.73 |
| 1:B:2253:TYR:CE2 | 1:B:2287:PRO:HB3 | 2.23 | 0.73 |
| 1:B:2379:MSE:SE | 1:B:2404:ARG:HD3 | 2.38 | 0.73 |
| 1:B:3928:PHE:HD2 | 1:B:3962:ARG:HH21 | 1.35 | 0.73 |
| 1:A:1132:ASP:HA | 1:A:1135:CYS:SG | 2.28 | 0.73 |
| 1:A:3176:MSE:HE1 | 1:A:3179:TRP:HE3 | 1.54 | 0.73 |
| 1:B:1073:PHE:CE2 | 1:B:3745:GLU:HA | 2.23 | 0.73 |
| 1:B:1985:LYS:HD2 | 1:B:2037:SER:HB3 | 1.69 | 0.73 |
| 1:B:2507:ILE:HA | 1:B:2510:LEU:HD12 | 1.69 | 0.73 |
| 1:A:2142:ILE:HA | 1:A:2145:PHE:HD2 | 1.51 | 0.73 |
| 1:A:2222:HIS:O | 1:A:2225:HIS:N | 2.16 | 0.73 |
| 1:A:760:LEU:HD13 | 1:A:802:THR:OG1 | 1.88 | 0.73 |
| 1:B:1342:MSE:HE2 | 1:B:1398:VAL:HG12 | 1.70 | 0.73 |
| 1:B:3493:TRP:HE3 | 1:B:3713:PRO:HB3 | 1.53 | 0.73 |
| 1:B:886:TRP:HD1 | 1:B:889:GLU:H | 1.35 | 0.73 |
| 1:B:363:ILE:O | 1:B:367:GLY:N | 2.18 | 0.73 |
| 1:A:2872:ASP:O | 1:A:2913:LYS:NZ | 2.21 | 0.73 |
| 1:B:2404:ARG:NH1 | 1:B:2412:TYR:CZ | 2.56 | 0.73 |
| 1:B:2917:PRO:HA | 1:B:2920:VAL:HG12 | 1.70 | 0.73 |
| 1:B:3432:SER:HB2 | 1:B:3435:ASP:HB2 | 1.69 | 0.73 |
| 1:A:2253:TYR:HB2 | 1:A:2291:GLN:HG2 | 1.70 | 0.73 |
| 1:A:4066:LEU:HG | 1:A:4075:ARG:HA | 1.71 | 0.73 |
| 1:B:1142:HIS:O | 1:B:1144:SER:N | 2.20 | 0.73 |
| 1:B:174:VAL:O | 1:B:178:LEU:HG | 1.88 | 0.73 |
| 1:B:2851:PHE:HA | 1:B:2854:PHE:CD2 | 2.24 | 0.73 |
| 1:B:3323:PHE:O | 1:B:3326:GLN:HG2 | 1.88 | 0.73 |
| 1:A:1115:HIS:O | 1:A:1119:LYS:N | 2.22 | 0.73 |
| 1:A:170:VAL:HG23 | 1:A:173:LYS:HD3 | 1.71 | 0.73 |
| 1:A:2883:SER:O | 1:A:2886:GLN:HG3 | 1.87 | 0.73 |
| 1:B:989:MSE:HE2 | 1:B:1031:ARG:HH12 | 1.54 | 0.73 |
| 1:B:2004:TYR:CD1 | 1:B:2054:TYR:HB3 | 2.23 | 0.73 |
| 1:B:3167:ARG:NH1 | 1:B:3167:ARG:HG3 | 2.02 | 0.73 |
| 1:B:4010:SER:O | 1:B:4015:ASN:N | 2.21 | 0.73 |
| 1:B:629:PHE:CZ | 1:B:666:PHE:HD1 | 2.07 | 0.73 |
| 1:A:70:ARG:HH22 | 1:A:117:LYS:HE3 | 1.54 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4010:SER:O | 1:A:4015:ASN:N | 2.22 | 0.73 |
| 1:A:567:GLU:OE2 | 1:A:1798:LEU:HB3 | 1.89 | 0.73 |
| 1:B:1070:PRO:HB2 | 1:B:1073:PHE:CZ | 2.24 | 0.73 |
| 1:B:153:PHE:HB2 | 1:B:157:TYR:CE2 | 2.24 | 0.73 |
| 1:B:2027:SER:HB2 | 1:B:2030:TYR:OH | 1.87 | 0.73 |
| 1:B:2321:GLU:OE2 | 1:B:2325:LEU:HD22 | 1.89 | 0.73 |
| 1:B:3944:HIS:HA | 1:B:4016:PHE:HZ | 1.53 | 0.73 |
| 1:A:1984:LEU:O | 1:A:1988:TYR:HB3 | 1.89 | 0.73 |
| 1:A:2571:ASP:O | 1:A:2789:SER:OG | 2.06 | 0.73 |
| 1:A:3167:ARG:O | 1:A:3186:ARG:NH2 | 2.22 | 0.73 |
| 1:B:1014:LEU:HB2 | 1:B:1078:ALA:HB1 | 1.71 | 0.73 |
| 1:B:1890:HIS:HB3 | 1:B:1937:ARG:HA | 1.69 | 0.73 |
| 1:A:1009:LEU:O | 1:A:1012:ALA:N | 2.22 | 0.73 |
| 1:A:1890:HIS:HB2 | 1:A:1937:ARG:HD2 | 1.71 | 0.73 |
| 1:A:19:LEU:O | 1:A:23:ASP:HB2 | 1.89 | 0.73 |
| 1:A:2157:PHE:CE1 | 1:A:2203:THR:HB | 2.23 | 0.73 |
| 1:A:2925:GLU:HB3 | 1:A:3121:LEU:HD11 | 1.70 | 0.73 |
| 1:B:730:LEU:HA | 1:B:733:LEU:HD12 | 1.71 | 0.73 |
| 1:A:3048:LYS:HD3 | 1:A:3061:LEU:HD23 | 1.71 | 0.72 |
| 1:A:609:ALA:O | 1:A:613:HIS:ND1 | 2.20 | 0.72 |
| 1:B:1651:LYS:O | 1:B:1655:ILE:HD12 | 1.89 | 0.72 |
| 1:B:2918:PRO:HA | 1:B:2921:LEU:HG | 1.70 | 0.72 |
| 1:A:1087:ARG:HD3 | 1:A:1134:LEU:HD22 | 1.71 | 0.72 |
| 1:A:1374:GLN:O | 1:A:1378:GLU:N | 2.21 | 0.72 |
| 1:A:253:LEU:HD11 | 1:A:297:LEU:HB3 | 1.71 | 0.72 |
| 1:A:3276:TRP:HB3 | 1:A:3280:TYR:CZ | 2.24 | 0.72 |
| 1:B:398:THR:HG22 | 1:B:1865:THR:HG21 | 1.70 | 0.72 |
| 1:B:2896:ALA:HA | 1:B:2899:ARG:NH2 | 2.04 | 0.72 |
| 1:B:3876:SER:HB3 | 1:B:4127:TRP:O | 1.87 | 0.72 |
| 1:B:535:LEU:HD22 | 1:B:626:LEU:HG | 1.72 | 0.72 |
| 1:B:990:GLN:HA | 1:B:993:HIS:CD2 | 2.24 | 0.72 |
| 1:A:1070:PRO:HG3 | 1:A:1075:ARG:HB2 | 1.70 | 0.72 |
| 1:A:1743:MSE:SE | 1:A:1880:MSE:SE | 3.07 | 0.72 |
| 1:B:1349:LEU:HD21 | 1:B:1359:LEU:HB2 | 1.70 | 0.72 |
| 1:B:471:LYS:HA | 1:B:1553:PHE:HE2 | 1.53 | 0.72 |
| 1:B:1886:LYS:NZ | 1:B:1948:ALA:HB2 | 2.05 | 0.72 |
| 1:B:2222:HIS:O | 1:B:2225:HIS:N | 2.19 | 0.72 |
| 1:A:2311:ARG:HG3 | 1:A:2363:CYS:HB2 | 1.69 | 0.72 |
| 1:A:3284:SER:HA | 1:A:3287:ARG:HE | 1.55 | 0.72 |
| 1:A:978:GLN:O | 1:A:981:ARG:HG2 | 1.89 | 0.72 |
| 1:B:1014:LEU:HA | 1:B:1025:LEU:HD13 | 1.69 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1115:HIS:O | 1:B:1119:LYS:N | 2.22 | 0.72 |
| 1:B:526:ASP:HB2 | 1:B:529:ASP:OD2 | 1.89 | 0.72 |
| 1:B:967:PRO:HA | 1:B:970:LEU:HD23 | 1.69 | 0.72 |
| 1:A:1456:LYS:HA | 1:A:1459:HIS:HD2 | 1.53 | 0.72 |
| 1:A:4082:ARG:HG3 | 1:A:4091:ALA:CB | 2.19 | 0.72 |
| 1:A:1456:LYS:HA | 1:A:1459:HIS:CD2 | 2.23 | 0.72 |
| 1:A:2260:PHE:O | 1:A:2262:GLY:N | 2.22 | 0.72 |
| 1:A:2542:LEU:HB2 | 1:A:2546:TYR:CE2 | 2.25 | 0.72 |
| 1:A:3045:ILE:O | 1:A:3048:LYS:HB3 | 1.89 | 0.72 |
| 1:A:3130:GLN:HG3 | 1:A:3178:ILE:HG12 | 1.72 | 0.72 |
| 1:B:2860:ASP:HB3 | 1:B:2868:LEU:HD22 | 1.72 | 0.72 |
| 1:A:1871:MSE:HA | 1:A:1874:TYR:HB2 | 1.71 | 0.72 |
| 1:A:2193:ILE:HA | 1:A:2196:TRP:CZ2 | 2.24 | 0.72 |
| 1:A:737:PRO:HA | 1:A:740:ILE:HD12 | 1.70 | 0.72 |
| 1:B:3583:LEU:O | 1:B:3587:ASP:HB2 | 1.88 | 0.72 |
| 1:A:3015:SER:O | 1:A:3019:ILE:N | 2.21 | 0.72 |
| 1:A:349:ILE:HG12 | 1:A:364:ARG:HD2 | 1.72 | 0.72 |
| 1:A:434:VAL:HA | 1:A:437:HIS:CE1 | 2.24 | 0.72 |
| 1:B:1802:TYR:O | 1:B:1805:PHE:N | 2.22 | 0.72 |
| 1:B:2177:ASN:HD22 | 1:B:2182:ILE:HG22 | 1.54 | 0.72 |
| 1:B:2563:LEU:O | 1:B:2567:SER:OG | 2.06 | 0.72 |
| 1:A:2300:PHE:HZ | 1:A:2341:LEU:HB2 | 1.54 | 0.72 |
| 1:A:3592:VAL:HG22 | 1:A:3609:MSE:SE | 2.40 | 0.72 |
| 1:B:2837:LEU:HA | 1:B:2840:PHE:CD2 | 2.25 | 0.72 |
| 1:B:3579:SER:OG | 1:B:3580:ASN:N | 2.22 | 0.72 |
| 1:B:868:LYS:HA | 1:B:871:LEU:HD12 | 1.71 | 0.72 |
| 1:A:3256:MSE:HE2 | 1:A:3282:ARG:NH1 | 2.03 | 0.72 |
| 1:A:3432:SER:HB2 | 1:A:3435:ASP:HB2 | 1.72 | 0.72 |
| 1:A:358:GLU:HA | 1:A:1858:LEU:HD22 | 1.71 | 0.72 |
| 1:A:871:LEU:HD11 | 1:A:3122:HIS:HE1 | 1.55 | 0.72 |
| 1:B:1090:ARG:HA | 1:B:1090:ARG:NE | 2.05 | 0.72 |
| 1:B:2313:LYS:HG3 | 1:B:2314:GLU:OE2 | 1.90 | 0.72 |
| 1:B:2961:ALA:HB1 | 1:B:3002:TYR:HD1 | 1.54 | 0.72 |
| 1:B:649:PHE:CE1 | 1:B:657:SER:HB2 | 2.25 | 0.72 |
| 1:B:721:TYR:CE1 | 1:B:1121:LEU:HD21 | 2.24 | 0.72 |
| 1:A:1870:LYS:HG2 | 1:A:1871:MSE:HE2 | 1.71 | 0.71 |
| 1:B:2239:LYS:HG3 | 1:B:2279:ILE:HG23 | 1.72 | 0.71 |
| 1:B:3326:GLN:OE1 | 1:B:3393:GLU:HA | 1.90 | 0.71 |
| 1:A:1306:ILE:HG12 | 1:A:1334:LYS:HB3 | 1.72 | 0.71 |
| 1:A:2323:LEU:HD21 | 1:A:2345:VAL:HG21 | 1.72 | 0.71 |
| 1:A:2423:VAL:HG13 | 1:A:2424:MSE:H | 1.55 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2433:LYS:HG3 | 1:A:2436:LEU:HD12 | 1.70 | 0.71 |
| 1:B:1032:CYS:HB3 | 1:B:1036:PHE:CZ | 2.25 | 0.71 |
| 1:B:932:GLU:HG3 | 1:B:2636:UNK:HA | 1.72 | 0.71 |
| 1:B:3593:ARG:HA | 1:B:3596:LEU:HD12 | 1.72 | 0.71 |
| 1:A:2312:TYR:HE2 | 1:A:2314:GLU:HG2 | 1.55 | 0.71 |
| 1:A:2453:GLU:O | 1:A:2457:PRO:HD3 | 1.90 | 0.71 |
| 1:A:3503:VAL:HG11 | 1:A:3535:ILE:HB | 1.72 | 0.71 |
| 1:A:3982:SER:O | 1:A:3986:HIS:ND1 | 2.22 | 0.71 |
| 1:B:1349:LEU:HA | 1:B:1353:PRO:HD2 | 1.71 | 0.71 |
| 1:B:1761:LEU:HD22 | 1:B:1860:GLU:HB3 | 1.73 | 0.71 |
| 1:B:2806:LYS:NZ | 1:B:2858:ILE:HG21 | 2.06 | 0.71 |
| 1:B:602:MSE:SE | 1:B:726:LEU:HD13 | 2.40 | 0.71 |
| 1:A:1977:ILE:O | 1:A:1979:GLU:N | 2.18 | 0.71 |
| 1:A:2070:GLU:HA | 1:A:2071:GLN:HB2 | 1.72 | 0.71 |
| 1:A:922:SER:HB3 | 1:A:926:THR:HG23 | 1.72 | 0.71 |
| 1:A:967:PRO:HA | 1:A:970:LEU:HD23 | 1.70 | 0.71 |
| 1:A:2281:MSE:HE2 | 1:A:2322:VAL:HA | 1.73 | 0.71 |
| 1:A:2435:CYS:O | 1:A:2439:ILE:HB | 1.89 | 0.71 |
| 1:A:3677:PRO:O | 1:A:3679:ASN:N | 2.22 | 0.71 |
| 1:A:616:LYS:HB3 | 1:A:617:PRO:HD2 | 1.72 | 0.71 |
| 1:B:1762:MSE:HB2 | 1:B:1896:ILE:HG12 | 1.72 | 0.71 |
| 1:B:2883:SER:O | 1:B:2885:GLN:N | 2.22 | 0.71 |
| 1:B:2884:LEU:HB3 | 1:B:3895:GLU:HG3 | 1.73 | 0.71 |
| 1:B:2970:LYS:NZ | 1:B:2974:GLU:OE2 | 2.22 | 0.71 |
| 1:B:3130:GLN:HG3 | 1:B:3178:ILE:HG12 | 1.73 | 0.71 |
| 1:B:491:CYS:SG | 1:B:492:SER:N | 2.62 | 0.71 |
| 1:B:560:LEU:HB3 | 1:B:616:LYS:HE2 | 1.73 | 0.71 |
| 1:A:2535:THR:O | 1:A:2538:ARG:HG2 | 1.89 | 0.71 |
| 1:B:204:LEU:HD22 | 1:B:219:VAL:HG12 | 1.71 | 0.71 |
| 1:B:3471:ILE:HG23 | 1:B:3472:ILE:HG13 | 1.73 | 0.71 |
| 1:B:553:VAL:HB | 1:B:637:LYS:HZ2 | 1.56 | 0.71 |
| 1:B:808:GLU:HG2 | 1:B:852:ARG:NH2 | 2.06 | 0.71 |
| 1:A:1256:TRP:O | 1:A:1260:LEU:N | 2.17 | 0.71 |
| 1:A:3257:LYS:HA | 1:A:3260:LYS:HD2 | 1.73 | 0.71 |
| 1:A:3427:GLU:HB3 | 1:A:3439:LEU:HD22 | 1.71 | 0.71 |
| 1:A:3835:PRO:HA | 1:A:3871:PHE:HE1 | 1.54 | 0.71 |
| 1:A:3875:GLU:HG2 | 1:A:4127:TRP:HB3 | 1.72 | 0.71 |
| 1:B:1702:LEU:O | 1:B:1706:SER:HB3 | 1.91 | 0.71 |
| 1:B:3587:ASP:HB3 | 1:B:4022:LYS:HZ2 | 1.55 | 0.71 |
| 1:A:1609:ALA:HB3 | 1:A:1806:ARG:NH2 | 2.06 | 0.71 |
| 1:A:1745:LYS:O | 1:A:1747:LEU:N | 2.24 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2538:ARG:HH12 | 1:A:2566:THR:H | 1.36 | 0.71 |
| 1:A:396:PHE:CZ | 1:A:397:LEU:HG | 2.25 | 0.71 |
| 1:A:705:ALA:HB1 | 1:A:1385:ASN:ND2 | 2.05 | 0.71 |
| 1:A:756:PHE:HA | 1:A:773:LEU:HD13 | 1.73 | 0.71 |
| 1:B:2043:PHE:O | 1:B:2047:THR:OG1 | 2.09 | 0.71 |
| 1:B:2200:ALA:HA | 1:B:2203:THR:HG22 | 1.73 | 0.71 |
| 1:A:2152:ASN:HB3 | 1:A:2153:THR:HA | 1.72 | 0.71 |
| 1:A:446:PHE:O | 1:A:533:HIS:NE2 | 2.24 | 0.71 |
| 1:A:621:SER:HB3 | 1:A:659:ARG:NH2 | 2.06 | 0.71 |
| 1:B:1798:LEU:O | 1:B:1802:TYR:HB2 | 1.90 | 0.71 |
| 1:B:3464:LYS:HG3 | 1:B:3468:LEU:HD11 | 1.72 | 0.71 |
| 1:B:454:GLN:HG3 | 1:B:533:HIS:HE1 | 1.54 | 0.71 |
| 1:A:1681:ASP:OD1 | 1:A:1682:THR:N | 2.23 | 0.71 |
| 1:A:2478:MSE:O | 1:A:2482:ASP:CB | 2.37 | 0.71 |
| 1:A:3813:LYS:HG2 | 1:A:3926:ASN:HA | 1.73 | 0.71 |
| 1:B:1267:TYR:O | 1:B:1271:ILE:HG13 | 1.90 | 0.71 |
| 1:B:1464:LEU:HB2 | 1:B:1468:LEU:HD12 | 1.73 | 0.71 |
| 1:B:3155:VAL:HG21 | 1:B:3159:ARG:NH2 | 2.06 | 0.71 |
| 1:B:3875:GLU:O | 1:B:3879:PRO:HD3 | 1.91 | 0.71 |
| 1:B:560:LEU:HD11 | 1:B:645:TRP:CZ2 | 2.26 | 0.71 |
| 1:A:1880:MSE:SE | 1:A:1881:TYR:HD1 | 2.23 | 0.70 |
| 1:A:2260:PHE:CZ | 1:A:2303:LEU:HA | 2.25 | 0.70 |
| 1:A:2312:TYR:CE2 | 1:A:2314:GLU:HG2 | 2.25 | 0.70 |
| 1:A:660:LEU:O | 1:A:664:SER:OG | 2.08 | 0.70 |
| 1:A:941:MSE:HB2 | 1:A:958:MSE:HE3 | 1.73 | 0.70 |
| 1:B:1060:PHE:HA | 1:B:1063:LEU:HD12 | 1.72 | 0.70 |
| 1:B:1138:ILE:HD13 | 1:B:1150:LYS:HE2 | 1.73 | 0.70 |
| 1:B:2161:ALA:HA | 1:B:2164:TRP:CD1 | 2.25 | 0.70 |
| 1:B:2227:LYS:HG3 | 1:B:2232:ARG:HA | 1.73 | 0.70 |
| 1:B:3772:ASN:ND2 | 1:B:3788:LEU:H | 1.89 | 0.70 |
| 1:B:4048:LYS:O | 1:B:4051:LEU:HB3 | 1.91 | 0.70 |
| 1:B:514:VAL:HG12 | 1:B:604:PRO:HG3 | 1.73 | 0.70 |
| 1:B:982:GLN:O | 1:B:986:PRO:HD3 | 1.91 | 0.70 |
| 1:A:1655:ILE:HG23 | 1:A:1677:SER:HB3 | 1.73 | 0.70 |
| 1:A:3498:TRP:HD1 | 1:A:3502:MSE:HB2 | 1.56 | 0.70 |
| 1:B:3340:ALA:O | 1:B:3343:SER:N | 2.24 | 0.70 |
| 1:B:575:ILE:HD11 | 1:B:579:LEU:HD22 | 1.70 | 0.70 |
| 1:B:913:ARG:NE | 1:B:916:GLU:OE2 | 2.24 | 0.70 |
| 1:A:1403:MSE:HE1 | 1:A:1419:LEU:HD21 | 1.73 | 0.70 |
| 1:A:2137:ILE:HB | 1:A:2170:GLN:HE22 | 1.55 | 0.70 |
| 1:A:3989:ARG:HH21 | 1:A:4100:GLU:HB3 | 1.55 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2086:ASP:HB3 | 1:B:2090:ARG:HH21 | 1.55 | 0.70 |
| 1:B:2896:ALA:HA | 1:B:2899:ARG:HH21 | 1.57 | 0.70 |
| 1:B:1472:SER:HA | 1:B:1476:HIS:CD2 | 2.26 | 0.70 |
| 1:B:2161:ALA:HB1 | 1:B:2211:LEU:HD13 | 1.71 | 0.70 |
| 1:B:2260:PHE:O | 1:B:2262:GLY:N | 2.24 | 0.70 |
| 1:A:1593:VAL:O | 1:A:1597:LEU:HB2 | 1.91 | 0.70 |
| 1:A:3044:MSE:O | 1:A:3047:SER:OG | 2.04 | 0.70 |
| 1:A:527:TYR:OH | 1:A:619:ASP:N | 2.22 | 0.70 |
| 1:B:989:MSE:HE2 | 1:B:1031:ARG:NH1 | 2.07 | 0.70 |
| 1:B:1155:ARG:NH2 | 1:B:1230:GLY:O | 2.24 | 0.70 |
| 1:B:2379:MSE:CE | 1:B:2404:ARG:HD3 | 2.20 | 0.70 |
| 1:A:446:PHE:H | 1:A:446:PHE:HD1 | 1.36 | 0.70 |
| 1:B:1017:ILE:HB | 1:B:1025:LEU:HB2 | 1.74 | 0.70 |
| 1:B:2412:TYR:HD2 | 1:B:2416:LYS:HE3 | 1.57 | 0.70 |
| 1:B:2936:TYR:HD2 | 1:B:3979:LEU:HD21 | 1.56 | 0.70 |
| 1:A:2030:TYR:HD1 | 1:A:2031:LEU:HG | 1.57 | 0.70 |
| 1:A:3917:ILE:HG22 | 1:A:3918:LEU:HD22 | 1.72 | 0.70 |
| 1:B:1416:GLU:O | 1:B:1420:ARG:HB2 | 1.91 | 0.70 |
| 1:B:2535:THR:O | 1:B:2538:ARG:HG2 | 1.92 | 0.70 |
| 1:B:2945:SER:O | 1:B:2949:THR:HG23 | 1.90 | 0.70 |
| 1:A:3592:VAL:HA | 1:A:3609:MSE:SE | 2.41 | 0.70 |
| 1:B:2112:GLN:OE1 | 1:B:2120:ARG:NH2 | 2.24 | 0.70 |
| 1:B:848:LEU:HA | 1:B:851:ILE:HD12 | 1.74 | 0.70 |
| 1:A:1592:MSE:O | 1:A:1594:SER:N | 2.24 | 0.70 |
| 1:B:1445:ARG:HA | 1:B:1448:LEU:HD12 | 1.74 | 0.70 |
| 1:B:2260:PHE:CE2 | 1:B:2303:LEU:HA | 2.27 | 0.70 |
| 1:B:3498:TRP:HE1 | 1:B:3502:MSE:SE | 2.25 | 0.70 |
| 1:B:3638:LYS:HA | 1:B:3641:ASP:OD2 | 1.91 | 0.70 |
| 1:B:3772:ASN:HB2 | 1:B:3787:GLN:CG | 2.19 | 0.70 |
| 1:B:932:GLU:HB3 | 1:B:2794:LEU:HD13 | 1.73 | 0.70 |
| 1:A:1014:LEU:HD13 | 1:A:1078:ALA:HB1 | 1.72 | 0.70 |
| 1:A:1918:LEU:HD22 | 1:A:1958:GLU:HB3 | 1.72 | 0.70 |
| 1:A:2239:LYS:HE2 | 1:A:2240:THR:HG22 | 1.73 | 0.70 |
| 1:A:527:TYR:CE1 | 1:A:615:ALA:HB1 | 2.26 | 0.70 |
| 1:B:177:LEU:O | 1:B:180:LEU:N | 2.25 | 0.70 |
| 1:B:19:LEU:HD22 | 1:B:30:ALA:HB1 | 1.72 | 0.70 |
| 1:B:970:LEU:CD2 | 1:B:1031:ARG:HH21 | 2.05 | 0.70 |
| 1:A:1249:SER:O | 1:A:1253:THR:HB | 1.92 | 0.69 |
| 1:A:114:VAL:HG11 | 1:A:130:LEU:HD11 | 1.72 | 0.69 |
| 1:A:1877:LEU:O | 1:A:1920:TYR:OH | 2.09 | 0.69 |
| 1:A:2781:PRO:HB2 | 1:A:2786:LYS:HD3 | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3687:MSE:O | 1:A:3689:ASP:N | 2.25 | 0.69 |
| 1:A:990:GLN:HA | 1:A:993:HIS:HD2 | 1.57 | 0.69 |
| 1:B:1985:LYS:O | 1:B:1989:ASN:ND2 | 2.22 | 0.69 |
| 1:B:2253:TYR:HB2 | 1:B:2291:GLN:CG | 2.22 | 0.69 |
| 1:B:2452:ARG:HA | 1:B:2455:LEU:HD12 | 1.73 | 0.69 |
| 1:B:3284:SER:HB2 | 1:B:3287:ARG:NH2 | 2.04 | 0.69 |
| 1:B:3119:VAL:HG21 | 1:B:3899:ALA:HB1 | 1.74 | 0.69 |
| 1:B:3910:LEU:O | 1:B:3914:SER:OG | 2.07 | 0.69 |
| 1:B:629:PHE:HZ | 1:B:666:PHE:HD1 | 1.40 | 0.69 |
| 1:A:1378:GLU:OE2 | 1:A:1382:ILE:HG23 | 1.92 | 0.69 |
| 1:A:1469:PRO:HA | 1:A:1472:SER:HB3 | 1.74 | 0.69 |
| 1:B:436:GLU:OE2 | 1:B:475:LEU:HD12 | 1.93 | 0.69 |
| 1:B:743:LEU:O | 1:B:746:ARG:NH1 | 2.25 | 0.69 |
| 1:A:1996:VAL:HG23 | 1:A:1997:PRO:CD | 2.22 | 0.69 |
| 1:A:2071:GLN:HA | 1:A:2074:PRO:HG2 | 1.73 | 0.69 |
| 1:A:2958:LEU:O | 1:A:3289:ARG:NH2 | 2.25 | 0.69 |
| 1:A:718:MSE:HE3 | 1:A:731:THR:HG22 | 1.74 | 0.69 |
| 1:A:718:MSE:HE2 | 1:A:754:MSE:HG3 | 1.75 | 0.69 |
| 1:B:660:LEU:O | 1:B:663:ILE:HG13 | 1.91 | 0.69 |
| 1:A:1583:MSE:SE | 1:A:1643:MSE:SE | 3.09 | 0.69 |
| 1:A:1651:LYS:O | 1:A:1655:ILE:HD12 | 1.92 | 0.69 |
| 1:A:2038:GLU:OE1 | 1:A:2076:VAL:HG22 | 1.93 | 0.69 |
| 1:A:2153:THR:OG1 | 1:A:2154:GLU:N | 2.18 | 0.69 |
| 1:B:1087:ARG:HD2 | 1:B:1137:ILE:HD11 | 1.74 | 0.69 |
| 1:B:1412:LYS:HA | 1:B:1415:LEU:HD12 | 1.72 | 0.69 |
| 1:B:3979:LEU:HA | 1:B:3981:TYR:HB3 | 1.74 | 0.69 |
| 1:B:512:GLY:HA2 | 1:B:602:MSE:HG3 | 1.73 | 0.69 |
| 1:B:629:PHE:CE2 | 1:B:668:LYS:HB2 | 2.28 | 0.69 |
| 1:A:334:HIS:CE1 | 1:A:338:LEU:HD21 | 2.28 | 0.69 |
| 1:B:2813:PHE:CD2 | 1:B:2859:GLN:HG3 | 2.25 | 0.69 |
| 1:B:272:LEU:HB3 | 1:B:319:PHE:CZ | 2.27 | 0.69 |
| 1:B:722:LYS:HB3 | 1:B:727:ALA:HA | 1.74 | 0.69 |
| 1:B:86:LEU:HD23 | 1:B:89:LEU:HD12 | 1.72 | 0.69 |
| 1:A:2216:LEU:HD22 | 1:A:2249:LEU:HD11 | 1.73 | 0.69 |
| 1:A:2452:ARG:HE | 1:A:2498:ILE:HD11 | 1.57 | 0.69 |
| 1:A:3810:VAL:HG23 | 1:A:3815:LEU:HD11 | 1.74 | 0.69 |
| 1:B:170:VAL:HG23 | 1:B:173:LYS:HZ1 | 1.57 | 0.69 |
| 1:B:2413:PHE:CE1 | 1:B:2442:MSE:HB3 | 2.27 | 0.69 |
| 1:B:2430:GLU:HG3 | 1:B:2465:PRO:HB3 | 1.74 | 0.69 |
| 1:B:2884:LEU:C | 1:B:2887:PRO:HD2 | 2.13 | 0.69 |
| 1:B:3574:ALA:HA | 1:B:3577:GLN:HB2 | 1.75 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1445:ARG:HA | 1:A:1448:LEU:HD12 | 1.74 | 0.69 |
| 1:A:2304:VAL:HG13 | 1:A:2348:GLN:HE21 | 1.57 | 0.69 |
| 1:A:2329:TYR:O | 1:A:2333:ARG:N | 2.25 | 0.69 |
| 1:A:2464:HIS:H | 1:A:2465:PRO:HD3 | 1.56 | 0.69 |
| 1:A:723:ASP:HB2 | 1:A:726:LEU:HD12 | 1.74 | 0.69 |
| 1:B:2196:TRP:HE1 | 1:B:2200:ALA:HB2 | 1.58 | 0.69 |
| 1:B:3654:MSE:SE | 1:B:3659:PHE:HB3 | 2.42 | 0.69 |
| 1:B:65:LEU:O | 1:B:69:VAL:HB | 1.93 | 0.69 |
| 1:A:1018:VAL:HB | 1:A:1074:LYS:HA | 1.75 | 0.69 |
| 1:A:1059:LEU:HD22 | 1:A:1063:LEU:HD11 | 1.75 | 0.69 |
| 1:A:1507:CYS:SG | 1:A:1508:LYS:N | 2.65 | 0.69 |
| 1:A:1685:ASP:HB2 | 1:A:1727:ARG:NH2 | 2.06 | 0.69 |
| 1:A:2125:TRP:O | 1:A:2127:LYS:N | 2.25 | 0.69 |
| 1:A:19:LEU:HB2 | 1:A:34:LEU:HD13 | 1.75 | 0.69 |
| 1:A:368:LEU:HD23 | 1:A:372:PRO:HG2 | 1.74 | 0.69 |
| 1:A:3974:MSE:HB3 | 1:A:3976:GLU:HB3 | 1.74 | 0.69 |
| 1:A:462:VAL:HG11 | 1:A:540:MSE:SE | 2.42 | 0.69 |
| 1:B:135:LEU:HD13 | 1:B:170:VAL:HB | 1.75 | 0.69 |
| 1:B:2351:GLN:O | 1:B:2355:THR:OG1 | 2.07 | 0.69 |
| 1:B:2555:LEU:O | 1:B:2558:ALA:HB3 | 1.92 | 0.69 |
| 1:A:602:MSE:SE | 1:A:726:LEU:HD13 | 2.42 | 0.69 |
| 1:B:414:LEU:HD23 | 1:B:460:ALA:HB1 | 1.74 | 0.69 |
| 1:B:434:VAL:HA | 1:B:437:HIS:CE1 | 2.28 | 0.69 |
| 1:A:2187:VAL:O | 1:A:2190:VAL:HG22 | 1.93 | 0.69 |
| 1:A:4121:TRP:HD1 | 1:A:4123:GLY:H | 1.40 | 0.69 |
| 1:A:870:LEU:HA | 1:A:873:VAL:HB | 1.75 | 0.69 |
| 1:B:1086:TYR:HD2 | 1:B:1090:ARG:HG2 | 1.58 | 0.69 |
| 1:B:1955:VAL:HG12 | 1:B:1957:ASN:HB2 | 1.75 | 0.69 |
| 1:A:1569:THR:O | 1:A:1573:LYS:HB2 | 1.93 | 0.69 |
| 1:A:3048:LYS:NZ | 1:A:3089:LEU:HB3 | 2.08 | 0.69 |
| 1:A:934:LEU:HD21 | 1:A:962:TYR:CE1 | 2.28 | 0.69 |
| 1:B:1799:GLU:HA | 1:B:1802:TYR:HB2 | 1.74 | 0.69 |
| 1:B:3587:ASP:HB3 | 1:B:4022:LYS:NZ | 2.08 | 0.69 |
| 1:B:3772:ASN:ND2 | 1:B:3788:LEU:O | 2.26 | 0.69 |
| 1:B:917:LEU:HD21 | 1:B:934:LEU:HD13 | 1.74 | 0.69 |
| 1:B:935:HIS:NE2 | 1:B:987:LEU:HG | 2.09 | 0.69 |
| 1:A:1763:THR:OG1 | 1:A:1864:ASP:OD2 | 2.09 | 0.68 |
| 1:A:3114:TYR:CE1 | 1:A:3128:LYS:HD3 | 2.28 | 0.68 |
| 1:A:970:LEU:HD22 | 1:A:1031:ARG:HH21 | 1.58 | 0.68 |
| 1:A:977:ASP:HB3 | 1:A:981:ARG:N | 2.08 | 0.68 |
| 1:B:999:LYS:HD3 | 1:B:1000:LYS:H | 1.58 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1080:LEU:CD1 | 1:B:1127:CYS:HB3 | 2.23 | 0.68 |
| 1:B:2074:PRO:O | 1:B:2077:HIS:N | 2.26 | 0.68 |
| 1:B:2283:ASN:O | 1:B:2287:PRO:HD3 | 1.92 | 0.68 |
| 1:B:2365:ASN:HD21 | 1:B:2382:VAL:HG11 | 1.58 | 0.68 |
| 1:B:2951:GLN:OE1 | 1:B:2972:TYR:OH | 2.10 | 0.68 |
| 1:A:3312:VAL:O | 1:A:3314:SER:N | 2.26 | 0.68 |
| 1:B:3631:LYS:HB3 | 1:B:3682:GLU:HA | 1.76 | 0.68 |
| 1:B:745:VAL:HG11 | 1:B:776:TRP:CZ2 | 2.27 | 0.68 |
| 1:A:1722:PHE:CD2 | 1:A:1754:GLN:HG2 | 2.29 | 0.68 |
| 1:B:3435:ASP:O | 1:B:3439:LEU:CB | 2.41 | 0.68 |
| 1:B:345:PHE:HD2 | 1:B:367:GLY:HA3 | 1.59 | 0.68 |
| 1:B:398:THR:O | 1:B:401:ASP:N | 2.24 | 0.68 |
| 1:A:2177:ASN:HD22 | 1:A:2182:ILE:HG22 | 1.57 | 0.68 |
| 1:A:2283:ASN:ND2 | 1:A:2284:ASP:OD2 | 2.26 | 0.68 |
| 1:B:1165:LEU:HA | 1:B:1168:LEU:HD12 | 1.76 | 0.68 |
| 1:B:2242:VAL:HG12 | 1:B:2246:LYS:HE3 | 1.75 | 0.68 |
| 1:A:1937:ARG:O | 1:A:1941:HIS:HB2 | 1.92 | 0.68 |
| 1:A:1917:LYS:HE2 | 1:A:1955:VAL:HB | 1.74 | 0.68 |
| 1:A:2271:SER:HB2 | 1:A:2314:GLU:HG3 | 1.75 | 0.68 |
| 1:A:2900:LEU:HB2 | 1:A:2910:VAL:HA | 1.75 | 0.68 |
| 1:A:3955:VAL:HG23 | 1:A:4121:TRP:CE3 | 2.28 | 0.68 |
| 1:B:1989:ASN:HB3 | 1:B:2040:MSE:HB3 | 1.75 | 0.68 |
| 1:B:2274:ILE:O | 1:B:2277:LEU:N | 2.27 | 0.68 |
| 1:B:4113:ASP:HB3 | 1:B:4116:ILE:HG13 | 1.75 | 0.68 |
| 1:B:721:TYR:HE1 | 1:B:1121:LEU:HD21 | 1.58 | 0.68 |
| 1:A:1382:ILE:HB | 1:A:1386:ILE:HD11 | 1.75 | 0.68 |
| 1:A:793:LEU:HG | 1:A:796:LEU:HD12 | 1.75 | 0.68 |
| 1:A:940:PHE:CZ | 1:A:2791:ILE:HG21 | 2.28 | 0.68 |
| 1:B:1682:THR:OG1 | 1:B:1727:ARG:NH2 | 2.27 | 0.68 |
| 1:B:1981:LEU:O | 1:B:1984:LEU:HG | 1.93 | 0.68 |
| 1:B:2423:VAL:HG23 | 1:B:2426:HIS:HB3 | 1.76 | 0.68 |
| 1:A:3583:LEU:O | 1:A:3587:ASP:HB2 | 1.92 | 0.68 |
| 1:A:3816:LEU:HD11 | 1:A:3883:LEU:HG | 1.74 | 0.68 |
| 1:A:4066:LEU:HD23 | 1:A:4075:ARG:HG3 | 1.76 | 0.68 |
| 1:A:543:SER:C | 1:A:545:LEU:H | 1.95 | 0.68 |
| 1:B:1403:MSE:HE1 | 1:B:1419:LEU:HD21 | 1.75 | 0.68 |
| 1:B:1643:MSE:HA | 1:B:1646:LEU:HG | 1.74 | 0.68 |
| 1:B:3084:GLN:OE1 | 1:B:3084:GLN:N | 2.21 | 0.68 |
| 1:B:3339:ASN:O | 1:B:3341:LEU:N | 2.26 | 0.68 |
| 1:B:3737:ARG:NH1 | 1:B:3739:ILE:HD11 | 2.07 | 0.68 |
| 1:B:3840:LYS:HE2 | 1:B:4122:GLU:HB3 | 1.76 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:669:LEU:HD22 | 1:B:672:ILE:HG13 | 1.75 | 0.68 |
| 1:B:926:THR:O | 1:B:930:ALA:HB3 | 1.92 | 0.68 |
| 1:A:2094:MSE:HE1 | 1:A:2143:ARG:HA | 1.75 | 0.68 |
| 1:A:2936:TYR:HB3 | 1:A:3979:LEU:HD11 | 1.75 | 0.68 |
| 1:A:484:HIS:CD2 | 1:A:616:LYS:HE3 | 2.29 | 0.68 |
| 1:A:580:ASP:OD1 | 1:A:581:LEU:N | 2.26 | 0.68 |
| 1:B:2477:LEU:HB3 | 1:B:2506:LEU:HD21 | 1.76 | 0.68 |
| 1:B:3031:TRP:CE3 | 1:B:3034:PRO:HD3 | 2.29 | 0.68 |
| 1:B:3981:TYR:OH | 1:B:4101:GLU:HB3 | 1.93 | 0.68 |
| 1:A:1437:TYR:CD2 | 1:A:1444:ASP:OD2 | 2.47 | 0.68 |
| 1:A:3830:SER:HB2 | 1:A:3835:PRO:HG3 | 1.76 | 0.68 |
| 1:B:2260:PHE:CZ | 1:B:2303:LEU:HA | 2.29 | 0.68 |
| 1:B:574:LYS:O | 1:B:577:GLU:HG2 | 1.94 | 0.68 |
| 1:A:1802:TYR:O | 1:A:1805:PHE:N | 2.27 | 0.68 |
| 1:A:265:TYR:O | 1:A:268:PRO:HD2 | 1.94 | 0.68 |
| 1:A:3049:LEU:HD13 | 1:A:3184:THR:HB | 1.76 | 0.68 |
| 1:A:3790:THR:HG22 | 1:A:3791:TYR:H | 1.58 | 0.68 |
| 1:A:882:SER:HB2 | 1:A:3892:THR:H | 1.59 | 0.68 |
| 1:A:3883:LEU:HD13 | 1:A:3970:LEU:HD13 | 1.74 | 0.68 |
| 1:B:1886:LYS:HZ3 | 1:B:1948:ALA:HB2 | 1.59 | 0.68 |
| 1:B:2316:TYR:CG | 1:B:2317:ALA:N | 2.62 | 0.68 |
| 1:B:655:LEU:O | 1:B:659:ARG:HG2 | 1.93 | 0.68 |
| 1:A:1080:LEU:HD12 | 1:A:1081:ALA:N | 2.08 | 0.67 |
| 1:A:260:ILE:HG22 | 1:A:264:ARG:HH12 | 1.59 | 0.67 |
| 1:B:2258:GLU:OE2 | 1:B:2295:GLN:NE2 | 2.22 | 0.67 |
| 1:B:2542:LEU:HB2 | 1:B:2546:TYR:CE2 | 2.29 | 0.67 |
| 1:B:3620:PRO:HA | 1:B:3625:LEU:HD12 | 1.76 | 0.67 |
| 1:B:411:PRO:HA | 1:B:414:LEU:HB3 | 1.75 | 0.67 |
| 1:B:968:VAL:HA | 1:B:971:ARG:HG2 | 1.76 | 0.67 |
| 1:A:1403:MSE:HA | 1:A:1406:LEU:HB2 | 1.76 | 0.67 |
| 1:A:172:GLU:O | 1:A:176:GLU:HG3 | 1.94 | 0.67 |
| 1:A:990:GLN:HA | 1:A:993:HIS:CD2 | 2.29 | 0.67 |
| 1:B:2390:HIS:HD1 | 1:B:2397:CYS:HG | 1.41 | 0.67 |
| 1:B:2440:TYR:HD2 | 1:B:2476:ILE:HD12 | 1.58 | 0.67 |
| 1:B:899:ARG:NH1 | 1:B:2570:PRO:HB2 | 2.00 | 0.67 |
| 1:B:4063:GLU:HA | 1:B:4066:LEU:HD22 | 1.75 | 0.67 |
| 1:A:323:VAL:O | 1:A:327:VAL:HB | 1.94 | 0.67 |
| 1:A:367:GLY:C | 1:A:369:PHE:H | 1.98 | 0.67 |
| 1:B:2776:ARG:HA | 1:B:2776:ARG:NH1 | 2.08 | 0.67 |
| 1:B:797:ASP:HA | 1:B:800:LEU:HD12 | 1.77 | 0.67 |
| 1:A:3788:LEU:HG | 1:A:3789:ARG:H | 1.58 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:376:ILE:HG13 | 1:A:381:VAL:CG2 | 2.24 | 0.67 |
| 1:A:848:LEU:HA | 1:A:851:ILE:HD12 | 1.76 | 0.67 |
| 1:A:909:VAL:HG13 | 1:A:913:ARG:NH1 | 2.09 | 0.67 |
| 1:B:3797:THR:HG22 | 1:B:3800:LEU:HG | 1.77 | 0.67 |
| 1:B:3761:ASP:HB3 | 1:B:3942:PHE:HB2 | 1.76 | 0.67 |
| 1:B:429:GLU:N | 1:B:429:GLU:OE1 | 2.27 | 0.67 |
| 1:B:554:ASN:CG | 1:B:637:LYS:HZ3 | 1.98 | 0.67 |
| 1:A:1163:LEU:HD13 | 1:A:1256:TRP:CD1 | 2.29 | 0.67 |
| 1:A:1723:PRO:C | 1:A:1725:GLN:H | 1.97 | 0.67 |
| 1:A:2239:LYS:HG3 | 1:A:2279:ILE:CG2 | 2.23 | 0.67 |
| 1:A:3174:ASP:OD2 | 1:A:3782:SER:HB3 | 1.94 | 0.67 |
| 1:A:3964:THR:O | 1:A:3967:PHE:HD1 | 1.78 | 0.67 |
| 1:A:3858:MSE:HB3 | 1:A:4119:ARG:NH2 | 2.10 | 0.67 |
| 1:A:411:PRO:HA | 1:A:414:LEU:HB3 | 1.76 | 0.67 |
| 1:A:571:SER:HB2 | 1:A:606:SER:H | 1.59 | 0.67 |
| 1:B:446:PHE:HD1 | 1:B:446:PHE:H | 1.42 | 0.67 |
| 1:B:969:LEU:O | 1:B:973:ALA:CB | 2.42 | 0.67 |
| 1:A:2538:ARG:HH11 | 1:A:2565:MSE:HB3 | 1.59 | 0.67 |
| 1:A:3959:MSE:HE1 | 1:A:4124:TRP:CD2 | 2.30 | 0.67 |
| 1:A:756:PHE:O | 1:A:760:LEU:HG | 1.95 | 0.67 |
| 1:B:1504:ASP:HA | 1:B:1507:CYS:HB3 | 1.76 | 0.67 |
| 1:B:550:PHE:HZ | 1:B:632:GLU:HG2 | 1.57 | 0.67 |
| 1:A:144:MSE:HE2 | 1:A:184:VAL:HG11 | 1.76 | 0.67 |
| 1:A:2477:LEU:HD13 | 1:A:2505:VAL:HG11 | 1.76 | 0.67 |
| 1:A:3974:MSE:HA | 1:A:3975:LYS:HB3 | 1.75 | 0.67 |
| 1:A:767:GLU:HG2 | 1:A:846:ILE:O | 1.94 | 0.67 |
| 1:B:1643:MSE:O | 1:B:1646:LEU:N | 2.27 | 0.67 |
| 1:A:1017:ILE:HD12 | 1:A:1025:LEU:HD22 | 1.77 | 0.67 |
| 1:A:1744:LYS:HA | 1:A:1880:MSE:HE3 | 1.75 | 0.67 |
| 1:A:2223:VAL:HB | 1:A:2238:ILE:HD12 | 1.76 | 0.67 |
| 1:A:2851:PHE:HA | 1:A:2854:PHE:CD2 | 2.29 | 0.67 |
| 1:A:3344:GLU:O | 1:A:3348:LEU:HG | 1.94 | 0.67 |
| 1:A:3505:LEU:HD12 | 1:A:3509:ASP:HB3 | 1.76 | 0.67 |
| 1:A:3583:LEU:HD11 | 1:A:3733:ARG:HD3 | 1.77 | 0.67 |
| 1:A:4066:LEU:HD11 | 1:A:4078:VAL:HG11 | 1.77 | 0.67 |
| 1:B:2140:LEU:HA | 1:B:2143:ARG:HD2 | 1.75 | 0.67 |
| 1:B:2420:PHE:HE1 | 1:B:2436:LEU:HD22 | 1.59 | 0.67 |
| 1:B:3812:LEU:HG | 1:B:3813:LYS:N | 2.08 | 0.67 |
| 1:B:406:ARG:O | 1:B:409:GLN:N | 2.26 | 0.67 |
| 1:B:463:LYS:O | 1:B:466:LEU:HB3 | 1.94 | 0.67 |
| 1:B:865:GLN:N | 1:B:865:GLN:OE1 | 2.25 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:709:LYS:NZ | 1:A:1328:GLU:OE2 | 2.24 | 0.67 |
| 1:A:173:LYS:O | 1:A:177:LEU:HG | 1.94 | 0.67 |
| 1:A:2253:TYR:CZ | 1:A:2287:PRO:HB3 | 2.30 | 0.67 |
| 1:B:1145:LEU:HB2 | 1:B:1149:LYS:NZ | 2.10 | 0.67 |
| 1:B:1344:PHE:O | 1:B:1348:LEU:CB | 2.33 | 0.67 |
| 1:B:1483:LEU:HA | 1:B:1500:LEU:HD21 | 1.75 | 0.67 |
| 1:B:1963:GLN:HE21 | 1:B:1995:GLU:HG2 | 1.60 | 0.67 |
| 1:B:2001:LYS:HA | 1:B:2054:TYR:CE2 | 2.29 | 0.67 |
| 1:B:2440:TYR:CD2 | 1:B:2476:ILE:HD12 | 2.29 | 0.67 |
| 1:B:2854:PHE:CG | 1:B:2882:ALA:HB2 | 2.30 | 0.67 |
| 1:B:327:VAL:HG22 | 1:B:338:LEU:HD22 | 1.77 | 0.67 |
| 1:B:985:GLU:HG3 | 1:B:1031:ARG:NH2 | 2.03 | 0.67 |
| 1:A:2033:ASP:O | 1:A:2037:SER:OG | 2.13 | 0.67 |
| 1:A:2224:PHE:CZ | 1:A:2276:LEU:HD22 | 2.30 | 0.67 |
| 1:A:2806:LYS:HA | 1:A:2809:PHE:CD2 | 2.30 | 0.67 |
| 1:A:3879:PRO:HB2 | 1:A:3966:GLN:OE1 | 1.94 | 0.67 |
| 1:B:1491:ILE:O | 1:B:1497:ARG:NH1 | 2.27 | 0.67 |
| 1:B:1751:GLU:OE2 | 1:B:1884:LEU:HD13 | 1.95 | 0.67 |
| 1:B:1894:SER:O | 1:B:1897:ASN:N | 2.21 | 0.67 |
| 1:B:2507:ILE:HG12 | 1:B:2548:PRO:HB2 | 1.77 | 0.67 |
| 1:B:794:PRO:HA | 1:B:869:ASN:HB3 | 1.77 | 0.67 |
| 1:A:1292:LYS:NZ | 1:A:1361:LYS:NZ | 2.44 | 0.66 |
| 1:A:1464:LEU:HB2 | 1:A:1468:LEU:HD12 | 1.75 | 0.66 |
| 1:A:1880:MSE:SE | 1:A:1881:TYR:CD1 | 2.98 | 0.66 |
| 1:A:2066:PHE:HB3 | 1:A:2067:ARG:HG2 | 1.76 | 0.66 |
| 1:A:2913:LYS:O | 1:A:2916:LEU:N | 2.22 | 0.66 |
| 1:A:646:VAL:HG22 | 1:A:660:LEU:HD23 | 1.76 | 0.66 |
| 1:A:76:ILE:HG13 | 1:A:77:GLU:H | 1.59 | 0.66 |
| 1:B:3007:GLU:O | 1:B:3010:SER:OG | 2.13 | 0.66 |
| 1:A:1036:PHE:CD1 | 1:A:1059:LEU:HD11 | 2.30 | 0.66 |
| 1:A:1214:GLU:HG2 | 1:A:1218:SER:HB3 | 1.77 | 0.66 |
| 1:A:2256:ILE:HD13 | 1:A:2276:LEU:HD11 | 1.77 | 0.66 |
| 1:A:3072:GLU:O | 1:A:3076:ALA:HB2 | 1.96 | 0.66 |
| 1:A:3471:ILE:HG23 | 1:A:3472:ILE:HG13 | 1.75 | 0.66 |
| 1:A:610:ALA:HA | 1:A:613:HIS:CE1 | 2.29 | 0.66 |
| 1:B:2323:LEU:HG | 1:B:2341:LEU:HD21 | 1.77 | 0.66 |
| 1:B:3414:MSE:HE1 | 1:B:3450:MSE:HA | 1.76 | 0.66 |
| 1:B:980:THR:CG2 | 1:B:984:TYR:HE2 | 2.09 | 0.66 |
| 1:A:3019:ILE:HG13 | 1:A:3020:ASP:H | 1.60 | 0.66 |
| 1:A:3467:ARG:HG3 | 1:A:3471:ILE:HD12 | 1.77 | 0.66 |
| 1:A:931:CYS:SG | 1:A:932:GLU:N | 2.68 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1103:ALA:O | 1:B:1106:ILE:HG12 | 1.95 | 0.66 |
| 1:B:2009:LYS:HG2 | 1:B:2011:ALA:H | 1.58 | 0.66 |
| 1:B:3042:PRO:HA | 1:B:3045:ILE:HG12 | 1.76 | 0.66 |
| 1:B:266:ALA:CB | 1:B:308:LEU:HG | 2.25 | 0.66 |
| 1:B:659:ARG:HH22 | 1:B:662:LEU:CG | 2.05 | 0.66 |
| 1:A:1548:GLY:O | 1:A:1552:HIS:ND1 | 2.28 | 0.66 |
| 1:A:2121:ASP:HA | 1:A:2126:MSE:HB3 | 1.77 | 0.66 |
| 1:A:3040:TYR:HA | 1:A:3043:TYR:CD2 | 2.31 | 0.66 |
| 1:A:3061:LEU:HD21 | 1:A:3089:LEU:HD13 | 1.76 | 0.66 |
| 1:A:3182:ILE:HB | 1:A:3186:ARG:HH11 | 1.58 | 0.66 |
| 1:A:3579:SER:OG | 1:A:3580:ASN:N | 2.25 | 0.66 |
| 1:A:3725:ARG:HH12 | 1:A:3737:ARG:HH22 | 1.43 | 0.66 |
| 1:A:3875:GLU:O | 1:A:3879:PRO:HD3 | 1.95 | 0.66 |
| 1:B:1113:LEU:HD13 | 1:B:1162:SER:HB3 | 1.76 | 0.66 |
| 1:B:1266:CYS:O | 1:B:1269:THR:OG1 | 2.12 | 0.66 |
| 1:B:1364:CYS:HB3 | 1:B:1367:HIS:ND1 | 2.10 | 0.66 |
| 1:B:1952:ILE:HG23 | 1:B:1953:CYS:O | 1.96 | 0.66 |
| 1:B:3606:ILE:HD13 | 1:B:3609:MSE:HE3 | 1.76 | 0.66 |
| 1:B:3820:MSE:HA | 1:B:3882:LEU:HD22 | 1.77 | 0.66 |
| 1:B:776:TRP:CZ2 | 1:B:780:ILE:HD12 | 2.30 | 0.66 |
| 1:A:1702:LEU:O | 1:A:1706:SER:HB3 | 1.95 | 0.66 |
| 1:A:2891:ARG:HD3 | 1:A:3972:LEU:HD22 | 1.77 | 0.66 |
| 1:A:3008:TRP:O | 1:A:3011:LEU:N | 2.22 | 0.66 |
| 1:A:3582:GLU:HB2 | 1:A:3674:SER:OG | 1.95 | 0.66 |
| 1:A:886:TRP:HZ3 | 1:A:954:GLY:O | 1.78 | 0.66 |
| 1:B:3160:LEU:O | 1:B:3163:THR:HG22 | 1.96 | 0.66 |
| 1:B:638:GLN:OE1 | 1:B:638:GLN:N | 2.25 | 0.66 |
| 1:A:657:SER:O | 1:A:661:PRO:HD3 | 1.95 | 0.66 |
| 1:B:2137:ILE:O | 1:B:2141:ASN:N | 2.27 | 0.66 |
| 1:B:2167:PRO:HB2 | 1:B:2171:LEU:HD22 | 1.77 | 0.66 |
| 1:B:3721:GLY:O | 1:B:3741:ARG:HB2 | 1.95 | 0.66 |
| 1:B:3842:TRP:CH2 | 1:B:3846:MSE:HE2 | 2.30 | 0.66 |
| 1:B:362:ALA:HB2 | 1:B:409:GLN:HE21 | 1.61 | 0.66 |
| 1:B:69:VAL:O | 1:B:73:LEU:HG | 1.96 | 0.66 |
| 1:A:1170:LYS:HA | 1:A:1173:LEU:HD12 | 1.77 | 0.66 |
| 1:A:2886:GLN:HG3 | 1:A:2887:PRO:HD3 | 1.77 | 0.66 |
| 1:A:3493:TRP:CE3 | 1:A:3496:ILE:HG13 | 2.30 | 0.66 |
| 1:A:514:VAL:HA | 1:A:604:PRO:HG3 | 1.78 | 0.66 |
| 1:B:4002:MSE:SE | 1:B:4048:LYS:HE3 | 2.46 | 0.66 |
| 1:B:793:LEU:HA | 1:B:796:LEU:HG | 1.78 | 0.66 |
| 1:A:1306:ILE:CG1 | 1:A:1334:LYS:HB3 | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1649:LEU:HA | 1:A:1652:ILE:HD12 | 1.76 | 0.66 |
| 1:A:175:TYR:HE1 | 1:A:200:PHE:HB3 | 1.59 | 0.66 |
| 1:A:2254:ARG:HG3 | 1:A:2255:LEU:H | 1.61 | 0.66 |
| 1:A:2549:LYS:HZ2 | 1:A:2554:PHE:HA | 1.59 | 0.66 |
| 1:A:260:ILE:HG23 | 1:A:263:LYS:HD2 | 1.75 | 0.66 |
| 1:A:3323:PHE:O | 1:A:3326:GLN:HG3 | 1.96 | 0.66 |
| 1:A:3703:GLY:O | 1:A:3706:ASP:HB2 | 1.95 | 0.66 |
| 1:A:612:LEU:O | 1:A:615:ALA:HB3 | 1.96 | 0.66 |
| 1:B:178:LEU:HB3 | 1:B:197:PHE:CZ | 2.30 | 0.66 |
| 1:B:2462:VAL:HG21 | 1:B:2473:MSE:SE | 2.46 | 0.66 |
| 1:B:3446:VAL:HA | 1:B:3449:LYS:HD2 | 1.78 | 0.66 |
| 1:B:3486:GLU:HG3 | 1:B:3487:ILE:N | 2.09 | 0.66 |
| 1:B:3725:ARG:HH12 | 1:B:3737:ARG:HH22 | 1.31 | 0.66 |
| 1:B:649:PHE:CZ | 1:B:657:SER:HB2 | 2.31 | 0.66 |
| 1:A:3125:ARG:O | 1:A:3128:LYS:N | 2.29 | 0.66 |
| 1:A:3414:MSE:HG3 | 1:A:3456:LEU:HD21 | 1.76 | 0.66 |
| 1:A:3460:GLU:HA | 1:A:3463:LEU:HD12 | 1.78 | 0.66 |
| 1:A:3619:ASP:HA | 1:A:3622:ALA:HB3 | 1.76 | 0.66 |
| 1:A:680:ILE:HG12 | 1:A:701:TYR:CD1 | 2.30 | 0.66 |
| 1:B:186:PRO:HB2 | 1:B:189:MSE:HB3 | 1.78 | 0.66 |
| 1:B:1993:GLU:O | 1:B:1997:PRO:HD2 | 1.96 | 0.66 |
| 1:B:2155:GLU:O | 1:B:2157:PHE:N | 2.29 | 0.66 |
| 1:B:2190:VAL:HG21 | 1:B:2241:LEU:HD13 | 1.76 | 0.66 |
| 1:B:2408:MSE:HE2 | 1:B:2408:MSE:HA | 1.78 | 0.66 |
| 1:B:294:PHE:HZ | 1:B:319:PHE:CD2 | 2.14 | 0.66 |
| 1:B:3887:PHE:HE2 | 1:B:3904:PHE:HD2 | 1.43 | 0.66 |
| 1:B:3944:HIS:CE1 | 1:B:4020:MSE:HE2 | 2.30 | 0.66 |
| 1:B:617:PRO:O | 1:B:620:PHE:N | 2.29 | 0.66 |
| 1:A:2382:VAL:HG21 | 1:A:2404:ARG:HG3 | 1.79 | 0.65 |
| 1:A:971:ARG:HB3 | 1:A:1027:ASP:OD2 | 1.96 | 0.65 |
| 1:B:1081:ALA:O | 1:B:1085:ILE:HG12 | 1.95 | 0.65 |
| 1:B:3262:LEU:HD21 | 1:B:3274:VAL:HG12 | 1.78 | 0.65 |
| 1:B:403:GLY:C | 1:B:405:ASP:H | 1.98 | 0.65 |
| 1:A:2011:ALA:O | 1:A:2013:GLU:N | 2.28 | 0.65 |
| 1:A:2023:SER:HA | 1:A:2070:GLU:OE2 | 1.96 | 0.65 |
| 1:A:2183:HIS:O | 1:A:2187:VAL:CB | 2.30 | 0.65 |
| 1:A:2962:ARG:HE | 1:A:3254:LEU:HA | 1.60 | 0.65 |
| 1:A:3042:PRO:HA | 1:A:3045:ILE:HG12 | 1.77 | 0.65 |
| 1:A:3287:ARG:HH11 | 1:A:3331:GLY:HA3 | 1.61 | 0.65 |
| 1:A:446:PHE:CD1 | 1:A:447:PRO:HD3 | 2.30 | 0.65 |
| 1:B:1681:ASP:OD1 | 1:B:1682:THR:N | 2.29 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2478:MSE:O | 1:B:2482:ASP:CB | 2.44 | 0.65 |
| 1:B:3589:SER:O | 1:B:3593:ARG:CB | 2.44 | 0.65 |
| 1:B:717:LYS:NZ | 1:B:1121:LEU:HD11 | 2.10 | 0.65 |
| 1:A:135:LEU:HD13 | 1:A:173:LYS:HB3 | 1.78 | 0.65 |
| 1:A:1802:TYR:HA | 1:A:1805:PHE:HD2 | 1.61 | 0.65 |
| 1:A:2794:LEU:HA | 1:A:2797:VAL:HG22 | 1.78 | 0.65 |
| 1:A:3847:SER:HA | 1:A:3857:LEU:HD13 | 1.77 | 0.65 |
| 1:B:2224:PHE:CZ | 1:B:2276:LEU:HD22 | 2.32 | 0.65 |
| 1:B:253:LEU:HD11 | 1:B:297:LEU:HB3 | 1.78 | 0.65 |
| 1:B:2571:ASP:O | 1:B:2789:SER:OG | 2.14 | 0.65 |
| 1:B:2935:GLU:HG3 | 1:B:2936:TYR:H | 1.62 | 0.65 |
| 1:B:3630:ARG:HG2 | 1:B:3686:TRP:NE1 | 2.11 | 0.65 |
| 1:B:393:LYS:HA | 1:B:396:PHE:CD1 | 2.31 | 0.65 |
| 1:B:3998:LEU:O | 1:B:4001:THR:OG1 | 2.13 | 0.65 |
| 1:B:649:PHE:O | 1:B:652:GLU:N | 2.15 | 0.65 |
| 1:A:1101:PHE:O | 1:A:1104:LEU:HB2 | 1.97 | 0.65 |
| 1:A:1934:LEU:CD1 | 1:A:1937:ARG:H | 2.09 | 0.65 |
| 1:A:3429:GLU:OE1 | 1:A:4046:TYR:OH | 2.13 | 0.65 |
| 1:A:3946:PHE:CE2 | 1:A:4048:LYS:HD2 | 2.31 | 0.65 |
| 1:A:939:MSE:HE2 | 1:A:942:LEU:HD13 | 1.79 | 0.65 |
| 1:B:1349:LEU:HD23 | 1:B:1353:PRO:HG2 | 1.78 | 0.65 |
| 1:B:1816:ARG:HB3 | 1:B:1819:PHE:HE1 | 1.60 | 0.65 |
| 1:A:1121:LEU:HG | 1:A:1122:GLY:N | 2.11 | 0.65 |
| 1:A:1292:LYS:NZ | 1:A:1361:LYS:HZ1 | 1.95 | 0.65 |
| 1:A:1423:ILE:HG13 | 1:A:1424:THR:H | 1.60 | 0.65 |
| 1:A:1718:ILE:HG23 | 1:A:1750:LEU:HD21 | 1.78 | 0.65 |
| 1:A:2034:SER:O | 1:A:2036:LEU:N | 2.29 | 0.65 |
| 1:A:2182:ILE:O | 1:A:2186:VAL:HG12 | 1.97 | 0.65 |
| 1:A:2253:TYR:HD1 | 1:A:2256:ILE:HD12 | 1.59 | 0.65 |
| 1:A:3480:LEU:O | 1:A:3484:THR:OG1 | 2.14 | 0.65 |
| 1:B:1101:PHE:CG | 1:B:1138:ILE:HG12 | 2.32 | 0.65 |
| 1:B:385:TYR:O | 1:B:389:ILE:HB | 1.95 | 0.65 |
| 1:B:753:GLN:O | 1:B:757:LYS:CB | 2.43 | 0.65 |
| 1:A:1737:ASN:C | 1:A:1739:TYR:H | 2.00 | 0.65 |
| 1:A:2049:VAL:O | 1:A:2052:TYR:N | 2.28 | 0.65 |
| 1:A:2507:ILE:HA | 1:A:2510:LEU:HD12 | 1.78 | 0.65 |
| 1:A:2886:GLN:OE1 | 1:A:2921:LEU:HB2 | 1.97 | 0.65 |
| 1:B:471:LYS:HA | 1:B:1553:PHE:CE2 | 2.31 | 0.65 |
| 1:B:173:LYS:O | 1:B:177:LEU:HG | 1.97 | 0.65 |
| 1:B:3677:PRO:O | 1:B:3679:ASN:N | 2.28 | 0.65 |
| 1:B:736:LEU:O | 1:B:740:ILE:HG13 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:938:VAL:HG21 | 1:B:962:TYR:CZ | 2.32 | 0.65 |
| 1:A:1346:THR:HG21 | 1:A:1401:ASN:HB3 | 1.79 | 0.65 |
| 1:A:2049:VAL:HA | 1:A:2052:TYR:CD2 | 2.30 | 0.65 |
| 1:A:2058:ASP:HB3 | 1:A:2059:PRO:HD3 | 1.78 | 0.65 |
| 1:A:2274:ILE:HA | 1:A:2277:LEU:HG | 1.76 | 0.65 |
| 1:A:2304:VAL:HG13 | 1:A:2348:GLN:NE2 | 2.10 | 0.65 |
| 1:A:3630:ARG:HA | 1:A:3686:TRP:CD1 | 2.32 | 0.65 |
| 1:A:393:LYS:HA | 1:A:396:PHE:CD1 | 2.32 | 0.65 |
| 1:A:4004:VAL:O | 1:A:4008:GLU:HB2 | 1.97 | 0.65 |
| 1:A:759:GLY:HA2 | 1:A:763:THR:OG1 | 1.95 | 0.65 |
| 1:A:895:ALA:HB3 | 1:A:904:VAL:HG21 | 1.78 | 0.65 |
| 1:B:1651:LYS:O | 1:B:1654:GLN:HB2 | 1.97 | 0.65 |
| 1:B:2062:ALA:HB1 | 1:B:2066:PHE:CE2 | 2.30 | 0.65 |
| 1:B:2937:ASP:OD1 | 1:B:3979:LEU:HD12 | 1.96 | 0.65 |
| 1:A:2240:THR:HG21 | 2:K:113:UNK:N | 2.12 | 0.65 |
| 1:A:1039:TRP:HZ2 | 1:A:1049:GLN:HA | 1.62 | 0.65 |
| 1:A:1107:TYR:O | 1:A:1111:LEU:N | 2.29 | 0.65 |
| 1:A:1138:ILE:HG21 | 1:A:1150:LYS:HE2 | 1.78 | 0.65 |
| 1:A:1373:VAL:HB | 1:A:1418:HIS:CE1 | 2.31 | 0.65 |
| 1:A:1437:TYR:CE2 | 1:A:1444:ASP:OD2 | 2.48 | 0.65 |
| 1:A:2854:PHE:CG | 1:A:2882:ALA:HB2 | 2.32 | 0.65 |
| 1:A:660:LEU:O | 1:A:663:ILE:HG13 | 1.96 | 0.65 |
| 1:A:757:LYS:HA | 1:A:760:LEU:HD12 | 1.78 | 0.65 |
| 1:B:1249:SER:O | 1:B:1253:THR:CB | 2.44 | 0.65 |
| 1:B:220:LEU:O | 1:B:224:LEU:HG | 1.97 | 0.65 |
| 1:B:3141:PHE:HE1 | 1:B:3193:ILE:HG13 | 1.62 | 0.65 |
| 1:B:3705:TYR:HE2 | 1:B:3708:ARG:NH1 | 1.95 | 0.65 |
| 1:B:4099:SER:O | 1:B:4103:GLN:NE2 | 2.27 | 0.65 |
| 1:A:1949:ILE:HD12 | 1:A:1952:ILE:HG21 | 1.79 | 0.65 |
| 1:A:2375:ALA:O | 1:A:2379:MSE:HB2 | 1.96 | 0.65 |
| 1:A:940:PHE:HE2 | 1:A:2576:MSE:SE | 2.29 | 0.65 |
| 1:A:3416:LEU:HD13 | 1:A:3446:VAL:HG12 | 1.78 | 0.65 |
| 1:A:909:VAL:HG13 | 1:A:913:ARG:HH11 | 1.62 | 0.65 |
| 1:B:2070:GLU:HB2 | 1:B:2072:ARG:N | 2.12 | 0.65 |
| 1:B:2270:ASN:O | 1:B:2274:ILE:HG23 | 1.95 | 0.65 |
| 1:B:2412:TYR:CD2 | 1:B:2416:LYS:HE3 | 2.31 | 0.65 |
| 1:B:3152:SER:HB2 | 1:B:3155:VAL:HB | 1.77 | 0.65 |
| 1:B:3257:LYS:HA | 1:B:3260:LYS:HD2 | 1.77 | 0.65 |
| 1:B:3722:PHE:CD1 | 1:B:3740:ILE:HA | 2.32 | 0.65 |
| 1:B:3704:GLN:HE21 | 1:B:3796:MSE:SE | 2.30 | 0.65 |
| 1:A:3176:MSE:HE1 | 1:A:3179:TRP:CE3 | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3843:LEU:HD22 | 1:A:3858:MSE:HE1 | 1.79 | 0.65 |
| 1:B:2196:TRP:CG | 1:B:2199:LEU:HD11 | 2.31 | 0.65 |
| 1:B:2413:PHE:CD2 | 1:B:2445:LYS:HG3 | 2.32 | 0.65 |
| 1:B:2883:SER:HA | 1:B:2886:GLN:HE21 | 1.62 | 0.65 |
| 1:B:2936:TYR:CE1 | 1:B:2949:THR:HG21 | 2.32 | 0.65 |
| 1:B:3499:ILE:HG13 | 1:B:3531:TYR:CZ | 2.32 | 0.65 |
| 1:B:3594:ALA:HB1 | 1:B:4028:ILE:HG21 | 1.79 | 0.65 |
| 1:B:4062:ASP:O | 1:B:4066:LEU:HD13 | 1.97 | 0.65 |
| 1:B:416:SER:O | 1:B:420:VAL:HB | 1.97 | 0.65 |
| 1:A:3141:PHE:HE1 | 1:A:3193:ILE:HG13 | 1.62 | 0.64 |
| 1:A:757:LYS:HA | 1:A:760:LEU:CD1 | 2.27 | 0.64 |
| 1:B:1094:SER:N | 1:B:1097:GLU:OE2 | 2.28 | 0.64 |
| 1:B:1163:LEU:HD22 | 1:B:1260:LEU:HD11 | 1.79 | 0.64 |
| 1:B:217:LEU:HD22 | 1:B:264:ARG:HG3 | 1.79 | 0.64 |
| 1:B:446:PHE:CZ | 1:B:530:LEU:HB3 | 2.32 | 0.64 |
| 1:A:1145:LEU:HD13 | 1:A:1149:LYS:HD3 | 1.80 | 0.64 |
| 1:A:1915:LEU:HD12 | 1:A:1916:ILE:HG13 | 1.78 | 0.64 |
| 1:A:3011:LEU:HD12 | 1:A:3047:SER:HB3 | 1.79 | 0.64 |
| 1:A:3421:ASP:OD2 | 1:A:3467:ARG:HD3 | 1.97 | 0.64 |
| 1:A:404:ASP:O | 1:A:406:ARG:N | 2.29 | 0.64 |
| 1:B:1655:ILE:HG13 | 1:B:1677:SER:HA | 1.79 | 0.64 |
| 1:B:172:GLU:O | 1:B:176:GLU:HG3 | 1.97 | 0.64 |
| 1:B:2538:ARG:NH1 | 1:B:2562:LEU:O | 2.30 | 0.64 |
| 1:B:2539:LEU:HA | 1:B:2542:LEU:HD23 | 1.79 | 0.64 |
| 1:B:3015:SER:O | 1:B:3019:ILE:N | 2.28 | 0.64 |
| 1:B:3931:ALA:O | 1:B:3935:GLY:CA | 2.43 | 0.64 |
| 1:A:1889:VAL:HG22 | 1:A:1900:PHE:CD2 | 2.33 | 0.64 |
| 1:A:2412:TYR:CE1 | 1:A:2415:LEU:HD23 | 2.32 | 0.64 |
| 1:B:171:LEU:HD13 | 1:B:219:VAL:HG13 | 1.80 | 0.64 |
| 1:B:1909:ASN:O | 1:B:1912:THR:HG23 | 1.98 | 0.64 |
| 1:B:385:TYR:CE1 | 1:B:421:LEU:HD23 | 2.31 | 0.64 |
| 1:A:2094:MSE:HE2 | 1:A:2142:ILE:HG22 | 1.79 | 0.64 |
| 1:A:183:GLU:HA | 1:A:233:ASN:HD21 | 1.62 | 0.64 |
| 1:A:2452:ARG:HG2 | 1:A:2498:ILE:HD11 | 1.79 | 0.64 |
| 1:A:3048:LYS:HZ2 | 1:A:3089:LEU:HB3 | 1.63 | 0.64 |
| 1:A:866:ILE:HB | 1:A:3129:LEU:HD13 | 1.78 | 0.64 |
| 1:A:3503:VAL:HG21 | 1:A:3535:ILE:O | 1.97 | 0.64 |
| 1:B:1649:LEU:HA | 1:B:1652:ILE:HD12 | 1.78 | 0.64 |
| 1:B:2999:LEU:HD12 | 1:B:3002:TYR:HE2 | 1.63 | 0.64 |
| 1:B:3496:ILE:O | 1:B:3498:TRP:N | 2.31 | 0.64 |
| 1:B:4020:MSE:HE3 | 1:B:4027:TRP:NE1 | 2.13 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:710:PHE:O | 1:B:714:VAL:HG23 | 1.96 | 0.64 |
| 1:A:1107:TYR:CE1 | 1:A:1111:LEU:HD13 | 2.33 | 0.64 |
| 1:A:1349:LEU:HD21 | 1:A:1359:LEU:HD13 | 1.78 | 0.64 |
| 1:A:2782:ASP:HA | 1:A:2786:LYS:HB2 | 1.80 | 0.64 |
| 1:A:3046:ARG:HH22 | 1:A:3181:ASP:CG | 1.99 | 0.64 |
| 1:A:3721:GLY:O | 1:A:3741:ARG:HB2 | 1.97 | 0.64 |
| 1:B:111:CYS:HA | 1:B:134:LEU:HD22 | 1.80 | 0.64 |
| 1:B:1279:LEU:HG | 1:B:1292:LYS:NZ | 2.13 | 0.64 |
| 1:B:3864:ARG:NH1 | 1:B:4115:ASN:OD1 | 2.30 | 0.64 |
| 1:A:1269:THR:HG22 | 1:A:1275:THR:HG21 | 1.78 | 0.64 |
| 1:A:1649:LEU:HD12 | 1:A:1652:ILE:HD12 | 1.78 | 0.64 |
| 1:A:3998:LEU:O | 1:A:4002:MSE:HG3 | 1.97 | 0.64 |
| 1:A:512:GLY:HA3 | 1:A:726:LEU:HD22 | 1.79 | 0.64 |
| 1:A:743:LEU:HG | 1:A:783:HIS:HE1 | 1.62 | 0.64 |
| 1:A:854:ARG:O | 1:A:858:MSE:HB2 | 1.98 | 0.64 |
| 1:B:1039:TRP:CZ2 | 1:B:1049:GLN:HA | 2.32 | 0.64 |
| 1:B:177:LEU:HA | 1:B:180:LEU:HB2 | 1.79 | 0.64 |
| 1:B:2467:THR:HB | 1:B:2518:GLN:HE22 | 1.62 | 0.64 |
| 1:B:2850:PHE:HB2 | 1:B:2853:PRO:HG2 | 1.80 | 0.64 |
| 1:B:2870:SER:O | 1:B:2872:ASP:N | 2.30 | 0.64 |
| 1:B:3974:MSE:SE | 1:B:3976:GLU:HB3 | 2.47 | 0.64 |
| 1:B:85:ILE:O | 1:B:89:LEU:HG | 1.97 | 0.64 |
| 1:A:1165:LEU:HB3 | 1:A:1169:VAL:HG23 | 1.79 | 0.64 |
| 1:A:1345:THR:HG21 | 1:A:1368:LEU:HD13 | 1.78 | 0.64 |
| 1:A:1609:ALA:HB3 | 1:A:1806:ARG:HH22 | 1.61 | 0.64 |
| 1:A:1890:HIS:CE1 | 1:A:1941:HIS:HA | 2.33 | 0.64 |
| 1:A:2307:MSE:HG2 | 1:A:2348:GLN:NE2 | 2.12 | 0.64 |
| 1:A:3589:SER:O | 1:A:3593:ARG:CB | 2.45 | 0.64 |
| 1:A:3676:PRO:O | 1:A:3679:ASN:ND2 | 2.30 | 0.64 |
| 1:A:3425:ARG:NH2 | 1:A:4000:ASN:OD1 | 2.31 | 0.64 |
| 1:B:2276:LEU:HA | 1:B:2279:ILE:HG12 | 1.80 | 0.64 |
| 1:B:2939:LEU:HD21 | 1:B:2994:TRP:CD2 | 2.33 | 0.64 |
| 1:A:1084:ASN:HD21 | 1:A:1131:ILE:HG22 | 1.63 | 0.64 |
| 1:A:720:GLN:HB3 | 1:A:1123:THR:HG21 | 1.78 | 0.64 |
| 1:A:2413:PHE:CE1 | 1:A:2442:MSE:HG2 | 2.33 | 0.64 |
| 1:A:2555:LEU:HD11 | 1:A:2803:ILE:HD11 | 1.79 | 0.64 |
| 1:A:3498:TRP:NE1 | 1:A:3502:MSE:SE | 2.81 | 0.64 |
| 1:B:1973:LYS:O | 1:B:1974:ASN:HB2 | 1.98 | 0.64 |
| 1:B:2423:VAL:HG13 | 1:B:2424:MSE:H | 1.63 | 0.64 |
| 1:B:2433:LYS:NZ | 1:B:2461:PHE:CZ | 2.65 | 0.64 |
| 1:B:2555:LEU:HD12 | 1:B:2556:SER:H | 1.62 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:272:LEU:HB3 | 1:B:319:PHE:HZ | 1.63 | 0.64 |
| 1:B:3705:TYR:CE2 | 1:B:3708:ARG:NH1 | 2.66 | 0.64 |
| 1:B:393:LYS:HA | 1:B:396:PHE:HD1 | 1.62 | 0.64 |
| 1:B:66:LEU:HD21 | 1:B:89:LEU:HD11 | 1.78 | 0.64 |
| 1:A:1700:THR:O | 1:A:1702:LEU:N | 2.30 | 0.64 |
| 1:A:884:VAL:HB | 1:A:3892:THR:OG1 | 1.98 | 0.64 |
| 1:A:995:PHE:CD1 | 1:A:1003:SER:HA | 2.33 | 0.64 |
| 1:B:101:ALA:HB3 | 1:B:102:PRO:HD3 | 1.80 | 0.64 |
| 1:B:1069:HIS:HB3 | 1:B:3741:ARG:CZ | 2.28 | 0.64 |
| 1:B:1598:ASN:CG | 1:B:1811:ARG:HG2 | 2.19 | 0.64 |
| 1:B:1696:LEU:HA | 1:B:1700:THR:HG21 | 1.79 | 0.64 |
| 1:B:3282:ARG:HB2 | 1:B:3282:ARG:NH1 | 2.13 | 0.64 |
| 1:B:345:PHE:CD2 | 1:B:367:GLY:HA3 | 2.32 | 0.64 |
| 1:B:3816:LEU:O | 1:B:3820:MSE:HB3 | 1.97 | 0.64 |
| 1:B:411:PRO:HG2 | 1:B:457:CYS:SG | 2.37 | 0.64 |
| 1:A:2253:TYR:HA | 1:A:2256:ILE:HB | 1.80 | 0.64 |
| 1:A:14:ARG:HB3 | 1:A:2359:LYS:HE2 | 1.79 | 0.64 |
| 1:A:3855:TYR:HB3 | 1:A:4074:PHE:CZ | 2.32 | 0.64 |
| 1:A:771:ASN:O | 1:A:773:LEU:N | 2.30 | 0.64 |
| 1:B:1471:GLN:O | 1:B:1475:LEU:HB3 | 1.98 | 0.64 |
| 1:B:207:GLN:O | 1:B:212:VAL:HG12 | 1.98 | 0.64 |
| 1:B:2379:MSE:HE1 | 1:B:2404:ARG:HH11 | 1.60 | 0.64 |
| 1:B:909:VAL:O | 1:B:913:ARG:HG2 | 1.98 | 0.64 |
| 1:A:1039:TRP:CZ2 | 1:A:1049:GLN:HA | 2.33 | 0.63 |
| 1:A:1939:LEU:HD13 | 1:A:1986:ARG:HH21 | 1.62 | 0.63 |
| 1:A:2194:LEU:HD13 | 1:A:2244:CYS:HB3 | 1.79 | 0.63 |
| 1:A:3110:PHE:O | 1:A:3114:TYR:HD1 | 1.81 | 0.63 |
| 1:A:2929:LEU:HG | 1:A:3784:ARG:HG2 | 1.79 | 0.63 |
| 1:A:3788:LEU:HG | 1:A:3789:ARG:N | 2.13 | 0.63 |
| 1:A:66:LEU:HD21 | 1:A:89:LEU:HD11 | 1.80 | 0.63 |
| 1:B:2912:GLY:HA2 | 1:B:2915:ARG:HH21 | 1.64 | 0.63 |
| 1:B:3725:ARG:NH1 | 1:B:3737:ARG:NH2 | 2.38 | 0.63 |
| 1:A:1640:GLU:O | 1:A:1644:ALA:CB | 2.46 | 0.63 |
| 1:A:2866:ALA:O | 1:A:2869:LEU:N | 2.31 | 0.63 |
| 1:A:3781:CYS:HA | 1:A:3786:LEU:HD12 | 1.78 | 0.63 |
| 1:A:3985:VAL:HG11 | 1:A:4101:GLU:HG2 | 1.79 | 0.63 |
| 1:A:493:LYS:HB3 | 1:A:494:PRO:HD2 | 1.80 | 0.63 |
| 1:B:139:ARG:HA | 1:B:173:LYS:HD3 | 1.80 | 0.63 |
| 1:B:1970:LYS:HE2 | 1:B:2017:GLY:HA3 | 1.80 | 0.63 |
| 1:B:4038:TRP:CH2 | 1:B:4040:PRO:HB3 | 2.32 | 0.63 |
| 1:A:1259:LEU:HD11 | 1:A:1337:VAL:HA | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2352:HIS:HB3 | 1:A:2360:PHE:HB3 | 1.78 | 0.63 |
| 1:B:2171:LEU:HG | 1:B:2177:ASN:HD21 | 1.63 | 0.63 |
| 1:B:3687:MSE:C | 1:B:3689:ASP:H | 1.99 | 0.63 |
| 1:B:617:PRO:HB3 | 1:B:659:ARG:HG3 | 1.80 | 0.63 |
| 1:A:132:ILE:HA | 1:A:135:LEU:HD12 | 1.80 | 0.63 |
| 1:A:1981:LEU:HD21 | 1:A:2031:LEU:O | 1.98 | 0.63 |
| 1:A:1982:ILE:HA | 1:A:1985:LYS:HE2 | 1.80 | 0.63 |
| 1:A:2281:MSE:SE | 1:A:2286:PRO:HB3 | 2.48 | 0.63 |
| 1:A:2404:ARG:NH1 | 1:A:2412:TYR:CZ | 2.67 | 0.63 |
| 1:A:3192:LYS:N | 1:A:3192:LYS:HD2 | 2.13 | 0.63 |
| 1:B:995:PHE:CD1 | 1:B:1003:SER:HA | 2.33 | 0.63 |
| 1:B:1296:PHE:O | 1:B:1299:GLU:N | 2.28 | 0.63 |
| 1:B:2145:PHE:HD1 | 1:B:2188:GLU:HG2 | 1.62 | 0.63 |
| 1:B:2433:LYS:HG3 | 1:B:2436:LEU:HD12 | 1.79 | 0.63 |
| 1:B:3974:MSE:HA | 1:B:3975:LYS:HB3 | 1.80 | 0.63 |
| 1:B:2933:ILE:HG23 | 1:B:3979:LEU:HB2 | 1.80 | 0.63 |
| 1:B:744:ASP:C | 1:B:746:ARG:H | 2.01 | 0.63 |
| 1:B:984:TYR:O | 1:B:988:VAL:HG13 | 1.99 | 0.63 |
| 1:A:1093:GLU:N | 1:A:1097:GLU:OE2 | 2.22 | 0.63 |
| 1:A:720:GLN:HG3 | 1:A:1121:LEU:HD22 | 1.81 | 0.63 |
| 1:A:1424:THR:O | 1:A:1427:SER:N | 2.28 | 0.63 |
| 1:A:1685:ASP:CB | 1:A:1727:ARG:HH22 | 2.06 | 0.63 |
| 1:A:278:HIS:O | 1:A:281:GLN:HB3 | 1.98 | 0.63 |
| 1:A:2936:TYR:CD1 | 1:A:2949:THR:HG21 | 2.33 | 0.63 |
| 1:A:904:VAL:O | 1:A:906:PHE:N | 2.32 | 0.63 |
| 1:B:1006:THR:HG22 | 1:B:1010:LEU:HG | 1.81 | 0.63 |
| 1:B:2022:PRO:HB2 | 1:B:2072:ARG:HH21 | 1.62 | 0.63 |
| 1:B:2144:LEU:HB3 | 1:B:2148:LYS:HE3 | 1.80 | 0.63 |
| 1:B:2449:VAL:HA | 1:B:2452:ARG:HD2 | 1.80 | 0.63 |
| 1:B:3155:VAL:HG23 | 1:B:3158:LYS:HD2 | 1.80 | 0.63 |
| 1:B:3630:ARG:HG2 | 1:B:3686:TRP:HE1 | 1.63 | 0.63 |
| 1:B:473:PRO:HA | 1:B:476:ARG:NH2 | 2.11 | 0.63 |
| 1:B:726:LEU:HD23 | 1:B:729:CYS:SG | 2.38 | 0.63 |
| 1:A:1070:PRO:HB2 | 1:A:1073:PHE:CE1 | 2.34 | 0.63 |
| 1:A:1729:PHE:CE2 | 1:A:1870:LYS:HG3 | 2.33 | 0.63 |
| 1:A:345:PHE:HD2 | 1:A:367:GLY:HA3 | 1.64 | 0.63 |
| 1:B:1251:GLN:O | 1:B:1255:CYS:HB2 | 1.98 | 0.63 |
| 1:B:2788:SER:O | 1:B:2791:ILE:HB | 1.98 | 0.63 |
| 1:B:3763:ARG:NH2 | 1:B:4009:PRO:HG3 | 2.13 | 0.63 |
| 1:B:3834:ALA:HB1 | 1:B:3838:GLU:OE1 | 1.98 | 0.63 |
| 1:B:766:ALA:O | 1:B:768:VAL:N | 2.28 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:256:ILE:HG22 | 1:A:257:ARG:HG3 | 1.80 | 0.63 |
| 1:A:3684:SER:OG | 1:A:3685:PRO:HD3 | 1.98 | 0.63 |
| 1:A:414:LEU:HD23 | 1:A:460:ALA:HB1 | 1.80 | 0.63 |
| 1:A:988:VAL:O | 1:A:992:ILE:HG23 | 1.99 | 0.63 |
| 1:B:1583:MSE:HE1 | 1:B:1640:GLU:OE2 | 1.98 | 0.63 |
| 1:B:1711:ARG:HG3 | 1:B:1712:ARG:N | 2.13 | 0.63 |
| 1:B:3919:GLY:H | 1:B:3946:PHE:H | 1.47 | 0.63 |
| 1:B:942:LEU:HD11 | 1:B:991:LEU:HD11 | 1.80 | 0.63 |
| 1:A:1419:LEU:O | 1:A:1421:GLU:N | 2.31 | 0.63 |
| 1:A:1575:LEU:HD13 | 1:A:1604:SER:HB3 | 1.80 | 0.63 |
| 1:A:1952:ILE:HG12 | 1:A:1953:CYS:H | 1.63 | 0.63 |
| 1:A:3816:LEU:HD13 | 1:A:3966:GLN:NE2 | 2.12 | 0.63 |
| 1:A:4050:LYS:HB3 | 1:A:4055:ASN:HD21 | 1.63 | 0.63 |
| 1:B:1100:VAL:O | 1:B:1104:LEU:N | 2.29 | 0.63 |
| 1:B:1279:LEU:HG | 1:B:1292:LYS:HZ1 | 1.62 | 0.63 |
| 1:B:1306:ILE:HG12 | 1:B:1334:LYS:HB3 | 1.81 | 0.63 |
| 1:B:3167:ARG:HG2 | 1:B:3186:ARG:NE | 2.14 | 0.63 |
| 1:B:3982:SER:O | 1:B:3986:HIS:ND1 | 2.32 | 0.63 |
| 1:B:4088:ASN:OD1 | 1:B:4091:ALA:HB3 | 1.99 | 0.63 |
| 1:B:988:VAL:O | 1:B:992:ILE:HG23 | 1.99 | 0.63 |
| 1:A:1887:ASP:OD1 | 1:A:1937:ARG:NH2 | 2.31 | 0.63 |
| 1:A:2256:ILE:HG21 | 1:A:2280:VAL:HG21 | 1.81 | 0.63 |
| 1:A:2327:LEU:O | 1:A:2331:MSE:HG2 | 1.99 | 0.63 |
| 1:B:114:VAL:CG1 | 1:B:130:LEU:HD11 | 2.29 | 0.63 |
| 1:B:2226:PRO:O | 1:B:2230:VAL:N | 2.27 | 0.63 |
| 1:B:2799:GLN:HG3 | 1:B:2808:LEU:HD11 | 1.81 | 0.63 |
| 1:B:2936:TYR:HE1 | 1:B:2949:THR:HG21 | 1.64 | 0.63 |
| 1:B:3045:ILE:O | 1:B:3048:LYS:HB2 | 1.99 | 0.63 |
| 1:B:4035:GLU:HG2 | 1:B:4038:TRP:CE3 | 2.34 | 0.63 |
| 1:B:559:SER:O | 1:B:563:LEU:HG | 1.98 | 0.63 |
| 1:A:999:LYS:HD3 | 1:A:1000:LYS:H | 1.64 | 0.62 |
| 1:A:1029:CYS:HB3 | 1:A:1085:ILE:HG13 | 1.81 | 0.62 |
| 1:A:2379:MSE:SE | 1:A:2408:MSE:SE | 3.17 | 0.62 |
| 1:A:31:GLY:O | 1:A:34:LEU:HB3 | 1.98 | 0.62 |
| 1:A:4048:LYS:O | 1:A:4051:LEU:HB3 | 1.99 | 0.62 |
| 1:A:649:PHE:O | 1:A:651:TYR:N | 2.32 | 0.62 |
| 1:A:802:THR:O | 1:A:806:SER:OG | 2.15 | 0.62 |
| 1:A:935:HIS:O | 1:A:938:VAL:HB | 1.99 | 0.62 |
| 1:B:3250:ASN:OD1 | 1:B:3285:HIS:HB3 | 1.98 | 0.62 |
| 1:A:1745:LYS:C | 1:A:1747:LEU:H | 2.02 | 0.62 |
| 1:A:4056:PRO:HG2 | 1:A:4094:PRO:HB3 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1459:HIS:CE1 | 1:B:1510:LEU:HG | 2.35 | 0.62 |
| 1:B:1604:SER:HB2 | 1:B:1632:TRP:HB3 | 1.80 | 0.62 |
| 1:B:2146:LEU:HA | 1:B:2149:LEU:HG | 1.80 | 0.62 |
| 1:B:3107:ILE:HA | 1:B:3110:PHE:CE2 | 2.34 | 0.62 |
| 1:B:3778:ASP:OD2 | 1:B:3781:CYS:N | 2.32 | 0.62 |
| 1:B:452:LYS:O | 1:B:455:LEU:HG | 1.99 | 0.62 |
| 1:B:585:ILE:HG22 | 1:B:586:GLN:H | 1.64 | 0.62 |
| 1:A:101:ALA:HB3 | 1:A:102:PRO:HD3 | 1.81 | 0.62 |
| 1:A:2147:ALA:HB1 | 1:A:2151:ILE:HD12 | 1.82 | 0.62 |
| 1:A:2378:PHE:CE1 | 1:A:2408:MSE:HE1 | 2.29 | 0.62 |
| 1:A:956:PRO:HB2 | 1:A:957:PRO:HD3 | 1.79 | 0.62 |
| 1:B:3592:VAL:HG13 | 1:B:3609:MSE:SE | 2.50 | 0.62 |
| 1:B:4046:TYR:CZ | 1:B:4049:ARG:NH2 | 2.68 | 0.62 |
| 1:A:2074:PRO:O | 1:A:2077:HIS:N | 2.32 | 0.62 |
| 1:A:252:VAL:HG11 | 1:A:265:TYR:HB2 | 1.81 | 0.62 |
| 1:A:2900:LEU:HD12 | 1:A:2905:LEU:HD21 | 1.80 | 0.62 |
| 1:A:3176:MSE:HE2 | 1:A:3251:ASN:HD22 | 1.64 | 0.62 |
| 1:A:3256:MSE:HE2 | 1:A:3282:ARG:HH12 | 1.62 | 0.62 |
| 1:A:3762:GLN:NE2 | 1:A:3763:ARG:NH1 | 2.46 | 0.62 |
| 1:A:3812:LEU:O | 1:A:3816:LEU:CB | 2.38 | 0.62 |
| 1:B:1637:SER:O | 1:B:1640:GLU:N | 2.32 | 0.62 |
| 1:B:154:SER:OG | 1:B:189:MSE:HG2 | 1.99 | 0.62 |
| 1:B:200:PHE:O | 1:B:204:LEU:HG | 1.98 | 0.62 |
| 1:B:2936:TYR:CD2 | 1:B:3979:LEU:HD21 | 2.33 | 0.62 |
| 1:B:2943:PHE:CD2 | 1:B:2944:THR:HG23 | 2.34 | 0.62 |
| 1:B:508:HIS:HD2 | 1:B:725:LEU:HD13 | 1.65 | 0.62 |
| 1:B:891:ARG:CD | 1:B:905:ILE:HG12 | 2.30 | 0.62 |
| 1:A:2239:LYS:HD3 | 2:K:110:UNK:CB | 2.30 | 0.62 |
| 1:A:2260:PHE:CD1 | 1:A:2274:ILE:HG22 | 2.35 | 0.62 |
| 1:A:2900:LEU:HB3 | 1:A:2905:LEU:HD11 | 1.80 | 0.62 |
| 1:A:3486:GLU:HG3 | 1:A:3487:ILE:H | 1.65 | 0.62 |
| 1:A:870:LEU:HD11 | 1:A:3125:ARG:HG3 | 1.80 | 0.62 |
| 1:B:1080:LEU:HD12 | 1:B:1081:ALA:N | 2.14 | 0.62 |
| 1:B:1708:GLU:HB2 | 1:B:1709:GLU:OE2 | 2.00 | 0.62 |
| 1:B:2386:LEU:O | 1:B:2390:HIS:HB2 | 2.00 | 0.62 |
| 1:B:3824:GLU:HB3 | 1:B:3829:LEU:HD11 | 1.81 | 0.62 |
| 1:A:971:ARG:HD2 | 1:A:1024:THR:HG23 | 1.80 | 0.62 |
| 1:A:1033:ILE:HB | 1:A:1085:ILE:HG22 | 1.81 | 0.62 |
| 1:A:1292:LYS:HZ2 | 1:A:1361:LYS:NZ | 1.96 | 0.62 |
| 1:A:2239:LYS:HD2 | 1:A:2279:ILE:HD12 | 1.81 | 0.62 |
| 1:A:245:SER:HA | 1:A:248:ILE:HD12 | 1.80 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2555:LEU:O | 1:A:2558:ALA:HB3 | 1.99 | 0.62 |
| 1:A:2837:LEU:HA | 1:A:2840:PHE:CD2 | 2.30 | 0.62 |
| 1:A:2869:LEU:HG | 1:A:2893:LEU:HD12 | 1.80 | 0.62 |
| 1:B:1265:GLU:O | 1:B:1269:THR:HG23 | 2.00 | 0.62 |
| 1:B:1293:ALA:HA | 1:B:1296:PHE:HD2 | 1.65 | 0.62 |
| 1:B:3174:ASP:OD2 | 1:B:3779:SER:HA | 2.00 | 0.62 |
| 1:B:3582:GLU:O | 1:B:3586:LYS:HB3 | 2.00 | 0.62 |
| 1:B:3630:ARG:HG2 | 1:B:3686:TRP:CD1 | 2.35 | 0.62 |
| 1:B:3812:LEU:HA | 1:B:3815:LEU:HD12 | 1.81 | 0.62 |
| 1:B:414:LEU:HA | 1:B:417:VAL:HB | 1.80 | 0.62 |
| 1:B:508:HIS:CD2 | 1:B:725:LEU:HD13 | 2.35 | 0.62 |
| 1:A:2847:THR:HB | 1:A:2850:PHE:HD2 | 1.65 | 0.62 |
| 1:A:345:PHE:CD2 | 1:A:367:GLY:HA3 | 2.34 | 0.62 |
| 1:A:3810:VAL:CG2 | 1:A:3815:LEU:HD11 | 2.29 | 0.62 |
| 1:A:3931:ALA:O | 1:A:3935:GLY:HA2 | 2.00 | 0.62 |
| 1:A:509:ARG:HB3 | 1:A:729:CYS:SG | 2.40 | 0.62 |
| 1:B:1574:ASN:HB3 | 1:B:1582:LEU:HD21 | 1.82 | 0.62 |
| 1:B:2925:GLU:HA | 1:B:3121:LEU:HD11 | 1.80 | 0.62 |
| 1:B:3393:GLU:OE1 | 1:B:3416:LEU:HD13 | 1.99 | 0.62 |
| 1:B:3872:ARG:HH11 | 1:B:3965:ARG:NH1 | 1.97 | 0.62 |
| 1:B:796:LEU:HA | 1:B:799:TYR:CE2 | 2.34 | 0.62 |
| 1:B:870:LEU:HA | 1:B:873:VAL:HB | 1.81 | 0.62 |
| 1:A:1119:LYS:HZ1 | 1:A:1256:TRP:HZ2 | 1.47 | 0.62 |
| 1:A:1220:LEU:HD13 | 1:A:1274:ARG:HG3 | 1.82 | 0.62 |
| 1:A:1216:GLY:HA3 | 1:A:1271:ILE:HG22 | 1.80 | 0.62 |
| 1:A:1342:MSE:SE | 1:A:1372:LEU:HB2 | 2.50 | 0.62 |
| 1:A:1429:GLU:O | 1:A:1433:ALA:CB | 2.46 | 0.62 |
| 1:A:1880:MSE:HE2 | 1:A:1884:LEU:HD11 | 1.81 | 0.62 |
| 1:A:2002:LYS:C | 1:A:2004:TYR:H | 2.03 | 0.62 |
| 1:A:2227:LYS:HA | 1:A:2234:ASN:HD22 | 1.64 | 0.62 |
| 1:A:2416:LYS:HB3 | 1:A:2442:MSE:SE | 2.49 | 0.62 |
| 1:A:3930:VAL:HG12 | 1:A:3937:VAL:HG22 | 1.81 | 0.62 |
| 1:A:398:THR:O | 1:A:401:ASP:N | 2.33 | 0.62 |
| 1:A:794:PRO:HA | 1:A:869:ASN:HB3 | 1.81 | 0.62 |
| 1:A:801:LYS:NZ | 1:A:877:ASP:OD2 | 2.29 | 0.62 |
| 1:B:1090:ARG:HA | 1:B:1090:ARG:HE | 1.64 | 0.62 |
| 1:B:1221:ILE:HG13 | 1:B:1274:ARG:NH1 | 2.14 | 0.62 |
| 1:B:2157:PHE:HE2 | 1:B:2199:LEU:CD1 | 2.12 | 0.62 |
| 1:B:2310:VAL:HG23 | 1:B:2315:VAL:HG21 | 1.81 | 0.62 |
| 1:B:2416:LYS:O | 1:B:2420:PHE:CB | 2.47 | 0.62 |
| 1:B:2776:ARG:HA | 1:B:2776:ARG:HH11 | 1.64 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3019:ILE:HG13 | 1:B:3020:ASP:H | 1.65 | 0.62 |
| 1:B:446:PHE:HA | 1:B:449:TYR:HE2 | 1.62 | 0.62 |
| 1:A:1449:ALA:HA | 1:A:1452:VAL:HB | 1.80 | 0.62 |
| 1:A:2283:ASN:O | 1:A:2287:PRO:HD3 | 2.00 | 0.62 |
| 1:A:3465:PHE:HA | 1:A:3468:LEU:HD12 | 1.81 | 0.62 |
| 1:A:572:VAL:HG13 | 1:A:573:LEU:H | 1.64 | 0.62 |
| 1:B:1269:THR:HG22 | 1:B:1275:THR:HG21 | 1.82 | 0.62 |
| 1:B:18:THR:O | 1:B:22:ALA:HB3 | 1.99 | 0.62 |
| 1:B:232:CYS:SG | 1:B:274:LEU:HD13 | 2.40 | 0.62 |
| 1:B:3228:SER:HA | 1:B:3231:ILE:HD12 | 1.80 | 0.62 |
| 1:B:3513:ALA:O | 1:B:3516:HIS:N | 2.33 | 0.62 |
| 1:B:634:LEU:HB3 | 1:B:638:GLN:HE22 | 1.65 | 0.62 |
| 1:A:2874:ALA:HB1 | 1:A:2878:ALA:HB3 | 1.81 | 0.62 |
| 1:A:2913:LYS:O | 1:A:2915:ARG:N | 2.32 | 0.62 |
| 1:A:538:ASP:O | 1:A:545:LEU:HD13 | 1.99 | 0.62 |
| 1:A:789:TYR:HA | 1:A:793:LEU:HD12 | 1.82 | 0.62 |
| 1:B:3243:ILE:HD13 | 1:B:3262:LEU:HD22 | 1.82 | 0.62 |
| 1:B:358:GLU:HG3 | 1:B:359:LEU:H | 1.64 | 0.62 |
| 1:A:1928:ALA:HB2 | 1:A:1941:HIS:CE1 | 2.35 | 0.61 |
| 1:A:242:PRO:O | 1:A:246:ARG:HB3 | 2.00 | 0.61 |
| 1:A:753:GLN:O | 1:A:757:LYS:CB | 2.48 | 0.61 |
| 1:A:935:HIS:HB2 | 1:A:984:TYR:HE2 | 1.65 | 0.61 |
| 1:B:1073:PHE:CZ | 1:B:3745:GLU:HA | 2.35 | 0.61 |
| 1:B:1280:GLN:HA | 1:B:1361:LYS:NZ | 2.15 | 0.61 |
| 1:B:1298:LEU:HA | 1:B:1301:ILE:HB | 1.82 | 0.61 |
| 1:B:732:PHE:HB2 | 1:B:733:LEU:HD23 | 1.82 | 0.61 |
| 1:A:1604:SER:HB2 | 1:A:1632:TRP:HB3 | 1.82 | 0.61 |
| 1:A:202:GLY:O | 1:A:206:THR:OG1 | 2.10 | 0.61 |
| 1:A:2399:GLU:O | 1:A:2402:LEU:HG | 2.00 | 0.61 |
| 1:A:2549:LYS:HZ1 | 1:A:2557:LEU:CD2 | 2.10 | 0.61 |
| 1:A:3008:TRP:HA | 1:A:3050:LYS:HG2 | 1.82 | 0.61 |
| 1:A:3684:SER:O | 1:A:3688:SER:OG | 2.14 | 0.61 |
| 1:A:3809:THR:HA | 1:A:3931:ALA:HA | 1.82 | 0.61 |
| 1:A:713:GLU:O | 1:A:717:LYS:HG2 | 2.00 | 0.61 |
| 1:B:1214:GLU:HB2 | 1:B:1218:SER:HB3 | 1.82 | 0.61 |
| 1:B:1374:GLN:O | 1:B:1378:GLU:HB2 | 2.00 | 0.61 |
| 1:B:2142:ILE:HA | 1:B:2145:PHE:HD2 | 1.62 | 0.61 |
| 1:B:592:GLU:HB3 | 1:B:601:TRP:HZ2 | 1.65 | 0.61 |
| 1:B:913:ARG:HG3 | 1:B:937:MSE:SE | 2.50 | 0.61 |
| 1:A:1108:MSE:O | 1:A:1112:ALA:N | 2.32 | 0.61 |
| 1:A:83:GLU:HG3 | 1:A:130:LEU:HD13 | 1.82 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1996:VAL:HG23 | 1:A:1997:PRO:HD2 | 1.82 | 0.61 |
| 1:A:2274:ILE:HD13 | 1:A:2318:ALA:HB2 | 1.81 | 0.61 |
| 1:A:287:LEU:C | 1:A:291:VAL:HB | 2.21 | 0.61 |
| 1:A:3037:GLN:HG3 | 1:A:3040:TYR:HE2 | 1.65 | 0.61 |
| 1:A:3578:LEU:HD13 | 1:A:3683:CYS:SG | 2.40 | 0.61 |
| 1:A:3924:HIS:H | 1:A:3927:ASN:HD22 | 1.46 | 0.61 |
| 1:B:1403:MSE:HA | 1:B:1406:LEU:HB2 | 1.81 | 0.61 |
| 1:B:2177:ASN:HD22 | 1:B:2182:ILE:CG2 | 2.12 | 0.61 |
| 1:B:2399:GLU:O | 1:B:2402:LEU:HG | 2.00 | 0.61 |
| 1:B:2957:LEU:HB3 | 1:B:3989:ARG:HH22 | 1.63 | 0.61 |
| 1:B:980:THR:HG22 | 1:B:984:TYR:HE2 | 1.66 | 0.61 |
| 1:A:2167:PRO:O | 1:A:2171:LEU:HB3 | 2.01 | 0.61 |
| 1:A:2925:GLU:O | 1:A:2927:ALA:N | 2.30 | 0.61 |
| 1:A:440:VAL:HG21 | 1:A:1814:PHE:CZ | 2.36 | 0.61 |
| 1:A:913:ARG:NE | 1:A:916:GLU:OE2 | 2.32 | 0.61 |
| 1:B:1431:LEU:HD11 | 1:B:1479:VAL:HG22 | 1.81 | 0.61 |
| 1:B:2538:ARG:HH11 | 1:B:2565:MSE:CB | 2.08 | 0.61 |
| 1:B:2961:ALA:HB1 | 1:B:3002:TYR:CD1 | 2.33 | 0.61 |
| 1:A:1086:TYR:CD2 | 1:A:1090:ARG:HG2 | 2.36 | 0.61 |
| 1:A:1574:ASN:HB3 | 1:A:1582:LEU:HD21 | 1.81 | 0.61 |
| 1:A:2936:TYR:O | 1:A:2940:ARG:HB2 | 2.00 | 0.61 |
| 1:A:3630:ARG:HD2 | 1:A:3633:ILE:HG12 | 1.83 | 0.61 |
| 1:A:3962:ARG:CZ | 1:A:3962:ARG:HB2 | 2.30 | 0.61 |
| 1:A:508:HIS:HD2 | 1:A:725:LEU:HD22 | 1.65 | 0.61 |
| 1:B:2220:MSE:SE | 1:B:2256:ILE:HD11 | 2.51 | 0.61 |
| 1:B:2849:SER:HB3 | 1:B:2881:LEU:HD12 | 1.82 | 0.61 |
| 1:B:3152:SER:HB3 | 1:B:3153:SER:CB | 2.31 | 0.61 |
| 1:B:3167:ARG:HD3 | 1:B:3186:ARG:HG2 | 1.82 | 0.61 |
| 1:A:1076:LEU:HD22 | 1:A:1111:LEU:HG | 1.83 | 0.61 |
| 1:A:2517:LEU:HA | 1:A:2520:ILE:HG22 | 1.82 | 0.61 |
| 1:A:3765:GLU:O | 1:A:3768:PHE:HB2 | 2.00 | 0.61 |
| 1:A:3962:ARG:NH1 | 1:A:4124:TRP:CZ3 | 2.66 | 0.61 |
| 1:A:575:ILE:HG12 | 1:A:579:LEU:HB2 | 1.81 | 0.61 |
| 1:B:1378:GLU:O | 1:B:1382:ILE:HG12 | 2.01 | 0.61 |
| 1:B:2011:ALA:O | 1:B:2013:GLU:N | 2.33 | 0.61 |
| 1:B:3435:ASP:O | 1:B:3439:LEU:HB3 | 2.01 | 0.61 |
| 1:B:4082:ARG:CG | 1:B:4091:ALA:HB2 | 2.30 | 0.61 |
| 1:B:612:LEU:O | 1:B:616:LYS:N | 2.31 | 0.61 |
| 1:A:1178:ARG:HB3 | 1:A:1179:PRO:HD3 | 1.82 | 0.61 |
| 1:A:2396:LEU:HA | 1:A:2400:VAL:HG23 | 1.82 | 0.61 |
| 1:A:3885:ARG:O | 1:A:3889:ARG:HB2 | 1.99 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:446:PHE:CE2 | 1:A:530:LEU:HB3 | 2.34 | 0.61 |
| 1:B:1108:MSE:O | 1:B:1112:ALA:N | 2.33 | 0.61 |
| 1:B:146:GLU:HB2 | 1:B:149:ILE:HB | 1.83 | 0.61 |
| 1:B:3314:SER:HB3 | 1:B:3318:LYS:HE3 | 1.82 | 0.61 |
| 1:B:3493:TRP:HB3 | 1:B:3711:PRO:HA | 1.81 | 0.61 |
| 1:B:3491:PRO:CB | 1:B:3711:PRO:HB3 | 2.30 | 0.61 |
| 1:A:1352:SER:HB3 | 1:A:1353:PRO:HD3 | 1.83 | 0.61 |
| 1:A:3435:ASP:O | 1:A:3439:LEU:CB | 2.49 | 0.61 |
| 1:A:3414:MSE:HE1 | 1:A:3450:MSE:HA | 1.82 | 0.61 |
| 1:A:3797:THR:HG22 | 1:A:3800:LEU:HG | 1.82 | 0.61 |
| 1:A:934:LEU:HA | 1:A:937:MSE:HE3 | 1.83 | 0.61 |
| 1:A:970:LEU:HD21 | 1:A:1031:ARG:HH21 | 1.65 | 0.61 |
| 1:B:1270:PHE:HZ | 1:B:1347:THR:HB | 1.66 | 0.61 |
| 1:B:2847:THR:HB | 1:B:2850:PHE:HD2 | 1.65 | 0.61 |
| 1:B:3047:SER:O | 1:B:3050:LYS:HG3 | 2.01 | 0.61 |
| 1:B:367:GLY:C | 1:B:369:PHE:H | 2.03 | 0.61 |
| 1:B:3729:MSE:HE2 | 1:B:3737:ARG:HB2 | 1.82 | 0.61 |
| 1:B:3835:PRO:HA | 1:B:3871:PHE:HE1 | 1.65 | 0.61 |
| 1:B:3923:ARG:CD | 1:B:3962:ARG:HH22 | 2.14 | 0.61 |
| 1:B:938:VAL:O | 1:B:942:LEU:HB2 | 2.00 | 0.61 |
| 1:A:1142:HIS:O | 1:A:1144:SER:N | 2.30 | 0.61 |
| 1:A:1270:PHE:CZ | 1:A:1347:THR:HG23 | 2.35 | 0.61 |
| 1:A:2204:GLY:HA2 | 1:A:2208:ASP:OD2 | 2.00 | 0.61 |
| 1:A:2479:TRP:CZ3 | 1:A:2480:ILE:HD13 | 2.36 | 0.61 |
| 1:A:349:ILE:CD1 | 1:A:368:LEU:HD12 | 2.31 | 0.61 |
| 1:A:3517:SER:HA | 1:A:3520:GLU:HB2 | 1.81 | 0.61 |
| 1:A:3543:LYS:HE2 | 1:A:3545:THR:HG22 | 1.82 | 0.61 |
| 1:A:1248:PHE:HB3 | 1:A:3695:LEU:HD23 | 1.83 | 0.61 |
| 1:A:935:HIS:HB2 | 1:A:984:TYR:CE2 | 2.34 | 0.61 |
| 1:B:1352:SER:O | 1:B:1354:GLU:N | 2.33 | 0.61 |
| 1:B:1587:VAL:HG23 | 1:B:1647:ALA:HB2 | 1.82 | 0.61 |
| 1:B:206:THR:HA | 1:B:209:THR:OG1 | 2.01 | 0.61 |
| 1:B:2814:SER:O | 1:B:2818:LYS:HB2 | 2.00 | 0.61 |
| 1:A:114:VAL:HG12 | 1:A:130:LEU:HD21 | 1.81 | 0.61 |
| 1:A:1740:VAL:O | 1:A:1743:MSE:HG3 | 1.99 | 0.61 |
| 1:A:239:GLU:HG3 | 1:A:240:GLU:HG3 | 1.83 | 0.61 |
| 1:A:273:ARG:HG3 | 1:A:274:LEU:N | 2.15 | 0.61 |
| 1:A:2960:GLU:HG2 | 1:A:3252:PHE:CD2 | 2.36 | 0.61 |
| 1:A:2933:ILE:HD13 | 1:A:3976:GLU:HG3 | 1.83 | 0.61 |
| 1:A:437:HIS:O | 1:A:440:VAL:HG22 | 2.00 | 0.61 |
| 1:A:484:HIS:CD2 | 1:A:556:SER:HB3 | 2.36 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:621:SER:HB3 | 1:A:659:ARG:CZ | 2.31 | 0.61 |
| 1:A:645:TRP:CE3 | 1:A:660:LEU:HD11 | 2.35 | 0.61 |
| 1:B:2157:PHE:HE2 | 1:B:2199:LEU:HD13 | 1.66 | 0.61 |
| 1:B:2345:VAL:O | 1:B:2349:LEU:HG | 2.01 | 0.61 |
| 1:B:2943:PHE:C | 1:B:2945:SER:H | 2.04 | 0.61 |
| 1:B:3247:ARG:NE | 1:B:3278:GLN:OE1 | 2.30 | 0.61 |
| 1:B:3614:TYR:O | 1:B:3618:GLY:N | 2.29 | 0.61 |
| 1:B:3631:LYS:HA | 1:B:3634:GLN:HB3 | 1.83 | 0.61 |
| 1:A:177:LEU:O | 1:A:180:LEU:N | 2.34 | 0.60 |
| 1:A:2183:HIS:CE1 | 1:A:2237:ILE:HD13 | 2.36 | 0.60 |
| 1:A:2260:PHE:HD1 | 1:A:2274:ILE:HG22 | 1.65 | 0.60 |
| 1:A:3915:HIS:O | 1:A:3918:LEU:N | 2.33 | 0.60 |
| 1:A:446:PHE:HD1 | 1:A:447:PRO:HD3 | 1.65 | 0.60 |
| 1:A:637:LYS:O | 1:A:641:PHE:HB3 | 2.01 | 0.60 |
| 1:B:1886:LYS:HE3 | 1:B:1924:THR:HG21 | 1.82 | 0.60 |
| 1:B:2274:ILE:HA | 1:B:2277:LEU:HG | 1.83 | 0.60 |
| 1:B:2481:HIS:HE1 | 1:B:2485:ARG:HH11 | 1.49 | 0.60 |
| 1:B:2575:PRO:HD2 | 1:B:2785:ILE:HD11 | 1.81 | 0.60 |
| 1:B:2806:LYS:HZ1 | 1:B:2858:ILE:HG21 | 1.64 | 0.60 |
| 1:B:3498:TRP:O | 1:B:3498:TRP:CD1 | 2.54 | 0.60 |
| 1:B:659:ARG:NH2 | 1:B:662:LEU:HG | 2.10 | 0.60 |
| 1:A:1087:ARG:HD2 | 1:A:1137:ILE:HD11 | 1.83 | 0.60 |
| 1:A:1118:GLU:HG3 | 1:A:3743:HIS:CE1 | 2.35 | 0.60 |
| 1:A:1155:ARG:O | 1:A:1158:PRO:HD2 | 2.01 | 0.60 |
| 1:A:135:LEU:HD21 | 1:A:173:LYS:HD2 | 1.83 | 0.60 |
| 1:A:1885:PRO:O | 1:A:1889:VAL:HG23 | 2.00 | 0.60 |
| 1:A:3117:ILE:HG13 | 1:A:3120:LEU:HB3 | 1.82 | 0.60 |
| 1:A:3283:LEU:HD11 | 1:A:3297:VAL:HG13 | 1.82 | 0.60 |
| 1:A:3788:LEU:HD13 | 1:A:3910:LEU:HD23 | 1.82 | 0.60 |
| 1:A:3947:GLY:O | 1:A:3950:THR:N | 2.34 | 0.60 |
| 1:B:1419:LEU:O | 1:B:1421:GLU:N | 2.34 | 0.60 |
| 1:B:1711:ARG:HG3 | 1:B:1712:ARG:H | 1.65 | 0.60 |
| 1:B:175:TYR:HA | 1:B:178:LEU:HD12 | 1.82 | 0.60 |
| 1:B:1903:SER:O | 1:B:1906:THR:OG1 | 2.18 | 0.60 |
| 1:B:2316:TYR:CZ | 1:B:2317:ALA:HB2 | 2.36 | 0.60 |
| 1:B:2989:ALA:O | 1:B:2993:PHE:N | 2.32 | 0.60 |
| 1:B:3595:GLU:HA | 1:B:3598:LYS:HD2 | 1.81 | 0.60 |
| 1:B:627:VAL:HG12 | 1:B:628:GLU:N | 2.15 | 0.60 |
| 1:B:775:GLU:O | 1:B:779:TYR:HD2 | 1.84 | 0.60 |
| 1:A:1424:THR:OG1 | 1:A:1425:ALA:N | 2.34 | 0.60 |
| 1:A:1452:VAL:HG11 | 1:A:1502:SER:HB3 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1805:PHE:HA | 1:A:1808:ASP:OD2 | 2.00 | 0.60 |
| 1:A:2167:PRO:HB2 | 1:A:2171:LEU:HD22 | 1.83 | 0.60 |
| 1:A:246:ARG:HA | 1:A:249:PHE:HD2 | 1.66 | 0.60 |
| 1:A:2813:PHE:HA | 1:A:2816:ILE:HG22 | 1.82 | 0.60 |
| 1:A:607:ASP:HA | 1:A:610:ALA:HB3 | 1.81 | 0.60 |
| 1:B:1762:MSE:HE2 | 1:B:1899:VAL:HG11 | 1.83 | 0.60 |
| 1:B:2353:GLN:HG2 | 1:B:2361:ILE:HD13 | 1.83 | 0.60 |
| 1:B:2775:TYR:HB3 | 1:B:2776:ARG:NH2 | 2.16 | 0.60 |
| 1:B:242:PRO:HB3 | 1:B:282:PHE:CD1 | 2.35 | 0.60 |
| 1:B:3048:LYS:O | 1:B:3052:LEU:N | 2.31 | 0.60 |
| 1:B:3265:GLU:HA | 1:B:3267:LYS:HE3 | 1.84 | 0.60 |
| 1:B:404:ASP:O | 1:B:406:ARG:N | 2.33 | 0.60 |
| 1:A:1761:LEU:HD22 | 1:A:1860:GLU:HB3 | 1.83 | 0.60 |
| 1:A:1981:LEU:O | 1:A:1985:LYS:HG2 | 2.02 | 0.60 |
| 1:A:2088:LEU:O | 1:A:2092:GLU:N | 2.34 | 0.60 |
| 1:A:3876:SER:O | 1:A:3879:PRO:HD2 | 2.00 | 0.60 |
| 1:A:390:GLN:O | 1:A:393:LYS:HG2 | 2.01 | 0.60 |
| 1:B:108:LYS:HG2 | 1:B:138:PHE:HA | 1.81 | 0.60 |
| 1:B:3065:ILE:HD13 | 1:B:3089:LEU:HD21 | 1.83 | 0.60 |
| 1:B:3594:ALA:HB1 | 1:B:4028:ILE:HD13 | 1.83 | 0.60 |
| 1:B:3954:PRO:HB3 | 1:B:4027:TRP:HA | 1.82 | 0.60 |
| 1:A:1131:ILE:HA | 1:A:1134:LEU:HG | 1.84 | 0.60 |
| 1:A:1978:PHE:O | 1:A:1981:LEU:HB3 | 2.01 | 0.60 |
| 1:A:1983:ASP:O | 1:A:1987:ARG:HB2 | 2.02 | 0.60 |
| 1:A:2430:GLU:OE2 | 1:A:2461:PHE:HD1 | 1.83 | 0.60 |
| 1:A:2413:PHE:CD1 | 1:A:2442:MSE:HG2 | 2.36 | 0.60 |
| 1:A:908:ASP:HB3 | 1:A:2807:GLN:OE1 | 2.01 | 0.60 |
| 1:A:3181:ASP:O | 1:A:3184:THR:OG1 | 2.13 | 0.60 |
| 1:A:4004:VAL:O | 1:A:4008:GLU:CB | 2.50 | 0.60 |
| 1:A:617:PRO:HB3 | 1:A:659:ARG:HG2 | 1.82 | 0.60 |
| 1:B:1259:LEU:HG | 1:B:1337:VAL:HG22 | 1.83 | 0.60 |
| 1:B:1743:MSE:HG2 | 1:B:1747:LEU:HD12 | 1.83 | 0.60 |
| 1:B:224:LEU:HD22 | 1:B:248:ILE:HD11 | 1.83 | 0.60 |
| 1:B:3389:VAL:HG11 | 1:B:3419:PHE:CZ | 2.35 | 0.60 |
| 1:B:327:VAL:HG22 | 1:B:338:LEU:HD13 | 1.83 | 0.60 |
| 1:B:3965:ARG:HE | 1:B:3969:ASN:HD21 | 1.49 | 0.60 |
| 1:B:730:LEU:HD23 | 1:B:733:LEU:HD12 | 1.83 | 0.60 |
| 1:A:1100:VAL:O | 1:A:1104:LEU:N | 2.33 | 0.60 |
| 1:A:1935:GLU:HB2 | 1:A:1986:ARG:CZ | 2.31 | 0.60 |
| 1:A:3155:VAL:N | 1:A:3156:PRO:HD2 | 2.17 | 0.60 |
| 1:A:3725:ARG:NH1 | 1:A:3737:ARG:HH22 | 1.99 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:403:GLY:C | 1:A:405:ASP:H | 2.04 | 0.60 |
| 1:A:966:PHE:O | 1:A:969:LEU:HB3 | 2.02 | 0.60 |
| 1:B:1742:CYS:HA | 1:B:1745:LYS:HD2 | 1.83 | 0.60 |
| 1:B:2472:GLN:O | 1:B:2476:ILE:HG23 | 2.02 | 0.60 |
| 1:B:3483:MSE:O | 1:B:3516:HIS:NE2 | 2.35 | 0.60 |
| 1:B:3670:MSE:O | 1:B:3674:SER:HB3 | 2.00 | 0.60 |
| 1:B:613:HIS:ND1 | 1:B:614:PRO:HD3 | 2.16 | 0.60 |
| 1:A:249:PHE:O | 1:A:253:LEU:HG | 2.01 | 0.60 |
| 1:A:3503:VAL:HG23 | 1:A:3536:SER:HA | 1.83 | 0.60 |
| 1:A:3760:GLN:OE1 | 1:A:3760:GLN:N | 2.34 | 0.60 |
| 1:A:566:ASP:OD2 | 1:A:1800:SER:HA | 2.02 | 0.60 |
| 1:B:1066:LEU:HA | 1:B:1069:HIS:CD2 | 2.36 | 0.60 |
| 1:B:1220:LEU:HD13 | 1:B:1274:ARG:HG3 | 1.81 | 0.60 |
| 1:B:1700:THR:OG1 | 1:B:1701:SER:N | 2.33 | 0.60 |
| 1:B:1946:ASN:O | 1:B:1949:ILE:HG22 | 2.02 | 0.60 |
| 1:B:2326:ILE:HG21 | 1:B:2341:LEU:HD23 | 1.82 | 0.60 |
| 1:B:3723:ASP:HB2 | 1:B:3741:ARG:HE | 1.66 | 0.60 |
| 1:A:3152:SER:HB3 | 1:A:3153:SER:CB | 2.32 | 0.60 |
| 1:A:3487:ILE:CG2 | 1:A:3495:PHE:HB2 | 2.31 | 0.60 |
| 1:A:752:LEU:HB2 | 1:A:756:PHE:CE1 | 2.37 | 0.60 |
| 1:A:936:SER:O | 1:A:939:MSE:N | 2.35 | 0.60 |
| 1:B:1130:ALA:O | 1:B:1134:LEU:HG | 2.01 | 0.60 |
| 1:B:1146:ASN:O | 1:B:1150:LYS:HB3 | 2.02 | 0.60 |
| 1:B:2975:ALA:C | 1:B:2977:ASN:H | 2.05 | 0.60 |
| 1:B:3344:GLU:O | 1:B:3348:LEU:HG | 2.02 | 0.60 |
| 1:B:3928:PHE:HE2 | 1:B:3962:ARG:HE | 1.47 | 0.60 |
| 1:B:3962:ARG:NH1 | 1:B:4124:TRP:CH2 | 2.70 | 0.60 |
| 1:B:649:PHE:HE1 | 1:B:653:LEU:H | 1.49 | 0.60 |
| 1:A:1063:LEU:HD13 | 1:A:1082:PHE:CZ | 2.37 | 0.60 |
| 1:A:1583:MSE:HE2 | 1:A:1639:LEU:HB2 | 1.83 | 0.60 |
| 1:A:2083:LEU:H | 1:A:2086:ASP:HB2 | 1.67 | 0.60 |
| 1:A:2274:ILE:CG1 | 1:A:2314:GLU:HB3 | 2.32 | 0.60 |
| 1:A:2554:PHE:O | 1:A:2557:LEU:N | 2.35 | 0.60 |
| 1:A:3351:ILE:O | 1:A:3355:LYS:HG2 | 2.02 | 0.60 |
| 1:A:416:SER:O | 1:A:420:VAL:HB | 2.01 | 0.60 |
| 1:A:999:LYS:HB3 | 1:A:1001:PHE:CE2 | 2.37 | 0.60 |
| 1:B:1520:ALA:O | 1:B:1524:LEU:HD13 | 2.01 | 0.60 |
| 1:B:3916:TRP:CE3 | 1:B:3917:ILE:HD12 | 2.36 | 0.60 |
| 1:B:3950:THR:OG1 | 1:B:3957:GLU:O | 2.09 | 0.60 |
| 1:A:2157:PHE:HE1 | 1:A:2203:THR:HB | 1.66 | 0.60 |
| 1:A:2389:PHE:CD2 | 1:A:2396:LEU:HD22 | 2.36 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:249:PHE:CD1 | 1:A:297:LEU:HD13 | 2.37 | 0.60 |
| 1:A:3971:MSE:HE1 | 1:A:3980:MSE:SE | 2.52 | 0.60 |
| 1:B:1762:MSE:HG2 | 1:B:1896:ILE:HA | 1.83 | 0.60 |
| 1:B:2145:PHE:HZ | 1:B:2185:MSE:HA | 1.66 | 0.60 |
| 1:B:2981:TRP:O | 1:B:2985:GLU:HB2 | 2.02 | 0.60 |
| 1:B:3444:ALA:HA | 1:B:3475:TYR:OH | 2.02 | 0.60 |
| 1:B:3571:PHE:O | 1:B:3575:LEU:CB | 2.49 | 0.60 |
| 1:A:2183:HIS:HE1 | 1:A:2237:ILE:HG21 | 1.67 | 0.59 |
| 1:A:2436:LEU:O | 1:A:2439:ILE:HG22 | 2.02 | 0.59 |
| 1:A:3498:TRP:HE1 | 1:A:3502:MSE:SE | 2.35 | 0.59 |
| 1:A:3572:ILE:O | 1:A:3575:LEU:HB2 | 2.01 | 0.59 |
| 1:A:3584:LEU:O | 1:A:3588:TRP:HB3 | 2.02 | 0.59 |
| 1:A:396:PHE:CD2 | 1:A:441:MSE:HG3 | 2.37 | 0.59 |
| 1:A:414:LEU:HA | 1:A:417:VAL:HB | 1.84 | 0.59 |
| 1:A:722:LYS:HB3 | 1:A:727:ALA:HA | 1.84 | 0.59 |
| 1:A:933:LEU:HD11 | 1:A:2795:GLN:OE1 | 2.02 | 0.59 |
| 1:B:1166:LEU:HB3 | 1:B:1170:LYS:NZ | 2.17 | 0.59 |
| 1:B:1569:THR:O | 1:B:1573:LYS:HB2 | 2.02 | 0.59 |
| 1:B:1750:LEU:O | 1:B:1754:GLN:HG3 | 2.02 | 0.59 |
| 1:B:18:THR:O | 1:B:22:ALA:CB | 2.49 | 0.59 |
| 1:B:3722:PHE:CE1 | 1:B:3740:ILE:HG12 | 2.23 | 0.59 |
| 1:B:913:ARG:HA | 1:B:916:GLU:CD | 2.23 | 0.59 |
| 1:A:1344:PHE:HA | 1:A:1347:THR:HB | 1.84 | 0.59 |
| 1:A:1438:GLY:O | 1:A:1441:ALA:HB2 | 2.01 | 0.59 |
| 1:A:1916:ILE:HG23 | 1:A:1920:TYR:CE1 | 2.36 | 0.59 |
| 1:A:2139:PRO:O | 1:A:2143:ARG:HD2 | 2.01 | 0.59 |
| 1:A:2352:HIS:HB2 | 1:A:2364:LEU:HD11 | 1.83 | 0.59 |
| 1:A:2549:LYS:NZ | 1:A:2557:LEU:HD22 | 2.11 | 0.59 |
| 1:A:3047:SER:HB2 | 1:A:3050:LYS:HE2 | 1.84 | 0.59 |
| 1:A:3435:ASP:O | 1:A:3439:LEU:HB3 | 2.02 | 0.59 |
| 1:A:3572:ILE:HA | 1:A:3575:LEU:HG | 1.82 | 0.59 |
| 1:A:3723:ASP:HB2 | 1:A:3741:ARG:HE | 1.67 | 0.59 |
| 1:B:2430:GLU:HG3 | 1:B:2465:PRO:CB | 2.32 | 0.59 |
| 1:B:850:GLU:OE2 | 1:B:854:ARG:NH2 | 2.34 | 0.59 |
| 1:B:977:ASP:HB3 | 1:B:981:ARG:H | 1.67 | 0.59 |
| 1:A:1651:LYS:O | 1:A:1654:GLN:HB2 | 2.02 | 0.59 |
| 1:A:2325:LEU:HG | 1:A:2329:TYR:CE2 | 2.37 | 0.59 |
| 1:A:393:LYS:HA | 1:A:396:PHE:HD1 | 1.67 | 0.59 |
| 1:A:3913:ILE:HD11 | 1:A:3984:MSE:HB3 | 1.83 | 0.59 |
| 1:A:3946:PHE:HE2 | 1:A:4048:LYS:HD2 | 1.68 | 0.59 |
| 1:A:913:ARG:CB | 1:A:934:LEU:HD12 | 2.32 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:980:THR:O | 1:A:984:TYR:HD1 | 1.85 | 0.59 |
| 1:B:1175:HIS:O | 1:B:1179:PRO:HD3 | 2.01 | 0.59 |
| 1:B:610:ALA:HA | 1:B:613:HIS:CE1 | 2.37 | 0.59 |
| 1:A:1029:CYS:SG | 1:A:1085:ILE:HG13 | 2.42 | 0.59 |
| 1:A:1142:HIS:C | 1:A:1144:SER:H | 2.05 | 0.59 |
| 1:A:1894:SER:HB2 | 1:A:1896:ILE:HG13 | 1.83 | 0.59 |
| 1:A:1996:VAL:HG21 | 1:A:2047:THR:OG1 | 2.02 | 0.59 |
| 1:A:2510:LEU:HG | 1:A:2522:ARG:HE | 1.68 | 0.59 |
| 1:A:3080:LEU:HB3 | 1:A:3102:TYR:CE1 | 2.37 | 0.59 |
| 1:A:3090:TYR:HB2 | 1:A:3099:ALA:HB2 | 1.84 | 0.59 |
| 1:A:3439:LEU:O | 1:A:3443:PRO:HD3 | 2.02 | 0.59 |
| 1:A:3583:LEU:HD13 | 1:A:3755:GLY:HA3 | 1.85 | 0.59 |
| 1:A:966:PHE:HB3 | 1:A:967:PRO:HD3 | 1.83 | 0.59 |
| 1:B:1005:ASP:OD1 | 1:B:1005:ASP:N | 2.34 | 0.59 |
| 1:B:108:LYS:HB3 | 1:B:138:PHE:CD1 | 2.37 | 0.59 |
| 1:B:2129:LEU:HD22 | 1:B:2144:LEU:HD11 | 1.83 | 0.59 |
| 1:B:2330:VAL:CG2 | 1:B:2335:ASN:HA | 2.28 | 0.59 |
| 1:B:2420:PHE:CZ | 1:B:2436:LEU:HB3 | 2.37 | 0.59 |
| 1:B:2542:LEU:CB | 1:B:2546:TYR:HE2 | 2.14 | 0.59 |
| 1:B:2886:GLN:CD | 1:B:2887:PRO:HD3 | 2.23 | 0.59 |
| 1:B:3333:THR:OG1 | 1:B:3385:LEU:HB3 | 2.01 | 0.59 |
| 1:B:3887:PHE:HE1 | 1:B:3900:LEU:HB3 | 1.67 | 0.59 |
| 2:S:217:UNK:HA | 2:S:220:MSE:SE | 2.52 | 0.59 |
| 1:A:136:GLN:HA | 1:A:139:ARG:HD3 | 1.84 | 0.59 |
| 1:A:2274:ILE:HG12 | 1:A:2314:GLU:HB3 | 1.83 | 0.59 |
| 1:A:2420:PHE:CZ | 1:A:2436:LEU:HB3 | 2.37 | 0.59 |
| 1:A:3811:THR:HG22 | 1:A:3929:MSE:SE | 2.53 | 0.59 |
| 1:A:4081:ALA:HA | 1:A:4113:ASP:OD2 | 2.02 | 0.59 |
| 1:B:1908:GLY:HA3 | 1:B:1952:ILE:HG13 | 1.84 | 0.59 |
| 1:B:232:CYS:HG | 1:B:275:PHE:HE1 | 1.50 | 0.59 |
| 1:B:3069:MSE:HA | 1:B:3072:GLU:HB3 | 1.84 | 0.59 |
| 1:B:3389:VAL:O | 1:B:3393:GLU:HG3 | 2.02 | 0.59 |
| 1:B:633:ILE:HG22 | 1:B:634:LEU:HD23 | 1.84 | 0.59 |
| 1:A:1416:GLU:O | 1:A:1420:ARG:HB2 | 2.03 | 0.59 |
| 1:A:1711:ARG:HB3 | 1:A:1739:TYR:HE1 | 1.68 | 0.59 |
| 1:A:1925:GLU:O | 1:A:1928:ALA:N | 2.32 | 0.59 |
| 1:A:2326:ILE:O | 1:A:2330:VAL:HB | 2.03 | 0.59 |
| 1:A:3156:PRO:HB2 | 1:A:3197:LEU:HD12 | 1.84 | 0.59 |
| 1:A:3581:PRO:O | 1:A:3585:PHE:HD1 | 1.85 | 0.59 |
| 1:B:1142:HIS:C | 1:B:1144:SER:H | 2.05 | 0.59 |
| 1:B:1368:LEU:HA | 1:B:1371:VAL:HG12 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:172:GLU:OE2 | 1:B:264:ARG:NH2 | 2.36 | 0.59 |
| 1:B:2239:LYS:O | 1:B:2242:VAL:HB | 2.02 | 0.59 |
| 1:B:2281:MSE:SE | 1:B:2286:PRO:HB3 | 2.52 | 0.59 |
| 1:B:2501:LEU:O | 1:B:2505:VAL:HG23 | 2.02 | 0.59 |
| 1:B:2921:LEU:HD12 | 1:B:2922:ARG:N | 2.17 | 0.59 |
| 1:B:3592:VAL:HA | 1:B:3609:MSE:SE | 2.53 | 0.59 |
| 1:A:1267:TYR:O | 1:A:1271:ILE:HG13 | 2.03 | 0.59 |
| 1:A:1467:ILE:HG13 | 1:A:1468:LEU:HG | 1.84 | 0.59 |
| 1:A:1962:TYR:O | 1:A:1965:PHE:N | 2.35 | 0.59 |
| 1:A:2299:TYR:O | 1:A:2302:ALA:N | 2.35 | 0.59 |
| 1:A:2319:ALA:O | 1:A:2323:LEU:HD12 | 2.03 | 0.59 |
| 1:A:2851:PHE:HA | 1:A:2854:PHE:CE2 | 2.38 | 0.59 |
| 1:A:2957:LEU:HB3 | 1:A:3989:ARG:HH12 | 1.63 | 0.59 |
| 1:A:253:LEU:HD21 | 1:A:297:LEU:HA | 1.84 | 0.59 |
| 1:A:3031:TRP:CE3 | 1:A:3034:PRO:HD3 | 2.37 | 0.59 |
| 1:A:3492:CYS:O | 1:A:3495:PHE:CB | 2.50 | 0.59 |
| 1:A:3612:ARG:HD3 | 1:A:3799:ARG:NH2 | 2.17 | 0.59 |
| 1:A:3963:LEU:HD12 | 1:A:3967:PHE:HZ | 1.66 | 0.59 |
| 1:A:940:PHE:CE1 | 1:A:2791:ILE:HG21 | 2.37 | 0.59 |
| 1:B:1594:SER:OG | 1:B:1683:LYS:HD3 | 2.02 | 0.59 |
| 1:B:2040:MSE:HA | 1:B:2043:PHE:HD1 | 1.68 | 0.59 |
| 1:B:2136:PRO:C | 1:B:2139:PRO:HD2 | 2.22 | 0.59 |
| 1:B:2144:LEU:HB3 | 1:B:2148:LYS:CE | 2.33 | 0.59 |
| 1:B:2291:GLN:O | 1:B:2293:GLY:N | 2.35 | 0.59 |
| 1:B:2638:UNK:O | 1:B:2790:LEU:HD13 | 2.02 | 0.59 |
| 1:B:3000:ASP:O | 1:B:3004:HIS:N | 2.35 | 0.59 |
| 1:B:327:VAL:HG13 | 1:B:338:LEU:HD13 | 1.84 | 0.59 |
| 1:A:2270:ASN:O | 1:A:2274:ILE:HG23 | 2.03 | 0.59 |
| 1:A:2543:ASN:HA | 1:A:2546:TYR:HD2 | 1.67 | 0.59 |
| 1:A:2960:GLU:CD | 1:A:3289:ARG:HH12 | 2.05 | 0.59 |
| 1:B:1655:ILE:HG12 | 1:B:1681:ASP:HB3 | 1.83 | 0.59 |
| 1:B:179:GLY:HA3 | 1:B:229:SER:HB3 | 1.84 | 0.59 |
| 1:B:2419:ASP:O | 1:B:2422:GLN:HB3 | 2.02 | 0.59 |
| 1:B:2645:UNK:HA | 1:B:2649:UNK:C | 2.33 | 0.59 |
| 1:B:270:ALA:O | 1:B:274:LEU:HG | 2.03 | 0.59 |
| 1:B:3273:LEU:O | 1:B:3277:VAL:HG12 | 2.03 | 0.59 |
| 1:B:4062:ASP:O | 1:B:4065:LEU:HG | 2.03 | 0.59 |
| 1:B:886:TRP:CH2 | 1:B:892:LEU:HD13 | 2.37 | 0.59 |
| 1:A:1060:PHE:O | 1:A:1064:TYR:HD2 | 1.85 | 0.59 |
| 1:A:1437:TYR:O | 1:A:1439:PRO:HD2 | 2.02 | 0.59 |
| 1:A:1571:LEU:HD13 | 1:A:1599:GLY:O | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1647:ALA:O | 1:A:1651:LYS:HE3 | 2.02 | 0.59 |
| 1:A:194:GLU:HA | 1:A:197:PHE:HD2 | 1.68 | 0.59 |
| 1:A:242:PRO:O | 1:A:246:ARG:CB | 2.50 | 0.59 |
| 1:A:2546:TYR:CE1 | 1:A:2558:ALA:HB2 | 2.38 | 0.59 |
| 1:A:2868:LEU:O | 1:A:2872:ASP:HB2 | 2.03 | 0.59 |
| 1:A:3269:ARG:HH11 | 1:A:3312:VAL:HA | 1.66 | 0.59 |
| 1:A:3638:LYS:O | 1:A:3641:ASP:N | 2.36 | 0.59 |
| 1:A:3811:THR:OG1 | 1:A:3811:THR:O | 2.19 | 0.59 |
| 1:A:4006:VAL:HA | 1:A:4012:ASP:OD2 | 2.03 | 0.59 |
| 1:A:980:THR:HG23 | 1:A:984:TYR:CE1 | 2.34 | 0.59 |
| 1:B:1018:VAL:HB | 1:B:1074:LYS:CB | 2.28 | 0.59 |
| 1:B:437:HIS:HA | 1:B:1814:PHE:CZ | 2.38 | 0.59 |
| 1:B:2185:MSE:O | 1:B:2189:ILE:HG13 | 2.02 | 0.59 |
| 1:B:197:PHE:CZ | 1:B:230:LEU:HD22 | 2.37 | 0.59 |
| 1:B:3753:LYS:HD3 | 1:B:3758:LEU:HD21 | 1.85 | 0.59 |
| 1:B:3909:ALA:HB2 | 1:B:3980:MSE:HE2 | 1.83 | 0.59 |
| 1:B:390:GLN:NE2 | 1:B:1723:PRO:HG2 | 2.18 | 0.59 |
| 1:B:392:CYS:HA | 1:B:395:MSE:HB2 | 1.83 | 0.59 |
| 1:B:767:GLU:HG2 | 1:B:846:ILE:O | 2.03 | 0.59 |
| 1:A:1866:GLN:O | 1:A:1870:LYS:HB2 | 2.03 | 0.59 |
| 1:A:1992:VAL:HG21 | 1:A:2044:ASP:OD1 | 2.03 | 0.59 |
| 1:A:2330:VAL:CG2 | 1:A:2335:ASN:HA | 2.31 | 0.59 |
| 1:A:3076:ALA:HB1 | 1:A:3080:LEU:HD11 | 1.85 | 0.59 |
| 1:A:3324:ARG:O | 1:A:3328:ILE:HG13 | 2.02 | 0.59 |
| 1:A:3505:LEU:HB3 | 1:A:3510:GLN:OE1 | 2.03 | 0.59 |
| 1:B:1016:GLY:O | 1:B:1019:ASP:HB2 | 2.03 | 0.59 |
| 1:B:1084:ASN:CG | 1:B:1134:LEU:HD11 | 2.22 | 0.59 |
| 1:B:3908:HIS:O | 1:B:3911:ILE:HG12 | 2.03 | 0.59 |
| 1:A:1736:PHE:O | 1:A:1740:VAL:HG23 | 2.02 | 0.58 |
| 1:A:2462:VAL:CB | 1:A:2473:MSE:SE | 3.00 | 0.58 |
| 1:A:3585:PHE:HE2 | 1:A:3617:LEU:HD11 | 1.68 | 0.58 |
| 1:A:535:LEU:HD13 | 1:A:626:LEU:HD21 | 1.84 | 0.58 |
| 1:A:982:GLN:O | 1:A:986:PRO:HD3 | 2.03 | 0.58 |
| 1:B:3149:GLY:HA3 | 1:B:3196:LYS:HE3 | 1.84 | 0.58 |
| 1:B:3351:ILE:HG23 | 1:B:3355:LYS:HE2 | 1.84 | 0.58 |
| 1:B:3503:VAL:HG22 | 1:B:3539:SER:HB2 | 1.84 | 0.58 |
| 1:B:3516:HIS:CG | 1:B:3517:SER:N | 2.70 | 0.58 |
| 1:B:673:THR:HG22 | 1:B:704:PHE:HE1 | 1.68 | 0.58 |
| 1:B:806:SER:O | 1:B:809:THR:N | 2.36 | 0.58 |
| 1:A:1102:GLU:HA | 1:A:1150:LYS:NZ | 2.18 | 0.58 |
| 1:A:1330:TYR:O | 1:A:1334:LYS:HG2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2058:ASP:H | 1:A:2061:PRO:HG2 | 1.68 | 0.58 |
| 1:A:2221:LYS:O | 1:A:2225:HIS:ND1 | 2.36 | 0.58 |
| 1:A:2560:ASN:OD1 | 1:A:2800:ARG:NH1 | 2.36 | 0.58 |
| 1:A:3274:VAL:O | 1:A:3277:VAL:HG22 | 2.04 | 0.58 |
| 1:A:3769:GLN:HA | 1:A:3772:ASN:OD1 | 2.03 | 0.58 |
| 1:A:3813:LYS:CE | 1:A:3926:ASN:HB2 | 2.31 | 0.58 |
| 1:A:3872:ARG:NH1 | 1:A:3965:ARG:HH12 | 1.98 | 0.58 |
| 1:A:2936:TYR:CD2 | 1:A:3979:LEU:HD21 | 2.38 | 0.58 |
| 1:A:437:HIS:CD2 | 1:A:438:LEU:N | 2.70 | 0.58 |
| 1:B:1036:PHE:CD1 | 1:B:1059:LEU:HD11 | 2.38 | 0.58 |
| 1:B:111:CYS:HB2 | 1:B:134:LEU:HB3 | 1.86 | 0.58 |
| 1:B:1648:LEU:HD13 | 1:B:1688:LEU:HD21 | 1.85 | 0.58 |
| 1:B:1737:ASN:C | 1:B:1739:TYR:H | 2.06 | 0.58 |
| 1:B:176:GLU:HG2 | 1:B:225:LYS:HD3 | 1.83 | 0.58 |
| 1:B:2145:PHE:CZ | 1:B:2185:MSE:HA | 2.39 | 0.58 |
| 1:B:3190:LEU:HD21 | 1:B:3235:LYS:HG2 | 1.85 | 0.58 |
| 1:B:3583:LEU:HD21 | 1:B:3733:ARG:HD3 | 1.84 | 0.58 |
| 1:B:3637:GLY:O | 1:B:3641:ASP:HB3 | 2.03 | 0.58 |
| 1:B:738:HIS:ND1 | 1:B:745:VAL:HG13 | 2.18 | 0.58 |
| 1:A:1386:ILE:HA | 1:A:1389:VAL:HB | 1.85 | 0.58 |
| 1:A:1454:ALA:O | 1:A:1457:GLN:HB2 | 2.03 | 0.58 |
| 1:A:2378:PHE:O | 1:A:2382:VAL:HG22 | 2.02 | 0.58 |
| 1:A:2942:ILE:HD12 | 1:A:2987:THR:HG22 | 1.85 | 0.58 |
| 1:A:3505:LEU:HA | 1:A:3509:ASP:HB2 | 1.84 | 0.58 |
| 1:A:368:LEU:CD2 | 1:A:384:MSE:HB2 | 2.18 | 0.58 |
| 1:B:143:LEU:O | 1:B:144:MSE:HB2 | 2.03 | 0.58 |
| 1:B:1918:LEU:HD13 | 1:B:1958:GLU:HB3 | 1.85 | 0.58 |
| 1:B:2003:LYS:O | 1:B:2007:ILE:HG13 | 2.03 | 0.58 |
| 1:B:2157:PHE:HA | 1:B:2160:TYR:CD2 | 2.38 | 0.58 |
| 1:B:2182:ILE:O | 1:B:2186:VAL:HG12 | 2.03 | 0.58 |
| 1:B:2775:TYR:HB3 | 1:B:2776:ARG:CZ | 2.33 | 0.58 |
| 1:B:2936:TYR:HA | 1:B:2939:LEU:HB2 | 1.85 | 0.58 |
| 1:B:321:LYS:O | 1:B:325:ASN:ND2 | 2.26 | 0.58 |
| 1:B:3427:GLU:HB3 | 1:B:3439:LEU:HD22 | 1.85 | 0.58 |
| 1:B:435:LEU:O | 1:B:439:VAL:HG23 | 2.03 | 0.58 |
| 1:B:535:LEU:HD21 | 1:B:622:ALA:O | 2.03 | 0.58 |
| 1:B:752:LEU:HA | 1:B:755:ALA:HB3 | 1.84 | 0.58 |
| 1:A:1296:PHE:HD1 | 1:A:1299:GLU:OE2 | 1.86 | 0.58 |
| 1:A:1711:ARG:HB3 | 1:A:1739:TYR:CE1 | 2.37 | 0.58 |
| 1:A:1919:CYS:O | 1:A:1923:PHE:CB | 2.50 | 0.58 |
| 1:A:2884:LEU:HD22 | 1:A:3895:GLU:OE2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3099:ALA:O | 1:A:3103:ILE:HB | 2.02 | 0.58 |
| 1:A:3454:LEU:HA | 1:A:3456:LEU:HD12 | 1.85 | 0.58 |
| 1:A:446:PHE:HA | 1:A:449:TYR:CE2 | 2.39 | 0.58 |
| 1:A:613:HIS:ND1 | 1:A:614:PRO:HD3 | 2.18 | 0.58 |
| 1:A:633:ILE:HG22 | 1:A:637:LYS:HG2 | 1.86 | 0.58 |
| 1:A:727:ALA:O | 1:A:731:THR:HG23 | 2.03 | 0.58 |
| 1:A:985:GLU:HB3 | 1:A:986:PRO:HD3 | 1.84 | 0.58 |
| 1:B:1963:GLN:NE2 | 1:B:1995:GLU:HG2 | 2.18 | 0.58 |
| 1:B:2070:GLU:HA | 1:B:2071:GLN:HB2 | 1.85 | 0.58 |
| 1:B:2913:LYS:HG3 | 1:B:2914:ALA:N | 2.18 | 0.58 |
| 1:B:571:SER:O | 1:B:605:THR:OG1 | 2.19 | 0.58 |
| 1:A:1386:ILE:HB | 1:A:1391:VAL:HG21 | 1.84 | 0.58 |
| 1:A:1959:LEU:HD13 | 1:A:1998:MSE:HE3 | 1.84 | 0.58 |
| 1:A:2420:PHE:CE1 | 1:A:2436:LEU:HB3 | 2.38 | 0.58 |
| 1:A:3092:LEU:HD22 | 1:A:3192:LYS:HE2 | 1.86 | 0.58 |
| 1:A:3587:ASP:HB3 | 1:A:4022:LYS:NZ | 2.19 | 0.58 |
| 1:B:971:ARG:HD2 | 1:B:1024:THR:OG1 | 2.04 | 0.58 |
| 1:B:1583:MSE:HE3 | 1:B:1643:MSE:CB | 2.33 | 0.58 |
| 1:B:503:SER:O | 1:B:507:ASP:HB2 | 2.02 | 0.58 |
| 1:B:713:GLU:O | 1:B:717:LYS:HG2 | 2.04 | 0.58 |
| 1:B:722:LYS:HD2 | 1:B:730:LEU:HB2 | 1.85 | 0.58 |
| 1:A:1648:LEU:HD22 | 1:A:1684:LEU:HD22 | 1.86 | 0.58 |
| 1:A:2275:GLN:O | 1:A:2279:ILE:HG12 | 2.03 | 0.58 |
| 1:A:2962:ARG:NH2 | 1:A:3006:ALA:HB1 | 2.18 | 0.58 |
| 1:A:3092:LEU:HD22 | 1:A:3192:LYS:CE | 2.33 | 0.58 |
| 1:A:3339:ASN:O | 1:A:3341:LEU:N | 2.36 | 0.58 |
| 1:A:450:SER:O | 1:A:454:GLN:HB2 | 2.04 | 0.58 |
| 1:A:566:ASP:O | 1:A:570:LYS:NZ | 2.36 | 0.58 |
| 1:A:491:CYS:SG | 1:A:615:ALA:HB2 | 2.43 | 0.58 |
| 1:B:1651:LYS:HB2 | 1:B:1684:LEU:CD1 | 2.29 | 0.58 |
| 1:B:2011:ALA:HB3 | 1:B:2014:ALA:CB | 2.29 | 0.58 |
| 1:B:2126:MSE:HE2 | 1:B:2156:VAL:HG22 | 1.86 | 0.58 |
| 1:B:2167:PRO:O | 1:B:2171:LEU:CB | 2.33 | 0.58 |
| 1:B:2900:LEU:HD12 | 1:B:2905:LEU:HD11 | 1.84 | 0.58 |
| 1:B:572:VAL:HG13 | 1:B:573:LEU:H | 1.67 | 0.58 |
| 1:A:1059:LEU:O | 1:A:1063:LEU:HG | 2.03 | 0.58 |
| 1:A:1101:PHE:CD2 | 1:A:1138:ILE:HG12 | 2.38 | 0.58 |
| 1:A:1327:GLY:O | 1:A:1330:TYR:HB3 | 2.04 | 0.58 |
| 1:A:1594:SER:HA | 1:A:1687:HIS:HE1 | 1.69 | 0.58 |
| 1:A:205:LYS:HA | 1:A:208:MSE:HG2 | 1.84 | 0.58 |
| 1:A:2085:MSE:SE | 1:A:2088:LEU:HD22 | 2.54 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2140:LEU:HA | 1:A:2143:ARG:HD3 | 1.86 | 0.58 |
| 1:A:2454:LEU:O | 1:A:2457:PRO:HD2 | 2.03 | 0.58 |
| 1:A:3910:LEU:O | 1:A:3914:SER:OG | 2.15 | 0.58 |
| 1:A:509:ARG:HD2 | 1:A:655:LEU:HD13 | 1.84 | 0.58 |
| 1:B:1063:LEU:HD13 | 1:B:1082:PHE:CE1 | 2.38 | 0.58 |
| 1:B:1086:TYR:HE2 | 1:B:1090:ARG:HE | 1.51 | 0.58 |
| 1:B:1644:ALA:HA | 1:B:1648:LEU:HD12 | 1.83 | 0.58 |
| 1:B:1925:GLU:OE2 | 1:B:1959:LEU:HG | 2.03 | 0.58 |
| 1:B:204:LEU:HD13 | 1:B:223:CYS:HB2 | 1.84 | 0.58 |
| 1:B:2358:ASP:HB2 | 1:B:2396:LEU:CD2 | 2.30 | 0.58 |
| 1:B:3463:LEU:HD13 | 1:B:4000:ASN:HB2 | 1.86 | 0.58 |
| 1:B:410:MSE:HE1 | 1:B:445:SER:HB3 | 1.85 | 0.58 |
| 1:B:446:PHE:CD1 | 1:B:447:PRO:HD3 | 2.38 | 0.58 |
| 1:B:903:PRO:HG2 | 1:B:2811:SER:HB2 | 1.85 | 0.58 |
| 1:A:1074:LYS:O | 1:A:1075:ARG:HG2 | 2.04 | 0.58 |
| 1:A:252:VAL:HG21 | 1:A:265:TYR:HB2 | 1.85 | 0.58 |
| 1:A:2920:VAL:HB | 1:A:3036:TYR:OH | 2.04 | 0.58 |
| 1:A:3454:LEU:O | 1:A:3494:GLN:NE2 | 2.34 | 0.58 |
| 1:A:3464:LYS:O | 1:A:3468:LEU:HG | 2.03 | 0.58 |
| 1:A:3525:TYR:O | 1:A:3529:ILE:HB | 2.03 | 0.58 |
| 1:A:3631:LYS:HE2 | 1:A:3634:GLN:HG2 | 1.86 | 0.58 |
| 1:A:3879:PRO:HA | 1:A:3882:LEU:HB2 | 1.86 | 0.58 |
| 1:A:617:PRO:O | 1:A:620:PHE:N | 2.36 | 0.58 |
| 1:B:1163:LEU:HA | 1:B:1260:LEU:HD21 | 1.84 | 0.58 |
| 1:B:1606:ARG:HH11 | 1:B:1806:ARG:HB3 | 1.69 | 0.58 |
| 1:B:175:TYR:HE1 | 1:B:200:PHE:HB3 | 1.68 | 0.58 |
| 1:B:2167:PRO:HA | 1:B:2171:LEU:HD13 | 1.86 | 0.58 |
| 1:B:419:SER:O | 1:B:422:LEU:HB2 | 2.04 | 0.58 |
| 1:A:2338:GLU:O | 1:A:2338:GLU:HG2 | 2.03 | 0.58 |
| 1:A:3047:SER:O | 1:A:3050:LYS:HG3 | 2.04 | 0.58 |
| 1:A:3322:ALA:O | 1:A:3325:ASP:HB3 | 2.04 | 0.58 |
| 1:A:352:VAL:HA | 1:A:355:ASN:O | 2.03 | 0.58 |
| 1:A:3772:ASN:O | 1:A:3787:GLN:NE2 | 2.24 | 0.58 |
| 1:A:549:ALA:O | 1:A:553:VAL:HG23 | 2.03 | 0.58 |
| 1:A:870:LEU:HD21 | 1:A:3129:LEU:HD11 | 1.86 | 0.58 |
| 1:B:2040:MSE:HA | 1:B:2043:PHE:CD1 | 2.38 | 0.58 |
| 1:B:2481:HIS:O | 1:B:2485:ARG:N | 2.37 | 0.58 |
| 1:B:2477:LEU:CB | 1:B:2506:LEU:HD21 | 2.34 | 0.58 |
| 1:B:3571:PHE:O | 1:B:3575:LEU:HB2 | 2.03 | 0.58 |
| 1:B:3974:MSE:HB3 | 1:B:3976:GLU:HB3 | 1.86 | 0.58 |
| 1:B:510:ALA:O | 1:B:513:GLU:HB2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1010:LEU:HA | 1:A:1013:ILE:CG1 | 2.30 | 0.58 |
| 1:A:1521:PHE:HB2 | 1:A:1589:ASN:OD1 | 2.04 | 0.58 |
| 1:A:2440:TYR:O | 1:A:2443:MSE:HE2 | 2.04 | 0.58 |
| 1:A:2430:GLU:HG3 | 1:A:2465:PRO:HB3 | 1.86 | 0.58 |
| 1:A:435:LEU:HD11 | 1:A:475:LEU:HD21 | 1.85 | 0.58 |
| 1:A:627:VAL:HG12 | 1:A:628:GLU:N | 2.17 | 0.58 |
| 1:A:806:SER:O | 1:A:809:THR:N | 2.26 | 0.58 |
| 1:B:1145:LEU:HB2 | 1:B:1149:LYS:HZ3 | 1.66 | 0.58 |
| 1:B:1883:ARG:HE | 1:B:1923:PHE:HZ | 1.50 | 0.58 |
| 1:B:3699:LEU:HB3 | 1:B:3718:ARG:HH12 | 1.69 | 0.58 |
| 1:B:669:LEU:O | 1:B:671:SER:N | 2.36 | 0.58 |
| 1:B:852:ARG:O | 1:B:855:VAL:HB | 2.04 | 0.58 |
| 1:A:2349:LEU:O | 1:A:2353:GLN:HG3 | 2.02 | 0.57 |
| 1:A:2440:TYR:OH | 1:A:2455:LEU:HG | 2.04 | 0.57 |
| 1:A:2474:TYR:HE2 | 1:A:2518:GLN:HB3 | 1.69 | 0.57 |
| 1:A:2993:PHE:O | 1:A:2997:ALA:N | 2.25 | 0.57 |
| 1:A:3451:LEU:HG | 1:A:3486:GLU:OE1 | 2.04 | 0.57 |
| 1:A:3649:SER:HA | 1:A:3652:LEU:HG | 1.86 | 0.57 |
| 1:A:3855:TYR:HB3 | 1:A:4074:PHE:HZ | 1.66 | 0.57 |
| 1:A:3944:HIS:CG | 1:A:3949:ALA:HA | 2.39 | 0.57 |
| 1:A:488:ILE:O | 1:A:612:LEU:HB2 | 2.04 | 0.57 |
| 1:A:852:ARG:O | 1:A:855:VAL:HB | 2.04 | 0.57 |
| 1:B:647:TYR:HE1 | 1:B:1389:VAL:HA | 1.68 | 0.57 |
| 1:B:1810:PRO:O | 1:B:1812:LEU:HG | 2.03 | 0.57 |
| 1:B:2568:MSE:HG3 | 1:B:2569:SER:H | 1.69 | 0.57 |
| 1:B:3104:GLN:HA | 1:B:3107:ILE:HD12 | 1.86 | 0.57 |
| 1:B:3464:LYS:HE3 | 1:B:3468:LEU:HD21 | 1.86 | 0.57 |
| 1:B:3501:HIS:HA | 1:B:4008:GLU:OE2 | 2.04 | 0.57 |
| 1:B:3981:TYR:CE1 | 1:B:4104:VAL:HB | 2.39 | 0.57 |
| 1:A:1139:GLU:HG3 | 1:A:1175:HIS:NE2 | 2.18 | 0.57 |
| 1:A:1400:VAL:O | 1:A:1404:LYS:HB2 | 2.04 | 0.57 |
| 1:A:1679:LEU:O | 1:A:1683:LYS:HG3 | 2.04 | 0.57 |
| 1:A:2065:ARG:HD3 | 1:A:2100:LEU:HD11 | 1.86 | 0.57 |
| 1:A:2495:SER:O | 1:A:2498:ILE:HB | 2.04 | 0.57 |
| 1:A:2538:ARG:HH11 | 1:A:2565:MSE:CB | 2.17 | 0.57 |
| 1:A:2782:ASP:HA | 1:A:2786:LYS:CB | 2.34 | 0.57 |
| 1:A:2950:LYS:HE2 | 1:A:4105:LYS:NZ | 2.18 | 0.57 |
| 1:B:1761:LEU:O | 1:B:1895:LYS:HB2 | 2.04 | 0.57 |
| 1:B:205:LYS:HA | 1:B:208:MSE:HE3 | 1.86 | 0.57 |
| 1:B:2323:LEU:HD21 | 1:B:2345:VAL:HG21 | 1.86 | 0.57 |
| 1:B:2374:LEU:CD1 | 1:B:2377:ARG:HB2 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:241:ASP:HB3 | 1:B:282:PHE:CE2 | 2.39 | 0.57 |
| 1:B:2837:LEU:HD12 | 1:B:2867:ALA:HB3 | 1.86 | 0.57 |
| 1:B:571:SER:HB2 | 1:B:606:SER:H | 1.68 | 0.57 |
| 1:B:781:ASP:OD2 | 1:B:862:LEU:HD21 | 2.03 | 0.57 |
| 1:B:966:PHE:O | 1:B:969:LEU:HB3 | 2.03 | 0.57 |
| 1:B:986:PRO:O | 1:B:989:MSE:N | 2.37 | 0.57 |
| 1:B:997:ASN:HA | 1:B:1042:LYS:HD3 | 1.86 | 0.57 |
| 1:A:1952:ILE:HG23 | 1:A:1953:CYS:O | 2.04 | 0.57 |
| 1:A:2286:PRO:HD3 | 1:A:2325:LEU:HD23 | 1.85 | 0.57 |
| 1:A:2809:PHE:HB3 | 1:A:2859:GLN:CD | 2.24 | 0.57 |
| 1:A:3287:ARG:NH1 | 1:A:3331:GLY:HA3 | 2.19 | 0.57 |
| 1:A:3496:ILE:O | 1:A:3498:TRP:N | 2.37 | 0.57 |
| 1:A:3686:TRP:CZ3 | 1:A:3687:MSE:HG3 | 2.39 | 0.57 |
| 1:A:75:SER:O | 1:A:77:GLU:N | 2.36 | 0.57 |
| 1:B:2094:MSE:HE1 | 1:B:2143:ARG:HA | 1.85 | 0.57 |
| 1:B:2927:ALA:HB2 | 1:B:2930:TYR:HD2 | 1.68 | 0.57 |
| 1:B:3181:ASP:HA | 1:B:3184:THR:HG23 | 1.86 | 0.57 |
| 1:B:3496:ILE:HG23 | 1:B:3499:ILE:HD11 | 1.86 | 0.57 |
| 1:B:3871:PHE:HB3 | 1:B:4127:TRP:CD1 | 2.39 | 0.57 |
| 1:B:450:SER:O | 1:B:454:GLN:HB2 | 2.03 | 0.57 |
| 1:B:2366:LYS:NZ | 2:S:101:UNK:HA | 2.19 | 0.57 |
| 1:A:1063:LEU:HD13 | 1:A:1082:PHE:CE1 | 2.39 | 0.57 |
| 1:A:1655:ILE:HG12 | 1:A:1677:SER:O | 2.05 | 0.57 |
| 1:A:1606:ARG:HA | 1:A:1806:ARG:HD3 | 1.87 | 0.57 |
| 1:A:205:LYS:NZ | 1:A:243:GLN:OE1 | 2.25 | 0.57 |
| 1:A:2562:LEU:O | 1:A:2566:THR:HG22 | 2.04 | 0.57 |
| 1:A:2960:GLU:HG2 | 1:A:3252:PHE:CG | 2.39 | 0.57 |
| 1:A:3034:PRO:O | 1:A:3038:GLU:HB3 | 2.05 | 0.57 |
| 1:A:368:LEU:HA | 1:A:372:PRO:HG2 | 1.86 | 0.57 |
| 1:A:756:PHE:O | 1:A:759:GLY:N | 2.36 | 0.57 |
| 1:A:871:LEU:HD21 | 1:A:3122:HIS:CE1 | 2.39 | 0.57 |
| 1:A:987:LEU:O | 1:A:991:LEU:HD13 | 2.05 | 0.57 |
| 1:B:1000:LYS:O | 1:B:1003:SER:N | 2.30 | 0.57 |
| 1:B:1090:ARG:HH22 | 1:B:1096:VAL:C | 2.07 | 0.57 |
| 1:B:1270:PHE:CZ | 1:B:1347:THR:HB | 2.38 | 0.57 |
| 1:B:1923:PHE:CE2 | 1:B:1927:MSE:HE1 | 2.40 | 0.57 |
| 1:B:1976:LEU:HD13 | 1:B:2031:LEU:CD2 | 2.34 | 0.57 |
| 1:B:2085:MSE:O | 1:B:2089:ASN:ND2 | 2.37 | 0.57 |
| 1:B:16:GLN:O | 1:B:20:SER:OG | 2.21 | 0.57 |
| 1:B:2886:GLN:OE1 | 1:B:2921:LEU:HB2 | 2.03 | 0.57 |
| 1:B:3174:ASP:H | 1:B:3175:PRO:HD2 | 1.67 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3568:ILE:O | 1:B:3571:PHE:N | 2.38 | 0.57 |
| 1:B:358:GLU:HA | 1:B:1858:LEU:HD22 | 1.85 | 0.57 |
| 1:B:473:PRO:CA | 1:B:476:ARG:HH22 | 2.12 | 0.57 |
| 1:B:886:TRP:HD1 | 1:B:889:GLU:N | 2.02 | 0.57 |
| 1:A:131:LEU:O | 1:A:135:LEU:HG | 2.05 | 0.57 |
| 1:A:2227:LYS:HZ1 | 1:A:2232:ARG:HB3 | 1.69 | 0.57 |
| 1:A:2503:LYS:O | 1:A:2507:ILE:HB | 2.04 | 0.57 |
| 1:A:805:LEU:CD2 | 1:A:3125:ARG:NH1 | 2.68 | 0.57 |
| 1:A:373:CYS:O | 1:A:423:TYR:OH | 2.20 | 0.57 |
| 1:A:4057:ALA:HB2 | 1:A:4090:ARG:O | 2.04 | 0.57 |
| 1:B:1238:GLN:HE22 | 1:B:1297:PHE:HD1 | 1.51 | 0.57 |
| 1:B:1632:TRP:HA | 1:B:1635:LYS:HD2 | 1.85 | 0.57 |
| 1:B:2190:VAL:O | 1:B:2193:ILE:HG22 | 2.04 | 0.57 |
| 1:B:2210:VAL:HG13 | 1:B:2211:LEU:H | 1.70 | 0.57 |
| 1:B:2321:GLU:O | 1:B:2324:GLY:N | 2.36 | 0.57 |
| 1:B:2555:LEU:HB2 | 1:B:2809:PHE:CE1 | 2.40 | 0.57 |
| 1:B:3767:LEU:O | 1:B:3771:MSE:HG3 | 2.04 | 0.57 |
| 1:B:3765:GLU:O | 1:B:3768:PHE:HB2 | 2.05 | 0.57 |
| 1:B:575:ILE:HD13 | 1:B:603:ILE:HB | 1.86 | 0.57 |
| 1:B:923:ASP:O | 1:B:927:LYS:HE2 | 2.03 | 0.57 |
| 1:A:2913:LYS:HG3 | 1:A:2914:ALA:N | 2.19 | 0.57 |
| 1:A:4027:TRP:HB3 | 1:A:4031:ILE:HD11 | 1.85 | 0.57 |
| 1:A:409:GLN:HG3 | 1:A:413:PHE:CZ | 2.39 | 0.57 |
| 1:A:414:LEU:HD22 | 1:A:442:GLN:HG2 | 1.85 | 0.57 |
| 1:A:704:PHE:HA | 1:A:707:PHE:CD1 | 2.39 | 0.57 |
| 1:A:797:ASP:HA | 1:A:800:LEU:HD12 | 1.86 | 0.57 |
| 1:B:1715:GLU:HA | 1:B:1718:ILE:HB | 1.85 | 0.57 |
| 1:B:2562:LEU:O | 1:B:2566:THR:HG22 | 2.04 | 0.57 |
| 1:B:3817:LEU:HA | 1:B:3820:MSE:HE3 | 1.87 | 0.57 |
| 1:B:610:ALA:HA | 1:B:613:HIS:ND1 | 2.19 | 0.57 |
| 1:A:2157:PHE:CZ | 1:A:2203:THR:HB | 2.40 | 0.57 |
| 1:A:2196:TRP:CG | 1:A:2199:LEU:HD11 | 2.39 | 0.57 |
| 1:A:2349:LEU:HD23 | 1:A:2364:LEU:HD22 | 1.86 | 0.57 |
| 1:A:737:PRO:O | 1:A:741:ILE:HG12 | 2.04 | 0.57 |
| 1:A:968:VAL:CG2 | 1:A:971:ARG:HD3 | 2.33 | 0.57 |
| 1:B:1681:ASP:HB2 | 1:B:1717:LEU:HD22 | 1.86 | 0.57 |
| 1:B:361:ILE:HD13 | 1:B:1858:LEU:HD23 | 1.86 | 0.57 |
| 1:B:2216:LEU:HD13 | 1:B:2249:LEU:HD21 | 1.85 | 0.57 |
| 1:B:2289:ASP:O | 1:B:2292:CYS:N | 2.24 | 0.57 |
| 1:B:262:LEU:HD22 | 1:B:306:VAL:HG12 | 1.86 | 0.57 |
| 1:B:680:ILE:HG12 | 1:B:701:TYR:HD2 | 1.69 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:798:GLY:HA2 | 1:B:873:VAL:HG11 | 1.87 | 0.57 |
| 1:B:969:LEU:O | 1:B:973:ALA:HB3 | 2.05 | 0.57 |
| 1:A:1982:ILE:O | 1:A:1986:ARG:HB2 | 2.04 | 0.57 |
| 1:A:182:GLY:O | 1:A:233:ASN:ND2 | 2.36 | 0.57 |
| 1:A:257:ARG:H | 1:A:258:PRO:CD | 2.17 | 0.57 |
| 1:A:3907:SER:CB | 1:A:3937:VAL:H | 2.17 | 0.57 |
| 1:A:567:GLU:HB3 | 1:A:606:SER:HB3 | 1.87 | 0.57 |
| 1:A:585:ILE:HG22 | 1:A:586:GLN:H | 1.68 | 0.57 |
| 1:B:1216:GLY:HA3 | 1:B:1271:ILE:CG2 | 2.35 | 0.57 |
| 1:B:2319:ALA:O | 1:B:2323:LEU:HD12 | 2.04 | 0.57 |
| 1:B:2801:ASP:HB2 | 1:B:2802:PRO:CD | 2.35 | 0.57 |
| 1:B:3267:LYS:N | 1:B:3271:ASP:OD2 | 2.37 | 0.57 |
| 1:B:3771:MSE:HE1 | 1:B:3917:ILE:HG21 | 1.85 | 0.57 |
| 1:B:990:GLN:HG3 | 1:B:2776:ARG:NH1 | 2.19 | 0.57 |
| 1:A:1635:LYS:O | 1:A:1639:LEU:HG | 2.05 | 0.57 |
| 1:A:1809:ASP:O | 1:A:1815:THR:HG22 | 2.05 | 0.57 |
| 1:A:1989:ASN:HB3 | 1:A:2040:MSE:HB3 | 1.86 | 0.57 |
| 1:A:2555:LEU:HD13 | 1:A:2809:PHE:CZ | 2.39 | 0.57 |
| 1:A:2883:SER:O | 1:A:2885:GLN:N | 2.38 | 0.57 |
| 1:A:3498:TRP:HB2 | 1:A:3501:HIS:HB2 | 1.86 | 0.57 |
| 1:A:3631:LYS:O | 1:A:3631:LYS:HD3 | 2.05 | 0.57 |
| 1:A:3687:MSE:C | 1:A:3689:ASP:H | 2.06 | 0.57 |
| 1:A:3839:TYR:HE1 | 1:A:3867:THR:HB | 1.70 | 0.57 |
| 1:A:576:VAL:HG13 | 1:A:601:TRP:CE3 | 2.40 | 0.57 |
| 1:B:1274:ARG:O | 1:B:1279:LEU:N | 2.28 | 0.57 |
| 1:B:1350:ASN:ND2 | 1:B:1404:LYS:HG2 | 2.18 | 0.57 |
| 1:B:1494:GLY:HA2 | 1:B:1497:ARG:HG3 | 1.87 | 0.57 |
| 1:B:2194:LEU:HD13 | 1:B:2244:CYS:SG | 2.45 | 0.57 |
| 1:B:2267:SER:HB2 | 1:B:2269:ASP:OD2 | 2.05 | 0.57 |
| 1:B:2927:ALA:CB | 1:B:2930:TYR:HD2 | 2.18 | 0.57 |
| 1:B:3903:HIS:O | 1:B:3907:SER:OG | 2.15 | 0.57 |
| 1:B:527:TYR:CE1 | 1:B:531:PHE:HZ | 2.21 | 0.57 |
| 1:B:752:LEU:HD13 | 1:B:776:TRP:CZ3 | 2.40 | 0.57 |
| 1:A:1006:THR:O | 1:A:1010:LEU:HG | 2.05 | 0.57 |
| 1:A:1146:ASN:O | 1:A:1150:LYS:HB3 | 2.05 | 0.57 |
| 1:A:283:SER:HA | 1:A:286:LEU:HG | 1.85 | 0.57 |
| 1:A:3167:ARG:HG2 | 1:A:3186:ARG:CZ | 2.35 | 0.57 |
| 1:A:3529:ILE:HG23 | 1:A:3532:PRO:HD2 | 1.86 | 0.57 |
| 1:A:3980:MSE:HB2 | 1:A:3983:ILE:HD12 | 1.86 | 0.57 |
| 1:A:575:ILE:HD11 | 1:A:579:LEU:HD13 | 1.87 | 0.57 |
| 1:A:891:ARG:HB2 | 1:A:905:ILE:HA | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:154:SER:HA | 1:B:181:LEU:HD22 | 1.87 | 0.57 |
| 1:B:2019:SER:O | 1:B:2023:SER:OG | 2.10 | 0.57 |
| 1:B:385:TYR:HD1 | 1:B:420:VAL:CG1 | 2.18 | 0.57 |
| 1:B:460:ALA:O | 1:B:464:VAL:HG12 | 2.05 | 0.57 |
| 1:B:566:ASP:O | 1:B:570:LYS:NZ | 2.38 | 0.57 |
| 1:B:70:ARG:HD3 | 1:B:82:ARG:HD3 | 1.87 | 0.57 |
| 1:A:175:TYR:CE1 | 1:A:200:PHE:HB3 | 2.39 | 0.56 |
| 1:A:2324:GLY:HA2 | 1:A:2371:PHE:HB3 | 1.87 | 0.56 |
| 1:A:2911:ARG:HG2 | 1:A:2914:ALA:HB3 | 1.87 | 0.56 |
| 1:A:3459:ASN:O | 1:A:3462:ARG:HG2 | 2.05 | 0.56 |
| 1:A:3483:MSE:C | 1:A:3516:HIS:HE2 | 2.08 | 0.56 |
| 1:A:2930:TYR:HH | 1:A:3902:SER:HG | 1.48 | 0.56 |
| 1:B:1007:VAL:O | 1:B:1011:GLU:HB3 | 2.04 | 0.56 |
| 1:B:1293:ALA:HA | 1:B:1296:PHE:CD2 | 2.40 | 0.56 |
| 1:B:144:MSE:HE2 | 1:B:144:MSE:HA | 1.86 | 0.56 |
| 1:B:2359:LYS:HA | 1:B:2362:VAL:HG13 | 1.87 | 0.56 |
| 1:B:2481:HIS:CE1 | 1:B:2485:ARG:NH1 | 2.65 | 0.56 |
| 1:B:3167:ARG:HG2 | 1:B:3186:ARG:CZ | 2.35 | 0.56 |
| 1:B:3238:MSE:O | 1:B:3242:MSE:HG3 | 2.05 | 0.56 |
| 1:B:3629:ARG:HH22 | 1:B:3638:LYS:CE | 2.18 | 0.56 |
| 1:B:647:TYR:O | 1:B:650:SER:OG | 2.12 | 0.56 |
| 1:B:909:VAL:CG1 | 1:B:913:ARG:HH11 | 2.05 | 0.56 |
| 1:A:1042:LYS:NZ | 1:A:1044:ILE:HD12 | 2.20 | 0.56 |
| 1:A:1343:GLU:O | 1:A:1347:THR:CB | 2.52 | 0.56 |
| 1:A:2193:ILE:HA | 1:A:2196:TRP:CE2 | 2.39 | 0.56 |
| 1:A:3493:TRP:CZ2 | 1:A:3496:ILE:HG21 | 2.40 | 0.56 |
| 1:A:4005:PHE:O | 1:A:4009:PRO:HD3 | 2.05 | 0.56 |
| 1:A:488:ILE:HG13 | 1:A:612:LEU:HD12 | 1.86 | 0.56 |
| 1:B:1475:LEU:O | 1:B:1479:VAL:HG23 | 2.04 | 0.56 |
| 1:B:2452:ARG:HE | 1:B:2498:ILE:HD11 | 1.71 | 0.56 |
| 1:B:2877:SER:C | 1:B:2879:GLY:H | 2.08 | 0.56 |
| 1:B:2967:GLU:O | 1:B:2971:GLN:NE2 | 2.38 | 0.56 |
| 1:B:3345:PRO:O | 1:B:3347:CYS:N | 2.34 | 0.56 |
| 1:B:3448:GLU:HG3 | 1:B:3449:LYS:HG3 | 1.87 | 0.56 |
| 1:B:3530:VAL:CG1 | 1:B:3702:PRO:HD3 | 2.31 | 0.56 |
| 1:A:1491:ILE:HG22 | 1:A:1497:ARG:HH22 | 1.70 | 0.56 |
| 1:A:1722:PHE:CE2 | 1:A:1754:GLN:HG2 | 2.39 | 0.56 |
| 1:A:205:LYS:HA | 1:A:208:MSE:HE3 | 1.86 | 0.56 |
| 1:A:2086:ASP:HB3 | 1:A:2090:ARG:NH2 | 2.20 | 0.56 |
| 1:A:3425:ARG:HH12 | 1:A:3999:THR:HG22 | 1.70 | 0.56 |
| 1:A:4063:GLU:HA | 1:A:4066:LEU:HD22 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:722:LYS:HD2 | 1:A:730:LEU:HB2 | 1.88 | 0.56 |
| 1:B:1046:PRO:O | 1:B:1049:GLN:HB3 | 2.05 | 0.56 |
| 1:B:1080:LEU:HB3 | 1:B:1111:LEU:CD2 | 2.36 | 0.56 |
| 1:B:1115:HIS:O | 1:B:1118:GLU:C | 2.44 | 0.56 |
| 1:B:1582:LEU:HD13 | 1:B:1600:MSE:SE | 2.55 | 0.56 |
| 1:B:1987:ARG:O | 1:B:1989:ASN:N | 2.38 | 0.56 |
| 1:B:2364:LEU:O | 1:B:2368:THR:OG1 | 2.11 | 0.56 |
| 1:B:2420:PHE:CE1 | 1:B:2439:ILE:HG21 | 2.40 | 0.56 |
| 1:B:2485:ARG:NH1 | 1:B:2530:ARG:CZ | 2.68 | 0.56 |
| 1:B:265:TYR:O | 1:B:268:PRO:HD2 | 2.05 | 0.56 |
| 1:B:2945:SER:O | 1:B:2949:THR:N | 2.36 | 0.56 |
| 1:B:3791:TYR:OH | 1:B:3942:PHE:HE2 | 1.88 | 0.56 |
| 1:B:4046:TYR:CE2 | 1:B:4049:ARG:NH2 | 2.74 | 0.56 |
| 1:B:642:PHE:CE2 | 1:B:710:PHE:HE2 | 2.23 | 0.56 |
| 1:B:657:SER:O | 1:B:661:PRO:HD3 | 2.04 | 0.56 |
| 1:A:1698:PHE:HD1 | 1:A:1699:PHE:N | 2.03 | 0.56 |
| 1:A:2808:LEU:O | 1:A:2812:LEU:HB2 | 2.06 | 0.56 |
| 1:A:3179:TRP:CH2 | 1:A:3258:LEU:HG | 2.39 | 0.56 |
| 1:A:369:PHE:CE1 | 1:A:419:SER:HB2 | 2.40 | 0.56 |
| 1:A:3907:SER:O | 1:A:3911:ILE:HG23 | 2.05 | 0.56 |
| 1:A:993:HIS:HB2 | 1:A:1038:LYS:HG2 | 1.86 | 0.56 |
| 1:B:2157:PHE:CE2 | 1:B:2199:LEU:HD13 | 2.40 | 0.56 |
| 1:B:242:PRO:HD3 | 1:B:282:PHE:CE2 | 2.41 | 0.56 |
| 1:B:3420:CYS:O | 1:B:3423:GLN:HB3 | 2.05 | 0.56 |
| 1:B:368:LEU:HD22 | 1:B:420:VAL:HG22 | 1.87 | 0.56 |
| 1:B:53:LEU:O | 1:B:56:SER:OG | 2.22 | 0.56 |
| 1:B:634:LEU:HD22 | 1:B:667:TYR:CD1 | 2.40 | 0.56 |
| 1:B:66:LEU:CD2 | 1:B:89:LEU:HD11 | 2.34 | 0.56 |
| 1:B:893:SER:OG | 1:B:906:PHE:HD2 | 1.88 | 0.56 |
| 1:A:852:ARG:NH1 | 1:A:3111:MSE:HE2 | 2.21 | 0.56 |
| 1:A:3762:GLN:HE22 | 1:A:3763:ARG:HH11 | 1.53 | 0.56 |
| 1:B:1000:LYS:O | 1:B:1002:GLU:N | 2.39 | 0.56 |
| 1:B:3279:SER:O | 1:B:3283:LEU:HB2 | 2.05 | 0.56 |
| 1:B:3397:GLN:OE1 | 1:B:3398:PRO:HD2 | 2.06 | 0.56 |
| 1:B:737:PRO:O | 1:B:741:ILE:HG13 | 2.06 | 0.56 |
| 1:B:778:ILE:HG13 | 1:B:858:MSE:SE | 2.56 | 0.56 |
| 1:A:1516:GLU:O | 1:A:1519:PHE:N | 2.38 | 0.56 |
| 1:A:164:LYS:HB3 | 1:A:166:ILE:HG13 | 1.88 | 0.56 |
| 1:A:2080:VAL:HG12 | 1:A:2081:LEU:H | 1.70 | 0.56 |
| 1:A:2236:GLU:HA | 1:A:2239:LYS:HB3 | 1.88 | 0.56 |
| 1:A:2538:ARG:NH1 | 1:A:2565:MSE:HB3 | 2.20 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3448:GLU:OE2 | 1:A:3449:LYS:HE3 | 2.04 | 0.56 |
| 1:A:3751:LEU:O | 1:A:3802:LEU:HG | 2.05 | 0.56 |
| 1:A:381:VAL:HB | 1:A:384:MSE:HG2 | 1.88 | 0.56 |
| 1:A:484:HIS:NE2 | 1:A:616:LYS:HE3 | 2.20 | 0.56 |
| 1:B:1017:ILE:HG23 | 1:B:1018:VAL:HG13 | 1.87 | 0.56 |
| 1:B:1374:GLN:O | 1:B:1378:GLU:N | 2.39 | 0.56 |
| 1:B:2265:PRO:HD3 | 1:B:2309:PHE:CZ | 2.41 | 0.56 |
| 1:B:3277:VAL:HB | 1:B:3321:LEU:HD21 | 1.88 | 0.56 |
| 1:B:797:ASP:HB3 | 1:B:870:LEU:HB3 | 1.88 | 0.56 |
| 1:B:909:VAL:HG22 | 1:B:2807:GLN:HG3 | 1.88 | 0.56 |
| 1:B:926:THR:O | 1:B:930:ALA:CB | 2.54 | 0.56 |
| 1:B:931:CYS:SG | 1:B:932:GLU:N | 2.78 | 0.56 |
| 1:B:964:ARG:HH12 | 1:B:968:VAL:HB | 1.70 | 0.56 |
| 1:A:1032:CYS:O | 1:A:1035:GLU:N | 2.37 | 0.56 |
| 1:A:1148:ALA:O | 1:A:1152:ARG:HG3 | 2.06 | 0.56 |
| 1:A:1598:ASN:O | 1:A:1602:ASP:HB3 | 2.05 | 0.56 |
| 1:A:168:ASP:O | 1:A:170:VAL:N | 2.36 | 0.56 |
| 1:A:1861:SER:O | 1:A:1864:ASP:HB3 | 2.06 | 0.56 |
| 1:A:1934:LEU:HD12 | 1:A:1937:ARG:H | 1.70 | 0.56 |
| 1:A:2799:GLN:HB3 | 1:A:2808:LEU:HD11 | 1.86 | 0.56 |
| 1:A:2879:GLY:HA2 | 1:A:2886:GLN:CG | 2.35 | 0.56 |
| 1:A:361:ILE:HG12 | 1:A:1858:LEU:CD2 | 2.36 | 0.56 |
| 1:A:3960:PRO:HG2 | 1:A:3961:PHE:CD2 | 2.41 | 0.56 |
| 1:A:654:ILE:HG13 | 1:A:655:LEU:H | 1.70 | 0.56 |
| 1:B:1090:ARG:NH2 | 1:B:1097:GLU:HA | 2.21 | 0.56 |
| 1:B:1431:LEU:O | 1:B:1434:VAL:HG12 | 2.05 | 0.56 |
| 1:B:2116:ASP:HB3 | 1:B:2119:PRO:HD2 | 1.88 | 0.56 |
| 1:B:313:LEU:HD11 | 1:B:359:LEU:HD21 | 1.88 | 0.56 |
| 1:A:3575:LEU:C | 1:A:3686:TRP:HH2 | 2.09 | 0.56 |
| 1:A:3590:ASN:OD1 | 1:A:3593:ARG:NH2 | 2.36 | 0.56 |
| 1:A:381:VAL:HB | 1:A:384:MSE:CG | 2.36 | 0.56 |
| 1:A:395:MSE:SE | 1:A:413:PHE:CE2 | 3.09 | 0.56 |
| 1:B:1128:CYS:HA | 1:B:1131:ILE:HG23 | 1.88 | 0.56 |
| 1:B:1587:VAL:HB | 1:B:1643:MSE:HE2 | 1.86 | 0.56 |
| 1:B:2330:VAL:HG21 | 1:B:2338:GLU:CB | 2.29 | 0.56 |
| 1:B:2450:GLU:O | 1:B:2454:LEU:HG | 2.06 | 0.56 |
| 1:B:2843:PHE:CE2 | 1:B:2853:PRO:HG3 | 2.41 | 0.56 |
| 1:B:3141:PHE:HZ | 1:B:3192:LYS:HB2 | 1.71 | 0.56 |
| 1:B:3331:GLY:O | 1:B:3335:ARG:HD2 | 2.05 | 0.56 |
| 1:B:3821:SER:OG | 1:B:3826:ALA:O | 2.22 | 0.56 |
| 1:B:993:HIS:CD2 | 1:B:2776:ARG:HD3 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1077:GLY:HA2 | 1:A:1080:LEU:HD21 | 1.86 | 0.56 |
| 1:A:155:LYS:O | 1:A:159:GLU:HG3 | 2.05 | 0.56 |
| 1:A:2073:ASP:HB3 | 1:A:2091:HIS:CE1 | 2.41 | 0.56 |
| 1:A:2093:CYS:HB3 | 1:A:2143:ARG:HH21 | 1.71 | 0.56 |
| 1:A:2552:VAL:CG2 | 1:A:2852:PRO:HG2 | 2.31 | 0.56 |
| 1:A:294:PHE:O | 1:A:298:LEU:HG | 2.05 | 0.56 |
| 1:A:3705:TYR:OH | 1:A:3765:GLU:OE1 | 2.20 | 0.56 |
| 1:B:1069:HIS:O | 1:B:3741:ARG:HD3 | 2.05 | 0.56 |
| 1:B:2810:SER:HA | 1:B:2813:PHE:CD2 | 2.41 | 0.56 |
| 1:B:2858:ILE:HD12 | 1:B:3894:PRO:HG2 | 1.86 | 0.56 |
| 1:B:3090:TYR:HB3 | 1:B:3095:ASP:OD2 | 2.05 | 0.56 |
| 1:B:3103:ILE:HD13 | 1:B:3139:GLN:OE1 | 2.06 | 0.56 |
| 1:B:3593:ARG:HD2 | 1:B:3660:ASN:O | 2.04 | 0.56 |
| 1:B:3847:SER:HA | 1:B:3857:LEU:HD13 | 1.86 | 0.56 |
| 1:B:3908:HIS:CD2 | 1:B:3912:CYS:SG | 2.99 | 0.56 |
| 1:B:3875:GLU:HG2 | 1:B:4127:TRP:HB3 | 1.88 | 0.56 |
| 1:B:886:TRP:CZ2 | 1:B:892:LEU:HD13 | 2.41 | 0.56 |
| 1:B:892:LEU:HB2 | 1:B:907:LEU:HD22 | 1.87 | 0.56 |
| 1:A:179:GLY:HA3 | 1:A:229:SER:HB3 | 1.86 | 0.56 |
| 1:A:2171:LEU:HG | 1:A:2177:ASN:ND2 | 2.21 | 0.56 |
| 1:A:2382:VAL:CG2 | 1:A:2404:ARG:HG3 | 2.36 | 0.56 |
| 1:A:3954:PRO:HG2 | 1:A:4027:TRP:HA | 1.88 | 0.56 |
| 1:A:855:VAL:O | 1:A:859:LEU:HG | 2.05 | 0.56 |
| 1:B:1348:LEU:HD23 | 1:B:1352:SER:HB3 | 1.87 | 0.56 |
| 1:B:1799:GLU:HA | 1:B:1802:TYR:CB | 2.36 | 0.56 |
| 1:B:4125:GLU:HA | 1:B:4127:TRP:HE3 | 1.70 | 0.56 |
| 1:A:131:LEU:HD21 | 1:A:170:VAL:HG23 | 1.86 | 0.56 |
| 1:A:2430:GLU:HG3 | 1:A:2465:PRO:CB | 2.36 | 0.56 |
| 1:A:2869:LEU:HB3 | 1:A:2893:LEU:HG | 1.88 | 0.56 |
| 1:B:1090:ARG:NH2 | 1:B:1096:VAL:O | 2.38 | 0.56 |
| 1:B:1131:ILE:HG12 | 1:B:1132:ASP:N | 2.19 | 0.56 |
| 1:B:1909:ASN:ND2 | 1:B:1951:VAL:O | 2.38 | 0.56 |
| 1:B:2886:GLN:CG | 1:B:2887:PRO:HD3 | 2.36 | 0.56 |
| 1:B:756:PHE:O | 1:B:760:LEU:HG | 2.06 | 0.56 |
| 1:B:759:GLY:HA3 | 1:B:773:LEU:CD1 | 2.36 | 0.56 |
| 1:B:964:ARG:NH1 | 1:B:968:VAL:HB | 2.21 | 0.56 |
| 1:B:978:GLN:H | 1:B:981:ARG:HD3 | 1.70 | 0.56 |
| 1:A:2842:ARG:O | 1:A:2846:THR:HG23 | 2.06 | 0.55 |
| 1:A:759:GLY:HA3 | 1:A:773:LEU:HD11 | 1.88 | 0.55 |
| 1:B:1805:PHE:HA | 1:B:1808:ASP:OD2 | 2.06 | 0.55 |
| 1:B:1977:ILE:C | 1:B:1979:GLU:H | 2.02 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2065:ARG:NH1 | 1:B:2097:LEU:HD21 | 2.21 | 0.55 |
| 1:B:176:GLU:HG2 | 1:B:225:LYS:CD | 2.36 | 0.55 |
| 1:B:2936:TYR:CE1 | 1:B:2940:ARG:HB2 | 2.40 | 0.55 |
| 1:B:3781:CYS:HA | 1:B:3786:LEU:HD12 | 1.87 | 0.55 |
| 1:B:3900:LEU:HD11 | 1:B:3934:THR:O | 2.05 | 0.55 |
| 1:B:3962:ARG:HB2 | 1:B:3962:ARG:CZ | 2.35 | 0.55 |
| 1:A:2186:VAL:O | 1:A:2190:VAL:HG13 | 2.06 | 0.55 |
| 1:A:2447:LYS:HA | 1:A:2451:LEU:HD12 | 1.89 | 0.55 |
| 1:A:2918:PRO:HA | 1:A:2921:LEU:HG | 1.88 | 0.55 |
| 1:A:3584:LEU:O | 1:A:3588:TRP:CB | 2.55 | 0.55 |
| 1:A:714:VAL:HG12 | 1:A:715:ALA:N | 2.21 | 0.55 |
| 1:B:2869:LEU:HG | 1:B:2893:LEU:HD12 | 1.88 | 0.55 |
| 1:B:392:CYS:SG | 1:B:438:LEU:HD21 | 2.46 | 0.55 |
| 1:B:3989:ARG:HH21 | 1:B:4100:GLU:CD | 2.09 | 0.55 |
| 1:B:411:PRO:HG3 | 1:B:442:GLN:HE22 | 1.71 | 0.55 |
| 1:A:1231:GLN:H | 1:A:1232:PRO:CD | 2.20 | 0.55 |
| 1:A:1952:ILE:HG12 | 1:A:1953:CYS:N | 2.21 | 0.55 |
| 1:A:2837:LEU:HD12 | 1:A:2867:ALA:HB3 | 1.89 | 0.55 |
| 1:A:3495:PHE:HZ | 1:A:3521:ILE:HG13 | 1.71 | 0.55 |
| 1:A:3499:ILE:O | 1:A:3503:VAL:HG12 | 2.07 | 0.55 |
| 1:A:4031:ILE:O | 1:A:4035:GLU:N | 2.37 | 0.55 |
| 1:A:4100:GLU:HG2 | 1:A:4101:GLU:H | 1.71 | 0.55 |
| 1:A:805:LEU:HD22 | 1:A:3125:ARG:NH1 | 2.20 | 0.55 |
| 1:A:913:ARG:HA | 1:A:916:GLU:CD | 2.27 | 0.55 |
| 1:A:989:MSE:O | 1:A:992:ILE:HG13 | 2.06 | 0.55 |
| 1:B:1292:LYS:O | 1:B:1295:ALA:HB3 | 2.05 | 0.55 |
| 1:B:1583:MSE:HE3 | 1:B:1643:MSE:HB2 | 1.87 | 0.55 |
| 1:B:1726:SER:HB2 | 1:B:1866:GLN:HE22 | 1.71 | 0.55 |
| 1:B:1733:THR:OG1 | 1:B:1877:LEU:HD13 | 2.06 | 0.55 |
| 1:B:2026:SER:HB3 | 2:S:207:UNK:CB | 2.37 | 0.55 |
| 1:B:2285:LEU:O | 1:B:2288:TYR:N | 2.39 | 0.55 |
| 1:B:2378:PHE:O | 1:B:2382:VAL:HG22 | 2.06 | 0.55 |
| 1:B:658:THR:HA | 1:B:733:LEU:CD2 | 2.32 | 0.55 |
| 1:B:968:VAL:HG22 | 1:B:972:LEU:HD23 | 1.87 | 0.55 |
| 1:A:204:LEU:HD13 | 1:A:223:CYS:HB2 | 1.87 | 0.55 |
| 1:A:2222:HIS:O | 1:A:2226:PRO:HD2 | 2.07 | 0.55 |
| 1:A:3144:PHE:CD1 | 1:A:3160:LEU:HD11 | 2.42 | 0.55 |
| 1:A:960:GLN:HG2 | 1:A:961:LEU:HD22 | 1.89 | 0.55 |
| 1:B:1442:GLN:HE22 | 1:B:1495:ASP:HB3 | 1.70 | 0.55 |
| 1:B:3106:GLY:HA2 | 1:B:3109:SER:HB2 | 1.88 | 0.55 |
| 1:B:3283:LEU:HG | 1:B:3300:VAL:HG21 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3966:GLN:H | 1:B:4128:MSE:C | 2.10 | 0.55 |
| 1:B:4125:GLU:HA | 1:B:4127:TRP:CE3 | 2.41 | 0.55 |
| 1:B:760:LEU:HD13 | 1:B:802:THR:OG1 | 2.06 | 0.55 |
| 1:B:985:GLU:O | 1:B:988:VAL:HG22 | 2.06 | 0.55 |
| 1:A:1636:ASP:O | 1:A:1640:GLU:HB2 | 2.06 | 0.55 |
| 1:A:1641:THR:O | 1:A:1645:VAL:HG23 | 2.07 | 0.55 |
| 1:A:1897:ASN:HB3 | 1:A:1901:HIS:HE1 | 1.71 | 0.55 |
| 1:A:2210:VAL:HG13 | 1:A:2211:LEU:H | 1.71 | 0.55 |
| 1:A:2575:PRO:HD2 | 1:A:2785:ILE:HD11 | 1.87 | 0.55 |
| 1:A:2890:ILE:HD12 | 1:A:2918:PRO:HB3 | 1.87 | 0.55 |
| 1:A:3994:ASP:OD2 | 1:A:3997:LEU:HD13 | 2.06 | 0.55 |
| 1:B:2031:LEU:C | 1:B:2033:ASP:H | 2.07 | 0.55 |
| 1:B:2375:ALA:O | 1:B:2379:MSE:HB2 | 2.04 | 0.55 |
| 1:B:2542:LEU:O | 1:B:2545:LEU:N | 2.38 | 0.55 |
| 1:B:2957:LEU:HB3 | 1:B:3989:ARG:NH2 | 2.22 | 0.55 |
| 1:B:3282:ARG:HB2 | 1:B:3282:ARG:HH11 | 1.70 | 0.55 |
| 1:B:4066:LEU:HD11 | 1:B:4078:VAL:HG11 | 1.88 | 0.55 |
| 1:B:922:SER:C | 1:B:924:ARG:H | 2.09 | 0.55 |
| 1:A:2236:GLU:HG2 | 2:K:110:UNK:CB | 2.36 | 0.55 |
| 1:A:1567:ILE:HG12 | 1:A:1571:LEU:HD11 | 1.87 | 0.55 |
| 1:A:2145:PHE:HD1 | 1:A:2188:GLU:HG2 | 1.71 | 0.55 |
| 1:A:2556:SER:O | 1:A:2559:THR:OG1 | 2.25 | 0.55 |
| 1:A:3722:PHE:CD1 | 1:A:3740:ILE:HA | 2.41 | 0.55 |
| 1:A:3981:TYR:OH | 1:A:4101:GLU:HB3 | 2.07 | 0.55 |
| 1:A:543:SER:O | 1:A:545:LEU:N | 2.34 | 0.55 |
| 1:A:793:LEU:HA | 1:A:796:LEU:CG | 2.33 | 0.55 |
| 1:B:1678:LEU:O | 1:B:1682:THR:HG22 | 2.07 | 0.55 |
| 1:B:1976:LEU:HD13 | 1:B:2031:LEU:HD23 | 1.89 | 0.55 |
| 1:B:2099:ALA:O | 1:B:2102:LYS:HB2 | 2.06 | 0.55 |
| 1:B:2239:LYS:HG3 | 1:B:2279:ILE:HD12 | 1.89 | 0.55 |
| 1:B:2289:ASP:O | 1:B:2291:GLN:N | 2.39 | 0.55 |
| 1:B:2806:LYS:HZ2 | 1:B:2858:ILE:HG13 | 1.71 | 0.55 |
| 1:A:1392:MSE:HA | 1:A:1395:LEU:HB3 | 1.89 | 0.55 |
| 1:A:1431:LEU:O | 1:A:1434:VAL:HG12 | 2.07 | 0.55 |
| 1:A:1946:ASN:HA | 1:A:1949:ILE:HG22 | 1.89 | 0.55 |
| 1:A:1982:ILE:HG23 | 1:A:1986:ARG:HE | 1.71 | 0.55 |
| 1:A:2271:SER:OG | 1:A:2272:VAL:N | 2.40 | 0.55 |
| 1:A:3499:ILE:CG2 | 1:A:3535:ILE:HG21 | 2.36 | 0.55 |
| 1:A:1069:HIS:O | 1:A:3741:ARG:HD3 | 2.07 | 0.55 |
| 1:B:1011:GLU:OE2 | 1:B:1062:ARG:CZ | 2.55 | 0.55 |
| 1:B:1102:GLU:HA | 1:B:1150:LYS:NZ | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2254:ARG:HB2 | 1:B:2295:GLN:OE1 | 2.06 | 0.55 |
| 1:B:279:ALA:HA | 1:B:282:PHE:CE2 | 2.41 | 0.55 |
| 1:B:2895:GLU:O | 1:B:2899:ARG:NH2 | 2.40 | 0.55 |
| 1:B:3578:LEU:HB3 | 1:B:3579:SER:HA | 1.89 | 0.55 |
| 1:B:629:PHE:CZ | 1:B:666:PHE:CD1 | 2.92 | 0.55 |
| 1:B:706:LEU:HB3 | 1:B:710:PHE:CZ | 2.42 | 0.55 |
| 1:B:776:TRP:CE2 | 1:B:780:ILE:HD12 | 2.41 | 0.55 |
| 1:A:1016:GLY:O | 1:A:1019:ASP:HB2 | 2.05 | 0.55 |
| 1:A:1083:ASN:HD21 | 1:A:1104:LEU:HD21 | 1.71 | 0.55 |
| 1:A:1400:VAL:O | 1:A:1404:LYS:CB | 2.55 | 0.55 |
| 1:A:1606:ARG:O | 1:A:1806:ARG:NH1 | 2.39 | 0.55 |
| 1:A:1880:MSE:O | 1:A:1883:ARG:N | 2.39 | 0.55 |
| 1:A:1918:LEU:HD11 | 1:A:1957:ASN:HB3 | 1.89 | 0.55 |
| 1:A:2098:THR:HG22 | 1:A:2146:LEU:HD13 | 1.89 | 0.55 |
| 1:A:2410:GLU:HA | 1:A:2413:PHE:CZ | 2.41 | 0.55 |
| 1:A:3424:LEU:HD13 | 1:A:3472:ILE:HD11 | 1.87 | 0.55 |
| 1:A:3472:ILE:HG22 | 1:A:3473:GLU:H | 1.71 | 0.55 |
| 1:A:3676:PRO:HG2 | 1:A:3677:PRO:HD3 | 1.89 | 0.55 |
| 1:A:3722:PHE:CE1 | 1:A:3740:ILE:HG12 | 2.34 | 0.55 |
| 1:A:2957:LEU:HD11 | 1:A:3985:VAL:HG11 | 1.87 | 0.55 |
| 1:A:446:PHE:N | 1:A:446:PHE:HD1 | 2.03 | 0.55 |
| 1:A:446:PHE:CZ | 1:A:530:LEU:HB3 | 2.41 | 0.55 |
| 1:A:743:LEU:HD21 | 1:A:784:VAL:HG21 | 1.89 | 0.55 |
| 1:B:1424:THR:OG1 | 1:B:1425:ALA:N | 2.40 | 0.55 |
| 1:B:1867:ILE:HG23 | 1:B:1871:MSE:HE3 | 1.89 | 0.55 |
| 1:B:2157:PHE:CE1 | 1:B:2203:THR:HB | 2.42 | 0.55 |
| 1:B:3592:VAL:HG22 | 1:B:3609:MSE:SE | 2.57 | 0.55 |
| 1:B:3791:TYR:HH | 1:B:3942:PHE:HE2 | 1.54 | 0.55 |
| 1:B:2929:LEU:HD22 | 1:B:3983:ILE:HG12 | 1.89 | 0.55 |
| 1:B:3964:THR:HB | 1:B:4128:MSE:O | 2.06 | 0.55 |
| 1:B:568:PHE:O | 1:B:571:SER:N | 2.39 | 0.55 |
| 1:B:612:LEU:CD2 | 1:B:1800:SER:HB3 | 2.36 | 0.55 |
| 1:B:612:LEU:HD12 | 1:B:613:HIS:N | 2.22 | 0.55 |
| 1:A:1335:CYS:HA | 1:A:1338:VAL:HG12 | 1.89 | 0.55 |
| 1:A:1423:ILE:O | 1:A:1427:SER:OG | 2.20 | 0.55 |
| 1:A:1573:LYS:O | 1:A:1576:ASP:HB3 | 2.07 | 0.55 |
| 1:A:1909:ASN:O | 1:A:1912:THR:HG23 | 2.07 | 0.55 |
| 1:A:2789:SER:O | 1:A:2793:PRO:HD3 | 2.07 | 0.55 |
| 1:A:2878:ALA:O | 1:A:2886:GLN:HB3 | 2.07 | 0.55 |
| 1:A:3487:ILE:HA | 1:A:3490:VAL:HG22 | 1.89 | 0.55 |
| 1:A:3901:ARG:HG2 | 1:A:3901:ARG:HH11 | 1.70 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3981:TYR:HE1 | 1:A:4105:LYS:N | 2.05 | 0.55 |
| 1:A:892:LEU:HD11 | 1:A:958:MSE:HB2 | 1.87 | 0.55 |
| 1:B:1087:ARG:HD3 | 1:B:1134:LEU:HD22 | 1.89 | 0.55 |
| 1:B:1167:ASP:O | 1:B:1171:TRP:HB2 | 2.06 | 0.55 |
| 1:B:1561:SER:HA | 1:B:1564:SER:HB2 | 1.89 | 0.55 |
| 1:B:2088:LEU:HD21 | 1:B:2095:ALA:HB2 | 1.89 | 0.55 |
| 1:B:2190:VAL:HA | 1:B:2193:ILE:HG22 | 1.88 | 0.55 |
| 1:B:3435:ASP:O | 1:B:3439:LEU:HB2 | 2.06 | 0.55 |
| 1:A:1217:VAL:O | 1:A:1221:ILE:HG13 | 2.07 | 0.55 |
| 1:A:1344:PHE:CE1 | 1:A:1348:LEU:HG | 2.42 | 0.55 |
| 1:A:1729:PHE:HZ | 1:A:1870:LYS:HG3 | 1.67 | 0.55 |
| 1:A:2046:SER:HB2 | 1:A:2096:PRO:HG2 | 1.89 | 0.55 |
| 1:A:2074:PRO:O | 1:A:2076:VAL:N | 2.40 | 0.55 |
| 1:A:2167:PRO:CA | 1:A:2171:LEU:HB2 | 2.36 | 0.55 |
| 1:A:2951:GLN:OE1 | 1:A:2972:TYR:OH | 2.18 | 0.55 |
| 1:A:3614:TYR:O | 1:A:3618:GLY:N | 2.29 | 0.55 |
| 1:A:3778:ASP:OD2 | 1:A:3781:CYS:N | 2.40 | 0.55 |
| 1:A:3816:LEU:O | 1:A:3820:MSE:HB3 | 2.07 | 0.55 |
| 1:A:4070:LYS:H | 1:A:4074:PHE:HD2 | 1.55 | 0.55 |
| 1:A:385:TYR:OH | 1:A:424:LEU:HD21 | 2.07 | 0.55 |
| 1:A:508:HIS:CD2 | 1:A:725:LEU:HD22 | 2.42 | 0.55 |
| 1:B:1346:THR:HG21 | 1:B:1401:ASN:CB | 2.35 | 0.55 |
| 1:B:174:VAL:HG12 | 1:B:178:LEU:HD11 | 1.87 | 0.55 |
| 1:B:2387:PRO:HA | 1:B:2390:HIS:HB3 | 1.88 | 0.55 |
| 1:B:3631:LYS:HA | 1:B:3634:GLN:CB | 2.37 | 0.55 |
| 1:B:3806:LEU:O | 1:B:3809:THR:HG22 | 2.07 | 0.55 |
| 1:B:3915:HIS:O | 1:B:3918:LEU:N | 2.40 | 0.55 |
| 1:B:2957:LEU:HD21 | 1:B:4101:GLU:CD | 2.27 | 0.55 |
| 1:B:431:TYR:HA | 1:B:434:VAL:CG1 | 2.36 | 0.55 |
| 1:B:756:PHE:O | 1:B:759:GLY:N | 2.40 | 0.55 |
| 1:A:1007:VAL:O | 1:A:1011:GLU:HB3 | 2.07 | 0.54 |
| 1:A:1080:LEU:HD22 | 1:A:1127:CYS:HB2 | 1.87 | 0.54 |
| 1:A:1253:THR:HA | 1:A:1257:LEU:HD12 | 1.89 | 0.54 |
| 1:A:86:LEU:HD13 | 1:A:134:LEU:HD21 | 1.88 | 0.54 |
| 1:A:2145:PHE:CD1 | 1:A:2188:GLU:HG2 | 2.41 | 0.54 |
| 1:A:220:LEU:O | 1:A:224:LEU:HG | 2.06 | 0.54 |
| 1:A:3699:LEU:HG | 1:A:3701:ILE:HG12 | 1.88 | 0.54 |
| 1:A:752:LEU:HA | 1:A:755:ALA:HB3 | 1.88 | 0.54 |
| 1:B:114:VAL:HG11 | 1:B:130:LEU:HD11 | 1.90 | 0.54 |
| 1:B:170:VAL:HG23 | 1:B:173:LYS:NZ | 2.21 | 0.54 |
| 1:B:1927:MSE:HG2 | 1:B:1941:HIS:CD2 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2213:ASN:HB2 | 1:B:2250:SER:HB2 | 1.90 | 0.54 |
| 1:B:2793:PRO:O | 1:B:2797:VAL:HG22 | 2.05 | 0.54 |
| 1:B:2944:THR:HG21 | 1:B:2983:ASP:OD2 | 2.07 | 0.54 |
| 1:B:358:GLU:N | 1:B:361:ILE:HG23 | 2.22 | 0.54 |
| 1:B:3872:ARG:NH1 | 1:B:3965:ARG:NH1 | 2.54 | 0.54 |
| 1:B:454:GLN:HG3 | 1:B:533:HIS:CE1 | 2.40 | 0.54 |
| 1:B:784:VAL:O | 1:B:787:PRO:HD2 | 2.07 | 0.54 |
| 1:A:1008:ALA:HA | 1:A:1011:GLU:OE1 | 2.07 | 0.54 |
| 1:A:1240:THR:HA | 1:A:1243:TYR:HD2 | 1.72 | 0.54 |
| 1:A:3122:HIS:O | 1:A:3125:ARG:N | 2.40 | 0.54 |
| 1:B:1276:VAL:HG13 | 1:B:1358:LEU:HD12 | 1.88 | 0.54 |
| 1:B:1378:GLU:HB3 | 1:B:1379:PRO:HD3 | 1.89 | 0.54 |
| 1:B:1636:ASP:O | 1:B:1640:GLU:HB2 | 2.07 | 0.54 |
| 1:B:1682:THR:HB | 1:B:1724:MSE:SE | 2.57 | 0.54 |
| 1:B:1797:LEU:HD13 | 1:B:1805:PHE:CE2 | 2.41 | 0.54 |
| 1:B:356:ASN:OD1 | 1:B:1859:ASN:HB2 | 2.06 | 0.54 |
| 1:B:197:PHE:CE2 | 1:B:230:LEU:HD22 | 2.42 | 0.54 |
| 1:B:2224:PHE:HB3 | 1:B:2272:VAL:CG1 | 2.38 | 0.54 |
| 1:B:2304:VAL:O | 1:B:2348:GLN:NE2 | 2.40 | 0.54 |
| 1:B:2352:HIS:CG | 1:B:2364:LEU:HD21 | 2.42 | 0.54 |
| 1:B:3704:GLN:NE2 | 1:B:3796:MSE:SE | 2.90 | 0.54 |
| 1:B:3493:TRP:CE3 | 1:B:3713:PRO:HB3 | 2.39 | 0.54 |
| 1:B:3876:SER:O | 1:B:3879:PRO:HD2 | 2.07 | 0.54 |
| 1:A:1279:LEU:HG | 1:A:1292:LYS:HZ3 | 1.72 | 0.54 |
| 1:A:1259:LEU:HG | 1:A:1337:VAL:HG22 | 1.90 | 0.54 |
| 1:A:1363:LEU:C | 1:A:1365:ASN:H | 2.11 | 0.54 |
| 1:A:1675:TYR:CZ | 1:A:1679:LEU:HD11 | 2.42 | 0.54 |
| 1:A:2040:MSE:HA | 1:A:2043:PHE:HD1 | 1.73 | 0.54 |
| 1:A:2056:SER:HA | 1:A:2061:PRO:HG3 | 1.88 | 0.54 |
| 1:A:2065:ARG:HB3 | 1:A:2125:TRP:CD1 | 2.42 | 0.54 |
| 1:A:245:SER:HB2 | 1:A:272:LEU:HD11 | 1.89 | 0.54 |
| 1:A:2796:ALA:O | 1:A:2800:ARG:HG3 | 2.06 | 0.54 |
| 1:A:2870:SER:O | 1:A:2872:ASP:N | 2.41 | 0.54 |
| 1:A:3273:LEU:HB3 | 1:A:3321:LEU:CD2 | 2.37 | 0.54 |
| 1:A:3413:TYR:HD2 | 1:A:3453:ALA:HB2 | 1.72 | 0.54 |
| 1:A:887:ASP:O | 1:A:3889:ARG:HG2 | 2.07 | 0.54 |
| 1:A:3967:PHE:CD1 | 1:A:3968:ILE:N | 2.75 | 0.54 |
| 1:B:2636:UNK:O | 1:B:2640:UNK:CB | 2.55 | 0.54 |
| 1:B:2801:ASP:HB2 | 1:B:2802:PRO:HD3 | 1.88 | 0.54 |
| 1:B:2894:GLU:HA | 1:B:2898:LEU:HB2 | 1.88 | 0.54 |
| 1:B:3464:LYS:O | 1:B:3468:LEU:HG | 2.08 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3864:ARG:HD2 | 1:B:4115:ASN:OD1 | 2.08 | 0.54 |
| 1:A:1018:VAL:HB | 1:A:1074:LYS:CA | 2.37 | 0.54 |
| 1:A:1064:TYR:CD1 | 1:A:1106:ILE:HD11 | 2.42 | 0.54 |
| 1:A:1296:PHE:O | 1:A:1299:GLU:N | 2.39 | 0.54 |
| 1:A:1462:GLY:C | 1:A:1464:LEU:H | 2.11 | 0.54 |
| 1:A:1551:ILE:HA | 1:A:1554:SER:HB3 | 1.89 | 0.54 |
| 1:A:15:LEU:HD23 | 1:A:2359:LYS:NZ | 2.22 | 0.54 |
| 1:A:2164:TRP:HH2 | 1:A:2190:VAL:HG12 | 1.70 | 0.54 |
| 1:A:2923:TRP:CD1 | 1:A:2931:ARG:HD3 | 2.42 | 0.54 |
| 1:A:3294:SER:HB3 | 1:A:3341:LEU:HD22 | 1.90 | 0.54 |
| 1:B:1216:GLY:HA3 | 1:B:1271:ILE:HG22 | 1.88 | 0.54 |
| 1:B:2462:VAL:HG11 | 1:B:2473:MSE:SE | 2.58 | 0.54 |
| 1:B:2474:TYR:CE1 | 1:B:2509:GLY:HA3 | 2.42 | 0.54 |
| 1:B:3472:ILE:HG22 | 1:B:3473:GLU:H | 1.73 | 0.54 |
| 1:B:409:GLN:HG3 | 1:B:413:PHE:CZ | 2.41 | 0.54 |
| 1:B:514:VAL:HA | 1:B:604:PRO:HG3 | 1.90 | 0.54 |
| 1:B:575:ILE:N | 1:B:605:THR:OG1 | 2.40 | 0.54 |
| 1:B:963:LYS:HB3 | 1:B:1009:LEU:HD11 | 1.88 | 0.54 |
| 1:A:1111:LEU:HA | 1:A:1114:ALA:HB3 | 1.90 | 0.54 |
| 1:A:401:ASP:HB2 | 1:A:1763:THR:OG1 | 2.07 | 0.54 |
| 1:A:2461:PHE:HE1 | 1:A:2469:CYS:HG | 1.55 | 0.54 |
| 1:A:2538:ARG:HH11 | 1:A:2565:MSE:CG | 2.21 | 0.54 |
| 1:A:3008:TRP:H | 1:A:3050:LYS:HG2 | 1.73 | 0.54 |
| 1:A:3114:TYR:OH | 1:A:3128:LYS:HB3 | 2.07 | 0.54 |
| 1:A:759:GLY:HA3 | 1:A:773:LEU:CD1 | 2.38 | 0.54 |
| 1:B:1019:ASP:HB3 | 1:B:1020:PRO:HD2 | 1.89 | 0.54 |
| 1:B:1639:LEU:HD12 | 1:B:1640:GLU:N | 2.23 | 0.54 |
| 1:B:3121:LEU:HB2 | 1:B:3124:SER:OG | 2.08 | 0.54 |
| 1:B:4027:TRP:HB3 | 1:B:4031:ILE:HD11 | 1.90 | 0.54 |
| 1:B:3864:ARG:NH2 | 1:B:4119:ARG:HH21 | 2.05 | 0.54 |
| 1:B:649:PHE:C | 1:B:651:TYR:N | 2.61 | 0.54 |
| 1:B:659:ARG:HH22 | 1:B:662:LEU:CB | 2.20 | 0.54 |
| 1:B:65:LEU:HD23 | 1:B:68:PHE:CE1 | 2.43 | 0.54 |
| 1:B:936:SER:HB3 | 1:B:2791:ILE:CG1 | 2.35 | 0.54 |
| 1:A:138:PHE:CD2 | 1:A:177:LEU:HD22 | 2.42 | 0.54 |
| 1:A:1424:THR:O | 1:A:1426:GLN:N | 2.41 | 0.54 |
| 1:A:1810:PRO:O | 1:A:1811:ARG:HG2 | 2.08 | 0.54 |
| 1:A:269:SER:HB2 | 1:A:315:ALA:HB2 | 1.90 | 0.54 |
| 1:B:1693:VAL:O | 1:B:1697:PRO:HD3 | 2.07 | 0.54 |
| 1:B:2039:GLU:HG2 | 1:B:2077:HIS:NE2 | 2.22 | 0.54 |
| 1:B:2220:MSE:SE | 1:B:2276:LEU:HD11 | 2.58 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2363:CYS:O | 1:B:2367:VAL:HG12 | 2.07 | 0.54 |
| 1:B:3907:SER:O | 1:B:3911:ILE:HG23 | 2.08 | 0.54 |
| 1:B:633:ILE:O | 1:B:637:LYS:HG2 | 2.08 | 0.54 |
| 1:B:897:PRO:HG2 | 1:B:898:PHE:CE1 | 2.43 | 0.54 |
| 1:A:1103:ALA:O | 1:A:1106:ILE:HG12 | 2.07 | 0.54 |
| 1:A:2030:TYR:CD1 | 1:A:2031:LEU:HG | 2.40 | 0.54 |
| 1:A:270:ALA:O | 1:A:274:LEU:HG | 2.08 | 0.54 |
| 1:A:2837:LEU:HD13 | 1:A:2868:LEU:N | 2.23 | 0.54 |
| 1:A:3390:GLN:O | 1:A:3394:GLU:HB2 | 2.08 | 0.54 |
| 1:A:3464:LYS:HE3 | 1:A:3468:LEU:HD21 | 1.88 | 0.54 |
| 1:A:3486:GLU:HG3 | 1:A:3487:ILE:N | 2.22 | 0.54 |
| 1:A:3701:ILE:O | 1:A:3701:ILE:HG13 | 2.08 | 0.54 |
| 1:A:3812:LEU:HG | 1:A:3813:LYS:N | 2.22 | 0.54 |
| 1:A:3963:LEU:HG | 1:A:3967:PHE:HE1 | 1.71 | 0.54 |
| 1:A:69:VAL:HG12 | 1:A:70:ARG:N | 2.22 | 0.54 |
| 1:B:2097:LEU:HA | 1:B:2100:LEU:HB3 | 1.89 | 0.54 |
| 1:B:2224:PHE:HZ | 1:B:2276:LEU:HD22 | 1.70 | 0.54 |
| 1:B:2386:LEU:HD11 | 1:B:2400:VAL:HG12 | 1.88 | 0.54 |
| 1:B:2543:ASN:HA | 1:B:2546:TYR:HD2 | 1.72 | 0.54 |
| 1:B:3840:LYS:CE | 1:B:4122:GLU:HB3 | 2.36 | 0.54 |
| 1:B:3858:MSE:HG2 | 1:B:4119:ARG:HD3 | 1.89 | 0.54 |
| 1:B:916:GLU:CB | 1:B:930:ALA:HB1 | 2.36 | 0.54 |
| 1:A:1087:ARG:CD | 1:A:1134:LEU:HD22 | 2.36 | 0.54 |
| 1:A:1406:LEU:HB3 | 1:A:1415:LEU:HD21 | 1.90 | 0.54 |
| 1:A:1609:ALA:HB2 | 1:A:1633:TRP:CZ2 | 2.42 | 0.54 |
| 1:A:2085:MSE:O | 1:A:2088:LEU:HB3 | 2.08 | 0.54 |
| 1:A:2416:LYS:HD3 | 1:A:2442:MSE:SE | 2.58 | 0.54 |
| 1:A:2935:GLU:HG3 | 1:A:2936:TYR:H | 1.73 | 0.54 |
| 1:A:83:GLU:O | 1:A:87:LYS:HG3 | 2.08 | 0.54 |
| 1:A:966:PHE:CZ | 1:A:988:VAL:HG12 | 2.43 | 0.54 |
| 1:A:971:ARG:NE | 1:A:1024:THR:OG1 | 2.40 | 0.54 |
| 1:B:2163:HIS:O | 1:B:2167:PRO:HD3 | 2.07 | 0.54 |
| 1:B:2312:TYR:CE2 | 1:B:2313:LYS:HG2 | 2.43 | 0.54 |
| 1:B:2352:HIS:HB2 | 1:B:2364:LEU:HD11 | 1.89 | 0.54 |
| 1:B:2820:MSE:SE | 1:B:2833:THR:HG21 | 2.58 | 0.54 |
| 1:B:3568:ILE:HD11 | 1:B:3691:LYS:HD2 | 1.90 | 0.54 |
| 1:B:649:PHE:C | 1:B:651:TYR:H | 2.10 | 0.54 |
| 1:B:855:VAL:O | 1:B:859:LEU:HG | 2.07 | 0.54 |
| 1:B:789:TYR:HD2 | 1:B:865:GLN:HG3 | 1.71 | 0.54 |
| 1:A:114:VAL:CG1 | 1:A:130:LEU:HD11 | 2.38 | 0.54 |
| 1:A:1886:LYS:HZ2 | 1:A:1924:THR:CB | 2.17 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1907:GLU:OE2 | 1:A:1911:LEU:HD11 | 2.08 | 0.54 |
| 1:A:2177:ASN:HD22 | 1:A:2182:ILE:CG2 | 2.21 | 0.54 |
| 1:A:2304:VAL:HG11 | 1:A:2344:LEU:HB3 | 1.90 | 0.54 |
| 1:A:2412:TYR:CE1 | 1:A:2415:LEU:HB3 | 2.43 | 0.54 |
| 1:A:262:LEU:HD13 | 1:A:306:VAL:HG12 | 1.88 | 0.54 |
| 1:A:3039:THR:O | 1:A:3042:PRO:HD2 | 2.08 | 0.54 |
| 1:A:3728:VAL:HG22 | 1:A:3736:LYS:HG3 | 1.89 | 0.54 |
| 1:A:3762:GLN:HE22 | 1:A:3763:ARG:NH1 | 2.05 | 0.54 |
| 1:B:87:LYS:HG2 | 1:B:133:LYS:HG3 | 1.89 | 0.54 |
| 1:B:1862:THR:O | 1:B:1865:THR:HG22 | 2.07 | 0.54 |
| 1:B:2049:VAL:HG11 | 1:B:2100:LEU:HD12 | 1.90 | 0.54 |
| 1:B:2238:ILE:O | 1:B:2242:VAL:HG23 | 2.08 | 0.54 |
| 1:B:276:ALA:HA | 1:B:280:SER:OG | 2.08 | 0.54 |
| 1:B:2806:LYS:HA | 1:B:2809:PHE:CD2 | 2.43 | 0.54 |
| 1:B:278:HIS:O | 1:B:281:GLN:HB3 | 2.08 | 0.54 |
| 1:B:2990:GLU:O | 1:B:2994:TRP:HB2 | 2.07 | 0.54 |
| 1:B:3048:LYS:NZ | 1:B:3064:PHE:CE2 | 2.74 | 0.54 |
| 1:B:3240:MSE:O | 1:B:3242:MSE:N | 2.41 | 0.54 |
| 1:B:39:GLY:HA2 | 1:B:92:PHE:HZ | 1.71 | 0.54 |
| 1:B:620:PHE:CE1 | 1:B:623:PHE:HD2 | 2.26 | 0.54 |
| 1:B:718:MSE:SE | 1:B:731:THR:HG22 | 2.58 | 0.54 |
| 1:B:981:ARG:HA | 1:B:984:TYR:HD2 | 1.71 | 0.54 |
| 1:B:2366:LYS:HZ2 | 2:S:101:UNK:HA | 1.73 | 0.54 |
| 1:A:1080:LEU:HD13 | 1:A:1127:CYS:CB | 2.38 | 0.54 |
| 1:A:1087:ARG:HD3 | 1:A:1134:LEU:HB3 | 1.89 | 0.54 |
| 1:A:1166:LEU:HB3 | 1:A:1170:LYS:NZ | 2.23 | 0.54 |
| 1:A:1582:LEU:O | 1:A:1585:SER:HB3 | 2.08 | 0.54 |
| 1:A:1718:ILE:HG23 | 1:A:1750:LEU:HD11 | 1.89 | 0.54 |
| 1:A:2039:GLU:HG2 | 1:A:2077:HIS:NE2 | 2.23 | 0.54 |
| 1:A:2200:ALA:HA | 1:A:2203:THR:HG22 | 1.89 | 0.54 |
| 1:A:2855:VAL:O | 1:A:2859:GLN:HB2 | 2.08 | 0.54 |
| 1:A:3518:VAL:HA | 1:A:3521:ILE:HG22 | 1.90 | 0.54 |
| 1:A:3857:LEU:HA | 1:A:3859:TYR:CE2 | 2.43 | 0.54 |
| 1:A:2891:ARG:HH22 | 1:A:3884:LYS:HE2 | 1.73 | 0.54 |
| 1:A:508:HIS:HB3 | 1:A:725:LEU:HB3 | 1.90 | 0.54 |
| 1:B:2798:ALA:HB3 | 1:B:2799:GLN:NE2 | 2.23 | 0.54 |
| 1:B:3578:LEU:HD22 | 1:B:3683:CYS:SG | 2.47 | 0.54 |
| 1:B:629:PHE:CZ | 1:B:666:PHE:O | 2.60 | 0.54 |
| 1:A:1008:ALA:O | 1:A:1011:GLU:HB3 | 2.08 | 0.53 |
| 1:A:1175:HIS:O | 1:A:1179:PRO:HD3 | 2.08 | 0.53 |
| 1:A:1804:MSE:O | 1:A:1808:ASP:HB3 | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1939:LEU:CD1 | 1:A:1986:ARG:HG2 | 2.38 | 0.53 |
| 1:A:2148:LYS:HD2 | 1:A:2188:GLU:OE2 | 2.08 | 0.53 |
| 1:A:3122:HIS:HB3 | 1:A:3126:LEU:HD13 | 1.89 | 0.53 |
| 1:A:3502:MSE:HE3 | 1:A:3517:SER:HB3 | 1.89 | 0.53 |
| 1:A:3525:TYR:CE1 | 1:A:3561:LYS:HD2 | 2.43 | 0.53 |
| 1:A:3974:MSE:HA | 1:A:3975:LYS:CB | 2.38 | 0.53 |
| 1:A:414:LEU:HG | 1:A:414:LEU:O | 2.01 | 0.53 |
| 1:A:548:GLU:O | 1:A:552:SER:OG | 2.21 | 0.53 |
| 1:B:1348:LEU:HD23 | 1:B:1353:PRO:HD3 | 1.90 | 0.53 |
| 1:B:1733:THR:HB | 1:B:1877:LEU:HD22 | 1.90 | 0.53 |
| 1:B:2813:PHE:HA | 1:B:2816:ILE:HG22 | 1.89 | 0.53 |
| 1:B:3047:SER:HB2 | 1:B:3050:LYS:HE2 | 1.90 | 0.53 |
| 1:B:3690:PHE:CZ | 1:B:3722:PHE:HD2 | 2.26 | 0.53 |
| 1:B:3917:ILE:O | 1:B:4048:LYS:CE | 2.56 | 0.53 |
| 1:B:3965:ARG:HG3 | 1:B:3969:ASN:OD1 | 2.09 | 0.53 |
| 2:S:217:UNK:O | 2:S:220:MSE:HG2 | 2.08 | 0.53 |
| 1:A:1817:GLN:HA | 1:A:1820:VAL:HG22 | 1.90 | 0.53 |
| 1:A:3789:ARG:HD3 | 1:A:3938:ILE:HG21 | 1.89 | 0.53 |
| 1:A:3794:VAL:HG11 | 1:A:3796:MSE:HE3 | 1.90 | 0.53 |
| 1:A:3819:THR:HG1 | 1:A:3889:ARG:HH12 | 1.46 | 0.53 |
| 1:B:1575:LEU:HD13 | 1:B:1604:SER:HB3 | 1.90 | 0.53 |
| 1:B:1648:LEU:HD22 | 1:B:1684:LEU:HD22 | 1.89 | 0.53 |
| 1:B:356:ASN:ND2 | 1:B:1859:ASN:H | 2.07 | 0.53 |
| 1:B:2049:VAL:HA | 1:B:2052:TYR:HD2 | 1.71 | 0.53 |
| 1:B:2870:SER:HA | 1:B:2897:LEU:HD22 | 1.89 | 0.53 |
| 1:B:294:PHE:O | 1:B:297:LEU:HG | 2.09 | 0.53 |
| 1:B:3469:LEU:O | 1:B:3474:ARG:HG2 | 2.08 | 0.53 |
| 1:B:3636:PHE:C | 1:B:3638:LYS:H | 2.12 | 0.53 |
| 1:B:3927:ASN:O | 1:B:3940:ILE:HG22 | 2.08 | 0.53 |
| 1:B:629:PHE:HZ | 1:B:666:PHE:O | 1.91 | 0.53 |
| 1:B:762:TYR:C | 1:B:764:PRO:HD3 | 2.29 | 0.53 |
| 1:A:1046:PRO:O | 1:A:1049:GLN:HB3 | 2.08 | 0.53 |
| 1:A:2078:ASP:HB3 | 1:A:2135:ASN:ND2 | 2.23 | 0.53 |
| 1:A:2168:LEU:HD13 | 1:A:2214:ARG:CZ | 2.37 | 0.53 |
| 1:A:368:LEU:HD23 | 1:A:372:PRO:CG | 2.37 | 0.53 |
| 1:A:489:ARG:HH22 | 1:A:492:SER:HB3 | 1.72 | 0.53 |
| 1:A:661:PRO:HG2 | 1:A:733:LEU:CA | 2.38 | 0.53 |
| 1:A:926:THR:O | 1:A:930:ALA:CB | 2.56 | 0.53 |
| 1:B:1590:THR:O | 1:B:1592:MSE:N | 2.41 | 0.53 |
| 1:B:1723:PRO:C | 1:B:1725:GLN:H | 2.12 | 0.53 |
| 1:B:2009:LYS:NZ | 1:B:2011:ALA:HA | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2196:TRP:CE2 | 1:B:2199:LEU:HD11 | 2.44 | 0.53 |
| 1:B:3585:PHE:HD1 | 1:B:3613:MSE:HE1 | 1.73 | 0.53 |
| 1:B:3790:THR:HG22 | 1:B:3791:TYR:H | 1.73 | 0.53 |
| 1:B:641:PHE:CE1 | 1:B:663:ILE:HG21 | 2.42 | 0.53 |
| 1:B:757:LYS:HA | 1:B:760:LEU:HD12 | 1.90 | 0.53 |
| 1:A:1032:CYS:HB3 | 1:A:1036:PHE:CZ | 2.44 | 0.53 |
| 1:A:1083:ASN:HB2 | 1:A:1107:TYR:HE2 | 1.74 | 0.53 |
| 1:A:1111:LEU:HD23 | 1:A:1128:CYS:SG | 2.48 | 0.53 |
| 1:A:306:VAL:O | 1:A:309:LYS:HG3 | 2.08 | 0.53 |
| 1:A:3141:PHE:HZ | 1:A:3192:LYS:HB2 | 1.73 | 0.53 |
| 1:A:3300:VAL:HG23 | 1:A:3328:ILE:HD13 | 1.89 | 0.53 |
| 1:A:3462:ARG:HE | 1:A:3501:HIS:CD2 | 2.27 | 0.53 |
| 1:A:361:ILE:HG13 | 1:A:362:ALA:N | 2.23 | 0.53 |
| 1:A:3944:HIS:NE2 | 1:A:4020:MSE:HE3 | 2.23 | 0.53 |
| 1:A:47:SER:H | 1:A:51:LEU:HD12 | 1.74 | 0.53 |
| 1:A:535:LEU:HB3 | 1:A:626:LEU:HD11 | 1.91 | 0.53 |
| 1:A:756:PHE:O | 1:A:759:GLY:C | 2.47 | 0.53 |
| 1:B:1275:THR:HA | 1:B:1279:LEU:HB2 | 1.90 | 0.53 |
| 1:B:1267:TYR:OH | 1:B:1340:ARG:NH2 | 2.41 | 0.53 |
| 1:B:1941:HIS:ND1 | 1:B:1941:HIS:O | 2.40 | 0.53 |
| 1:B:2300:PHE:CE2 | 1:B:2341:LEU:HB2 | 2.44 | 0.53 |
| 1:B:3311:ASN:O | 1:B:3313:SER:N | 2.39 | 0.53 |
| 1:B:3458:SER:OG | 1:B:3494:GLN:NE2 | 2.42 | 0.53 |
| 1:B:3530:VAL:HA | 1:B:3533:PHE:CD2 | 2.43 | 0.53 |
| 1:B:3629:ARG:NH2 | 1:B:3638:LYS:NZ | 2.53 | 0.53 |
| 1:B:3699:LEU:HG | 1:B:3701:ILE:HG23 | 1.90 | 0.53 |
| 1:B:969:LEU:O | 1:B:973:ALA:HB2 | 2.07 | 0.53 |
| 1:B:977:ASP:O | 1:B:980:THR:HB | 2.09 | 0.53 |
| 1:A:1221:ILE:HG12 | 1:A:1274:ARG:NH1 | 2.24 | 0.53 |
| 1:A:1288:SER:O | 1:A:1290:LEU:N | 2.42 | 0.53 |
| 1:A:1306:ILE:HG22 | 1:A:1381:SER:HB3 | 1.90 | 0.53 |
| 1:A:1758:LEU:HD13 | 1:A:1860:GLU:HG2 | 1.89 | 0.53 |
| 1:A:2094:MSE:HE1 | 1:A:2143:ARG:CA | 2.38 | 0.53 |
| 1:A:2352:HIS:CG | 1:A:2364:LEU:HD21 | 2.44 | 0.53 |
| 1:A:276:ALA:HA | 1:A:280:SER:OG | 2.09 | 0.53 |
| 1:A:3529:ILE:HG13 | 1:A:3532:PRO:HG2 | 1.89 | 0.53 |
| 1:A:567:GLU:HB3 | 1:A:606:SER:CB | 2.39 | 0.53 |
| 1:B:1015:ASP:HA | 1:B:1018:VAL:HG22 | 1.90 | 0.53 |
| 1:B:1044:ILE:O | 1:B:1045:THR:OG1 | 2.25 | 0.53 |
| 1:B:430:VAL:HG21 | 1:B:1682:THR:HG23 | 1.90 | 0.53 |
| 1:B:397:LEU:HD21 | 1:B:1813:SER:HB3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3259:LEU:O | 1:B:3263:HIS:CB | 2.53 | 0.53 |
| 1:B:3605:ASN:O | 1:B:3609:MSE:HG3 | 2.07 | 0.53 |
| 1:A:1348:LEU:O | 1:A:1352:SER:N | 2.35 | 0.53 |
| 1:A:2129:LEU:HB3 | 1:A:2156:VAL:HG13 | 1.90 | 0.53 |
| 1:A:3266:SER:HB2 | 1:A:3271:ASP:CG | 2.29 | 0.53 |
| 1:A:3486:GLU:O | 1:A:3489:SER:N | 2.41 | 0.53 |
| 1:A:3617:LEU:HD13 | 1:A:3644:PHE:HD2 | 1.74 | 0.53 |
| 1:A:364:ARG:O | 1:A:368:LEU:N | 2.24 | 0.53 |
| 1:A:965:THR:HA | 1:A:968:VAL:HG12 | 1.90 | 0.53 |
| 1:B:110:THR:O | 1:B:114:VAL:HG23 | 2.07 | 0.53 |
| 1:B:1756:PRO:C | 1:B:1758:LEU:H | 2.11 | 0.53 |
| 1:B:2280:VAL:HG13 | 1:B:2287:PRO:HB2 | 1.91 | 0.53 |
| 1:B:3530:VAL:HG11 | 1:B:3700:GLU:O | 2.09 | 0.53 |
| 1:B:4017:GLU:N | 1:B:4017:GLU:OE1 | 2.39 | 0.53 |
| 1:B:69:VAL:HG12 | 1:B:70:ARG:N | 2.24 | 0.53 |
| 1:B:884:VAL:HG11 | 1:B:3889:ARG:O | 2.08 | 0.53 |
| 1:A:1004:GLN:O | 1:A:1008:ALA:CB | 2.56 | 0.53 |
| 1:A:1513:GLY:O | 1:A:1517:LEU:HG | 2.07 | 0.53 |
| 1:A:1567:ILE:O | 1:A:1571:LEU:HG | 2.09 | 0.53 |
| 1:A:1976:LEU:HD22 | 1:A:1981:LEU:HD22 | 1.91 | 0.53 |
| 1:A:2870:SER:C | 1:A:2872:ASP:H | 2.11 | 0.53 |
| 1:A:3464:LYS:HG3 | 1:A:3468:LEU:HD11 | 1.91 | 0.53 |
| 1:A:3493:TRP:HB2 | 1:A:3713:PRO:HG3 | 1.91 | 0.53 |
| 1:A:3818:ASN:O | 1:A:3821:SER:HB3 | 2.08 | 0.53 |
| 1:A:361:ILE:HD11 | 1:A:413:PHE:CZ | 2.44 | 0.53 |
| 1:A:947:GLN:HB2 | 1:A:949:PRO:HD3 | 1.89 | 0.53 |
| 1:B:1256:TRP:O | 1:B:1260:LEU:HG | 2.08 | 0.53 |
| 1:B:150:GLY:HA2 | 1:B:153:PHE:CE2 | 2.43 | 0.53 |
| 1:B:1914:THR:HG22 | 1:B:1955:VAL:HG21 | 1.89 | 0.53 |
| 1:B:1988:TYR:OH | 1:B:2044:ASP:OD2 | 2.24 | 0.53 |
| 1:B:2349:LEU:HD23 | 1:B:2364:LEU:HD22 | 1.90 | 0.53 |
| 1:B:2798:ALA:O | 1:B:2802:PRO:HD2 | 2.09 | 0.53 |
| 1:B:2890:ILE:HD12 | 1:B:2918:PRO:HB3 | 1.90 | 0.53 |
| 1:B:3588:TRP:O | 1:B:3592:VAL:HG23 | 2.09 | 0.53 |
| 1:B:3459:ASN:ND2 | 1:B:3710:LYS:NZ | 2.57 | 0.53 |
| 1:B:75:SER:O | 1:B:77:GLU:N | 2.41 | 0.53 |
| 1:A:995:PHE:CE1 | 1:A:1003:SER:HA | 2.43 | 0.53 |
| 1:A:995:PHE:HZ | 1:A:1006:THR:HB | 1.74 | 0.53 |
| 1:A:1067:ALA:HB1 | 1:A:1111:LEU:CD1 | 2.38 | 0.53 |
| 1:A:361:ILE:HG12 | 1:A:1858:LEU:HD23 | 1.91 | 0.53 |
| 1:A:2094:MSE:HA | 1:A:2094:MSE:HE3 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:313:LEU:O | 1:A:316:LEU:N | 2.42 | 0.53 |
| 1:A:321:LYS:O | 1:A:325:ASN:ND2 | 2.33 | 0.53 |
| 1:A:3280:TYR:O | 1:A:3283:LEU:HB3 | 2.09 | 0.53 |
| 1:A:3620:PRO:HG2 | 1:A:3641:ASP:OD2 | 2.08 | 0.53 |
| 1:A:4002:MSE:SE | 1:A:4048:LYS:HE3 | 2.58 | 0.53 |
| 1:A:771:ASN:C | 1:A:773:LEU:H | 2.12 | 0.53 |
| 1:B:1158:PRO:HB2 | 1:B:1159:PRO:HD3 | 1.91 | 0.53 |
| 1:B:1685:ASP:OD1 | 1:B:1717:LEU:HD13 | 2.09 | 0.53 |
| 1:B:179:GLY:O | 1:B:183:GLU:HG3 | 2.08 | 0.53 |
| 1:B:2502:ALA:O | 1:B:2506:LEU:HG | 2.08 | 0.53 |
| 1:B:3133:GLN:O | 1:B:3137:GLU:HG2 | 2.09 | 0.53 |
| 1:B:3487:ILE:HD11 | 1:B:3498:TRP:HH2 | 1.74 | 0.53 |
| 1:B:3908:HIS:CG | 1:B:3967:PHE:CZ | 2.97 | 0.53 |
| 1:B:3997:LEU:H | 1:B:3997:LEU:HD12 | 1.73 | 0.53 |
| 1:B:808:GLU:OE1 | 1:B:3114:TYR:HB3 | 2.08 | 0.53 |
| 1:A:2186:VAL:HG21 | 1:A:2219:LEU:HD21 | 1.91 | 0.53 |
| 1:A:3024:PRO:HB2 | 1:A:3067:LYS:NZ | 2.23 | 0.53 |
| 1:A:3251:ASN:ND2 | 1:A:3254:LEU:HB2 | 2.24 | 0.53 |
| 1:A:3578:LEU:HD11 | 1:A:3686:TRP:CZ3 | 2.43 | 0.53 |
| 1:A:3457:ASN:CG | 1:A:3710:LYS:HZ2 | 2.12 | 0.53 |
| 1:B:1802:TYR:HA | 1:B:1805:PHE:CD2 | 2.37 | 0.53 |
| 1:B:1916:ILE:O | 1:B:1920:TYR:HD1 | 1.92 | 0.53 |
| 1:B:2009:LYS:HG2 | 1:B:2011:ALA:N | 2.24 | 0.53 |
| 1:B:2379:MSE:SE | 1:B:2408:MSE:SE | 3.27 | 0.53 |
| 1:B:2532:PRO:HG2 | 1:B:2538:ARG:N | 2.23 | 0.53 |
| 1:B:2870:SER:C | 1:B:2872:ASP:H | 2.04 | 0.53 |
| 1:B:2877:SER:O | 1:B:2879:GLY:N | 2.28 | 0.53 |
| 1:B:3080:LEU:HA | 1:B:3086:LEU:HD22 | 1.91 | 0.53 |
| 1:B:3719:ILE:HG23 | 1:B:3720:ALA:H | 1.73 | 0.53 |
| 1:B:3879:PRO:HG2 | 1:B:4128:MSE:HE3 | 1.91 | 0.53 |
| 1:B:3946:PHE:CE2 | 1:B:4048:LYS:HD2 | 2.44 | 0.53 |
| 1:B:3972:LEU:HB2 | 1:B:3974:MSE:HE2 | 1.91 | 0.53 |
| 1:B:531:PHE:CZ | 1:B:619:ASP:HB2 | 2.43 | 0.53 |
| 1:B:550:PHE:CZ | 1:B:632:GLU:HG2 | 2.42 | 0.53 |
| 1:A:1382:ILE:HD12 | 1:A:1386:ILE:HD11 | 1.91 | 0.53 |
| 1:A:139:ARG:O | 1:A:141:SER:N | 2.39 | 0.53 |
| 1:A:1982:ILE:HG23 | 1:A:1986:ARG:NE | 2.24 | 0.53 |
| 1:A:2083:LEU:N | 1:A:2086:ASP:HB2 | 2.24 | 0.53 |
| 1:A:2412:TYR:HD2 | 1:A:2416:LYS:HZ2 | 1.57 | 0.53 |
| 1:A:3238:MSE:O | 1:A:3242:MSE:HG3 | 2.08 | 0.53 |
| 1:A:3498:TRP:NE1 | 1:A:3502:MSE:HB2 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3696:ARG:O | 1:A:3699:LEU:HB2 | 2.09 | 0.53 |
| 1:A:558:GLU:HA | 1:A:561:ASN:ND2 | 2.24 | 0.53 |
| 1:A:562:HIS:HA | 1:A:565:TYR:HB3 | 1.91 | 0.53 |
| 1:B:1349:LEU:CD2 | 1:B:1359:LEU:HB2 | 2.38 | 0.53 |
| 1:B:1652:ILE:HG13 | 1:B:1684:LEU:HD12 | 1.90 | 0.53 |
| 1:B:244:THR:O | 1:B:248:ILE:HG13 | 2.09 | 0.53 |
| 1:B:2517:LEU:H | 1:B:2517:LEU:HD23 | 1.73 | 0.53 |
| 1:B:3012:GLU:HB2 | 1:B:3050:LYS:HZ3 | 1.69 | 0.53 |
| 1:B:3425:ARG:NH1 | 1:B:4003:ASP:OD2 | 2.42 | 0.53 |
| 1:B:658:THR:N | 1:B:733:LEU:HD13 | 2.24 | 0.53 |
| 1:A:1550:VAL:HG23 | 1:A:1551:ILE:H | 1.74 | 0.52 |
| 1:A:1560:TYR:O | 1:A:1563:PHE:N | 2.30 | 0.52 |
| 1:A:1729:PHE:H | 1:A:1730:PRO:HD2 | 1.74 | 0.52 |
| 1:A:3145:ILE:HG23 | 1:A:3196:LYS:HG2 | 1.91 | 0.52 |
| 1:A:3640:PHE:HB3 | 1:A:3644:PHE:CE2 | 2.44 | 0.52 |
| 1:A:659:ARG:NH2 | 1:A:662:LEU:HG | 2.18 | 0.52 |
| 1:B:1733:THR:N | 1:B:1734:PRO:HD3 | 2.24 | 0.52 |
| 1:B:1933:LEU:HD22 | 1:B:1937:ARG:HG2 | 1.90 | 0.52 |
| 1:B:2273:GLY:O | 1:B:2276:LEU:HB3 | 2.09 | 0.52 |
| 1:B:2420:PHE:CE2 | 1:B:2424:MSE:HE3 | 2.44 | 0.52 |
| 1:B:3175:PRO:HB2 | 1:B:3178:ILE:HG13 | 1.90 | 0.52 |
| 1:B:357:LYS:HB2 | 1:B:361:ILE:HG22 | 1.89 | 0.52 |
| 1:B:385:TYR:CE2 | 1:B:424:LEU:HD21 | 2.44 | 0.52 |
| 1:B:986:PRO:O | 1:B:990:GLN:HG2 | 2.10 | 0.52 |
| 1:A:1111:LEU:O | 1:A:1114:ALA:HB3 | 2.09 | 0.52 |
| 1:A:2462:VAL:HG11 | 1:A:2473:MSE:HE1 | 1.91 | 0.52 |
| 1:A:3007:GLU:HA | 1:A:3011:LEU:HB2 | 1.90 | 0.52 |
| 1:A:3051:LEU:HD22 | 1:A:3058:ASP:HB2 | 1.91 | 0.52 |
| 1:A:3170:ASP:O | 1:A:3172:LYS:NZ | 2.39 | 0.52 |
| 1:A:3397:GLN:NE2 | 1:A:3449:LYS:HD3 | 2.21 | 0.52 |
| 1:A:3498:TRP:O | 1:A:3498:TRP:CD1 | 2.61 | 0.52 |
| 1:A:4081:ALA:HB2 | 1:A:4116:ILE:HD11 | 1.90 | 0.52 |
| 1:B:1096:VAL:HG23 | 1:B:1099:PHE:HE2 | 1.73 | 0.52 |
| 1:B:1356:TRP:HZ2 | 1:B:1409:SER:HB3 | 1.72 | 0.52 |
| 1:B:138:PHE:CD2 | 1:B:173:LYS:HE3 | 2.38 | 0.52 |
| 1:B:2223:VAL:HB | 1:B:2238:ILE:HD12 | 1.92 | 0.52 |
| 1:B:245:SER:O | 1:B:248:ILE:N | 2.42 | 0.52 |
| 1:B:2461:PHE:O | 1:B:2465:PRO:HD3 | 2.09 | 0.52 |
| 1:B:2999:LEU:HA | 1:B:3002:TYR:CE2 | 2.44 | 0.52 |
| 1:B:3461:ALA:O | 1:B:3464:LYS:N | 2.41 | 0.52 |
| 1:B:396:PHE:CZ | 1:B:397:LEU:HG | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:730:LEU:HA | 1:B:733:LEU:CD1 | 2.39 | 0.52 |
| 1:B:933:LEU:O | 1:B:936:SER:N | 2.41 | 0.52 |
| 1:A:104:SER:HA | 1:A:107:ILE:HD12 | 1.92 | 0.52 |
| 1:A:103:TYR:O | 1:A:107:ILE:HG13 | 2.09 | 0.52 |
| 1:A:1520:ALA:O | 1:A:1524:LEU:HD13 | 2.09 | 0.52 |
| 1:A:1725:GLN:OE1 | 1:A:1754:GLN:NE2 | 2.43 | 0.52 |
| 1:A:175:TYR:HE1 | 1:A:200:PHE:CB | 2.23 | 0.52 |
| 1:A:1760:GLU:CB | 1:A:1894:SER:HA | 2.40 | 0.52 |
| 1:A:2281:MSE:SE | 1:A:2286:PRO:CB | 3.07 | 0.52 |
| 1:A:2395:THR:O | 1:A:2399:GLU:HB2 | 2.09 | 0.52 |
| 1:A:2420:PHE:HE1 | 1:A:2436:LEU:HD22 | 1.75 | 0.52 |
| 1:A:231:LEU:HB2 | 1:A:275:PHE:CZ | 2.44 | 0.52 |
| 1:A:3117:ILE:HD12 | 1:A:3125:ARG:NH1 | 2.23 | 0.52 |
| 1:A:4071:ALA:O | 1:A:4075:ARG:CB | 2.55 | 0.52 |
| 1:A:535:LEU:HD22 | 1:A:626:LEU:HG | 1.91 | 0.52 |
| 1:B:1073:PHE:CD1 | 1:B:1074:LYS:N | 2.74 | 0.52 |
| 1:B:1880:MSE:HE2 | 1:B:1884:LEU:HD21 | 1.92 | 0.52 |
| 1:B:217:LEU:N | 1:B:218:PRO:HD2 | 2.23 | 0.52 |
| 1:B:249:PHE:HD1 | 1:B:265:TYR:CE1 | 2.27 | 0.52 |
| 1:B:3684:SER:OG | 1:B:3685:PRO:HD3 | 2.10 | 0.52 |
| 1:B:580:ASP:OD1 | 1:B:581:LEU:N | 2.42 | 0.52 |
| 1:B:70:ARG:HG3 | 1:B:78:PHE:HB3 | 1.90 | 0.52 |
| 1:B:922:SER:O | 1:B:924:ARG:N | 2.42 | 0.52 |
| 1:A:1369:MSE:HE1 | 1:A:1414:ILE:O | 2.10 | 0.52 |
| 1:A:178:LEU:HB3 | 1:A:197:PHE:CZ | 2.45 | 0.52 |
| 1:A:2542:LEU:CB | 1:A:2546:TYR:HE2 | 2.18 | 0.52 |
| 1:A:3033:GLU:OE2 | 1:A:3079:GLU:OE2 | 2.27 | 0.52 |
| 1:A:307:GLU:H | 1:A:307:GLU:CD | 2.12 | 0.52 |
| 1:A:3416:LEU:CD1 | 1:A:3446:VAL:HG12 | 2.40 | 0.52 |
| 1:A:654:ILE:O | 1:A:657:SER:N | 2.42 | 0.52 |
| 1:A:703:CYS:O | 1:A:707:PHE:HD1 | 1.92 | 0.52 |
| 1:A:947:GLN:C | 1:A:949:PRO:HD3 | 2.30 | 0.52 |
| 1:B:1104:LEU:HD22 | 1:B:1135:CYS:SG | 2.49 | 0.52 |
| 1:B:1698:PHE:HD1 | 1:B:1699:PHE:N | 2.07 | 0.52 |
| 1:B:2464:HIS:H | 1:B:2465:PRO:HD3 | 1.74 | 0.52 |
| 1:B:2824:LYS:O | 1:B:2826:LEU:HG | 2.09 | 0.52 |
| 1:B:937:MSE:O | 1:B:941:MSE:HG3 | 2.08 | 0.52 |
| 1:A:1090:ARG:HH22 | 1:A:1096:VAL:HG22 | 1.74 | 0.52 |
| 1:A:608:PRO:HB2 | 1:A:1800:SER:HB2 | 1.91 | 0.52 |
| 1:A:2799:GLN:CB | 1:A:2808:LEU:HD11 | 2.40 | 0.52 |
| 1:A:3331:GLY:O | 1:A:3335:ARG:HD2 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3503:VAL:CG2 | 1:A:3536:SER:HA | 2.39 | 0.52 |
| 1:A:3588:TRP:O | 1:A:3592:VAL:HG23 | 2.08 | 0.52 |
| 1:A:3620:PRO:CB | 1:A:3633:ILE:HG23 | 2.39 | 0.52 |
| 1:A:368:LEU:C | 1:A:372:PRO:HG2 | 2.30 | 0.52 |
| 1:A:3769:GLN:O | 1:A:3773:GLY:HA3 | 2.10 | 0.52 |
| 1:A:385:TYR:CE1 | 1:A:421:LEU:HD23 | 2.45 | 0.52 |
| 1:A:730:LEU:HA | 1:A:733:LEU:HD12 | 1.90 | 0.52 |
| 1:B:1883:ARG:HB2 | 1:B:1923:PHE:CZ | 2.44 | 0.52 |
| 1:B:1911:LEU:O | 1:B:1913:LYS:N | 2.37 | 0.52 |
| 1:B:1913:LYS:HG3 | 1:B:1916:ILE:HD12 | 1.91 | 0.52 |
| 1:B:194:GLU:HA | 1:B:197:PHE:HD2 | 1.74 | 0.52 |
| 1:B:2002:LYS:O | 1:B:2004:TYR:N | 2.43 | 0.52 |
| 1:B:2308:SER:H | 1:B:2348:GLN:NE2 | 2.08 | 0.52 |
| 1:B:2854:PHE:CZ | 1:B:2881:LEU:HB2 | 2.45 | 0.52 |
| 1:B:2987:THR:HB | 1:B:2991:LYS:N | 2.20 | 0.52 |
| 1:B:3005:LEU:C | 1:B:3254:LEU:HD21 | 2.28 | 0.52 |
| 1:B:3625:LEU:HD13 | 1:B:3633:ILE:HG13 | 1.91 | 0.52 |
| 1:B:1244:LEU:HD13 | 1:B:3698:GLU:OE2 | 2.10 | 0.52 |
| 1:B:88:PHE:O | 1:B:91:ILE:HG13 | 2.09 | 0.52 |
| 1:B:981:ARG:CG | 1:B:982:GLN:N | 2.72 | 0.52 |
| 1:A:985:GLU:HG3 | 1:A:1031:ARG:NH2 | 2.25 | 0.52 |
| 1:A:1076:LEU:C | 1:A:1078:ALA:H | 2.12 | 0.52 |
| 1:A:1675:TYR:OH | 1:A:1679:LEU:HD11 | 2.10 | 0.52 |
| 1:A:2405:VAL:O | 1:A:2408:MSE:HB2 | 2.08 | 0.52 |
| 1:A:2854:PHE:CZ | 1:A:2881:LEU:HB2 | 2.44 | 0.52 |
| 1:A:3251:ASN:HD21 | 1:A:3254:LEU:HD13 | 1.75 | 0.52 |
| 1:A:3464:LYS:HD2 | 1:A:3467:ARG:HD2 | 1.91 | 0.52 |
| 1:A:3602:ASN:HA | 1:A:3606:ILE:HG12 | 1.92 | 0.52 |
| 1:A:3775:LEU:HB2 | 1:A:3787:GLN:NE2 | 2.24 | 0.52 |
| 1:A:476:ARG:O | 1:A:479:ILE:HB | 2.10 | 0.52 |
| 1:A:446:PHE:HB2 | 1:A:533:HIS:CD2 | 2.44 | 0.52 |
| 1:A:612:LEU:HD23 | 1:A:613:HIS:N | 2.24 | 0.52 |
| 1:A:913:ARG:HB3 | 1:A:934:LEU:HD12 | 1.90 | 0.52 |
| 1:B:2002:LYS:C | 1:B:2004:TYR:H | 2.12 | 0.52 |
| 1:B:1993:GLU:HG2 | 1:B:2043:PHE:CD2 | 2.44 | 0.52 |
| 1:B:2210:VAL:HG13 | 1:B:2211:LEU:HG | 1.90 | 0.52 |
| 1:B:2546:TYR:CE1 | 1:B:2558:ALA:CB | 2.90 | 0.52 |
| 1:B:2546:TYR:HE1 | 1:B:2558:ALA:CB | 2.20 | 0.52 |
| 1:B:2573:PRO:C | 1:B:2575:PRO:HD3 | 2.30 | 0.52 |
| 1:B:3064:PHE:CG | 1:B:3065:ILE:N | 2.74 | 0.52 |
| 1:B:4077:TYR:CZ | 1:B:4119:ARG:HG2 | 2.44 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:567:GLU:O | 1:B:571:SER:N | 2.42 | 0.52 |
| 1:B:580:ASP:O | 1:B:584:GLU:N | 2.43 | 0.52 |
| 1:B:631:ARG:HG2 | 1:B:669:LEU:HD11 | 1.91 | 0.52 |
| 1:B:658:THR:CG2 | 1:B:659:ARG:HH11 | 2.17 | 0.52 |
| 1:A:1067:ALA:HB1 | 1:A:1111:LEU:HD11 | 1.91 | 0.52 |
| 1:A:3280:TYR:CD1 | 1:A:3328:ILE:HD11 | 2.44 | 0.52 |
| 1:A:408:TYR:HB2 | 1:A:453:MSE:HG2 | 1.91 | 0.52 |
| 1:A:736:LEU:O | 1:A:740:ILE:HG13 | 2.10 | 0.52 |
| 1:A:967:PRO:O | 1:A:970:LEU:N | 2.42 | 0.52 |
| 1:B:1352:SER:HB3 | 1:B:1353:PRO:HD3 | 1.92 | 0.52 |
| 1:B:1399:CYS:O | 1:B:1403:MSE:HG3 | 2.10 | 0.52 |
| 1:B:1885:PRO:O | 1:B:1888:ASP:N | 2.42 | 0.52 |
| 1:B:2031:LEU:CB | 1:B:2033:ASP:HB2 | 2.37 | 0.52 |
| 1:B:2365:ASN:ND2 | 1:B:2382:VAL:HG11 | 2.24 | 0.52 |
| 1:B:2803:ILE:O | 1:B:2805:ALA:N | 2.43 | 0.52 |
| 1:B:2942:ILE:HG22 | 1:B:2943:PHE:CD1 | 2.45 | 0.52 |
| 1:B:3280:TYR:O | 1:B:3283:LEU:HB3 | 2.09 | 0.52 |
| 1:B:3575:LEU:HG | 1:B:3687:MSE:CG | 2.36 | 0.52 |
| 1:B:3649:SER:HA | 1:B:3652:LEU:HG | 1.92 | 0.52 |
| 1:B:552:SER:O | 1:B:556:SER:HB2 | 2.09 | 0.52 |
| 1:A:1733:THR:OG1 | 1:A:1877:LEU:HD13 | 2.09 | 0.52 |
| 1:A:2125:TRP:CZ2 | 1:A:2128:PHE:HB2 | 2.45 | 0.52 |
| 1:A:2427:ARG:HD3 | 1:A:2436:LEU:HD11 | 1.91 | 0.52 |
| 1:A:2538:ARG:HH11 | 1:A:2565:MSE:HG3 | 1.74 | 0.52 |
| 1:A:3461:ALA:O | 1:A:3464:LYS:N | 2.43 | 0.52 |
| 1:A:3496:ILE:HG23 | 1:A:3499:ILE:HD11 | 1.91 | 0.52 |
| 1:A:3964:THR:O | 1:A:3967:PHE:CD1 | 2.59 | 0.52 |
| 1:A:433:PRO:HB2 | 1:A:1812:LEU:HA | 1.91 | 0.52 |
| 1:A:653:LEU:HD12 | 1:A:656:GLN:HG3 | 1.92 | 0.52 |
| 1:B:1412:LYS:O | 1:B:1415:LEU:HB2 | 2.10 | 0.52 |
| 1:A:14:ARG:HE | 1:A:2396:LEU:CD1 | 2.23 | 0.52 |
| 1:A:2289:ASP:O | 1:A:2291:GLN:N | 2.43 | 0.52 |
| 1:A:2886:GLN:CG | 1:A:2887:PRO:HD3 | 2.39 | 0.52 |
| 1:A:3109:SER:O | 1:A:3112:GLN:HB3 | 2.10 | 0.52 |
| 1:A:3398:PRO:HG2 | 1:A:3399:PRO:HD3 | 1.92 | 0.52 |
| 1:A:872:THR:O | 1:A:876:SER:HB2 | 2.09 | 0.52 |
| 1:B:1006:THR:HA | 1:B:1009:LEU:HD12 | 1.91 | 0.52 |
| 1:B:2361:ILE:HA | 1:B:2364:LEU:HG | 1.92 | 0.52 |
| 1:B:3475:TYR:O | 1:B:3479:THR:HG22 | 2.09 | 0.52 |
| 1:B:358:GLU:O | 1:B:361:ILE:HG12 | 2.10 | 0.52 |
| 1:B:3840:LYS:O | 1:B:3844:THR:HG23 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:627:VAL:CG1 | 1:B:628:GLU:H | 2.17 | 0.52 |
| 1:B:865:GLN:HB2 | 1:B:869:ASN:OD1 | 2.10 | 0.52 |
| 1:A:1070:PRO:O | 1:A:1072:ALA:N | 2.43 | 0.52 |
| 1:A:1574:ASN:CG | 1:A:1582:LEU:HD21 | 2.30 | 0.52 |
| 1:A:1711:ARG:O | 1:A:1715:GLU:HG3 | 2.10 | 0.52 |
| 1:A:181:LEU:CD1 | 1:A:189:MSE:HE2 | 2.39 | 0.52 |
| 1:A:3856:MSE:O | 1:A:3859:TYR:OH | 2.10 | 0.52 |
| 1:A:493:LYS:HB3 | 1:A:494:PRO:CD | 2.39 | 0.52 |
| 1:A:611:ASN:C | 1:A:614:PRO:HD2 | 2.30 | 0.52 |
| 1:B:2058:ASP:C | 1:B:2061:PRO:HD2 | 2.30 | 0.52 |
| 1:B:2097:LEU:HD23 | 1:B:2100:LEU:HD22 | 1.90 | 0.52 |
| 1:B:2154:GLU:O | 1:B:2157:PHE:HB2 | 2.10 | 0.52 |
| 1:B:2183:HIS:O | 1:B:2187:VAL:CB | 2.26 | 0.52 |
| 1:B:2199:LEU:HA | 1:B:2202:PRO:HD2 | 1.92 | 0.52 |
| 1:B:2440:TYR:O | 1:B:2443:MSE:HE2 | 2.10 | 0.52 |
| 1:B:3058:ASP:OD1 | 1:B:3060:SER:N | 2.43 | 0.52 |
| 1:B:3277:VAL:HG23 | 1:B:3324:ARG:CD | 2.40 | 0.52 |
| 1:B:3487:ILE:HA | 1:B:3490:VAL:HG22 | 1.92 | 0.52 |
| 1:B:359:LEU:O | 1:B:362:ALA:HB3 | 2.10 | 0.52 |
| 1:B:413:PHE:O | 1:B:417:VAL:HG23 | 2.10 | 0.52 |
| 1:B:658:THR:O | 1:B:661:PRO:HD2 | 2.09 | 0.52 |
| 1:B:805:LEU:HA | 1:B:808:GLU:OE1 | 2.10 | 0.52 |
| 1:A:1010:LEU:HB2 | 1:A:1028:PHE:CE1 | 2.44 | 0.51 |
| 1:A:1014:LEU:HA | 1:A:1025:LEU:HD13 | 1.91 | 0.51 |
| 1:A:111:CYS:HA | 1:A:134:LEU:HD22 | 1.91 | 0.51 |
| 1:A:1632:TRP:HA | 1:A:1635:LYS:HD2 | 1.91 | 0.51 |
| 1:A:3311:ASN:O | 1:A:3313:SER:N | 2.43 | 0.51 |
| 1:A:3333:THR:OG1 | 1:A:3385:LEU:HB3 | 2.10 | 0.51 |
| 1:A:3912:CYS:HB2 | 1:A:3984:MSE:HE2 | 1.91 | 0.51 |
| 1:A:655:LEU:HD12 | 1:A:658:THR:HB | 1.91 | 0.51 |
| 1:B:1106:ILE:O | 1:B:1109:GLU:HB3 | 2.11 | 0.51 |
| 1:B:1132:ASP:HA | 1:B:1135:CYS:SG | 2.50 | 0.51 |
| 1:B:1524:LEU:HD11 | 1:B:1592:MSE:HE3 | 1.92 | 0.51 |
| 1:B:1640:GLU:HG2 | 1:B:1691:GLN:HG2 | 1.92 | 0.51 |
| 1:B:1747:LEU:HD23 | 1:B:1750:LEU:HD12 | 1.92 | 0.51 |
| 1:B:1758:LEU:HD22 | 1:B:1759:LEU:HD22 | 1.92 | 0.51 |
| 1:B:1957:ASN:O | 1:B:1961:PHE:N | 2.43 | 0.51 |
| 1:B:2454:LEU:O | 1:B:2457:PRO:HD2 | 2.10 | 0.51 |
| 1:B:2575:PRO:C | 1:B:2576:MSE:HG3 | 2.31 | 0.51 |
| 1:B:2884:LEU:O | 1:B:2887:PRO:HD2 | 2.10 | 0.51 |
| 1:B:2933:ILE:HG12 | 1:B:3979:LEU:O | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3781:CYS:SG | 1:B:3786:LEU:HB2 | 2.50 | 0.51 |
| 1:A:1101:PHE:CG | 1:A:1138:ILE:HG12 | 2.45 | 0.51 |
| 1:A:1330:TYR:O | 1:A:1333:SER:OG | 2.28 | 0.51 |
| 1:A:1590:THR:HG23 | 1:A:1591:LYS:N | 2.25 | 0.51 |
| 1:A:2003:LYS:O | 1:A:2007:ILE:HG13 | 2.11 | 0.51 |
| 1:A:2185:MSE:O | 1:A:2189:ILE:HG12 | 2.11 | 0.51 |
| 1:A:2298:GLU:HB3 | 1:A:2301:GLN:HB3 | 1.92 | 0.51 |
| 1:A:2379:MSE:HE3 | 1:A:2383:PHE:HD1 | 1.75 | 0.51 |
| 1:A:3462:ARG:HH21 | 1:A:3501:HIS:CD2 | 2.28 | 0.51 |
| 1:A:3505:LEU:O | 1:A:3510:GLN:HB2 | 2.11 | 0.51 |
| 1:A:3516:HIS:CG | 1:A:3517:SER:N | 2.77 | 0.51 |
| 1:A:3585:PHE:CE2 | 1:A:3613:MSE:SE | 3.13 | 0.51 |
| 1:A:3631:LYS:HD2 | 1:A:3682:GLU:HG2 | 1.91 | 0.51 |
| 1:A:3659:PHE:CD1 | 1:A:3662:ILE:HD12 | 2.45 | 0.51 |
| 1:A:3705:TYR:HD2 | 1:A:3792:SER:HB2 | 1.74 | 0.51 |
| 1:A:4088:ASN:OD1 | 1:A:4091:ALA:HB3 | 2.09 | 0.51 |
| 1:A:557:SER:O | 1:A:560:LEU:N | 2.42 | 0.51 |
| 1:A:760:LEU:HD11 | 1:A:799:TYR:HB2 | 1.92 | 0.51 |
| 1:A:939:MSE:CE | 1:A:942:LEU:HD13 | 2.40 | 0.51 |
| 1:B:1213:LYS:O | 1:B:1215:GLU:N | 2.43 | 0.51 |
| 1:B:1263:ALA:O | 1:B:1267:TYR:HD1 | 1.94 | 0.51 |
| 1:B:1905:ILE:HG12 | 1:B:1951:VAL:HG11 | 1.92 | 0.51 |
| 1:B:2177:ASN:HB3 | 1:B:2182:ILE:N | 2.24 | 0.51 |
| 1:B:2307:MSE:HB3 | 1:B:2348:GLN:NE2 | 2.17 | 0.51 |
| 1:B:2374:LEU:HD13 | 1:B:2377:ARG:HB2 | 1.91 | 0.51 |
| 1:B:276:ALA:HB2 | 1:B:318:SER:OG | 2.10 | 0.51 |
| 1:B:2796:ALA:O | 1:B:2800:ARG:HG3 | 2.10 | 0.51 |
| 1:B:3343:SER:O | 1:B:3345:PRO:HD3 | 2.10 | 0.51 |
| 1:B:613:HIS:CE1 | 1:B:614:PRO:HD3 | 2.45 | 0.51 |
| 1:B:886:TRP:HZ3 | 1:B:954:GLY:O | 1.93 | 0.51 |
| 1:A:127:ALA:O | 1:A:131:LEU:HB2 | 2.11 | 0.51 |
| 1:A:135:LEU:CD2 | 1:A:173:LYS:HD2 | 2.40 | 0.51 |
| 1:A:1376:LEU:HD23 | 1:A:1376:LEU:H | 1.75 | 0.51 |
| 1:A:17:GLU:OE2 | 1:A:61:ARG:NH1 | 2.43 | 0.51 |
| 1:A:1970:LYS:NZ | 1:A:2017:GLY:HA3 | 2.24 | 0.51 |
| 1:A:21:ALA:O | 1:A:24:ARG:HB2 | 2.11 | 0.51 |
| 1:A:352:VAL:HB | 1:A:357:LYS:HG2 | 1.92 | 0.51 |
| 1:A:3909:ALA:HB2 | 1:A:3980:MSE:HE3 | 1.92 | 0.51 |
| 1:A:576:VAL:HG13 | 1:A:601:TRP:HE3 | 1.76 | 0.51 |
| 1:A:649:PHE:HE1 | 1:A:653:LEU:H | 1.57 | 0.51 |
| 1:A:659:ARG:HH22 | 1:A:662:LEU:CG | 2.19 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:681:LYS:HD2 | 1:A:746:ARG:HE | 1.75 | 0.51 |
| 1:B:1029:CYS:CB | 1:B:1085:ILE:HG13 | 2.36 | 0.51 |
| 1:B:1275:THR:HA | 1:B:1279:LEU:CB | 2.41 | 0.51 |
| 1:B:1579:VAL:HG12 | 1:B:1635:LYS:HG2 | 1.91 | 0.51 |
| 1:B:208:MSE:SE | 1:B:220:LEU:HD21 | 2.61 | 0.51 |
| 1:B:2874:ALA:O | 1:B:2877:SER:N | 2.44 | 0.51 |
| 1:B:3107:ILE:HG23 | 1:B:3110:PHE:CZ | 2.45 | 0.51 |
| 1:B:384:MSE:O | 1:B:385:TYR:HB3 | 2.11 | 0.51 |
| 1:B:649:PHE:O | 1:B:651:TYR:N | 2.43 | 0.51 |
| 1:A:1072:ALA:HB1 | 1:A:1076:LEU:HD11 | 1.92 | 0.51 |
| 1:A:1266:CYS:O | 1:A:1269:THR:OG1 | 2.25 | 0.51 |
| 1:A:1750:LEU:O | 1:A:1754:GLN:HG3 | 2.10 | 0.51 |
| 1:A:2203:THR:O | 1:A:2208:ASP:N | 2.43 | 0.51 |
| 1:A:2450:GLU:O | 1:A:2454:LEU:HG | 2.11 | 0.51 |
| 1:A:2452:ARG:HG2 | 1:A:2498:ILE:CD1 | 2.40 | 0.51 |
| 1:A:266:ALA:CB | 1:A:308:LEU:HG | 2.41 | 0.51 |
| 1:A:3283:LEU:HD21 | 1:A:3297:VAL:HG22 | 1.92 | 0.51 |
| 1:A:3772:ASN:HB3 | 1:A:3788:LEU:H | 1.74 | 0.51 |
| 1:A:906:PHE:O | 1:A:909:VAL:N | 2.35 | 0.51 |
| 1:B:1298:LEU:O | 1:B:1302:ALA:HB2 | 2.10 | 0.51 |
| 1:B:111:CYS:O | 1:B:134:LEU:HD13 | 2.10 | 0.51 |
| 1:B:2436:LEU:O | 1:B:2439:ILE:HG22 | 2.10 | 0.51 |
| 1:B:3493:TRP:NE1 | 1:B:3708:ARG:O | 2.40 | 0.51 |
| 1:B:3794:VAL:HB | 1:B:3802:LEU:H | 1.76 | 0.51 |
| 1:B:3967:PHE:O | 1:B:3970:LEU:HD23 | 2.10 | 0.51 |
| 1:B:2957:LEU:CB | 1:B:3989:ARG:HH22 | 2.22 | 0.51 |
| 1:B:4013:TRP:CZ3 | 1:B:4014:LYS:HB2 | 2.45 | 0.51 |
| 1:A:1503:LEU:O | 1:A:1507:CYS:HB3 | 2.11 | 0.51 |
| 1:A:3588:TRP:HD1 | 1:A:3612:ARG:HD2 | 1.75 | 0.51 |
| 1:A:4019:LYS:HA | 1:A:4019:LYS:HE2 | 1.93 | 0.51 |
| 1:A:413:PHE:O | 1:A:417:VAL:HG23 | 2.11 | 0.51 |
| 1:A:863:GLY:HA2 | 1:A:866:ILE:HD11 | 1.91 | 0.51 |
| 1:B:1405:ALA:O | 1:B:1410:PRO:HD3 | 2.10 | 0.51 |
| 1:B:1970:LYS:CE | 1:B:2017:GLY:HA3 | 2.40 | 0.51 |
| 1:B:2094:MSE:SE | 1:B:2143:ARG:HG3 | 2.60 | 0.51 |
| 1:B:2355:THR:O | 1:B:2356:MSE:HG3 | 2.11 | 0.51 |
| 1:B:407:VAL:O | 1:B:411:PRO:HD3 | 2.10 | 0.51 |
| 1:B:941:MSE:HE3 | 1:B:958:MSE:CG | 2.40 | 0.51 |
| 1:A:1465:HIS:HA | 1:A:1469:PRO:CD | 2.41 | 0.51 |
| 1:A:2037:SER:O | 1:A:2041:SER:HB3 | 2.10 | 0.51 |
| 1:A:2114:GLU:HG3 | 1:A:2116:ASP:H | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2224:PHE:HZ | 1:A:2276:LEU:HD22 | 1.73 | 0.51 |
| 1:A:3147:LYS:O | 1:A:3151:LEU:HG | 2.10 | 0.51 |
| 1:A:3189:PHE:O | 1:A:3193:ILE:HB | 2.10 | 0.51 |
| 1:A:3813:LYS:HB3 | 1:A:3925:LEU:HG | 1.93 | 0.51 |
| 1:A:4062:ASP:HB3 | 1:A:4078:VAL:HG21 | 1.93 | 0.51 |
| 1:A:543:SER:C | 1:A:545:LEU:N | 2.63 | 0.51 |
| 1:A:609:ALA:HB2 | 1:A:1800:SER:OG | 2.11 | 0.51 |
| 1:A:619:ASP:O | 1:A:621:SER:N | 2.44 | 0.51 |
| 1:B:1266:CYS:HA | 1:B:1344:PHE:CE1 | 2.46 | 0.51 |
| 1:B:1879:VAL:C | 1:B:1882:SER:H | 2.14 | 0.51 |
| 1:B:3134:ALA:O | 1:B:3138:ILE:HG12 | 2.11 | 0.51 |
| 1:B:3298:LEU:HD11 | 1:B:3351:ILE:HD13 | 1.93 | 0.51 |
| 1:B:3525:TYR:CZ | 1:B:3533:PHE:HE1 | 2.29 | 0.51 |
| 1:B:3954:PRO:HB2 | 1:B:4027:TRP:CD1 | 2.45 | 0.51 |
| 1:B:511:SER:HB2 | 1:B:515:ARG:HG2 | 1.93 | 0.51 |
| 1:A:1378:GLU:O | 1:A:1382:ILE:HG12 | 2.11 | 0.51 |
| 1:A:1865:THR:HA | 1:A:1868:THR:OG1 | 2.10 | 0.51 |
| 1:A:1876:ILE:O | 1:A:1876:ILE:HG12 | 2.11 | 0.51 |
| 1:A:1993:GLU:O | 1:A:1997:PRO:HD2 | 2.10 | 0.51 |
| 1:A:19:LEU:HD22 | 1:A:30:ALA:HB1 | 1.93 | 0.51 |
| 1:A:3173:MSE:HB3 | 1:A:3175:PRO:HD2 | 1.93 | 0.51 |
| 1:A:3173:MSE:HG2 | 1:A:3174:ASP:OD1 | 2.11 | 0.51 |
| 1:A:3518:VAL:O | 1:A:3522:THR:OG1 | 2.10 | 0.51 |
| 1:A:514:VAL:HG11 | 1:A:610:ALA:O | 2.10 | 0.51 |
| 1:A:917:LEU:HD22 | 1:A:969:LEU:HG | 1.93 | 0.51 |
| 1:A:969:LEU:O | 1:A:973:ALA:HB2 | 2.10 | 0.51 |
| 1:B:153:PHE:O | 1:B:157:TYR:HD2 | 1.94 | 0.51 |
| 1:B:1975:LEU:HA | 1:B:1976:LEU:HB3 | 1.91 | 0.51 |
| 1:B:3142:ILE:O | 1:B:3145:ILE:HG22 | 2.11 | 0.51 |
| 1:B:3451:LEU:HD21 | 1:B:3483:MSE:HG2 | 1.93 | 0.51 |
| 1:B:3583:LEU:O | 1:B:3587:ASP:CB | 2.58 | 0.51 |
| 1:B:887:ASP:O | 1:B:3889:ARG:HB3 | 2.11 | 0.51 |
| 1:B:798:GLY:HA2 | 1:B:873:VAL:CG1 | 2.41 | 0.51 |
| 1:A:1073:PHE:CD1 | 1:A:1074:LYS:N | 2.76 | 0.51 |
| 1:A:1894:SER:C | 1:A:1896:ILE:N | 2.64 | 0.51 |
| 1:A:901:MSE:HG2 | 1:A:2819:GLU:HG2 | 1.92 | 0.51 |
| 1:A:2952:ILE:O | 1:A:2955:SER:OG | 2.18 | 0.51 |
| 1:A:3044:MSE:HE3 | 1:A:3060:SER:OG | 2.11 | 0.51 |
| 1:A:3354:ASP:O | 1:A:3357:ARG:HB2 | 2.11 | 0.51 |
| 1:A:371:GLY:O | 1:A:375:VAL:N | 2.44 | 0.51 |
| 1:A:3780:ALA:HB1 | 1:A:3784:ARG:NH1 | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3954:PRO:CG | 1:A:4027:TRP:HA | 2.41 | 0.51 |
| 1:A:421:LEU:C | 1:A:423:TYR:H | 2.13 | 0.51 |
| 1:A:968:VAL:HA | 1:A:971:ARG:HG2 | 1.93 | 0.51 |
| 1:B:1729:PHE:H | 1:B:1730:PRO:HD2 | 1.75 | 0.51 |
| 1:B:2038:GLU:HB3 | 1:B:2076:VAL:HG21 | 1.93 | 0.51 |
| 1:B:2365:ASN:HB2 | 1:B:2400:VAL:HG13 | 1.93 | 0.51 |
| 1:B:2470:ARG:HB3 | 1:B:2474:TYR:CE2 | 2.45 | 0.51 |
| 1:B:273:ARG:HE | 1:B:314:SER:HB3 | 1.76 | 0.51 |
| 1:B:2923:TRP:HD1 | 1:B:2926:LEU:HD21 | 1.76 | 0.51 |
| 1:B:3450:MSE:HG2 | 1:B:3464:LYS:HG2 | 1.93 | 0.51 |
| 1:B:3448:GLU:HA | 1:B:3451:LEU:HD22 | 1.91 | 0.51 |
| 1:B:19:LEU:HB2 | 1:B:34:LEU:HD22 | 1.92 | 0.51 |
| 1:B:3723:ASP:HB2 | 1:B:3741:ARG:NE | 2.26 | 0.51 |
| 1:B:981:ARG:HG2 | 1:B:982:GLN:N | 2.26 | 0.51 |
| 1:A:963:LYS:HB3 | 1:A:1009:LEU:HD11 | 1.93 | 0.51 |
| 1:A:2274:ILE:HD11 | 1:A:2314:GLU:HB3 | 1.92 | 0.51 |
| 1:A:2375:ALA:HB1 | 1:A:2411:LEU:HD22 | 1.93 | 0.51 |
| 1:A:2936:TYR:O | 1:A:2940:ARG:CB | 2.58 | 0.51 |
| 1:A:3705:TYR:CD2 | 1:A:3792:SER:HB2 | 2.46 | 0.51 |
| 1:A:3905:ALA:O | 1:A:3908:HIS:N | 2.44 | 0.51 |
| 1:A:479:ILE:O | 1:A:483:VAL:HG13 | 2.11 | 0.51 |
| 1:B:1132:ASP:O | 1:B:1135:CYS:N | 2.44 | 0.51 |
| 1:B:125:ILE:H | 1:B:126:PRO:CD | 2.24 | 0.51 |
| 1:B:83:GLU:HG3 | 1:B:130:LEU:HD13 | 1.91 | 0.51 |
| 1:B:1700:THR:O | 1:B:1702:LEU:N | 2.44 | 0.51 |
| 1:B:178:LEU:HB3 | 1:B:197:PHE:HZ | 1.75 | 0.51 |
| 1:B:287:LEU:C | 1:B:291:VAL:HB | 2.30 | 0.51 |
| 1:B:306:VAL:HG23 | 1:B:308:LEU:H | 1.75 | 0.51 |
| 1:B:3696:ARG:O | 1:B:3699:LEU:HB2 | 2.11 | 0.51 |
| 1:B:3751:LEU:HD13 | 1:B:3805:TRP:HB2 | 1.92 | 0.51 |
| 1:B:2928:LYS:HD2 | 1:B:3783:GLN:HB3 | 1.93 | 0.51 |
| 1:B:3883:LEU:HG | 1:B:3970:LEU:HD13 | 1.93 | 0.51 |
| 1:B:3989:ARG:HH21 | 1:B:4100:GLU:CB | 2.24 | 0.51 |
| 1:B:714:VAL:CG1 | 1:B:734:LEU:HD21 | 2.41 | 0.51 |
| 1:B:913:ARG:HE | 1:B:916:GLU:CD | 2.14 | 0.51 |
| 1:A:1004:GLN:O | 1:A:1008:ALA:HB2 | 2.11 | 0.51 |
| 1:A:100:ILE:O | 1:A:104:SER:N | 2.44 | 0.51 |
| 1:A:2205:VAL:HB | 1:A:2206:PRO:HD3 | 1.92 | 0.51 |
| 1:A:2356:MSE:SE | 1:A:2360:PHE:CZ | 3.14 | 0.51 |
| 1:A:273:ARG:HG3 | 1:A:274:LEU:H | 1.76 | 0.51 |
| 1:A:3614:TYR:CE1 | 1:A:3618:GLY:HA3 | 2.46 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:540:MSE:HG2 | 1:A:541:MSE:H | 1.76 | 0.51 |
| 1:A:743:LEU:HD22 | 1:A:746:ARG:HH12 | 1.76 | 0.51 |
| 1:A:877:ASP:O | 1:A:879:MSE:N | 2.44 | 0.51 |
| 1:B:716:VAL:HG11 | 1:B:1121:LEU:HD13 | 1.93 | 0.51 |
| 1:B:1122:GLY:O | 1:B:1123:THR:OG1 | 2.23 | 0.51 |
| 1:B:2495:SER:O | 1:B:2498:ILE:HB | 2.10 | 0.51 |
| 1:B:2890:ILE:HG21 | 1:B:2922:ARG:HH12 | 1.76 | 0.51 |
| 1:B:2943:PHE:O | 1:B:2945:SER:N | 2.41 | 0.51 |
| 1:B:3518:VAL:HG13 | 1:B:3554:PHE:CZ | 2.46 | 0.51 |
| 1:B:3568:ILE:HD11 | 1:B:3691:LYS:CD | 2.41 | 0.51 |
| 1:B:3572:ILE:HA | 1:B:3575:LEU:HB3 | 1.93 | 0.51 |
| 1:B:3901:ARG:HG2 | 1:B:3901:ARG:HH11 | 1.75 | 0.51 |
| 1:B:4077:TYR:OH | 1:B:4119:ARG:HG2 | 2.11 | 0.51 |
| 1:B:538:ASP:CB | 1:B:627:VAL:HG13 | 2.39 | 0.51 |
| 1:B:63:PHE:CD1 | 1:B:89:LEU:HD13 | 2.46 | 0.51 |
| 1:B:947:GLN:C | 1:B:949:PRO:HD3 | 2.32 | 0.51 |
| 1:A:1347:THR:O | 1:A:1351:THR:OG1 | 2.27 | 0.50 |
| 1:A:1342:MSE:HE2 | 1:A:1398:VAL:HG12 | 1.93 | 0.50 |
| 1:A:1472:SER:HA | 1:A:1476:HIS:CD2 | 2.46 | 0.50 |
| 1:A:1521:PHE:O | 1:A:1524:LEU:HB2 | 2.11 | 0.50 |
| 1:A:2323:LEU:HD11 | 1:A:2345:VAL:HG21 | 1.93 | 0.50 |
| 1:A:2443:MSE:SE | 1:A:2480:ILE:HG21 | 2.61 | 0.50 |
| 1:A:2464:HIS:H | 1:A:2465:PRO:CD | 2.24 | 0.50 |
| 1:A:2501:LEU:O | 1:A:2505:VAL:HG23 | 2.10 | 0.50 |
| 1:A:2884:LEU:C | 1:A:2887:PRO:HD2 | 2.32 | 0.50 |
| 1:A:3167:ARG:HG2 | 1:A:3186:ARG:NE | 2.26 | 0.50 |
| 1:A:3280:TYR:CZ | 1:A:3304:VAL:HG23 | 2.46 | 0.50 |
| 1:A:3979:LEU:CA | 1:A:3981:TYR:HB3 | 2.39 | 0.50 |
| 1:A:4038:TRP:CH2 | 1:A:4040:PRO:HB3 | 2.46 | 0.50 |
| 1:A:406:ARG:O | 1:A:409:GLN:N | 2.27 | 0.50 |
| 1:A:575:ILE:HD11 | 1:A:579:LEU:HD22 | 1.93 | 0.50 |
| 1:A:87:LYS:HG2 | 1:A:133:LYS:CG | 2.38 | 0.50 |
| 1:A:84:GLU:O | 1:A:88:PHE:HD1 | 1.94 | 0.50 |
| 1:B:2152:ASN:CB | 1:B:2153:THR:HA | 2.36 | 0.50 |
| 1:B:2204:GLY:HA2 | 1:B:2208:ASP:OD2 | 2.12 | 0.50 |
| 1:B:217:LEU:O | 1:B:221:ALA:HB2 | 2.10 | 0.50 |
| 1:B:3487:ILE:CG2 | 1:B:3495:PHE:HB2 | 2.37 | 0.50 |
| 1:B:3505:LEU:HD12 | 1:B:3509:ASP:HB3 | 1.91 | 0.50 |
| 1:B:2928:LYS:HG3 | 1:B:3783:GLN:O | 2.11 | 0.50 |
| 1:B:3820:MSE:HB2 | 1:B:3882:LEU:HD13 | 1.94 | 0.50 |
| 1:B:3915:HIS:ND1 | 1:B:3920:ILE:HD12 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:886:TRP:CD1 | 1:B:889:GLU:N | 2.69 | 0.50 |
| 1:B:929:ALA:O | 1:B:933:LEU:HB2 | 2.11 | 0.50 |
| 1:B:928:VAL:O | 1:B:932:GLU:HB2 | 2.11 | 0.50 |
| 1:A:1017:ILE:HG23 | 1:A:1018:VAL:HG13 | 1.92 | 0.50 |
| 1:A:1063:LEU:O | 1:A:1066:LEU:HB3 | 2.11 | 0.50 |
| 1:A:1584:GLN:O | 1:A:1588:ASP:OD1 | 2.29 | 0.50 |
| 1:A:1789:GLY:O | 1:A:1793:THR:HG23 | 2.12 | 0.50 |
| 1:A:3011:LEU:HB3 | 1:A:3047:SER:HB3 | 1.94 | 0.50 |
| 1:A:3768:PHE:O | 1:A:3771:MSE:N | 2.44 | 0.50 |
| 1:A:3981:TYR:CE1 | 1:A:4104:VAL:HB | 2.46 | 0.50 |
| 1:A:489:ARG:O | 1:A:489:ARG:CZ | 2.59 | 0.50 |
| 1:B:1376:LEU:HG | 1:B:1377:CYS:N | 2.26 | 0.50 |
| 1:B:1596:VAL:O | 1:B:1600:MSE:HG3 | 2.11 | 0.50 |
| 1:B:2031:LEU:C | 1:B:2033:ASP:N | 2.64 | 0.50 |
| 1:B:2390:HIS:ND1 | 1:B:2397:CYS:SG | 2.74 | 0.50 |
| 1:B:2462:VAL:CB | 1:B:2473:MSE:SE | 3.09 | 0.50 |
| 1:B:2935:GLU:O | 1:B:2939:LEU:HG | 2.10 | 0.50 |
| 1:B:348:ILE:HG23 | 1:B:357:LYS:HG3 | 1.93 | 0.50 |
| 1:B:3705:TYR:HE2 | 1:B:3708:ARG:HH12 | 1.60 | 0.50 |
| 1:B:3762:GLN:OE1 | 1:B:3795:PRO:HG3 | 2.11 | 0.50 |
| 1:B:390:GLN:O | 1:B:393:LYS:HG2 | 2.11 | 0.50 |
| 1:B:411:PRO:O | 1:B:415:GLN:HB2 | 2.12 | 0.50 |
| 1:B:419:SER:HA | 1:B:422:LEU:HG | 1.94 | 0.50 |
| 1:B:743:LEU:O | 1:B:746:ARG:HG2 | 2.11 | 0.50 |
| 1:B:796:LEU:HD22 | 1:B:799:TYR:HE2 | 1.76 | 0.50 |
| 1:A:1042:LYS:HZ1 | 1:A:1044:ILE:HD12 | 1.76 | 0.50 |
| 1:A:1350:ASN:ND2 | 1:A:1404:LYS:HG2 | 2.27 | 0.50 |
| 1:A:1698:PHE:CD1 | 1:A:1699:PHE:N | 2.79 | 0.50 |
| 1:A:173:LYS:HA | 1:A:176:GLU:OE1 | 2.11 | 0.50 |
| 1:A:1815:THR:C | 1:A:1816:ARG:HE | 2.14 | 0.50 |
| 1:A:2095:ALA:HB3 | 1:A:2096:PRO:HD3 | 1.92 | 0.50 |
| 1:A:2190:VAL:HA | 1:A:2193:ILE:HG22 | 1.93 | 0.50 |
| 1:A:2216:LEU:O | 1:A:2220:MSE:HG3 | 2.11 | 0.50 |
| 1:A:2254:ARG:HG3 | 1:A:2255:LEU:N | 2.27 | 0.50 |
| 1:A:2339:GLU:O | 1:A:2343:GLU:HG3 | 2.10 | 0.50 |
| 1:A:237:SER:O | 1:A:278:HIS:HB3 | 2.10 | 0.50 |
| 1:A:3007:GLU:OE2 | 1:A:3046:ARG:HD3 | 2.10 | 0.50 |
| 1:A:3108:GLN:HA | 1:A:3111:MSE:HG3 | 1.94 | 0.50 |
| 1:A:3780:ALA:HB1 | 1:A:3784:ARG:HH12 | 1.77 | 0.50 |
| 1:A:703:CYS:O | 1:A:706:LEU:HB2 | 2.11 | 0.50 |
| 1:B:1036:PHE:CZ | 1:B:1082:PHE:HE2 | 2.29 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1076:LEU:HD11 | 1:B:1114:ALA:HB1 | 1.93 | 0.50 |
| 1:B:1238:GLN:HB2 | 1:B:1239:PRO:HD3 | 1.94 | 0.50 |
| 1:B:1469:PRO:HA | 1:B:1472:SER:CB | 2.38 | 0.50 |
| 1:B:2088:LEU:O | 1:B:2092:GLU:N | 2.43 | 0.50 |
| 1:B:2145:PHE:CE1 | 1:B:2188:GLU:HB3 | 2.47 | 0.50 |
| 1:B:3072:GLU:HG3 | 1:B:3080:LEU:HD11 | 1.94 | 0.50 |
| 1:B:3789:ARG:NH2 | 1:B:3806:LEU:HD22 | 2.26 | 0.50 |
| 1:B:410:MSE:HE1 | 1:B:445:SER:CB | 2.42 | 0.50 |
| 1:A:964:ARG:N | 1:A:1009:LEU:HD13 | 2.26 | 0.50 |
| 1:A:1265:GLU:O | 1:A:1269:THR:HG23 | 2.10 | 0.50 |
| 1:A:1751:GLU:HG2 | 1:A:1870:LYS:CE | 2.39 | 0.50 |
| 1:A:1856:THR:O | 1:A:1860:GLU:HB2 | 2.12 | 0.50 |
| 1:A:1882:SER:C | 1:A:1885:PRO:HD2 | 2.32 | 0.50 |
| 1:A:2000:ARG:HG2 | 1:A:2001:LYS:HG3 | 1.92 | 0.50 |
| 1:A:2097:LEU:HD13 | 1:A:2143:ARG:HG2 | 1.93 | 0.50 |
| 1:A:232:CYS:SG | 1:A:274:LEU:HD13 | 2.51 | 0.50 |
| 1:A:2379:MSE:O | 1:A:2383:PHE:HB2 | 2.11 | 0.50 |
| 1:A:2386:LEU:HD11 | 1:A:2400:VAL:HG12 | 1.94 | 0.50 |
| 1:A:2956:ALA:HA | 1:A:2965:TYR:OH | 2.11 | 0.50 |
| 1:A:367:GLY:C | 1:A:369:PHE:N | 2.64 | 0.50 |
| 1:A:568:PHE:CZ | 1:A:653:LEU:HG | 2.47 | 0.50 |
| 1:A:767:GLU:O | 1:A:771:ASN:HB2 | 2.10 | 0.50 |
| 1:B:1162:SER:N | 1:B:1165:LEU:HD12 | 2.20 | 0.50 |
| 1:B:1220:LEU:HD13 | 1:B:1274:ARG:CG | 2.41 | 0.50 |
| 1:B:1503:LEU:O | 1:B:1507:CYS:HB3 | 2.11 | 0.50 |
| 1:B:1956:PHE:HB3 | 1:B:1998:MSE:HE1 | 1.93 | 0.50 |
| 1:B:2129:LEU:HD13 | 1:B:2156:VAL:HG13 | 1.93 | 0.50 |
| 1:B:2220:MSE:SE | 1:B:2256:ILE:CD1 | 3.10 | 0.50 |
| 1:B:3962:ARG:HD3 | 1:B:4124:TRP:CE3 | 2.46 | 0.50 |
| 1:B:554:ASN:O | 1:B:557:SER:HB2 | 2.11 | 0.50 |
| 1:B:852:ARG:CZ | 1:B:3111:MSE:SE | 3.09 | 0.50 |
| 1:A:1102:GLU:O | 1:A:1105:VAL:HG22 | 2.12 | 0.50 |
| 1:A:1107:TYR:HE1 | 1:A:1111:LEU:HD13 | 1.75 | 0.50 |
| 1:A:1678:LEU:O | 1:A:1682:THR:HG22 | 2.12 | 0.50 |
| 1:A:1922:ALA:HA | 1:A:1925:GLU:OE2 | 2.11 | 0.50 |
| 1:A:1886:LYS:NZ | 1:A:1924:THR:HB | 2.23 | 0.50 |
| 1:A:3593:ARG:HD2 | 1:A:3660:ASN:O | 2.12 | 0.50 |
| 1:A:3763:ARG:O | 1:A:3767:LEU:HB2 | 2.12 | 0.50 |
| 1:A:3901:ARG:HG2 | 1:A:3901:ARG:NH1 | 2.26 | 0.50 |
| 1:A:3981:TYR:O | 1:A:3985:VAL:HG23 | 2.11 | 0.50 |
| 1:A:3962:ARG:HD3 | 1:A:4124:TRP:CE3 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:487:LEU:O | 1:A:490:ILE:HG22 | 2.11 | 0.50 |
| 1:B:1039:TRP:HH2 | 1:B:1052:SER:HB3 | 1.76 | 0.50 |
| 1:B:1101:PHE:O | 1:B:1104:LEU:HB2 | 2.12 | 0.50 |
| 1:B:3151:LEU:O | 1:B:3156:PRO:HD3 | 2.11 | 0.50 |
| 1:B:3810:VAL:HG23 | 1:B:3815:LEU:HD11 | 1.93 | 0.50 |
| 1:B:385:TYR:CD1 | 1:B:420:VAL:HG13 | 2.40 | 0.50 |
| 1:B:527:TYR:CE1 | 1:B:615:ALA:HA | 2.46 | 0.50 |
| 1:B:67:VAL:O | 1:B:71:LYS:CB | 2.41 | 0.50 |
| 1:A:1502:SER:O | 1:A:1505:LEU:N | 2.43 | 0.50 |
| 1:A:175:TYR:OH | 1:A:204:LEU:HD11 | 2.10 | 0.50 |
| 1:A:2166:SER:O | 1:A:2170:GLN:HB3 | 2.12 | 0.50 |
| 1:A:288:ASP:N | 1:A:288:ASP:OD1 | 2.43 | 0.50 |
| 1:A:3674:SER:O | 1:A:3677:PRO:HD2 | 2.12 | 0.50 |
| 1:A:4007:LYS:CG | 1:A:4041:ARG:HD2 | 2.35 | 0.50 |
| 1:A:801:LYS:O | 1:A:805:LEU:HB2 | 2.11 | 0.50 |
| 1:A:85:ILE:O | 1:A:89:LEU:HG | 2.10 | 0.50 |
| 1:A:913:ARG:HB2 | 1:A:934:LEU:HD12 | 1.93 | 0.50 |
| 1:A:954:GLY:O | 1:A:957:PRO:HD2 | 2.12 | 0.50 |
| 1:B:1406:LEU:HA | 1:B:1410:PRO:HG3 | 1.94 | 0.50 |
| 1:B:1406:LEU:O | 1:B:1415:LEU:HD21 | 2.12 | 0.50 |
| 1:B:2352:HIS:CD2 | 1:B:2364:LEU:HD21 | 2.47 | 0.50 |
| 1:B:2430:GLU:OE1 | 1:B:2433:LYS:HE3 | 2.11 | 0.50 |
| 1:B:2936:TYR:CZ | 1:B:2940:ARG:HD2 | 2.47 | 0.50 |
| 1:B:3648:GLY:O | 1:B:3651:LEU:HB2 | 2.11 | 0.50 |
| 1:B:3766:GLN:O | 1:B:3770:VAL:HG23 | 2.11 | 0.50 |
| 1:B:512:GLY:CA | 1:B:602:MSE:HG3 | 2.40 | 0.50 |
| 1:B:68:PHE:O | 1:B:72:SER:OG | 2.10 | 0.50 |
| 1:B:722:LYS:HB3 | 1:B:727:ALA:CA | 2.42 | 0.50 |
| 1:B:734:LEU:C | 1:B:737:PRO:HD2 | 2.32 | 0.50 |
| 1:A:1036:PHE:CZ | 1:A:1082:PHE:HE2 | 2.30 | 0.50 |
| 1:A:1741:ASP:O | 1:A:1745:LYS:HG3 | 2.11 | 0.50 |
| 1:A:2318:ALA:O | 1:A:2322:VAL:HB | 2.12 | 0.50 |
| 1:A:3049:LEU:HA | 1:A:3188:PHE:CZ | 2.46 | 0.50 |
| 1:A:334:HIS:O | 1:A:338:LEU:HD11 | 2.12 | 0.50 |
| 1:A:3525:TYR:CZ | 1:A:3533:PHE:HE1 | 2.30 | 0.50 |
| 1:A:3998:LEU:O | 1:A:4001:THR:OG1 | 2.28 | 0.50 |
| 1:A:676:ASN:O | 1:A:680:ILE:HG13 | 2.11 | 0.50 |
| 1:A:743:LEU:HG | 1:A:783:HIS:CE1 | 2.44 | 0.50 |
| 1:A:66:LEU:CD2 | 1:A:89:LEU:HD11 | 2.42 | 0.50 |
| 1:B:1357:LYS:HG3 | 1:B:1360:LYS:NZ | 2.26 | 0.50 |
| 1:B:152:LEU:O | 1:B:156:PHE:HD1 | 1.95 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1696:LEU:HD23 | 1:B:1700:THR:HG21 | 1.92 | 0.50 |
| 1:B:1756:PRO:O | 1:B:1758:LEU:N | 2.34 | 0.50 |
| 1:B:1894:SER:O | 1:B:1896:ILE:N | 2.44 | 0.50 |
| 1:B:1972:GLU:CD | 1:B:1987:ARG:HH12 | 2.14 | 0.50 |
| 1:B:2320:ALA:HB1 | 1:B:2370:SER:OG | 2.10 | 0.50 |
| 1:B:2389:PHE:CD2 | 1:B:2396:LEU:HD22 | 2.46 | 0.50 |
| 1:B:2536:LEU:O | 1:B:2539:LEU:HB2 | 2.11 | 0.50 |
| 1:B:368:LEU:HA | 1:B:372:PRO:HG2 | 1.94 | 0.50 |
| 1:B:3726:VAL:HG21 | 1:B:3736:LYS:HD3 | 1.93 | 0.50 |
| 1:B:4066:LEU:HD23 | 1:B:4075:ARG:HG3 | 1.94 | 0.50 |
| 1:B:888:ARG:HA | 1:B:907:LEU:HD21 | 1.94 | 0.50 |
| 1:A:1086:TYR:HD2 | 1:A:1090:ARG:HG2 | 1.76 | 0.50 |
| 1:A:1106:ILE:O | 1:A:1109:GLU:HB3 | 2.12 | 0.50 |
| 1:A:1298:LEU:HA | 1:A:1301:ILE:HB | 1.94 | 0.50 |
| 1:A:1433:ALA:O | 1:A:1437:TYR:CD2 | 2.65 | 0.50 |
| 1:A:1604:SER:HA | 1:A:1632:TRP:CE3 | 2.47 | 0.50 |
| 1:A:1956:PHE:HB3 | 1:A:1998:MSE:CE | 2.41 | 0.50 |
| 1:A:2512:ASP:H | 1:A:2519:LEU:HD12 | 1.76 | 0.50 |
| 1:A:2814:SER:O | 1:A:2818:LYS:HB2 | 2.11 | 0.50 |
| 1:A:293:LEU:O | 1:A:296:VAL:HG12 | 2.12 | 0.50 |
| 1:A:3464:LYS:O | 1:A:3467:ARG:HB3 | 2.12 | 0.50 |
| 1:A:3498:TRP:HD1 | 1:A:3498:TRP:O | 1.95 | 0.50 |
| 1:A:3789:ARG:CZ | 1:A:3806:LEU:HD22 | 2.40 | 0.50 |
| 1:A:4066:LEU:HD21 | 1:A:4078:VAL:HG21 | 1.94 | 0.50 |
| 1:A:741:ILE:O | 1:A:743:LEU:N | 2.45 | 0.50 |
| 1:A:969:LEU:O | 1:A:973:ALA:CB | 2.60 | 0.50 |
| 1:B:1074:LYS:O | 1:B:1075:ARG:HG3 | 2.12 | 0.50 |
| 1:B:1586:SER:HB3 | 1:B:1643:MSE:HE1 | 1.94 | 0.50 |
| 1:B:1736:PHE:O | 1:B:1740:VAL:HG23 | 2.11 | 0.50 |
| 1:B:175:TYR:HD2 | 1:B:222:GLY:HA3 | 1.76 | 0.50 |
| 1:B:1816:ARG:HB3 | 1:B:1819:PHE:CE1 | 2.45 | 0.50 |
| 1:B:2080:VAL:HG12 | 1:B:2081:LEU:H | 1.75 | 0.50 |
| 1:B:2212:ALA:O | 1:B:2215:LEU:N | 2.44 | 0.50 |
| 1:B:2879:GLY:HA2 | 1:B:2886:GLN:CG | 2.29 | 0.50 |
| 1:B:2964:ASP:O | 1:B:2968:ALA:HB2 | 2.12 | 0.50 |
| 1:B:2960:GLU:O | 1:B:2965:TYR:CD1 | 2.65 | 0.50 |
| 1:B:3179:TRP:CZ2 | 1:B:3258:LEU:HG | 2.47 | 0.50 |
| 1:B:3383:GLN:HG3 | 1:B:3438:GLU:OE2 | 2.12 | 0.50 |
| 1:B:3510:GLN:O | 1:B:3512:VAL:N | 2.34 | 0.50 |
| 1:B:3572:ILE:HD13 | 1:B:3575:LEU:HD22 | 1.94 | 0.50 |
| 1:B:898:PHE:CE2 | 1:B:2566:THR:HG21 | 2.47 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:966:PHE:CE2 | 1:B:988:VAL:HG12 | 2.47 | 0.50 |
| 1:A:1655:ILE:CD1 | 1:A:1681:ASP:HB3 | 2.40 | 0.50 |
| 1:A:1747:LEU:O | 1:A:1750:LEU:N | 2.41 | 0.50 |
| 1:A:1935:GLU:HB2 | 1:A:1986:ARG:NH2 | 2.27 | 0.50 |
| 1:A:2171:LEU:CG | 1:A:2177:ASN:HD21 | 2.25 | 0.50 |
| 1:A:2416:LYS:O | 1:A:2420:PHE:HB3 | 2.12 | 0.50 |
| 1:A:2538:ARG:HH22 | 1:A:2566:THR:CG2 | 2.25 | 0.50 |
| 1:A:3495:PHE:CZ | 1:A:3521:ILE:HG13 | 2.47 | 0.50 |
| 1:A:3865:THR:O | 1:A:3869:THR:OG1 | 2.14 | 0.50 |
| 1:A:629:PHE:HA | 1:A:634:LEU:HD21 | 1.91 | 0.50 |
| 1:B:1299:GLU:OE2 | 1:B:1367:HIS:HB2 | 2.12 | 0.50 |
| 1:B:1348:LEU:O | 1:B:1352:SER:N | 2.34 | 0.50 |
| 1:B:1455:CYS:O | 1:B:1458:LEU:HB2 | 2.11 | 0.50 |
| 1:B:1882:SER:C | 1:B:1885:PRO:HD2 | 2.33 | 0.50 |
| 1:B:2922:ARG:HD3 | 1:B:2930:TYR:HD1 | 1.77 | 0.50 |
| 1:B:3141:PHE:CZ | 1:B:3192:LYS:HB2 | 2.47 | 0.50 |
| 1:B:3277:VAL:HG23 | 1:B:3324:ARG:HD2 | 1.94 | 0.50 |
| 1:B:3507:ASP:CG | 1:B:3540:TYR:HA | 2.32 | 0.50 |
| 1:B:3503:VAL:HG21 | 1:B:3535:ILE:O | 2.12 | 0.50 |
| 1:B:12:LEU:HD13 | 1:B:42:CYS:SG | 2.52 | 0.50 |
| 1:A:1014:LEU:HB2 | 1:A:1078:ALA:CB | 2.41 | 0.49 |
| 1:A:2135:ASN:N | 1:A:2136:PRO:CD | 2.75 | 0.49 |
| 1:A:2196:TRP:HE1 | 1:A:2200:ALA:HB2 | 1.77 | 0.49 |
| 1:A:2373:PRO:HA | 1:A:2378:PHE:HZ | 1.77 | 0.49 |
| 1:A:242:PRO:HD3 | 1:A:282:PHE:CD2 | 2.47 | 0.49 |
| 1:A:232:CYS:HG | 1:A:275:PHE:HE1 | 1.60 | 0.49 |
| 1:A:3397:GLN:HB3 | 1:A:3398:PRO:CD | 2.42 | 0.49 |
| 1:A:3989:ARG:HH21 | 1:A:4100:GLU:HB2 | 1.77 | 0.49 |
| 1:A:4090:ARG:NH1 | 1:A:4106:CYS:HA | 2.20 | 0.49 |
| 1:A:569:VAL:HG13 | 1:A:570:LYS:H | 1.77 | 0.49 |
| 1:B:1553:PHE:O | 1:B:1557:GLU:HB2 | 2.12 | 0.49 |
| 1:B:428:PRO:HB3 | 1:B:1679:LEU:HD13 | 1.94 | 0.49 |
| 1:B:2157:PHE:O | 1:B:2160:TYR:N | 2.45 | 0.49 |
| 1:B:2373:PRO:HB3 | 1:B:2407:GLY:O | 2.11 | 0.49 |
| 1:B:2485:ARG:HH11 | 1:B:2530:ARG:CZ | 2.25 | 0.49 |
| 1:B:294:PHE:CZ | 1:B:319:PHE:CD2 | 2.96 | 0.49 |
| 1:B:2957:LEU:CA | 1:B:3989:ARG:HH22 | 2.24 | 0.49 |
| 1:B:2939:LEU:HD21 | 1:B:2994:TRP:CE2 | 2.47 | 0.49 |
| 1:B:3484:THR:HA | 1:B:3516:HIS:HE2 | 1.77 | 0.49 |
| 1:B:3858:MSE:HG3 | 1:B:4119:ARG:NE | 2.27 | 0.49 |
| 1:B:661:PRO:HG2 | 1:B:733:LEU:HA | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1905:ILE:HG23 | 1:A:1951:VAL:HG21 | 1.94 | 0.49 |
| 1:A:2066:PHE:HB3 | 1:A:2067:ARG:CG | 2.41 | 0.49 |
| 1:A:2177:ASN:ND2 | 1:A:2182:ILE:HA | 2.28 | 0.49 |
| 1:A:2168:LEU:HD13 | 1:A:2214:ARG:NE | 2.27 | 0.49 |
| 1:A:2255:LEU:HA | 1:A:2258:GLU:HB2 | 1.94 | 0.49 |
| 1:A:3531:TYR:HB3 | 1:A:3532:PRO:HD3 | 1.93 | 0.49 |
| 1:A:3578:LEU:HD11 | 1:A:3686:TRP:HZ3 | 1.77 | 0.49 |
| 1:A:2936:TYR:HB3 | 1:A:3979:LEU:CD1 | 2.41 | 0.49 |
| 1:A:455:LEU:HD13 | 1:A:459:ARG:CZ | 2.42 | 0.49 |
| 1:A:476:ARG:HA | 1:A:479:ILE:HD12 | 1.93 | 0.49 |
| 1:A:617:PRO:HB3 | 1:A:659:ARG:CG | 2.41 | 0.49 |
| 1:A:63:PHE:O | 1:A:66:LEU:HG | 2.13 | 0.49 |
| 1:A:730:LEU:O | 1:A:734:LEU:HG | 2.12 | 0.49 |
| 1:B:114:VAL:HG12 | 1:B:130:LEU:HD21 | 1.94 | 0.49 |
| 1:B:1927:MSE:C | 1:B:1929:GLY:H | 2.15 | 0.49 |
| 1:B:1965:PHE:O | 1:B:1968:SER:OG | 2.18 | 0.49 |
| 1:B:2220:MSE:HB3 | 1:B:2224:PHE:CZ | 2.47 | 0.49 |
| 1:B:2447:LYS:N | 1:B:2448:PRO:HD2 | 2.28 | 0.49 |
| 1:B:2458:VAL:HA | 1:B:2461:PHE:CD2 | 2.45 | 0.49 |
| 1:B:2961:ALA:HB1 | 1:B:3002:TYR:HB2 | 1.94 | 0.49 |
| 1:B:3272:TRP:CE3 | 1:B:3307:LEU:HD21 | 2.46 | 0.49 |
| 1:B:3280:TYR:CZ | 1:B:3304:VAL:HG23 | 2.47 | 0.49 |
| 1:B:3774:ILE:HG22 | 1:B:3775:LEU:HD23 | 1.94 | 0.49 |
| 1:B:805:LEU:HD23 | 1:B:808:GLU:OE2 | 2.13 | 0.49 |
| 1:A:1119:LYS:NZ | 1:A:1256:TRP:HZ2 | 2.10 | 0.49 |
| 1:A:1389:VAL:HG12 | 1:A:1389:VAL:O | 2.12 | 0.49 |
| 1:A:1469:PRO:HA | 1:A:1472:SER:CB | 2.42 | 0.49 |
| 1:A:1574:ASN:CB | 1:A:1582:LEU:HD21 | 2.40 | 0.49 |
| 1:A:2393:LEU:HD13 | 1:A:2426:HIS:CD2 | 2.46 | 0.49 |
| 1:A:282:PHE:CD1 | 1:A:283:SER:N | 2.80 | 0.49 |
| 1:A:3005:LEU:O | 1:A:3180:ASP:OD2 | 2.30 | 0.49 |
| 1:A:3012:GLU:HB2 | 1:A:3050:LYS:NZ | 2.27 | 0.49 |
| 1:A:39:GLY:O | 1:A:43:VAL:HG23 | 2.12 | 0.49 |
| 1:A:47:SER:N | 1:A:51:LEU:HD12 | 2.27 | 0.49 |
| 1:A:884:VAL:HG22 | 1:A:888:ARG:HG2 | 1.93 | 0.49 |
| 1:A:965:THR:HA | 1:A:968:VAL:CG1 | 2.42 | 0.49 |
| 1:A:986:PRO:O | 1:A:990:GLN:HG2 | 2.12 | 0.49 |
| 1:B:1010:LEU:HD13 | 1:B:1028:PHE:CE1 | 2.28 | 0.49 |
| 1:B:1907:GLU:O | 1:B:1911:LEU:HG | 2.11 | 0.49 |
| 1:B:2328:ARG:O | 1:B:2332:GLU:HG2 | 2.13 | 0.49 |
| 1:B:319:PHE:O | 1:B:323:VAL:HG23 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3326:GLN:CB | 1:B:3393:GLU:HG2 | 2.38 | 0.49 |
| 1:B:3493:TRP:CD1 | 1:B:3710:LYS:O | 2.65 | 0.49 |
| 1:B:3923:ARG:HB3 | 1:B:3962:ARG:HH12 | 1.78 | 0.49 |
| 1:B:533:HIS:O | 1:B:537:SER:HB3 | 2.13 | 0.49 |
| 1:B:941:MSE:HE3 | 1:B:958:MSE:HG3 | 1.95 | 0.49 |
| 1:A:1121:LEU:HG | 1:A:1122:GLY:H | 1.75 | 0.49 |
| 1:A:86:LEU:HD13 | 1:A:134:LEU:CD2 | 2.42 | 0.49 |
| 1:A:1491:ILE:N | 1:A:1497:ARG:HH12 | 2.10 | 0.49 |
| 1:A:390:GLN:NE2 | 1:A:1723:PRO:HG2 | 2.28 | 0.49 |
| 1:A:1751:GLU:OE2 | 1:A:1884:LEU:HD13 | 2.11 | 0.49 |
| 1:A:1811:ARG:O | 1:A:1815:THR:HG23 | 2.12 | 0.49 |
| 1:A:2280:VAL:HG13 | 1:A:2287:PRO:HB2 | 1.93 | 0.49 |
| 1:A:2420:PHE:CE1 | 1:A:2439:ILE:HG21 | 2.46 | 0.49 |
| 1:A:2927:ALA:HB2 | 1:A:3121:LEU:HD22 | 1.93 | 0.49 |
| 1:A:3174:ASP:N | 1:A:3175:PRO:HD2 | 2.17 | 0.49 |
| 1:A:318:SER:O | 1:A:321:LYS:HB2 | 2.12 | 0.49 |
| 1:A:3620:PRO:HB3 | 1:A:3633:ILE:HD12 | 1.94 | 0.49 |
| 1:A:481:THR:HG23 | 1:A:559:SER:OG | 2.13 | 0.49 |
| 1:A:680:ILE:HG12 | 1:A:701:TYR:CE1 | 2.48 | 0.49 |
| 1:B:103:TYR:O | 1:B:107:ILE:HG13 | 2.13 | 0.49 |
| 1:B:1086:TYR:CE2 | 1:B:1090:ARG:HG2 | 2.48 | 0.49 |
| 1:B:1139:GLU:HG3 | 1:B:1175:HIS:CD2 | 2.47 | 0.49 |
| 1:B:1702:LEU:O | 1:B:1706:SER:CB | 2.61 | 0.49 |
| 1:B:2193:ILE:HA | 1:B:2196:TRP:CE2 | 2.48 | 0.49 |
| 1:B:2847:THR:HB | 1:B:2850:PHE:CD2 | 2.47 | 0.49 |
| 1:B:3163:THR:OG1 | 1:B:3167:ARG:NH2 | 2.43 | 0.49 |
| 1:B:3323:PHE:CE1 | 1:B:3324:ARG:HG3 | 2.48 | 0.49 |
| 1:B:334:HIS:O | 1:B:338:LEU:HD11 | 2.12 | 0.49 |
| 1:B:560:LEU:HD11 | 1:B:645:TRP:HZ2 | 1.74 | 0.49 |
| 1:B:954:GLY:O | 1:B:957:PRO:HD2 | 2.11 | 0.49 |
| 1:A:1145:LEU:HD22 | 1:A:1149:LYS:HZ3 | 1.78 | 0.49 |
| 1:A:1155:ARG:HH12 | 1:A:1159:PRO:CD | 2.21 | 0.49 |
| 1:A:1158:PRO:HB2 | 1:A:1159:PRO:HD3 | 1.95 | 0.49 |
| 1:A:1475:LEU:O | 1:A:1478:SER:HB3 | 2.13 | 0.49 |
| 1:A:1808:ASP:OD1 | 1:A:1809:ASP:N | 2.45 | 0.49 |
| 1:A:2027:SER:HB2 | 1:A:2030:TYR:OH | 2.12 | 0.49 |
| 1:A:2144:LEU:C | 1:A:2148:LYS:HE3 | 2.33 | 0.49 |
| 1:A:2944:THR:HG21 | 1:A:2983:ASP:OD2 | 2.12 | 0.49 |
| 1:A:2970:LYS:NZ | 1:A:3013:TYR:OH | 2.44 | 0.49 |
| 1:A:396:PHE:CG | 1:A:397:LEU:N | 2.80 | 0.49 |
| 1:A:4012:ASP:C | 1:A:4016:PHE:HB2 | 2.33 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:745:VAL:HG11 | 1:A:776:TRP:HZ2 | 1.78 | 0.49 |
| 1:A:808:GLU:OE1 | 1:A:3114:TYR:HB3 | 2.13 | 0.49 |
| 1:A:767:GLU:CG | 1:A:851:ILE:HD11 | 2.40 | 0.49 |
| 1:B:1645:VAL:HG22 | 1:B:1709:GLU:OE1 | 2.13 | 0.49 |
| 1:B:1945:TYR:CD1 | 1:B:1948:ALA:HB3 | 2.47 | 0.49 |
| 1:B:2094:MSE:O | 1:B:2098:THR:HG23 | 2.13 | 0.49 |
| 1:B:2358:ASP:O | 1:B:2361:ILE:HG22 | 2.12 | 0.49 |
| 1:B:2423:VAL:HG22 | 1:B:2424:MSE:N | 2.27 | 0.49 |
| 1:B:2806:LYS:NZ | 1:B:2858:ILE:HG13 | 2.26 | 0.49 |
| 1:B:2913:LYS:O | 1:B:2915:ARG:N | 2.45 | 0.49 |
| 1:B:3259:LEU:HD21 | 1:B:3279:SER:HB2 | 1.94 | 0.49 |
| 1:B:3696:ARG:HB2 | 1:B:3699:LEU:HB2 | 1.95 | 0.49 |
| 1:B:3825:LYS:HB2 | 1:B:3829:LEU:HD13 | 1.93 | 0.49 |
| 1:B:437:HIS:CD2 | 1:B:438:LEU:N | 2.80 | 0.49 |
| 1:B:407:VAL:O | 1:B:449:TYR:HE1 | 1.95 | 0.49 |
| 1:B:604:PRO:HG2 | 1:B:607:ASP:OD1 | 2.13 | 0.49 |
| 1:B:638:GLN:HG3 | 1:B:667:TYR:CD2 | 2.48 | 0.49 |
| 1:B:708:VAL:HG22 | 1:B:744:ASP:OD2 | 2.12 | 0.49 |
| 1:B:855:VAL:HG12 | 1:B:859:LEU:HD11 | 1.93 | 0.49 |
| 1:B:964:ARG:O | 1:B:967:PRO:HD2 | 2.11 | 0.49 |
| 1:B:978:GLN:HA | 1:B:981:ARG:NE | 2.21 | 0.49 |
| 1:B:977:ASP:HB3 | 1:B:981:ARG:N | 2.26 | 0.49 |
| 1:A:1060:PHE:HB3 | 1:A:1064:TYR:HE2 | 1.78 | 0.49 |
| 1:A:203:GLU:O | 1:A:207:GLN:CB | 2.55 | 0.49 |
| 1:A:2352:HIS:CD2 | 1:A:2364:LEU:HD21 | 2.48 | 0.49 |
| 1:A:2320:ALA:CA | 1:A:2367:VAL:HG23 | 2.42 | 0.49 |
| 1:A:2960:GLU:HG3 | 1:A:3289:ARG:HH22 | 1.77 | 0.49 |
| 1:A:3356:ALA:CB | 1:A:3384:HIS:HB3 | 2.43 | 0.49 |
| 1:A:704:PHE:O | 1:A:707:PHE:HB2 | 2.11 | 0.49 |
| 1:A:871:LEU:HD11 | 1:A:3122:HIS:CE1 | 2.42 | 0.49 |
| 1:B:992:ILE:HD13 | 1:B:1031:ARG:HB3 | 1.95 | 0.49 |
| 1:B:1107:TYR:O | 1:B:1111:LEU:N | 2.40 | 0.49 |
| 1:B:2452:ARG:HG2 | 1:B:2498:ILE:HD11 | 1.94 | 0.49 |
| 1:B:3266:SER:HB2 | 1:B:3271:ASP:OD1 | 2.12 | 0.49 |
| 1:B:352:VAL:HG23 | 1:B:357:LYS:H | 1.77 | 0.49 |
| 1:B:3793:VAL:O | 1:B:3795:PRO:HD3 | 2.12 | 0.49 |
| 1:B:63:PHE:CE1 | 1:B:89:LEU:HD22 | 2.47 | 0.49 |
| 1:B:903:PRO:O | 1:B:905:ILE:HG13 | 2.12 | 0.49 |
| 1:A:1102:GLU:O | 1:A:1105:VAL:HG13 | 2.13 | 0.49 |
| 1:A:1643:MSE:O | 1:A:1646:LEU:N | 2.46 | 0.49 |
| 1:A:1723:PRO:C | 1:A:1725:GLN:N | 2.66 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2097:LEU:HA | 1:A:2100:LEU:HB3 | 1.94 | 0.49 |
| 1:A:2148:LYS:NZ | 1:A:2188:GLU:HG2 | 2.27 | 0.49 |
| 1:A:21:ALA:HA | 1:A:24:ARG:HG3 | 1.94 | 0.49 |
| 1:A:2511:ILE:HA | 1:A:2519:LEU:HD12 | 1.94 | 0.49 |
| 1:A:2542:LEU:HD12 | 1:A:2543:ASN:N | 2.28 | 0.49 |
| 1:A:2567:SER:O | 1:A:2571:ASP:HB2 | 2.11 | 0.49 |
| 1:A:933:LEU:HD22 | 1:A:2795:GLN:HA | 1.93 | 0.49 |
| 1:A:3152:SER:HB2 | 1:A:3155:VAL:HB | 1.94 | 0.49 |
| 1:A:899:ARG:HH22 | 1:A:2570:PRO:CB | 2.25 | 0.49 |
| 1:A:892:LEU:H | 1:A:907:LEU:HD22 | 1.78 | 0.49 |
| 1:B:1033:ILE:HA | 1:B:1036:PHE:CD2 | 2.48 | 0.49 |
| 1:B:1960:LYS:HA | 1:B:1963:GLN:OE1 | 2.13 | 0.49 |
| 1:B:2222:HIS:O | 1:B:2226:PRO:HD2 | 2.12 | 0.49 |
| 1:B:2854:PHE:CE1 | 1:B:2878:ALA:HA | 2.48 | 0.49 |
| 1:B:2999:LEU:HD12 | 1:B:3002:TYR:CE2 | 2.46 | 0.49 |
| 1:B:3003:ASN:O | 1:B:3006:ALA:N | 2.46 | 0.49 |
| 1:B:3163:THR:O | 1:B:3167:ARG:HB2 | 2.13 | 0.49 |
| 1:B:3501:HIS:O | 1:B:3505:LEU:HD13 | 2.12 | 0.49 |
| 1:B:3576:ASP:C | 1:B:3578:LEU:HG | 2.33 | 0.49 |
| 1:B:3667:LEU:HA | 1:B:3670:MSE:HG2 | 1.92 | 0.49 |
| 1:B:3906:SER:O | 1:B:3910:LEU:HD13 | 2.12 | 0.49 |
| 1:B:388:LEU:HG | 1:B:420:VAL:HG21 | 1.94 | 0.49 |
| 1:B:479:ILE:O | 1:B:483:VAL:HG13 | 2.12 | 0.49 |
| 1:B:789:TYR:CD2 | 1:B:865:GLN:HG3 | 2.47 | 0.49 |
| 1:A:1044:ILE:O | 1:A:1045:THR:OG1 | 2.28 | 0.49 |
| 1:A:134:LEU:O | 1:A:137:THR:OG1 | 2.25 | 0.49 |
| 1:A:1407:LYS:HG2 | 1:A:1462:GLY:N | 2.28 | 0.49 |
| 1:A:2245:TRP:CE3 | 1:A:2245:TRP:HA | 2.48 | 0.49 |
| 1:A:2365:ASN:HA | 1:A:2368:THR:HB | 1.94 | 0.49 |
| 1:A:2412:TYR:CD2 | 1:A:2416:LYS:HG3 | 2.47 | 0.49 |
| 1:A:270:ALA:HA | 1:A:273:ARG:HG2 | 1.95 | 0.49 |
| 1:A:3052:LEU:HD13 | 1:A:3061:LEU:HG | 1.94 | 0.49 |
| 1:A:3179:TRP:CZ2 | 1:A:3258:LEU:HG | 2.46 | 0.49 |
| 1:A:3510:GLN:OE1 | 1:A:3513:ALA:HB2 | 2.13 | 0.49 |
| 1:A:3525:TYR:OH | 1:A:3561:LYS:HB2 | 2.13 | 0.49 |
| 1:A:3885:ARG:HG3 | 1:A:3889:ARG:HD3 | 1.95 | 0.49 |
| 1:A:3929:MSE:O | 1:A:3938:ILE:HG13 | 2.12 | 0.49 |
| 1:A:729:CYS:HA | 1:A:732:PHE:CE2 | 2.48 | 0.49 |
| 1:B:1007:VAL:HA | 1:B:1010:LEU:CD1 | 2.43 | 0.49 |
| 1:B:1220:LEU:O | 1:B:1223:THR:OG1 | 2.26 | 0.49 |
| 1:B:1280:GLN:HA | 1:B:1361:LYS:HZ2 | 1.75 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1459:HIS:NE2 | 1:B:1509:GLN:O | 2.46 | 0.49 |
| 1:B:1751:GLU:O | 1:B:1755:SER:N | 2.42 | 0.49 |
| 1:B:1726:SER:HB2 | 1:B:1869:LYS:HD2 | 1.94 | 0.49 |
| 1:B:3117:ILE:CD1 | 1:B:3125:ARG:HH11 | 2.06 | 0.49 |
| 1:B:3293:CYS:O | 1:B:3297:VAL:HB | 2.13 | 0.49 |
| 1:B:3570:ASP:O | 1:B:3573:ASN:HB3 | 2.13 | 0.49 |
| 1:B:3657:SER:O | 1:B:3660:ASN:HB2 | 2.13 | 0.49 |
| 1:B:3971:MSE:HE2 | 1:B:3976:GLU:OE2 | 2.13 | 0.49 |
| 1:B:712:LYS:O | 1:B:716:VAL:HG23 | 2.13 | 0.49 |
| 1:B:63:PHE:HD1 | 1:B:89:LEU:HD13 | 1.78 | 0.49 |
| 1:A:1139:GLU:HG3 | 1:A:1175:HIS:CD2 | 2.48 | 0.49 |
| 1:A:1684:LEU:HA | 1:A:1687:HIS:HD2 | 1.77 | 0.49 |
| 1:A:175:TYR:HB2 | 1:A:222:GLY:C | 2.33 | 0.49 |
| 1:A:2274:ILE:CD1 | 1:A:2314:GLU:HB3 | 2.43 | 0.49 |
| 1:A:3103:ILE:HD13 | 1:A:3139:GLN:OE1 | 2.13 | 0.49 |
| 1:A:3984:MSE:SE | 1:A:4108:MSE:HE2 | 2.63 | 0.49 |
| 1:A:442:GLN:HA | 1:A:445:SER:OG | 2.12 | 0.49 |
| 1:B:1493:PRO:HG2 | 1:B:1495:ASP:HB2 | 1.94 | 0.49 |
| 1:B:2161:ALA:CB | 1:B:2211:LEU:HD13 | 2.39 | 0.49 |
| 1:B:2357:GLU:OE1 | 1:B:2388:LYS:NZ | 2.42 | 0.49 |
| 1:B:2778:GLY:O | 1:B:2781:PRO:HD2 | 2.13 | 0.49 |
| 1:B:249:PHE:HB3 | 1:B:297:LEU:HD13 | 1.93 | 0.49 |
| 1:B:3522:THR:O | 1:B:3526:PRO:HD3 | 2.13 | 0.49 |
| 1:B:3974:MSE:CG | 1:B:3976:GLU:HB3 | 2.43 | 0.49 |
| 1:B:4041:ARG:HB2 | 1:B:4042:GLN:OE1 | 2.12 | 0.49 |
| 1:B:793:LEU:HA | 1:B:796:LEU:HB2 | 1.94 | 0.49 |
| 1:B:891:ARG:HD2 | 1:B:905:ILE:HG12 | 1.94 | 0.49 |
| 1:A:1113:LEU:HA | 1:A:1116:ALA:HB3 | 1.94 | 0.49 |
| 1:A:1695:LEU:HA | 1:A:1698:PHE:CE2 | 2.48 | 0.49 |
| 1:A:1762:MSE:HE3 | 1:A:1864:ASP:OD1 | 2.13 | 0.49 |
| 1:A:3045:ILE:O | 1:A:3048:LYS:HE2 | 2.13 | 0.49 |
| 1:A:3186:ARG:HD3 | 1:A:3242:MSE:SE | 2.63 | 0.49 |
| 1:A:3247:ARG:HH21 | 1:A:3277:VAL:HG23 | 1.78 | 0.49 |
| 1:A:3651:LEU:HA | 1:A:3654:MSE:HB2 | 1.95 | 0.49 |
| 1:A:3962:ARG:NH1 | 1:A:4124:TRP:CH2 | 2.81 | 0.49 |
| 1:A:903:PRO:HD2 | 1:A:904:VAL:HG23 | 1.95 | 0.49 |
| 1:A:927:LYS:HD3 | 1:A:976:VAL:HG12 | 1.94 | 0.49 |
| 1:B:1219:PHE:O | 1:B:1223:THR:HG23 | 2.13 | 0.49 |
| 1:B:2467:THR:HA | 1:B:2470:ARG:HG3 | 1.93 | 0.49 |
| 1:B:2842:ARG:O | 1:B:2846:THR:HG23 | 2.11 | 0.49 |
| 1:B:2887:PRO:CB | 1:B:2922:ARG:HH11 | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3034:PRO:CG | 1:B:3037:GLN:HB2 | 2.39 | 0.49 |
| 1:B:485:GLN:HA | 1:B:488:ILE:HG12 | 1.94 | 0.49 |
| 1:B:567:GLU:HB3 | 1:B:606:SER:CB | 2.43 | 0.49 |
| 1:B:990:GLN:HA | 1:B:993:HIS:HD2 | 1.77 | 0.49 |
| 1:A:174:VAL:O | 1:A:178:LEU:HG | 2.13 | 0.48 |
| 1:A:181:LEU:HD13 | 1:A:189:MSE:HE2 | 1.95 | 0.48 |
| 1:A:2990:GLU:O | 1:A:2994:TRP:HD1 | 1.96 | 0.48 |
| 1:A:3468:LEU:HD13 | 1:A:3483:MSE:HE1 | 1.93 | 0.48 |
| 1:A:3547:THR:HG21 | 1:A:3552:LYS:HB2 | 1.94 | 0.48 |
| 1:A:3648:GLY:O | 1:A:3651:LEU:HB2 | 2.13 | 0.48 |
| 1:A:760:LEU:HD23 | 1:A:803:SER:HB3 | 1.95 | 0.48 |
| 1:A:901:MSE:HE1 | 1:A:2539:LEU:CD2 | 2.43 | 0.48 |
| 1:A:925:GLN:OE1 | 1:A:925:GLN:N | 2.39 | 0.48 |
| 1:B:1059:LEU:O | 1:B:1063:LEU:HG | 2.13 | 0.48 |
| 1:B:13:LEU:O | 1:B:16:GLN:HG2 | 2.13 | 0.48 |
| 1:B:1976:LEU:HG | 1:B:1978:PHE:H | 1.77 | 0.48 |
| 1:B:1959:LEU:CD1 | 1:B:1998:MSE:HE3 | 2.32 | 0.48 |
| 1:B:20:SER:HB2 | 1:B:65:LEU:HD22 | 1.95 | 0.48 |
| 1:B:2602:UNK:CB | 1:B:2793:PRO:HG3 | 2.43 | 0.48 |
| 1:B:3061:LEU:HD21 | 1:B:3089:LEU:HD13 | 1.95 | 0.48 |
| 1:B:3155:VAL:N | 1:B:3156:PRO:HD2 | 2.28 | 0.48 |
| 1:B:3972:LEU:O | 1:B:3974:MSE:HG2 | 2.13 | 0.48 |
| 1:B:4085:LYS:HA | 1:B:4088:ASN:CB | 2.43 | 0.48 |
| 1:B:613:HIS:O | 1:B:617:PRO:HG2 | 2.13 | 0.48 |
| 1:A:1122:GLY:O | 1:A:1123:THR:OG1 | 2.29 | 0.48 |
| 1:A:1170:LYS:HD3 | 1:A:1267:TYR:CG | 2.48 | 0.48 |
| 1:A:1722:PHE:H | 1:A:1723:PRO:CD | 2.26 | 0.48 |
| 1:A:398:THR:HG22 | 1:A:1865:THR:HG21 | 1.94 | 0.48 |
| 1:A:1869:LYS:O | 1:A:1873:TYR:HD1 | 1.96 | 0.48 |
| 1:A:2110:PRO:HB2 | 1:A:2111:PRO:HD3 | 1.95 | 0.48 |
| 1:A:2171:LEU:HG | 1:A:2177:ASN:HD21 | 1.78 | 0.48 |
| 1:A:2193:ILE:HD11 | 1:A:2245:TRP:CZ2 | 2.48 | 0.48 |
| 1:A:14:ARG:HD2 | 1:A:2358:ASP:OD2 | 2.13 | 0.48 |
| 1:A:3247:ARG:NH2 | 1:A:3277:VAL:HG23 | 2.27 | 0.48 |
| 1:A:3684:SER:HB3 | 1:A:3726:VAL:CG1 | 2.42 | 0.48 |
| 1:A:3950:THR:OG1 | 1:A:3957:GLU:O | 2.22 | 0.48 |
| 1:A:3963:LEU:HG | 1:A:3967:PHE:CE1 | 2.47 | 0.48 |
| 1:A:3974:MSE:HB3 | 1:A:3976:GLU:N | 2.23 | 0.48 |
| 1:A:4103:GLN:H | 1:A:4103:GLN:CD | 2.17 | 0.48 |
| 1:A:531:PHE:CE2 | 1:A:619:ASP:HB2 | 2.47 | 0.48 |
| 1:B:1076:LEU:C | 1:B:1078:ALA:H | 2.16 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1238:GLN:NE2 | 1:B:1298:LEU:HG | 2.28 | 0.48 |
| 1:B:1365:ASN:HA | 1:B:1368:LEU:HD21 | 1.94 | 0.48 |
| 1:B:1708:GLU:HB2 | 1:B:1709:GLU:CD | 2.33 | 0.48 |
| 1:B:1996:VAL:CG1 | 1:B:2048:GLY:HA2 | 2.37 | 0.48 |
| 1:B:2322:VAL:O | 1:B:2326:ILE:HG12 | 2.13 | 0.48 |
| 1:B:3228:SER:O | 1:B:3231:ILE:HB | 2.13 | 0.48 |
| 1:B:280:SER:HB3 | 1:B:322:GLN:HB2 | 1.95 | 0.48 |
| 1:B:3284:SER:HA | 1:B:3287:ARG:NE | 2.09 | 0.48 |
| 1:B:3788:LEU:HD13 | 1:B:3907:SER:HA | 1.96 | 0.48 |
| 1:B:3901:ARG:NH1 | 1:B:3901:ARG:HG2 | 2.27 | 0.48 |
| 1:B:4066:LEU:HG | 1:B:4075:ARG:HA | 1.95 | 0.48 |
| 1:B:575:ILE:HG12 | 1:B:579:LEU:HB2 | 1.95 | 0.48 |
| 1:B:669:LEU:HD13 | 1:B:672:ILE:HD12 | 1.95 | 0.48 |
| 1:A:2213:ASN:HB2 | 1:A:2250:SER:HB2 | 1.95 | 0.48 |
| 1:A:940:PHE:HZ | 1:A:2791:ILE:HG21 | 1.73 | 0.48 |
| 1:A:583:LEU:HD23 | 1:A:592:GLU:OE2 | 2.13 | 0.48 |
| 1:A:848:LEU:HA | 1:A:851:ILE:CD1 | 2.44 | 0.48 |
| 1:B:1299:GLU:HA | 1:B:1302:ALA:CB | 2.44 | 0.48 |
| 1:B:1330:TYR:O | 1:B:1333:SER:OG | 2.27 | 0.48 |
| 1:B:1889:VAL:HG13 | 1:B:1900:PHE:CD2 | 2.48 | 0.48 |
| 1:B:2031:LEU:HB2 | 1:B:2033:ASP:CB | 2.40 | 0.48 |
| 1:B:2059:PRO:O | 1:B:2062:ALA:HB3 | 2.13 | 0.48 |
| 1:B:2291:GLN:NE2 | 1:B:2294:ILE:HG13 | 2.28 | 0.48 |
| 1:B:2299:TYR:O | 1:B:2302:ALA:N | 2.46 | 0.48 |
| 1:B:2387:PRO:O | 1:B:2390:HIS:HB3 | 2.12 | 0.48 |
| 1:B:249:PHE:O | 1:B:253:LEU:HG | 2.13 | 0.48 |
| 1:B:2459:VAL:HG11 | 1:B:2505:VAL:HG22 | 1.95 | 0.48 |
| 1:B:2549:LYS:HD2 | 1:B:2554:PHE:HB3 | 1.95 | 0.48 |
| 1:B:2851:PHE:O | 1:B:2855:VAL:HG23 | 2.13 | 0.48 |
| 1:B:293:LEU:O | 1:B:296:VAL:HG12 | 2.12 | 0.48 |
| 1:B:856:VAL:HG21 | 1:B:3110:PHE:CE1 | 2.48 | 0.48 |
| 1:B:3398:PRO:HG2 | 1:B:3399:PRO:HD3 | 1.94 | 0.48 |
| 1:B:358:GLU:HG3 | 1:B:359:LEU:N | 2.27 | 0.48 |
| 1:B:3989:ARG:HE | 1:B:4100:GLU:CB | 2.26 | 0.48 |
| 1:B:611:ASN:C | 1:B:614:PRO:HD2 | 2.33 | 0.48 |
| 1:B:758:LEU:O | 1:B:762:TYR:HB3 | 2.13 | 0.48 |
| 1:B:884:VAL:HG22 | 1:B:888:ARG:HG2 | 1.95 | 0.48 |
| 1:B:892:LEU:HD12 | 1:B:892:LEU:O | 2.13 | 0.48 |
| 1:B:996:THR:O | 1:B:1042:LYS:HG2 | 2.12 | 0.48 |
| 1:A:1001:PHE:CD1 | 1:A:1002:GLU:N | 2.82 | 0.48 |
| 1:A:1075:ARG:O | 1:A:1078:ALA:HB3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1029:CYS:CB | 1:A:1085:ILE:HG13 | 2.43 | 0.48 |
| 1:A:1231:GLN:H | 1:A:1232:PRO:HD3 | 1.78 | 0.48 |
| 1:A:1387:GLY:HA2 | 1:A:1392:MSE:SE | 2.63 | 0.48 |
| 1:A:1889:VAL:HG22 | 1:A:1900:PHE:CE2 | 2.49 | 0.48 |
| 1:A:2122:LEU:HA | 1:A:2127:LYS:HE2 | 1.96 | 0.48 |
| 1:A:2161:ALA:HB1 | 1:A:2211:LEU:HD13 | 1.95 | 0.48 |
| 1:A:2166:SER:N | 1:A:2167:PRO:HD2 | 2.28 | 0.48 |
| 1:A:2573:PRO:C | 1:A:2575:PRO:HD3 | 2.32 | 0.48 |
| 1:A:2778:GLY:O | 1:A:2781:PRO:HD2 | 2.14 | 0.48 |
| 1:A:3020:ASP:HB3 | 1:A:3027:LEU:HD12 | 1.95 | 0.48 |
| 1:A:3612:ARG:O | 1:A:3615:ALA:HB3 | 2.14 | 0.48 |
| 1:A:4117:LEU:HB3 | 1:A:4126:PRO:HB2 | 1.96 | 0.48 |
| 1:B:1741:ASP:O | 1:B:1745:LYS:HG3 | 2.14 | 0.48 |
| 1:B:1884:LEU:HB2 | 1:B:1885:PRO:HD3 | 1.95 | 0.48 |
| 1:B:2086:ASP:CB | 1:B:2090:ARG:HH21 | 2.24 | 0.48 |
| 1:B:2148:LYS:HD3 | 1:B:2160:TYR:HE1 | 1.78 | 0.48 |
| 1:B:2227:LYS:HD2 | 1:B:2235:LEU:CG | 2.35 | 0.48 |
| 1:B:3076:ALA:O | 1:B:3080:LEU:HG | 2.14 | 0.48 |
| 1:B:3498:TRP:NE1 | 1:B:3502:MSE:HB2 | 2.28 | 0.48 |
| 1:B:3764:VAL:O | 1:B:3768:PHE:HD1 | 1.96 | 0.48 |
| 1:B:3972:LEU:O | 1:B:3974:MSE:N | 2.46 | 0.48 |
| 1:B:706:LEU:HA | 1:B:709:LYS:HB2 | 1.94 | 0.48 |
| 1:B:793:LEU:HA | 1:B:796:LEU:CG | 2.43 | 0.48 |
| 1:A:1389:VAL:O | 1:A:1390:GLN:HB2 | 2.13 | 0.48 |
| 1:A:19:LEU:HA | 1:A:22:ALA:HB3 | 1.95 | 0.48 |
| 1:A:2196:TRP:CE2 | 1:A:2199:LEU:HD11 | 2.47 | 0.48 |
| 1:A:2241:LEU:HA | 1:A:2244:CYS:SG | 2.53 | 0.48 |
| 1:A:2386:LEU:HD13 | 1:A:2401:VAL:HA | 1.95 | 0.48 |
| 1:A:2437:ASP:HB3 | 1:A:2472:GLN:HG2 | 1.95 | 0.48 |
| 1:A:2532:PRO:O | 1:A:2565:MSE:HE2 | 2.14 | 0.48 |
| 1:A:322:GLN:HA | 1:A:325:ASN:HB2 | 1.95 | 0.48 |
| 1:A:3409:VAL:HB | 1:A:3413:TYR:CE2 | 2.48 | 0.48 |
| 1:A:49:ALA:O | 1:A:53:LEU:HB2 | 2.12 | 0.48 |
| 1:A:88:PHE:O | 1:A:91:ILE:HG13 | 2.13 | 0.48 |
| 1:A:979:VAL:O | 1:A:982:GLN:HB3 | 2.12 | 0.48 |
| 1:B:1228:GLY:O | 1:B:1282:LEU:HD11 | 2.14 | 0.48 |
| 1:B:1698:PHE:CD1 | 1:B:1699:PHE:N | 2.82 | 0.48 |
| 1:B:2063:THR:HA | 1:B:2066:PHE:HB2 | 1.95 | 0.48 |
| 1:B:2085:MSE:O | 1:B:2088:LEU:HB3 | 2.13 | 0.48 |
| 1:B:2837:LEU:HD22 | 1:B:2868:LEU:CG | 2.41 | 0.48 |
| 1:B:3045:ILE:HB | 1:B:3048:LYS:HZ1 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3420:CYS:SG | 1:B:3421:ASP:N | 2.86 | 0.48 |
| 1:B:3629:ARG:HH22 | 1:B:3638:LYS:HE3 | 1.78 | 0.48 |
| 1:B:3771:MSE:O | 1:B:3775:LEU:HG | 2.14 | 0.48 |
| 1:B:3881:ASP:HA | 1:B:3884:LYS:HD2 | 1.96 | 0.48 |
| 1:B:417:VAL:O | 1:B:421:LEU:HG | 2.14 | 0.48 |
| 1:B:629:PHE:CD2 | 1:B:668:LYS:HE2 | 2.48 | 0.48 |
| 1:B:741:ILE:O | 1:B:743:LEU:N | 2.46 | 0.48 |
| 1:A:1136:ARG:HG2 | 1:A:1171:TRP:CH2 | 2.48 | 0.48 |
| 1:A:1385:ASN:O | 1:A:1389:VAL:HG23 | 2.13 | 0.48 |
| 1:A:1430:GLU:HA | 1:A:1433:ALA:HB3 | 1.95 | 0.48 |
| 1:A:3464:LYS:CD | 1:A:3467:ARG:HD2 | 2.43 | 0.48 |
| 1:A:3617:LEU:HD13 | 1:A:3644:PHE:CD2 | 2.49 | 0.48 |
| 1:A:3762:GLN:OE1 | 1:A:3795:PRO:HG3 | 2.13 | 0.48 |
| 1:A:4085:LYS:HA | 1:A:4088:ASN:CB | 2.43 | 0.48 |
| 1:A:65:LEU:HD23 | 1:A:68:PHE:CE1 | 2.48 | 0.48 |
| 1:A:934:LEU:C | 1:A:934:LEU:HD23 | 2.33 | 0.48 |
| 1:A:978:GLN:HA | 1:A:981:ARG:NE | 2.23 | 0.48 |
| 1:B:1390:GLN:O | 1:B:1393:ALA:HB3 | 2.14 | 0.48 |
| 1:B:1414:ILE:O | 1:B:1418:HIS:HB2 | 2.13 | 0.48 |
| 1:B:1571:LEU:HD22 | 1:B:1600:MSE:HA | 1.96 | 0.48 |
| 1:B:1894:SER:C | 1:B:1896:ILE:N | 2.66 | 0.48 |
| 1:B:1890:HIS:NE2 | 1:B:1941:HIS:HA | 2.29 | 0.48 |
| 1:B:2231:PHE:CE1 | 1:B:2233:HIS:HB2 | 2.49 | 0.48 |
| 1:B:2782:ASP:HA | 1:B:2786:LYS:HB3 | 1.96 | 0.48 |
| 1:B:3319:ASN:O | 1:B:3323:PHE:HD2 | 1.95 | 0.48 |
| 1:B:3427:GLU:OE1 | 1:B:3435:ASP:HB3 | 2.14 | 0.48 |
| 1:B:3495:PHE:CZ | 1:B:3521:ILE:HG13 | 2.49 | 0.48 |
| 1:B:3538:GLU:HG2 | 1:B:3759:ARG:NH1 | 2.29 | 0.48 |
| 1:B:3629:ARG:NH2 | 1:B:3634:GLN:HA | 2.28 | 0.48 |
| 1:B:361:ILE:HA | 1:B:364:ARG:HG2 | 1.94 | 0.48 |
| 1:B:3575:LEU:HD21 | 1:B:3687:MSE:SE | 2.63 | 0.48 |
| 1:B:3981:TYR:O | 1:B:3985:VAL:HG23 | 2.14 | 0.48 |
| 1:B:46:SER:H | 1:B:51:LEU:HD13 | 1.78 | 0.48 |
| 1:B:749:VAL:N | 1:B:750:PRO:CD | 2.77 | 0.48 |
| 1:B:757:LYS:HA | 1:B:760:LEU:CD1 | 2.44 | 0.48 |
| 1:B:938:VAL:HG21 | 1:B:962:TYR:OH | 2.13 | 0.48 |
| 1:A:1340:ARG:NH1 | 1:A:1343:GLU:HG2 | 2.29 | 0.48 |
| 1:A:1465:HIS:HA | 1:A:1469:PRO:HD2 | 1.95 | 0.48 |
| 1:A:2230:VAL:HB | 1:A:2234:ASN:HD21 | 1.79 | 0.48 |
| 1:A:2467:THR:HB | 1:A:2518:GLN:NE2 | 2.16 | 0.48 |
| 1:A:2890:ILE:CG2 | 1:A:2922:ARG:HH12 | 2.23 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:295:GLU:HA | 1:A:298:LEU:HD12 | 1.96 | 0.48 |
| 1:A:3454:LEU:HD12 | 1:A:3490:VAL:HG11 | 1.95 | 0.48 |
| 1:A:358:GLU:N | 1:A:361:ILE:HG23 | 2.29 | 0.48 |
| 1:A:449:TYR:CZ | 1:A:457:CYS:SG | 3.05 | 0.48 |
| 1:B:1007:VAL:O | 1:B:1011:GLU:CB | 2.61 | 0.48 |
| 1:B:1055:ASN:HA | 1:B:1059:LEU:HG | 1.94 | 0.48 |
| 1:B:1080:LEU:HB2 | 1:B:1131:ILE:HG22 | 1.94 | 0.48 |
| 1:B:1165:LEU:HB3 | 1:B:1169:VAL:HG23 | 1.96 | 0.48 |
| 1:B:86:LEU:HD13 | 1:B:134:LEU:HD21 | 1.95 | 0.48 |
| 1:B:1387:GLY:HA2 | 1:B:1392:MSE:HB2 | 1.94 | 0.48 |
| 1:B:1692:ALA:O | 1:B:1695:LEU:HB2 | 2.14 | 0.48 |
| 1:B:1711:ARG:O | 1:B:1715:GLU:HG3 | 2.12 | 0.48 |
| 1:B:1946:ASN:O | 1:B:1949:ILE:N | 2.35 | 0.48 |
| 1:B:1970:LYS:HB3 | 1:B:1971:PRO:HD3 | 1.95 | 0.48 |
| 1:B:1978:PHE:O | 1:B:1981:LEU:HB3 | 2.13 | 0.48 |
| 1:B:2462:VAL:HB | 1:B:2473:MSE:SE | 2.63 | 0.48 |
| 1:B:901:MSE:HE1 | 1:B:2535:THR:HG21 | 1.96 | 0.48 |
| 1:B:3463:LEU:HD21 | 1:B:4001:THR:HA | 1.96 | 0.48 |
| 1:B:3582:GLU:HB2 | 1:B:3674:SER:OG | 2.14 | 0.48 |
| 1:B:3675:LYS:N | 1:B:3676:PRO:HD2 | 2.29 | 0.48 |
| 1:B:3916:TRP:HE3 | 1:B:3917:ILE:HD12 | 1.77 | 0.48 |
| 1:B:4103:GLN:H | 1:B:4103:GLN:CD | 2.16 | 0.48 |
| 1:A:1066:LEU:HA | 1:A:1069:HIS:CD2 | 2.49 | 0.48 |
| 1:A:1086:TYR:HE2 | 1:A:1090:ARG:NE | 2.08 | 0.48 |
| 1:A:1105:VAL:HB | 1:A:1153:LEU:HD22 | 1.95 | 0.48 |
| 1:A:1080:LEU:HD13 | 1:A:1127:CYS:HB3 | 1.96 | 0.48 |
| 1:A:1651:LYS:HD2 | 1:A:1684:LEU:CG | 2.44 | 0.48 |
| 1:A:1737:ASN:O | 1:A:1739:TYR:N | 2.44 | 0.48 |
| 1:A:2224:PHE:CE2 | 1:A:2259:LYS:HD3 | 2.48 | 0.48 |
| 1:A:2467:THR:CB | 1:A:2518:GLN:HE22 | 2.17 | 0.48 |
| 1:A:2911:ARG:CG | 1:A:2914:ALA:HB3 | 2.43 | 0.48 |
| 1:A:2890:ILE:HD13 | 1:A:2922:ARG:HH12 | 1.78 | 0.48 |
| 1:A:3806:LEU:O | 1:A:3809:THR:HG22 | 2.14 | 0.48 |
| 1:A:3917:ILE:O | 1:A:4048:LYS:NZ | 2.46 | 0.48 |
| 1:A:440:VAL:HG12 | 1:A:483:VAL:HG12 | 1.94 | 0.48 |
| 1:A:634:LEU:HD22 | 1:A:667:TYR:HD1 | 1.79 | 0.48 |
| 1:A:722:LYS:HB3 | 1:A:727:ALA:CA | 2.44 | 0.48 |
| 1:A:883:TYR:CE2 | 1:A:961:LEU:HD12 | 2.49 | 0.48 |
| 1:B:1306:ILE:CG1 | 1:B:1334:LYS:HB3 | 2.42 | 0.48 |
| 1:B:429:GLU:OE2 | 1:B:1595:ALA:HB2 | 2.13 | 0.48 |
| 1:B:1916:ILE:HG23 | 1:B:1920:TYR:CE1 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2073:ASP:N | 1:B:2074:PRO:CD | 2.77 | 0.48 |
| 1:B:2142:ILE:HG12 | 1:B:2145:PHE:CE2 | 2.49 | 0.48 |
| 1:B:2164:TRP:HH2 | 1:B:2190:VAL:HG12 | 1.79 | 0.48 |
| 1:B:2304:VAL:HG13 | 1:B:2348:GLN:NE2 | 2.28 | 0.48 |
| 1:B:2877:SER:C | 1:B:2879:GLY:N | 2.67 | 0.48 |
| 1:B:2915:ARG:HG3 | 1:B:2915:ARG:HH11 | 1.78 | 0.48 |
| 1:B:3145:ILE:HG12 | 1:B:3196:LYS:HG2 | 1.95 | 0.48 |
| 1:B:3175:PRO:HG2 | 1:B:3178:ILE:HD11 | 1.95 | 0.48 |
| 1:B:345:PHE:O | 1:B:349:ILE:HG13 | 2.13 | 0.48 |
| 1:B:3825:LYS:HD2 | 1:B:3829:LEU:HA | 1.95 | 0.48 |
| 1:B:3835:PRO:HA | 1:B:3871:PHE:CE1 | 2.47 | 0.48 |
| 1:B:3913:ILE:O | 1:B:3917:ILE:HD13 | 2.14 | 0.48 |
| 1:B:645:TRP:CZ3 | 1:B:659:ARG:CB | 2.97 | 0.48 |
| 1:B:994:TRP:HA | 1:B:994:TRP:CE3 | 2.48 | 0.48 |
| 1:A:1042:LYS:HE3 | 1:A:1044:ILE:HG21 | 1.95 | 0.48 |
| 1:A:1072:ALA:CB | 1:A:1114:ALA:HB1 | 2.44 | 0.48 |
| 1:A:1165:LEU:O | 1:A:1168:LEU:N | 2.46 | 0.48 |
| 1:A:1175:HIS:O | 1:A:1178:ARG:HB3 | 2.13 | 0.48 |
| 1:A:1434:VAL:HB | 1:A:1448:LEU:HD11 | 1.94 | 0.48 |
| 1:A:2193:ILE:CD1 | 1:A:2245:TRP:CZ2 | 2.97 | 0.48 |
| 1:A:2232:ARG:NH2 | 1:A:2313:LYS:NZ | 2.62 | 0.48 |
| 1:A:2256:ILE:HG12 | 1:A:2276:LEU:HD21 | 1.96 | 0.48 |
| 1:A:2820:MSE:HE3 | 1:A:2829:LYS:HB3 | 1.96 | 0.48 |
| 1:A:280:SER:O | 1:A:322:GLN:HG2 | 2.14 | 0.48 |
| 1:A:3638:LYS:C | 1:A:3641:ASP:H | 2.16 | 0.48 |
| 1:A:542:ASP:HA | 1:A:545:LEU:CD1 | 2.44 | 0.48 |
| 1:A:611:ASN:O | 1:A:614:PRO:HD2 | 2.13 | 0.48 |
| 1:A:509:ARG:CB | 1:A:729:CYS:SG | 3.02 | 0.48 |
| 1:A:889:GLU:OE2 | 1:A:950:GLU:HG2 | 2.13 | 0.48 |
| 1:B:1109:GLU:O | 1:B:1113:LEU:HB3 | 2.14 | 0.48 |
| 1:B:1303:MSE:O | 1:B:1307:ILE:HG13 | 2.13 | 0.48 |
| 1:B:1476:HIS:CE1 | 1:B:1507:CYS:HA | 2.49 | 0.48 |
| 1:B:1574:ASN:CB | 1:B:1582:LEU:HD21 | 2.42 | 0.48 |
| 1:B:1923:PHE:HE2 | 1:B:1927:MSE:HE1 | 1.79 | 0.48 |
| 1:B:19:LEU:HA | 1:B:22:ALA:HB3 | 1.96 | 0.48 |
| 1:B:2146:LEU:HD22 | 1:B:2149:LEU:HD11 | 1.95 | 0.48 |
| 1:B:231:LEU:HD23 | 1:B:234:PHE:HB3 | 1.94 | 0.48 |
| 1:B:3460:GLU:HA | 1:B:3463:LEU:HD12 | 1.96 | 0.48 |
| 1:B:39:GLY:O | 1:B:43:VAL:HG23 | 2.13 | 0.48 |
| 1:B:446:PHE:HD2 | 1:B:533:HIS:CB | 2.25 | 0.48 |
| 1:B:641:PHE:CZ | 1:B:645:TRP:NE1 | 2.82 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:929:ALA:O | 1:B:933:LEU:CB | 2.62 | 0.48 |
| 1:A:1373:VAL:C | 1:A:1375:THR:H | 2.16 | 0.48 |
| 1:A:1723:PRO:O | 1:A:1725:GLN:N | 2.47 | 0.48 |
| 1:A:1984:LEU:HD12 | 1:A:1985:LYS:N | 2.29 | 0.48 |
| 1:A:2004:TYR:CE1 | 1:A:2054:TYR:O | 2.67 | 0.48 |
| 1:A:2328:ARG:O | 1:A:2332:GLU:HG3 | 2.13 | 0.48 |
| 1:A:2854:PHE:HZ | 1:A:2881:LEU:HB2 | 1.77 | 0.48 |
| 1:A:290:TYR:CD1 | 1:A:293:LEU:HD13 | 2.48 | 0.48 |
| 1:A:2979:GLN:O | 1:A:2982:VAL:HG22 | 2.14 | 0.48 |
| 1:A:3008:TRP:CG | 1:A:3257:LYS:NZ | 2.81 | 0.48 |
| 1:A:3326:GLN:CB | 1:A:3393:GLU:HG2 | 2.37 | 0.48 |
| 1:A:3806:LEU:HG | 1:A:3807:GLU:O | 2.13 | 0.48 |
| 1:A:3900:LEU:HD11 | 1:A:3934:THR:O | 2.13 | 0.48 |
| 1:A:3980:MSE:HA | 1:A:3983:ILE:HG13 | 1.94 | 0.48 |
| 1:B:1025:LEU:HA | 1:B:1025:LEU:HD12 | 1.60 | 0.48 |
| 1:B:1087:ARG:CD | 1:B:1134:LEU:HD22 | 2.44 | 0.48 |
| 1:B:1253:THR:HA | 1:B:1257:LEU:HD12 | 1.95 | 0.48 |
| 1:B:2222:HIS:O | 1:B:2224:PHE:N | 2.47 | 0.48 |
| 1:B:2912:GLY:HA2 | 1:B:2915:ARG:NH2 | 2.28 | 0.48 |
| 1:B:2913:LYS:HG3 | 1:B:2914:ALA:H | 1.76 | 0.48 |
| 1:B:3571:PHE:O | 1:B:3575:LEU:HB3 | 2.13 | 0.48 |
| 1:B:3758:LEU:HD22 | 1:B:3761:ASP:OD2 | 2.13 | 0.48 |
| 1:B:3862:ALA:O | 1:B:3865:THR:OG1 | 2.27 | 0.48 |
| 1:B:3816:LEU:HD11 | 1:B:3883:LEU:HD22 | 1.96 | 0.48 |
| 1:A:157:TYR:HA | 1:A:160:LEU:HG | 1.96 | 0.47 |
| 1:A:1762:MSE:SE | 1:A:1867:ILE:HG21 | 2.64 | 0.47 |
| 1:A:1918:LEU:HD11 | 1:A:1957:ASN:ND2 | 2.29 | 0.47 |
| 1:A:1977:ILE:C | 1:A:1979:GLU:H | 2.13 | 0.47 |
| 1:A:2074:PRO:CB | 1:A:2136:PRO:HB3 | 2.43 | 0.47 |
| 1:A:2358:ASP:N | 1:A:2358:ASP:OD1 | 2.46 | 0.47 |
| 1:A:2390:HIS:ND1 | 1:A:2397:CYS:SG | 2.64 | 0.47 |
| 1:A:2538:ARG:HG3 | 1:A:2539:LEU:N | 2.28 | 0.47 |
| 1:A:3128:LYS:C | 1:A:3130:GLN:H | 2.15 | 0.47 |
| 1:A:3425:ARG:NH1 | 1:A:3999:THR:HG22 | 2.29 | 0.47 |
| 1:A:3725:ARG:HH12 | 1:A:3737:ARG:NH2 | 2.11 | 0.47 |
| 1:A:3870:SER:OG | 1:A:3871:PHE:N | 2.46 | 0.47 |
| 1:A:65:LEU:O | 1:A:69:VAL:HB | 2.14 | 0.47 |
| 1:B:1018:VAL:HB | 1:B:1074:LYS:CA | 2.44 | 0.47 |
| 1:B:1036:PHE:CZ | 1:B:1082:PHE:CE2 | 3.02 | 0.47 |
| 1:B:1268:ASN:HA | 1:B:1271:ILE:HD12 | 1.95 | 0.47 |
| 1:B:1299:GLU:C | 1:B:1302:ALA:H | 2.17 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1946:ASN:HA | 1:B:1949:ILE:HG22 | 1.96 | 0.47 |
| 1:B:2193:ILE:HG13 | 1:B:2196:TRP:CZ2 | 2.49 | 0.47 |
| 1:B:2382:VAL:CG2 | 1:B:2404:ARG:HG3 | 2.40 | 0.47 |
| 1:B:2538:ARG:HG3 | 1:B:2539:LEU:N | 2.28 | 0.47 |
| 1:B:2782:ASP:HA | 1:B:2786:LYS:CB | 2.44 | 0.47 |
| 1:B:3003:ASN:ND2 | 1:B:3010:SER:HB2 | 2.28 | 0.47 |
| 1:B:3110:PHE:HB2 | 1:B:3114:TYR:HE1 | 1.78 | 0.47 |
| 1:B:3136:THR:O | 1:B:3140:GLU:HB2 | 2.14 | 0.47 |
| 1:B:3268:THR:H | 1:B:3271:ASP:HB3 | 1.79 | 0.47 |
| 1:B:3525:TYR:HA | 1:B:3529:ILE:HG21 | 1.96 | 0.47 |
| 1:B:3531:TYR:HB3 | 1:B:3532:PRO:HD3 | 1.95 | 0.47 |
| 1:B:3789:ARG:CZ | 1:B:3806:LEU:HD22 | 2.44 | 0.47 |
| 1:B:3896:ALA:O | 1:B:3899:ALA:HB3 | 2.14 | 0.47 |
| 1:B:4062:ASP:HA | 1:B:4065:LEU:CD2 | 2.44 | 0.47 |
| 1:B:645:TRP:CZ3 | 1:B:659:ARG:HB3 | 2.49 | 0.47 |
| 1:B:76:ILE:HG13 | 1:B:77:GLU:H | 1.79 | 0.47 |
| 1:B:989:MSE:HB2 | 1:B:990:GLN:NE2 | 2.29 | 0.47 |
| 1:B:942:LEU:HD11 | 1:B:991:LEU:CD1 | 2.44 | 0.47 |
| 1:A:1716:GLN:O | 1:A:1719:VAL:N | 2.40 | 0.47 |
| 1:A:1733:THR:N | 1:A:1734:PRO:CD | 2.77 | 0.47 |
| 1:A:2291:GLN:NE2 | 1:A:2294:ILE:HG21 | 2.29 | 0.47 |
| 1:A:290:TYR:O | 1:A:294:PHE:HD1 | 1.97 | 0.47 |
| 1:A:335:LYS:HA | 1:A:338:LEU:HD12 | 1.94 | 0.47 |
| 1:A:3493:TRP:CZ3 | 1:A:3496:ILE:HG13 | 2.49 | 0.47 |
| 1:A:1073:PHE:CZ | 1:A:3745:GLU:HA | 2.49 | 0.47 |
| 1:A:3954:PRO:HG3 | 1:A:4030:GLU:HB2 | 1.95 | 0.47 |
| 1:A:419:SER:O | 1:A:422:LEU:HB2 | 2.15 | 0.47 |
| 1:A:31:GLY:HA3 | 1:A:81:CYS:SG | 2.54 | 0.47 |
| 1:A:935:HIS:NE2 | 1:A:987:LEU:HG | 2.29 | 0.47 |
| 1:B:1438:GLY:O | 1:B:1441:ALA:HB2 | 2.14 | 0.47 |
| 1:B:1869:LYS:O | 1:B:1873:TYR:HD1 | 1.96 | 0.47 |
| 1:B:2420:PHE:HZ | 1:B:2436:LEU:HB3 | 1.76 | 0.47 |
| 1:B:2482:ASP:HA | 1:B:2485:ARG:HB3 | 1.95 | 0.47 |
| 1:B:2911:ARG:O | 1:B:2915:ARG:NE | 2.47 | 0.47 |
| 1:B:3522:THR:HA | 1:B:3525:TYR:HB3 | 1.96 | 0.47 |
| 1:B:3842:TRP:HH2 | 1:B:3846:MSE:HE2 | 1.73 | 0.47 |
| 1:B:58:VAL:O | 1:B:62:ASP:HB2 | 2.14 | 0.47 |
| 1:B:650:SER:HA | 1:B:652:GLU:OE2 | 2.13 | 0.47 |
| 1:B:659:ARG:HH12 | 1:B:662:LEU:CD2 | 2.28 | 0.47 |
| 1:B:922:SER:O | 1:B:926:THR:OG1 | 2.28 | 0.47 |
| 1:A:292:SER:O | 1:A:296:VAL:HB | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2960:GLU:HA | 1:A:3251:ASN:O | 2.14 | 0.47 |
| 1:A:3301:LEU:HB2 | 1:A:3328:ILE:CG2 | 2.44 | 0.47 |
| 1:A:3493:TRP:CE3 | 1:A:3713:PRO:HB3 | 2.49 | 0.47 |
| 1:A:3606:ILE:HD13 | 1:A:3609:MSE:HE3 | 1.96 | 0.47 |
| 1:B:1111:LEU:HD22 | 1:B:1131:ILE:HD13 | 1.96 | 0.47 |
| 1:B:1397:ASP:O | 1:B:1400:VAL:HB | 2.13 | 0.47 |
| 1:B:1501:PRO:O | 1:B:1505:LEU:HB2 | 2.14 | 0.47 |
| 1:B:187:SER:O | 1:B:190:ILE:HG22 | 2.13 | 0.47 |
| 1:B:2440:TYR:O | 1:B:2440:TYR:CG | 2.67 | 0.47 |
| 1:B:3334:TYR:CE1 | 1:B:3426:LYS:HD3 | 2.49 | 0.47 |
| 1:B:3797:THR:CG2 | 1:B:3800:LEU:HG | 2.43 | 0.47 |
| 1:B:634:LEU:O | 1:B:669:LEU:HD12 | 2.14 | 0.47 |
| 1:B:714:VAL:HG11 | 1:B:734:LEU:HD21 | 1.96 | 0.47 |
| 1:A:14:ARG:HH12 | 1:A:2392:VAL:HG21 | 1.79 | 0.47 |
| 1:A:2003:LYS:HG2 | 1:A:2006:GLU:OE1 | 2.14 | 0.47 |
| 1:A:2776:ARG:CZ | 1:A:2776:ARG:HA | 2.44 | 0.47 |
| 1:A:2841:ASN:OD1 | 1:A:2844:LEU:HD12 | 2.15 | 0.47 |
| 1:A:2917:PRO:HB2 | 1:A:2918:PRO:HD3 | 1.95 | 0.47 |
| 1:A:2940:ARG:HD3 | 1:A:3975:LYS:CD | 2.44 | 0.47 |
| 1:A:3487:ILE:HG21 | 1:A:3524:ASN:HD21 | 1.78 | 0.47 |
| 1:A:368:LEU:CA | 1:A:372:PRO:HG2 | 2.44 | 0.47 |
| 1:A:3878:VAL:HB | 1:A:3879:PRO:HD3 | 1.96 | 0.47 |
| 1:A:403:GLY:O | 1:A:405:ASP:N | 2.44 | 0.47 |
| 1:A:455:LEU:O | 1:A:459:ARG:HG3 | 2.15 | 0.47 |
| 1:A:69:VAL:O | 1:A:73:LEU:HG | 2.13 | 0.47 |
| 1:A:718:MSE:O | 1:A:722:LYS:HB2 | 2.15 | 0.47 |
| 1:A:892:LEU:HD21 | 1:A:958:MSE:HG3 | 1.96 | 0.47 |
| 1:B:1080:LEU:HB2 | 1:B:1131:ILE:CG2 | 2.45 | 0.47 |
| 1:B:1472:SER:OG | 1:B:1473:THR:N | 2.48 | 0.47 |
| 1:B:2155:GLU:HB3 | 1:B:2156:VAL:H | 1.40 | 0.47 |
| 1:B:2186:VAL:O | 1:B:2190:VAL:HG13 | 2.13 | 0.47 |
| 1:B:2193:ILE:HG12 | 1:B:2193:ILE:O | 2.14 | 0.47 |
| 1:B:2200:ALA:CA | 1:B:2203:THR:HG22 | 2.41 | 0.47 |
| 1:B:2212:ALA:O | 1:B:2215:LEU:HB3 | 2.15 | 0.47 |
| 1:B:2257:PHE:CE1 | 1:B:2299:TYR:HB3 | 2.49 | 0.47 |
| 1:B:3498:TRP:HD1 | 1:B:3502:MSE:HB2 | 1.77 | 0.47 |
| 1:B:3514:VAL:HG21 | 1:B:3551:ASN:HB3 | 1.95 | 0.47 |
| 1:B:3839:TYR:HB2 | 1:B:3871:PHE:CE1 | 2.49 | 0.47 |
| 1:B:411:PRO:O | 1:B:415:GLN:CB | 2.62 | 0.47 |
| 1:B:612:LEU:HD21 | 1:B:1800:SER:HB3 | 1.96 | 0.47 |
| 1:B:887:ASP:O | 1:B:3889:ARG:NE | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:927:LYS:O | 1:B:931:CYS:SG | 2.73 | 0.47 |
| 1:A:1216:GLY:HA3 | 1:A:1271:ILE:CG2 | 2.45 | 0.47 |
| 1:A:1292:LYS:H | 1:A:1292:LYS:HG3 | 1.52 | 0.47 |
| 1:A:1508:LYS:C | 1:A:1510:LEU:H | 2.18 | 0.47 |
| 1:A:1809:ASP:HA | 1:A:1815:THR:HA | 1.96 | 0.47 |
| 1:A:2549:LYS:HZ3 | 1:A:2554:PHE:HA | 1.75 | 0.47 |
| 1:A:3008:TRP:CE3 | 1:A:3050:LYS:HB2 | 2.50 | 0.47 |
| 1:A:3114:TYR:CE2 | 1:A:3125:ARG:NH2 | 2.83 | 0.47 |
| 1:A:3775:LEU:HB3 | 1:A:3781:CYS:SG | 2.53 | 0.47 |
| 1:A:3834:ALA:HB1 | 1:A:3838:GLU:OE1 | 2.14 | 0.47 |
| 1:A:749:VAL:N | 1:A:750:PRO:HD3 | 2.30 | 0.47 |
| 1:B:1001:PHE:CD1 | 1:B:1002:GLU:N | 2.81 | 0.47 |
| 1:B:1090:ARG:HH12 | 1:B:1096:VAL:CG1 | 2.22 | 0.47 |
| 1:B:205:LYS:HE3 | 1:B:243:GLN:HB3 | 1.96 | 0.47 |
| 1:B:2508:GLN:HG2 | 1:B:2508:GLN:O | 2.14 | 0.47 |
| 1:B:2539:LEU:HG | 1:B:2816:ILE:HG13 | 1.95 | 0.47 |
| 1:B:2603:UNK:CB | 1:B:2793:PRO:HB2 | 2.44 | 0.47 |
| 1:B:3128:LYS:O | 1:B:3132:VAL:HG13 | 2.14 | 0.47 |
| 1:B:3160:LEU:HA | 1:B:3160:LEU:HD12 | 1.75 | 0.47 |
| 1:B:3330:LEU:C | 1:B:3332:THR:H | 2.17 | 0.47 |
| 1:B:3820:MSE:O | 1:B:3824:GLU:N | 2.41 | 0.47 |
| 1:B:428:PRO:O | 1:B:430:VAL:HG23 | 2.14 | 0.47 |
| 1:B:539:GLN:HG3 | 1:B:626:LEU:O | 2.14 | 0.47 |
| 1:B:756:PHE:O | 1:B:759:GLY:C | 2.52 | 0.47 |
| 1:B:801:LYS:HB2 | 1:B:805:LEU:HD12 | 1.96 | 0.47 |
| 1:B:927:LYS:HE3 | 1:B:928:VAL:HG13 | 1.96 | 0.47 |
| 1:A:1213:LYS:O | 1:A:1215:GLU:N | 2.48 | 0.47 |
| 1:A:82:ARG:NH2 | 1:A:130:LEU:HD22 | 2.30 | 0.47 |
| 1:A:1372:LEU:HG | 1:A:1373:VAL:N | 2.29 | 0.47 |
| 1:A:1396:PRO:O | 1:A:1400:VAL:HG23 | 2.14 | 0.47 |
| 1:A:2164:TRP:CH2 | 1:A:2190:VAL:HG12 | 2.49 | 0.47 |
| 1:A:2325:LEU:HG | 1:A:2329:TYR:CD2 | 2.49 | 0.47 |
| 1:A:238:MSE:HG3 | 1:A:239:GLU:HG2 | 1.96 | 0.47 |
| 1:A:3524:ASN:O | 1:A:3529:ILE:HD13 | 2.14 | 0.47 |
| 1:A:3719:ILE:HG23 | 1:A:3720:ALA:H | 1.79 | 0.47 |
| 1:A:3846:MSE:O | 1:A:3857:LEU:HD22 | 2.14 | 0.47 |
| 1:A:4077:TYR:CG | 1:A:4119:ARG:NH1 | 2.82 | 0.47 |
| 1:A:410:MSE:HE2 | 1:A:441:MSE:CE | 2.44 | 0.47 |
| 1:A:977:ASP:O | 1:A:980:THR:HB | 2.14 | 0.47 |
| 1:B:1290:LEU:HD12 | 1:B:1294:VAL:HG21 | 1.97 | 0.47 |
| 1:B:1570:GLU:HA | 1:B:1573:LYS:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1726:SER:CB | 1:B:1866:GLN:HE22 | 2.27 | 0.47 |
| 1:B:2420:PHE:CZ | 1:B:2424:MSE:HE3 | 2.49 | 0.47 |
| 1:B:2803:ILE:O | 1:B:2803:ILE:HG12 | 2.14 | 0.47 |
| 1:B:2884:LEU:O | 1:B:2888:VAL:HG23 | 2.15 | 0.47 |
| 1:B:2989:ALA:HB1 | 1:B:2993:PHE:CD2 | 2.49 | 0.47 |
| 1:B:3128:LYS:C | 1:B:3130:GLN:H | 2.17 | 0.47 |
| 1:B:324:SER:HB3 | 1:B:370:ALA:O | 2.15 | 0.47 |
| 1:B:3762:GLN:HA | 1:B:3793:VAL:CG2 | 2.36 | 0.47 |
| 1:B:458:CYS:SG | 1:B:540:MSE:SE | 3.23 | 0.47 |
| 1:B:749:VAL:N | 1:B:750:PRO:HD3 | 2.30 | 0.47 |
| 2:K:215:UNK:O | 2:K:219:UNK:N | 2.48 | 0.47 |
| 1:A:1013:ILE:O | 1:A:1016:GLY:N | 2.48 | 0.47 |
| 1:A:1033:ILE:CG1 | 1:A:1089:PHE:HE2 | 2.27 | 0.47 |
| 1:A:1715:GLU:HA | 1:A:1718:ILE:HB | 1.95 | 0.47 |
| 1:A:1816:ARG:HD3 | 1:A:1819:PHE:CE1 | 2.49 | 0.47 |
| 1:A:2224:PHE:HB3 | 1:A:2272:VAL:HG13 | 1.96 | 0.47 |
| 1:A:2257:PHE:CD1 | 1:A:2299:TYR:HB3 | 2.49 | 0.47 |
| 1:A:2313:LYS:HA | 1:A:2316:TYR:CD2 | 2.50 | 0.47 |
| 1:A:2390:HIS:CE1 | 1:A:2397:CYS:HG | 2.33 | 0.47 |
| 1:A:2538:ARG:HD2 | 1:A:2562:LEU:HD22 | 1.96 | 0.47 |
| 1:A:282:PHE:CD1 | 1:A:282:PHE:C | 2.88 | 0.47 |
| 1:A:2861:ILE:HD13 | 1:A:2889:GLY:HA2 | 1.96 | 0.47 |
| 1:A:2936:TYR:HD1 | 1:A:2949:THR:HG21 | 1.80 | 0.47 |
| 1:A:2939:LEU:HD21 | 1:A:2994:TRP:CD1 | 2.49 | 0.47 |
| 1:A:3090:TYR:O | 1:A:3092:LEU:N | 2.48 | 0.47 |
| 1:A:3284:SER:HB2 | 1:A:3287:ARG:HH21 | 1.79 | 0.47 |
| 1:A:3757:ASP:OD2 | 1:A:3759:ARG:HD3 | 2.14 | 0.47 |
| 1:A:4083:GLY:O | 1:A:4088:ASN:ND2 | 2.44 | 0.47 |
| 1:A:4085:LYS:HA | 1:A:4088:ASN:HB2 | 1.97 | 0.47 |
| 1:A:527:TYR:O | 1:A:531:PHE:CE2 | 2.67 | 0.47 |
| 1:A:729:CYS:HA | 1:A:732:PHE:CD2 | 2.50 | 0.47 |
| 1:B:1492:ALA:HB1 | 1:B:1493:PRO:CD | 2.45 | 0.47 |
| 1:B:2549:LYS:HD2 | 1:B:2554:PHE:CB | 2.44 | 0.47 |
| 1:B:3187:CYS:O | 1:B:3190:LEU:N | 2.48 | 0.47 |
| 1:B:3503:VAL:HG23 | 1:B:3536:SER:HA | 1.96 | 0.47 |
| 1:B:3834:ALA:H | 1:B:3835:PRO:HD3 | 1.79 | 0.47 |
| 1:B:3887:PHE:CE1 | 1:B:3900:LEU:HB3 | 2.47 | 0.47 |
| 1:B:3919:GLY:N | 1:B:3946:PHE:H | 2.09 | 0.47 |
| 1:A:1116:ALA:O | 1:A:1119:LYS:HG2 | 2.14 | 0.47 |
| 1:A:1162:SER:H | 1:A:1165:LEU:HD12 | 1.80 | 0.47 |
| 1:A:1689:LYS:O | 1:A:1693:VAL:HG23 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1879:VAL:O | 1:A:1882:SER:HB3 | 2.15 | 0.47 |
| 1:A:2023:SER:HB2 | 1:A:2024:TYR:CD1 | 2.49 | 0.47 |
| 1:A:2216:LEU:HD13 | 1:A:2249:LEU:HD21 | 1.97 | 0.47 |
| 1:A:2462:VAL:HG11 | 1:A:2473:MSE:CE | 2.44 | 0.47 |
| 1:A:3447:VAL:HG11 | 1:A:3475:TYR:OH | 2.15 | 0.47 |
| 1:A:3741:ARG:HG2 | 1:A:3741:ARG:NH1 | 2.29 | 0.47 |
| 1:A:3820:MSE:CB | 1:A:3882:LEU:HD13 | 2.44 | 0.47 |
| 1:A:2936:TYR:HD2 | 1:A:3979:LEU:HD11 | 1.78 | 0.47 |
| 1:A:557:SER:O | 1:A:560:LEU:HG | 2.14 | 0.47 |
| 1:A:63:PHE:O | 1:A:67:VAL:HG23 | 2.14 | 0.47 |
| 1:B:1076:LEU:HD11 | 1:B:1114:ALA:CB | 2.45 | 0.47 |
| 1:B:1705:GLY:HA2 | 1:B:1739:TYR:OH | 2.15 | 0.47 |
| 1:B:170:VAL:HG23 | 1:B:173:LYS:CE | 2.44 | 0.47 |
| 1:B:1718:ILE:HA | 1:B:1725:GLN:OE1 | 2.14 | 0.47 |
| 1:B:1737:ASN:O | 1:B:1739:TYR:N | 2.46 | 0.47 |
| 1:B:1760:GLU:HB2 | 1:B:1894:SER:HA | 1.97 | 0.47 |
| 1:B:1945:TYR:OH | 1:B:1959:LEU:HD12 | 2.15 | 0.47 |
| 1:B:2187:VAL:O | 1:B:2190:VAL:HG22 | 2.14 | 0.47 |
| 1:B:2320:ALA:HA | 1:B:2367:VAL:HG23 | 1.96 | 0.47 |
| 1:B:2809:PHE:HB3 | 1:B:2859:GLN:OE1 | 2.14 | 0.47 |
| 1:B:3011:LEU:O | 1:B:3014:CYS:HB2 | 2.14 | 0.47 |
| 1:B:3196:LYS:C | 1:B:3199:PRO:HD2 | 2.35 | 0.47 |
| 1:B:3499:ILE:HG13 | 1:B:3531:TYR:OH | 2.15 | 0.47 |
| 1:B:3792:SER:OG | 1:B:3804:GLU:HB2 | 2.14 | 0.47 |
| 1:B:2933:ILE:HG21 | 1:B:3976:GLU:HG3 | 1.96 | 0.47 |
| 1:B:895:ALA:HB2 | 1:B:904:VAL:HG21 | 1.96 | 0.47 |
| 1:B:966:PHE:CD1 | 1:B:969:LEU:HD13 | 2.50 | 0.47 |
| 1:B:986:PRO:C | 1:B:990:GLN:HE21 | 2.18 | 0.47 |
| 2:K:217:UNK:O | 2:K:220:MSE:HG2 | 2.15 | 0.47 |
| 1:A:1575:LEU:O | 1:A:1635:LYS:NZ | 2.39 | 0.47 |
| 1:A:1729:PHE:CE2 | 1:A:1873:TYR:CE1 | 3.03 | 0.47 |
| 1:A:174:VAL:HG12 | 1:A:178:LEU:HD11 | 1.96 | 0.47 |
| 1:A:2134:GLY:H | 1:A:2137:ILE:HD11 | 1.80 | 0.47 |
| 1:A:2404:ARG:NH1 | 1:A:2412:TYR:CE1 | 2.82 | 0.47 |
| 1:A:2430:GLU:OE2 | 1:A:2461:PHE:CD1 | 2.65 | 0.47 |
| 1:A:3420:CYS:HB2 | 1:A:3446:VAL:HG11 | 1.96 | 0.47 |
| 1:A:3467:ARG:CG | 1:A:3471:ILE:HD12 | 2.45 | 0.47 |
| 1:A:3920:ILE:HG13 | 1:A:3923:ARG:CD | 2.45 | 0.47 |
| 1:A:3944:HIS:CD2 | 1:A:4020:MSE:HE3 | 2.49 | 0.47 |
| 1:A:3985:VAL:HG22 | 1:A:4104:VAL:HG21 | 1.95 | 0.47 |
| 1:A:4069:GLU:OE2 | 1:A:4070:LYS:HG3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:68:PHE:O | 1:A:72:SER:OG | 2.23 | 0.47 |
| 1:A:798:GLY:HA2 | 1:A:873:VAL:HG11 | 1.96 | 0.47 |
| 1:B:1118:GLU:O | 1:B:1120:SER:N | 2.47 | 0.47 |
| 1:B:2385:LEU:HG | 1:B:2389:PHE:CE2 | 2.49 | 0.47 |
| 1:B:3040:TYR:HA | 1:B:3043:TYR:CD2 | 2.50 | 0.47 |
| 1:B:3122:HIS:O | 1:B:3125:ARG:N | 2.47 | 0.47 |
| 1:B:3251:ASN:HD21 | 1:B:3254:LEU:HD13 | 1.80 | 0.47 |
| 1:B:3247:ARG:HD3 | 1:B:3281:CYS:SG | 2.55 | 0.47 |
| 1:B:3459:ASN:ND2 | 1:B:3710:LYS:HZ3 | 2.12 | 0.47 |
| 1:B:3659:PHE:CD1 | 1:B:3662:ILE:HD12 | 2.50 | 0.47 |
| 1:B:704:PHE:HA | 1:B:707:PHE:CD1 | 2.50 | 0.47 |
| 1:B:858:MSE:O | 1:B:861:SER:N | 2.48 | 0.47 |
| 1:A:1036:PHE:CZ | 1:A:1082:PHE:CE2 | 3.03 | 0.47 |
| 1:A:1131:ILE:HG12 | 1:A:1132:ASP:N | 2.29 | 0.47 |
| 1:A:1701:SER:OG | 1:A:1702:LEU:N | 2.48 | 0.47 |
| 1:A:1970:LYS:HZ1 | 1:A:2018:ASP:N | 2.13 | 0.47 |
| 1:A:205:LYS:O | 1:A:208:MSE:HG2 | 2.15 | 0.47 |
| 1:A:257:ARG:H | 1:A:258:PRO:HD2 | 1.78 | 0.47 |
| 1:A:241:ASP:HB2 | 1:A:282:PHE:HE2 | 1.80 | 0.47 |
| 1:A:3080:LEU:HD13 | 1:A:3102:TYR:OH | 2.15 | 0.47 |
| 1:A:3386:SER:HA | 1:A:3389:VAL:HG12 | 1.97 | 0.47 |
| 1:A:3393:GLU:OE1 | 1:A:3416:LEU:HD23 | 2.15 | 0.47 |
| 1:A:3510:GLN:CD | 1:A:3513:ALA:HB2 | 2.35 | 0.47 |
| 1:A:3583:LEU:HD11 | 1:A:3733:ARG:CB | 2.42 | 0.47 |
| 1:A:384:MSE:O | 1:A:385:TYR:HB3 | 2.15 | 0.47 |
| 1:A:2891:ARG:HH21 | 1:A:3884:LYS:HD3 | 1.76 | 0.47 |
| 1:A:667:TYR:O | 1:A:669:LEU:N | 2.47 | 0.47 |
| 1:A:776:TRP:CZ2 | 1:A:780:ILE:HD12 | 2.50 | 0.47 |
| 1:A:928:VAL:HG23 | 1:A:929:ALA:N | 2.29 | 0.47 |
| 1:B:963:LYS:HG3 | 1:B:1009:LEU:CD1 | 2.45 | 0.47 |
| 1:B:1036:PHE:HD1 | 1:B:1059:LEU:HD11 | 1.79 | 0.47 |
| 1:B:1068:LEU:HD11 | 1:B:1110:SER:OG | 2.15 | 0.47 |
| 1:B:1302:ALA:O | 1:B:1306:ILE:HB | 2.15 | 0.47 |
| 1:B:2239:LYS:CG | 1:B:2279:ILE:HD12 | 2.45 | 0.47 |
| 1:B:2254:ARG:HB2 | 1:B:2295:GLN:HB2 | 1.97 | 0.47 |
| 1:B:2379:MSE:HG2 | 1:B:2408:MSE:SE | 2.65 | 0.47 |
| 1:B:2407:GLY:O | 1:B:2409:THR:HG23 | 2.15 | 0.47 |
| 1:B:2987:THR:O | 1:B:2990:GLU:HB2 | 2.14 | 0.47 |
| 1:B:3160:LEU:HB3 | 1:B:3164:TRP:CZ3 | 2.50 | 0.47 |
| 1:B:3243:ILE:HG23 | 1:B:3258:LEU:HD12 | 1.96 | 0.47 |
| 1:B:3244:ASP:O | 1:B:3247:ARG:HB3 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3503:VAL:CG2 | 1:B:3536:SER:HA | 2.45 | 0.47 |
| 1:B:3720:ALA:HB2 | 1:B:3743:HIS:HB2 | 1.96 | 0.47 |
| 1:B:3944:HIS:ND1 | 1:B:3949:ALA:HA | 2.29 | 0.47 |
| 1:B:777:SER:HB2 | 1:B:858:MSE:HE1 | 1.97 | 0.47 |
| 1:B:943:GLY:O | 1:B:945:ALA:N | 2.45 | 0.47 |
| 1:B:987:LEU:O | 1:B:991:LEU:HD13 | 2.15 | 0.47 |
| 1:A:1251:GLN:HE21 | 1:A:1329:ARG:NH1 | 2.13 | 0.47 |
| 1:A:125:ILE:H | 1:A:126:PRO:CD | 2.28 | 0.47 |
| 1:A:1292:LYS:O | 1:A:1295:ALA:HB3 | 2.15 | 0.47 |
| 1:A:1335:CYS:SG | 1:A:1382:ILE:HG21 | 2.55 | 0.47 |
| 1:A:474:VAL:HG11 | 1:A:1564:SER:HB2 | 1.97 | 0.47 |
| 1:A:1685:ASP:CB | 1:A:1727:ARG:NH2 | 2.74 | 0.47 |
| 1:A:1745:LYS:C | 1:A:1747:LEU:N | 2.68 | 0.47 |
| 1:A:1598:ASN:ND2 | 1:A:1811:ARG:HB3 | 2.30 | 0.47 |
| 1:A:2260:PHE:HA | 1:A:2273:GLY:HA3 | 1.96 | 0.47 |
| 1:A:234:PHE:O | 1:A:235:THR:OG1 | 2.22 | 0.47 |
| 1:A:2637:UNK:O | 1:A:2641:UNK:CB | 2.63 | 0.47 |
| 1:A:2856:SER:O | 1:A:2859:GLN:HB3 | 2.15 | 0.47 |
| 1:A:3011:LEU:HD11 | 1:A:3043:TYR:O | 2.15 | 0.47 |
| 1:A:3053:LEU:HD11 | 1:A:3187:CYS:HB3 | 1.96 | 0.47 |
| 1:A:3147:LYS:O | 1:A:3151:LEU:N | 2.48 | 0.47 |
| 1:A:3533:PHE:CD1 | 1:A:3562:LEU:HB3 | 2.50 | 0.47 |
| 1:A:544:ILE:O | 1:A:548:GLU:HB2 | 2.14 | 0.47 |
| 1:A:927:LYS:O | 1:A:931:CYS:SG | 2.73 | 0.47 |
| 1:B:1350:ASN:HD22 | 1:B:1404:LYS:HE3 | 1.79 | 0.47 |
| 1:B:1349:LEU:CA | 1:B:1353:PRO:HD2 | 2.44 | 0.47 |
| 1:B:133:LYS:O | 1:B:137:THR:HG23 | 2.15 | 0.47 |
| 1:B:1583:MSE:SE | 1:B:1643:MSE:SE | 3.32 | 0.47 |
| 1:B:1952:ILE:HG12 | 1:B:1953:CYS:H | 1.79 | 0.47 |
| 1:B:2097:LEU:CD2 | 1:B:2100:LEU:HD22 | 2.45 | 0.47 |
| 1:B:257:ARG:N | 1:B:258:PRO:CD | 2.77 | 0.47 |
| 1:B:260:ILE:O | 1:B:264:ARG:HG2 | 2.15 | 0.47 |
| 1:B:2970:LYS:O | 1:B:2974:GLU:HG2 | 2.14 | 0.47 |
| 1:B:3059:GLN:CD | 1:B:3059:GLN:H | 2.17 | 0.47 |
| 1:B:3284:SER:CA | 1:B:3287:ARG:HE | 2.12 | 0.47 |
| 1:B:3298:LEU:HD11 | 1:B:3351:ILE:CD1 | 2.45 | 0.47 |
| 1:B:3585:PHE:HE1 | 1:B:3617:LEU:HD11 | 1.79 | 0.47 |
| 1:B:3904:PHE:CE1 | 1:B:3967:PHE:HE1 | 2.32 | 0.47 |
| 1:B:3965:ARG:HE | 1:B:3969:ASN:ND2 | 2.14 | 0.47 |
| 1:B:3981:TYR:HA | 1:B:4108:MSE:HE1 | 1.96 | 0.47 |
| 1:B:912:PRO:HB2 | 1:B:913:ARG:CZ | 2.45 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1059:LEU:O | 1:A:1062:ARG:N | 2.48 | 0.46 |
| 1:A:1601:LEU:O | 1:A:1605:PHE:HB2 | 2.14 | 0.46 |
| 1:A:1583:MSE:HE2 | 1:A:1639:LEU:HD13 | 1.97 | 0.46 |
| 1:A:1687:HIS:HB3 | 1:A:1691:GLN:NE2 | 2.30 | 0.46 |
| 1:A:2323:LEU:HD13 | 1:A:2371:PHE:CZ | 2.50 | 0.46 |
| 1:A:2473:MSE:O | 1:A:2476:ILE:HG12 | 2.14 | 0.46 |
| 1:A:2514:ASN:H | 1:A:2515:PRO:CD | 2.29 | 0.46 |
| 1:A:242:PRO:HD3 | 1:A:282:PHE:CE2 | 2.50 | 0.46 |
| 1:A:358:GLU:OE1 | 1:A:1858:LEU:HD13 | 2.15 | 0.46 |
| 1:A:3620:PRO:HB2 | 1:A:3633:ILE:HG23 | 1.95 | 0.46 |
| 1:A:3699:LEU:O | 1:A:3718:ARG:NH1 | 2.47 | 0.46 |
| 1:A:3887:PHE:HZ | 1:A:3904:PHE:CD2 | 2.33 | 0.46 |
| 1:A:3928:PHE:C | 1:A:3928:PHE:CD1 | 2.88 | 0.46 |
| 1:A:443:ILE:HD11 | 1:A:465:PHE:HE2 | 1.80 | 0.46 |
| 1:A:797:ASP:HA | 1:A:800:LEU:HB2 | 1.96 | 0.46 |
| 1:A:934:LEU:HD21 | 1:A:962:TYR:CZ | 2.49 | 0.46 |
| 1:B:1563:PHE:CD1 | 1:B:1567:ILE:HG13 | 2.50 | 0.46 |
| 1:B:2404:ARG:NH1 | 1:B:2412:TYR:CE2 | 2.83 | 0.46 |
| 1:B:2439:ILE:HG21 | 1:B:2439:ILE:HD13 | 1.64 | 0.46 |
| 1:B:2554:PHE:O | 1:B:2557:LEU:N | 2.48 | 0.46 |
| 1:B:277:LEU:HD22 | 1:B:278:HIS:CD2 | 2.51 | 0.46 |
| 1:B:361:ILE:HB | 1:B:364:ARG:NH2 | 2.30 | 0.46 |
| 1:B:3457:ASN:O | 1:B:3710:LYS:NZ | 2.47 | 0.46 |
| 1:B:3722:PHE:HD1 | 1:B:3740:ILE:HA | 1.80 | 0.46 |
| 1:B:4081:ALA:HA | 1:B:4113:ASP:OD2 | 2.13 | 0.46 |
| 1:B:670:LEU:HG | 1:B:740:ILE:HG23 | 1.97 | 0.46 |
| 1:B:732:PHE:CE1 | 1:B:768:VAL:HG12 | 2.50 | 0.46 |
| 1:B:965:THR:HA | 1:B:968:VAL:HG12 | 1.95 | 0.46 |
| 1:A:1010:LEU:O | 1:A:1013:ILE:N | 2.39 | 0.46 |
| 1:A:1373:VAL:O | 1:A:1375:THR:N | 2.41 | 0.46 |
| 1:A:186:PRO:O | 1:A:189:MSE:HB3 | 2.16 | 0.46 |
| 1:A:1976:LEU:HD11 | 1:A:2031:LEU:CB | 2.44 | 0.46 |
| 1:A:2186:VAL:O | 1:A:2189:ILE:HG13 | 2.15 | 0.46 |
| 1:A:2199:LEU:HA | 1:A:2202:PRO:HD2 | 1.97 | 0.46 |
| 1:A:2418:LYS:O | 1:A:2421:VAL:HG12 | 2.15 | 0.46 |
| 1:A:2554:PHE:O | 1:A:2557:LEU:HB2 | 2.16 | 0.46 |
| 1:A:2900:LEU:HD23 | 1:A:2910:VAL:HA | 1.97 | 0.46 |
| 1:A:3008:TRP:CA | 1:A:3050:LYS:HG2 | 2.44 | 0.46 |
| 1:A:348:ILE:O | 1:A:364:ARG:HD3 | 2.16 | 0.46 |
| 1:A:3674:SER:C | 1:A:3677:PRO:HD2 | 2.35 | 0.46 |
| 1:A:3931:ALA:HB3 | 1:A:3936:GLY:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:4069:GLU:HA | 1:A:4070:LYS:HA | 1.64 | 0.46 |
| 1:B:1231:GLN:H | 1:B:1232:PRO:CD | 2.28 | 0.46 |
| 1:B:1259:LEU:HD11 | 1:B:1337:VAL:HA | 1.97 | 0.46 |
| 1:B:135:LEU:O | 1:B:139:ARG:HG3 | 2.15 | 0.46 |
| 1:B:401:ASP:HB2 | 1:B:1763:THR:HB | 1.98 | 0.46 |
| 1:B:1874:TYR:OH | 1:B:1884:LEU:HD12 | 2.15 | 0.46 |
| 1:B:2289:ASP:O | 1:B:2290:PRO:C | 2.53 | 0.46 |
| 1:B:381:VAL:O | 1:B:384:MSE:HG2 | 2.14 | 0.46 |
| 1:B:763:THR:HG21 | 1:B:769:GLY:HA3 | 1.97 | 0.46 |
| 1:A:135:LEU:HD22 | 1:A:173:LYS:HB2 | 1.97 | 0.46 |
| 1:A:1376:LEU:HG | 1:A:1377:CYS:N | 2.30 | 0.46 |
| 1:A:1495:ASP:O | 1:A:1498:GLN:HB2 | 2.15 | 0.46 |
| 1:A:1696:LEU:HD23 | 1:A:1700:THR:HG21 | 1.97 | 0.46 |
| 1:A:1985:LYS:HD2 | 1:A:2037:SER:HB3 | 1.98 | 0.46 |
| 1:A:2233:HIS:O | 1:A:2237:ILE:HG13 | 2.15 | 0.46 |
| 1:A:2823:PHE:CG | 1:A:2824:LYS:N | 2.83 | 0.46 |
| 1:A:2949:THR:O | 1:A:2952:ILE:N | 2.46 | 0.46 |
| 1:A:3141:PHE:CE1 | 1:A:3189:PHE:HA | 2.51 | 0.46 |
| 1:A:3762:GLN:HA | 1:A:3793:VAL:CG2 | 2.41 | 0.46 |
| 1:A:399:GLN:OE1 | 1:A:405:ASP:HB2 | 2.16 | 0.46 |
| 1:A:385:TYR:HE1 | 1:A:421:LEU:HD23 | 1.79 | 0.46 |
| 1:A:436:GLU:OE2 | 1:A:475:LEU:CD1 | 2.63 | 0.46 |
| 1:A:777:SER:O | 1:A:781:ASP:N | 2.48 | 0.46 |
| 1:B:1455:CYS:O | 1:B:1458:LEU:N | 2.49 | 0.46 |
| 1:B:1602:ASP:HB2 | 1:B:1810:PRO:HB3 | 1.98 | 0.46 |
| 1:B:2009:LYS:HG3 | 1:B:2012:ARG:NH1 | 2.30 | 0.46 |
| 1:B:2067:ARG:O | 1:B:2068:ARG:HB2 | 2.14 | 0.46 |
| 1:B:222:GLY:O | 1:B:225:LYS:N | 2.49 | 0.46 |
| 1:B:3616:ALA:O | 1:B:3617:LEU:HD23 | 2.16 | 0.46 |
| 1:B:4002:MSE:SE | 1:B:4048:LYS:CE | 3.12 | 0.46 |
| 1:B:3855:TYR:HB3 | 1:B:4074:PHE:HZ | 1.80 | 0.46 |
| 1:B:431:TYR:N | 1:B:431:TYR:CD1 | 2.79 | 0.46 |
| 1:B:487:LEU:HD21 | 1:B:530:LEU:HB2 | 1.97 | 0.46 |
| 1:B:543:SER:O | 1:B:545:LEU:N | 2.37 | 0.46 |
| 1:B:789:TYR:HB2 | 1:B:865:GLN:HE21 | 1.81 | 0.46 |
| 1:A:1395:LEU:N | 1:A:1396:PRO:HD2 | 2.30 | 0.46 |
| 1:A:1476:HIS:CE1 | 1:A:1507:CYS:HA | 2.50 | 0.46 |
| 1:A:1589:ASN:O | 1:A:1590:THR:HG22 | 2.16 | 0.46 |
| 1:A:1602:ASP:HB2 | 1:A:1810:PRO:HB3 | 1.96 | 0.46 |
| 1:A:1604:SER:CB | 1:A:1632:TRP:HE3 | 2.28 | 0.46 |
| 1:A:1874:TYR:HD2 | 1:A:1885:PRO:HG3 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2177:ASN:HB3 | 1:A:2182:ILE:N | 2.30 | 0.46 |
| 1:A:2310:VAL:HG23 | 1:A:2315:VAL:HG21 | 1.98 | 0.46 |
| 1:A:2834:GLN:O | 1:A:2837:LEU:HG | 2.15 | 0.46 |
| 1:A:350:ARG:NH1 | 1:A:387:GLU:OE1 | 2.49 | 0.46 |
| 1:A:730:LEU:HA | 1:A:730:LEU:HD23 | 1.82 | 0.46 |
| 1:A:764:PRO:HB3 | 1:A:770:LEU:HD11 | 1.97 | 0.46 |
| 1:A:849:GLU:H | 1:A:849:GLU:CD | 2.18 | 0.46 |
| 1:B:158:GLY:O | 1:B:162:LEU:HD13 | 2.15 | 0.46 |
| 1:B:1809:ASP:O | 1:B:1815:THR:HG22 | 2.14 | 0.46 |
| 1:B:1917:LYS:HE2 | 1:B:1953:CYS:O | 2.14 | 0.46 |
| 1:B:2312:TYR:CZ | 1:B:2313:LYS:HG2 | 2.50 | 0.46 |
| 1:B:241:ASP:HB3 | 1:B:282:PHE:HE2 | 1.78 | 0.46 |
| 1:B:3160:LEU:HD23 | 1:B:3164:TRP:CH2 | 2.51 | 0.46 |
| 1:B:3283:LEU:O | 1:B:3283:LEU:HD22 | 2.16 | 0.46 |
| 1:B:3740:ILE:HD12 | 1:B:3750:PHE:CE1 | 2.51 | 0.46 |
| 1:B:3816:LEU:O | 1:B:3820:MSE:CB | 2.64 | 0.46 |
| 1:B:3463:LEU:HD13 | 1:B:4000:ASN:CB | 2.45 | 0.46 |
| 1:B:70:ARG:HH12 | 1:B:117:LYS:HD2 | 1.80 | 0.46 |
| 1:B:852:ARG:HH12 | 1:B:3111:MSE:HG2 | 1.79 | 0.46 |
| 1:B:892:LEU:HD11 | 1:B:958:MSE:HG3 | 1.98 | 0.46 |
| 1:B:898:PHE:CD2 | 1:B:2566:THR:HG21 | 2.50 | 0.46 |
| 1:A:2240:THR:HG21 | 2:K:112:UNK:HA | 1.98 | 0.46 |
| 1:A:964:ARG:CB | 1:A:1009:LEU:HD22 | 2.35 | 0.46 |
| 1:A:1012:ALA:O | 1:A:1015:ASP:HB3 | 2.15 | 0.46 |
| 1:A:993:HIS:HB2 | 1:A:1038:LYS:CG | 2.45 | 0.46 |
| 1:A:1072:ALA:HB1 | 1:A:1076:LEU:CD1 | 2.46 | 0.46 |
| 1:A:1494:GLY:O | 1:A:1498:GLN:HG3 | 2.15 | 0.46 |
| 1:A:1593:VAL:O | 1:A:1597:LEU:CB | 2.62 | 0.46 |
| 1:A:429:GLU:HG2 | 1:A:1594:SER:HB2 | 1.97 | 0.46 |
| 1:A:1636:ASP:HA | 1:A:1639:LEU:HD11 | 1.98 | 0.46 |
| 1:A:1651:LYS:HD2 | 1:A:1684:LEU:HG | 1.98 | 0.46 |
| 1:A:1897:ASN:HB3 | 1:A:1901:HIS:CE1 | 2.50 | 0.46 |
| 1:A:1933:LEU:H | 1:A:1938:ARG:NH2 | 2.13 | 0.46 |
| 1:A:1934:LEU:HD11 | 1:A:1937:ARG:H | 1.80 | 0.46 |
| 1:A:2923:TRP:CD1 | 1:A:2926:LEU:HD23 | 2.50 | 0.46 |
| 1:A:3121:LEU:O | 1:A:3124:SER:HB2 | 2.14 | 0.46 |
| 1:A:3297:VAL:HG11 | 1:A:3332:THR:HG23 | 1.97 | 0.46 |
| 1:B:1423:ILE:HG13 | 1:B:1424:THR:H | 1.81 | 0.46 |
| 1:B:1447:ARG:O | 1:B:1451:VAL:HG23 | 2.15 | 0.46 |
| 1:B:1592:MSE:O | 1:B:1596:VAL:HG12 | 2.16 | 0.46 |
| 1:B:1865:THR:O | 1:B:1869:LYS:HG3 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:178:LEU:HB3 | 1:B:197:PHE:CE1 | 2.49 | 0.46 |
| 1:B:2383:PHE:CE1 | 1:B:2412:TYR:HD1 | 2.34 | 0.46 |
| 1:B:2413:PHE:HD2 | 1:B:2445:LYS:HG3 | 1.76 | 0.46 |
| 1:B:3334:TYR:HE1 | 1:B:3426:LYS:HD3 | 1.81 | 0.46 |
| 1:B:3813:LYS:HE3 | 1:B:3926:ASN:HB2 | 1.98 | 0.46 |
| 1:B:368:LEU:HD21 | 1:B:384:MSE:SE | 2.66 | 0.46 |
| 1:B:4057:ALA:C | 1:B:4059:ILE:N | 2.69 | 0.46 |
| 1:B:4085:LYS:HA | 1:B:4088:ASN:HB3 | 1.98 | 0.46 |
| 1:B:648:SER:O | 1:B:651:TYR:HB2 | 2.15 | 0.46 |
| 1:A:1917:LYS:HD2 | 1:A:1953:CYS:HB3 | 1.98 | 0.46 |
| 1:A:2177:ASN:HB2 | 1:A:2182:ILE:HG23 | 1.97 | 0.46 |
| 1:A:2232:ARG:O | 1:A:2234:ASN:N | 2.49 | 0.46 |
| 1:A:2260:PHE:CZ | 1:A:2306:ASN:HB2 | 2.51 | 0.46 |
| 1:A:2371:PHE:CG | 1:A:2372:PRO:HD3 | 2.51 | 0.46 |
| 1:A:2555:LEU:HD12 | 1:A:2556:SER:H | 1.79 | 0.46 |
| 1:A:2776:ARG:O | 1:A:2780:LEU:HD23 | 2.15 | 0.46 |
| 1:A:2575:PRO:HB3 | 1:A:2789:SER:N | 2.31 | 0.46 |
| 1:A:3463:LEU:HD13 | 1:A:4000:ASN:HB2 | 1.97 | 0.46 |
| 1:A:3549:HIS:NE2 | 1:A:3553:GLU:HG3 | 2.30 | 0.46 |
| 1:A:3578:LEU:HB3 | 1:A:3579:SER:HA | 1.97 | 0.46 |
| 1:A:3722:PHE:CE1 | 1:A:3740:ILE:HA | 2.51 | 0.46 |
| 1:A:3817:LEU:HD23 | 1:A:3820:MSE:CE | 2.45 | 0.46 |
| 1:A:3966:GLN:HG2 | 1:A:4128:MSE:O | 2.15 | 0.46 |
| 1:A:3944:HIS:HA | 1:A:4016:PHE:HZ | 1.81 | 0.46 |
| 1:A:434:VAL:HG23 | 1:A:437:HIS:CE1 | 2.51 | 0.46 |
| 1:A:471:LYS:HG3 | 1:A:1553:PHE:HZ | 1.81 | 0.46 |
| 1:A:512:GLY:HA2 | 1:A:602:MSE:CE | 2.45 | 0.46 |
| 1:A:649:PHE:C | 1:A:651:TYR:H | 2.18 | 0.46 |
| 1:A:749:VAL:N | 1:A:750:PRO:CD | 2.79 | 0.46 |
| 1:A:89:LEU:HA | 1:A:92:PHE:CD2 | 2.50 | 0.46 |
| 1:B:1565:GLU:HG2 | 1:B:1566:THR:HG23 | 1.97 | 0.46 |
| 1:B:2142:ILE:O | 1:B:2145:PHE:HB2 | 2.16 | 0.46 |
| 1:B:2159:PRO:HA | 1:B:2162:LYS:HB2 | 1.98 | 0.46 |
| 1:B:2539:LEU:HB3 | 1:B:2816:ILE:CD1 | 2.46 | 0.46 |
| 1:B:3092:LEU:O | 1:B:3192:LYS:NZ | 2.42 | 0.46 |
| 1:B:3167:ARG:CD | 1:B:3186:ARG:HG2 | 2.45 | 0.46 |
| 1:B:3578:LEU:HD13 | 1:B:3683:CYS:SG | 2.56 | 0.46 |
| 1:B:3701:ILE:HG13 | 1:B:3701:ILE:O | 2.15 | 0.46 |
| 1:B:12:LEU:HD12 | 1:B:58:VAL:HG21 | 1.97 | 0.46 |
| 1:B:617:PRO:CB | 1:B:659:ARG:HD2 | 2.45 | 0.46 |
| 1:A:1138:ILE:HD13 | 1:A:1150:LYS:CE | 2.39 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1382:ILE:HB | 1:A:1386:ILE:CD1 | 2.44 | 0.46 |
| 1:A:1633:TRP:HA | 1:A:1636:ASP:OD2 | 2.15 | 0.46 |
| 1:A:2004:TYR:C | 1:A:2004:TYR:CD1 | 2.88 | 0.46 |
| 1:A:2097:LEU:HA | 1:A:2097:LEU:HD23 | 1.77 | 0.46 |
| 1:A:2190:VAL:O | 1:A:2193:ILE:HG22 | 2.16 | 0.46 |
| 1:A:2220:MSE:O | 1:A:2223:VAL:HG12 | 2.16 | 0.46 |
| 1:A:2252:PRO:HA | 1:A:2254:ARG:NH1 | 2.31 | 0.46 |
| 1:A:231:LEU:HD23 | 1:A:234:PHE:HB3 | 1.98 | 0.46 |
| 1:A:2433:LYS:HG3 | 1:A:2436:LEU:CD1 | 2.42 | 0.46 |
| 1:A:2861:ILE:HD12 | 1:A:2892:LEU:HD23 | 1.97 | 0.46 |
| 1:A:852:ARG:HH12 | 1:A:3110:PHE:HE1 | 1.61 | 0.46 |
| 1:A:3971:MSE:HE1 | 1:A:3980:MSE:HE1 | 1.97 | 0.46 |
| 1:A:4066:LEU:HD21 | 1:A:4078:VAL:CG2 | 2.46 | 0.46 |
| 1:A:608:PRO:HG2 | 1:A:1798:LEU:HD12 | 1.97 | 0.46 |
| 1:B:598:PRO:HG3 | 1:B:1022:ASP:O | 2.16 | 0.46 |
| 1:B:1119:LYS:NZ | 1:B:1256:TRP:HE1 | 2.13 | 0.46 |
| 1:B:1449:ALA:HA | 1:B:1452:VAL:HB | 1.96 | 0.46 |
| 1:B:2002:LYS:C | 1:B:2004:TYR:N | 2.68 | 0.46 |
| 1:B:2374:LEU:N | 1:B:2378:PHE:HE1 | 2.14 | 0.46 |
| 1:B:2926:LEU:HD22 | 1:B:2931:ARG:NE | 2.31 | 0.46 |
| 1:B:2962:ARG:HG3 | 1:B:3253:SER:OG | 2.16 | 0.46 |
| 1:B:3173:MSE:HG2 | 1:B:3174:ASP:OD1 | 2.15 | 0.46 |
| 1:B:3323:PHE:O | 1:B:3326:GLN:N | 2.48 | 0.46 |
| 1:B:3630:ARG:HD2 | 1:B:3633:ILE:HG12 | 1.98 | 0.46 |
| 1:B:3878:VAL:HB | 1:B:3879:PRO:HD3 | 1.98 | 0.46 |
| 1:B:655:LEU:HA | 1:B:655:LEU:HD12 | 1.60 | 0.46 |
| 1:A:1132:ASP:O | 1:A:1135:CYS:N | 2.49 | 0.46 |
| 1:A:1378:GLU:O | 1:A:1381:SER:N | 2.49 | 0.46 |
| 1:A:1521:PHE:HA | 1:A:1524:LEU:HD22 | 1.98 | 0.46 |
| 1:A:1652:ILE:HA | 1:A:1655:ILE:HD12 | 1.97 | 0.46 |
| 1:A:2011:ALA:HB3 | 1:A:2014:ALA:HB2 | 1.98 | 0.46 |
| 1:A:2221:LYS:O | 1:A:2225:HIS:CE1 | 2.69 | 0.46 |
| 1:A:2385:LEU:HG | 1:A:2389:PHE:CZ | 2.51 | 0.46 |
| 1:A:2828:GLU:O | 1:A:2832:ILE:HG13 | 2.15 | 0.46 |
| 1:A:3024:PRO:N | 1:A:3025:PRO:HD3 | 2.31 | 0.46 |
| 1:A:3059:GLN:H | 1:A:3059:GLN:CD | 2.19 | 0.46 |
| 1:A:3292:GLY:O | 1:A:3297:VAL:HG23 | 2.15 | 0.46 |
| 1:A:3593:ARG:HH11 | 1:A:3593:ARG:HG2 | 1.81 | 0.46 |
| 1:A:3771:MSE:SE | 1:A:3991:PHE:HE1 | 2.49 | 0.46 |
| 1:A:4077:TYR:CZ | 1:A:4119:ARG:HD2 | 2.51 | 0.46 |
| 1:A:513:GLU:OE1 | 1:A:655:LEU:HB3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1690:GLY:O | 1:B:1694:THR:HG22 | 2.16 | 0.46 |
| 1:B:2000:ARG:HG2 | 1:B:2001:LYS:HG3 | 1.97 | 0.46 |
| 1:B:2369:LYS:HE3 | 1:B:2406:GLU:OE1 | 2.16 | 0.46 |
| 1:B:239:GLU:C | 1:B:242:PRO:HD2 | 2.36 | 0.46 |
| 1:B:2869:LEU:HB3 | 1:B:2893:LEU:HG | 1.96 | 0.46 |
| 1:B:3052:LEU:HD11 | 1:B:3092:LEU:HG | 1.97 | 0.46 |
| 1:B:3241:LYS:C | 1:B:3243:ILE:H | 2.18 | 0.46 |
| 1:B:3272:TRP:CZ3 | 1:B:3307:LEU:HD21 | 2.51 | 0.46 |
| 1:B:3439:LEU:O | 1:B:3443:PRO:HD3 | 2.16 | 0.46 |
| 1:B:3499:ILE:CG2 | 1:B:3535:ILE:HD13 | 2.41 | 0.46 |
| 1:B:3868:VAL:HG13 | 1:B:3872:ARG:HB2 | 1.98 | 0.46 |
| 1:B:575:ILE:HB | 1:B:605:THR:CA | 2.46 | 0.46 |
| 1:A:67:VAL:HG22 | 1:A:110:THR:HG21 | 1.97 | 0.46 |
| 1:A:1455:CYS:O | 1:A:1458:LEU:HB2 | 2.16 | 0.46 |
| 1:A:1563:PHE:CE1 | 1:A:1567:ILE:HG13 | 2.51 | 0.46 |
| 1:A:1652:ILE:HG21 | 1:A:1716:GLN:OE1 | 2.15 | 0.46 |
| 1:A:1760:GLU:HB2 | 1:A:1894:SER:HA | 1.97 | 0.46 |
| 1:A:2100:LEU:O | 1:A:2104:MSE:HB2 | 2.16 | 0.46 |
| 1:A:2183:HIS:C | 1:A:2187:VAL:HB | 2.26 | 0.46 |
| 1:A:2164:TRP:HH2 | 1:A:2190:VAL:CG1 | 2.29 | 0.46 |
| 1:A:2232:ARG:HH22 | 1:A:2313:LYS:NZ | 2.13 | 0.46 |
| 1:A:2255:LEU:HD12 | 1:A:2258:GLU:HB2 | 1.98 | 0.46 |
| 1:A:2517:LEU:HD23 | 1:A:2517:LEU:H | 1.80 | 0.46 |
| 1:A:2801:ASP:HB2 | 1:A:2802:PRO:HD3 | 1.98 | 0.46 |
| 1:A:3092:LEU:O | 1:A:3192:LYS:NZ | 2.45 | 0.46 |
| 1:A:295:GLU:CD | 1:A:341:PHE:HE1 | 2.19 | 0.46 |
| 1:A:3694:PHE:CD2 | 1:A:3697:ASN:HA | 2.51 | 0.46 |
| 1:A:431:TYR:CD1 | 1:A:431:TYR:N | 2.84 | 0.46 |
| 1:A:805:LEU:HD13 | 1:A:3117:ILE:HD13 | 1.98 | 0.46 |
| 1:A:878:GLU:C | 1:A:880:MSE:H | 2.19 | 0.46 |
| 1:A:971:ARG:CG | 1:A:972:LEU:N | 2.69 | 0.46 |
| 1:A:973:ALA:HB1 | 1:A:977:ASP:OD2 | 2.16 | 0.46 |
| 1:B:172:GLU:HG2 | 1:B:221:ALA:HB3 | 1.98 | 0.46 |
| 1:B:1747:LEU:HA | 1:B:1747:LEU:HD23 | 1.77 | 0.46 |
| 1:B:2312:TYR:CG | 1:B:2313:LYS:N | 2.83 | 0.46 |
| 1:B:2900:LEU:HD23 | 1:B:2910:VAL:HA | 1.98 | 0.46 |
| 1:B:3091:LEU:O | 1:B:3192:LYS:HE2 | 2.15 | 0.46 |
| 1:B:3141:PHE:HA | 1:B:3144:PHE:CE2 | 2.51 | 0.46 |
| 1:B:3408:GLY:O | 1:B:3411:ASP:HB2 | 2.16 | 0.46 |
| 1:B:3534:ILE:H | 1:B:3534:ILE:HD12 | 1.79 | 0.46 |
| 1:B:3829:LEU:HA | 1:B:3829:LEU:HD12 | 1.60 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:398:THR:C | 1:B:400:THR:N | 2.68 | 0.46 |
| 1:B:403:GLY:C | 1:B:405:ASP:N | 2.67 | 0.46 |
| 1:B:560:LEU:CB | 1:B:616:LYS:HG2 | 2.46 | 0.46 |
| 1:A:2069:ARG:HG2 | 2:K:204:UNK:CB | 2.46 | 0.46 |
| 1:A:1133:HIS:CG | 1:A:1133:HIS:O | 2.68 | 0.46 |
| 1:A:1856:THR:HB | 1:A:1860:GLU:OE1 | 2.16 | 0.46 |
| 1:A:1927:MSE:HE3 | 1:A:1927:MSE:HB2 | 1.62 | 0.46 |
| 1:A:2129:LEU:HD22 | 1:A:2144:LEU:HD11 | 1.96 | 0.46 |
| 1:A:2313:LYS:HA | 1:A:2316:TYR:HE2 | 1.79 | 0.46 |
| 1:A:3583:LEU:HD21 | 1:A:3733:ARG:NH1 | 2.31 | 0.46 |
| 1:A:3780:ALA:CB | 1:A:3784:ARG:HH12 | 2.29 | 0.46 |
| 1:A:3819:THR:O | 1:A:3823:GLU:HG2 | 2.16 | 0.46 |
| 1:A:3900:LEU:HA | 1:A:3900:LEU:HD12 | 1.80 | 0.46 |
| 1:A:4062:ASP:O | 1:A:4066:LEU:HD13 | 2.16 | 0.46 |
| 1:A:982:GLN:O | 1:A:986:PRO:CD | 2.63 | 0.46 |
| 1:B:1430:GLU:OE1 | 1:B:1448:LEU:HA | 2.16 | 0.46 |
| 1:B:1810:PRO:O | 1:B:1811:ARG:HD2 | 2.16 | 0.46 |
| 1:B:1889:VAL:HG22 | 1:B:1900:PHE:CD2 | 2.51 | 0.46 |
| 1:B:1911:LEU:HD13 | 1:B:1916:ILE:HG22 | 1.97 | 0.46 |
| 1:B:2135:ASN:N | 1:B:2136:PRO:CD | 2.79 | 0.46 |
| 1:B:2161:ALA:O | 1:B:2164:TRP:HB2 | 2.16 | 0.46 |
| 1:B:2241:LEU:H | 1:B:2241:LEU:HG | 1.53 | 0.46 |
| 1:B:2352:HIS:O | 1:B:2360:PHE:HD2 | 1.99 | 0.46 |
| 1:B:2373:PRO:HA | 1:B:2378:PHE:HZ | 1.80 | 0.46 |
| 1:B:2386:LEU:O | 1:B:2390:HIS:CB | 2.64 | 0.46 |
| 1:B:257:ARG:H | 1:B:258:PRO:CD | 2.29 | 0.46 |
| 1:B:3483:MSE:O | 1:B:3516:HIS:CE1 | 2.69 | 0.46 |
| 1:B:3872:ARG:O | 1:B:3876:SER:CB | 2.64 | 0.46 |
| 1:B:408:TYR:C | 1:B:408:TYR:CD1 | 2.90 | 0.46 |
| 1:B:2957:LEU:HB3 | 1:B:4100:GLU:OE2 | 2.16 | 0.46 |
| 1:B:504:GLU:O | 1:B:508:HIS:CG | 2.69 | 0.46 |
| 1:B:578:LYS:O | 1:B:581:LEU:HB2 | 2.16 | 0.46 |
| 1:B:620:PHE:HE1 | 1:B:623:PHE:HD2 | 1.64 | 0.46 |
| 1:B:752:LEU:HB2 | 1:B:756:PHE:CE1 | 2.51 | 0.46 |
| 1:A:1426:GLN:O | 1:A:1430:GLU:HG3 | 2.16 | 0.45 |
| 1:A:1802:TYR:HA | 1:A:1805:PHE:CD2 | 2.48 | 0.45 |
| 1:A:2035:THR:O | 1:A:2039:GLU:HG3 | 2.16 | 0.45 |
| 1:A:2147:ALA:O | 1:A:2151:ILE:N | 2.49 | 0.45 |
| 1:A:2223:VAL:HG21 | 1:A:2238:ILE:HB | 1.98 | 0.45 |
| 1:A:2356:MSE:HE2 | 1:A:2359:LYS:HD2 | 1.97 | 0.45 |
| 1:A:252:VAL:HB | 1:A:265:TYR:HD1 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2874:ALA:O | 1:A:2878:ALA:N | 2.50 | 0.45 |
| 1:A:2921:LEU:HD12 | 1:A:2922:ARG:N | 2.31 | 0.45 |
| 1:A:3326:GLN:OE1 | 1:A:3393:GLU:OE2 | 2.34 | 0.45 |
| 1:A:3413:TYR:CD1 | 1:A:3449:LYS:HB3 | 2.51 | 0.45 |
| 1:A:3564:GLN:C | 1:A:3566:GLY:H | 2.19 | 0.45 |
| 1:A:382:ASP:O | 1:A:386:VAL:CB | 2.58 | 0.45 |
| 1:A:3997:LEU:O | 1:A:4001:THR:HG23 | 2.17 | 0.45 |
| 1:A:752:LEU:HB2 | 1:A:756:PHE:HE1 | 1.79 | 0.45 |
| 1:A:93:LEU:HD23 | 1:A:93:LEU:HA | 1.78 | 0.45 |
| 1:B:1014:LEU:HB2 | 1:B:1078:ALA:CB | 2.43 | 0.45 |
| 1:B:1630:ASP:HA | 1:B:1633:TRP:HE3 | 1.81 | 0.45 |
| 1:B:1879:VAL:HG23 | 1:B:1920:TYR:CD2 | 2.51 | 0.45 |
| 1:B:1989:ASN:HB3 | 1:B:2040:MSE:SE | 2.66 | 0.45 |
| 1:B:2373:PRO:HA | 1:B:2378:PHE:CZ | 2.51 | 0.45 |
| 1:B:2389:PHE:CG | 1:B:2396:LEU:HD22 | 2.51 | 0.45 |
| 1:B:2405:VAL:O | 1:B:2408:MSE:HB2 | 2.16 | 0.45 |
| 1:B:2538:ARG:NH1 | 1:B:2562:LEU:HA | 2.31 | 0.45 |
| 1:B:2908:LYS:HA | 1:B:2908:LYS:HD3 | 1.72 | 0.45 |
| 1:B:3582:GLU:OE2 | 1:B:3675:LYS:HG3 | 2.16 | 0.45 |
| 1:B:3703:GLY:H | 1:B:3717:VAL:HG13 | 1.80 | 0.45 |
| 1:B:3866:GLU:HA | 1:B:3869:THR:OG1 | 2.16 | 0.45 |
| 1:B:3954:PRO:CB | 1:B:4027:TRP:HA | 2.46 | 0.45 |
| 1:B:406:ARG:HB3 | 1:B:408:TYR:CD2 | 2.51 | 0.45 |
| 1:B:528:VAL:HA | 1:B:531:PHE:CE2 | 2.51 | 0.45 |
| 1:B:634:LEU:O | 1:B:638:GLN:NE2 | 2.49 | 0.45 |
| 1:B:756:PHE:CD2 | 1:B:773:LEU:HB3 | 2.51 | 0.45 |
| 1:A:992:ILE:HD13 | 1:A:1035:GLU:HB2 | 1.98 | 0.45 |
| 1:A:1076:LEU:HD21 | 1:A:1114:ALA:HB1 | 1.99 | 0.45 |
| 1:A:1334:LYS:HA | 1:A:1334:LYS:HD3 | 1.82 | 0.45 |
| 1:A:1386:ILE:HB | 1:A:1391:VAL:CG2 | 2.45 | 0.45 |
| 1:A:1460:ARG:HD2 | 1:A:1460:ARG:H | 1.81 | 0.45 |
| 1:A:1894:SER:O | 1:A:1897:ASN:N | 2.33 | 0.45 |
| 1:A:1966:LEU:HD22 | 1:A:1991:PRO:CB | 2.42 | 0.45 |
| 1:A:2423:VAL:O | 1:A:2425:ARG:N | 2.50 | 0.45 |
| 1:A:264:ARG:O | 1:A:268:PRO:HD3 | 2.15 | 0.45 |
| 1:A:2785:ILE:O | 1:A:2785:ILE:HG12 | 2.16 | 0.45 |
| 1:A:2806:LYS:O | 1:A:2806:LYS:HG2 | 2.15 | 0.45 |
| 1:A:3141:PHE:HA | 1:A:3144:PHE:CE2 | 2.51 | 0.45 |
| 1:A:3530:VAL:HA | 1:A:3533:PHE:CD2 | 2.51 | 0.45 |
| 1:A:356:ASN:OD1 | 1:A:1859:ASN:HB2 | 2.16 | 0.45 |
| 1:A:44:LEU:HG | 1:A:44:LEU:H | 1.54 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:760:LEU:O | 1:A:764:PRO:HG3 | 2.16 | 0.45 |
| 1:A:968:VAL:O | 1:A:971:ARG:HG2 | 2.16 | 0.45 |
| 1:B:1559:PHE:CE1 | 1:B:1592:MSE:HE2 | 2.52 | 0.45 |
| 1:B:1875:LYS:HG3 | 1:B:1876:ILE:HB | 1.99 | 0.45 |
| 1:B:2157:PHE:CD1 | 1:B:2157:PHE:C | 2.90 | 0.45 |
| 1:B:2316:TYR:O | 1:B:2319:ALA:HB3 | 2.17 | 0.45 |
| 1:B:2893:LEU:O | 1:B:2897:LEU:N | 2.47 | 0.45 |
| 1:B:2957:LEU:HD21 | 1:B:4101:GLU:HG3 | 1.97 | 0.45 |
| 1:B:3243:ILE:HG12 | 1:B:3258:LEU:CD1 | 2.40 | 0.45 |
| 1:B:3393:GLU:O | 1:B:3397:GLN:OE1 | 2.34 | 0.45 |
| 1:B:3920:ILE:HD13 | 1:B:3961:PHE:HA | 1.98 | 0.45 |
| 1:B:3808:ASN:HB3 | 1:B:3933:GLU:HG2 | 1.98 | 0.45 |
| 1:B:4090:ARG:HD3 | 1:B:4090:ARG:HA | 1.71 | 0.45 |
| 1:B:392:CYS:SG | 1:B:438:LEU:HD11 | 2.57 | 0.45 |
| 1:B:637:LYS:O | 1:B:641:PHE:CB | 2.58 | 0.45 |
| 1:B:657:SER:O | 1:B:660:LEU:HB2 | 2.16 | 0.45 |
| 1:B:910:PHE:HE2 | 1:B:941:MSE:SE | 2.49 | 0.45 |
| 1:A:1099:PHE:CG | 1:A:1100:VAL:N | 2.84 | 0.45 |
| 1:A:1416:GLU:HB3 | 1:A:1420:ARG:HD2 | 1.97 | 0.45 |
| 1:A:1604:SER:HA | 1:A:1632:TRP:HE3 | 1.80 | 0.45 |
| 1:A:1939:LEU:HD13 | 1:A:1986:ARG:NH2 | 2.30 | 0.45 |
| 1:A:19:LEU:O | 1:A:23:ASP:CB | 2.62 | 0.45 |
| 1:A:2074:PRO:HB3 | 1:A:2136:PRO:HB3 | 1.98 | 0.45 |
| 1:A:2126:MSE:HE2 | 1:A:2126:MSE:HB2 | 1.79 | 0.45 |
| 1:A:2260:PHE:HZ | 1:A:2306:ASN:HB2 | 1.82 | 0.45 |
| 1:A:252:VAL:C | 1:A:254:LYS:H | 2.20 | 0.45 |
| 1:A:2940:ARG:HD3 | 1:A:3975:LYS:HD2 | 1.97 | 0.45 |
| 1:A:313:LEU:HD22 | 1:A:317:GLU:OE2 | 2.16 | 0.45 |
| 1:A:3291:GLN:NE2 | 1:A:3294:SER:OG | 2.50 | 0.45 |
| 1:A:3477:GLU:HA | 1:A:3480:LEU:HG | 1.98 | 0.45 |
| 1:A:3513:ALA:O | 1:A:3516:HIS:N | 2.49 | 0.45 |
| 1:A:3771:MSE:HE1 | 1:A:3917:ILE:HG21 | 1.97 | 0.45 |
| 1:A:3612:ARG:HD3 | 1:A:3799:ARG:HH21 | 1.82 | 0.45 |
| 1:A:3853:GLY:C | 1:A:3855:TYR:H | 2.18 | 0.45 |
| 1:A:3981:TYR:CE1 | 1:A:4105:LYS:HA | 2.51 | 0.45 |
| 1:B:1014:LEU:HD23 | 1:B:1028:PHE:CE2 | 2.51 | 0.45 |
| 1:B:1651:LYS:CE | 1:B:1684:LEU:HD21 | 2.46 | 0.45 |
| 1:B:1801:VAL:HG12 | 1:B:1805:PHE:CE2 | 2.52 | 0.45 |
| 1:B:226:GLY:O | 1:B:230:LEU:HD23 | 2.16 | 0.45 |
| 1:B:264:ARG:HA | 1:B:264:ARG:HD3 | 1.75 | 0.45 |
| 1:B:2912:GLY:O | 1:B:2915:ARG:CZ | 2.65 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3459:ASN:CG | 1:B:3710:LYS:HZ3 | 2.19 | 0.45 |
| 1:B:11:SER:OG | 1:B:41:GLU:OE1 | 2.34 | 0.45 |
| 1:B:488:ILE:HG21 | 1:B:616:LYS:CD | 2.38 | 0.45 |
| 1:B:617:PRO:HB3 | 1:B:659:ARG:CG | 2.46 | 0.45 |
| 1:B:706:LEU:CD2 | 1:B:1385:ASN:HD22 | 2.29 | 0.45 |
| 1:B:789:TYR:HD2 | 1:B:865:GLN:CG | 2.29 | 0.45 |
| 1:A:1685:ASP:HA | 1:A:1728:GLU:OE2 | 2.16 | 0.45 |
| 1:A:1727:ARG:NH1 | 1:A:1728:GLU:OE1 | 2.50 | 0.45 |
| 1:A:185:HIS:N | 1:A:186:PRO:HD2 | 2.18 | 0.45 |
| 1:A:2286:PRO:HD2 | 1:A:2329:TYR:CE2 | 2.50 | 0.45 |
| 1:A:244:THR:O | 1:A:248:ILE:HG13 | 2.16 | 0.45 |
| 1:A:249:PHE:CG | 1:A:297:LEU:HD13 | 2.52 | 0.45 |
| 1:A:2539:LEU:HA | 1:A:2542:LEU:HD23 | 1.98 | 0.45 |
| 1:A:2563:LEU:O | 1:A:2567:SER:CB | 2.65 | 0.45 |
| 1:A:2553:HIS:ND1 | 1:A:2803:ILE:HD12 | 2.32 | 0.45 |
| 1:A:3141:PHE:HZ | 1:A:3192:LYS:CB | 2.30 | 0.45 |
| 1:A:3868:VAL:HG12 | 1:A:3872:ARG:HE | 1.81 | 0.45 |
| 1:A:4059:ILE:HD11 | 1:A:4082:ARG:HD2 | 1.99 | 0.45 |
| 1:A:443:ILE:HD11 | 1:A:465:PHE:CE2 | 2.52 | 0.45 |
| 1:A:48:PRO:O | 1:A:50:VAL:N | 2.50 | 0.45 |
| 1:B:1093:GLU:O | 1:B:1096:VAL:HG12 | 2.17 | 0.45 |
| 1:B:1577:LEU:HD12 | 1:B:1578:ALA:HB2 | 1.99 | 0.45 |
| 1:B:1879:VAL:O | 1:B:1882:SER:N | 2.48 | 0.45 |
| 1:B:2038:GLU:OE1 | 1:B:2076:VAL:HG22 | 2.17 | 0.45 |
| 1:B:2271:SER:OG | 1:B:2272:VAL:N | 2.50 | 0.45 |
| 1:B:396:PHE:CG | 1:B:397:LEU:N | 2.83 | 0.45 |
| 1:B:4108:MSE:O | 1:B:4111:ALA:N | 2.44 | 0.45 |
| 1:B:433:PRO:CB | 1:B:1812:LEU:HB3 | 2.47 | 0.45 |
| 1:B:764:PRO:CB | 1:B:848:LEU:HD11 | 2.46 | 0.45 |
| 1:A:1090:ARG:NH2 | 1:A:1100:VAL:HG11 | 2.17 | 0.45 |
| 1:A:1363:LEU:HA | 1:A:1363:LEU:HD23 | 1.70 | 0.45 |
| 1:A:1479:VAL:O | 1:A:1482:GLU:HB2 | 2.15 | 0.45 |
| 1:A:1894:SER:O | 1:A:1896:ILE:N | 2.49 | 0.45 |
| 1:A:2137:ILE:HG22 | 1:A:2141:ASN:HD21 | 1.82 | 0.45 |
| 1:A:2164:TRP:HZ3 | 1:A:2186:VAL:HG23 | 1.81 | 0.45 |
| 1:A:2196:TRP:NE1 | 1:A:2200:ALA:HB2 | 2.31 | 0.45 |
| 1:A:2538:ARG:NH1 | 1:A:2566:THR:N | 2.64 | 0.45 |
| 1:A:933:LEU:HD21 | 1:A:2795:GLN:NE2 | 2.31 | 0.45 |
| 1:A:2808:LEU:O | 1:A:2811:SER:OG | 2.31 | 0.45 |
| 1:A:3764:VAL:O | 1:A:3768:PHE:HD1 | 2.00 | 0.45 |
| 1:A:910:PHE:H | 1:A:912:PRO:HD2 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1468:LEU:O | 1:B:1472:SER:N | 2.50 | 0.45 |
| 1:B:1686:LEU:HA | 1:B:1686:LEU:HD23 | 1.56 | 0.45 |
| 1:B:1971:PRO:O | 1:B:1972:GLU:HG2 | 2.16 | 0.45 |
| 1:B:2028:LEU:HB2 | 1:B:2030:TYR:CE2 | 2.52 | 0.45 |
| 1:B:2193:ILE:CD1 | 1:B:2245:TRP:CZ2 | 2.99 | 0.45 |
| 1:B:2524:PHE:HA | 1:B:2527:HIS:HB3 | 1.98 | 0.45 |
| 1:B:2937:ASP:OD2 | 1:B:3976:GLU:HB2 | 2.16 | 0.45 |
| 1:B:3005:LEU:HG | 1:B:3005:LEU:H | 1.60 | 0.45 |
| 1:B:3048:LYS:HB2 | 1:B:3048:LYS:HE3 | 1.77 | 0.45 |
| 1:B:3160:LEU:HB3 | 1:B:3164:TRP:CH2 | 2.52 | 0.45 |
| 1:B:3454:LEU:HA | 1:B:3454:LEU:HD23 | 1.59 | 0.45 |
| 1:B:3881:ASP:OD1 | 1:B:3884:LYS:NZ | 2.47 | 0.45 |
| 1:B:4066:LEU:CD2 | 1:B:4075:ARG:HG3 | 2.46 | 0.45 |
| 1:B:437:HIS:HA | 1:B:1814:PHE:CE2 | 2.52 | 0.45 |
| 1:B:733:LEU:HD23 | 1:B:733:LEU:N | 2.31 | 0.45 |
| 1:B:906:PHE:HA | 1:B:909:VAL:HB | 1.98 | 0.45 |
| 1:A:1147:LYS:O | 1:A:1151:ARG:NE | 2.50 | 0.45 |
| 1:A:1161:ALA:O | 1:A:1260:LEU:HD13 | 2.17 | 0.45 |
| 1:A:706:LEU:HD21 | 1:A:1388:ASP:OD2 | 2.15 | 0.45 |
| 1:A:1917:LYS:HD2 | 1:A:1953:CYS:SG | 2.57 | 0.45 |
| 1:A:2327:LEU:HA | 1:A:2330:VAL:HG12 | 1.98 | 0.45 |
| 1:A:2379:MSE:HE1 | 1:A:2404:ARG:NH1 | 2.26 | 0.45 |
| 1:A:2427:ARG:HB3 | 1:A:2433:LYS:HB2 | 1.98 | 0.45 |
| 1:A:260:ILE:HG22 | 1:A:264:ARG:NH1 | 2.27 | 0.45 |
| 1:A:2806:LYS:HA | 1:A:2809:PHE:CE2 | 2.50 | 0.45 |
| 1:A:2950:LYS:HE2 | 1:A:4105:LYS:HZ1 | 1.80 | 0.45 |
| 1:A:3944:HIS:CE1 | 1:A:4020:MSE:HE3 | 2.52 | 0.45 |
| 1:A:4013:TRP:HB2 | 1:A:4040:PRO:HG2 | 1.98 | 0.45 |
| 1:A:763:THR:HG21 | 1:A:769:GLY:HA3 | 1.99 | 0.45 |
| 1:A:971:ARG:HD2 | 1:A:1024:THR:CG2 | 2.44 | 0.45 |
| 1:A:977:ASP:CB | 1:A:981:ARG:H | 2.24 | 0.45 |
| 1:B:1299:GLU:HA | 1:B:1302:ALA:HB3 | 1.99 | 0.45 |
| 1:B:1652:ILE:HG12 | 1:B:1717:LEU:HD11 | 1.99 | 0.45 |
| 1:B:279:ALA:HA | 1:B:282:PHE:CD2 | 2.52 | 0.45 |
| 1:B:2913:LYS:O | 1:B:2916:LEU:N | 2.25 | 0.45 |
| 1:B:3268:THR:O | 1:B:3271:ASP:HB3 | 2.17 | 0.45 |
| 1:B:3518:VAL:HA | 1:B:3521:ILE:HG22 | 1.98 | 0.45 |
| 1:B:3890:MSE:O | 1:B:3891:SER:OG | 2.33 | 0.45 |
| 1:B:3916:TRP:CZ3 | 1:B:3917:ILE:HD12 | 2.52 | 0.45 |
| 1:B:3880:ALA:HB1 | 1:B:3969:ASN:HB3 | 1.99 | 0.45 |
| 1:B:542:ASP:HA | 1:B:545:LEU:CD1 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:560:LEU:HA | 1:B:563:LEU:HB2 | 1.99 | 0.45 |
| 1:B:586:GLN:OE1 | 1:B:1088:GLU:HG2 | 2.17 | 0.45 |
| 1:B:763:THR:N | 1:B:764:PRO:HD3 | 2.31 | 0.45 |
| 1:B:982:GLN:O | 1:B:986:PRO:CD | 2.64 | 0.45 |
| 1:A:1147:LYS:HG2 | 1:A:1180:GLN:HG2 | 1.97 | 0.45 |
| 1:A:1996:VAL:HG23 | 1:A:1997:PRO:HD3 | 1.98 | 0.45 |
| 1:A:2004:TYR:OH | 1:A:2055:SER:HB3 | 2.16 | 0.45 |
| 1:A:2077:HIS:HB3 | 1:A:2081:LEU:HG | 1.99 | 0.45 |
| 1:A:2236:GLU:HG3 | 1:A:2236:GLU:H | 1.46 | 0.45 |
| 1:A:2485:ARG:HA | 1:A:2499:PHE:HE2 | 1.82 | 0.45 |
| 1:A:3077:ILE:O | 1:A:3081:HIS:CG | 2.70 | 0.45 |
| 1:A:313:LEU:HD13 | 1:A:317:GLU:OE2 | 2.16 | 0.45 |
| 1:A:3244:ASP:O | 1:A:3247:ARG:HB3 | 2.16 | 0.45 |
| 1:A:3458:SER:OG | 1:A:3494:GLN:NE2 | 2.49 | 0.45 |
| 1:A:3572:ILE:HD13 | 1:A:3575:LEU:HD12 | 1.97 | 0.45 |
| 1:A:3575:LEU:C | 1:A:3577:GLN:H | 2.18 | 0.45 |
| 1:A:3619:ASP:N | 1:A:3620:PRO:CD | 2.80 | 0.45 |
| 1:A:3670:MSE:HE3 | 1:A:3670:MSE:HB2 | 1.78 | 0.45 |
| 1:A:3834:ALA:H | 1:A:3835:PRO:HD3 | 1.81 | 0.45 |
| 1:A:3955:VAL:HG12 | 1:A:4027:TRP:NE1 | 2.24 | 0.45 |
| 1:A:3958:LEU:O | 1:A:3958:LEU:HD12 | 2.17 | 0.45 |
| 1:A:4077:TYR:OH | 1:A:4116:ILE:HA | 2.17 | 0.45 |
| 1:A:575:ILE:N | 1:A:605:THR:OG1 | 2.50 | 0.45 |
| 1:A:65:LEU:HD23 | 1:A:68:PHE:CZ | 2.52 | 0.45 |
| 1:A:799:TYR:O | 1:A:801:LYS:N | 2.50 | 0.45 |
| 1:A:916:GLU:HA | 1:A:919:LEU:HG | 1.99 | 0.45 |
| 1:B:1039:TRP:CH2 | 1:B:1052:SER:HB3 | 2.51 | 0.45 |
| 1:B:1269:THR:CG2 | 1:B:1275:THR:HG21 | 2.46 | 0.45 |
| 1:B:1378:GLU:HB3 | 1:B:1379:PRO:CD | 2.46 | 0.45 |
| 1:B:1517:LEU:HD13 | 1:B:1585:SER:HB2 | 1.99 | 0.45 |
| 1:B:1876:ILE:O | 1:B:1877:LEU:HG | 2.16 | 0.45 |
| 1:B:2265:PRO:HD3 | 1:B:2309:PHE:HZ | 1.79 | 0.45 |
| 1:B:2459:VAL:HG13 | 1:B:2505:VAL:HG13 | 1.98 | 0.45 |
| 1:B:2462:VAL:CG2 | 1:B:2473:MSE:SE | 3.13 | 0.45 |
| 1:B:215:PRO:HB3 | 1:B:251:PHE:CD2 | 2.51 | 0.45 |
| 1:B:901:MSE:HG3 | 1:B:2819:GLU:HB2 | 1.98 | 0.45 |
| 1:B:3312:VAL:O | 1:B:3314:SER:N | 2.50 | 0.45 |
| 1:B:3315:TYR:CG | 1:B:3316:LEU:N | 2.84 | 0.45 |
| 1:B:348:ILE:HG23 | 1:B:357:LYS:HE3 | 1.98 | 0.45 |
| 1:B:3813:LYS:CE | 1:B:3926:ASN:HB2 | 2.46 | 0.45 |
| 1:B:3812:LEU:O | 1:B:3816:LEU:HB2 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:743:LEU:HD23 | 1:B:783:HIS:HE1 | 1.82 | 0.45 |
| 1:B:980:THR:HG23 | 1:B:984:TYR:HE2 | 1.80 | 0.45 |
| 1:A:1027:ASP:O | 1:A:1031:ARG:HG2 | 2.17 | 0.45 |
| 1:A:1033:ILE:HG13 | 1:A:1089:PHE:HE2 | 1.82 | 0.45 |
| 1:A:1737:ASN:C | 1:A:1739:TYR:N | 2.69 | 0.45 |
| 1:A:2222:HIS:O | 1:A:2224:PHE:N | 2.49 | 0.45 |
| 1:A:2327:LEU:HD12 | 1:A:2371:PHE:HB2 | 1.98 | 0.45 |
| 1:A:3273:LEU:HD13 | 1:A:3321:LEU:HD13 | 1.99 | 0.45 |
| 1:A:3516:HIS:CE1 | 1:A:3517:SER:HG | 2.34 | 0.45 |
| 1:A:3784:ARG:HB2 | 1:A:3786:LEU:HG | 1.99 | 0.45 |
| 1:A:3820:MSE:HB2 | 1:A:3882:LEU:HD13 | 1.98 | 0.45 |
| 1:A:3967:PHE:CG | 1:A:3968:ILE:N | 2.84 | 0.45 |
| 1:A:436:GLU:O | 1:A:440:VAL:HG13 | 2.17 | 0.45 |
| 1:A:460:ALA:O | 1:A:464:VAL:HG12 | 2.17 | 0.45 |
| 1:A:557:SER:HA | 1:A:560:LEU:CD2 | 2.47 | 0.45 |
| 1:A:933:LEU:HD12 | 1:A:933:LEU:HA | 1.56 | 0.45 |
| 1:B:2196:TRP:NE1 | 1:B:2200:ALA:HB2 | 2.30 | 0.45 |
| 1:B:2402:LEU:HA | 1:B:2405:VAL:HG22 | 1.97 | 0.45 |
| 1:B:252:VAL:C | 1:B:254:LYS:H | 2.20 | 0.45 |
| 1:B:3168:TYR:HB3 | 1:B:3169:PRO:HD3 | 1.99 | 0.45 |
| 1:B:3181:ASP:HA | 1:B:3184:THR:CG2 | 2.45 | 0.45 |
| 1:B:3438:GLU:HB3 | 1:B:3442:TYR:HE2 | 1.82 | 0.45 |
| 1:B:3525:TYR:OH | 1:B:3561:LYS:HB2 | 2.17 | 0.45 |
| 1:B:3594:ALA:CB | 1:B:4028:ILE:HD13 | 2.45 | 0.45 |
| 1:B:3961:PHE:CE1 | 1:B:3963:LEU:HB2 | 2.51 | 0.45 |
| 1:B:4077:TYR:HB2 | 1:B:4119:ARG:NH2 | 2.32 | 0.45 |
| 1:B:63:PHE:O | 1:B:66:LEU:HG | 2.17 | 0.45 |
| 1:B:759:GLY:HA3 | 1:B:773:LEU:HD11 | 1.98 | 0.45 |
| 1:A:1402:LEU:O | 1:A:1406:LEU:HD23 | 2.17 | 0.45 |
| 1:A:1685:ASP:HB3 | 1:A:1728:GLU:OE1 | 2.16 | 0.45 |
| 1:A:1762:MSE:HG2 | 1:A:1864:ASP:OD1 | 2.17 | 0.45 |
| 1:A:1858:LEU:O | 1:A:1861:SER:HB2 | 2.16 | 0.45 |
| 1:A:1911:LEU:HD13 | 1:A:1916:ILE:CG2 | 2.45 | 0.45 |
| 1:A:1975:LEU:HA | 1:A:1976:LEU:HD23 | 1.98 | 0.45 |
| 1:A:2226:PRO:O | 1:A:2230:VAL:N | 2.43 | 0.45 |
| 1:A:2253:TYR:HE1 | 1:A:2280:VAL:HG22 | 1.82 | 0.45 |
| 1:A:2439:ILE:C | 1:A:2441:LYS:H | 2.20 | 0.45 |
| 1:A:2777:HIS:O | 1:A:2781:PRO:HD3 | 2.17 | 0.45 |
| 1:A:3930:VAL:HA | 1:A:3937:VAL:HG13 | 1.98 | 0.45 |
| 1:A:16:GLN:OE1 | 1:A:61:ARG:HB2 | 2.17 | 0.45 |
| 1:A:513:GLU:HG2 | 1:A:653:LEU:HD11 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:114:VAL:HG12 | 1:B:130:LEU:HD11 | 1.98 | 0.45 |
| 1:B:1598:ASN:ND2 | 1:B:1811:ARG:HG2 | 2.32 | 0.45 |
| 1:B:1886:LYS:NZ | 1:B:1944:ALA:O | 2.47 | 0.45 |
| 1:B:2039:GLU:HG2 | 1:B:2077:HIS:CE1 | 2.52 | 0.45 |
| 1:B:2087:GLU:OE2 | 1:B:2138:VAL:HG12 | 2.17 | 0.45 |
| 1:B:262:LEU:H | 1:B:262:LEU:HG | 1.60 | 0.45 |
| 1:B:3110:PHE:C | 1:B:3114:TYR:HD1 | 2.20 | 0.45 |
| 1:B:321:LYS:O | 1:B:325:ASN:HB2 | 2.17 | 0.45 |
| 1:B:3498:TRP:HB2 | 1:B:3501:HIS:HB2 | 1.99 | 0.45 |
| 1:B:3550:LYS:HZ3 | 1:B:3554:PHE:HD2 | 1.58 | 0.45 |
| 1:B:3863:ASN:O | 1:B:3867:THR:HG23 | 2.16 | 0.45 |
| 1:B:396:PHE:CZ | 1:B:437:HIS:CD2 | 3.05 | 0.45 |
| 1:B:4056:PRO:HD2 | 1:B:4059:ILE:HG22 | 1.99 | 0.45 |
| 1:B:468:LEU:HD22 | 1:B:475:LEU:CD2 | 2.46 | 0.45 |
| 1:B:633:ILE:HG22 | 1:B:634:LEU:CD2 | 2.46 | 0.45 |
| 1:B:912:PRO:O | 1:B:916:GLU:HG3 | 2.16 | 0.45 |
| 1:B:927:LYS:HE2 | 1:B:927:LYS:HB3 | 1.80 | 0.45 |
| 1:A:111:CYS:HB3 | 1:A:134:LEU:HB3 | 1.98 | 0.45 |
| 1:A:1300:SER:O | 1:A:1304:HIS:ND1 | 2.36 | 0.45 |
| 1:A:1305:ASP:OD1 | 1:A:1306:ILE:N | 2.50 | 0.45 |
| 1:A:1357:LYS:HG2 | 1:A:1357:LYS:O | 2.17 | 0.45 |
| 1:A:1464:LEU:O | 1:A:1468:LEU:N | 2.43 | 0.45 |
| 1:A:1645:VAL:HG22 | 1:A:1709:GLU:OE1 | 2.17 | 0.45 |
| 1:A:1806:ARG:O | 1:A:1810:PRO:HD3 | 2.17 | 0.45 |
| 1:A:1915:LEU:CD1 | 1:A:1916:ILE:HG13 | 2.46 | 0.45 |
| 1:A:1991:PRO:HD2 | 1:A:1992:VAL:H | 1.81 | 0.45 |
| 1:A:2356:MSE:SE | 1:A:2360:PHE:CE1 | 3.20 | 0.45 |
| 1:A:275:PHE:O | 1:A:277:LEU:N | 2.50 | 0.45 |
| 1:A:2959:ALA:O | 1:A:3251:ASN:HA | 2.17 | 0.45 |
| 1:A:2972:TYR:CE2 | 1:A:2991:LYS:NZ | 2.84 | 0.45 |
| 1:A:3425:ARG:NH2 | 1:A:3467:ARG:NH1 | 2.65 | 0.45 |
| 1:A:763:THR:OG1 | 1:A:770:LEU:HD23 | 2.17 | 0.45 |
| 1:B:1032:CYS:HB3 | 1:B:1036:PHE:HZ | 1.77 | 0.45 |
| 1:B:1301:ILE:HA | 1:B:1304:HIS:HB2 | 1.99 | 0.45 |
| 1:B:1583:MSE:HE3 | 1:B:1643:MSE:HB3 | 1.98 | 0.45 |
| 1:B:1655:ILE:CG1 | 1:B:1681:ASP:HB3 | 2.47 | 0.45 |
| 1:B:2070:GLU:HG3 | 1:B:2072:ARG:CG | 2.38 | 0.45 |
| 1:B:2164:TRP:HH2 | 1:B:2190:VAL:CG1 | 2.30 | 0.45 |
| 1:B:2219:LEU:HA | 1:B:2219:LEU:HD23 | 1.76 | 0.45 |
| 1:B:2220:MSE:HE1 | 1:B:2256:ILE:HD11 | 1.98 | 0.45 |
| 1:B:2313:LYS:O | 1:B:2316:TYR:HE1 | 2.00 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2555:LEU:HD22 | 1:B:2809:PHE:CE2 | 2.52 | 0.45 |
| 1:B:2883:SER:HA | 1:B:2886:GLN:NE2 | 2.30 | 0.45 |
| 1:B:3493:TRP:CZ2 | 1:B:3496:ILE:HG21 | 2.52 | 0.45 |
| 1:B:362:ALA:HB2 | 1:B:409:GLN:NE2 | 2.29 | 0.45 |
| 1:A:1249:SER:O | 1:A:1253:THR:CB | 2.63 | 0.44 |
| 1:A:437:HIS:CE1 | 1:A:1813:SER:HG | 2.35 | 0.44 |
| 1:A:2145:PHE:CE2 | 1:A:2185:MSE:SE | 3.20 | 0.44 |
| 1:A:2203:THR:HG23 | 1:A:2245:TRP:HH2 | 1.82 | 0.44 |
| 1:A:2634:UNK:O | 1:A:2637:UNK:N | 2.50 | 0.44 |
| 1:A:3186:ARG:O | 1:A:3189:PHE:HB2 | 2.17 | 0.44 |
| 1:A:1249:SER:HA | 1:A:3698:GLU:OE2 | 2.17 | 0.44 |
| 1:A:3751:LEU:HD13 | 1:A:3805:TRP:HB2 | 1.98 | 0.44 |
| 1:A:3872:ARG:O | 1:A:3876:SER:CB | 2.65 | 0.44 |
| 1:A:3961:PHE:HE1 | 1:A:3963:LEU:HB2 | 1.76 | 0.44 |
| 1:A:4025:GLY:O | 1:A:4028:ILE:HG22 | 2.17 | 0.44 |
| 1:A:4090:ARG:HD3 | 1:A:4090:ARG:HA | 1.83 | 0.44 |
| 1:A:601:TRP:HE3 | 1:A:601:TRP:H | 1.65 | 0.44 |
| 1:A:865:GLN:OE1 | 1:A:865:GLN:N | 2.49 | 0.44 |
| 1:A:868:LYS:HA | 1:A:871:LEU:HD12 | 1.99 | 0.44 |
| 1:A:909:VAL:HG12 | 1:A:937:MSE:SE | 2.67 | 0.44 |
| 1:B:109:ASN:HA | 1:B:112:THR:HG22 | 1.99 | 0.44 |
| 1:B:1137:ILE:O | 1:B:1140:LYS:HD2 | 2.18 | 0.44 |
| 1:B:82:ARG:NH1 | 1:B:114:VAL:HG13 | 2.32 | 0.44 |
| 1:B:1438:GLY:HA2 | 1:B:1491:ILE:HD11 | 1.99 | 0.44 |
| 1:B:2147:ALA:O | 1:B:2151:ILE:HG13 | 2.17 | 0.44 |
| 1:B:2960:GLU:O | 1:B:2965:TYR:HD1 | 2.00 | 0.44 |
| 1:B:2970:LYS:CE | 1:B:2974:GLU:OE2 | 2.65 | 0.44 |
| 1:B:3479:THR:OG1 | 1:B:3483:MSE:SE | 2.85 | 0.44 |
| 1:B:3862:ALA:O | 1:B:3866:GLU:HG3 | 2.17 | 0.44 |
| 1:B:4121:TRP:CG | 1:B:4122:GLU:N | 2.85 | 0.44 |
| 1:B:550:PHE:CE1 | 1:B:633:ILE:HA | 2.52 | 0.44 |
| 1:B:805:LEU:HD13 | 1:B:3117:ILE:CD1 | 2.46 | 0.44 |
| 1:B:989:MSE:HG2 | 1:B:1031:ARG:NH1 | 2.32 | 0.44 |
| 1:A:1358:LEU:HD23 | 1:A:1358:LEU:O | 2.17 | 0.44 |
| 1:A:1684:LEU:HD23 | 1:A:1687:HIS:HD2 | 1.83 | 0.44 |
| 1:A:187:SER:O | 1:A:190:ILE:HG22 | 2.16 | 0.44 |
| 1:A:1918:LEU:HD11 | 1:A:1957:ASN:HD22 | 1.81 | 0.44 |
| 1:A:2227:LYS:C | 1:A:2229:ALA:H | 2.21 | 0.44 |
| 1:A:2866:ALA:O | 1:A:2869:LEU:HB2 | 2.17 | 0.44 |
| 1:A:3172:LYS:HG3 | 1:A:3178:ILE:HG21 | 1.99 | 0.44 |
| 1:A:3427:GLU:HG3 | 1:A:3439:LEU:HD13 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:567:GLU:OE1 | 1:A:1798:LEU:HD13 | 2.18 | 0.44 |
| 1:A:74:ASN:HB3 | 1:A:75:SER:H | 1.44 | 0.44 |
| 1:B:1701:SER:OG | 1:B:1702:LEU:N | 2.51 | 0.44 |
| 1:B:2007:ILE:HG22 | 1:B:2009:LYS:CB | 2.47 | 0.44 |
| 1:B:2004:TYR:CG | 1:B:2054:TYR:HB3 | 2.52 | 0.44 |
| 1:B:2093:CYS:C | 1:B:2096:PRO:HD2 | 2.37 | 0.44 |
| 1:B:2442:MSE:H | 1:B:2442:MSE:HG2 | 1.62 | 0.44 |
| 1:B:3619:ASP:N | 1:B:3620:PRO:CD | 2.80 | 0.44 |
| 1:B:3912:CYS:HB3 | 1:B:3961:PHE:CG | 2.52 | 0.44 |
| 1:B:3764:VAL:HG13 | 1:B:3918:LEU:HD21 | 1.99 | 0.44 |
| 1:B:3974:MSE:HB3 | 1:B:3976:GLU:N | 2.32 | 0.44 |
| 1:B:414:LEU:O | 1:B:414:LEU:HG | 2.14 | 0.44 |
| 1:B:732:PHE:HB2 | 1:B:733:LEU:CD2 | 2.47 | 0.44 |
| 1:B:84:GLU:O | 1:B:88:PHE:HD2 | 2.01 | 0.44 |
| 1:B:89:LEU:HA | 1:B:92:PHE:CD2 | 2.52 | 0.44 |
| 1:B:934:LEU:O | 1:B:938:VAL:HG23 | 2.17 | 0.44 |
| 1:B:955:ALA:O | 1:B:959:TYR:CB | 2.66 | 0.44 |
| 1:B:91:ILE:O | 1:B:95:LYS:HG3 | 2.17 | 0.44 |
| 1:A:1282:LEU:HD12 | 1:A:1282:LEU:HA | 1.69 | 0.44 |
| 1:A:1476:HIS:HB2 | 1:A:1511:ALA:HB2 | 2.00 | 0.44 |
| 1:A:1583:MSE:HE1 | 1:A:1640:GLU:CD | 2.37 | 0.44 |
| 1:A:1752:LEU:HD23 | 1:A:1752:LEU:HA | 1.74 | 0.44 |
| 1:A:433:PRO:CB | 1:A:1812:LEU:HA | 2.48 | 0.44 |
| 1:A:185:HIS:H | 1:A:186:PRO:CD | 2.19 | 0.44 |
| 1:A:172:GLU:HA | 1:A:222:GLY:HA3 | 1.99 | 0.44 |
| 1:A:2277:LEU:O | 1:A:2280:VAL:HB | 2.17 | 0.44 |
| 1:A:2310:VAL:O | 1:A:2315:VAL:HG21 | 2.18 | 0.44 |
| 1:A:2320:ALA:HB2 | 1:A:2367:VAL:HA | 1.99 | 0.44 |
| 1:A:3501:HIS:O | 1:A:3505:LEU:HD13 | 2.18 | 0.44 |
| 1:A:3578:LEU:HD22 | 1:A:3683:CYS:SG | 2.57 | 0.44 |
| 1:A:3739:ILE:CD1 | 1:A:3749:PRO:HB3 | 2.48 | 0.44 |
| 1:A:409:GLN:HG3 | 1:A:413:PHE:CE2 | 2.53 | 0.44 |
| 1:A:385:TYR:OH | 1:A:421:LEU:HD23 | 2.18 | 0.44 |
| 1:A:456:VAL:O | 1:A:459:ARG:HB2 | 2.18 | 0.44 |
| 1:B:1005:ASP:HB2 | 1:B:1006:THR:H | 1.51 | 0.44 |
| 1:B:1119:LYS:HZ3 | 1:B:1256:TRP:HE1 | 1.64 | 0.44 |
| 1:B:1342:MSE:HG2 | 1:B:1402:LEU:HD23 | 1.99 | 0.44 |
| 1:B:1651:LYS:HD2 | 1:B:1684:LEU:HD21 | 2.00 | 0.44 |
| 1:B:2416:LYS:HE2 | 1:B:2439:ILE:HG12 | 1.99 | 0.44 |
| 1:B:307:GLU:O | 1:B:308:LEU:HD13 | 2.17 | 0.44 |
| 1:B:3156:PRO:HB2 | 1:B:3197:LEU:HD12 | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3477:GLU:O | 1:B:3481:SER:HB2 | 2.17 | 0.44 |
| 1:B:3972:LEU:C | 1:B:3974:MSE:HG2 | 2.38 | 0.44 |
| 1:B:4056:PRO:O | 1:B:4058:VAL:N | 2.51 | 0.44 |
| 1:B:487:LEU:HD23 | 1:B:530:LEU:HD12 | 1.99 | 0.44 |
| 1:B:527:TYR:HH | 1:B:619:ASP:N | 2.12 | 0.44 |
| 1:B:654:ILE:HG21 | 1:B:726:LEU:HB3 | 1.99 | 0.44 |
| 1:B:734:LEU:HD23 | 1:B:734:LEU:HA | 1.52 | 0.44 |
| 1:A:1147:LYS:CG | 1:A:1180:GLN:HG2 | 2.47 | 0.44 |
| 1:A:1583:MSE:SE | 1:A:1643:MSE:HE3 | 2.67 | 0.44 |
| 1:A:1802:TYR:O | 1:A:1805:PHE:HB2 | 2.17 | 0.44 |
| 1:A:1908:GLY:CA | 1:A:1952:ILE:HG13 | 2.47 | 0.44 |
| 1:A:2506:LEU:H | 1:A:2506:LEU:HG | 1.56 | 0.44 |
| 1:A:939:MSE:SE | 1:A:2783:ILE:HG23 | 2.67 | 0.44 |
| 1:A:334:HIS:ND1 | 1:A:338:LEU:HD21 | 2.31 | 0.44 |
| 1:A:3443:PRO:C | 1:A:3445:LEU:H | 2.20 | 0.44 |
| 1:A:352:VAL:HG23 | 1:A:357:LYS:N | 2.23 | 0.44 |
| 1:A:368:LEU:O | 1:A:420:VAL:HG23 | 2.17 | 0.44 |
| 1:A:3717:VAL:HG22 | 1:A:3718:ARG:H | 1.83 | 0.44 |
| 1:A:3583:LEU:CD1 | 1:A:3733:ARG:HB3 | 2.43 | 0.44 |
| 1:A:3903:HIS:ND1 | 1:A:3934:THR:OG1 | 2.51 | 0.44 |
| 1:A:3966:GLN:HG2 | 1:A:4128:MSE:C | 2.38 | 0.44 |
| 1:A:487:LEU:HG | 1:A:530:LEU:HD13 | 2.00 | 0.44 |
| 1:A:658:THR:N | 1:A:733:LEU:HD13 | 2.33 | 0.44 |
| 1:B:1101:PHE:HA | 1:B:1104:LEU:HD12 | 1.98 | 0.44 |
| 1:B:1272:GLY:C | 1:B:1274:ARG:H | 2.21 | 0.44 |
| 1:B:1373:VAL:HG13 | 1:B:1374:GLN:HG2 | 2.00 | 0.44 |
| 1:B:1692:ALA:HA | 1:B:1695:LEU:HD12 | 1.98 | 0.44 |
| 1:B:1949:ILE:HD12 | 1:B:1952:ILE:CG2 | 2.35 | 0.44 |
| 1:B:1958:GLU:HA | 1:B:1961:PHE:HB3 | 2.00 | 0.44 |
| 1:B:2307:MSE:HE1 | 1:B:2367:VAL:HG11 | 1.98 | 0.44 |
| 1:B:2359:LYS:H | 1:B:2359:LYS:HG3 | 1.62 | 0.44 |
| 1:B:2917:PRO:HB2 | 1:B:2918:PRO:HD3 | 1.99 | 0.44 |
| 1:B:481:THR:O | 1:B:485:GLN:HG2 | 2.17 | 0.44 |
| 1:B:65:LEU:O | 1:B:69:VAL:CB | 2.64 | 0.44 |
| 1:B:669:LEU:C | 1:B:671:SER:N | 2.70 | 0.44 |
| 1:B:771:ASN:O | 1:B:773:LEU:N | 2.51 | 0.44 |
| 1:B:797:ASP:OD2 | 1:B:869:ASN:HB2 | 2.18 | 0.44 |
| 1:A:1076:LEU:O | 1:A:1078:ALA:N | 2.51 | 0.44 |
| 1:A:1086:TYR:CE1 | 1:A:1089:PHE:HB2 | 2.53 | 0.44 |
| 1:A:1115:HIS:O | 1:A:1118:GLU:C | 2.56 | 0.44 |
| 1:A:1151:ARG:O | 1:A:1154:PRO:HD2 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:153:PHE:HB2 | 1:A:157:TYR:HE2 | 1.82 | 0.44 |
| 1:A:189:MSE:HE3 | 1:A:193:ALA:HB2 | 1.99 | 0.44 |
| 1:A:2145:PHE:CE1 | 1:A:2188:GLU:HB3 | 2.53 | 0.44 |
| 1:A:224:LEU:HD22 | 1:A:248:ILE:HD11 | 2.00 | 0.44 |
| 1:A:2379:MSE:HE1 | 1:A:2404:ARG:HD3 | 1.99 | 0.44 |
| 1:A:3125:ARG:HH21 | 1:A:3128:LYS:HD2 | 1.82 | 0.44 |
| 1:A:3835:PRO:HA | 1:A:3871:PHE:CE1 | 2.43 | 0.44 |
| 1:A:432:THR:HB | 1:A:433:PRO:CD | 2.48 | 0.44 |
| 1:A:863:GLY:CA | 1:A:866:ILE:HD11 | 2.47 | 0.44 |
| 1:B:1025:LEU:CD1 | 1:B:1028:PHE:HD2 | 2.30 | 0.44 |
| 1:B:1108:MSE:HB2 | 1:B:1132:ASP:OD1 | 2.17 | 0.44 |
| 1:B:2058:ASP:HB3 | 1:B:2059:PRO:HD3 | 1.98 | 0.44 |
| 1:B:2205:VAL:HB | 1:B:2206:PRO:HD3 | 1.99 | 0.44 |
| 1:B:2539:LEU:O | 1:B:2542:LEU:HG | 2.18 | 0.44 |
| 1:B:602:MSE:SE | 1:B:726:LEU:CD1 | 3.14 | 0.44 |
| 1:B:63:PHE:O | 1:B:67:VAL:HG23 | 2.18 | 0.44 |
| 1:B:729:CYS:O | 1:B:733:LEU:HG | 2.17 | 0.44 |
| 1:B:954:GLY:O | 1:B:958:MSE:HB3 | 2.17 | 0.44 |
| 1:B:971:ARG:CG | 1:B:972:LEU:N | 2.71 | 0.44 |
| 1:A:1340:ARG:O | 1:A:1343:GLU:HB3 | 2.18 | 0.44 |
| 1:A:1433:ALA:O | 1:A:1437:TYR:CG | 2.71 | 0.44 |
| 1:A:1455:CYS:O | 1:A:1458:LEU:N | 2.50 | 0.44 |
| 1:A:1504:ASP:HA | 1:A:1507:CYS:SG | 2.57 | 0.44 |
| 1:A:2147:ALA:CB | 1:A:2151:ILE:HD12 | 2.47 | 0.44 |
| 1:A:2164:TRP:CE3 | 1:A:2189:ILE:HD12 | 2.52 | 0.44 |
| 1:A:2167:PRO:C | 1:A:2171:LEU:HB2 | 2.37 | 0.44 |
| 1:A:2253:TYR:CE1 | 1:A:2280:VAL:HG22 | 2.53 | 0.44 |
| 1:A:2320:ALA:HA | 1:A:2367:VAL:HG23 | 1.99 | 0.44 |
| 1:A:249:PHE:HD1 | 1:A:265:TYR:CE1 | 2.36 | 0.44 |
| 1:A:268:PRO:O | 1:A:271:GLY:N | 2.51 | 0.44 |
| 1:A:3045:ILE:HG21 | 1:A:3064:PHE:CZ | 2.52 | 0.44 |
| 1:A:3073:LEU:H | 1:A:3073:LEU:HG | 1.63 | 0.44 |
| 1:A:3155:VAL:HG11 | 1:A:3159:ARG:CZ | 2.47 | 0.44 |
| 1:A:3168:TYR:HB3 | 1:A:3169:PRO:HD3 | 2.00 | 0.44 |
| 1:A:3283:LEU:HD22 | 1:A:3283:LEU:O | 2.17 | 0.44 |
| 1:A:3305:SER:HA | 1:A:3308:ASP:CB | 2.45 | 0.44 |
| 1:A:3345:PRO:HB2 | 1:A:3346:ALA:H | 1.58 | 0.44 |
| 1:A:3534:ILE:HG13 | 1:A:3569:GLN:OE1 | 2.17 | 0.44 |
| 1:A:430:VAL:HG11 | 1:A:1682:THR:HG21 | 2.00 | 0.44 |
| 1:A:530:LEU:HG | 1:A:530:LEU:H | 1.44 | 0.44 |
| 1:B:1485:SER:HA | 1:B:1488:TYR:CD2 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1568:ASN:N | 1:B:1568:ASN:OD1 | 2.51 | 0.44 |
| 1:B:180:LEU:HD23 | 1:B:183:GLU:OE1 | 2.17 | 0.44 |
| 1:B:1906:THR:O | 1:B:1910:GLU:HB2 | 2.18 | 0.44 |
| 1:B:2083:LEU:HD22 | 1:B:2184:TYR:HD2 | 1.82 | 0.44 |
| 1:B:901:MSE:HE1 | 1:B:2535:THR:CG2 | 2.47 | 0.44 |
| 1:B:2536:LEU:HA | 1:B:2539:LEU:HB2 | 1.99 | 0.44 |
| 1:B:2817:LEU:HA | 1:B:2820:MSE:HE2 | 1.99 | 0.44 |
| 1:B:2936:TYR:HD2 | 1:B:3979:LEU:CD2 | 2.28 | 0.44 |
| 1:B:3103:ILE:HD11 | 1:B:3138:ILE:HG21 | 2.00 | 0.44 |
| 1:B:3243:ILE:HG22 | 1:B:3278:GLN:HE21 | 1.83 | 0.44 |
| 1:B:3631:LYS:HG3 | 1:B:3685:PRO:HG2 | 1.99 | 0.44 |
| 1:B:3720:ALA:HB3 | 1:B:3741:ARG:O | 2.17 | 0.44 |
| 1:B:3771:MSE:O | 1:B:3774:ILE:HB | 2.17 | 0.44 |
| 1:B:4013:TRP:CE3 | 1:B:4014:LYS:HB2 | 2.53 | 0.44 |
| 1:B:4074:PHE:O | 1:B:4077:TYR:HB3 | 2.17 | 0.44 |
| 1:B:3984:MSE:SE | 1:B:4108:MSE:HE2 | 2.68 | 0.44 |
| 1:B:612:LEU:O | 1:B:615:ALA:HB3 | 2.18 | 0.44 |
| 1:B:625:ASN:HA | 1:B:666:PHE:CE1 | 2.53 | 0.44 |
| 1:B:886:TRP:HH2 | 1:B:958:MSE:HB2 | 1.82 | 0.44 |
| 1:B:894:PHE:O | 1:B:940:PHE:CZ | 2.71 | 0.44 |
| 1:A:1076:LEU:HD23 | 1:A:1076:LEU:HA | 1.65 | 0.44 |
| 1:A:1072:ALA:HB1 | 1:A:1076:LEU:HG | 2.00 | 0.44 |
| 1:A:82:ARG:HD2 | 1:A:114:VAL:CG1 | 2.48 | 0.44 |
| 1:A:1387:GLY:HA2 | 1:A:1392:MSE:HG3 | 1.99 | 0.44 |
| 1:A:1582:LEU:HA | 1:A:1582:LEU:HD23 | 1.77 | 0.44 |
| 1:A:1722:PHE:HE2 | 1:A:1754:GLN:HA | 1.81 | 0.44 |
| 1:A:1946:ASN:O | 1:A:1949:ILE:N | 2.31 | 0.44 |
| 1:A:2028:LEU:HB2 | 1:A:2030:TYR:HE2 | 1.82 | 0.44 |
| 1:A:2068:ARG:O | 1:A:2070:GLU:N | 2.50 | 0.44 |
| 1:A:2453:GLU:HA | 1:A:2456:ASN:ND2 | 2.33 | 0.44 |
| 1:A:2936:TYR:CD2 | 1:A:3979:LEU:HD11 | 2.52 | 0.44 |
| 1:A:321:LYS:C | 1:A:325:ASN:HD22 | 2.20 | 0.44 |
| 1:A:3247:ARG:HB2 | 1:A:3278:GLN:NE2 | 2.32 | 0.44 |
| 1:A:452:LYS:O | 1:A:455:LEU:HG | 2.17 | 0.44 |
| 1:A:760:LEU:CD2 | 1:A:803:SER:HB3 | 2.47 | 0.44 |
| 1:A:948:MSE:N | 1:A:949:PRO:HD3 | 2.33 | 0.44 |
| 1:B:1087:ARG:NE | 1:B:1134:LEU:HD22 | 2.33 | 0.44 |
| 1:B:1424:THR:O | 1:B:1426:GLN:N | 2.51 | 0.44 |
| 1:B:175:TYR:HB3 | 1:B:226:GLY:HA3 | 1.98 | 0.44 |
| 1:B:1913:LYS:HB2 | 1:B:1916:ILE:HB | 2.00 | 0.44 |
| 1:B:197:PHE:O | 1:B:201:LEU:HG | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2177:ASN:HB2 | 1:B:2182:ILE:HG23 | 1.99 | 0.44 |
| 1:B:2211:LEU:H | 1:B:2211:LEU:HG | 1.49 | 0.44 |
| 1:B:2224:PHE:CE2 | 1:B:2259:LYS:HD3 | 2.53 | 0.44 |
| 1:B:2318:ALA:O | 1:B:2322:VAL:HB | 2.18 | 0.44 |
| 1:B:2505:VAL:O | 1:B:2508:GLN:N | 2.50 | 0.44 |
| 1:B:320:LEU:O | 1:B:323:VAL:HB | 2.17 | 0.44 |
| 1:B:3413:TYR:CD1 | 1:B:3449:LYS:HB3 | 2.53 | 0.44 |
| 1:B:3699:LEU:HA | 1:B:3699:LEU:HD12 | 1.83 | 0.44 |
| 1:B:563:LEU:O | 1:B:566:ASP:HB2 | 2.18 | 0.44 |
| 1:B:571:SER:HB2 | 1:B:605:THR:H | 1.83 | 0.44 |
| 1:B:638:GLN:NE2 | 1:B:667:TYR:HB3 | 2.32 | 0.44 |
| 1:B:653:LEU:HD23 | 1:B:653:LEU:HA | 1.50 | 0.44 |
| 1:B:727:ALA:O | 1:B:731:THR:HG23 | 2.18 | 0.44 |
| 1:B:78:PHE:O | 1:B:81:CYS:N | 2.51 | 0.44 |
| 1:B:966:PHE:CE1 | 1:B:969:LEU:HD13 | 2.53 | 0.44 |
| 1:A:1022:ASP:CG | 1:A:1023:SER:H | 2.21 | 0.44 |
| 1:A:1032:CYS:HB3 | 1:A:1036:PHE:CE2 | 2.52 | 0.44 |
| 1:A:993:HIS:ND1 | 1:A:1038:LYS:HE2 | 2.33 | 0.44 |
| 1:A:2183:HIS:HE1 | 1:A:2237:ILE:HD13 | 1.82 | 0.44 |
| 1:A:2271:SER:HB2 | 1:A:2314:GLU:CG | 2.47 | 0.44 |
| 1:A:2461:PHE:CE1 | 1:A:2462:VAL:HG23 | 2.52 | 0.44 |
| 1:A:271:GLY:O | 1:A:274:LEU:HD12 | 2.18 | 0.44 |
| 1:A:294:PHE:HZ | 1:A:341:PHE:CZ | 2.36 | 0.44 |
| 1:A:3155:VAL:HG11 | 1:A:3159:ARG:NH1 | 2.32 | 0.44 |
| 1:A:3186:ARG:HA | 1:A:3189:PHE:CD2 | 2.52 | 0.44 |
| 1:A:3266:SER:HB2 | 1:A:3271:ASP:OD1 | 2.17 | 0.44 |
| 1:A:3276:TRP:HB3 | 1:A:3280:TYR:CE2 | 2.52 | 0.44 |
| 1:A:3455:LYS:H | 1:A:3455:LYS:HG3 | 1.62 | 0.44 |
| 1:A:366:TYR:C | 1:A:369:PHE:HB3 | 2.36 | 0.44 |
| 1:A:3857:LEU:HG | 1:A:3859:TYR:CD2 | 2.53 | 0.44 |
| 1:A:82:ARG:HH21 | 1:A:83:GLU:HG3 | 1.83 | 0.44 |
| 1:B:1334:LYS:HD3 | 1:B:1334:LYS:HA | 1.45 | 0.44 |
| 1:B:1369:MSE:SE | 1:B:1418:HIS:ND1 | 3.01 | 0.44 |
| 1:B:1471:GLN:OE1 | 1:B:1471:GLN:N | 2.51 | 0.44 |
| 1:B:1684:LEU:HA | 1:B:1684:LEU:HD23 | 1.71 | 0.44 |
| 1:B:1761:LEU:HD13 | 1:B:1860:GLU:OE1 | 2.18 | 0.44 |
| 1:B:1999:GLU:HB3 | 1:B:2051:SER:HB3 | 2.00 | 0.44 |
| 1:B:2093:CYS:CA | 1:B:2096:PRO:HD2 | 2.48 | 0.44 |
| 1:B:2164:TRP:C | 1:B:2167:PRO:HD2 | 2.38 | 0.44 |
| 1:B:2232:ARG:O | 1:B:2234:ASN:N | 2.51 | 0.44 |
| 1:B:2213:ASN:CG | 1:B:2250:SER:HB2 | 2.38 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2854:PHE:HZ | 1:B:2881:LEU:HB2 | 1.81 | 0.44 |
| 1:B:2886:GLN:HG3 | 1:B:2887:PRO:HD3 | 1.99 | 0.44 |
| 1:B:2916:LEU:HB3 | 1:B:2917:PRO:HD3 | 2.00 | 0.44 |
| 1:B:3475:TYR:HB2 | 1:B:3479:THR:H | 1.83 | 0.44 |
| 1:B:3636:PHE:C | 1:B:3638:LYS:N | 2.71 | 0.44 |
| 1:B:3819:THR:HG1 | 1:B:3889:ARG:NH1 | 2.10 | 0.44 |
| 1:B:3974:MSE:HB3 | 1:B:3976:GLU:CB | 2.48 | 0.44 |
| 1:B:3975:LYS:HE3 | 1:B:3975:LYS:HB2 | 1.81 | 0.44 |
| 1:B:848:LEU:HD12 | 1:B:848:LEU:HA | 1.78 | 0.44 |
| 1:B:928:VAL:HG23 | 1:B:929:ALA:N | 2.33 | 0.44 |
| 1:A:1014:LEU:HD23 | 1:A:1028:PHE:HE2 | 1.83 | 0.44 |
| 1:A:1733:THR:HG23 | 1:A:1881:TYR:CE2 | 2.53 | 0.44 |
| 1:A:2021:GLY:N | 1:A:2022:PRO:HD2 | 2.32 | 0.44 |
| 1:A:2004:TYR:CD1 | 1:A:2054:TYR:HB3 | 2.52 | 0.44 |
| 1:A:3720:ALA:HB3 | 1:A:3741:ARG:O | 2.18 | 0.44 |
| 1:A:3960:PRO:HG2 | 1:A:3961:PHE:CE2 | 2.52 | 0.44 |
| 1:A:446:PHE:N | 1:A:447:PRO:CD | 2.81 | 0.44 |
| 1:A:447:PRO:HD2 | 1:A:448:GLN:H | 1.82 | 0.44 |
| 1:B:1017:ILE:HD12 | 1:B:1025:LEU:HD23 | 2.00 | 0.44 |
| 1:B:1070:PRO:O | 1:B:1073:PHE:CE2 | 2.71 | 0.44 |
| 1:B:1368:LEU:HA | 1:B:1371:VAL:CG1 | 2.48 | 0.44 |
| 1:B:1937:ARG:O | 1:B:1941:HIS:HB2 | 2.18 | 0.44 |
| 1:B:2028:LEU:HB2 | 1:B:2030:TYR:HE2 | 1.81 | 0.44 |
| 1:B:2164:TRP:CH2 | 1:B:2190:VAL:HG12 | 2.53 | 0.44 |
| 1:B:2316:TYR:CE2 | 1:B:2317:ALA:HB2 | 2.53 | 0.44 |
| 1:B:2473:MSE:O | 1:B:2477:LEU:HG | 2.17 | 0.44 |
| 1:B:271:GLY:O | 1:B:274:LEU:HD12 | 2.18 | 0.44 |
| 1:B:290:TYR:O | 1:B:294:PHE:HB3 | 2.17 | 0.44 |
| 1:B:2983:ASP:O | 1:B:2986:PRO:HD2 | 2.18 | 0.44 |
| 1:B:3109:SER:O | 1:B:3112:GLN:HB3 | 2.17 | 0.44 |
| 1:B:856:VAL:HG21 | 1:B:3110:PHE:CZ | 2.53 | 0.44 |
| 1:B:3842:TRP:HA | 1:B:3845:LYS:HB2 | 2.00 | 0.44 |
| 1:B:393:LYS:O | 1:B:397:LEU:HB2 | 2.18 | 0.44 |
| 1:B:12:LEU:HD21 | 1:B:41:GLU:HB2 | 2.00 | 0.44 |
| 1:B:13:LEU:HD22 | 1:B:61:ARG:HD2 | 2.00 | 0.44 |
| 1:B:927:LYS:HE3 | 1:B:928:VAL:CG1 | 2.47 | 0.44 |
| 1:A:1017:ILE:HB | 1:A:1025:LEU:HB2 | 2.00 | 0.43 |
| 1:A:1073:PHE:HD1 | 1:A:1074:LYS:N | 2.06 | 0.43 |
| 1:A:1163:LEU:HA | 1:A:1260:LEU:HD21 | 2.00 | 0.43 |
| 1:A:12:LEU:HD21 | 1:A:41:GLU:HB2 | 2.00 | 0.43 |
| 1:A:1471:GLN:O | 1:A:1475:LEU:CB | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1804:MSE:HE1 | 1:A:1822:ARG:HH11 | 1.82 | 0.43 |
| 1:A:1762:MSE:SE | 1:A:1896:ILE:HG12 | 2.67 | 0.43 |
| 1:A:1945:TYR:O | 1:A:1948:ALA:HB3 | 2.18 | 0.43 |
| 1:A:266:ALA:HB2 | 1:A:308:LEU:HG | 1.99 | 0.43 |
| 1:A:3092:LEU:HD22 | 1:A:3192:LYS:HE3 | 2.00 | 0.43 |
| 1:A:3259:LEU:HD21 | 1:A:3279:SER:HB2 | 1.99 | 0.43 |
| 1:A:360:SER:O | 1:A:363:ILE:HB | 2.18 | 0.43 |
| 1:A:3887:PHE:HZ | 1:A:3904:PHE:CE2 | 2.36 | 0.43 |
| 1:A:3908:HIS:O | 1:A:3911:ILE:HG12 | 2.17 | 0.43 |
| 1:A:3915:HIS:CD2 | 1:A:3920:ILE:HD12 | 2.53 | 0.43 |
| 1:A:3810:VAL:O | 1:A:3929:MSE:HG3 | 2.18 | 0.43 |
| 1:A:3961:PHE:CZ | 1:A:3963:LEU:HD13 | 2.53 | 0.43 |
| 1:A:646:VAL:HG11 | 1:A:710:PHE:CG | 2.54 | 0.43 |
| 1:A:764:PRO:HB2 | 1:A:848:LEU:HD11 | 2.00 | 0.43 |
| 1:A:992:ILE:CD1 | 1:A:1035:GLU:HB2 | 2.48 | 0.43 |
| 1:B:1015:ASP:HA | 1:B:1018:VAL:CG2 | 2.47 | 0.43 |
| 1:B:1079:SER:O | 1:B:1082:PHE:HB3 | 2.17 | 0.43 |
| 1:B:1153:LEU:HB3 | 1:B:1154:PRO:HD3 | 2.01 | 0.43 |
| 1:B:1218:SER:OG | 1:B:1219:PHE:N | 2.51 | 0.43 |
| 1:B:13:LEU:HA | 1:B:16:GLN:HG2 | 2.00 | 0.43 |
| 1:B:1876:ILE:O | 1:B:1876:ILE:HG12 | 2.17 | 0.43 |
| 1:B:217:LEU:HB3 | 1:B:264:ARG:HG3 | 2.00 | 0.43 |
| 1:B:2554:PHE:O | 1:B:2557:LEU:HB2 | 2.18 | 0.43 |
| 1:B:280:SER:O | 1:B:322:GLN:HG2 | 2.17 | 0.43 |
| 1:B:2923:TRP:CD1 | 1:B:2931:ARG:HD3 | 2.53 | 0.43 |
| 1:B:2979:GLN:H | 1:B:2979:GLN:CD | 2.22 | 0.43 |
| 1:B:3107:ILE:HG22 | 1:B:3111:MSE:HE2 | 1.98 | 0.43 |
| 1:B:3454:LEU:HD21 | 1:B:3461:ALA:HB2 | 1.99 | 0.43 |
| 1:B:3610:TYR:O | 1:B:3613:MSE:HB3 | 2.18 | 0.43 |
| 1:B:3631:LYS:HB2 | 1:B:3685:PRO:HB2 | 2.00 | 0.43 |
| 1:B:3872:ARG:NH1 | 1:B:3965:ARG:HH12 | 2.16 | 0.43 |
| 1:B:70:ARG:HG3 | 1:B:78:PHE:CB | 2.48 | 0.43 |
| 1:B:733:LEU:O | 1:B:737:PRO:HG3 | 2.18 | 0.43 |
| 1:A:1073:PHE:CE1 | 1:A:3745:GLU:HA | 2.53 | 0.43 |
| 1:A:1067:ALA:HA | 1:A:1079:SER:HB2 | 2.00 | 0.43 |
| 1:A:1354:GLU:C | 1:A:1356:TRP:H | 2.21 | 0.43 |
| 1:A:1583:MSE:HE1 | 1:A:1640:GLU:OE2 | 2.17 | 0.43 |
| 1:A:1733:THR:N | 1:A:1734:PRO:HD3 | 2.33 | 0.43 |
| 1:A:1747:LEU:HD13 | 1:A:1880:MSE:HE1 | 2.00 | 0.43 |
| 1:A:1950:SER:O | 1:A:2000:ARG:NH1 | 2.51 | 0.43 |
| 1:A:2373:PRO:HA | 1:A:2378:PHE:CZ | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2415:LEU:HD11 | 1:A:2419:ASP:OD2 | 2.17 | 0.43 |
| 1:A:2795:GLN:O | 1:A:2799:GLN:HG2 | 2.18 | 0.43 |
| 1:A:2860:ASP:HB3 | 1:A:2868:LEU:HD22 | 2.00 | 0.43 |
| 1:A:2963:SER:O | 1:A:2967:GLU:HG2 | 2.18 | 0.43 |
| 1:A:3547:THR:HB | 1:A:3548:GLY:O | 2.18 | 0.43 |
| 1:A:3921:GLY:C | 1:A:3923:ARG:N | 2.71 | 0.43 |
| 1:A:733:LEU:H | 1:A:733:LEU:HG | 1.61 | 0.43 |
| 1:A:681:LYS:HD2 | 1:A:746:ARG:NE | 2.33 | 0.43 |
| 1:A:739:ASN:OD1 | 1:A:776:TRP:HA | 2.19 | 0.43 |
| 1:A:784:VAL:O | 1:A:787:PRO:HD2 | 2.18 | 0.43 |
| 1:B:1010:LEU:HA | 1:B:1013:ILE:HG12 | 1.99 | 0.43 |
| 1:B:1039:TRP:CG | 1:B:1055:ASN:HB2 | 2.53 | 0.43 |
| 1:B:1087:ARG:HD3 | 1:B:1134:LEU:CB | 2.38 | 0.43 |
| 1:B:1945:TYR:O | 1:B:1946:ASN:C | 2.56 | 0.43 |
| 1:B:1945:TYR:O | 1:B:1948:ALA:N | 2.50 | 0.43 |
| 1:B:2110:PRO:HB2 | 1:B:2111:PRO:HD3 | 1.99 | 0.43 |
| 1:B:2286:PRO:HB2 | 1:B:2289:ASP:CA | 2.40 | 0.43 |
| 1:B:2464:HIS:H | 1:B:2465:PRO:CD | 2.31 | 0.43 |
| 1:B:2927:ALA:HB2 | 1:B:2930:TYR:CD2 | 2.52 | 0.43 |
| 1:B:3110:PHE:CD1 | 1:B:3111:MSE:N | 2.86 | 0.43 |
| 1:B:358:GLU:CG | 1:B:359:LEU:N | 2.81 | 0.43 |
| 1:B:3847:SER:HA | 1:B:3857:LEU:HD22 | 2.00 | 0.43 |
| 1:B:3880:ALA:O | 1:B:3884:LYS:HG3 | 2.18 | 0.43 |
| 1:B:4113:ASP:O | 1:B:4116:ILE:N | 2.47 | 0.43 |
| 1:B:451:PRO:O | 1:B:454:GLN:HB3 | 2.18 | 0.43 |
| 1:B:572:VAL:HG13 | 1:B:573:LEU:N | 2.33 | 0.43 |
| 1:A:1365:ASN:O | 1:A:1369:MSE:HG2 | 2.17 | 0.43 |
| 1:A:1577:LEU:HD12 | 1:A:1578:ALA:HB2 | 2.01 | 0.43 |
| 1:A:1996:VAL:HG21 | 1:A:2047:THR:CB | 2.48 | 0.43 |
| 1:A:2358:ASP:O | 1:A:2361:ILE:HG22 | 2.18 | 0.43 |
| 1:A:3033:GLU:HB3 | 1:A:3038:GLU:OE1 | 2.19 | 0.43 |
| 1:A:342:MSE:O | 1:A:345:PHE:HB2 | 2.18 | 0.43 |
| 1:A:348:ILE:HG23 | 1:A:357:LYS:HE3 | 1.99 | 0.43 |
| 1:A:3829:LEU:HA | 1:A:3829:LEU:HD12 | 1.70 | 0.43 |
| 1:A:929:ALA:O | 1:A:933:LEU:HB2 | 2.18 | 0.43 |
| 1:A:939:MSE:O | 1:A:942:LEU:HB3 | 2.19 | 0.43 |
| 1:A:966:PHE:CE1 | 1:A:988:VAL:HG12 | 2.54 | 0.43 |
| 1:B:1107:TYR:CD2 | 1:B:1131:ILE:HD12 | 2.53 | 0.43 |
| 1:B:1147:LYS:O | 1:B:1151:ARG:NE | 2.52 | 0.43 |
| 1:B:1356:TRP:HA | 1:B:1356:TRP:CE3 | 2.52 | 0.43 |
| 1:B:1550:VAL:HG23 | 1:B:1551:ILE:H | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1722:PHE:HB3 | 1:B:1723:PRO:HD3 | 1.99 | 0.43 |
| 1:B:2126:MSE:HE2 | 1:B:2156:VAL:CG2 | 2.48 | 0.43 |
| 1:B:2171:LEU:HG | 1:B:2177:ASN:ND2 | 2.30 | 0.43 |
| 1:B:2323:LEU:CD2 | 1:B:2345:VAL:HG21 | 2.48 | 0.43 |
| 1:B:2408:MSE:HA | 1:B:2408:MSE:CE | 2.41 | 0.43 |
| 1:B:275:PHE:O | 1:B:277:LEU:N | 2.52 | 0.43 |
| 1:B:2788:SER:HA | 1:B:2791:ILE:HG13 | 2.01 | 0.43 |
| 1:B:2923:TRP:CD1 | 1:B:2926:LEU:HD21 | 2.53 | 0.43 |
| 1:B:3008:TRP:H | 1:B:3050:LYS:HG2 | 1.83 | 0.43 |
| 1:B:352:VAL:HG23 | 1:B:357:LYS:HG2 | 2.01 | 0.43 |
| 1:B:2937:ASP:OD1 | 1:B:3976:GLU:HA | 2.18 | 0.43 |
| 1:B:554:ASN:O | 1:B:558:GLU:OE2 | 2.37 | 0.43 |
| 1:B:620:PHE:HE2 | 1:B:641:PHE:CE2 | 2.37 | 0.43 |
| 1:B:717:LYS:HA | 1:B:717:LYS:HD3 | 1.84 | 0.43 |
| 1:B:785:MSE:HB3 | 1:B:785:MSE:HE2 | 1.68 | 0.43 |
| 1:A:1087:ARG:HD3 | 1:A:1134:LEU:CD2 | 2.45 | 0.43 |
| 1:A:1652:ILE:CD1 | 1:A:1713:VAL:HG13 | 2.48 | 0.43 |
| 1:A:2915:ARG:O | 1:A:2938:VAL:HG21 | 2.19 | 0.43 |
| 1:A:3008:TRP:N | 1:A:3050:LYS:HG2 | 2.33 | 0.43 |
| 1:A:3583:LEU:HA | 1:A:3583:LEU:HD23 | 1.85 | 0.43 |
| 1:A:732:PHE:HB2 | 1:A:733:LEU:CD2 | 2.48 | 0.43 |
| 1:B:139:ARG:HG3 | 1:B:173:LYS:HZ2 | 1.84 | 0.43 |
| 1:B:1633:TRP:NE1 | 1:B:1697:PRO:HG2 | 2.33 | 0.43 |
| 1:B:1856:THR:O | 1:B:1860:GLU:HB2 | 2.18 | 0.43 |
| 1:B:2356:MSE:SE | 1:B:2360:PHE:CZ | 3.21 | 0.43 |
| 1:B:2926:LEU:HD12 | 1:B:3123:GLN:CD | 2.38 | 0.43 |
| 1:B:3271:ASP:OD2 | 1:B:3272:TRP:CD1 | 2.72 | 0.43 |
| 1:B:3498:TRP:NE1 | 1:B:3502:MSE:SE | 2.99 | 0.43 |
| 1:B:3480:LEU:HD22 | 1:B:3516:HIS:HB3 | 1.99 | 0.43 |
| 1:B:3682:GLU:C | 1:B:3685:PRO:HD2 | 2.38 | 0.43 |
| 1:B:389:ILE:HG22 | 1:B:390:GLN:N | 2.33 | 0.43 |
| 1:B:3904:PHE:HE1 | 1:B:3967:PHE:HE1 | 1.66 | 0.43 |
| 1:B:485:GLN:O | 1:B:488:ILE:HG12 | 2.19 | 0.43 |
| 1:B:575:ILE:HD12 | 1:B:604:PRO:O | 2.18 | 0.43 |
| 1:B:74:ASN:HB3 | 1:B:75:SER:H | 1.45 | 0.43 |
| 1:B:910:PHE:CE2 | 1:B:941:MSE:SE | 3.22 | 0.43 |
| 1:B:981:ARG:HA | 1:B:984:TYR:CD2 | 2.52 | 0.43 |
| 1:A:1056:THR:OG1 | 1:A:1057:LYS:N | 2.51 | 0.43 |
| 1:A:1014:LEU:HB2 | 1:A:1078:ALA:HA | 2.01 | 0.43 |
| 1:A:1087:ARG:NE | 1:A:1134:LEU:HD22 | 2.32 | 0.43 |
| 1:A:1645:VAL:HG12 | 1:A:1646:LEU:HD23 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1942:CYS:HB2 | 1:A:1990:PHE:CD1 | 2.54 | 0.43 |
| 1:A:226:GLY:O | 1:A:230:LEU:HD23 | 2.19 | 0.43 |
| 1:A:2359:LYS:O | 1:A:2362:VAL:HG22 | 2.18 | 0.43 |
| 1:A:2365:ASN:HB2 | 1:A:2400:VAL:HG13 | 1.99 | 0.43 |
| 1:A:2461:PHE:HE1 | 1:A:2469:CYS:SG | 2.42 | 0.43 |
| 1:A:2463:SER:O | 1:A:2464:HIS:ND1 | 2.51 | 0.43 |
| 1:A:2794:LEU:HA | 1:A:2797:VAL:CG2 | 2.46 | 0.43 |
| 1:A:241:ASP:HB2 | 1:A:282:PHE:CE2 | 2.53 | 0.43 |
| 1:A:3052:LEU:HD23 | 1:A:3188:PHE:CZ | 2.54 | 0.43 |
| 1:A:3253:SER:HA | 1:A:3256:MSE:HB2 | 2.00 | 0.43 |
| 1:A:3683:CYS:SG | 1:A:3736:LYS:NZ | 2.90 | 0.43 |
| 1:A:3759:ARG:C | 1:A:3761:ASP:H | 2.21 | 0.43 |
| 1:A:448:GLN:O | 1:A:449:TYR:CD1 | 2.71 | 0.43 |
| 1:A:572:VAL:HG13 | 1:A:573:LEU:N | 2.29 | 0.43 |
| 1:A:963:LYS:HB3 | 1:A:1009:LEU:CD1 | 2.48 | 0.43 |
| 1:B:1401:ASN:O | 1:B:1404:LYS:HB3 | 2.19 | 0.43 |
| 1:B:1916:ILE:O | 1:B:1920:TYR:CD1 | 2.71 | 0.43 |
| 1:B:2040:MSE:HE2 | 1:B:2040:MSE:HB3 | 1.96 | 0.43 |
| 1:B:2066:PHE:HB3 | 1:B:2067:ARG:HG2 | 2.00 | 0.43 |
| 1:B:2311:ARG:HG3 | 1:B:2363:CYS:CB | 2.43 | 0.43 |
| 1:B:2908:LYS:NZ | 1:B:2986:PRO:CG | 2.81 | 0.43 |
| 1:B:273:ARG:HA | 1:B:318:SER:OG | 2.19 | 0.43 |
| 1:B:3443:PRO:C | 1:B:3445:LEU:H | 2.21 | 0.43 |
| 1:B:3656:LEU:O | 1:B:3659:PHE:HB2 | 2.19 | 0.43 |
| 1:B:3908:HIS:CD2 | 1:B:3967:PHE:CZ | 3.06 | 0.43 |
| 1:B:657:SER:C | 1:B:733:LEU:HD13 | 2.38 | 0.43 |
| 1:B:714:VAL:O | 1:B:717:LYS:N | 2.52 | 0.43 |
| 1:A:1332:TYR:CZ | 1:A:1386:ILE:HG22 | 2.54 | 0.43 |
| 1:A:1565:GLU:HG2 | 1:A:1566:THR:HG23 | 2.00 | 0.43 |
| 1:A:1687:HIS:HB3 | 1:A:1691:GLN:HE22 | 1.83 | 0.43 |
| 1:A:185:HIS:O | 1:A:186:PRO:C | 2.56 | 0.43 |
| 1:A:2012:ARG:HA | 1:A:2012:ARG:HD3 | 1.69 | 0.43 |
| 1:A:2227:LYS:HZ2 | 1:A:2232:ARG:C | 2.21 | 0.43 |
| 1:A:2216:LEU:HD22 | 1:A:2249:LEU:HD21 | 2.01 | 0.43 |
| 1:A:224:LEU:HD13 | 1:A:248:ILE:HD13 | 2.01 | 0.43 |
| 1:A:2473:MSE:O | 1:A:2477:LEU:HG | 2.17 | 0.43 |
| 1:A:2538:ARG:NH1 | 1:A:2566:THR:H | 2.08 | 0.43 |
| 1:A:2804:ILE:O | 1:A:2806:LYS:N | 2.46 | 0.43 |
| 1:A:3506:LEU:HD11 | 1:A:3555:VAL:HG13 | 2.00 | 0.43 |
| 1:A:3835:PRO:HB2 | 1:A:3836:PRO:HD3 | 2.00 | 0.43 |
| 1:A:3842:TRP:CZ3 | 1:A:3843:LEU:HD23 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:473:PRO:CA | 1:A:476:ARG:HH22 | 2.18 | 0.43 |
| 1:A:680:ILE:HG12 | 1:A:701:TYR:HD1 | 1.79 | 0.43 |
| 1:B:112:THR:O | 1:B:116:THR:OG1 | 2.25 | 0.43 |
| 1:B:1165:LEU:O | 1:B:1168:LEU:N | 2.50 | 0.43 |
| 1:B:1174:ALA:O | 1:B:1178:ARG:HB2 | 2.18 | 0.43 |
| 1:B:1256:TRP:O | 1:B:1259:LEU:N | 2.51 | 0.43 |
| 1:B:1266:CYS:O | 1:B:1270:PHE:CD2 | 2.72 | 0.43 |
| 1:B:1354:GLU:C | 1:B:1356:TRP:H | 2.22 | 0.43 |
| 1:B:390:GLN:NE2 | 1:B:1724:MSE:HB2 | 2.33 | 0.43 |
| 1:B:1885:PRO:O | 1:B:1886:LYS:C | 2.57 | 0.43 |
| 1:B:1920:TYR:O | 1:B:1923:PHE:HB3 | 2.18 | 0.43 |
| 1:B:2083:LEU:HD13 | 1:B:2184:TYR:HE2 | 1.83 | 0.43 |
| 1:B:2482:ASP:CG | 1:B:2485:ARG:HH21 | 2.21 | 0.43 |
| 1:B:2517:LEU:HA | 1:B:2520:ILE:HG22 | 2.00 | 0.43 |
| 1:B:2557:LEU:HB3 | 1:B:2561:PHE:CZ | 2.53 | 0.43 |
| 1:B:2936:TYR:CD2 | 1:B:3979:LEU:HD11 | 2.54 | 0.43 |
| 1:B:334:HIS:ND1 | 1:B:338:LEU:HD21 | 2.33 | 0.43 |
| 1:B:3564:GLN:C | 1:B:3566:GLY:H | 2.22 | 0.43 |
| 1:B:3572:ILE:CA | 1:B:3575:LEU:HB3 | 2.49 | 0.43 |
| 1:B:3789:ARG:HB3 | 1:B:3938:ILE:CG2 | 2.49 | 0.43 |
| 1:B:3944:HIS:NE2 | 1:B:3948:SER:O | 2.51 | 0.43 |
| 1:B:4075:ARG:O | 1:B:4078:VAL:HG22 | 2.19 | 0.43 |
| 1:B:553:VAL:HB | 1:B:637:LYS:NZ | 2.31 | 0.43 |
| 1:B:669:LEU:HA | 1:B:669:LEU:HD23 | 1.74 | 0.43 |
| 1:B:913:ARG:CB | 1:B:934:LEU:HD12 | 2.48 | 0.43 |
| 1:A:2239:LYS:NZ | 2:K:109:UNK:O | 2.35 | 0.43 |
| 2:S:212:UNK:O | 2:S:215:UNK:N | 2.52 | 0.43 |
| 1:A:1112:ALA:HA | 1:A:1115:HIS:CE1 | 2.54 | 0.43 |
| 1:A:1153:LEU:HB3 | 1:A:1154:PRO:HD3 | 2.00 | 0.43 |
| 1:A:1253:THR:HB | 1:A:1254:LEU:HG | 2.00 | 0.43 |
| 1:A:1330:TYR:CE1 | 1:A:1334:LYS:HE3 | 2.53 | 0.43 |
| 1:A:1433:ALA:HB1 | 1:A:1437:TYR:CZ | 2.53 | 0.43 |
| 1:A:1808:ASP:CB | 1:A:1814:PHE:HB3 | 2.30 | 0.43 |
| 1:A:2009:LYS:O | 1:A:2010:GLU:HG3 | 2.18 | 0.43 |
| 1:A:2192:THR:HA | 1:A:2195:SER:OG | 2.19 | 0.43 |
| 1:A:257:ARG:N | 1:A:258:PRO:CD | 2.81 | 0.43 |
| 1:A:2876:VAL:HG22 | 1:A:3035:PHE:CZ | 2.53 | 0.43 |
| 1:A:3272:TRP:CE3 | 1:A:3307:LEU:HD21 | 2.53 | 0.43 |
| 1:A:3283:LEU:HG | 1:A:3300:VAL:CG2 | 2.48 | 0.43 |
| 1:A:3344:GLU:HB2 | 1:A:3348:LEU:CD1 | 2.48 | 0.43 |
| 1:A:3359:ILE:CG2 | 1:A:3391:ALA:HB3 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3427:GLU:OE1 | 1:A:3435:ASP:HB3 | 2.19 | 0.43 |
| 1:A:3445:LEU:O | 1:A:3449:LYS:NZ | 2.42 | 0.43 |
| 1:A:474:VAL:HG21 | 1:A:1564:SER:OG | 2.19 | 0.43 |
| 1:A:562:HIS:O | 1:A:562:HIS:ND1 | 2.50 | 0.43 |
| 1:A:742:GLU:HB3 | 1:A:783:HIS:CG | 2.54 | 0.43 |
| 1:B:963:LYS:CG | 1:B:1009:LEU:HD11 | 2.49 | 0.43 |
| 1:B:1091:GLU:CG | 1:B:1137:ILE:HD13 | 2.49 | 0.43 |
| 1:B:1214:GLU:O | 1:B:1218:SER:OG | 2.23 | 0.43 |
| 1:B:1349:LEU:HA | 1:B:1353:PRO:CD | 2.45 | 0.43 |
| 1:B:1353:PRO:HA | 1:B:1358:LEU:CB | 2.48 | 0.43 |
| 1:B:1725:GLN:O | 1:B:1725:GLN:HG2 | 2.18 | 0.43 |
| 1:B:1991:PRO:HA | 1:B:1994:VAL:HG12 | 2.00 | 0.43 |
| 1:B:1989:ASN:HB3 | 1:B:2040:MSE:HE2 | 2.01 | 0.43 |
| 1:B:2071:GLN:HA | 1:B:2074:PRO:HG2 | 2.01 | 0.43 |
| 1:B:2257:PHE:CD1 | 1:B:2299:TYR:HB3 | 2.54 | 0.43 |
| 1:B:2437:ASP:O | 1:B:2440:TYR:HB3 | 2.18 | 0.43 |
| 1:B:2515:PRO:HG2 | 1:B:2518:GLN:HE22 | 1.84 | 0.43 |
| 1:B:2548:PRO:O | 1:B:2550:ILE:HG13 | 2.19 | 0.43 |
| 1:B:2987:THR:OG1 | 1:B:2991:LYS:HB2 | 2.19 | 0.43 |
| 1:B:3179:TRP:HZ2 | 1:B:3258:LEU:HG | 1.83 | 0.43 |
| 1:B:3287:ARG:NH1 | 1:B:3328:ILE:HA | 2.33 | 0.43 |
| 1:B:3319:ASN:O | 1:B:3323:PHE:CD2 | 2.71 | 0.43 |
| 1:B:3498:TRP:HE1 | 1:B:3502:MSE:CG | 2.32 | 0.43 |
| 1:B:3499:ILE:HD13 | 1:B:3499:ILE:HA | 1.76 | 0.43 |
| 1:B:3630:ARG:O | 1:B:3634:GLN:N | 2.50 | 0.43 |
| 1:B:3696:ARG:HB2 | 1:B:3699:LEU:CB | 2.48 | 0.43 |
| 1:B:744:ASP:C | 1:B:746:ARG:N | 2.70 | 0.43 |
| 1:B:767:GLU:HG3 | 1:B:851:ILE:HD11 | 2.01 | 0.43 |
| 1:B:892:LEU:HD23 | 1:B:907:LEU:HD13 | 2.01 | 0.43 |
| 1:A:1116:ALA:CB | 1:A:1164:CYS:HB3 | 2.49 | 0.43 |
| 1:A:1508:LYS:NZ | 1:A:1516:GLU:HG3 | 2.33 | 0.43 |
| 1:A:175:TYR:CZ | 1:A:204:LEU:HD11 | 2.54 | 0.43 |
| 1:A:2312:TYR:O | 1:A:2315:VAL:HG22 | 2.19 | 0.43 |
| 1:A:2837:LEU:HG | 1:A:2837:LEU:H | 1.51 | 0.43 |
| 1:A:3252:PHE:HA | 1:A:3282:ARG:CZ | 2.48 | 0.43 |
| 1:A:342:MSE:O | 1:A:342:MSE:HG2 | 2.17 | 0.43 |
| 1:A:3884:LYS:N | 1:A:3970:LEU:HD12 | 2.34 | 0.43 |
| 1:A:3955:VAL:O | 1:A:3955:VAL:HG13 | 2.18 | 0.43 |
| 1:A:4066:LEU:CD2 | 1:A:4075:ARG:HG3 | 2.45 | 0.43 |
| 1:A:568:PHE:HZ | 1:A:653:LEU:HG | 1.84 | 0.43 |
| 1:A:595:ASP:CG | 1:A:1026:ARG:HG3 | 2.39 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:798:GLY:O | 1:A:801:LYS:HE2 | 2.19 | 0.43 |
| 1:A:901:MSE:HE1 | 1:A:2539:LEU:HD21 | 2.00 | 0.43 |
| 1:A:937:MSE:HA | 1:A:940:PHE:CD1 | 2.53 | 0.43 |
| 1:A:984:TYR:O | 1:A:988:VAL:HG13 | 2.19 | 0.43 |
| 1:B:1038:LYS:HA | 1:B:1038:LYS:HD2 | 1.85 | 0.43 |
| 1:B:993:HIS:CB | 1:B:1038:LYS:HG2 | 2.37 | 0.43 |
| 1:B:14:ARG:O | 1:B:18:THR:HG23 | 2.18 | 0.43 |
| 1:B:1871:MSE:CA | 1:B:1874:TYR:HB2 | 2.45 | 0.43 |
| 1:B:2138:VAL:HA | 1:B:2141:ASN:ND2 | 2.34 | 0.43 |
| 1:B:224:LEU:O | 1:B:228:SER:OG | 2.34 | 0.43 |
| 1:B:2276:LEU:O | 1:B:2279:ILE:HB | 2.18 | 0.43 |
| 1:B:197:PHE:CE1 | 1:B:230:LEU:HD22 | 2.53 | 0.43 |
| 1:B:2401:VAL:O | 1:B:2405:VAL:HG13 | 2.19 | 0.43 |
| 1:B:2433:LYS:O | 1:B:2436:LEU:N | 2.44 | 0.43 |
| 1:B:2443:MSE:HB3 | 1:B:2480:ILE:CG1 | 2.43 | 0.43 |
| 1:B:2510:LEU:HG | 1:B:2522:ARG:HE | 1.84 | 0.43 |
| 1:B:2575:PRO:HG3 | 1:B:2789:SER:OG | 2.18 | 0.43 |
| 1:B:2989:ALA:HA | 1:B:2992:ASP:HB2 | 1.99 | 0.43 |
| 1:B:3329:LEU:HA | 1:B:3329:LEU:HD23 | 1.80 | 0.43 |
| 1:B:3503:VAL:HG21 | 1:B:3535:ILE:C | 2.39 | 0.43 |
| 1:B:3531:TYR:CD2 | 1:B:3707:GLY:HA3 | 2.53 | 0.43 |
| 1:B:3788:LEU:HD12 | 1:B:3788:LEU:HA | 1.74 | 0.43 |
| 1:B:458:CYS:HA | 1:B:461:ILE:HD12 | 2.01 | 0.43 |
| 1:B:766:ALA:HB1 | 1:B:768:VAL:HG23 | 2.00 | 0.43 |
| 1:B:948:MSE:N | 1:B:949:PRO:HD3 | 2.34 | 0.43 |
| 1:A:996:THR:O | 1:A:1042:LYS:HG2 | 2.19 | 0.43 |
| 1:A:175:TYR:HA | 1:A:178:LEU:HD12 | 2.00 | 0.43 |
| 1:A:1883:ARG:HG3 | 1:A:1884:LEU:N | 2.33 | 0.43 |
| 1:A:1949:ILE:CD1 | 1:A:1952:ILE:HG21 | 2.48 | 0.43 |
| 1:A:2379:MSE:SE | 1:A:2404:ARG:HD3 | 2.69 | 0.43 |
| 1:A:2439:ILE:O | 1:A:2441:LYS:N | 2.52 | 0.43 |
| 1:A:3155:VAL:N | 1:A:3156:PRO:CD | 2.82 | 0.43 |
| 1:A:3314:SER:HB2 | 1:A:3315:TYR:O | 2.19 | 0.43 |
| 1:A:3495:PHE:HA | 1:A:3498:TRP:CZ2 | 2.54 | 0.43 |
| 1:A:3651:LEU:HA | 1:A:3654:MSE:HE3 | 2.01 | 0.43 |
| 1:A:514:VAL:CG1 | 1:A:610:ALA:HB1 | 2.49 | 0.43 |
| 1:A:763:THR:N | 1:A:764:PRO:HD3 | 2.34 | 0.43 |
| 1:A:745:VAL:HG11 | 1:A:776:TRP:CZ2 | 2.54 | 0.43 |
| 1:A:905:ILE:O | 1:A:906:PHE:HB2 | 2.18 | 0.43 |
| 1:A:981:ARG:CG | 1:A:982:GLN:N | 2.81 | 0.43 |
| 1:B:103:TYR:O | 1:B:106:GLU:HB2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1222:ASN:O | 1:B:1225:GLU:HB2 | 2.18 | 0.43 |
| 1:B:125:ILE:H | 1:B:126:PRO:HD2 | 1.84 | 0.43 |
| 1:B:130:LEU:HD12 | 1:B:130:LEU:HA | 1.65 | 0.43 |
| 1:B:173:LYS:O | 1:B:174:VAL:C | 2.57 | 0.43 |
| 1:B:2253:TYR:HA | 1:B:2256:ILE:HB | 2.01 | 0.43 |
| 1:B:2526:SER:O | 1:B:2530:ARG:HB3 | 2.19 | 0.43 |
| 1:B:2841:ASN:HD22 | 1:B:2871:LEU:HD23 | 1.84 | 0.43 |
| 1:B:2943:PHE:CE2 | 1:B:2944:THR:HG23 | 2.54 | 0.43 |
| 1:B:3262:LEU:HD12 | 1:B:3266:SER:OG | 2.18 | 0.43 |
| 1:B:3424:LEU:CD1 | 1:B:3439:LEU:HD11 | 2.49 | 0.43 |
| 1:B:3480:LEU:HB3 | 1:B:3516:HIS:HB2 | 2.01 | 0.43 |
| 1:B:3525:TYR:O | 1:B:3529:ILE:HB | 2.19 | 0.43 |
| 1:B:3174:ASP:OD2 | 1:B:3783:GLN:HG3 | 2.19 | 0.43 |
| 1:B:385:TYR:HA | 1:B:388:LEU:HB3 | 2.00 | 0.43 |
| 1:B:3984:MSE:O | 1:B:3987:ALA:HB3 | 2.18 | 0.43 |
| 1:B:4020:MSE:HE3 | 1:B:4027:TRP:HE1 | 1.84 | 0.43 |
| 1:B:892:LEU:HD11 | 1:B:958:MSE:CG | 2.49 | 0.43 |
| 1:B:933:LEU:HD11 | 1:B:2795:GLN:OE1 | 2.19 | 0.43 |
| 1:A:1133:HIS:ND1 | 1:A:1136:ARG:HD2 | 2.34 | 0.43 |
| 1:A:184:VAL:O | 1:A:185:HIS:CG | 2.72 | 0.43 |
| 1:A:2399:GLU:HA | 1:A:2402:LEU:HD23 | 2.01 | 0.43 |
| 1:A:3167:ARG:HG2 | 1:A:3186:ARG:NH2 | 2.33 | 0.43 |
| 1:A:3141:PHE:CE1 | 1:A:3193:ILE:HG13 | 2.49 | 0.43 |
| 1:A:3617:LEU:CD1 | 1:A:3644:PHE:HD2 | 2.30 | 0.43 |
| 1:A:3908:HIS:CD2 | 1:A:3912:CYS:SG | 3.12 | 0.43 |
| 1:A:3917:ILE:O | 1:A:4048:LYS:HE2 | 2.19 | 0.43 |
| 1:A:3951:GLN:NE2 | 1:A:4068:HIS:CE1 | 2.87 | 0.43 |
| 1:A:4074:PHE:O | 1:A:4077:TYR:HB3 | 2.19 | 0.43 |
| 1:A:435:LEU:O | 1:A:439:VAL:HG23 | 2.19 | 0.43 |
| 1:A:47:SER:O | 1:A:51:LEU:HB2 | 2.19 | 0.43 |
| 1:A:634:LEU:HD22 | 1:A:667:TYR:CD1 | 2.53 | 0.43 |
| 1:A:70:ARG:CD | 1:A:82:ARG:HD3 | 2.38 | 0.43 |
| 1:A:939:MSE:HA | 1:A:939:MSE:HE3 | 2.01 | 0.43 |
| 1:B:1017:ILE:HA | 1:B:1021:VAL:O | 2.18 | 0.43 |
| 1:B:1027:ASP:O | 1:B:1031:ARG:HG2 | 2.19 | 0.43 |
| 1:B:1296:PHE:CE1 | 1:B:1362:ASP:HB2 | 2.53 | 0.43 |
| 1:B:1296:PHE:CZ | 1:B:1362:ASP:HB2 | 2.54 | 0.43 |
| 1:B:1449:ALA:O | 1:B:1453:SER:OG | 2.28 | 0.43 |
| 1:B:1874:TYR:CE1 | 1:B:1881:TYR:CG | 3.06 | 0.43 |
| 1:B:2167:PRO:CB | 1:B:2171:LEU:HD22 | 2.47 | 0.43 |
| 1:B:2461:PHE:HA | 1:B:2464:HIS:ND1 | 2.34 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2871:LEU:O | 1:B:2873:PRO:HD3 | 2.19 | 0.43 |
| 1:B:2879:GLY:CA | 1:B:2886:GLN:HG2 | 2.31 | 0.43 |
| 1:B:3020:ASP:OD2 | 1:B:3024:PRO:HA | 2.18 | 0.43 |
| 1:B:3179:TRP:CG | 1:B:3179:TRP:O | 2.71 | 0.43 |
| 1:B:3266:SER:HB3 | 1:B:3271:ASP:HB2 | 2.01 | 0.43 |
| 1:B:348:ILE:O | 1:B:364:ARG:HD3 | 2.19 | 0.43 |
| 1:B:3575:LEU:HB2 | 1:B:3686:TRP:CZ3 | 2.54 | 0.43 |
| 1:B:3830:SER:O | 1:B:3833:ARG:N | 2.50 | 0.43 |
| 1:B:2858:ILE:HG23 | 1:B:3894:PRO:HG3 | 2.00 | 0.43 |
| 1:B:396:PHE:CE1 | 1:B:397:LEU:HG | 2.54 | 0.43 |
| 1:B:3989:ARG:HE | 1:B:4100:GLU:HB3 | 1.83 | 0.43 |
| 1:B:4003:ASP:O | 1:B:4006:VAL:HG22 | 2.19 | 0.43 |
| 1:B:408:TYR:O | 1:B:411:PRO:HD2 | 2.19 | 0.43 |
| 1:B:560:LEU:HA | 1:B:563:LEU:HD12 | 2.00 | 0.43 |
| 1:B:719:LYS:HE3 | 1:B:750:PRO:HB2 | 2.01 | 0.43 |
| 1:A:971:ARG:HD2 | 1:A:1024:THR:OG1 | 2.18 | 0.42 |
| 1:A:1073:PHE:HD1 | 1:A:1074:LYS:CG | 2.31 | 0.42 |
| 1:A:1305:ASP:OD1 | 1:A:1334:LYS:HD2 | 2.18 | 0.42 |
| 1:A:1913:LYS:O | 1:A:1915:LEU:N | 2.52 | 0.42 |
| 1:A:194:GLU:HA | 1:A:197:PHE:CD2 | 2.51 | 0.42 |
| 1:A:2299:TYR:O | 1:A:2302:ALA:HB3 | 2.19 | 0.42 |
| 1:A:2645:UNK:HA | 1:A:2649:UNK:O | 2.20 | 0.42 |
| 1:A:3049:LEU:HA | 1:A:3188:PHE:HZ | 1.82 | 0.42 |
| 1:A:3076:ALA:HB1 | 1:A:3080:LEU:CD1 | 2.48 | 0.42 |
| 1:A:3144:PHE:HZ | 1:A:3193:ILE:HD11 | 1.84 | 0.42 |
| 1:A:3619:ASP:O | 1:A:3625:LEU:HB2 | 2.19 | 0.42 |
| 1:A:3675:LYS:N | 1:A:3676:PRO:HD2 | 2.33 | 0.42 |
| 1:A:3690:PHE:CD1 | 1:A:3692:VAL:HG23 | 2.54 | 0.42 |
| 1:A:3906:SER:O | 1:A:3910:LEU:HD13 | 2.18 | 0.42 |
| 1:A:3955:VAL:CG1 | 1:A:4027:TRP:HE1 | 2.25 | 0.42 |
| 1:A:4113:ASP:HB3 | 1:A:4116:ILE:HG13 | 2.00 | 0.42 |
| 1:A:446:PHE:CD1 | 1:A:446:PHE:N | 2.75 | 0.42 |
| 1:A:892:LEU:HG | 1:A:958:MSE:SE | 2.69 | 0.42 |
| 1:B:1033:ILE:HD11 | 1:B:1089:PHE:HE2 | 1.84 | 0.42 |
| 1:B:1455:CYS:HA | 1:B:1458:LEU:HD12 | 2.00 | 0.42 |
| 1:B:146:GLU:HG3 | 1:B:149:ILE:HD12 | 2.00 | 0.42 |
| 1:B:1574:ASN:CG | 1:B:1582:LEU:HD21 | 2.40 | 0.42 |
| 1:B:1718:ILE:CG2 | 1:B:1750:LEU:HD11 | 2.40 | 0.42 |
| 1:B:1812:LEU:HD13 | 1:B:1814:PHE:HD2 | 1.84 | 0.42 |
| 1:B:1981:LEU:HA | 1:B:1984:LEU:CD2 | 2.48 | 0.42 |
| 1:B:2452:ARG:O | 1:B:2455:LEU:HB2 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2804:ILE:O | 1:B:2806:LYS:N | 2.50 | 0.42 |
| 1:B:3104:GLN:O | 1:B:3107:ILE:HB | 2.19 | 0.42 |
| 1:B:856:VAL:HG11 | 1:B:3110:PHE:CZ | 2.54 | 0.42 |
| 1:B:3252:PHE:CE2 | 1:B:3289:ARG:NH2 | 2.87 | 0.42 |
| 1:B:3390:GLN:O | 1:B:3394:GLU:HB2 | 2.18 | 0.42 |
| 1:B:3483:MSE:O | 1:B:3486:GLU:HG2 | 2.19 | 0.42 |
| 1:B:3525:TYR:HA | 1:B:3529:ILE:CG2 | 2.49 | 0.42 |
| 1:B:381:VAL:HB | 1:B:384:MSE:SE | 2.68 | 0.42 |
| 1:B:3985:VAL:O | 1:B:3988:LEU:N | 2.51 | 0.42 |
| 1:B:4077:TYR:CG | 1:B:4119:ARG:NH2 | 2.87 | 0.42 |
| 1:B:4093:GLU:O | 1:B:4095:GLU:HG2 | 2.19 | 0.42 |
| 1:B:432:THR:HB | 1:B:433:PRO:CD | 2.48 | 0.42 |
| 1:B:963:LYS:O | 1:B:967:PRO:HD3 | 2.20 | 0.42 |
| 1:B:993:HIS:C | 1:B:993:HIS:ND1 | 2.73 | 0.42 |
| 1:A:1812:LEU:O | 1:A:1815:THR:HG23 | 2.19 | 0.42 |
| 1:A:361:ILE:HG21 | 1:A:1858:LEU:HD23 | 2.01 | 0.42 |
| 1:A:1882:SER:O | 1:A:1885:PRO:HD2 | 2.19 | 0.42 |
| 1:A:2070:GLU:CG | 1:A:2072:ARG:HG3 | 2.33 | 0.42 |
| 1:A:2251:ILE:HG23 | 1:A:2288:TYR:HD2 | 1.84 | 0.42 |
| 1:A:2358:ASP:HB3 | 1:A:2389:PHE:CE1 | 2.54 | 0.42 |
| 1:A:2552:VAL:HG22 | 1:A:2553:HIS:ND1 | 2.35 | 0.42 |
| 1:A:262:LEU:H | 1:A:262:LEU:HG | 1.62 | 0.42 |
| 1:A:2943:PHE:O | 1:A:2945:SER:N | 2.45 | 0.42 |
| 1:A:293:LEU:HA | 1:A:296:VAL:HG12 | 2.00 | 0.42 |
| 1:A:3174:ASP:HA | 1:A:3249:GLN:NE2 | 2.34 | 0.42 |
| 1:A:3397:GLN:HE21 | 1:A:3413:TYR:HD1 | 1.63 | 0.42 |
| 1:A:3435:ASP:O | 1:A:3439:LEU:HB2 | 2.18 | 0.42 |
| 1:A:3583:LEU:HD22 | 1:A:3587:ASP:OD2 | 2.19 | 0.42 |
| 1:A:349:ILE:HD12 | 1:A:368:LEU:HD12 | 1.99 | 0.42 |
| 1:A:3806:LEU:HG | 1:A:3807:GLU:N | 2.33 | 0.42 |
| 1:B:1157:PHE:HB3 | 1:B:1169:VAL:HG22 | 2.02 | 0.42 |
| 1:B:1263:ALA:HB1 | 1:B:1267:TYR:HE1 | 1.84 | 0.42 |
| 1:B:1389:VAL:O | 1:B:1389:VAL:HG12 | 2.19 | 0.42 |
| 1:B:138:PHE:HD2 | 1:B:173:LYS:CE | 2.25 | 0.42 |
| 1:B:1583:MSE:HE2 | 1:B:1639:LEU:C | 2.40 | 0.42 |
| 1:B:1727:ARG:O | 1:B:1730:PRO:HD2 | 2.19 | 0.42 |
| 1:B:1992:VAL:HG11 | 1:B:2044:ASP:OD1 | 2.19 | 0.42 |
| 1:B:2125:TRP:CZ3 | 1:B:2129:LEU:HD21 | 2.55 | 0.42 |
| 1:B:2255:LEU:HD12 | 1:B:2258:GLU:HB2 | 2.01 | 0.42 |
| 1:B:2291:GLN:O | 1:B:2294:ILE:N | 2.53 | 0.42 |
| 1:B:2325:LEU:O | 1:B:2329:TYR:HB2 | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2320:ALA:CA | 1:B:2367:VAL:HG23 | 2.49 | 0.42 |
| 1:B:2776:ARG:H | 1:B:2776:ARG:HG2 | 1.59 | 0.42 |
| 1:B:3047:SER:HB2 | 1:B:3050:LYS:CE | 2.48 | 0.42 |
| 1:B:346:TYR:HA | 1:B:349:ILE:HD12 | 2.01 | 0.42 |
| 1:B:3470:GLN:HG2 | 1:B:3474:ARG:HH11 | 1.83 | 0.42 |
| 1:B:367:GLY:C | 1:B:369:PHE:N | 2.69 | 0.42 |
| 1:B:3987:ALA:O | 1:B:3991:PHE:HD1 | 2.01 | 0.42 |
| 1:B:4019:LYS:HA | 1:B:4019:LYS:HE2 | 2.01 | 0.42 |
| 1:B:44:LEU:H | 1:B:44:LEU:HG | 1.71 | 0.42 |
| 1:B:487:LEU:CD2 | 1:B:530:LEU:HB2 | 2.49 | 0.42 |
| 1:B:560:LEU:HB2 | 1:B:616:LYS:HG2 | 2.01 | 0.42 |
| 1:B:775:GLU:O | 1:B:779:TYR:CD2 | 2.70 | 0.42 |
| 1:B:970:LEU:CD2 | 1:B:1031:ARG:NH2 | 2.78 | 0.42 |
| 2:S:212:UNK:C | 2:S:214:UNK:N | 2.82 | 0.42 |
| 1:A:131:LEU:HD23 | 1:A:135:LEU:HD11 | 2.02 | 0.42 |
| 1:A:1345:THR:HG22 | 1:A:1349:LEU:HD12 | 2.01 | 0.42 |
| 1:A:143:LEU:CD1 | 1:A:143:LEU:H | 2.25 | 0.42 |
| 1:A:1798:LEU:O | 1:A:1802:TYR:HB2 | 2.19 | 0.42 |
| 1:A:1955:VAL:HA | 1:A:2003:LYS:HZ2 | 1.85 | 0.42 |
| 1:A:2167:PRO:HA | 1:A:2171:LEU:H | 1.84 | 0.42 |
| 1:A:2300:PHE:HZ | 1:A:2341:LEU:HD22 | 1.83 | 0.42 |
| 1:A:14:ARG:HH12 | 1:A:2392:VAL:HG11 | 1.83 | 0.42 |
| 1:A:2462:VAL:HG13 | 1:A:2470:ARG:HE | 1.84 | 0.42 |
| 1:A:3069:MSE:HA | 1:A:3072:GLU:HB3 | 2.02 | 0.42 |
| 1:A:3465:PHE:HD1 | 1:A:3483:MSE:SE | 2.52 | 0.42 |
| 1:A:3557:ARG:O | 1:A:3560:SER:HB3 | 2.19 | 0.42 |
| 1:A:3587:ASP:HB3 | 1:A:4022:LYS:HZ2 | 1.85 | 0.42 |
| 1:A:3640:PHE:O | 1:A:3644:PHE:CG | 2.72 | 0.42 |
| 1:A:3568:ILE:HG21 | 1:A:3699:LEU:HD21 | 2.01 | 0.42 |
| 1:A:3972:LEU:HD12 | 1:A:3974:MSE:HE3 | 2.01 | 0.42 |
| 1:A:568:PHE:O | 1:A:571:SER:N | 2.52 | 0.42 |
| 1:A:658:THR:HA | 1:A:733:LEU:CD2 | 2.38 | 0.42 |
| 1:A:901:MSE:SE | 1:A:2536:LEU:HD21 | 2.69 | 0.42 |
| 1:B:1163:LEU:CD2 | 1:B:1260:LEU:HD11 | 2.47 | 0.42 |
| 1:B:1353:PRO:HG3 | 1:B:1358:LEU:HB3 | 2.02 | 0.42 |
| 1:B:2012:ARG:HA | 1:B:2012:ARG:HD3 | 1.79 | 0.42 |
| 1:B:2171:LEU:CD2 | 1:B:2177:ASN:HD21 | 2.32 | 0.42 |
| 1:B:2424:MSE:HA | 1:B:2436:LEU:HD12 | 2.01 | 0.42 |
| 1:B:2928:LYS:HB3 | 1:B:3784:ARG:CG | 2.49 | 0.42 |
| 1:B:294:PHE:CE2 | 1:B:298:LEU:HD21 | 2.55 | 0.42 |
| 1:B:3624:GLY:O | 1:B:3625:LEU:HD23 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3754:GLY:HA2 | 1:B:3800:LEU:HB2 | 2.02 | 0.42 |
| 1:B:3946:PHE:HE2 | 1:B:4048:LYS:HD2 | 1.84 | 0.42 |
| 1:B:403:GLY:O | 1:B:405:ASP:N | 2.52 | 0.42 |
| 1:B:557:SER:O | 1:B:560:LEU:HG | 2.19 | 0.42 |
| 1:B:808:GLU:CD | 1:B:3114:TYR:HB3 | 2.40 | 0.42 |
| 1:B:892:LEU:HD11 | 1:B:958:MSE:CB | 2.49 | 0.42 |
| 1:B:932:GLU:O | 1:B:935:HIS:HB3 | 2.18 | 0.42 |
| 1:A:1475:LEU:O | 1:A:1479:VAL:HG23 | 2.20 | 0.42 |
| 1:A:153:PHE:HA | 1:A:156:PHE:CD2 | 2.54 | 0.42 |
| 1:A:1632:TRP:N | 1:A:1632:TRP:CD1 | 2.86 | 0.42 |
| 1:A:177:LEU:HA | 1:A:180:LEU:HD12 | 2.01 | 0.42 |
| 1:A:1968:SER:O | 1:A:1971:PRO:HD2 | 2.19 | 0.42 |
| 1:A:1999:GLU:OE1 | 1:A:2051:SER:HB2 | 2.20 | 0.42 |
| 1:A:2023:SER:HB2 | 1:A:2024:TYR:CE1 | 2.54 | 0.42 |
| 1:A:2386:LEU:HA | 1:A:2386:LEU:HD23 | 1.75 | 0.42 |
| 1:A:2473:MSE:HE2 | 1:A:2473:MSE:HB3 | 1.90 | 0.42 |
| 1:A:2797:VAL:HG12 | 1:A:2800:ARG:NH1 | 2.34 | 0.42 |
| 1:A:2926:LEU:HD22 | 1:A:2931:ARG:NE | 2.34 | 0.42 |
| 1:A:3247:ARG:NE | 1:A:3278:GLN:OE1 | 2.50 | 0.42 |
| 1:A:3272:TRP:CZ3 | 1:A:3307:LEU:HD11 | 2.55 | 0.42 |
| 1:A:3315:TYR:CG | 1:A:3316:LEU:N | 2.88 | 0.42 |
| 1:A:438:LEU:HA | 1:A:438:LEU:HD12 | 1.87 | 0.42 |
| 1:A:560:LEU:CB | 1:A:616:LYS:HZ3 | 2.05 | 0.42 |
| 1:B:1064:TYR:CD1 | 1:B:1106:ILE:HD11 | 2.55 | 0.42 |
| 1:B:1300:SER:O | 1:B:1304:HIS:ND1 | 2.35 | 0.42 |
| 1:B:1493:PRO:O | 1:B:1497:ARG:HG2 | 2.20 | 0.42 |
| 1:B:1596:VAL:HG13 | 1:B:1597:LEU:H | 1.83 | 0.42 |
| 1:B:1608:ARG:NE | 1:B:1608:ARG:O | 2.51 | 0.42 |
| 1:B:2360:PHE:O | 1:B:2364:LEU:HG | 2.19 | 0.42 |
| 1:B:2379:MSE:HE1 | 1:B:2404:ARG:CD | 2.42 | 0.42 |
| 1:B:2424:MSE:HA | 1:B:2436:LEU:CD1 | 2.49 | 0.42 |
| 1:B:3005:LEU:O | 1:B:3254:LEU:HD21 | 2.20 | 0.42 |
| 1:B:3118:ASP:N | 1:B:3118:ASP:OD1 | 2.51 | 0.42 |
| 1:B:3251:ASN:ND2 | 1:B:3254:LEU:HD13 | 2.35 | 0.42 |
| 1:B:3324:ARG:O | 1:B:3328:ILE:HG13 | 2.20 | 0.42 |
| 1:B:3479:THR:O | 1:B:3483:MSE:CB | 2.63 | 0.42 |
| 1:B:3570:ASP:HA | 1:B:3573:ASN:HB3 | 2.02 | 0.42 |
| 1:B:3612:ARG:O | 1:B:3615:ALA:HB3 | 2.19 | 0.42 |
| 1:B:3704:GLN:HG3 | 1:B:3796:MSE:SE | 2.68 | 0.42 |
| 1:B:3775:LEU:HD13 | 1:B:3781:CYS:SG | 2.59 | 0.42 |
| 1:B:3705:TYR:HD2 | 1:B:3792:SER:HB2 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3819:THR:O | 1:B:3823:GLU:HG2 | 2.18 | 0.42 |
| 1:B:3501:HIS:ND1 | 1:B:4008:GLU:OE1 | 2.52 | 0.42 |
| 1:B:436:GLU:O | 1:B:439:VAL:HB | 2.20 | 0.42 |
| 1:B:493:LYS:HB3 | 1:B:494:PRO:HD2 | 2.00 | 0.42 |
| 1:B:742:GLU:HA | 1:B:745:VAL:HG23 | 2.01 | 0.42 |
| 1:B:766:ALA:C | 1:B:768:VAL:H | 2.17 | 0.42 |
| 1:B:88:PHE:HB3 | 1:B:92:PHE:CZ | 2.55 | 0.42 |
| 1:B:971:ARG:O | 1:B:974:CYS:HB3 | 2.19 | 0.42 |
| 1:A:1019:ASP:HB2 | 1:A:1021:VAL:HG23 | 2.00 | 0.42 |
| 1:A:1238:GLN:HG3 | 1:A:1298:LEU:HD21 | 2.01 | 0.42 |
| 1:A:1469:PRO:HG3 | 1:A:1510:LEU:HD21 | 2.00 | 0.42 |
| 1:A:1718:ILE:CG2 | 1:A:1750:LEU:HD11 | 2.48 | 0.42 |
| 1:A:1970:LYS:HZ3 | 1:A:2017:GLY:HA3 | 1.85 | 0.42 |
| 1:A:2136:PRO:C | 1:A:2139:PRO:HD2 | 2.39 | 0.42 |
| 1:A:2322:VAL:HG12 | 1:A:2323:LEU:N | 2.35 | 0.42 |
| 1:A:2367:VAL:O | 1:A:2371:PHE:HE1 | 2.03 | 0.42 |
| 1:A:2357:GLU:CD | 1:A:2388:LYS:HZ1 | 2.22 | 0.42 |
| 1:A:2408:MSE:O | 1:A:2409:THR:OG1 | 2.31 | 0.42 |
| 1:A:2548:PRO:O | 1:A:2550:ILE:HG13 | 2.18 | 0.42 |
| 1:A:2869:LEU:HD23 | 1:A:2893:LEU:HA | 2.01 | 0.42 |
| 1:A:866:ILE:HG21 | 1:A:3129:LEU:HD22 | 2.02 | 0.42 |
| 1:A:2961:ALA:HB3 | 1:A:3254:LEU:CD1 | 2.49 | 0.42 |
| 1:A:3343:SER:O | 1:A:3345:PRO:HD3 | 2.19 | 0.42 |
| 1:A:367:GLY:O | 1:A:369:PHE:N | 2.52 | 0.42 |
| 1:A:3766:GLN:O | 1:A:3770:VAL:HG23 | 2.20 | 0.42 |
| 1:A:4037:ASN:O | 1:A:4037:ASN:ND2 | 2.53 | 0.42 |
| 1:A:463:LYS:O | 1:A:466:LEU:HB3 | 2.19 | 0.42 |
| 1:A:481:THR:O | 1:A:485:GLN:HG2 | 2.18 | 0.42 |
| 1:A:560:LEU:HA | 1:A:563:LEU:HD12 | 2.01 | 0.42 |
| 1:A:736:LEU:HA | 1:A:739:ASN:HB2 | 2.02 | 0.42 |
| 1:A:678:LYS:HB2 | 1:A:743:LEU:HD13 | 2.02 | 0.42 |
| 1:A:924:ARG:H | 1:A:924:ARG:HG2 | 1.74 | 0.42 |
| 1:B:1726:SER:O | 1:B:1729:PHE:HB3 | 2.19 | 0.42 |
| 1:B:177:LEU:H | 1:B:177:LEU:HG | 1.63 | 0.42 |
| 1:B:1890:HIS:HE1 | 1:B:1941:HIS:CD2 | 2.38 | 0.42 |
| 1:B:1952:ILE:HG12 | 1:B:1953:CYS:N | 2.35 | 0.42 |
| 1:B:224:LEU:HD13 | 1:B:248:ILE:HD13 | 2.00 | 0.42 |
| 1:B:2555:LEU:HD12 | 1:B:2556:SER:N | 2.32 | 0.42 |
| 1:B:2646:UNK:HA | 1:B:2778:GLY:HA3 | 2.00 | 0.42 |
| 1:B:2794:LEU:HA | 1:B:2794:LEU:HD23 | 1.80 | 0.42 |
| 1:B:2957:LEU:HD21 | 1:B:4101:GLU:CG | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3119:VAL:HG21 | 1:B:3899:ALA:CB | 2.48 | 0.42 |
| 1:B:356:ASN:CG | 1:B:1859:ASN:H | 2.23 | 0.42 |
| 1:B:3629:ARG:NH2 | 1:B:3638:LYS:HZ1 | 2.17 | 0.42 |
| 1:B:3631:LYS:HD2 | 1:B:3681:LYS:O | 2.19 | 0.42 |
| 1:B:3824:GLU:O | 1:B:3829:LEU:HD13 | 2.19 | 0.42 |
| 1:B:3850:HIS:H | 1:B:3850:HIS:CD2 | 2.37 | 0.42 |
| 1:B:3791:TYR:OH | 1:B:3942:PHE:CE2 | 2.70 | 0.42 |
| 1:B:575:ILE:HG13 | 1:B:579:LEU:HD13 | 2.01 | 0.42 |
| 1:B:957:PRO:O | 1:B:961:LEU:HB2 | 2.20 | 0.42 |
| 1:A:1700:THR:OG1 | 1:A:1701:SER:N | 2.48 | 0.42 |
| 1:A:172:GLU:HG3 | 1:A:173:LYS:N | 2.35 | 0.42 |
| 1:A:402:THR:HB | 1:A:1763:THR:HB | 2.02 | 0.42 |
| 1:A:154:SER:OG | 1:A:181:LEU:HD13 | 2.19 | 0.42 |
| 1:A:1915:LEU:HD12 | 1:A:1916:ILE:N | 2.34 | 0.42 |
| 1:A:1890:HIS:CB | 1:A:1937:ARG:HD2 | 2.46 | 0.42 |
| 1:A:1970:LYS:NZ | 1:A:2017:GLY:CA | 2.83 | 0.42 |
| 1:A:2311:ARG:O | 1:A:2311:ARG:HG2 | 2.19 | 0.42 |
| 1:A:899:ARG:HH22 | 1:A:2570:PRO:HB2 | 1.83 | 0.42 |
| 1:A:2813:PHE:HA | 1:A:2816:ILE:CG2 | 2.47 | 0.42 |
| 1:A:3034:PRO:C | 1:A:3036:TYR:H | 2.23 | 0.42 |
| 1:A:3101:TYR:HE2 | 1:A:3102:TYR:CE1 | 2.38 | 0.42 |
| 1:A:3198:THR:OG1 | 1:A:3199:PRO:HD3 | 2.19 | 0.42 |
| 1:A:3530:VAL:HG11 | 1:A:3700:GLU:O | 2.18 | 0.42 |
| 1:A:3771:MSE:O | 1:A:3775:LEU:HG | 2.20 | 0.42 |
| 1:A:3923:ARG:CG | 1:A:3962:ARG:HH22 | 2.00 | 0.42 |
| 1:A:396:PHE:CZ | 1:A:437:HIS:CD2 | 3.07 | 0.42 |
| 1:A:655:LEU:HA | 1:A:658:THR:OG1 | 2.18 | 0.42 |
| 1:A:774:GLU:OE2 | 1:A:854:ARG:HB2 | 2.19 | 0.42 |
| 1:A:952:GLY:C | 1:A:954:GLY:H | 2.23 | 0.42 |
| 1:B:1166:LEU:HB3 | 1:B:1170:LYS:HZ1 | 1.83 | 0.42 |
| 1:B:1270:PHE:HZ | 1:B:1347:THR:C | 2.23 | 0.42 |
| 1:B:1437:TYR:O | 1:B:1439:PRO:HD2 | 2.20 | 0.42 |
| 1:B:1718:ILE:HG23 | 1:B:1750:LEU:CD1 | 2.40 | 0.42 |
| 1:B:1751:GLU:H | 1:B:1751:GLU:HG3 | 1.57 | 0.42 |
| 1:B:1763:THR:N | 1:B:1864:ASP:OD2 | 2.52 | 0.42 |
| 1:B:1889:VAL:HG22 | 1:B:1900:PHE:CE2 | 2.54 | 0.42 |
| 1:B:1927:MSE:C | 1:B:1929:GLY:N | 2.72 | 0.42 |
| 1:B:2074:PRO:HB2 | 1:B:2075:THR:H | 1.75 | 0.42 |
| 1:B:2168:LEU:HG | 1:B:2168:LEU:H | 1.56 | 0.42 |
| 1:B:2602:UNK:CB | 1:B:2790:LEU:HD23 | 2.49 | 0.42 |
| 1:B:2823:PHE:CG | 1:B:2824:LYS:N | 2.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2900:LEU:HD12 | 1:B:2905:LEU:HD21 | 2.02 | 0.42 |
| 1:B:3034:PRO:C | 1:B:3036:TYR:H | 2.23 | 0.42 |
| 1:B:3039:THR:O | 1:B:3042:PRO:HD2 | 2.19 | 0.42 |
| 1:B:3141:PHE:HZ | 1:B:3192:LYS:CB | 2.31 | 0.42 |
| 1:B:3167:ARG:NH1 | 1:B:3167:ARG:CG | 2.71 | 0.42 |
| 1:B:3255:ALA:HB1 | 1:B:3282:ARG:CZ | 2.49 | 0.42 |
| 1:B:3585:PHE:CD1 | 1:B:3613:MSE:HE1 | 2.53 | 0.42 |
| 1:B:3588:TRP:NE1 | 1:B:3609:MSE:O | 2.39 | 0.42 |
| 1:B:3763:ARG:HH21 | 1:B:4009:PRO:HG3 | 1.85 | 0.42 |
| 1:B:627:VAL:CG1 | 1:B:628:GLU:N | 2.81 | 0.42 |
| 1:B:890:LYS:HD3 | 1:B:890:LYS:HA | 1.85 | 0.42 |
| 1:B:898:PHE:HD2 | 1:B:2566:THR:OG1 | 2.02 | 0.42 |
| 1:A:1002:GLU:O | 1:A:1005:ASP:OD2 | 2.38 | 0.42 |
| 1:A:1069:HIS:H | 1:A:1070:PRO:CD | 2.32 | 0.42 |
| 1:A:1093:GLU:HB3 | 1:A:1096:VAL:CG1 | 2.50 | 0.42 |
| 1:A:1360:LYS:HG3 | 1:A:1360:LYS:H | 1.52 | 0.42 |
| 1:A:1372:LEU:HG | 1:A:1418:HIS:HE1 | 1.85 | 0.42 |
| 1:A:136:GLN:HG2 | 1:A:139:ARG:HH11 | 1.84 | 0.42 |
| 1:A:170:VAL:CG2 | 1:A:173:LYS:HD3 | 2.47 | 0.42 |
| 1:A:1817:GLN:NE2 | 1:A:1821:ASP:HB2 | 2.35 | 0.42 |
| 1:A:1960:LYS:HB2 | 1:A:1998:MSE:SE | 2.70 | 0.42 |
| 1:A:2065:ARG:HB3 | 1:A:2125:TRP:HD1 | 1.82 | 0.42 |
| 1:A:2292:CYS:CB | 1:A:2300:PHE:HB2 | 2.38 | 0.42 |
| 1:A:197:PHE:CZ | 1:A:230:LEU:HD22 | 2.54 | 0.42 |
| 1:A:2375:ALA:HB1 | 1:A:2411:LEU:CD2 | 2.49 | 0.42 |
| 1:A:2384:PHE:C | 1:A:2387:PRO:HD2 | 2.39 | 0.42 |
| 1:A:2411:LEU:HG | 1:A:2412:TYR:N | 2.34 | 0.42 |
| 1:A:2433:LYS:O | 1:A:2436:LEU:N | 2.46 | 0.42 |
| 1:A:2434:VAL:O | 1:A:2438:ILE:HG13 | 2.19 | 0.42 |
| 1:A:2990:GLU:O | 1:A:2994:TRP:CD1 | 2.72 | 0.42 |
| 1:A:3181:ASP:HA | 1:A:3184:THR:HG23 | 2.02 | 0.42 |
| 1:A:3450:MSE:O | 1:A:3454:LEU:HG | 2.20 | 0.42 |
| 1:A:3503:VAL:HG21 | 1:A:3535:ILE:C | 2.40 | 0.42 |
| 1:A:3513:ALA:O | 1:A:3518:VAL:HB | 2.20 | 0.42 |
| 1:A:3575:LEU:O | 1:A:3686:TRP:HH2 | 2.03 | 0.42 |
| 1:A:3619:ASP:N | 1:A:3620:PRO:HD2 | 2.34 | 0.42 |
| 1:A:3745:GLU:O | 1:A:3745:GLU:HG2 | 2.20 | 0.42 |
| 1:A:3839:TYR:CE2 | 1:A:3843:LEU:HD11 | 2.54 | 0.42 |
| 1:A:3955:VAL:HG22 | 1:A:3957:GLU:HG3 | 2.01 | 0.42 |
| 1:A:580:ASP:O | 1:A:584:GLU:N | 2.53 | 0.42 |
| 1:A:649:PHE:C | 1:A:651:TYR:N | 2.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:742:GLU:OE1 | 1:A:783:HIS:CD2 | 2.72 | 0.42 |
| 1:A:929:ALA:O | 1:A:933:LEU:CB | 2.67 | 0.42 |
| 1:A:927:LYS:HE2 | 1:A:976:VAL:HG12 | 2.02 | 0.42 |
| 1:B:963:LYS:HG3 | 1:B:1009:LEU:HD11 | 2.00 | 0.42 |
| 1:B:1580:LEU:HD13 | 1:B:1639:LEU:HB3 | 2.00 | 0.42 |
| 1:B:1655:ILE:HD12 | 1:B:1655:ILE:H | 1.85 | 0.42 |
| 1:B:1679:LEU:O | 1:B:1683:LYS:HG3 | 2.19 | 0.42 |
| 1:B:1756:PRO:C | 1:B:1758:LEU:N | 2.71 | 0.42 |
| 1:B:2255:LEU:HD13 | 1:B:2258:GLU:OE1 | 2.20 | 0.42 |
| 1:B:2405:VAL:HB | 1:B:2439:ILE:CD1 | 2.49 | 0.42 |
| 1:B:2411:LEU:HG | 1:B:2412:TYR:N | 2.35 | 0.42 |
| 1:B:2474:TYR:O | 1:B:2478:MSE:HG3 | 2.19 | 0.42 |
| 1:B:2520:ILE:HG13 | 1:B:2524:PHE:CE2 | 2.55 | 0.42 |
| 1:B:2637:UNK:O | 1:B:2641:UNK:CB | 2.67 | 0.42 |
| 1:B:2933:ILE:HG22 | 1:B:2937:ASP:OD2 | 2.20 | 0.42 |
| 1:B:3258:LEU:HA | 1:B:3258:LEU:HD22 | 1.75 | 0.42 |
| 1:B:3427:GLU:HG3 | 1:B:3439:LEU:HD13 | 2.01 | 0.42 |
| 1:B:3522:THR:OG1 | 1:B:3558:ILE:HD11 | 2.20 | 0.42 |
| 1:B:3816:LEU:HD23 | 1:B:3816:LEU:HA | 1.84 | 0.42 |
| 1:B:558:GLU:HA | 1:B:561:ASN:ND2 | 2.35 | 0.42 |
| 1:B:576:VAL:HG13 | 1:B:601:TRP:CE3 | 2.41 | 0.42 |
| 1:B:38:LEU:HD13 | 1:B:62:ASP:OD2 | 2.20 | 0.42 |
| 2:S:114:UNK:O | 2:S:116:UNK:N | 2.53 | 0.42 |
| 1:A:1463:LEU:O | 1:A:1467:ILE:HG12 | 2.20 | 0.42 |
| 1:A:1498:GLN:C | 1:A:1501:PRO:HD2 | 2.40 | 0.42 |
| 1:A:1608:ARG:NE | 1:A:1608:ARG:O | 2.52 | 0.42 |
| 1:A:1655:ILE:HD13 | 1:A:1681:ASP:CB | 2.45 | 0.42 |
| 1:A:1889:VAL:HG22 | 1:A:1900:PHE:CG | 2.54 | 0.42 |
| 1:A:2066:PHE:CD1 | 1:A:2128:PHE:HE1 | 2.38 | 0.42 |
| 1:A:2210:VAL:HG13 | 1:A:2211:LEU:HG | 2.01 | 0.42 |
| 1:A:2300:PHE:CE2 | 1:A:2341:LEU:HB2 | 2.54 | 0.42 |
| 1:A:2943:PHE:CE1 | 1:A:2984:GLY:HA2 | 2.55 | 0.42 |
| 1:A:35:ILE:HG21 | 1:A:84:GLU:HB3 | 2.02 | 0.42 |
| 1:A:3690:PHE:HD1 | 1:A:3692:VAL:HG23 | 1.84 | 0.42 |
| 1:A:3872:ARG:HD2 | 1:A:3965:ARG:NH1 | 2.35 | 0.42 |
| 1:A:3982:SER:HB3 | 1:A:3986:HIS:HE1 | 1.83 | 0.42 |
| 1:A:453:MSE:SE | 1:A:456:VAL:HG11 | 2.70 | 0.42 |
| 1:A:781:ASP:OD2 | 1:A:862:LEU:HD21 | 2.20 | 0.42 |
| 1:A:961:LEU:HA | 1:A:961:LEU:HD13 | 1.81 | 0.42 |
| 1:B:107:ILE:O | 1:B:110:THR:HB | 2.20 | 0.42 |
| 1:B:1551:ILE:HA | 1:B:1554:SER:HB3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1686:LEU:CD2 | 1:B:1727:ARG:NH1 | 2.83 | 0.42 |
| 1:B:1861:SER:O | 1:B:1864:ASP:HB3 | 2.20 | 0.42 |
| 1:B:2135:ASN:N | 1:B:2136:PRO:HD3 | 2.35 | 0.42 |
| 1:B:2166:SER:O | 1:B:2170:GLN:CB | 2.50 | 0.42 |
| 1:B:2171:LEU:CG | 1:B:2177:ASN:HD21 | 2.29 | 0.42 |
| 1:B:2326:ILE:HA | 1:B:2326:ILE:HD13 | 1.89 | 0.42 |
| 1:B:2443:MSE:N | 1:B:2444:PRO:HD2 | 2.35 | 0.42 |
| 1:B:2531:LEU:HA | 1:B:2531:LEU:HD12 | 1.89 | 0.42 |
| 1:B:2541:ALA:O | 1:B:2545:LEU:HG | 2.20 | 0.42 |
| 1:B:2905:LEU:HB2 | 1:B:2906:PRO:CD | 2.50 | 0.42 |
| 1:B:2875:ALA:HB2 | 1:B:2921:LEU:HD23 | 2.01 | 0.42 |
| 1:B:3283:LEU:HD13 | 1:B:3287:ARG:CZ | 2.50 | 0.42 |
| 1:B:3283:LEU:HD13 | 1:B:3287:ARG:NE | 2.34 | 0.42 |
| 1:B:3529:ILE:HG22 | 1:B:3529:ILE:O | 2.19 | 0.42 |
| 1:B:3694:PHE:CD2 | 1:B:3697:ASN:HA | 2.54 | 0.42 |
| 1:B:3577:GLN:HG3 | 1:B:3800:LEU:CD2 | 2.50 | 0.42 |
| 1:B:3885:ARG:O | 1:B:3888:VAL:HG12 | 2.20 | 0.42 |
| 1:B:617:PRO:HB3 | 1:B:659:ARG:CD | 2.50 | 0.42 |
| 1:B:792:ILE:O | 1:B:796:LEU:HG | 2.19 | 0.42 |
| 1:B:886:TRP:CH2 | 1:B:958:MSE:HB2 | 2.54 | 0.42 |
| 1:B:980:THR:HG22 | 1:B:984:TYR:CE2 | 2.52 | 0.42 |
| 1:A:971:ARG:HD2 | 1:A:1024:THR:CB | 2.50 | 0.42 |
| 1:A:1127:CYS:O | 1:A:1131:ILE:HG23 | 2.20 | 0.42 |
| 1:A:1279:LEU:HG | 1:A:1292:LYS:NZ | 2.33 | 0.42 |
| 1:A:1651:LYS:HB2 | 1:A:1684:LEU:CD1 | 2.50 | 0.42 |
| 1:A:1686:LEU:HD23 | 1:A:1727:ARG:CZ | 2.50 | 0.42 |
| 1:A:1939:LEU:O | 1:A:1942:CYS:N | 2.53 | 0.42 |
| 1:A:1981:LEU:O | 1:A:1984:LEU:HG | 2.19 | 0.42 |
| 1:A:2166:SER:N | 1:A:2167:PRO:CD | 2.82 | 0.42 |
| 1:A:2154:GLU:N | 1:A:2199:LEU:HD22 | 2.34 | 0.42 |
| 1:A:2233:HIS:HA | 1:A:2236:GLU:CD | 2.40 | 0.42 |
| 1:A:2913:LYS:HG3 | 1:A:2914:ALA:H | 1.82 | 0.42 |
| 1:A:3454:LEU:HD21 | 1:A:3461:ALA:HB2 | 2.01 | 0.42 |
| 1:A:3789:ARG:HH22 | 1:A:3806:LEU:CD2 | 2.23 | 0.42 |
| 1:A:403:GLY:C | 1:A:405:ASP:N | 2.71 | 0.42 |
| 1:A:575:ILE:HD13 | 1:A:603:ILE:HB | 2.01 | 0.42 |
| 1:A:758:LEU:HA | 1:A:758:LEU:HD12 | 1.91 | 0.42 |
| 1:B:1007:VAL:HA | 1:B:1010:LEU:HD11 | 2.02 | 0.42 |
| 1:B:1017:ILE:HB | 1:B:1025:LEU:CB | 2.47 | 0.42 |
| 1:B:1349:LEU:CD2 | 1:B:1353:PRO:HG2 | 2.49 | 0.42 |
| 1:B:1467:ILE:HG13 | 1:B:1468:LEU:HG | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2327:LEU:HA | 1:B:2330:VAL:HG12 | 2.01 | 0.42 |
| 1:B:2877:SER:O | 1:B:2880:CYS:N | 2.36 | 0.42 |
| 1:B:3053:LEU:HD23 | 1:B:3053:LEU:HA | 1.55 | 0.42 |
| 1:B:3293:CYS:HA | 1:B:3297:VAL:CG2 | 2.50 | 0.42 |
| 1:B:62:ASP:O | 1:B:66:LEU:HD23 | 2.20 | 0.42 |
| 1:B:642:PHE:HE2 | 1:B:710:PHE:HE2 | 1.66 | 0.42 |
| 1:B:992:ILE:HA | 1:B:995:PHE:CE2 | 2.54 | 0.42 |
| 1:A:1015:ASP:HA | 1:A:1018:VAL:HG22 | 2.01 | 0.42 |
| 1:A:1083:ASN:HD21 | 1:A:1104:LEU:CD2 | 2.32 | 0.42 |
| 1:A:1303:MSE:HB2 | 1:A:1371:VAL:HG23 | 2.01 | 0.42 |
| 1:A:147:PHE:CD2 | 1:A:148:LYS:HG3 | 2.55 | 0.42 |
| 1:A:1715:GLU:O | 1:A:1719:VAL:HG23 | 2.19 | 0.42 |
| 1:A:2035:THR:HG22 | 1:A:2076:VAL:HG13 | 2.02 | 0.42 |
| 1:A:2276:LEU:O | 1:A:2279:ILE:HB | 2.19 | 0.42 |
| 1:A:2387:PRO:O | 1:A:2390:HIS:HB3 | 2.20 | 0.42 |
| 1:A:2472:GLN:O | 1:A:2476:ILE:HG12 | 2.19 | 0.42 |
| 1:A:2520:ILE:HD12 | 1:A:2607:UNK:CB | 2.50 | 0.42 |
| 1:A:2538:ARG:NH1 | 1:A:2565:MSE:HG3 | 2.35 | 0.42 |
| 1:A:2843:PHE:HE2 | 1:A:2853:PRO:HG3 | 1.85 | 0.42 |
| 1:A:281:GLN:HA | 1:A:326:MSE:SE | 2.70 | 0.42 |
| 1:A:3280:TYR:CG | 1:A:3328:ILE:HD11 | 2.55 | 0.42 |
| 1:A:356:ASN:CG | 1:A:1859:ASN:HB2 | 2.40 | 0.42 |
| 1:A:393:LYS:HA | 1:A:396:PHE:CE1 | 2.54 | 0.42 |
| 1:A:429:GLU:N | 1:A:429:GLU:OE1 | 2.53 | 0.42 |
| 1:A:436:GLU:OE2 | 1:A:475:LEU:HD11 | 2.19 | 0.42 |
| 1:A:654:ILE:HG23 | 1:A:722:LYS:NZ | 2.35 | 0.42 |
| 1:A:846:ILE:HG23 | 1:A:854:ARG:NH1 | 2.35 | 0.42 |
| 1:B:1335:CYS:HA | 1:B:1338:VAL:HG12 | 2.01 | 0.42 |
| 1:B:149:ILE:O | 1:B:152:LEU:HG | 2.20 | 0.42 |
| 1:B:1681:ASP:HB2 | 1:B:1717:LEU:CD2 | 2.50 | 0.42 |
| 1:B:1809:ASP:N | 1:B:1810:PRO:HD3 | 2.35 | 0.42 |
| 1:B:2385:LEU:HG | 1:B:2389:PHE:CZ | 2.55 | 0.42 |
| 1:B:2398:LEU:O | 1:B:2402:LEU:HD23 | 2.20 | 0.42 |
| 1:B:3148:GLN:HE22 | 1:B:3160:LEU:HD22 | 1.85 | 0.42 |
| 1:B:3283:LEU:HG | 1:B:3300:VAL:CG2 | 2.49 | 0.42 |
| 1:B:3978:GLY:O | 1:B:3979:LEU:HD23 | 2.19 | 0.42 |
| 1:B:446:PHE:HD2 | 1:B:533:HIS:CG | 2.37 | 0.42 |
| 1:B:617:PRO:HB3 | 1:B:659:ARG:HD2 | 2.02 | 0.42 |
| 1:B:913:ARG:O | 1:B:917:LEU:HG | 2.20 | 0.42 |
| 1:B:977:ASP:HB3 | 1:B:980:THR:HG22 | 2.02 | 0.42 |
| 1:A:1080:LEU:HD23 | 1:A:1128:CYS:SG | 2.61 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1060:PHE:CD2 | 1:A:1099:PHE:HZ | 2.38 | 0.41 |
| 1:A:82:ARG:NH1 | 1:A:114:VAL:HG13 | 2.35 | 0.41 |
| 1:A:1747:LEU:O | 1:A:1748:ASP:C | 2.58 | 0.41 |
| 1:A:1763:THR:N | 1:A:1864:ASP:OD2 | 2.43 | 0.41 |
| 1:A:2082:GLU:HB2 | 1:A:2086:ASP:CB | 2.50 | 0.41 |
| 1:A:2534:ASN:HB3 | 1:A:2537:ASP:HB2 | 2.01 | 0.41 |
| 1:A:279:ALA:HA | 1:A:282:PHE:CD2 | 2.55 | 0.41 |
| 1:A:2943:PHE:CD1 | 1:A:2944:THR:N | 2.79 | 0.41 |
| 1:A:3386:SER:O | 1:A:3390:GLN:HB2 | 2.19 | 0.41 |
| 1:A:345:PHE:O | 1:A:348:ILE:N | 2.53 | 0.41 |
| 1:A:381:VAL:HB | 1:A:384:MSE:SE | 2.70 | 0.41 |
| 1:A:3995:PRO:O | 1:A:3999:THR:OG1 | 2.17 | 0.41 |
| 1:A:398:THR:HA | 1:A:400:THR:HG22 | 2.02 | 0.41 |
| 1:A:417:VAL:O | 1:A:420:VAL:HG12 | 2.20 | 0.41 |
| 1:A:489:ARG:HA | 1:A:612:LEU:HB2 | 2.02 | 0.41 |
| 1:A:513:GLU:OE1 | 1:A:653:LEU:HD11 | 2.19 | 0.41 |
| 1:B:2047:THR:O | 1:B:2050:GLN:HB2 | 2.20 | 0.41 |
| 1:B:2190:VAL:HG21 | 1:B:2241:LEU:CD1 | 2.47 | 0.41 |
| 1:B:2843:PHE:HE2 | 1:B:2853:PRO:HG3 | 1.84 | 0.41 |
| 1:B:3585:PHE:O | 1:B:3589:SER:OG | 2.30 | 0.41 |
| 1:B:368:LEU:HD13 | 1:B:388:LEU:HD23 | 2.00 | 0.41 |
| 1:B:3577:GLN:HA | 1:B:3800:LEU:HD22 | 2.02 | 0.41 |
| 1:B:454:GLN:CG | 1:B:533:HIS:HE1 | 2.29 | 0.41 |
| 1:A:100:ILE:HG22 | 1:A:100:ILE:O | 2.20 | 0.41 |
| 1:A:997:ASN:HA | 1:A:1042:LYS:HD3 | 2.03 | 0.41 |
| 1:A:1503:LEU:HA | 1:A:1503:LEU:HD23 | 1.88 | 0.41 |
| 1:A:1569:THR:O | 1:A:1573:LYS:CB | 2.67 | 0.41 |
| 1:A:1711:ARG:HG3 | 1:A:1712:ARG:N | 2.35 | 0.41 |
| 1:A:1722:PHE:O | 1:A:1725:GLN:HB3 | 2.20 | 0.41 |
| 1:A:2263:LYS:HB3 | 1:A:2264:ASP:H | 1.61 | 0.41 |
| 1:A:2458:VAL:HG12 | 1:A:2473:MSE:HG3 | 2.01 | 0.41 |
| 1:A:2482:ASP:HB2 | 1:A:2485:ARG:NH2 | 2.35 | 0.41 |
| 1:A:2502:ALA:O | 1:A:2506:LEU:HG | 2.19 | 0.41 |
| 1:A:3351:ILE:HG23 | 1:A:3355:LYS:CE | 2.49 | 0.41 |
| 1:A:3454:LEU:HD21 | 1:A:3461:ALA:CB | 2.50 | 0.41 |
| 1:A:3505:LEU:HD12 | 1:A:3509:ASP:CB | 2.45 | 0.41 |
| 1:A:560:LEU:HA | 1:A:563:LEU:CG | 2.50 | 0.41 |
| 1:B:1354:GLU:C | 1:B:1356:TRP:N | 2.74 | 0.41 |
| 1:B:2010:GLU:C | 1:B:2012:ARG:N | 2.73 | 0.41 |
| 1:B:2166:SER:N | 1:B:2167:PRO:HD2 | 2.35 | 0.41 |
| 1:B:2193:ILE:HD12 | 1:B:2245:TRP:CZ2 | 2.54 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2277:LEU:O | 1:B:2280:VAL:HB | 2.20 | 0.41 |
| 1:B:2337:LEU:HD12 | 1:B:2337:LEU:HA | 1.86 | 0.41 |
| 1:B:2359:LYS:O | 1:B:2362:VAL:HG22 | 2.20 | 0.41 |
| 1:B:2365:ASN:HA | 1:B:2368:THR:HB | 2.00 | 0.41 |
| 1:B:2473:MSE:HB3 | 1:B:2473:MSE:HE2 | 1.82 | 0.41 |
| 1:B:271:GLY:HA2 | 1:B:274:LEU:HD11 | 2.02 | 0.41 |
| 1:B:2837:LEU:HD13 | 1:B:2868:LEU:N | 2.35 | 0.41 |
| 1:B:2886:GLN:H | 1:B:2886:GLN:HG3 | 1.48 | 0.41 |
| 1:B:3241:LYS:O | 1:B:3243:ILE:N | 2.41 | 0.41 |
| 1:B:389:ILE:HG23 | 1:B:434:VAL:HG21 | 2.00 | 0.41 |
| 1:B:3929:MSE:HB3 | 1:B:3938:ILE:HD12 | 2.02 | 0.41 |
| 1:B:43:VAL:O | 1:B:45:SER:N | 2.52 | 0.41 |
| 1:A:1163:LEU:HD23 | 1:A:1260:LEU:HD11 | 2.03 | 0.41 |
| 1:A:1251:GLN:O | 1:A:1255:CYS:HB2 | 2.20 | 0.41 |
| 1:A:1582:LEU:O | 1:A:1583:MSE:C | 2.59 | 0.41 |
| 1:A:1684:LEU:HA | 1:A:1684:LEU:HD23 | 1.82 | 0.41 |
| 1:A:1695:LEU:O | 1:A:1700:THR:HB | 2.20 | 0.41 |
| 1:A:2103:HIS:HA | 1:A:2106:ARG:HB2 | 2.02 | 0.41 |
| 1:A:2168:LEU:HD13 | 1:A:2214:ARG:NH2 | 2.35 | 0.41 |
| 1:A:2462:VAL:HA | 1:A:2465:PRO:HD3 | 2.02 | 0.41 |
| 1:A:2443:MSE:CE | 1:A:2476:ILE:HB | 2.34 | 0.41 |
| 1:A:2841:ASN:HD22 | 1:A:2871:LEU:HG | 1.86 | 0.41 |
| 1:A:3011:LEU:O | 1:A:3011:LEU:HD13 | 2.19 | 0.41 |
| 1:A:3056:GLU:HA | 1:A:3092:LEU:HD11 | 2.02 | 0.41 |
| 1:A:349:ILE:HG12 | 1:A:364:ARG:HB2 | 2.01 | 0.41 |
| 1:A:3621:LYS:HB3 | 1:A:3638:LYS:HE2 | 2.02 | 0.41 |
| 1:A:398:THR:C | 1:A:400:THR:N | 2.74 | 0.41 |
| 1:A:513:GLU:OE2 | 1:A:655:LEU:HD23 | 2.21 | 0.41 |
| 1:A:592:GLU:HB3 | 1:A:601:TRP:HZ2 | 1.84 | 0.41 |
| 1:A:922:SER:OG | 1:A:925:GLN:OE1 | 2.19 | 0.41 |
| 1:A:955:ALA:O | 1:A:959:TYR:HB3 | 2.19 | 0.41 |
| 1:A:999:LYS:HD2 | 1:A:1001:PHE:CE2 | 2.55 | 0.41 |
| 1:B:1025:LEU:HD12 | 1:B:1028:PHE:HD2 | 1.84 | 0.41 |
| 1:B:113:SER:O | 1:B:116:THR:HB | 2.20 | 0.41 |
| 1:B:1164:CYS:O | 1:B:1164:CYS:SG | 2.77 | 0.41 |
| 1:B:1648:LEU:O | 1:B:1652:ILE:HD12 | 2.20 | 0.41 |
| 1:B:162:LEU:HD21 | 1:B:196:LEU:HD13 | 2.01 | 0.41 |
| 1:B:2160:TYR:HA | 1:B:2163:HIS:CD2 | 2.55 | 0.41 |
| 1:B:2213:ASN:CB | 1:B:2250:SER:HB2 | 2.50 | 0.41 |
| 1:B:2367:VAL:HG22 | 1:B:2371:PHE:CE1 | 2.55 | 0.41 |
| 1:B:2396:LEU:H | 1:B:2396:LEU:HD12 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:259:GLN:C | 1:B:260:ILE:HG13 | 2.41 | 0.41 |
| 1:B:2647:UNK:HA | 1:B:2775:TYR:HD1 | 1.85 | 0.41 |
| 1:B:2806:LYS:HD3 | 1:B:2855:VAL:CG1 | 2.43 | 0.41 |
| 1:B:19:LEU:HB2 | 1:B:34:LEU:HD13 | 2.02 | 0.41 |
| 1:B:61:ARG:O | 1:B:65:LEU:CB | 2.54 | 0.41 |
| 1:B:646:VAL:HG11 | 1:B:710:PHE:CZ | 2.54 | 0.41 |
| 1:B:850:GLU:CD | 1:B:854:ARG:HH21 | 2.21 | 0.41 |
| 1:A:1060:PHE:HB3 | 1:A:1064:TYR:CE2 | 2.56 | 0.41 |
| 1:A:166:ILE:HG22 | 1:A:167:PRO:HD2 | 2.02 | 0.41 |
| 1:A:1640:GLU:HG2 | 1:A:1691:GLN:HG2 | 2.01 | 0.41 |
| 1:A:1729:PHE:HZ | 1:A:1870:LYS:HZ3 | 1.69 | 0.41 |
| 1:A:1997:PRO:HA | 1:A:2000:ARG:N | 2.36 | 0.41 |
| 1:A:2813:PHE:O | 1:A:2816:ILE:HG22 | 2.20 | 0.41 |
| 1:A:3151:LEU:HA | 1:A:3152:SER:HA | 1.85 | 0.41 |
| 1:A:449:TYR:CD2 | 1:A:454:GLN:HA | 2.55 | 0.41 |
| 1:A:51:LEU:H | 1:A:51:LEU:HG | 1.62 | 0.41 |
| 1:A:488:ILE:HD12 | 1:A:616:LYS:HD3 | 2.02 | 0.41 |
| 1:A:741:ILE:HB | 1:A:744:ASP:CG | 2.40 | 0.41 |
| 1:A:851:ILE:O | 1:A:855:VAL:HG23 | 2.19 | 0.41 |
| 1:B:1006:THR:O | 1:B:1010:LEU:HG | 2.21 | 0.41 |
| 1:B:1092:GLU:O | 1:B:1093:GLU:HB2 | 2.20 | 0.41 |
| 1:B:1289:SER:OG | 1:B:1289:SER:O | 2.39 | 0.41 |
| 1:B:1735:ARG:O | 1:B:1736:PHE:HB2 | 2.20 | 0.41 |
| 1:B:1761:LEU:HD23 | 1:B:1762:MSE:N | 2.36 | 0.41 |
| 1:B:1931:ASN:OD1 | 1:B:1932:GLN:N | 2.53 | 0.41 |
| 1:B:1945:TYR:HD1 | 1:B:1948:ALA:HB3 | 1.86 | 0.41 |
| 1:B:2003:LYS:HA | 1:B:2006:GLU:HB2 | 2.03 | 0.41 |
| 1:B:2066:PHE:HB3 | 1:B:2067:ARG:HA | 2.02 | 0.41 |
| 1:B:2386:LEU:HA | 1:B:2386:LEU:HD23 | 1.80 | 0.41 |
| 1:B:2870:SER:C | 1:B:2872:ASP:N | 2.71 | 0.41 |
| 1:B:2995:GLU:O | 1:B:2998:SER:HB3 | 2.20 | 0.41 |
| 1:B:3778:ASP:OD1 | 1:B:3780:ALA:N | 2.53 | 0.41 |
| 1:B:3944:HIS:CG | 1:B:3949:ALA:HA | 2.55 | 0.41 |
| 1:B:3953:LEU:HD13 | 1:B:4069:GLU:HB3 | 2.01 | 0.41 |
| 1:B:4028:ILE:HA | 1:B:4031:ILE:HD12 | 2.02 | 0.41 |
| 1:A:1025:LEU:HD12 | 1:A:1025:LEU:HA | 1.78 | 0.41 |
| 1:A:2083:LEU:HA | 1:A:2083:LEU:HD23 | 1.81 | 0.41 |
| 1:A:2163:HIS:O | 1:A:2167:PRO:HD3 | 2.21 | 0.41 |
| 1:A:2239:LYS:HE2 | 1:A:2240:THR:CG2 | 2.45 | 0.41 |
| 1:A:249:PHE:HZ | 1:A:272:LEU:HD12 | 1.86 | 0.41 |
| 1:A:2512:ASP:HB2 | 1:A:2515:PRO:HD2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3002:TYR:CE1 | 1:A:3003:ASN:HB3 | 2.55 | 0.41 |
| 1:A:3048:LYS:HZ3 | 1:A:3089:LEU:HB3 | 1.85 | 0.41 |
| 1:A:3135:LEU:O | 1:A:3138:ILE:HB | 2.20 | 0.41 |
| 1:A:3640:PHE:HB3 | 1:A:3644:PHE:CD2 | 2.56 | 0.41 |
| 1:A:3687:MSE:C | 1:A:3689:ASP:N | 2.70 | 0.41 |
| 1:A:3710:LYS:HA | 1:A:3710:LYS:HD3 | 1.95 | 0.41 |
| 1:A:703:CYS:O | 1:A:707:PHE:CD1 | 2.73 | 0.41 |
| 1:B:1076:LEU:HA | 1:B:1076:LEU:HD23 | 1.75 | 0.41 |
| 1:B:1255:CYS:SG | 1:B:1333:SER:HB3 | 2.60 | 0.41 |
| 1:B:1366:THR:O | 1:B:1369:MSE:HB2 | 2.20 | 0.41 |
| 1:B:1608:ARG:HD3 | 1:B:1631:SER:H | 1.86 | 0.41 |
| 1:B:567:GLU:OE2 | 1:B:1798:LEU:HD22 | 2.21 | 0.41 |
| 1:B:2129:LEU:HD13 | 1:B:2156:VAL:CG1 | 2.51 | 0.41 |
| 1:B:2427:ARG:HB3 | 1:B:2433:LYS:HB2 | 2.02 | 0.41 |
| 1:B:2634:UNK:O | 1:B:2637:UNK:N | 2.53 | 0.41 |
| 1:B:2789:SER:O | 1:B:2793:PRO:HD3 | 2.21 | 0.41 |
| 1:B:2970:LYS:HE3 | 1:B:2974:GLU:OE2 | 2.21 | 0.41 |
| 1:B:3026:ASP:O | 1:B:3030:ILE:HG13 | 2.20 | 0.41 |
| 1:B:3072:GLU:HA | 1:B:3076:ALA:HA | 2.03 | 0.41 |
| 1:B:31:GLY:O | 1:B:34:LEU:HB3 | 2.20 | 0.41 |
| 1:B:3006:ALA:HB2 | 1:B:3254:LEU:HD11 | 2.03 | 0.41 |
| 1:B:368:LEU:C | 1:B:372:PRO:HG2 | 2.41 | 0.41 |
| 1:B:3974:MSE:CB | 1:B:3976:GLU:HB3 | 2.49 | 0.41 |
| 1:B:394:GLN:O | 1:B:398:THR:HG23 | 2.20 | 0.41 |
| 1:B:476:ARG:HA | 1:B:479:ILE:CG1 | 2.50 | 0.41 |
| 1:B:633:ILE:HG23 | 1:B:637:LYS:CE | 2.51 | 0.41 |
| 1:B:906:PHE:O | 1:B:909:VAL:HB | 2.21 | 0.41 |
| 1:A:1014:LEU:O | 1:A:1078:ALA:HB2 | 2.19 | 0.41 |
| 1:A:1116:ALA:HB2 | 1:A:1164:CYS:HB3 | 2.03 | 0.41 |
| 1:A:1220:LEU:HD13 | 1:A:1274:ARG:CG | 2.49 | 0.41 |
| 1:A:1359:LEU:HD11 | 1:A:1365:ASN:OD1 | 2.20 | 0.41 |
| 1:A:197:PHE:CE2 | 1:A:230:LEU:HD22 | 2.56 | 0.41 |
| 1:A:2412:TYR:HD2 | 1:A:2416:LYS:NZ | 2.17 | 0.41 |
| 1:A:246:ARG:CA | 1:A:249:PHE:HD2 | 2.32 | 0.41 |
| 1:A:2520:ILE:HG23 | 1:A:2521:ILE:N | 2.36 | 0.41 |
| 1:A:2858:ILE:CD1 | 1:A:2888:VAL:HB | 2.51 | 0.41 |
| 1:A:2887:PRO:HG3 | 1:A:2921:LEU:HD13 | 2.03 | 0.41 |
| 1:A:2962:ARG:HH22 | 1:A:3006:ALA:HB1 | 1.85 | 0.41 |
| 1:A:3614:TYR:CD1 | 1:A:3618:GLY:HA3 | 2.56 | 0.41 |
| 1:A:3622:ALA:HB1 | 1:A:3623:PRO:HD2 | 2.02 | 0.41 |
| 1:A:3723:ASP:HB2 | 1:A:3741:ARG:NE | 2.33 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3766:GLN:O | 1:A:3769:GLN:HG2 | 2.21 | 0.41 |
| 1:A:3920:ILE:HG13 | 1:A:3923:ARG:HD3 | 2.02 | 0.41 |
| 1:A:2936:TYR:HD2 | 1:A:3979:LEU:HD21 | 1.83 | 0.41 |
| 1:A:504:GLU:O | 1:A:508:HIS:CG | 2.74 | 0.41 |
| 1:A:752:LEU:O | 1:A:756:PHE:HD1 | 2.02 | 0.41 |
| 1:A:75:SER:HA | 1:A:79:ARG:HG3 | 2.01 | 0.41 |
| 1:A:923:ASP:O | 1:A:927:LYS:HE3 | 2.20 | 0.41 |
| 1:B:989:MSE:SE | 1:B:1030:GLY:O | 2.89 | 0.41 |
| 1:B:717:LYS:HZ3 | 1:B:1121:LEU:HD11 | 1.83 | 0.41 |
| 1:B:168:ASP:O | 1:B:170:VAL:N | 2.47 | 0.41 |
| 1:B:1880:MSE:O | 1:B:1883:ARG:N | 2.51 | 0.41 |
| 1:B:204:LEU:HG | 1:B:204:LEU:H | 1.53 | 0.41 |
| 1:B:204:LEU:HD22 | 1:B:219:VAL:CG1 | 2.46 | 0.41 |
| 1:B:2066:PHE:CD1 | 1:B:2128:PHE:HE1 | 2.39 | 0.41 |
| 1:B:2164:TRP:CZ3 | 1:B:2186:VAL:HG23 | 2.55 | 0.41 |
| 1:B:2542:LEU:HD13 | 1:B:2546:TYR:CE2 | 2.56 | 0.41 |
| 1:B:3329:LEU:O | 1:B:3332:THR:OG1 | 2.32 | 0.41 |
| 1:B:3494:GLN:O | 1:B:3498:TRP:CZ3 | 2.73 | 0.41 |
| 1:B:3736:LYS:HB3 | 1:B:3752:VAL:HB | 2.02 | 0.41 |
| 1:B:3772:ASN:HA | 1:B:3775:LEU:HG | 2.02 | 0.41 |
| 1:B:431:TYR:CA | 1:B:434:VAL:HG12 | 2.44 | 0.41 |
| 1:B:527:TYR:CD1 | 1:B:531:PHE:HZ | 2.38 | 0.41 |
| 1:A:1165:LEU:O | 1:A:1166:LEU:C | 2.59 | 0.41 |
| 1:A:1168:LEU:O | 1:A:1171:TRP:HB3 | 2.21 | 0.41 |
| 1:A:1364:CYS:C | 1:A:1366:THR:N | 2.74 | 0.41 |
| 1:A:1500:LEU:HB3 | 1:A:1501:PRO:HD3 | 2.03 | 0.41 |
| 1:A:160:LEU:O | 1:A:164:LYS:HG2 | 2.20 | 0.41 |
| 1:A:1816:ARG:HD3 | 1:A:1819:PHE:HE1 | 1.86 | 0.41 |
| 1:A:1949:ILE:HD12 | 1:A:1949:ILE:HA | 1.88 | 0.41 |
| 1:A:1992:VAL:HG23 | 1:A:1993:GLU:N | 2.35 | 0.41 |
| 1:A:2040:MSE:HA | 1:A:2043:PHE:CD1 | 2.55 | 0.41 |
| 1:A:2070:GLU:HB2 | 1:A:2072:ARG:N | 2.36 | 0.41 |
| 1:A:217:LEU:N | 1:A:218:PRO:HD2 | 2.36 | 0.41 |
| 1:A:2219:LEU:HB3 | 1:A:2238:ILE:HG21 | 2.02 | 0.41 |
| 1:A:2238:ILE:O | 1:A:2242:VAL:HG23 | 2.21 | 0.41 |
| 1:A:2344:LEU:O | 1:A:2347:LYS:HB2 | 2.21 | 0.41 |
| 1:A:2541:ALA:O | 1:A:2545:LEU:HG | 2.20 | 0.41 |
| 1:A:2824:LYS:HB3 | 1:A:2825:THR:H | 1.69 | 0.41 |
| 1:A:2863:CYS:O | 1:A:2865:HIS:N | 2.54 | 0.41 |
| 1:A:2920:VAL:O | 1:A:2923:TRP:HB3 | 2.21 | 0.41 |
| 1:A:3033:GLU:OE2 | 1:A:3079:GLU:CD | 2.59 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:3356:ALA:HB1 | 1:A:3384:HIS:HB3 | 2.02 | 0.41 |
| 1:A:3502:MSE:CE | 1:A:3517:SER:HB3 | 2.51 | 0.41 |
| 1:A:3529:ILE:HG22 | 1:A:3529:ILE:O | 2.21 | 0.41 |
| 1:A:3676:PRO:CG | 1:A:3677:PRO:HD3 | 2.50 | 0.41 |
| 1:A:3928:PHE:O | 1:A:3928:PHE:CD1 | 2.74 | 0.41 |
| 1:A:396:PHE:CE1 | 1:A:437:HIS:CD2 | 3.08 | 0.41 |
| 1:A:474:VAL:HG11 | 1:A:1564:SER:CB | 2.50 | 0.41 |
| 1:A:481:THR:HG22 | 1:A:482:VAL:N | 2.35 | 0.41 |
| 1:A:560:LEU:O | 1:A:563:LEU:N | 2.54 | 0.41 |
| 1:A:704:PHE:HA | 1:A:707:PHE:CG | 2.56 | 0.41 |
| 1:A:508:HIS:CD2 | 1:A:725:LEU:HD13 | 2.55 | 0.41 |
| 1:A:959:TYR:O | 1:A:963:LYS:CB | 2.62 | 0.41 |
| 1:A:980:THR:CG2 | 1:A:984:TYR:CE1 | 3.01 | 0.41 |
| 1:B:989:MSE:CG | 1:B:1031:ARG:NH1 | 2.83 | 0.41 |
| 1:B:1273:GLU:HG2 | 1:B:1276:VAL:HB | 2.02 | 0.41 |
| 1:B:1513:GLY:O | 1:B:1517:LEU:HG | 2.19 | 0.41 |
| 1:B:1909:ASN:ND2 | 1:B:1909:ASN:N | 2.69 | 0.41 |
| 1:B:1911:LEU:HD22 | 1:B:1916:ILE:HG21 | 2.03 | 0.41 |
| 1:B:1946:ASN:ND2 | 1:B:1993:GLU:OE2 | 2.40 | 0.41 |
| 1:B:1996:VAL:HG23 | 1:B:1997:PRO:CD | 2.51 | 0.41 |
| 1:B:2062:ALA:O | 1:B:2066:PHE:N | 2.53 | 0.41 |
| 1:B:2412:TYR:CG | 1:B:2412:TYR:O | 2.73 | 0.41 |
| 1:B:2565:MSE:SE | 1:B:2565:MSE:O | 2.88 | 0.41 |
| 1:B:2787:HIS:HB3 | 1:B:2790:LEU:HD12 | 2.02 | 0.41 |
| 1:B:2870:SER:HA | 1:B:2897:LEU:CD2 | 2.51 | 0.41 |
| 1:B:2975:ALA:C | 1:B:2977:ASN:N | 2.74 | 0.41 |
| 1:B:2925:GLU:HB3 | 1:B:3121:LEU:HD21 | 2.02 | 0.41 |
| 1:B:3136:THR:O | 1:B:3140:GLU:CB | 2.68 | 0.41 |
| 1:B:3259:LEU:HD11 | 1:B:3275:SER:O | 2.21 | 0.41 |
| 1:B:3291:GLN:O | 1:B:3294:SER:OG | 2.39 | 0.41 |
| 1:B:3492:CYS:HB2 | 1:B:3713:PRO:HG3 | 2.03 | 0.41 |
| 1:B:4002:MSE:O | 1:B:4006:VAL:HG13 | 2.21 | 0.41 |
| 1:B:4082:ARG:HG3 | 1:B:4091:ALA:CB | 2.37 | 0.41 |
| 1:B:752:LEU:HA | 1:B:755:ALA:CB | 2.50 | 0.41 |
| 1:A:1111:LEU:N | 1:A:1111:LEU:HD12 | 2.35 | 0.41 |
| 1:A:1894:SER:C | 1:A:1896:ILE:H | 2.24 | 0.41 |
| 1:A:2138:VAL:HB | 1:A:2139:PRO:HD3 | 2.03 | 0.41 |
| 1:A:2330:VAL:CG2 | 1:A:2338:GLU:HB3 | 2.35 | 0.41 |
| 1:A:2423:VAL:HG22 | 1:A:2424:MSE:N | 2.36 | 0.41 |
| 1:A:2640:UNK:O | 1:A:2641:UNK:C | 2.68 | 0.41 |
| 1:A:265:TYR:C | 1:A:268:PRO:HD2 | 2.40 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2999:LEU:HD12 | 1:A:3002:TYR:HE2 | 1.86 | 0.41 |
| 1:A:3048:LYS:HE2 | 1:A:3048:LYS:HB3 | 1.68 | 0.41 |
| 1:A:3190:LEU:O | 1:A:3194:GLU:HB2 | 2.21 | 0.41 |
| 1:A:4070:LYS:HB3 | 1:A:4073:ALA:HB3 | 2.02 | 0.41 |
| 1:B:1463:LEU:O | 1:B:1463:LEU:HD23 | 2.21 | 0.41 |
| 1:B:1548:GLY:O | 1:B:1552:HIS:ND1 | 2.53 | 0.41 |
| 1:B:1606:ARG:NH1 | 1:B:1806:ARG:HB3 | 2.36 | 0.41 |
| 1:B:1880:MSE:CE | 1:B:1884:LEU:HD11 | 2.51 | 0.41 |
| 1:B:1874:TYR:HD2 | 1:B:1885:PRO:HG3 | 1.85 | 0.41 |
| 1:B:2009:LYS:CG | 1:B:2010:GLU:H | 2.34 | 0.41 |
| 1:B:2083:LEU:HD23 | 1:B:2083:LEU:HA | 1.82 | 0.41 |
| 1:B:2164:TRP:CE3 | 1:B:2215:LEU:HG | 2.55 | 0.41 |
| 1:B:2367:VAL:O | 1:B:2371:PHE:HE1 | 2.04 | 0.41 |
| 1:B:2371:PHE:CG | 1:B:2372:PRO:HD3 | 2.56 | 0.41 |
| 1:B:2440:TYR:CE2 | 1:B:2443:MSE:SE | 3.24 | 0.41 |
| 1:B:2943:PHE:C | 1:B:2945:SER:N | 2.73 | 0.41 |
| 1:B:3031:TRP:CD2 | 1:B:3034:PRO:HD3 | 2.56 | 0.41 |
| 1:B:3148:GLN:NE2 | 1:B:3197:LEU:HD12 | 2.36 | 0.41 |
| 1:B:3839:TYR:CE1 | 1:B:3867:THR:HB | 2.29 | 0.41 |
| 1:B:46:SER:H | 1:B:51:LEU:CD1 | 2.34 | 0.41 |
| 1:B:476:ARG:HA | 1:B:479:ILE:HG13 | 2.03 | 0.41 |
| 1:B:634:LEU:CB | 1:B:638:GLN:HE22 | 2.32 | 0.41 |
| 1:B:70:ARG:NH2 | 1:B:79:ARG:HG2 | 2.35 | 0.41 |
| 1:B:911:LEU:O | 1:B:915:THR:HG23 | 2.20 | 0.41 |
| 1:A:1005:ASP:HB2 | 1:A:1006:THR:H | 1.63 | 0.41 |
| 1:A:995:PHE:HZ | 1:A:1006:THR:HG1 | 1.69 | 0.41 |
| 1:A:1013:ILE:HG21 | 1:A:1028:PHE:HB2 | 2.02 | 0.41 |
| 1:A:1147:LYS:CD | 1:A:1180:GLN:HG2 | 2.50 | 0.41 |
| 1:A:1369:MSE:CE | 1:A:1418:HIS:HB2 | 2.51 | 0.41 |
| 1:A:1431:LEU:HD11 | 1:A:1479:VAL:HG22 | 2.01 | 0.41 |
| 1:A:1938:ARG:O | 1:A:1941:HIS:HB3 | 2.21 | 0.41 |
| 1:A:2439:ILE:HG12 | 1:A:2442:MSE:CE | 2.51 | 0.41 |
| 1:A:2445:LYS:HD3 | 1:A:2445:LYS:HA | 1.78 | 0.41 |
| 1:A:2514:ASN:H | 1:A:2515:PRO:HD3 | 1.86 | 0.41 |
| 1:A:2884:LEU:HD12 | 1:A:2884:LEU:H | 1.86 | 0.41 |
| 1:A:2943:PHE:HE1 | 1:A:2984:GLY:HA2 | 1.86 | 0.41 |
| 1:A:3425:ARG:NH1 | 1:A:3999:THR:CG2 | 2.84 | 0.41 |
| 1:A:3567:VAL:HG22 | 1:A:3571:PHE:CZ | 2.56 | 0.41 |
| 1:A:3736:LYS:HD2 | 1:A:3752:VAL:HG21 | 2.03 | 0.41 |
| 1:A:3779:SER:O | 1:A:3782:SER:N | 2.54 | 0.41 |
| 1:A:3972:LEU:HD12 | 1:A:3974:MSE:CE | 2.51 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:100:ILE:O | 1:B:104:SER:HB3 | 2.20 | 0.41 |
| 1:B:1145:LEU:HD13 | 1:B:1149:LYS:HD3 | 2.02 | 0.41 |
| 1:B:1359:LEU:O | 1:B:1362:ASP:OD1 | 2.39 | 0.41 |
| 1:B:1374:GLN:HA | 1:B:1374:GLN:OE1 | 2.21 | 0.41 |
| 1:B:1583:MSE:HE3 | 1:B:1643:MSE:SE | 2.70 | 0.41 |
| 1:B:1949:ILE:O | 1:B:1952:ILE:HG22 | 2.20 | 0.41 |
| 1:B:1981:LEU:HA | 1:B:1984:LEU:HD23 | 2.01 | 0.41 |
| 1:B:2386:LEU:HD12 | 1:B:2404:ARG:HE | 1.84 | 0.41 |
| 1:B:3147:LYS:O | 1:B:3151:LEU:HG | 2.20 | 0.41 |
| 1:B:3155:VAL:HG21 | 1:B:3159:ARG:HH21 | 1.83 | 0.41 |
| 1:B:3231:ILE:HG23 | 1:B:3235:LYS:HE3 | 2.02 | 0.41 |
| 1:B:3319:ASN:ND2 | 1:B:3400:SER:HA | 2.35 | 0.41 |
| 1:B:3632:PHE:HE2 | 1:B:3683:CYS:SG | 2.43 | 0.41 |
| 1:B:3575:LEU:CD2 | 1:B:3687:MSE:SE | 3.18 | 0.41 |
| 1:B:3705:TYR:CD2 | 1:B:3792:SER:HB2 | 2.56 | 0.41 |
| 1:B:4106:CYS:O | 1:B:4108:MSE:N | 2.54 | 0.41 |
| 1:B:804:ALA:O | 1:B:806:SER:N | 2.53 | 0.41 |
| 1:B:922:SER:C | 1:B:924:ARG:N | 2.74 | 0.41 |
| 1:B:978:GLN:N | 1:B:981:ARG:HD3 | 2.34 | 0.41 |
| 1:A:1069:HIS:N | 1:A:1070:PRO:CD | 2.84 | 0.41 |
| 1:A:1385:ASN:O | 1:A:1388:ASP:N | 2.46 | 0.41 |
| 1:A:15:LEU:HA | 1:A:2359:LYS:NZ | 2.36 | 0.41 |
| 1:A:1874:TYR:CD2 | 1:A:1885:PRO:HG3 | 2.56 | 0.41 |
| 1:A:178:LEU:HB3 | 1:A:197:PHE:CE1 | 2.56 | 0.41 |
| 1:A:2165:LEU:HD11 | 1:A:2211:LEU:HD22 | 2.03 | 0.41 |
| 1:A:2239:LYS:CD | 1:A:2279:ILE:HD12 | 2.49 | 0.41 |
| 1:A:2646:UNK:CB | 1:A:2779:ASP:HA | 2.51 | 0.41 |
| 1:A:2797:VAL:HG23 | 1:A:2798:ALA:N | 2.36 | 0.41 |
| 1:A:2876:VAL:HG13 | 1:A:3035:PHE:CE1 | 2.56 | 0.41 |
| 1:A:295:GLU:HA | 1:A:298:LEU:HB2 | 2.02 | 0.41 |
| 1:A:298:LEU:O | 1:A:301:CYS:HB3 | 2.21 | 0.41 |
| 1:A:3027:LEU:HB3 | 1:A:3031:TRP:CZ2 | 2.56 | 0.41 |
| 1:A:3311:ASN:HB3 | 1:A:3312:VAL:H | 1.62 | 0.41 |
| 1:A:3356:ALA:HB2 | 1:A:3384:HIS:HB3 | 2.03 | 0.41 |
| 1:A:340:TYR:O | 1:A:344:GLN:HG3 | 2.21 | 0.41 |
| 1:A:3741:ARG:HG2 | 1:A:3741:ARG:HH11 | 1.84 | 0.41 |
| 1:A:3850:HIS:H | 1:A:3850:HIS:CD2 | 2.39 | 0.41 |
| 1:A:3887:PHE:O | 1:A:3890:MSE:HG2 | 2.20 | 0.41 |
| 1:B:1165:LEU:O | 1:B:1166:LEU:C | 2.60 | 0.41 |
| 1:B:1338:VAL:HA | 1:B:1341:ILE:HD12 | 2.03 | 0.41 |
| 1:B:153:PHE:CD1 | 1:B:154:SER:N | 2.88 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1752:LEU:C | 1:B:1754:GLN:H | 2.23 | 0.41 |
| 1:B:185:HIS:N | 1:B:186:PRO:HD2 | 2.27 | 0.41 |
| 1:B:2009:LYS:HE2 | 1:B:2012:ARG:HH11 | 1.86 | 0.41 |
| 1:B:214:GLU:HB3 | 1:B:215:PRO:HD2 | 2.02 | 0.41 |
| 1:B:2220:MSE:O | 1:B:2221:LYS:C | 2.59 | 0.41 |
| 1:B:175:TYR:CD2 | 1:B:222:GLY:HA3 | 2.54 | 0.41 |
| 1:B:2849:SER:O | 1:B:2850:PHE:CD1 | 2.74 | 0.41 |
| 1:B:3151:LEU:HA | 1:B:3152:SER:HA | 1.73 | 0.41 |
| 1:B:3186:ARG:HH11 | 1:B:3186:ARG:HG3 | 1.85 | 0.41 |
| 1:B:3292:GLY:HA2 | 1:B:3296:GLN:HG2 | 2.03 | 0.41 |
| 1:B:3503:VAL:HG22 | 1:B:3539:SER:CB | 2.51 | 0.41 |
| 1:B:3694:PHE:O | 1:B:3697:ASN:N | 2.54 | 0.41 |
| 1:B:3950:THR:OG1 | 1:B:4065:LEU:HD22 | 2.20 | 0.41 |
| 1:B:553:VAL:O | 1:B:556:SER:HB3 | 2.21 | 0.41 |
| 1:B:613:HIS:CG | 1:B:614:PRO:HD3 | 2.56 | 0.41 |
| 1:B:806:SER:O | 1:B:808:GLU:N | 2.54 | 0.41 |
| 1:B:850:GLU:CD | 1:B:854:ARG:NH2 | 2.75 | 0.41 |
| 1:A:960:GLN:CG | 1:A:1009:LEU:HD21 | 2.44 | 0.41 |
| 1:A:1342:MSE:HE3 | 1:A:1402:LEU:HD23 | 2.03 | 0.41 |
| 1:A:1678:LEU:O | 1:A:1681:ASP:OD1 | 2.38 | 0.41 |
| 1:A:1692:ALA:HA | 1:A:1695:LEU:HD12 | 2.02 | 0.41 |
| 1:A:1955:VAL:HA | 1:A:2003:LYS:NZ | 2.36 | 0.41 |
| 1:A:2256:ILE:CD1 | 1:A:2276:LEU:HD11 | 2.49 | 0.41 |
| 1:A:2442:MSE:O | 1:A:2451:LEU:HD21 | 2.21 | 0.41 |
| 1:A:2536:LEU:HA | 1:A:2536:LEU:HD23 | 1.81 | 0.41 |
| 1:A:2826:LEU:O | 1:A:2830:ASN:HB2 | 2.21 | 0.41 |
| 1:A:3174:ASP:N | 1:A:3175:PRO:CD | 2.84 | 0.41 |
| 1:A:3301:LEU:HB2 | 1:A:3328:ILE:HG21 | 2.03 | 0.41 |
| 1:A:3454:LEU:C | 1:A:3456:LEU:H | 2.25 | 0.41 |
| 1:A:3629:ARG:O | 1:A:3686:TRP:NE1 | 2.51 | 0.41 |
| 1:A:3630:ARG:HA | 1:A:3686:TRP:NE1 | 2.36 | 0.41 |
| 1:A:3683:CYS:O | 1:A:3687:MSE:HB2 | 2.21 | 0.41 |
| 1:A:34:LEU:HD11 | 1:A:38:LEU:HD11 | 2.03 | 0.41 |
| 1:A:591:GLN:HB3 | 1:A:1026:ARG:HD3 | 2.03 | 0.41 |
| 1:A:617:PRO:O | 1:A:659:ARG:HD2 | 2.21 | 0.41 |
| 1:A:671:SER:O | 1:A:675:ARG:HB2 | 2.21 | 0.41 |
| 1:A:776:TRP:CE2 | 1:A:780:ILE:HD12 | 2.55 | 0.41 |
| 1:A:846:ILE:HG23 | 1:A:854:ARG:HH12 | 1.86 | 0.41 |
| 1:B:1010:LEU:HD12 | 1:B:1011:GLU:H | 1.85 | 0.41 |
| 1:B:115:TYR:O | 1:B:118:ASP:HB3 | 2.21 | 0.41 |
| 1:B:1452:VAL:HG11 | 1:B:1502:SER:HB3 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:155:LYS:O | 1:B:159:GLU:HG3 | 2.21 | 0.41 |
| 1:B:2044:ASP:O | 1:B:2048:GLY:HA3 | 2.20 | 0.41 |
| 1:B:2795:GLN:O | 1:B:2799:GLN:HG2 | 2.21 | 0.41 |
| 1:B:2915:ARG:O | 1:B:2938:VAL:HG21 | 2.21 | 0.41 |
| 1:B:2991:LYS:O | 1:B:2995:GLU:HG2 | 2.21 | 0.41 |
| 1:B:3593:ARG:HD3 | 1:B:3663:THR:HG21 | 2.03 | 0.41 |
| 1:B:3600:PRO:C | 1:B:3602:ASN:N | 2.75 | 0.41 |
| 1:B:3601:VAL:O | 1:B:3605:ASN:HB2 | 2.21 | 0.41 |
| 1:B:3654:MSE:SE | 1:B:3659:PHE:CB | 3.17 | 0.41 |
| 1:B:3839:TYR:HB2 | 1:B:3871:PHE:CZ | 2.56 | 0.41 |
| 1:B:3920:ILE:CG1 | 1:B:3923:ARG:HD2 | 2.35 | 0.41 |
| 1:B:710:PHE:O | 1:B:711:GLY:C | 2.59 | 0.41 |
| 1:B:892:LEU:CD2 | 1:B:907:LEU:HD13 | 2.50 | 0.41 |
| 1:A:127:ALA:O | 1:A:131:LEU:CB | 2.69 | 0.40 |
| 1:A:1462:GLY:O | 1:A:1464:LEU:N | 2.54 | 0.40 |
| 1:A:1507:CYS:SG | 1:A:1508:LYS:HG2 | 2.61 | 0.40 |
| 1:A:1710:LEU:HD23 | 1:A:1710:LEU:HA | 1.68 | 0.40 |
| 1:A:1960:LYS:HG2 | 1:A:1963:GLN:OE1 | 2.20 | 0.40 |
| 1:A:197:PHE:O | 1:A:201:LEU:HG | 2.21 | 0.40 |
| 1:A:2120:ARG:NE | 1:A:2120:ARG:HA | 2.36 | 0.40 |
| 1:A:225:LYS:O | 1:A:228:SER:OG | 2.31 | 0.40 |
| 1:A:2775:TYR:N | 1:A:2775:TYR:CD1 | 2.89 | 0.40 |
| 1:A:2576:MSE:HE3 | 1:A:2788:SER:HB2 | 2.02 | 0.40 |
| 1:A:3024:PRO:N | 1:A:3025:PRO:CD | 2.84 | 0.40 |
| 1:A:3076:ALA:O | 1:A:3080:LEU:HG | 2.21 | 0.40 |
| 1:A:3065:ILE:HD13 | 1:A:3089:LEU:HD21 | 2.02 | 0.40 |
| 1:A:3008:TRP:HB2 | 1:A:3257:LYS:NZ | 2.36 | 0.40 |
| 1:A:3503:VAL:HG13 | 1:A:3504:ALA:H | 1.87 | 0.40 |
| 1:A:3636:PHE:O | 1:A:3640:PHE:HB2 | 2.21 | 0.40 |
| 1:A:3664:ASN:O | 1:A:3668:LEU:HB2 | 2.21 | 0.40 |
| 1:A:4059:ILE:HD13 | 1:A:4059:ILE:HG21 | 1.82 | 0.40 |
| 1:A:4066:LEU:HG | 1:A:4075:ARG:CA | 2.44 | 0.40 |
| 1:A:797:ASP:OD1 | 1:A:800:LEU:HD12 | 2.21 | 0.40 |
| 1:A:913:ARG:HE | 1:A:916:GLU:CD | 2.24 | 0.40 |
| 1:B:1032:CYS:O | 1:B:1035:GLU:N | 2.54 | 0.40 |
| 1:B:1142:HIS:C | 1:B:1144:SER:N | 2.73 | 0.40 |
| 1:B:1291:LEU:HB3 | 1:B:1292:LYS:H | 1.65 | 0.40 |
| 1:B:1426:GLN:O | 1:B:1430:GLU:HG3 | 2.21 | 0.40 |
| 1:B:1651:LYS:HB3 | 1:B:1680:ALA:HB1 | 2.02 | 0.40 |
| 1:B:2042:GLN:HG3 | 1:B:2046:SER:HB3 | 2.03 | 0.40 |
| 1:B:2226:PRO:HA | 1:B:2229:ALA:HB3 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2298:GLU:HB3 | 1:B:2301:GLN:HB3 | 2.03 | 0.40 |
| 1:B:2368:THR:HA | 1:B:2371:PHE:CE1 | 2.56 | 0.40 |
| 1:B:2374:LEU:O | 1:B:2374:LEU:HD12 | 2.21 | 0.40 |
| 1:B:2374:LEU:H | 1:B:2378:PHE:HE1 | 1.69 | 0.40 |
| 1:B:2481:HIS:CE1 | 1:B:2485:ARG:HD3 | 2.56 | 0.40 |
| 1:B:2852:PRO:O | 1:B:2855:VAL:HB | 2.22 | 0.40 |
| 1:B:281:GLN:HG3 | 1:B:326:MSE:HE1 | 2.02 | 0.40 |
| 1:B:4058:VAL:HG12 | 1:B:4061:CYS:HB3 | 2.03 | 0.40 |
| 1:B:783:HIS:C | 1:B:785:MSE:H | 2.24 | 0.40 |
| 1:B:805:LEU:H | 1:B:805:LEU:HG | 1.71 | 0.40 |
| 1:B:952:GLY:C | 1:B:954:GLY:H | 2.25 | 0.40 |
| 1:B:979:VAL:O | 1:B:982:GLN:HB3 | 2.21 | 0.40 |
| 1:A:1350:ASN:OD1 | 1:A:1405:ALA:HA | 2.20 | 0.40 |
| 1:A:1797:LEU:HA | 1:A:1797:LEU:HD23 | 1.83 | 0.40 |
| 1:A:2296:SER:OG | 1:A:2297:SER:N | 2.52 | 0.40 |
| 1:A:2260:PHE:CE2 | 1:A:2303:LEU:HA | 2.57 | 0.40 |
| 1:A:2308:SER:HA | 1:A:2352:HIS:NE2 | 2.36 | 0.40 |
| 1:A:2424:MSE:HA | 1:A:2436:LEU:CD1 | 2.51 | 0.40 |
| 1:A:979:VAL:HG21 | 1:A:2656:UNK:HA | 2.02 | 0.40 |
| 1:A:2882:ALA:HB1 | 1:A:2885:GLN:HB2 | 2.03 | 0.40 |
| 1:A:3052:LEU:HG | 1:A:3092:LEU:CD2 | 2.50 | 0.40 |
| 1:A:3125:ARG:HA | 1:A:3125:ARG:HD3 | 1.57 | 0.40 |
| 1:A:3811:THR:O | 1:A:3814:ASP:N | 2.54 | 0.40 |
| 1:A:385:TYR:CZ | 1:A:424:LEU:HD21 | 2.56 | 0.40 |
| 1:A:3880:ALA:HB1 | 1:A:3884:LYS:NZ | 2.36 | 0.40 |
| 1:A:463:LYS:O | 1:A:466:LEU:N | 2.54 | 0.40 |
| 1:A:513:GLU:HA | 1:A:653:LEU:HD21 | 2.03 | 0.40 |
| 1:A:654:ILE:CG2 | 1:A:729:CYS:HB2 | 2.51 | 0.40 |
| 1:A:757:LYS:HA | 1:A:760:LEU:HD11 | 2.01 | 0.40 |
| 1:A:766:ALA:O | 1:A:768:VAL:HG23 | 2.22 | 0.40 |
| 1:A:971:ARG:CG | 1:A:972:LEU:H | 2.27 | 0.40 |
| 1:B:104:SER:HA | 1:B:107:ILE:HD12 | 2.02 | 0.40 |
| 1:B:1087:ARG:CD | 1:B:1134:LEU:HB3 | 2.40 | 0.40 |
| 1:B:82:ARG:HD2 | 1:B:114:VAL:HG13 | 2.03 | 0.40 |
| 1:B:1229:CYS:SG | 1:B:1282:LEU:HG | 2.61 | 0.40 |
| 1:B:1357:LYS:HG3 | 1:B:1360:LYS:HZ1 | 1.86 | 0.40 |
| 1:B:1419:LEU:HD23 | 1:B:1419:LEU:HA | 1.81 | 0.40 |
| 1:B:1465:HIS:HA | 1:B:1469:PRO:CD | 2.51 | 0.40 |
| 1:B:2077:HIS:O | 1:B:2081:LEU:HG | 2.21 | 0.40 |
| 1:B:2200:ALA:O | 1:B:2204:GLY:N | 2.55 | 0.40 |
| 1:B:2349:LEU:HA | 1:B:2364:LEU:HD13 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:2480:ILE:HA | 1:B:2480:ILE:HD12 | 1.83 | 0.40 |
| 1:B:280:SER:C | 1:B:322:GLN:HG2 | 2.42 | 0.40 |
| 1:B:2939:LEU:HD11 | 1:B:2994:TRP:CZ3 | 2.56 | 0.40 |
| 1:B:2960:GLU:HG2 | 1:B:3289:ARG:HH22 | 1.86 | 0.40 |
| 1:B:3602:ASN:O | 1:B:3606:ILE:HB | 2.21 | 0.40 |
| 1:B:3824:GLU:HG2 | 1:B:3882:LEU:HD21 | 2.03 | 0.40 |
| 1:B:4063:GLU:O | 1:B:4066:LEU:HB2 | 2.20 | 0.40 |
| 1:B:487:LEU:O | 1:B:490:ILE:HG22 | 2.20 | 0.40 |
| 1:B:491:CYS:HB2 | 1:B:527:TYR:CD1 | 2.56 | 0.40 |
| 1:B:560:LEU:O | 1:B:563:LEU:N | 2.54 | 0.40 |
| 1:B:560:LEU:HA | 1:B:563:LEU:CG | 2.52 | 0.40 |
| 1:B:593:ASN:ND2 | 1:B:1084:ASN:HB2 | 2.37 | 0.40 |
| 1:B:86:LEU:HD13 | 1:B:134:LEU:CD2 | 2.52 | 0.40 |
| 1:B:934:LEU:HD21 | 1:B:962:TYR:OH | 2.22 | 0.40 |
| 1:A:1424:THR:HA | 1:A:1427:SER:HB2 | 2.02 | 0.40 |
| 1:A:1597:LEU:HA | 1:A:1600:MSE:HB2 | 2.03 | 0.40 |
| 1:A:1604:SER:OG | 1:A:1605:PHE:N | 2.54 | 0.40 |
| 1:A:178:LEU:HD13 | 1:A:197:PHE:CE1 | 2.57 | 0.40 |
| 1:A:2420:PHE:CZ | 1:A:2424:MSE:HG3 | 2.57 | 0.40 |
| 1:A:2531:LEU:HA | 1:A:2531:LEU:HD12 | 1.91 | 0.40 |
| 1:A:257:ARG:N | 1:A:258:PRO:HD2 | 2.37 | 0.40 |
| 1:A:294:PHE:CG | 1:A:295:GLU:N | 2.89 | 0.40 |
| 1:A:2960:GLU:O | 1:A:2965:TYR:CD1 | 2.74 | 0.40 |
| 1:A:294:PHE:O | 1:A:297:LEU:HG | 2.21 | 0.40 |
| 1:A:2989:ALA:O | 1:A:2993:PHE:N | 2.49 | 0.40 |
| 1:A:3173:MSE:HB3 | 1:A:3174:ASP:H | 1.58 | 0.40 |
| 1:A:2960:GLU:CG | 1:A:3289:ARG:HH22 | 2.34 | 0.40 |
| 1:A:3495:PHE:CE1 | 1:A:3521:ILE:HA | 2.56 | 0.40 |
| 1:A:3762:GLN:HE21 | 1:A:3763:ARG:HH11 | 1.67 | 0.40 |
| 1:A:3771:MSE:SE | 1:A:3991:PHE:CE1 | 3.24 | 0.40 |
| 1:A:4062:ASP:C | 1:A:4066:LEU:HD22 | 2.42 | 0.40 |
| 1:B:1014:LEU:HD23 | 1:B:1028:PHE:HE2 | 1.86 | 0.40 |
| 1:B:1741:ASP:HB3 | 1:B:1745:LYS:HE3 | 2.03 | 0.40 |
| 1:B:2088:LEU:HG | 1:B:2095:ALA:H | 1.87 | 0.40 |
| 1:B:2065:ARG:CZ | 1:B:2097:LEU:HD21 | 2.52 | 0.40 |
| 1:B:2957:LEU:HD22 | 1:B:3989:ARG:NH2 | 2.36 | 0.40 |
| 1:B:3356:ALA:CB | 1:B:3384:HIS:HB3 | 2.51 | 0.40 |
| 1:B:3447:VAL:HG21 | 1:B:3475:TYR:CE2 | 2.56 | 0.40 |
| 1:B:3479:THR:HG23 | 1:B:3480:LEU:HD23 | 2.03 | 0.40 |
| 1:B:3606:ILE:HG22 | 1:B:3610:TYR:CE2 | 2.56 | 0.40 |
| 1:B:3896:ALA:HA | 1:B:3899:ALA:HB3 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3907:SER:HB2 | 1:B:3937:VAL:H | 1.86 | 0.40 |
| 1:B:3964:THR:O | 1:B:3967:PHE:HB3 | 2.21 | 0.40 |
| 1:B:3974:MSE:HA | 1:B:3975:LYS:CB | 2.47 | 0.40 |
| 1:B:4055:ASN:HA | 1:B:4056:PRO:HD3 | 1.91 | 0.40 |
| 1:B:480:SER:O | 1:B:484:HIS:HB2 | 2.21 | 0.40 |
| 1:B:542:ASP:HA | 1:B:545:LEU:HD12 | 2.04 | 0.40 |
| 1:B:661:PRO:CG | 1:B:733:LEU:HA | 2.51 | 0.40 |
| 1:B:667:TYR:O | 1:B:669:LEU:N | 2.39 | 0.40 |
| 1:B:676:ASN:O | 1:B:680:ILE:HG13 | 2.21 | 0.40 |
| 1:B:75:SER:HA | 1:B:79:ARG:HG3 | 2.03 | 0.40 |
| 1:B:932:GLU:HB3 | 1:B:2794:LEU:CD1 | 2.45 | 0.40 |
| 1:A:1056:THR:O | 1:A:1059:LEU:HB2 | 2.22 | 0.40 |
| 1:A:1106:ILE:HA | 1:A:1109:GLU:HB3 | 2.04 | 0.40 |
| 1:A:1084:ASN:ND2 | 1:A:1131:ILE:HG22 | 2.33 | 0.40 |
| 1:A:136:GLN:HG2 | 1:A:139:ARG:NH1 | 2.37 | 0.40 |
| 1:A:1492:ALA:HB1 | 1:A:1493:PRO:HD2 | 2.02 | 0.40 |
| 1:A:1524:LEU:HG | 1:A:1559:PHE:CD1 | 2.56 | 0.40 |
| 1:A:1583:MSE:HB3 | 1:A:1584:GLN:H | 1.70 | 0.40 |
| 1:A:2142:ILE:O | 1:A:2145:PHE:HB2 | 2.22 | 0.40 |
| 1:A:2640:UNK:O | 1:A:2643:UNK:N | 2.54 | 0.40 |
| 1:A:286:LEU:HD22 | 1:A:290:TYR:HD2 | 1.87 | 0.40 |
| 1:A:3011:LEU:HD11 | 1:A:3043:TYR:C | 2.42 | 0.40 |
| 1:A:3448:GLU:O | 1:A:3451:LEU:HB2 | 2.21 | 0.40 |
| 1:A:3425:ARG:NH2 | 1:A:3467:ARG:HH12 | 2.18 | 0.40 |
| 1:A:3812:LEU:HD22 | 1:A:3928:PHE:CE1 | 2.57 | 0.40 |
| 1:A:3930:VAL:HA | 1:A:3937:VAL:HA | 2.02 | 0.40 |
| 1:A:396:PHE:CE1 | 1:A:437:HIS:NE2 | 2.90 | 0.40 |
| 1:B:1128:CYS:O | 1:B:1131:ILE:HG23 | 2.21 | 0.40 |
| 1:B:1682:THR:CB | 1:B:1724:MSE:SE | 3.18 | 0.40 |
| 1:B:2007:ILE:HD13 | 1:B:2007:ILE:HG21 | 1.72 | 0.40 |
| 1:B:2065:ARG:HD3 | 1:B:2100:LEU:HD11 | 2.02 | 0.40 |
| 1:B:2485:ARG:HH11 | 1:B:2530:ARG:NH2 | 2.18 | 0.40 |
| 1:B:262:LEU:HD22 | 1:B:306:VAL:CG1 | 2.51 | 0.40 |
| 1:B:2813:PHE:CD1 | 1:B:2814:SER:N | 2.90 | 0.40 |
| 1:B:3176:MSE:HG2 | 1:B:3249:GLN:HG2 | 2.03 | 0.40 |
| 1:B:3230:LEU:O | 1:B:3234:CYS:HB2 | 2.22 | 0.40 |
| 1:B:3564:GLN:C | 1:B:3566:GLY:N | 2.73 | 0.40 |
| 1:B:3736:LYS:HB2 | 1:B:3736:LYS:HE3 | 1.87 | 0.40 |
| 1:B:3860:LYS:O | 1:B:3864:ARG:HG3 | 2.22 | 0.40 |
| 1:B:3959:MSE:SE | 1:B:4124:TRP:CZ3 | 3.25 | 0.40 |
| 1:B:3981:TYR:HE1 | 1:B:4105:LYS:N | 2.19 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:410:MSE:HE3 | 1:B:410:MSE:HB3 | 1.84 | 0.40 |
| 1:B:435:LEU:HD12 | 1:B:436:GLU:N | 2.36 | 0.40 |
| 1:B:484:HIS:O | 1:B:488:ILE:HG23 | 2.22 | 0.40 |
| 1:B:506:GLU:O | 1:B:509:ARG:HG2 | 2.20 | 0.40 |
| 1:B:544:ILE:O | 1:B:546:ALA:N | 2.55 | 0.40 |
| 1:B:611:ASN:O | 1:B:614:PRO:HD2 | 2.20 | 0.40 |
| 1:B:742:GLU:HB3 | 1:B:783:HIS:CD2 | 2.56 | 0.40 |
| 1:B:763:THR:HB | 1:B:770:LEU:HD23 | 2.02 | 0.40 |
| 1:A:1639:LEU:HD12 | 1:A:1640:GLU:N | 2.37 | 0.40 |
| 1:A:1727:ARG:O | 1:A:1730:PRO:HD2 | 2.21 | 0.40 |
| 1:A:1602:ASP:HB2 | 1:A:1810:PRO:CB | 2.52 | 0.40 |
| 1:A:1916:ILE:HG23 | 1:A:1920:TYR:HE1 | 1.85 | 0.40 |
| 1:A:2065:ARG:CZ | 1:A:2097:LEU:HD21 | 2.50 | 0.40 |
| 1:A:2307:MSE:O | 1:A:2310:VAL:O | 2.40 | 0.40 |
| 1:A:2325:LEU:HD12 | 1:A:2325:LEU:HA | 1.82 | 0.40 |
| 1:A:2926:LEU:HB2 | 1:A:3123:GLN:CD | 2.42 | 0.40 |
| 1:A:3042:PRO:HA | 1:A:3045:ILE:CG1 | 2.49 | 0.40 |
| 1:A:3144:PHE:CZ | 1:A:3193:ILE:HD11 | 2.57 | 0.40 |
| 1:A:323:VAL:O | 1:A:327:VAL:CB | 2.66 | 0.40 |
| 1:A:2960:GLU:HG2 | 1:A:3252:PHE:CB | 2.51 | 0.40 |
| 1:A:3251:ASN:HD21 | 1:A:3254:LEU:HD22 | 1.87 | 0.40 |
| 1:A:2929:LEU:HD21 | 1:A:3784:ARG:HB3 | 2.04 | 0.40 |
| 1:A:882:SER:HB2 | 1:A:3892:THR:CB | 2.52 | 0.40 |
| 1:A:3933:GLU:C | 1:A:3935:GLY:H | 2.24 | 0.40 |
| 1:A:442:GLN:OE1 | 1:A:457:CYS:HB3 | 2.22 | 0.40 |
| 1:B:1017:ILE:HD12 | 1:B:1025:LEU:CD2 | 2.52 | 0.40 |
| 1:B:101:ALA:O | 1:B:104:SER:OG | 2.17 | 0.40 |
| 1:B:1353:PRO:HA | 1:B:1358:LEU:HB3 | 2.03 | 0.40 |
| 1:B:1571:LEU:HD13 | 1:B:1599:GLY:O | 2.21 | 0.40 |
| 1:B:1737:ASN:C | 1:B:1739:TYR:N | 2.73 | 0.40 |
| 1:B:1762:MSE:CB | 1:B:1896:ILE:HG12 | 2.48 | 0.40 |
| 1:B:1916:ILE:HG23 | 1:B:1920:TYR:HE1 | 1.85 | 0.40 |
| 1:B:2379:MSE:HE3 | 1:B:2383:PHE:HD1 | 1.87 | 0.40 |
| 1:B:2461:PHE:CE1 | 1:B:2462:VAL:HG23 | 2.57 | 0.40 |
| 1:B:2894:GLU:CD | 1:B:3973:PRO:HG2 | 2.41 | 0.40 |
| 1:B:2950:LYS:O | 1:B:2954:GLN:HB2 | 2.22 | 0.40 |
| 1:B:3159:ARG:C | 1:B:3161:LEU:H | 2.25 | 0.40 |
| 1:B:350:ARG:NH1 | 1:B:387:GLU:CD | 2.74 | 0.40 |
| 1:B:3605:ASN:HB3 | 1:B:3609:MSE:CE | 2.52 | 0.40 |
| 1:B:376:ILE:HG13 | 1:B:381:VAL:HG21 | 2.03 | 0.40 |
| 1:B:3775:LEU:HB3 | 1:B:3781:CYS:SG | 2.61 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:B:3870:SER:OG | 1:B:3871:PHE:N | 2.54 | 0.40 |
| 1:B:509:ARG:HB3 | 1:B:729:CYS:SG | 2.62 | 0.40 |
| 1:B:567:GLU:HB3 | 1:B:606:SER:HB2 | 2.04 | 0.40 |
| 1:B:869:ASN:O | 1:B:873:VAL:HG23 | 2.21 | 0.40 |
| 1:B:971:ARG:CG | 1:B:972:LEU:H | 2.29 | 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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|------------|----------|-------------|-----|
| 1 | A | 3631/4128 (88%) | 2664 (73%) | 724 (20%) | 243 (7%) | 1 | 18 |
| 1 | B | 3631/4128 (88%) | 2657 (73%) | 723 (20%) | 251 (7%) | 1 | 17 |
| 2 | K | 1/194 (0%) | 1 (100%) | 0 | 0 | 100 | 100 |
| 2 | S | 1/194 (0%) | 1 (100%) | 0 | 0 | 100 | 100 |
| All | All | 7264/8644 (84%) | 5323 (73%) | 1447 (20%) | 494 (7%) | 1 | 17 |

All (494) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 49 | ALA |
| 1 | A | 76 | ILE |
| 1 | A | 147 | PHE |
| 1 | A | 167 | PRO |
| 1 | A | 184 | VAL |
| 1 | A | 185 | HIS |
| 1 | A | 276 | ALA |
| 1 | A | 325 | ASN |
| 1 | A | 405 | ASP |
| 1 | A | 428 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 430 | VAL |
| 1 | A | 544 | ILE |
| 1 | A | 546 | ALA |
| 1 | A | 566 | ASP |
| 1 | A | 635 | PRO |
| 1 | A | 650 | SER |
| 1 | A | 742 | GLU |
| 1 | A | 755 | ALA |
| 1 | A | 767 | GLU |
| 1 | A | 885 | ALA |
| 1 | A | 897 | PRO |
| 1 | A | 903 | PRO |
| 1 | A | 905 | ILE |
| 1 | A | 958 | MSE |
| 1 | A | 1001 | PHE |
| 1 | A | 1005 | ASP |
| 1 | A | 1053 | PRO |
| 1 | A | 1094 | SER |
| 1 | A | 1110 | SER |
| 1 | A | 1141 | LYS |
| 1 | A | 1143 | VAL |
| 1 | A | 1271 | ILE |
| 1 | A | 1324 | PRO |
| 1 | A | 1425 | ALA |
| 1 | A | 1583 | MSE |
| 1 | A | 1591 | LYS |
| 1 | A | 1593 | VAL |
| 1 | A | 1733 | THR |
| 1 | A | 1746 | PHE |
| 1 | A | 1762 | MSE |
| 1 | A | 1978 | PHE |
| 1 | A | 2003 | LYS |
| 1 | A | 2012 | ARG |
| 1 | A | 2029 | SER |
| 1 | A | 2030 | TYR |
| 1 | A | 2058 | ASP |
| 1 | A | 2068 | ARG |
| 1 | A | 2069 | ARG |
| 1 | A | 2074 | PRO |
| 1 | A | 2075 | THR |
| 1 | A | 2126 | MSE |
| 1 | A | 2155 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 2177 | ASN |
| 1 | A | 2248 | CYS |
| 1 | A | 2261 | SER |
| 1 | A | 2286 | PRO |
| 1 | A | 2287 | PRO |
| 1 | A | 2290 | PRO |
| 1 | A | 2357 | GLU |
| 1 | A | 2373 | PRO |
| 1 | A | 2424 | MSE |
| 1 | A | 2464 | HIS |
| 1 | A | 2785 | ILE |
| 1 | A | 2878 | ALA |
| 1 | A | 2926 | LEU |
| 1 | A | 2927 | ALA |
| 1 | A | 3173 | MSE |
| 1 | A | 3313 | SER |
| 1 | A | 3345 | PRO |
| 1 | A | 3576 | ASP |
| 1 | A | 3600 | PRO |
| 1 | A | 3603 | LYS |
| 1 | A | 3688 | SER |
| 1 | A | 3716 | HIS |
| 1 | A | 3835 | PRO |
| 1 | A | 3933 | GLU |
| 1 | B | 76 | ILE |
| 1 | B | 167 | PRO |
| 1 | B | 184 | VAL |
| 1 | B | 185 | HIS |
| 1 | B | 238 | MSE |
| 1 | B | 260 | ILE |
| 1 | B | 276 | ALA |
| 1 | B | 395 | MSE |
| 1 | B | 405 | ASP |
| 1 | B | 430 | VAL |
| 1 | B | 540 | MSE |
| 1 | B | 546 | ALA |
| 1 | B | 566 | ASP |
| 1 | B | 635 | PRO |
| 1 | B | 670 | LEU |
| 1 | B | 742 | GLU |
| 1 | B | 746 | ARG |
| 1 | B | 767 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 784 | VAL |
| 1 | B | 871 | LEU |
| 1 | B | 885 | ALA |
| 1 | B | 897 | PRO |
| 1 | B | 903 | PRO |
| 1 | B | 923 | ASP |
| 1 | B | 1001 | PHE |
| 1 | B | 1005 | ASP |
| 1 | B | 1073 | PHE |
| 1 | B | 1093 | GLU |
| 1 | B | 1110 | SER |
| 1 | B | 1119 | LYS |
| 1 | B | 1122 | GLY |
| 1 | B | 1141 | LYS |
| 1 | B | 1143 | VAL |
| 1 | B | 1214 | GLU |
| 1 | B | 1271 | ILE |
| 1 | B | 1324 | PRO |
| 1 | B | 1408 | MSE |
| 1 | B | 1591 | LYS |
| 1 | B | 1762 | MSE |
| 1 | B | 1957 | ASN |
| 1 | B | 1974 | ASN |
| 1 | B | 1978 | PHE |
| 1 | B | 2012 | ARG |
| 1 | B | 2029 | SER |
| 1 | B | 2058 | ASP |
| 1 | B | 2068 | ARG |
| 1 | B | 2069 | ARG |
| 1 | B | 2074 | PRO |
| 1 | B | 2075 | THR |
| 1 | B | 2155 | GLU |
| 1 | B | 2156 | VAL |
| 1 | B | 2177 | ASN |
| 1 | B | 2248 | CYS |
| 1 | B | 2261 | SER |
| 1 | B | 2263 | LYS |
| 1 | B | 2286 | PRO |
| 1 | B | 2287 | PRO |
| 1 | B | 2290 | PRO |
| 1 | B | 2373 | PRO |
| 1 | B | 2424 | MSE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 2785 | ILE |
| 1 | B | 2878 | ALA |
| 1 | B | 2884 | LEU |
| 1 | B | 3240 | MSE |
| 1 | B | 3241 | LYS |
| 1 | B | 3313 | SER |
| 1 | B | 3340 | ALA |
| 1 | B | 3600 | PRO |
| 1 | B | 3603 | LYS |
| 1 | B | 3688 | SER |
| 1 | B | 3711 | PRO |
| 1 | B | 3835 | PRO |
| 1 | A | 97 | GLY |
| 1 | A | 169 | THR |
| 1 | A | 170 | VAL |
| 1 | A | 186 | PRO |
| 1 | A | 187 | SER |
| 1 | A | 260 | ILE |
| 1 | A | 602 | MSE |
| 1 | A | 608 | PRO |
| 1 | A | 746 | ARG |
| 1 | A | 772 | ALA |
| 1 | A | 871 | LEU |
| 1 | A | 923 | ASP |
| 1 | A | 957 | PRO |
| 1 | A | 1000 | LYS |
| 1 | A | 1075 | ARG |
| 1 | A | 1093 | GLU |
| 1 | A | 1112 | ALA |
| 1 | A | 1119 | LYS |
| 1 | A | 1122 | GLY |
| 1 | A | 1169 | VAL |
| 1 | A | 1214 | GLU |
| 1 | A | 1231 | GLN |
| 1 | A | 1237 | ALA |
| 1 | A | 1290 | LEU |
| 1 | A | 1590 | THR |
| 1 | A | 1700 | THR |
| 1 | A | 1724 | MSE |
| 1 | A | 1745 | LYS |
| 1 | A | 1934 | LEU |
| 1 | A | 1957 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1963 | GLN |
| 1 | A | 2002 | LYS |
| 1 | A | 2011 | ALA |
| 1 | A | 2016 | ASN |
| 1 | A | 2072 | ARG |
| 1 | A | 2168 | LEU |
| 1 | A | 2282 | ALA |
| 1 | A | 2423 | VAL |
| 1 | A | 2514 | ASN |
| 1 | A | 2824 | LYS |
| 1 | A | 2884 | LEU |
| 1 | A | 3311 | ASN |
| 1 | A | 3312 | VAL |
| 1 | A | 3340 | ALA |
| 1 | A | 3456 | LEU |
| 1 | A | 3575 | LEU |
| 1 | A | 3678 | GLY |
| 1 | A | 3973 | PRO |
| 1 | B | 325 | ASN |
| 1 | B | 394 | GLN |
| 1 | B | 428 | PRO |
| 1 | B | 545 | LEU |
| 1 | B | 654 | ILE |
| 1 | B | 671 | SER |
| 1 | B | 712 | LYS |
| 1 | B | 755 | ALA |
| 1 | B | 958 | MSE |
| 1 | B | 1053 | PRO |
| 1 | B | 1075 | ARG |
| 1 | B | 1094 | SER |
| 1 | B | 1290 | LEU |
| 1 | B | 1420 | ARG |
| 1 | B | 1425 | ALA |
| 1 | B | 1709 | GLU |
| 1 | B | 1733 | THR |
| 1 | B | 1811 | ARG |
| 1 | B | 2002 | LYS |
| 1 | B | 2030 | TYR |
| 1 | B | 2072 | ARG |
| 1 | B | 2168 | LEU |
| 1 | B | 2423 | VAL |
| 1 | B | 2570 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 2801 | ASP |
| 1 | B | 2824 | LYS |
| 1 | B | 2871 | LEU |
| 1 | B | 2926 | LEU |
| 1 | B | 2944 | THR |
| 1 | B | 3064 | PHE |
| 1 | B | 3242 | MSE |
| 1 | B | 3345 | PRO |
| 1 | B | 3403 | CYS |
| 1 | B | 3456 | LEU |
| 1 | B | 3499 | ILE |
| 1 | B | 3678 | GLY |
| 1 | B | 3826 | ALA |
| 1 | B | 3933 | GLU |
| 1 | A | 28 | ALA |
| 1 | A | 30 | ALA |
| 1 | A | 48 | PRO |
| 1 | A | 404 | ASP |
| 1 | A | 425 | ASP |
| 1 | A | 604 | PRO |
| 1 | A | 628 | GLU |
| 1 | A | 654 | ILE |
| 1 | A | 1045 | THR |
| 1 | A | 1077 | GLY |
| 1 | A | 1238 | GLN |
| 1 | A | 1289 | SER |
| 1 | A | 1408 | MSE |
| 1 | A | 1420 | ARG |
| 1 | A | 1722 | PHE |
| 1 | A | 1811 | ARG |
| 1 | A | 1962 | TYR |
| 1 | A | 2034 | SER |
| 1 | A | 2096 | PRO |
| 1 | A | 2206 | PRO |
| 1 | A | 2263 | LYS |
| 1 | A | 2280 | VAL |
| 1 | A | 2371 | PHE |
| 1 | A | 2823 | PHE |
| 1 | A | 2914 | ALA |
| 1 | A | 3314 | SER |
| 1 | A | 3545 | THR |
| 1 | A | 3598 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 3796 | MSE |
| 1 | A | 3826 | ALA |
| 1 | A | 3857 | LEU |
| 1 | A | 3978 | GLY |
| 1 | B | 27 | ALA |
| 1 | B | 48 | PRO |
| 1 | B | 101 | ALA |
| 1 | B | 125 | ILE |
| 1 | B | 144 | MSE |
| 1 | B | 186 | PRO |
| 1 | B | 257 | ARG |
| 1 | B | 368 | LEU |
| 1 | B | 404 | ASP |
| 1 | B | 425 | ASP |
| 1 | B | 513 | GLU |
| 1 | B | 650 | SER |
| 1 | B | 957 | PRO |
| 1 | B | 1215 | GLU |
| 1 | B | 1231 | GLN |
| 1 | B | 1237 | ALA |
| 1 | B | 1238 | GLN |
| 1 | B | 1492 | ALA |
| 1 | B | 1565 | GLU |
| 1 | B | 1583 | MSE |
| 1 | B | 1700 | THR |
| 1 | B | 1722 | PHE |
| 1 | B | 1917 | LYS |
| 1 | B | 2003 | LYS |
| 1 | B | 2011 | ALA |
| 1 | B | 2080 | VAL |
| 1 | B | 2096 | PRO |
| 1 | B | 2206 | PRO |
| 1 | B | 2357 | GLU |
| 1 | B | 2371 | PHE |
| 1 | B | 2465 | PRO |
| 1 | B | 2514 | ASN |
| 1 | B | 2575 | PRO |
| 1 | B | 2795 | GLN |
| 1 | B | 2823 | PHE |
| 1 | B | 2927 | ALA |
| 1 | B | 3174 | ASP |
| 1 | B | 3311 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 3601 | VAL |
| 1 | B | 3716 | HIS |
| 1 | B | 3796 | MSE |
| 1 | B | 4120 | THR |
| 1 | A | 27 | ALA |
| 1 | A | 125 | ILE |
| 1 | A | 257 | ARG |
| 1 | A | 277 | LEU |
| 1 | A | 515 | ARG |
| 1 | A | 543 | SER |
| 1 | A | 712 | LYS |
| 1 | A | 784 | VAL |
| 1 | A | 878 | GLU |
| 1 | A | 949 | PRO |
| 1 | A | 1073 | PHE |
| 1 | A | 1463 | LEU |
| 1 | A | 1492 | ALA |
| 1 | A | 1565 | GLU |
| 1 | A | 1647 | ALA |
| 1 | A | 1723 | PRO |
| 1 | A | 2010 | GLU |
| 1 | A | 2080 | VAL |
| 1 | A | 2176 | ASN |
| 1 | A | 2542 | LEU |
| 1 | A | 2795 | GLN |
| 1 | A | 2871 | LEU |
| 1 | A | 2873 | PRO |
| 1 | A | 2879 | GLY |
| 1 | A | 3064 | PHE |
| 1 | A | 3240 | MSE |
| 1 | A | 3443 | PRO |
| 1 | A | 3472 | ILE |
| 1 | A | 3760 | GLN |
| 1 | A | 3860 | LYS |
| 1 | B | 49 | ALA |
| 1 | B | 69 | VAL |
| 1 | B | 169 | THR |
| 1 | B | 277 | LEU |
| 1 | B | 411 | PRO |
| 1 | B | 604 | PRO |
| 1 | B | 910 | PHE |
| 1 | B | 947 | GLN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 1000 | LYS |
| 1 | B | 1045 | THR |
| 1 | B | 1069 | HIS |
| 1 | B | 1077 | GLY |
| 1 | B | 1112 | ALA |
| 1 | B | 1348 | LEU |
| 1 | B | 1590 | THR |
| 1 | B | 1723 | PRO |
| 1 | B | 1757 | MSE |
| 1 | B | 1891 | ALA |
| 1 | B | 1895 | LYS |
| 1 | B | 1934 | LEU |
| 1 | B | 1962 | TYR |
| 1 | B | 1987 | ARG |
| 1 | B | 2098 | THR |
| 1 | B | 2464 | HIS |
| 1 | B | 3075 | LYS |
| 1 | B | 3486 | GLU |
| 1 | B | 3497 | SER |
| 1 | B | 3637 | GLY |
| 1 | B | 3654 | MSE |
| 1 | B | 3720 | ALA |
| 1 | B | 3760 | GLN |
| 1 | B | 3847 | SER |
| 1 | B | 3860 | LYS |
| 1 | B | 3973 | PRO |
| 1 | A | 368 | LEU |
| 1 | A | 540 | MSE |
| 1 | A | 598 | PRO |
| 1 | A | 634 | LEU |
| 1 | A | 900 | GLU |
| 1 | A | 1069 | HIS |
| 1 | A | 1364 | CYS |
| 1 | A | 1510 | LEU |
| 1 | A | 1891 | ALA |
| 1 | A | 1895 | LYS |
| 1 | A | 2448 | PRO |
| 1 | A | 2465 | PRO |
| 1 | A | 2569 | SER |
| 1 | A | 2805 | ALA |
| 1 | A | 3091 | LEU |
| 1 | A | 3654 | MSE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 3720 | ALA |
| 1 | A | 3732 | LEU |
| 1 | A | 4058 | VAL |
| 1 | B | 30 | ALA |
| 1 | B | 74 | ASN |
| 1 | B | 745 | VAL |
| 1 | B | 763 | THR |
| 1 | B | 878 | GLU |
| 1 | B | 997 | ASN |
| 1 | B | 1071 | ASN |
| 1 | B | 1169 | VAL |
| 1 | B | 1247 | PRO |
| 1 | B | 1346 | THR |
| 1 | B | 1423 | ILE |
| 1 | B | 1593 | VAL |
| 1 | B | 1631 | SER |
| 1 | B | 1701 | SER |
| 1 | B | 1707 | LEU |
| 1 | B | 1812 | LEU |
| 1 | B | 1963 | GLN |
| 1 | B | 2016 | ASN |
| 1 | B | 2280 | VAL |
| 1 | B | 2289 | ASP |
| 1 | B | 2292 | CYS |
| 1 | B | 2879 | GLY |
| 1 | B | 2914 | ALA |
| 1 | B | 3129 | LEU |
| 1 | B | 3243 | ILE |
| 1 | B | 3312 | VAL |
| 1 | B | 3472 | ILE |
| 1 | B | 3978 | GLY |
| 1 | A | 74 | ASN |
| 1 | A | 298 | LEU |
| 1 | A | 627 | VAL |
| 1 | A | 763 | THR |
| 1 | A | 1520 | ALA |
| 1 | A | 2289 | ASP |
| 1 | A | 2942 | ILE |
| 1 | A | 3117 | ILE |
| 1 | A | 3317 | SER |
| 1 | A | 3499 | ILE |
| 1 | A | 3711 | PRO |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 3981 | TYR |
| 1 | B | 187 | SER |
| 1 | B | 298 | LEU |
| 1 | B | 323 | VAL |
| 1 | B | 427 | VAL |
| 1 | B | 627 | VAL |
| 1 | B | 718 | MSE |
| 1 | B | 748 | TYR |
| 1 | B | 1364 | CYS |
| 1 | B | 1738 | ASN |
| 1 | B | 2291 | GLN |
| 1 | B | 2873 | PRO |
| 1 | B | 2976 | LEU |
| 1 | B | 3443 | PRO |
| 1 | B | 4068 | HIS |
| 1 | A | 256 | ILE |
| 1 | A | 411 | PRO |
| 1 | A | 553 | VAL |
| 1 | A | 1637 | SER |
| 1 | A | 2076 | VAL |
| 1 | A | 2505 | VAL |
| 1 | A | 2552 | VAL |
| 1 | A | 2575 | PRO |
| 1 | A | 3025 | PRO |
| 1 | A | 3601 | VAL |
| 1 | B | 50 | VAL |
| 1 | B | 67 | VAL |
| 1 | B | 170 | VAL |
| 1 | B | 2552 | VAL |
| 1 | B | 4058 | VAL |
| 1 | A | 50 | VAL |
| 1 | A | 69 | VAL |
| 1 | A | 1382 | ILE |
| 1 | A | 2156 | VAL |
| 1 | A | 3174 | ASP |
| 1 | B | 948 | MSE |
| 1 | B | 1382 | ILE |
| 1 | B | 2448 | PRO |
| 1 | B | 3331 | GLY |
| 1 | A | 67 | VAL |
| 1 | A | 381 | VAL |
| 1 | A | 447 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 2059 | PRO |
| 1 | A | 2230 | VAL |
| 1 | A | 2324 | GLY |
| 1 | A | 3919 | GLY |
| 1 | B | 381 | VAL |
| 1 | B | 495 | VAL |
| 1 | B | 2230 | VAL |
| 1 | B | 2569 | SER |
| 1 | B | 3919 | GLY |
| 1 | A | 1247 | PRO |
| 1 | A | 1729 | PHE |
| 1 | B | 174 | VAL |
| 1 | B | 544 | ILE |
| 1 | B | 884 | VAL |
| 1 | B | 905 | ILE |
| 1 | B | 1637 | SER |
| 1 | B | 2804 | ILE |
| 1 | A | 1468 | LEU |
| 1 | A | 3178 | ILE |
| 1 | B | 256 | ILE |
| 1 | B | 2802 | PRO |
| 1 | B | 2942 | ILE |

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 X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1 | A | 3259/3384 (96%) | 3089 (95%) | 170 (5%) | 23 | 50 |
| 1 | B | 3259/3384 (96%) | 3084 (95%) | 175 (5%) | 22 | 50 |
| 2 | K | - | 1 (100%) | 0 | 100 | 100 |
| 2 | S | - | 1 (100%) | 0 | 100 | 100 |
| All | All | 6520/6768 (96%) | 6175 (95%) | 345 (5%) | 22 | 50 |

All (345) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 143 | LEU |
| 1 | A | 156 | PHE |
| 1 | A | 274 | LEU |
| 1 | A | 277 | LEU |
| 1 | A | 294 | PHE |
| 1 | A | 326 | MSE |
| 1 | A | 342 | MSE |
| 1 | A | 360 | SER |
| 1 | A | 361 | ILE |
| 1 | A | 368 | LEU |
| 1 | A | 392 | CYS |
| 1 | A | 393 | LYS |
| 1 | A | 396 | PHE |
| 1 | A | 405 | ASP |
| 1 | A | 420 | VAL |
| 1 | A | 444 | ASP |
| 1 | A | 445 | SER |
| 1 | A | 446 | PHE |
| 1 | A | 556 | SER |
| 1 | A | 559 | SER |
| 1 | A | 564 | LEU |
| 1 | A | 595 | ASP |
| 1 | A | 603 | ILE |
| 1 | A | 612 | LEU |
| 1 | A | 620 | PHE |
| 1 | A | 625 | ASN |
| 1 | A | 630 | CYS |
| 1 | A | 631 | ARG |
| 1 | A | 754 | MSE |
| 1 | A | 763 | THR |
| 1 | A | 793 | LEU |
| 1 | A | 858 | MSE |
| 1 | A | 866 | ILE |
| 1 | A | 879 | MSE |
| 1 | A | 884 | VAL |
| 1 | A | 891 | ARG |
| 1 | A | 898 | PHE |
| 1 | A | 907 | LEU |
| 1 | A | 924 | ARG |
| 1 | A | 939 | MSE |
| 1 | A | 963 | LYS |
| 1 | A | 965 | THR |
| 1 | A | 966 | PHE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 970 | LEU |
| 1 | A | 975 | ASP |
| 1 | A | 983 | LEU |
| 1 | A | 988 | VAL |
| 1 | A | 989 | MSE |
| 1 | A | 993 | HIS |
| 1 | A | 1005 | ASP |
| 1 | A | 1010 | LEU |
| 1 | A | 1014 | LEU |
| 1 | A | 1017 | ILE |
| 1 | A | 1024 | THR |
| 1 | A | 1068 | LEU |
| 1 | A | 1070 | PRO |
| 1 | A | 1105 | VAL |
| 1 | A | 1107 | TYR |
| 1 | A | 1108 | MSE |
| 1 | A | 1121 | LEU |
| 1 | A | 1131 | ILE |
| 1 | A | 1180 | GLN |
| 1 | A | 1288 | SER |
| 1 | A | 1291 | LEU |
| 1 | A | 1347 | THR |
| 1 | A | 1364 | CYS |
| 1 | A | 1372 | LEU |
| 1 | A | 1403 | MSE |
| 1 | A | 1430 | GLU |
| 1 | A | 1444 | ASP |
| 1 | A | 1507 | CYS |
| 1 | A | 1526 | GLU |
| 1 | A | 1583 | MSE |
| 1 | A | 1590 | THR |
| 1 | A | 1592 | MSE |
| 1 | A | 1597 | LEU |
| 1 | A | 1600 | MSE |
| 1 | A | 1640 | GLU |
| 1 | A | 1643 | MSE |
| 1 | A | 1721 | HIS |
| 1 | A | 1737 | ASN |
| 1 | A | 1743 | MSE |
| 1 | A | 1757 | MSE |
| 1 | A | 1758 | LEU |
| 1 | A | 1759 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 1761 | LEU |
| 1 | A | 1812 | LEU |
| 1 | A | 1883 | ARG |
| 1 | A | 1886 | LYS |
| 1 | A | 1919 | CYS |
| 1 | A | 1942 | CYS |
| 1 | A | 1947 | CYS |
| 1 | A | 1950 | SER |
| 1 | A | 1959 | LEU |
| 1 | A | 1986 | ARG |
| 1 | A | 1993 | GLU |
| 1 | A | 1998 | MSE |
| 1 | A | 2012 | ARG |
| 1 | A | 2104 | MSE |
| 1 | A | 2155 | GLU |
| 1 | A | 2189 | ILE |
| 1 | A | 2239 | LYS |
| 1 | A | 2241 | LEU |
| 1 | A | 2245 | TRP |
| 1 | A | 2277 | LEU |
| 1 | A | 2287 | PRO |
| 1 | A | 2307 | MSE |
| 1 | A | 2330 | VAL |
| 1 | A | 2337 | LEU |
| 1 | A | 2338 | GLU |
| 1 | A | 2355 | THR |
| 1 | A | 2362 | VAL |
| 1 | A | 2370 | SER |
| 1 | A | 2402 | LEU |
| 1 | A | 2404 | ARG |
| 1 | A | 2473 | MSE |
| 1 | A | 2555 | LEU |
| 1 | A | 2568 | MSE |
| 1 | A | 2574 | ASN |
| 1 | A | 2788 | SER |
| 1 | A | 2886 | GLN |
| 1 | A | 2890 | ILE |
| 1 | A | 2921 | LEU |
| 1 | A | 2943 | PHE |
| 1 | A | 2991 | LYS |
| 1 | A | 3011 | LEU |
| 1 | A | 3050 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 3051 | LEU |
| 1 | A | 3084 | GLN |
| 1 | A | 3145 | ILE |
| 1 | A | 3173 | MSE |
| 1 | A | 3256 | MSE |
| 1 | A | 3278 | GLN |
| 1 | A | 3283 | LEU |
| 1 | A | 3326 | GLN |
| 1 | A | 3416 | LEU |
| 1 | A | 3451 | LEU |
| 1 | A | 3481 | SER |
| 1 | A | 3509 | ASP |
| 1 | A | 3518 | VAL |
| 1 | A | 3575 | LEU |
| 1 | A | 3636 | PHE |
| 1 | A | 3641 | ASP |
| 1 | A | 3670 | MSE |
| 1 | A | 3687 | MSE |
| 1 | A | 3706 | ASP |
| 1 | A | 3729 | MSE |
| 1 | A | 3771 | MSE |
| 1 | A | 3781 | CYS |
| 1 | A | 3810 | VAL |
| 1 | A | 3811 | THR |
| 1 | A | 3813 | LYS |
| 1 | A | 3824 | GLU |
| 1 | A | 3831 | ASP |
| 1 | A | 3846 | MSE |
| 1 | A | 3883 | LEU |
| 1 | A | 3893 | SER |
| 1 | A | 3895 | GLU |
| 1 | A | 3926 | ASN |
| 1 | A | 3928 | PHE |
| 1 | A | 3929 | MSE |
| 1 | A | 3944 | HIS |
| 1 | A | 3959 | MSE |
| 1 | A | 3963 | LEU |
| 1 | A | 3964 | THR |
| 1 | A | 3967 | PHE |
| 1 | A | 4066 | LEU |
| 1 | A | 4078 | VAL |
| 1 | A | 4104 | VAL |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 4128 | MSE |
| 1 | B | 42 | CYS |
| 1 | B | 111 | CYS |
| 1 | B | 143 | LEU |
| 1 | B | 145 | ASP |
| 1 | B | 156 | PHE |
| 1 | B | 274 | LEU |
| 1 | B | 298 | LEU |
| 1 | B | 322 | GLN |
| 1 | B | 360 | SER |
| 1 | B | 361 | ILE |
| 1 | B | 368 | LEU |
| 1 | B | 389 | ILE |
| 1 | B | 393 | LYS |
| 1 | B | 395 | MSE |
| 1 | B | 396 | PHE |
| 1 | B | 405 | ASP |
| 1 | B | 408 | TYR |
| 1 | B | 410 | MSE |
| 1 | B | 420 | VAL |
| 1 | B | 444 | ASP |
| 1 | B | 446 | PHE |
| 1 | B | 487 | LEU |
| 1 | B | 491 | CYS |
| 1 | B | 559 | SER |
| 1 | B | 564 | LEU |
| 1 | B | 603 | ILE |
| 1 | B | 612 | LEU |
| 1 | B | 620 | PHE |
| 1 | B | 633 | ILE |
| 1 | B | 653 | LEU |
| 1 | B | 666 | PHE |
| 1 | B | 733 | LEU |
| 1 | B | 741 | ILE |
| 1 | B | 763 | THR |
| 1 | B | 793 | LEU |
| 1 | B | 865 | GLN |
| 1 | B | 898 | PHE |
| 1 | B | 901 | MSE |
| 1 | B | 924 | ARG |
| 1 | B | 963 | LYS |
| 1 | B | 965 | THR |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 966 | PHE |
| 1 | B | 970 | LEU |
| 1 | B | 989 | MSE |
| 1 | B | 993 | HIS |
| 1 | B | 1000 | LYS |
| 1 | B | 1005 | ASP |
| 1 | B | 1009 | LEU |
| 1 | B | 1010 | LEU |
| 1 | B | 1017 | ILE |
| 1 | B | 1024 | THR |
| 1 | B | 1036 | PHE |
| 1 | B | 1070 | PRO |
| 1 | B | 1108 | MSE |
| 1 | B | 1121 | LEU |
| 1 | B | 1131 | ILE |
| 1 | B | 1287 | GLN |
| 1 | B | 1347 | THR |
| 1 | B | 1354 | GLU |
| 1 | B | 1372 | LEU |
| 1 | B | 1392 | MSE |
| 1 | B | 1399 | CYS |
| 1 | B | 1430 | GLU |
| 1 | B | 1471 | GLN |
| 1 | B | 1507 | CYS |
| 1 | B | 1583 | MSE |
| 1 | B | 1590 | THR |
| 1 | B | 1597 | LEU |
| 1 | B | 1602 | ASP |
| 1 | B | 1639 | LEU |
| 1 | B | 1725 | GLN |
| 1 | B | 1733 | THR |
| 1 | B | 1743 | MSE |
| 1 | B | 1758 | LEU |
| 1 | B | 1759 | LEU |
| 1 | B | 1761 | LEU |
| 1 | B | 1802 | TYR |
| 1 | B | 1812 | LEU |
| 1 | B | 1819 | PHE |
| 1 | B | 1858 | LEU |
| 1 | B | 1909 | ASN |
| 1 | B | 1927 | MSE |
| 1 | B | 1930 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 1942 | CYS |
| 1 | B | 1950 | SER |
| 1 | B | 1959 | LEU |
| 1 | B | 1973 | LYS |
| 1 | B | 1974 | ASN |
| 1 | B | 1976 | LEU |
| 1 | B | 1986 | ARG |
| 1 | B | 1993 | GLU |
| 1 | B | 1998 | MSE |
| 1 | B | 1999 | GLU |
| 1 | B | 2012 | ARG |
| 1 | B | 2023 | SER |
| 1 | B | 2104 | MSE |
| 1 | B | 2126 | MSE |
| 1 | B | 2155 | GLU |
| 1 | B | 2239 | LYS |
| 1 | B | 2245 | TRP |
| 1 | B | 2265 | PRO |
| 1 | B | 2277 | LEU |
| 1 | B | 2287 | PRO |
| 1 | B | 2325 | LEU |
| 1 | B | 2330 | VAL |
| 1 | B | 2338 | GLU |
| 1 | B | 2355 | THR |
| 1 | B | 2362 | VAL |
| 1 | B | 2370 | SER |
| 1 | B | 2374 | LEU |
| 1 | B | 2402 | LEU |
| 1 | B | 2481 | HIS |
| 1 | B | 2555 | LEU |
| 1 | B | 2559 | THR |
| 1 | B | 2576 | MSE |
| 1 | B | 2776 | ARG |
| 1 | B | 2788 | SER |
| 1 | B | 2820 | MSE |
| 1 | B | 2865 | HIS |
| 1 | B | 2886 | GLN |
| 1 | B | 2890 | ILE |
| 1 | B | 2921 | LEU |
| 1 | B | 2929 | LEU |
| 1 | B | 2943 | PHE |
| 1 | B | 2991 | LYS |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 3044 | MSE |
| 1 | B | 3050 | LYS |
| 1 | B | 3051 | LEU |
| 1 | B | 3058 | ASP |
| 1 | B | 3118 | ASP |
| 1 | B | 3120 | LEU |
| 1 | B | 3133 | GLN |
| 1 | B | 3145 | ILE |
| 1 | B | 3155 | VAL |
| 1 | B | 3238 | MSE |
| 1 | B | 3242 | MSE |
| 1 | B | 3258 | LEU |
| 1 | B | 3282 | ARG |
| 1 | B | 3283 | LEU |
| 1 | B | 3311 | ASN |
| 1 | B | 3397 | GLN |
| 1 | B | 3403 | CYS |
| 1 | B | 3416 | LEU |
| 1 | B | 3450 | MSE |
| 1 | B | 3451 | LEU |
| 1 | B | 3467 | ARG |
| 1 | B | 3509 | ASP |
| 1 | B | 3518 | VAL |
| 1 | B | 3636 | PHE |
| 1 | B | 3641 | ASP |
| 1 | B | 3763 | ARG |
| 1 | B | 3782 | SER |
| 1 | B | 3796 | MSE |
| 1 | B | 3810 | VAL |
| 1 | B | 3813 | LYS |
| 1 | B | 3820 | MSE |
| 1 | B | 3835 | PRO |
| 1 | B | 3846 | MSE |
| 1 | B | 3856 | MSE |
| 1 | B | 3858 | MSE |
| 1 | B | 3883 | LEU |
| 1 | B | 3895 | GLU |
| 1 | B | 3904 | PHE |
| 1 | B | 3926 | ASN |
| 1 | B | 3944 | HIS |
| 1 | B | 3959 | MSE |
| 1 | B | 3963 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | B | 3970 | LEU |
| 1 | B | 4016 | PHE |
| 1 | B | 4020 | MSE |
| 1 | B | 4029 | GLN |
| 1 | B | 4066 | LEU |
| 1 | B | 4090 | ARG |
| 1 | B | 4104 | VAL |
| 1 | B | 4119 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | A | 233 | ASN |
| 1 | A | 334 | HIS |
| 1 | A | 508 | HIS |
| 1 | A | 783 | HIS |
| 1 | A | 1069 | HIS |
| 1 | A | 1083 | ASN |
| 1 | A | 1146 | ASN |
| 1 | A | 1385 | ASN |
| 1 | A | 1418 | HIS |
| 1 | A | 1457 | GLN |
| 1 | A | 1459 | HIS |
| 1 | A | 1476 | HIS |
| 1 | A | 1574 | ASN |
| 1 | A | 1687 | HIS |
| 1 | A | 1725 | GLN |
| 1 | A | 1754 | GLN |
| 1 | A | 1890 | HIS |
| 1 | A | 2170 | GLN |
| 1 | A | 2177 | ASN |
| 1 | A | 2183 | HIS |
| 1 | A | 2234 | ASN |
| 1 | A | 2426 | HIS |
| 1 | A | 2518 | GLN |
| 1 | A | 3003 | ASN |
| 1 | A | 3081 | HIS |
| 1 | A | 3122 | HIS |
| 1 | A | 3251 | ASN |
| 1 | A | 3291 | GLN |
| 1 | A | 3319 | ASN |
| 1 | A | 3501 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 3524 | ASN |
| 1 | A | 3762 | GLN |
| 1 | A | 3927 | ASN |
| 1 | A | 3951 | GLN |
| 1 | A | 4068 | HIS |
| 1 | B | 390 | GLN |
| 1 | B | 409 | GLN |
| 1 | B | 437 | HIS |
| 1 | B | 442 | GLN |
| 1 | B | 508 | HIS |
| 1 | B | 593 | ASN |
| 1 | B | 990 | GLN |
| 1 | B | 993 | HIS |
| 1 | B | 1055 | ASN |
| 1 | B | 1238 | GLN |
| 1 | B | 1350 | ASN |
| 1 | B | 1476 | HIS |
| 1 | B | 1574 | ASN |
| 1 | B | 1687 | HIS |
| 1 | B | 1866 | GLN |
| 1 | B | 1890 | HIS |
| 1 | B | 1897 | ASN |
| 1 | B | 1974 | ASN |
| 1 | B | 2077 | HIS |
| 1 | B | 2177 | ASN |
| 1 | B | 2348 | GLN |
| 1 | B | 2365 | ASN |
| 1 | B | 2481 | HIS |
| 1 | B | 2518 | GLN |
| 1 | B | 3251 | ASN |
| 1 | B | 3459 | ASN |
| 1 | B | 3494 | GLN |
| 1 | B | 3524 | ASN |
| 1 | B | 3772 | ASN |
| 1 | B | 3908 | HIS |
| 1 | B | 3926 | ASN |
| 1 | B | 4018 | GLN |
| 1 | B | 4110 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1 | B | 1 |
| 1 | A | 1 |
| 2 | K | 1 |
| 2 | S | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | K | 133:UNK | C | 201:UNK | N | 46.74 |
| 1 | S | 133:UNK | C | 201:UNK | N | 41.40 |
| 1 | B | 3794:VAL | C | 3795:PRO | N | 1.18 |
| 1 | A | 1069:HIS | C | 1070:PRO | N | 1.15 |

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 1 | A | 3551/4128 (86%) | 0.25 | 220 (6%) 20 17 | 83, 248, 332, 443 | 0 |
| 1 | B | 3551/4128 (86%) | 0.30 | 240 (6%) 17 14 | 117, 251, 358, 507 | 0 |
| 2 | K | 0/194 | - | - | - | - |
| 2 | S | 0/194 | - | - | - | - |
| All | All | 7102/8644 (82%) | 0.28 | 460 (6%) 18 15 | 83, 249, 343, 507 | 0 |

All (460) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 122 | LYS | 12.8 |
| 1 | B | 31 | GLY | 9.6 |
| 1 | B | 1355 | GLY | 9.6 |
| 1 | B | 145 | ASP | 9.1 |
| 1 | A | 126 | PRO | 8.7 |
| 1 | A | 123 | CYS | 8.6 |
| 1 | A | 1290 | LEU | 8.2 |
| 1 | B | 586 | GLN | 8.2 |
| 1 | A | 1286 | ALA | 8.1 |
| 1 | A | 1763 | THR | 7.7 |
| 1 | B | 3026 | ASP | 7.5 |
| 1 | A | 1287 | GLN | 7.5 |
| 1 | A | 121 | ALA | 7.4 |
| 1 | B | 30 | ALA | 7.2 |
| 1 | B | 3358 | ARG | 6.9 |
| 1 | A | 1289 | SER | 6.7 |
| 1 | B | 215 | PRO | 6.7 |
| 1 | B | 3023 | ASN | 6.6 |
| 1 | A | 1523 | GLY | 6.6 |
| 1 | A | 2910 | VAL | 6.4 |
| 1 | B | 24 | ARG | 6.4 |
| 1 | A | 1285 | GLU | 6.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 215 | PRO | 6.4 |
| 1 | A | 589 | GLY | 6.3 |
| 1 | A | 953 | GLN | 6.3 |
| 1 | B | 25 | CYS | 6.2 |
| 1 | B | 153 | PHE | 6.2 |
| 1 | B | 3029 | LYS | 6.2 |
| 1 | B | 2263 | LYS | 6.1 |
| 1 | A | 590 | GLU | 6.1 |
| 1 | B | 1357 | LYS | 6.1 |
| 1 | B | 3025 | PRO | 6.0 |
| 1 | B | 3033 | GLU | 6.0 |
| 1 | B | 3028 | ASN | 6.0 |
| 1 | A | 2906 | PRO | 5.9 |
| 1 | B | 3027 | LEU | 5.9 |
| 1 | B | 22 | ALA | 5.8 |
| 1 | A | 1761 | LEU | 5.7 |
| 1 | A | 2898 | LEU | 5.6 |
| 1 | B | 100 | ILE | 5.6 |
| 1 | B | 3515 | GLN | 5.6 |
| 1 | A | 125 | ILE | 5.5 |
| 1 | A | 2202 | PRO | 5.5 |
| 1 | A | 124 | LYS | 5.4 |
| 1 | A | 2113 | GLY | 5.3 |
| 1 | A | 2905 | LEU | 5.3 |
| 1 | B | 280 | SER | 5.1 |
| 1 | A | 3152 | SER | 5.0 |
| 1 | A | 503 | SER | 5.0 |
| 1 | A | 3403 | CYS | 4.9 |
| 1 | B | 32 | HIS | 4.9 |
| 1 | B | 3359 | ILE | 4.9 |
| 1 | A | 1288 | SER | 4.9 |
| 1 | A | 3029 | LYS | 4.9 |
| 1 | B | 3153 | SER | 4.8 |
| 1 | A | 2897 | LEU | 4.7 |
| 1 | B | 26 | GLY | 4.7 |
| 1 | B | 3528 | ALA | 4.7 |
| 1 | B | 2900 | LEU | 4.7 |
| 1 | B | 2430 | GLU | 4.6 |
| 1 | B | 3675 | LYS | 4.6 |
| 1 | A | 950 | GLU | 4.6 |
| 1 | A | 237 | SER | 4.6 |
| 1 | A | 2900 | LEU | 4.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | B | 23 | ASP | 4.6 |
| 1 | B | 1044 | ILE | 4.6 |
| 1 | B | 10 | CYS | 4.5 |
| 1 | B | 253 | LEU | 4.5 |
| 1 | A | 3402 | SER | 4.4 |
| 1 | B | 1761 | LEU | 4.4 |
| 1 | A | 3510 | GLN | 4.4 |
| 1 | B | 125 | ILE | 4.4 |
| 1 | A | 2250 | SER | 4.4 |
| 1 | A | 127 | ALA | 4.3 |
| 1 | B | 3152 | SER | 4.3 |
| 1 | B | 495 | VAL | 4.3 |
| 1 | A | 2183 | HIS | 4.3 |
| 1 | A | 2821 | ASP | 4.3 |
| 1 | B | 1763 | THR | 4.3 |
| 1 | A | 3311 | ASN | 4.3 |
| 1 | A | 670 | LEU | 4.3 |
| 1 | A | 951 | GLY | 4.3 |
| 1 | B | 3976 | GLU | 4.3 |
| 1 | B | 257 | ARG | 4.3 |
| 1 | A | 3308 | ASP | 4.2 |
| 1 | B | 3499 | ILE | 4.2 |
| 1 | B | 3024 | PRO | 4.1 |
| 1 | B | 3020 | ASP | 4.1 |
| 1 | B | 3406 | ALA | 4.1 |
| 1 | B | 1286 | ALA | 4.1 |
| 1 | B | 72 | SER | 4.1 |
| 1 | B | 3074 | GLN | 4.1 |
| 1 | A | 2985 | GLU | 4.1 |
| 1 | B | 279 | ALA | 4.1 |
| 1 | A | 1284 | THR | 4.1 |
| 1 | B | 1856 | THR | 4.1 |
| 1 | B | 582 | THR | 4.1 |
| 1 | B | 126 | PRO | 4.0 |
| 1 | A | 280 | SER | 4.0 |
| 1 | A | 216 | LYS | 4.0 |
| 1 | A | 128 | LEU | 4.0 |
| 1 | A | 2868 | LEU | 4.0 |
| 1 | A | 2203 | THR | 4.0 |
| 1 | B | 3623 | PRO | 3.9 |
| 1 | A | 952 | GLY | 3.9 |
| 1 | B | 216 | LYS | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 1589 | ASN | 3.9 |
| 1 | A | 3272 | TRP | 3.9 |
| 1 | B | 123 | CYS | 3.9 |
| 1 | A | 3478 | GLU | 3.8 |
| 1 | A | 2782 | ASP | 3.8 |
| 1 | A | 3509 | ASP | 3.8 |
| 1 | B | 27 | ALA | 3.8 |
| 1 | A | 171 | LEU | 3.8 |
| 1 | A | 897 | PRO | 3.8 |
| 1 | B | 2116 | ASP | 3.8 |
| 1 | A | 3357 | ARG | 3.8 |
| 1 | A | 3196 | LYS | 3.8 |
| 1 | A | 671 | SER | 3.7 |
| 1 | A | 1489 | LYS | 3.7 |
| 1 | B | 122 | LYS | 3.7 |
| 1 | B | 1354 | GLU | 3.7 |
| 1 | B | 3676 | PRO | 3.7 |
| 1 | A | 3150 | ASN | 3.6 |
| 1 | A | 956 | PRO | 3.6 |
| 1 | A | 2984 | GLY | 3.6 |
| 1 | A | 2986 | PRO | 3.6 |
| 1 | A | 3269 | ARG | 3.6 |
| 1 | A | 3317 | SER | 3.6 |
| 1 | B | 1043 | GLN | 3.6 |
| 1 | B | 4039 | TYR | 3.6 |
| 1 | A | 588 | VAL | 3.6 |
| 1 | A | 1357 | LYS | 3.5 |
| 1 | A | 3199 | PRO | 3.5 |
| 1 | A | 591 | GLN | 3.5 |
| 1 | A | 1673 | THR | 3.5 |
| 1 | B | 154 | SER | 3.5 |
| 1 | A | 3358 | ARG | 3.5 |
| 1 | A | 3149 | GLY | 3.5 |
| 1 | B | 3405 | PRO | 3.5 |
| 1 | B | 116 | THR | 3.5 |
| 1 | A | 153 | PHE | 3.5 |
| 1 | B | 542 | ASP | 3.5 |
| 1 | A | 3515 | GLN | 3.5 |
| 1 | B | 157 | TYR | 3.4 |
| 1 | B | 1287 | GLN | 3.4 |
| 1 | A | 506 | GLU | 3.4 |
| 1 | A | 2201 | THR | 3.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | B | 1671 | VAL | 3.4 |
| 1 | B | 2942 | ILE | 3.4 |
| 1 | B | 1356 | TRP | 3.4 |
| 1 | A | 214 | GLU | 3.3 |
| 1 | B | 2175 | GLU | 3.3 |
| 1 | B | 628 | GLU | 3.3 |
| 1 | A | 129 | ASP | 3.3 |
| 1 | B | 2067 | ARG | 3.3 |
| 1 | B | 668 | LYS | 3.3 |
| 1 | B | 3936 | GLY | 3.3 |
| 1 | A | 1526 | GLU | 3.3 |
| 1 | B | 2981 | TRP | 3.3 |
| 1 | A | 2978 | LYS | 3.3 |
| 1 | A | 2527 | HIS | 3.3 |
| 1 | B | 631 | ARG | 3.2 |
| 1 | B | 190 | ILE | 3.2 |
| 1 | B | 213 | ARG | 3.2 |
| 1 | B | 3056 | GLU | 3.2 |
| 1 | B | 2980 | ASP | 3.2 |
| 1 | A | 1436 | LEU | 3.1 |
| 1 | B | 3550 | LYS | 3.1 |
| 1 | B | 3035 | PHE | 3.1 |
| 1 | B | 4082 | ARG | 3.1 |
| 1 | B | 3355 | LYS | 3.1 |
| 1 | A | 1586 | SER | 3.1 |
| 1 | A | 739 | ASN | 3.1 |
| 1 | A | 2867 | ALA | 3.1 |
| 1 | A | 2308 | SER | 3.1 |
| 1 | B | 2464 | HIS | 3.1 |
| 1 | B | 3514 | VAL | 3.1 |
| 1 | B | 92 | PHE | 3.1 |
| 1 | B | 3674 | SER | 3.1 |
| 1 | A | 2988 | GLU | 3.1 |
| 1 | A | 892 | LEU | 3.1 |
| 1 | B | 3510 | GLN | 3.1 |
| 1 | B | 3624 | GLY | 3.1 |
| 1 | A | 2197 | THR | 3.1 |
| 1 | B | 1290 | LEU | 3.0 |
| 1 | B | 2264 | ASP | 3.0 |
| 1 | A | 3098 | ARG | 3.0 |
| 1 | B | 2090 | ARG | 3.0 |
| 1 | A | 3153 | SER | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 1435 | ASN | 3.0 |
| 1 | A | 2068 | ARG | 3.0 |
| 1 | B | 14 | ARG | 3.0 |
| 1 | A | 157 | TYR | 3.0 |
| 1 | A | 2444 | PRO | 3.0 |
| 1 | B | 3809 | THR | 3.0 |
| 1 | A | 252 | VAL | 3.0 |
| 1 | B | 265 | TYR | 3.0 |
| 1 | B | 3540 | TYR | 3.0 |
| 1 | A | 3102 | TYR | 3.0 |
| 1 | B | 104 | SER | 3.0 |
| 1 | B | 2533 | SER | 2.9 |
| 1 | B | 627 | VAL | 2.9 |
| 1 | B | 1672 | PHE | 2.9 |
| 1 | A | 604 | PRO | 2.9 |
| 1 | A | 2267 | SER | 2.9 |
| 1 | A | 120 | ALA | 2.9 |
| 1 | A | 2980 | ASP | 2.9 |
| 1 | A | 3700 | GLU | 2.9 |
| 1 | A | 2907 | ALA | 2.9 |
| 1 | B | 86 | LEU | 2.9 |
| 1 | B | 103 | TYR | 2.9 |
| 1 | B | 101 | ALA | 2.9 |
| 1 | A | 505 | SER | 2.9 |
| 1 | B | 2822 | LYS | 2.9 |
| 1 | A | 213 | ARG | 2.9 |
| 1 | A | 1488 | TYR | 2.9 |
| 1 | A | 3026 | ASP | 2.9 |
| 1 | B | 124 | LYS | 2.8 |
| 1 | A | 355 | ASN | 2.8 |
| 1 | A | 809 | THR | 2.8 |
| 1 | A | 18 | THR | 2.8 |
| 1 | B | 1437 | TYR | 2.8 |
| 1 | A | 1604 | SER | 2.8 |
| 1 | A | 896 | VAL | 2.8 |
| 1 | A | 3976 | GLU | 2.8 |
| 1 | B | 950 | GLU | 2.8 |
| 1 | A | 81 | CYS | 2.8 |
| 1 | B | 585 | ILE | 2.8 |
| 1 | B | 3070 | HIS | 2.8 |
| 1 | A | 3273 | LEU | 2.8 |
| 1 | A | 259 | GLN | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | B | 3841 | ASP | 2.8 |
| 1 | A | 2496 | GLN | 2.8 |
| 1 | B | 908 | ASP | 2.8 |
| 1 | B | 3830 | SER | 2.8 |
| 1 | B | 262 | LEU | 2.8 |
| 1 | B | 2078 | ASP | 2.8 |
| 1 | B | 3822 | GLN | 2.8 |
| 1 | B | 3879 | PRO | 2.8 |
| 1 | B | 472 | GLY | 2.8 |
| 1 | A | 2899 | ARG | 2.8 |
| 1 | B | 35 | ILE | 2.8 |
| 1 | A | 1522 | GLY | 2.7 |
| 1 | B | 2427 | ARG | 2.7 |
| 1 | B | 3341 | LEU | 2.7 |
| 1 | B | 21 | ALA | 2.7 |
| 1 | A | 513 | GLU | 2.7 |
| 1 | A | 781 | ASP | 2.7 |
| 1 | B | 71 | LYS | 2.7 |
| 1 | A | 3633 | ILE | 2.7 |
| 1 | B | 1548 | GLY | 2.7 |
| 1 | B | 1822 | ARG | 2.7 |
| 1 | B | 2411 | LEU | 2.7 |
| 1 | A | 3312 | VAL | 2.7 |
| 1 | A | 3624 | GLY | 2.7 |
| 1 | B | 34 | LEU | 2.7 |
| 1 | B | 330 | ASN | 2.7 |
| 1 | B | 59 | PHE | 2.7 |
| 1 | B | 3486 | GLU | 2.7 |
| 1 | A | 1699 | PHE | 2.7 |
| 1 | A | 2975 | ALA | 2.7 |
| 1 | A | 3828 | TYR | 2.7 |
| 1 | B | 115 | TYR | 2.7 |
| 1 | B | 191 | ASN | 2.7 |
| 1 | A | 3404 | GLY | 2.7 |
| 1 | B | 2930 | TYR | 2.7 |
| 1 | A | 3318 | LYS | 2.6 |
| 1 | B | 2412 | TYR | 2.6 |
| 1 | A | 782 | ARG | 2.6 |
| 1 | B | 252 | VAL | 2.6 |
| 1 | B | 2898 | LEU | 2.6 |
| 1 | B | 2176 | ASN | 2.6 |
| 1 | B | 2390 | HIS | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 1698 | PHE | 2.6 |
| 1 | A | 2208 | ASP | 2.6 |
| 1 | B | 3432 | SER | 2.6 |
| 1 | B | 1101 | PHE | 2.6 |
| 1 | B | 2465 | PRO | 2.6 |
| 1 | B | 146 | GLU | 2.6 |
| 1 | B | 3553 | GLU | 2.6 |
| 1 | A | 3603 | LYS | 2.6 |
| 1 | B | 3580 | ASN | 2.6 |
| 1 | B | 4115 | ASN | 2.6 |
| 1 | B | 2899 | ARG | 2.6 |
| 1 | A | 890 | LYS | 2.6 |
| 1 | B | 38 | LEU | 2.6 |
| 1 | A | 2421 | VAL | 2.5 |
| 1 | B | 4081 | ALA | 2.5 |
| 1 | B | 3875 | GLU | 2.5 |
| 1 | A | 3875 | GLU | 2.5 |
| 1 | B | 1732 | GLY | 2.5 |
| 1 | A | 1558 | TYR | 2.5 |
| 1 | B | 1816 | ARG | 2.5 |
| 1 | B | 3828 | TYR | 2.5 |
| 1 | A | 3443 | PRO | 2.5 |
| 1 | B | 183 | GLU | 2.5 |
| 1 | B | 11 | SER | 2.5 |
| 1 | B | 1284 | THR | 2.5 |
| 1 | B | 2081 | LEU | 2.5 |
| 1 | A | 1907 | GLU | 2.5 |
| 1 | B | 1002 | GLU | 2.5 |
| 1 | B | 1799 | GLU | 2.5 |
| 1 | A | 2781 | PRO | 2.5 |
| 1 | B | 877 | ASP | 2.5 |
| 1 | B | 3549 | HIS | 2.5 |
| 1 | B | 1426 | GLN | 2.5 |
| 1 | B | 99 | LYS | 2.4 |
| 1 | A | 2263 | LYS | 2.4 |
| 1 | A | 3393 | GLU | 2.4 |
| 1 | B | 494 | PRO | 2.4 |
| 1 | A | 543 | SER | 2.4 |
| 1 | A | 62 | ASP | 2.4 |
| 1 | A | 3695 | LEU | 2.4 |
| 1 | B | 2461 | PHE | 2.4 |
| 1 | A | 3698 | GLU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | B | 1509 | GLN | 2.4 |
| 1 | A | 2259 | LYS | 2.4 |
| 1 | A | 80 | GLU | 2.4 |
| 1 | A | 2114 | GLU | 2.4 |
| 1 | B | 1255 | CYS | 2.4 |
| 1 | B | 2905 | LEU | 2.4 |
| 1 | A | 593 | ASN | 2.4 |
| 1 | A | 3629 | ARG | 2.4 |
| 1 | B | 20 | SER | 2.4 |
| 1 | B | 2084 | GLU | 2.4 |
| 1 | A | 2893 | LEU | 2.4 |
| 1 | B | 68 | PHE | 2.4 |
| 1 | B | 2821 | ASP | 2.4 |
| 1 | A | 3627 | ALA | 2.4 |
| 1 | A | 3159 | ARG | 2.4 |
| 1 | A | 262 | LEU | 2.4 |
| 1 | B | 1589 | ASN | 2.4 |
| 1 | A | 3300 | VAL | 2.4 |
| 1 | B | 3105 | ASN | 2.4 |
| 1 | B | 3346 | ALA | 2.3 |
| 1 | B | 583 | LEU | 2.3 |
| 1 | A | 3879 | PRO | 2.3 |
| 1 | B | 3380 | ARG | 2.3 |
| 1 | A | 587 | THR | 2.3 |
| 1 | B | 2904 | GLU | 2.3 |
| 1 | A | 799 | TYR | 2.3 |
| 1 | A | 3610 | TYR | 2.3 |
| 1 | A | 2461 | PHE | 2.3 |
| 1 | A | 3326 | GLN | 2.3 |
| 1 | B | 3500 | SER | 2.3 |
| 1 | A | 2979 | GLN | 2.3 |
| 1 | B | 136 | GLN | 2.3 |
| 1 | A | 2869 | LEU | 2.3 |
| 1 | A | 4092 | GLN | 2.3 |
| 1 | A | 3052 | LEU | 2.3 |
| 1 | B | 2077 | HIS | 2.3 |
| 1 | A | 119 | ARG | 2.3 |
| 1 | B | 82 | ARG | 2.3 |
| 1 | B | 2488 | GLU | 2.3 |
| 1 | A | 2195 | SER | 2.3 |
| 1 | B | 60 | SER | 2.3 |
| 1 | B | 1051 | LYS | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 194 | GLU | 2.3 |
| 1 | A | 2440 | TYR | 2.3 |
| 1 | B | 2486 | ASP | 2.3 |
| 1 | A | 3708 | ARG | 2.3 |
| 1 | B | 1350 | ASN | 2.3 |
| 1 | B | 1138 | ILE | 2.3 |
| 1 | B | 3546 | SER | 2.3 |
| 1 | B | 28 | ALA | 2.3 |
| 1 | A | 2492 | ASP | 2.3 |
| 1 | A | 1788 | ARG | 2.3 |
| 1 | A | 2909 | ARG | 2.3 |
| 1 | B | 2943 | PHE | 2.3 |
| 1 | B | 150 | GLY | 2.2 |
| 1 | A | 3105 | ASN | 2.2 |
| 1 | A | 27 | ALA | 2.2 |
| 1 | B | 516 | THR | 2.2 |
| 1 | B | 2184 | TYR | 2.2 |
| 1 | A | 2464 | HIS | 2.2 |
| 1 | A | 3405 | PRO | 2.2 |
| 1 | B | 167 | PRO | 2.2 |
| 1 | A | 1277 | GLY | 2.2 |
| 1 | A | 2939 | LEU | 2.2 |
| 1 | B | 1020 | PRO | 2.2 |
| 1 | B | 2491 | THR | 2.2 |
| 1 | B | 2986 | PRO | 2.2 |
| 1 | A | 514 | VAL | 2.2 |
| 1 | A | 580 | ASP | 2.2 |
| 1 | B | 2391 | GLY | 2.2 |
| 1 | A | 2067 | ARG | 2.2 |
| 1 | B | 2201 | THR | 2.2 |
| 1 | B | 3551 | ASN | 2.2 |
| 1 | B | 47 | SER | 2.2 |
| 1 | B | 4118 | GLY | 2.2 |
| 1 | A | 356 | ASN | 2.2 |
| 1 | A | 585 | ILE | 2.2 |
| 1 | A | 3630 | ARG | 2.2 |
| 1 | B | 63 | PHE | 2.2 |
| 1 | B | 81 | CYS | 2.2 |
| 1 | A | 3406 | ALA | 2.2 |
| 1 | B | 3199 | PRO | 2.2 |
| 1 | B | 3350 | GLU | 2.2 |
| 1 | A | 3007 | GLU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | A | 2333 | ARG | 2.2 |
| 1 | B | 867 | ASN | 2.2 |
| 1 | A | 3382 | PHE | 2.2 |
| 1 | B | 117 | LYS | 2.2 |
| 1 | B | 738 | HIS | 2.2 |
| 1 | B | 3489 | SER | 2.2 |
| 1 | A | 3310 | ASN | 2.2 |
| 1 | B | 1512 | SER | 2.2 |
| 1 | A | 3696 | ARG | 2.2 |
| 1 | A | 582 | THR | 2.2 |
| 1 | B | 341 | PHE | 2.1 |
| 1 | A | 1506 | SER | 2.1 |
| 1 | A | 3058 | ASP | 2.1 |
| 1 | B | 3407 | ALA | 2.1 |
| 1 | B | 95 | LYS | 2.1 |
| 1 | A | 3197 | LEU | 2.1 |
| 1 | A | 3400 | SER | 2.1 |
| 1 | B | 1675 | TYR | 2.1 |
| 1 | A | 3493 | TRP | 2.1 |
| 1 | A | 672 | ILE | 2.1 |
| 1 | A | 2112 | GLN | 2.1 |
| 1 | A | 3849 | LYS | 2.1 |
| 1 | A | 3252 | PHE | 2.1 |
| 1 | A | 3476 | PRO | 2.1 |
| 1 | B | 1818 | SER | 2.1 |
| 1 | B | 3373 | VAL | 2.1 |
| 1 | A | 3439 | LEU | 2.1 |
| 1 | B | 579 | LEU | 2.1 |
| 1 | B | 1052 | SER | 2.1 |
| 1 | A | 1088 | GLU | 2.1 |
| 1 | B | 676 | ASN | 2.1 |
| 1 | B | 1442 | GLN | 2.1 |
| 1 | A | 2082 | GLU | 2.1 |
| 1 | B | 132 | ILE | 2.1 |
| 1 | B | 1031 | ARG | 2.1 |
| 1 | B | 37 | GLY | 2.1 |
| 1 | B | 3527 | GLN | 2.1 |
| 1 | B | 1471 | GLN | 2.1 |
| 1 | B | 2308 | SER | 2.1 |
| 1 | A | 61 | ARG | 2.0 |
| 1 | B | 3625 | LEU | 2.0 |
| 1 | A | 803 | SER | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 3104 | GLN | 2.0 |
| 1 | B | 29 | LEU | 2.0 |
| 1 | B | 2174 | SER | 2.0 |
| 1 | A | 1437 | TYR | 2.0 |
| 1 | A | 63 | PHE | 2.0 |
| 1 | A | 3699 | LEU | 2.0 |
| 1 | A | 130 | LEU | 2.0 |
| 1 | A | 1463 | LEU | 2.0 |
| 1 | B | 1360 | LYS | 2.0 |
| 1 | A | 3604 | LYS | 2.0 |
| 1 | B | 3975 | LYS | 2.0 |
| 1 | B | 79 | ARG | 2.0 |
| 1 | B | 3617 | LEU | 2.0 |
| 1 | B | 258 | PRO | 2.0 |
| 1 | A | 2430 | GLU | 2.0 |
| 1 | A | 4093 | GLU | 2.0 |
| 1 | B | 868 | LYS | 2.0 |
| 1 | B | 3622 | ALA | 2.0 |

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.