# Full wwPDB EM Validation Report ⓘ

Nov 14, 2023 – 12:50 PM EST

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|---|---|---|
| PDB ID | : | 8UXE |
| EMDB ID | : | EMD-42761 |
| Title | : | Structure of PKA phosphorylated human RyR2-R420Q in the closed state in the presence of ARM210 |
| Authors | : | Miotto, M.C.; Marks, A.R. |
| Deposited on | : | 2023-11-09 |
| Resolution | : | 3.53 Å(reported) |
| Based on initial model | : | 7UA5 |

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

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

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

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

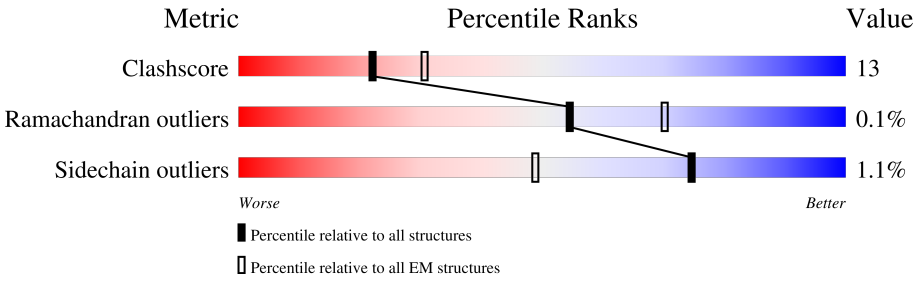
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.53 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 108 | 75% 23% |
| 1 | F | 108 | 74% 24% |
| 1 | G | 108 | 74% 24% |
| 1 | H | 108 | 74% 24% |
| 2 | A | 4967 | 12% 61% 23% 15% |
| 2 | B | 4967 | 12% 61% 23% 15% |
| 2 | C | 4967 | 12% 61% 23% 15% |
| 2 | D | 4967 | 12% 61% 23% 15% |

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 138692 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called Ryanodine receptor 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 4224 | Total | C | N | O | S | 2 | 0 |
| | | | 33769 | 21515 | 5743 | 6281 | 230 | | |
| 2 | B | 4224 | Total | C | N | O | S | 2 | 0 |
| | | | 33769 | 21515 | 5743 | 6281 | 230 | | |
| 2 | C | 4224 | Total | C | N | O | S | 2 | 0 |
| | | | 33769 | 21515 | 5743 | 6281 | 230 | | |
| 2 | D | 4224 | Total | C | N | O | S | 2 | 0 |
| | | | 33769 | 21515 | 5743 | 6281 | 230 | | |

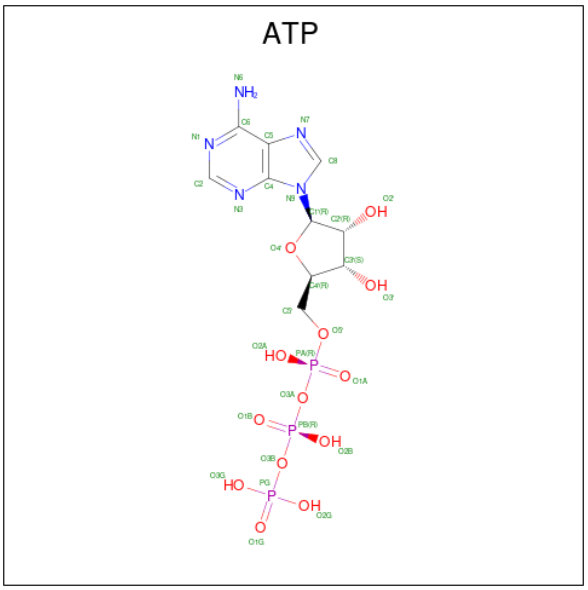
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 420 | GLN | ARG | conflict | UNP Q92736 |
| B | 420 | GLN | ARG | conflict | UNP Q92736 |
| C | 420 | GLN | ARG | conflict | UNP Q92736 |
| D | 420 | GLN | ARG | conflict | UNP Q92736 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 3 | A | 1 | Total Zn<br>1 1 | 0 |
| 3 | B | 1 | Total Zn<br>1 1 | 0 |
| 3 | C | 1 | Total Zn<br>1 1 | 0 |
| 3 | D | 1 | Total Zn<br>1 1 | 0 |

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 4 | A | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | A | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | B | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | B | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | C | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | C | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 4 | D | 1 | Total C N O P<br>31 10 5 13 3 | 0 |

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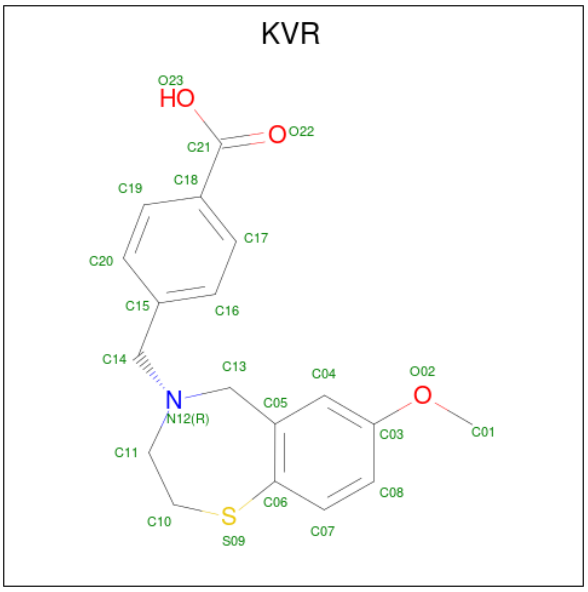
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 4 | D | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: $C_{18}H_{19}NO_3S$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 5 | A | 1 | Total | C | N | O | S | 0 |
| | | | 23 | 18 | 1 | 3 | 1 | |
| 5 | B | 1 | Total | C | N | O | S | 0 |
| | | | 23 | 18 | 1 | 3 | 1 | |
| 5 | C | 1 | Total | C | N | O | S | 0 |
| | | | 23 | 18 | 1 | 3 | 1 | |
| 5 | D | 1 | Total | C | N | O | S | 0 |
| | | | 23 | 18 | 1 | 3 | 1 | |

# 3 Residue-property plots (i)

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

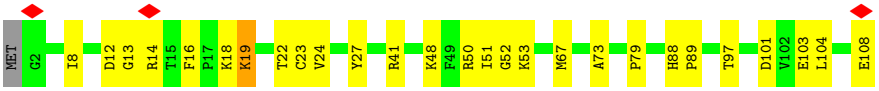
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



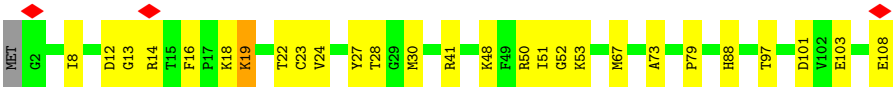
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:

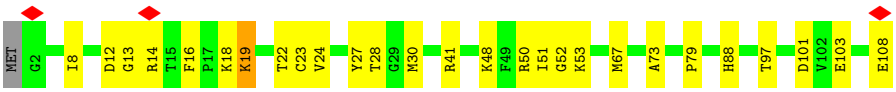

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:

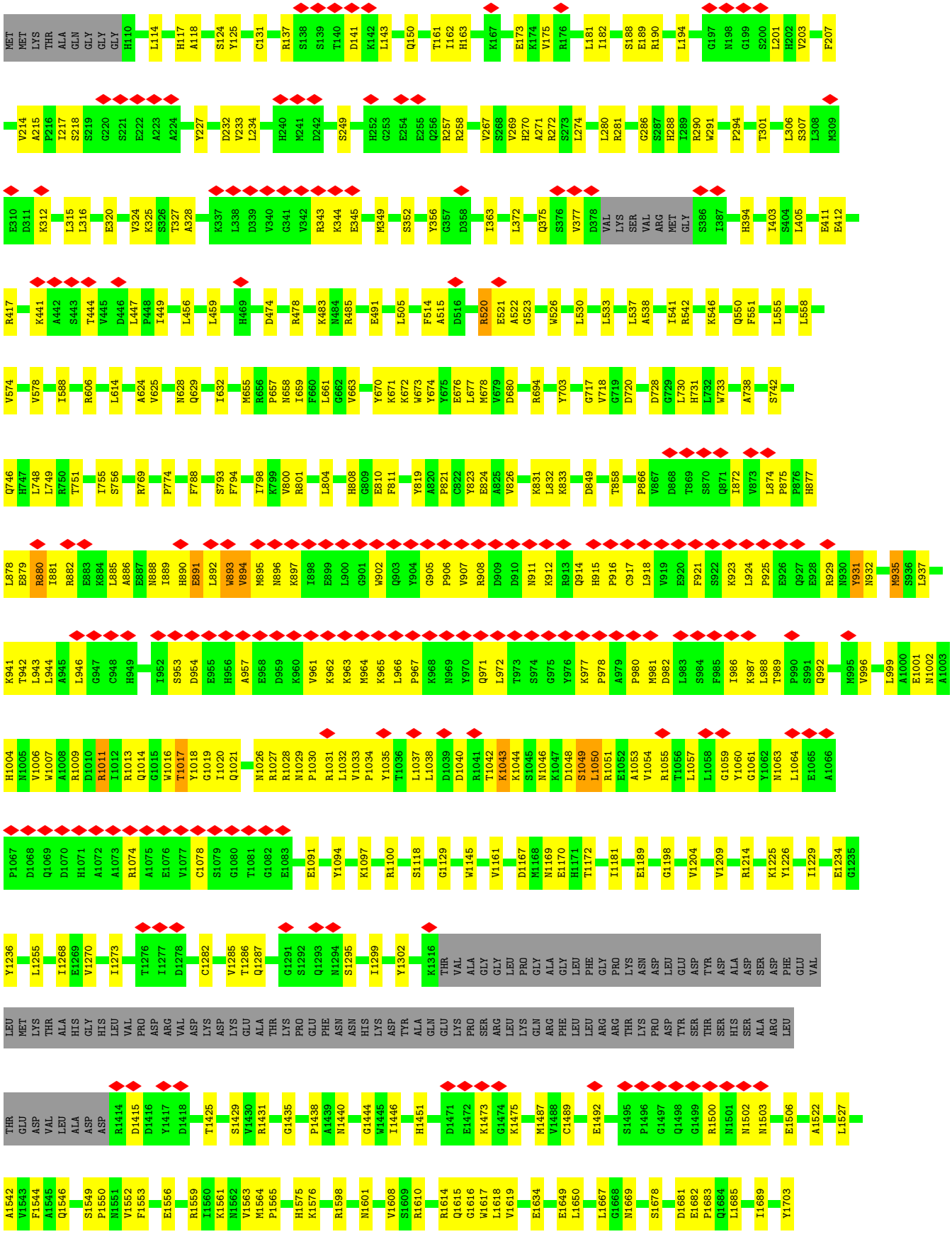

• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

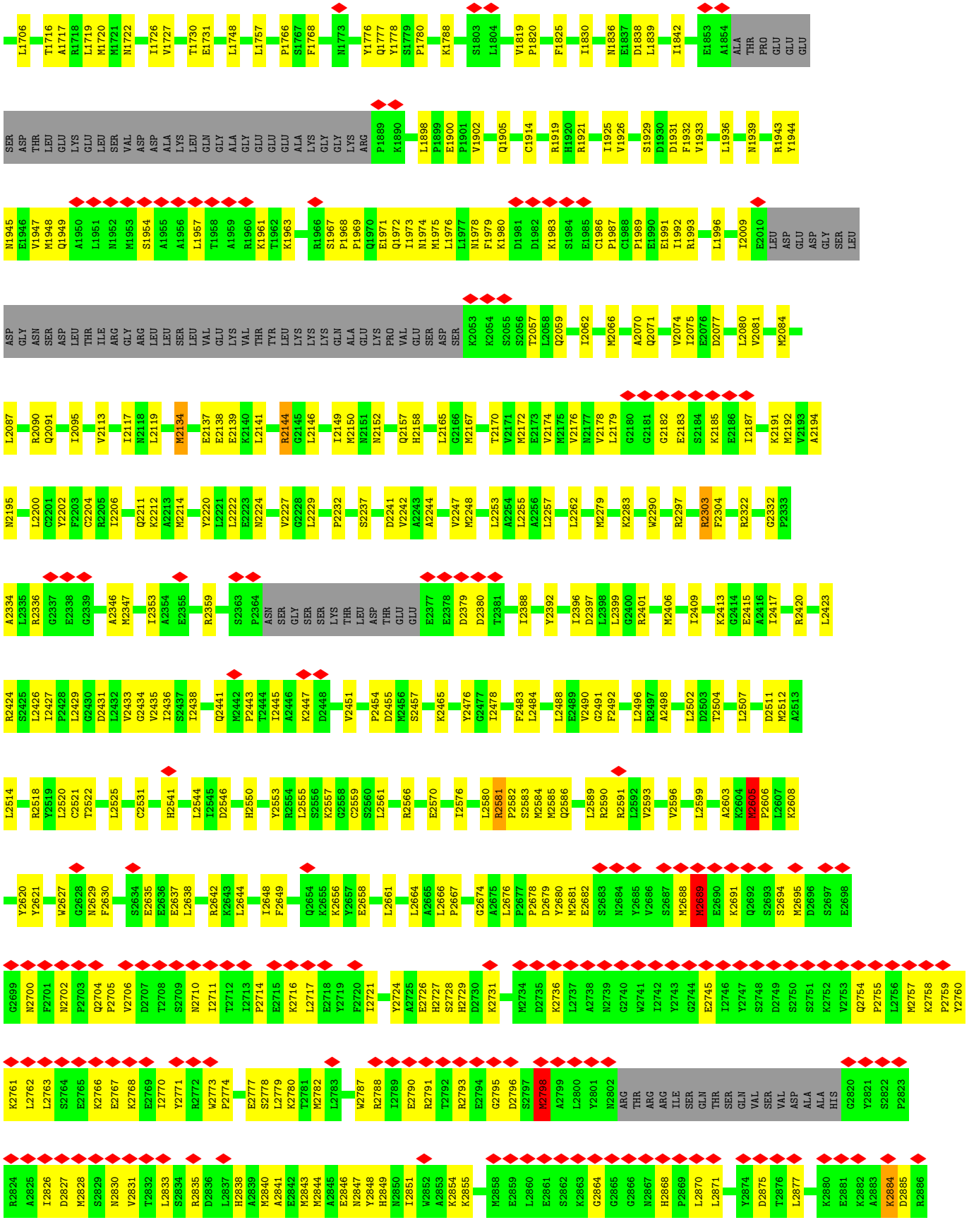
Chain H:

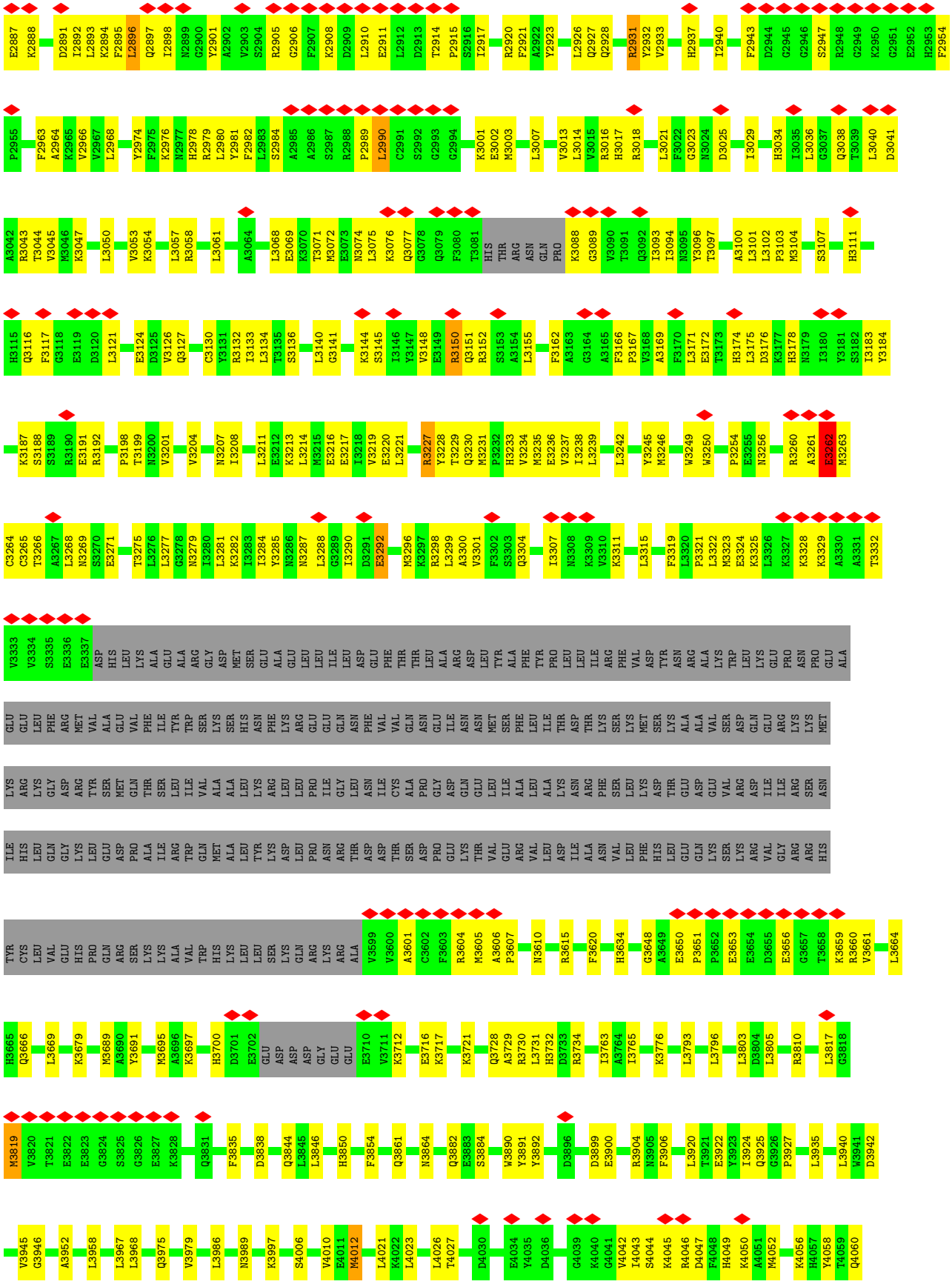



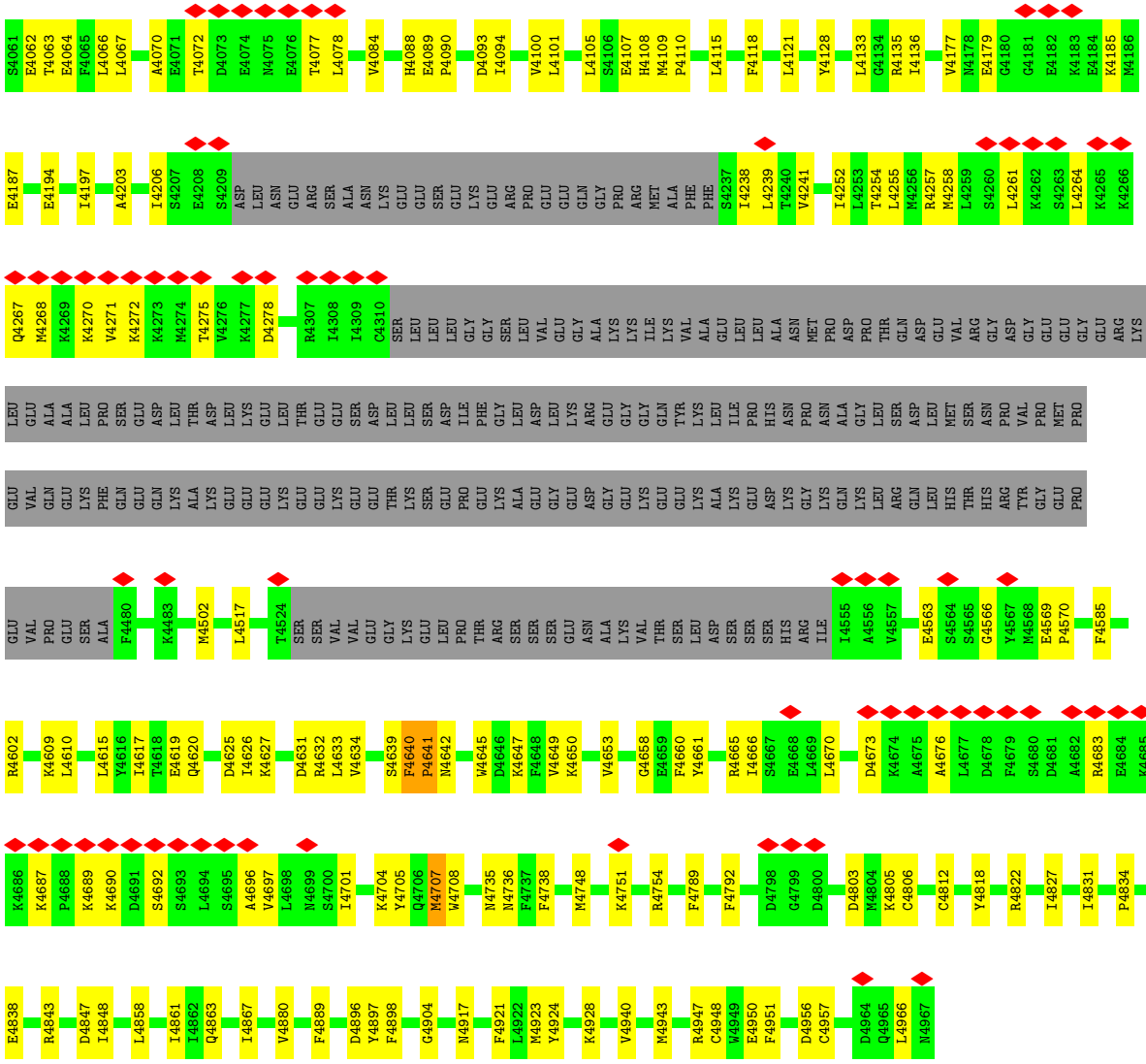

• Molecule 2: Ryanodine receptor 2

Chain A:

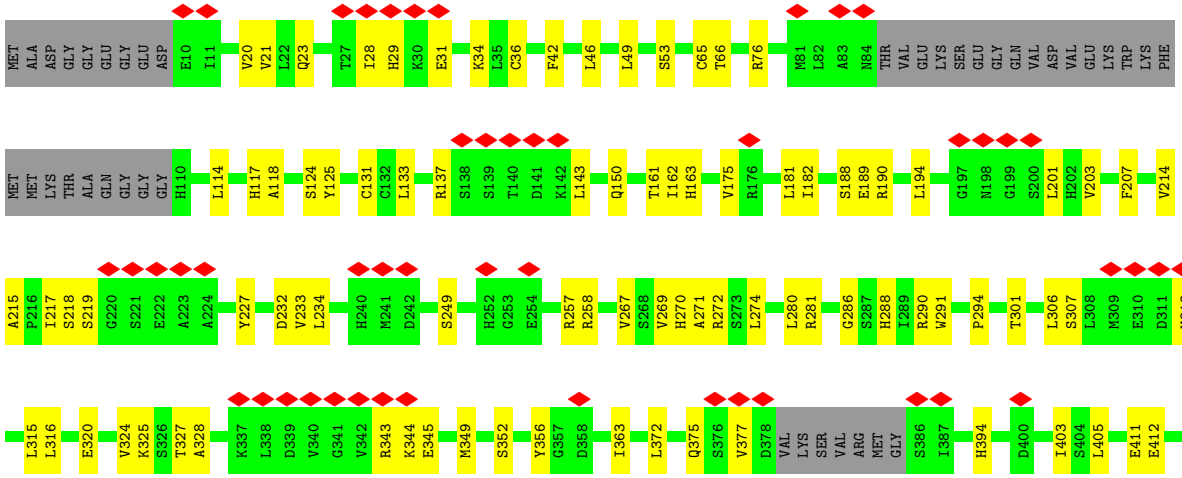


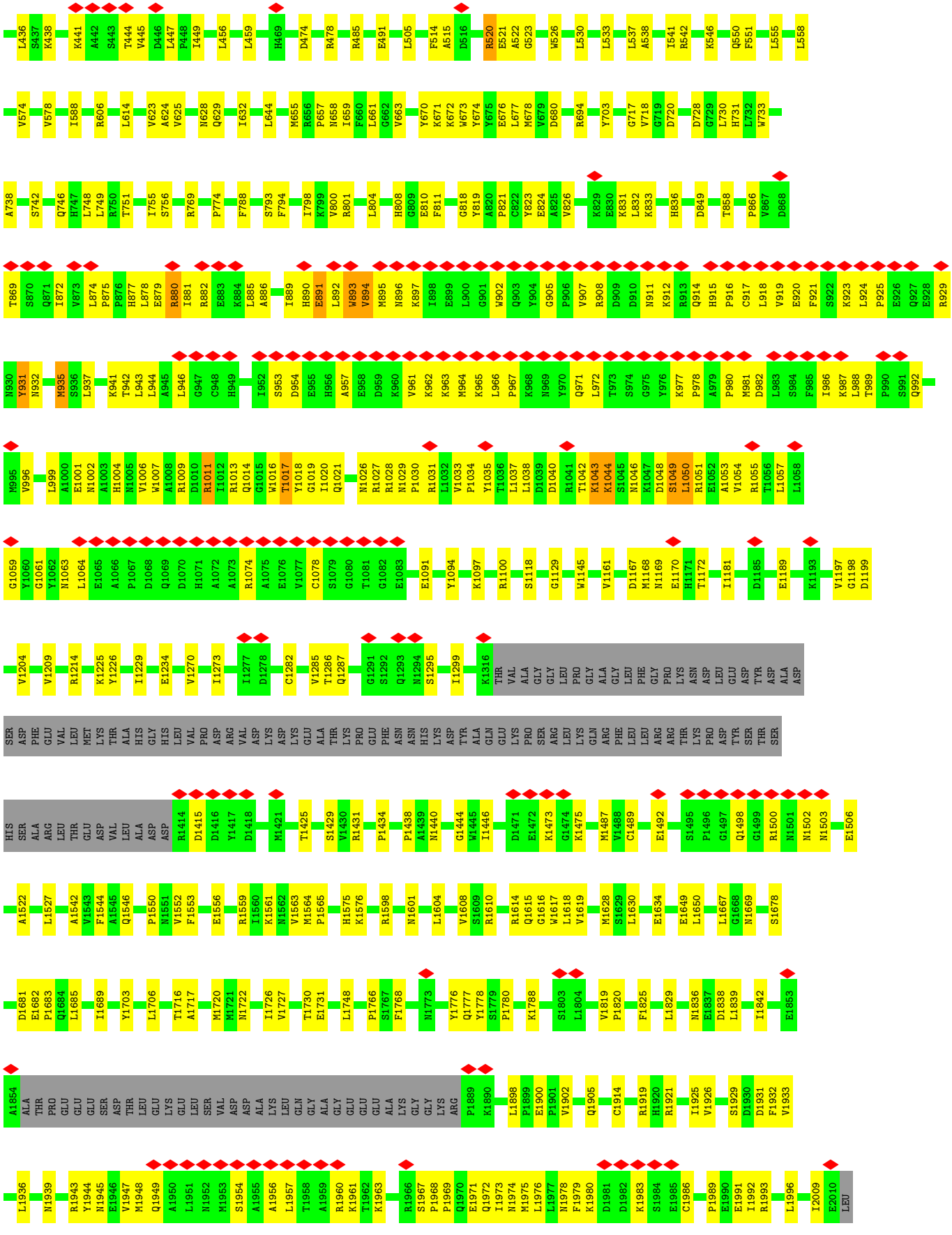


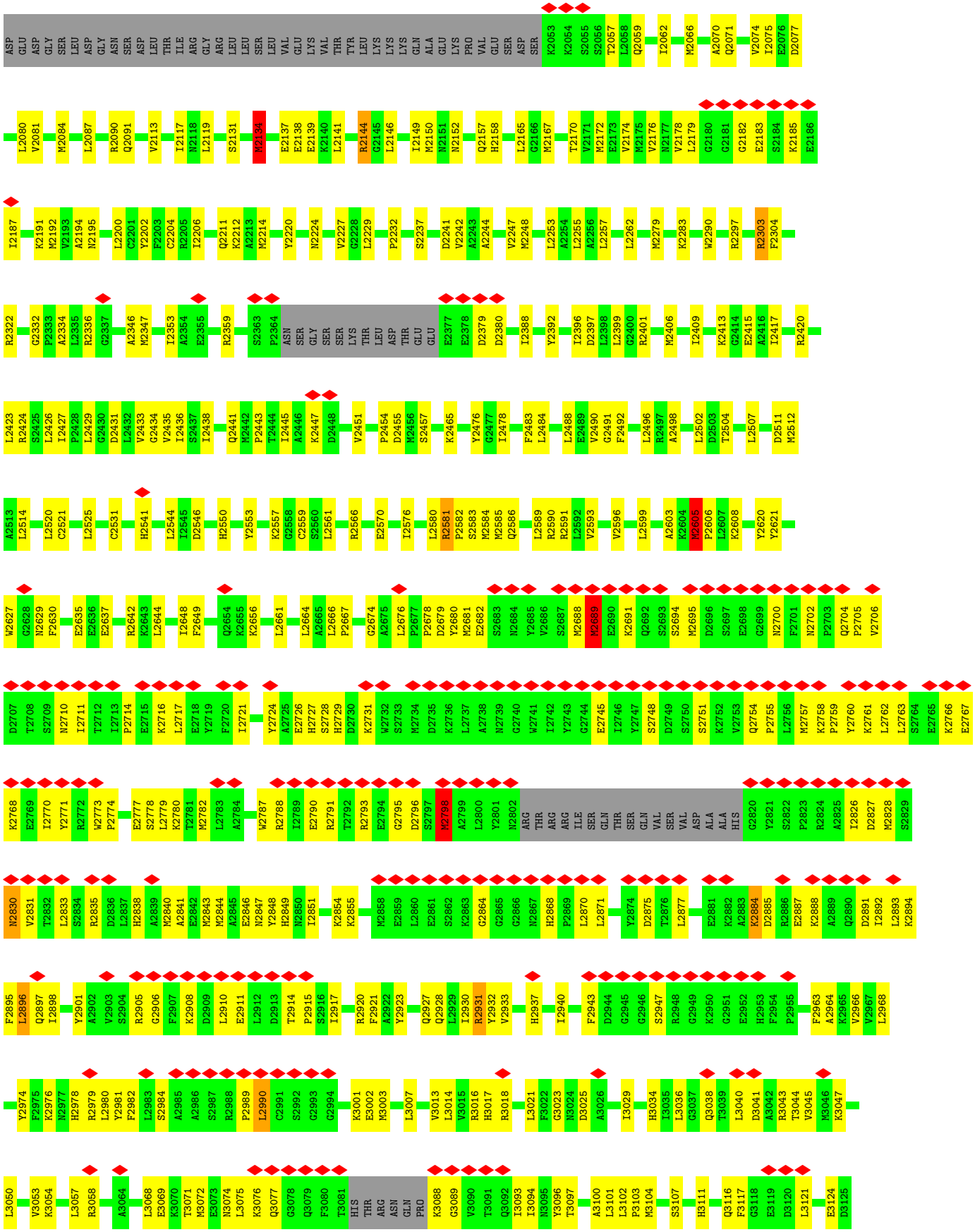


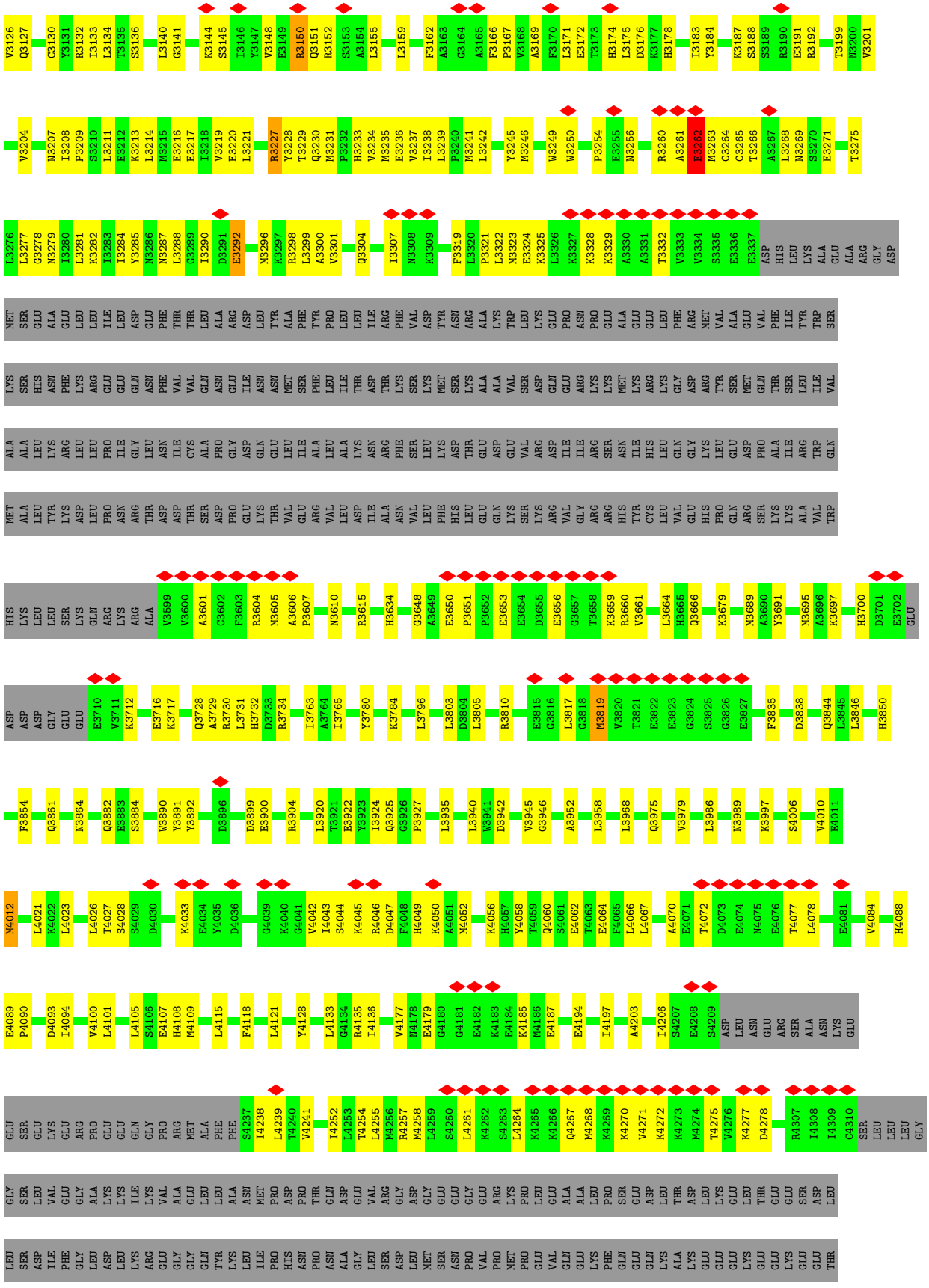
• Molecule 2: Ryanodine receptor 2

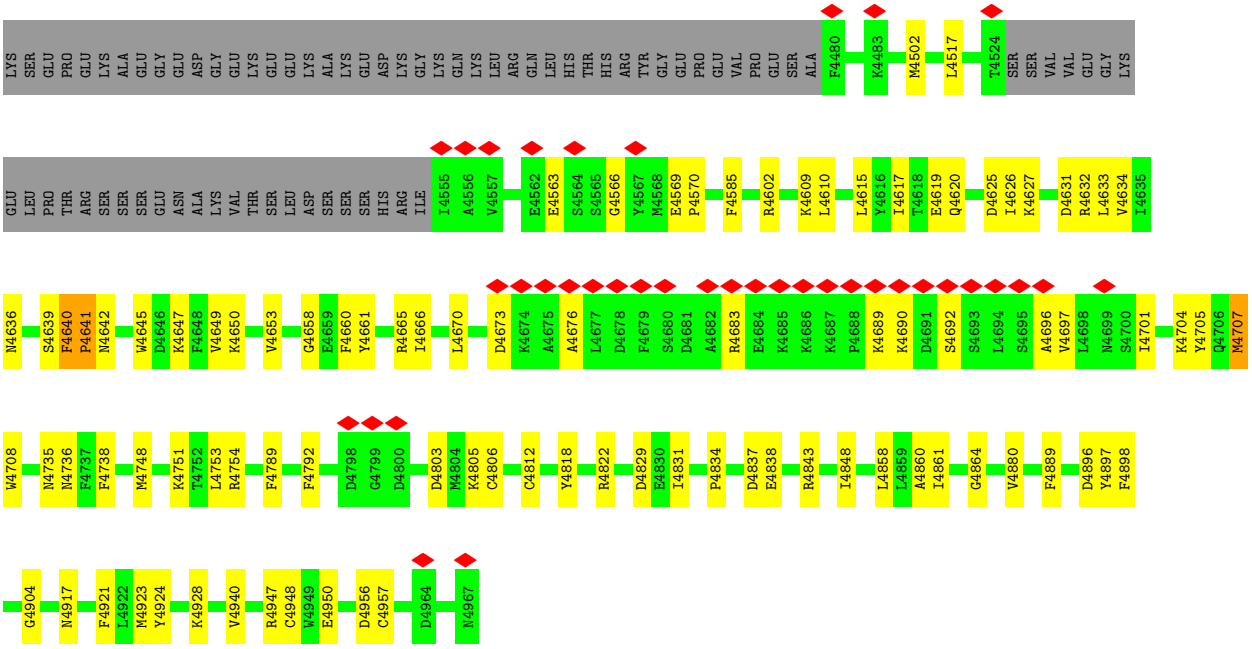
Chain B:


L436 S437 K438 K441 A442 S443 T444 V445 D446 L447 P448 I449 L456 L459 H469 D474 R478 R485 E491 L505 F514 A515 D516 R520 E521 A522 G523 W526 L530 L533 L537 A538 I541 R542 K546 Q550 F551 L555 L558
V574 V578 I588 R606 L614 V623 A624 V625 N628 Q629 I632 L644 M655 R656 P657 N658 I659 F660 L661 G662 V663 Y670 K671 K672 W673 Y674 Y675 E676 L677 M678 V679 D680 R694 Y703 G717 V718 G719 D720 D728 G729 L730 H731 L732 W733
A738 S742 Q746 H747 L748 L749 R750 T751 I755 S756 R769 P774 F788 S793 F794 I798 K799 V800 R801 L804 H808 G809 E810 F811 G818 Y819 A820 P821 C822 Y823 E824 A825 V826 K829 E830 K831 L832 K833 H836 D849 T858 P866 V867 D868
T869 S870 Q871 I872 V873 L874 P875 P876 H877 L878 E879 R880 I881 R882 E883 K884 L885 A886 I889 H890 E891 L892 W893 V894 M895 N896 K897 I898 E899 L900 G901 W902 Q903 Y904 G905 P906 V907 R908 D909 D910 N911 K912 R913 Q914 H915 P916 C917 L918 V919 E920 F921 S922 K923 L924 P925 E926 Q927 E928 R929
N930 Y931 N932 M935 S936 L937 K941 T942 L943 L944 A945 L946 G947 C948 H949 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992
M995 V996 L999 A1000 E1001 N1002 A1003 H1004 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 T1017 Y1018 G1019 I1020 Q1021 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058
G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066 P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 E1091 Y1094 K1097 R1100 S1118 G1129 W1145 V1161 D1167 M1168 N1169 E1170 H1171 T1172 I1181 D1185 E1189 K1193 V1197 G1198 D1199
V1204 V1209 R1214 K1225 Y1226 I1229 E1234 V1270 I1273 I1277 D1278 C1282 V1285 T1286 Q1287 G1291 S1292 Q1293 N1294 S1295 I1299 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP
SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER
HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 M1421 T1425 S1429 V1430 R1431 P1434 P1438 A1439 N1440 G1444 W1445 I1446 D1471 E1472 K1473 G1474 K1475 M1487 V1488 C1489 E1492 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 E1506
A1522 L1527 A1542 V1543 F1544 A1545 Q1546 P1550 N1551 V1552 F1553 E1556 R1559 I1560 K1561 N1562 V1563 M1564 P1565 H1575 K1576 R1598 N1601 L1604 V1608 S1609 R1610 R1614 Q1615 G1616 W1617 L1618 V1619 M1628 S1629 L1630 E1634 E1649 L1650 L1667 G1668 N1669 S1678
D1681 E1682 P1683 Q1684 L1685 I1689 Y1703 L1706 T1716 A1717 M1720 M1721 N1722 I1726 V1727 T1730 E1731 L1748 P1766 S1767 F1768 N1773 Y1776 Q1777 Y1778 S1779 P1780 K1788 S1803 L1804 V1819 P1820 F1825 L1829 N1836 E1837 D1838 L1839 I1842 E1863
A1854 ALA THR PRO GLU GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 L1898 P1899 E1900 P1901 V1902 Q1905 C1914 R1919 H1920 R1921 I1925 V1926 S1929 D1930 D1931 F1932 V1933
L1936 N1939 R1943 Y1944 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 R1966 S1967 P1968 P1969 Q1970 E1971 Q1972 I1973 N1974 M1975 L1976 L1977 N1978 F1979 K1980 D1981 D1982 K1983 S1984 E1985 C1986 P1989 E1990 E1991 I1992 R1993 L1996 I2009 E2010 LEU

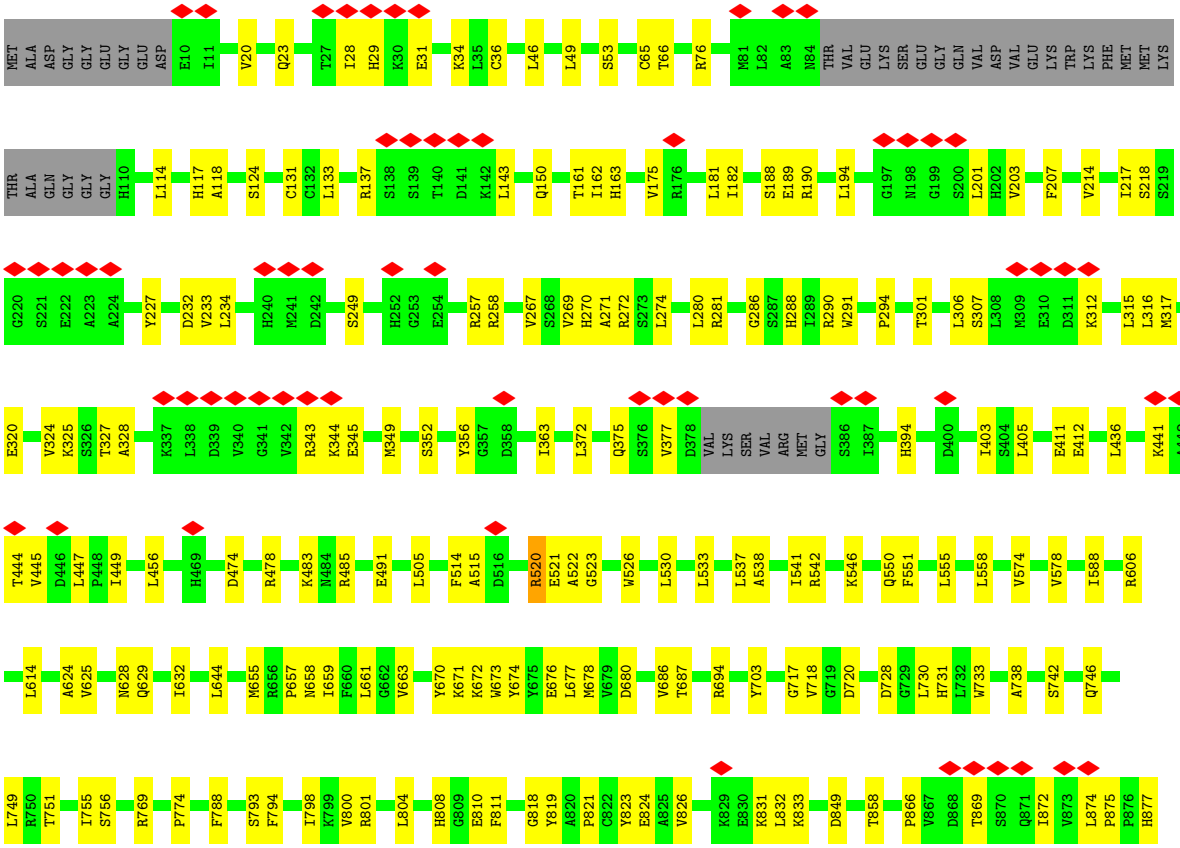


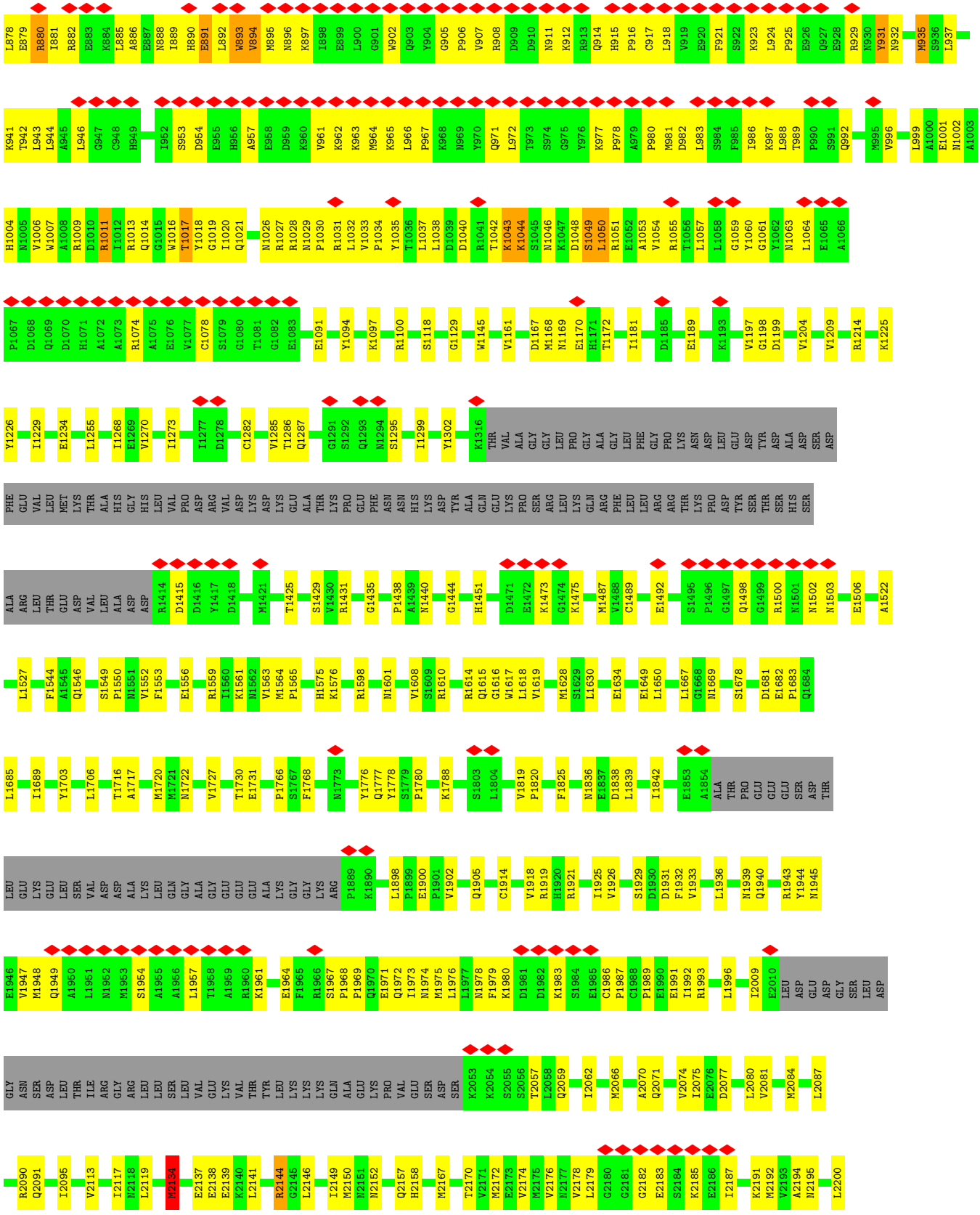




• Molecule 2: Ryanodine receptor 2

Chain C: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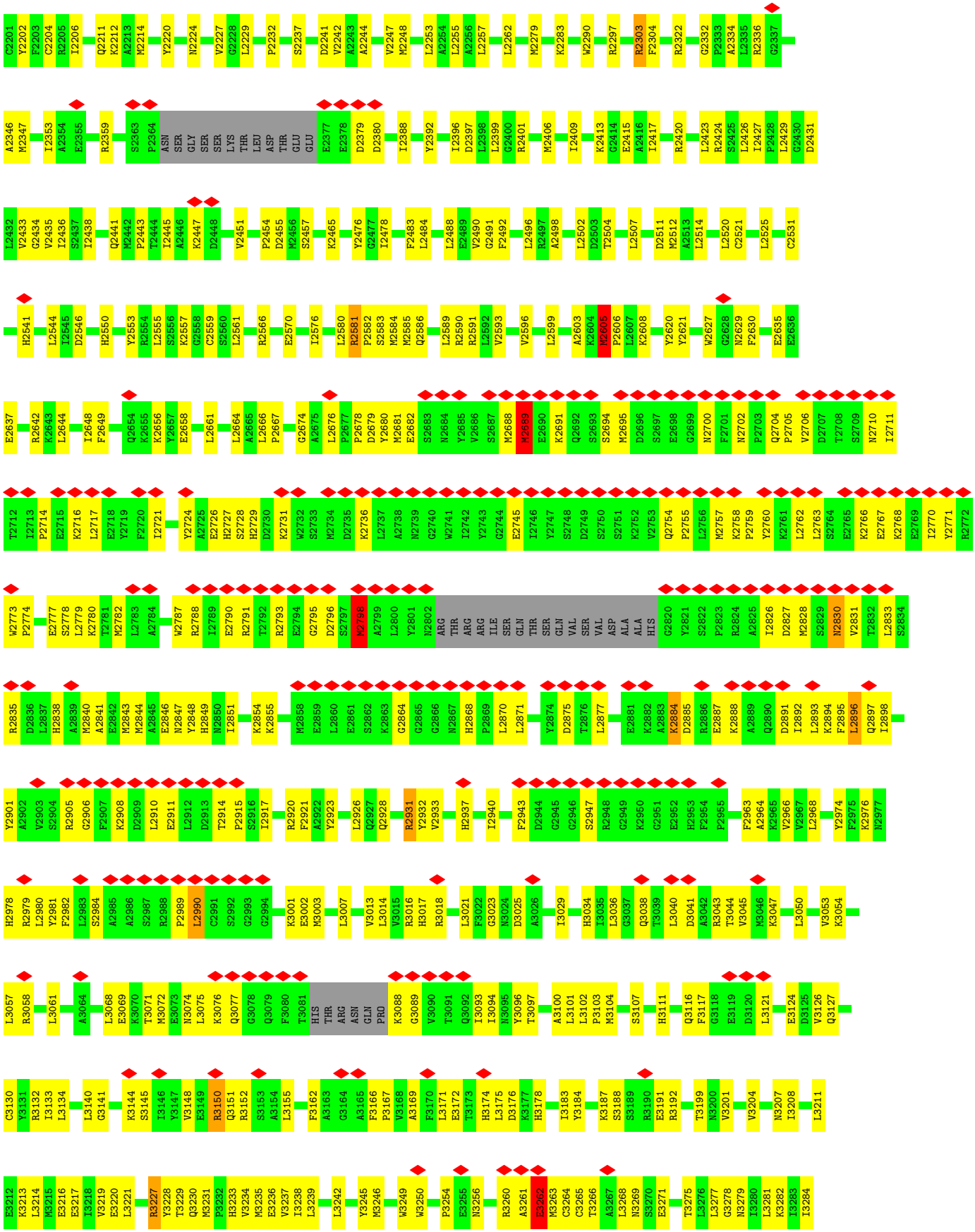
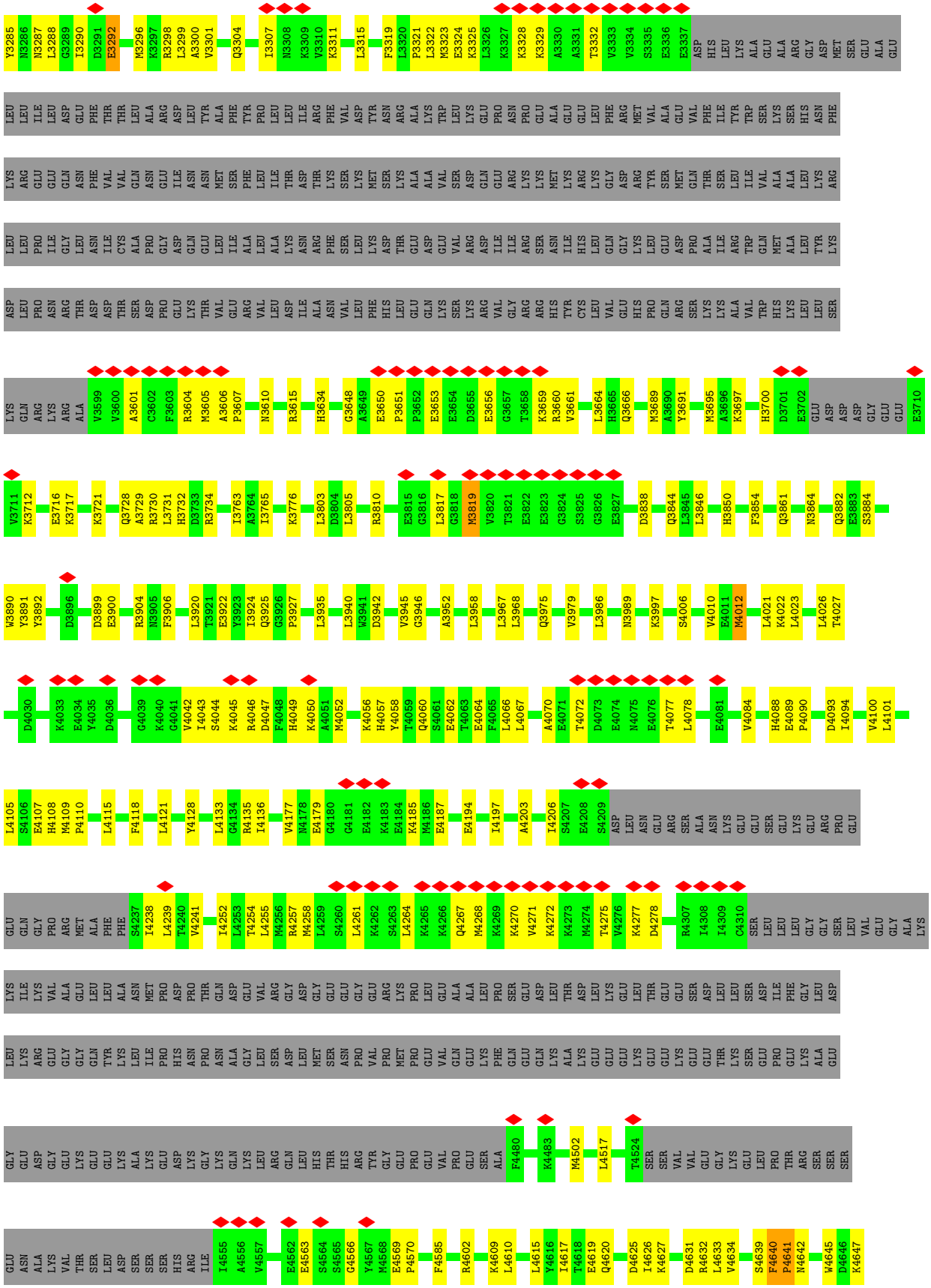
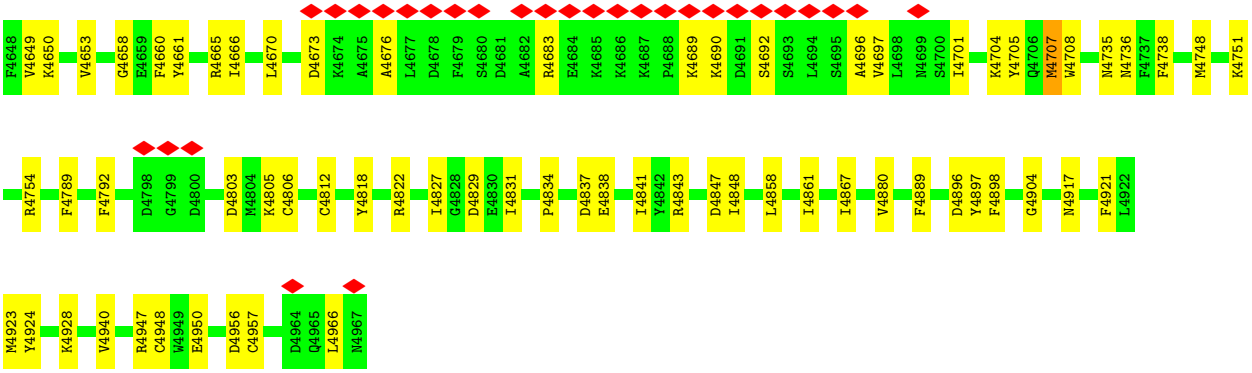
K941 T942 L943 L944 A945 L946 G947 C948 H949 I952 S953 D954 E955 H956 A957 E958 D959 K960 V961 K962 K963 M964 K965 L966 P967 K968 N969 Y970 Q971 L972 T973 S974 G975 Y976 K977 P978 A979 P980 M981 D982 L983 S984 F985 I986 K987 L988 T989 P990 S991 Q992 M995 V996 L999 A1000 E1001 N1002 A1003
H1004 N1005 V1006 W1007 A1008 R1009 D1010 R1011 I1012 R1013 Q1014 G1015 W1016 T1017 Y1018 G1019 I1020 Q1021 N1026 R1027 R1028 N1029 P1030 R1031 L1032 V1033 P1034 Y1035 T1036 L1037 L1038 D1039 D1040 R1041 T1042 K1043 K1044 S1045 N1046 K1047 D1048 S1049 L1050 R1051 E1052 A1053 V1054 R1055 T1056 L1057 L1058 G1059 Y1060 G1061 Y1062 N1063 L1064 E1065 A1066
P1067 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 E1091 Y1094 K1097 R1100 S1118 G1129 W1145 V1161 D1167 M1168 N1169 E1170 H1171 T1172 I1181 D1185 E1189 K1193 V1197 G1198 D1199 V1204 V1209 R1214 K1225
Y1226 I1229 E1234 L1255 I1268 E1269 V1270 I1273 I1277 D1278 C1282 V1285 T1286 Q1287 G1291 S1292 Q1293 N1294 S1295 I1299 Y1302 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP
PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER
ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 M1421 T1425 S1429 V1430 R1431 G1435 P1438 A1439 N1440 G1444 H1451 D1471 E1472 K1473 G1474 K1475 M1487 Y1488 C1489 E1492 S1496 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503 E1506 A1522
L1527 F1544 A1545 Q1546 S1549 P1550 N1551 V1552 F1553 E1556 R1559 I1560 K1561 N1562 V1563 M1564 P1565 H1575 K1576 R1598 N1601 V1608 S1609 R1610 R1614 Q1615 G1616 W1617 L1618 V1619 M1628 S1629 L1630 E1634 E1649 L1650 L1667 G1668 N1669 S1678 D1681 E1682 P1683 Q1684
L1685 I1689 Y1703 L1706 T1716 A1717 M1720 M1721 N1722 V1727 T1730 E1731 P1766 S1767 F1768 N1773 Y1776 Q1777 Y1778 S1779 P1780 K1788 S1803 L1804 V1819 P1820 F1825 N1836 E1837 D1838 L1839 I1842 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR
LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 L1898 P1899 E1900 P1901 V1902 Q1905 C1914 V1918 R1919 H1920 R1921 I1925 V1926 S1929 D1930 D1931 F1932 V1933 L1936 N1939 Q1940 R1943 Y1944 N1945
E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 E1964 F1965 R1966 S1967 P1968 P1969 Q1970 E1971 Q1972 I1973 N1974 M1975 L1976 L1977 N1978 F1979 K1980 D1981 D1982 K1983 S1984 E1985 C1986 P1987 C1988 P1989 E1990 E1991 I1992 R1993 L1996 I2009 E2010 LEU ASP GLU ASP GLY SER LEU ASP
GLY ASN SER ASP LEU LEU THR ILE ARG GLY ARG LEU LEU LEU SER LEU LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 S2056 T2057 L2058 Q2059 I2062 M2066 A2070 Q2071 V2074 I2075 E2076 D2077 L2080 V2081 M2084 L2087
R2090 Q2091 I2095 V2113 I2117 N2118 L2119 M2134 E2137 E2138 E2139 K2140 L2141 R2144 G2145 L2146 I2149 M2150 N2151 N2152 Q2157 H2158 M2167 T2170 V2171 M2172 E2173 V2174 M2175 V2176 N2177 V2178 L2179 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 K2191 M2192 V2193 A2194 N2195 L2200





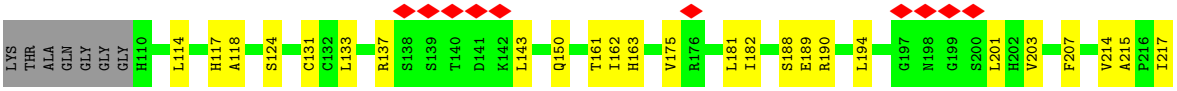


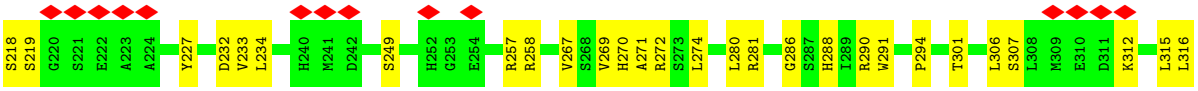


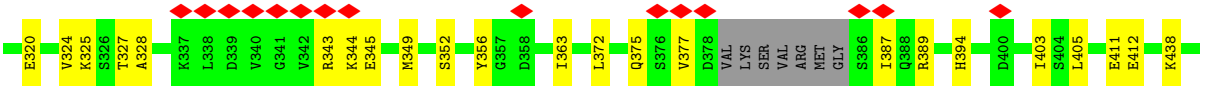


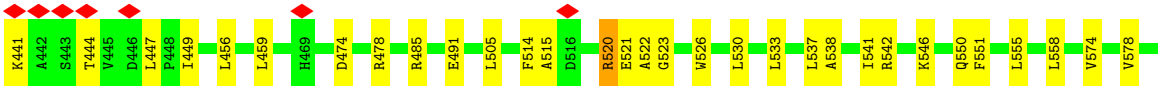
• Molecule 2: Ryanodine receptor 2

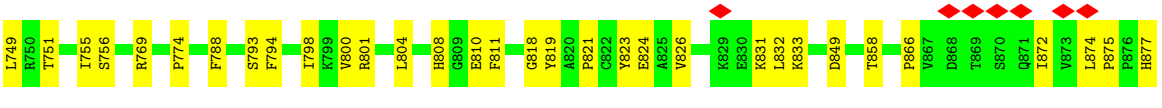
Chain D:

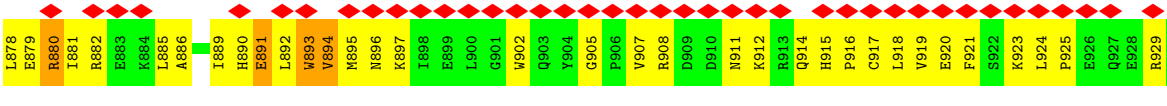



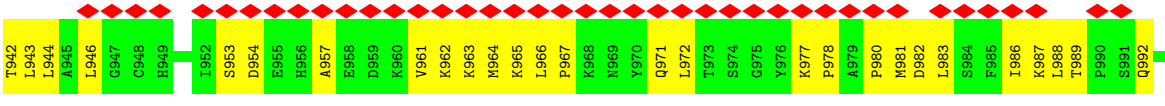


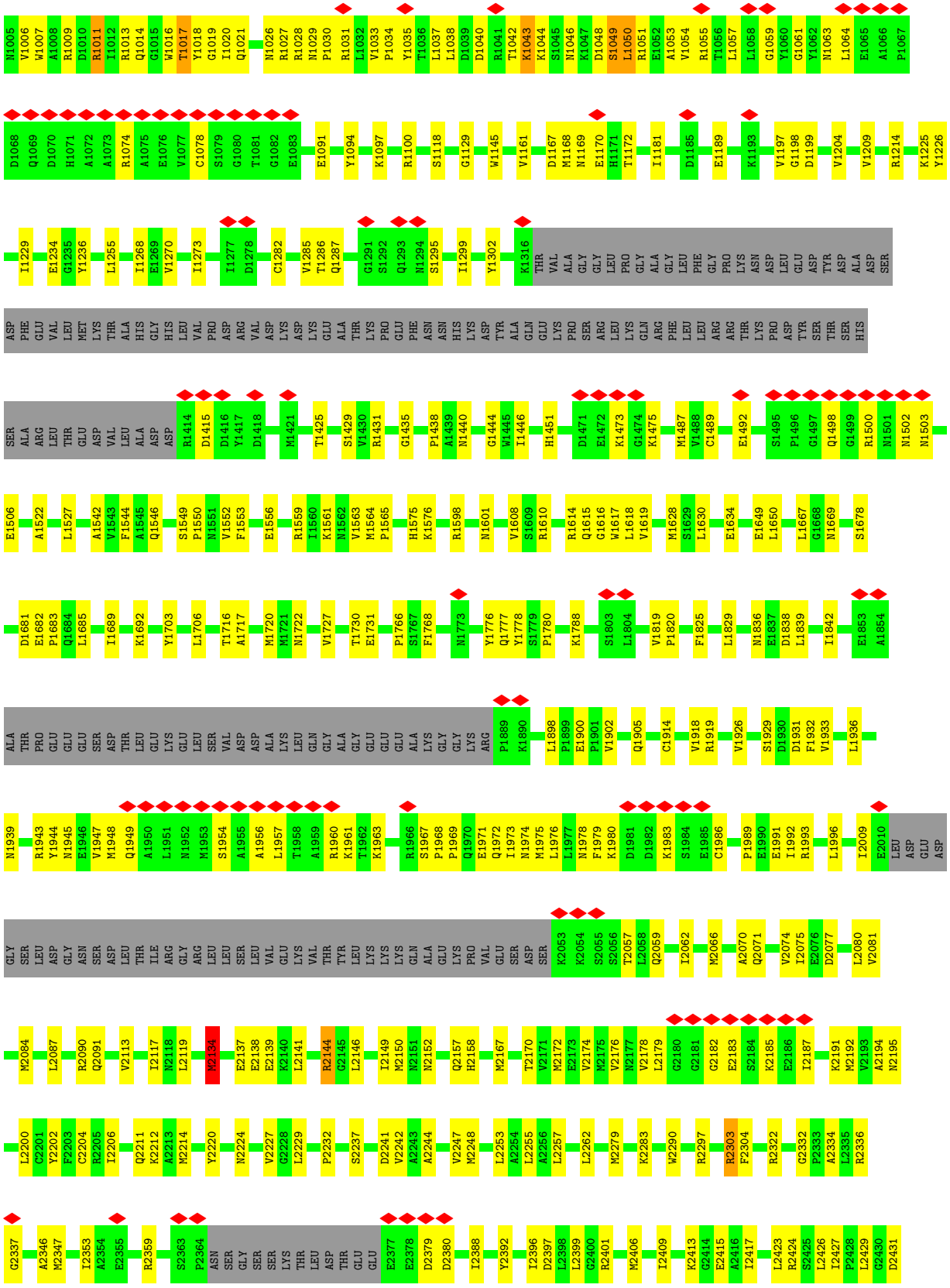








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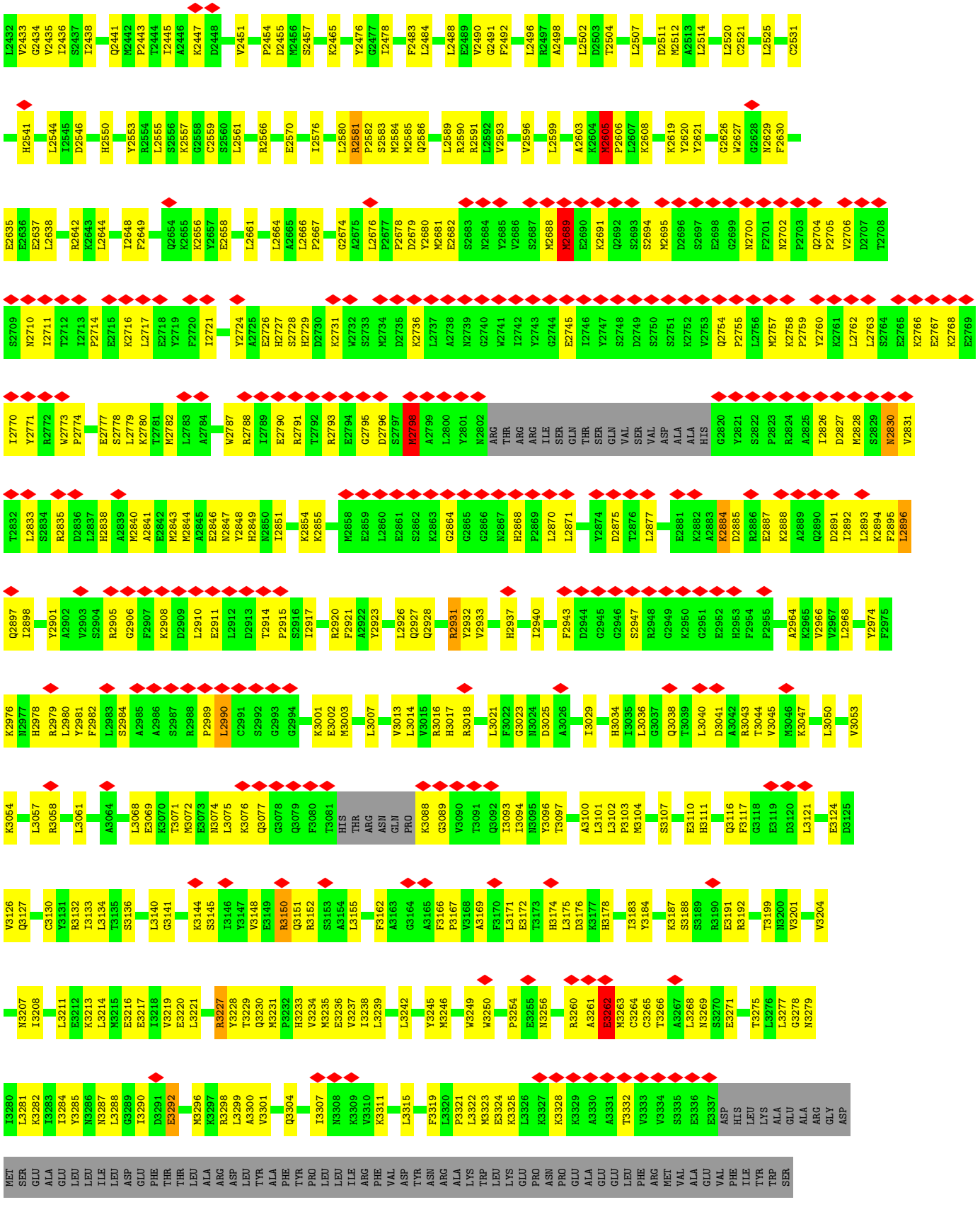
D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 S1079 G1080 T1081 G1082 E1083 E1091 Y1094 K1097 R1100 S1118 G1129 W1145 V1161 D1167 M1168 N1169 E1170 H1171 T1172 I1181 D1185 E1189 K1193 V1197 G1198 D1199 V1204 V1209 R1214 K1225 Y1226
I1229 E1234 G1235 Y1236 L1255 I1268 E1269 V1270 I1273 I1277 D1278 C1282 V1285 T1286 Q1287 G1291 S1292 Q1293 N1294 S1295 I1299 Y1302 K1316
THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER
ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS
SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 D1416 Y1417 D1418 M1421 T1425 S1429 V1430 R1431 G1435 P1438 A1439 N1440 G1444 W1445 I1446 H1451 D1471 E1472 K1473 G1474 K1475 M1487 V1488 C1489 E1492 S1495 P1496 G1497 Q1498 G1499 R1500 N1501 N1502 N1503
E1506 A1522 L1527 A1542 V1543 F1544 A1545 Q1546 S1549 P1550 N1551 V1552 F1553 E1556 R1559 I1560 K1561 N1562 V1563 M1564 P1565 H1575 K1576 R1598 N1601 V1608 S1609 R1610 R1614 Q1615 G1616 W1617 L1618 V1619 M1628 S1629 L1630 E1634 E1649 L1650 L1667 G1668 N1669 S1678
D1681 E1682 P1683 Q1684 L1685 I1689 K1692 Y1703 L1706 T1716 A1717 M1720 M1721 N1722 V1727 T1730 E1731 P1766 S1767 F1768 N1773 Y1776 Q1777 Y1778 S1779 P1780 K1788 S1803 L1804 V1819 P1820 F1825 L1829 N1836 E1837 D1838 L1839 I1842 E1853 A1854
ALA THR PRO GLU GLU GLU SER ASP THR LEU LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 K1890 L1898 P1899 E1900 P1901 V1902 Q1905 C1914 V1918 R1919 V1926 S1929 D1930 D1931 F1932 V1933 L1936
N1939 R1943 Y1944 N1945 E1946 V1947 M1948 Q1949 A1950 L1951 N1952 M1953 S1954 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 R1966 S1967 P1968 P1969 Q1970 E1971 Q1972 I1973 N1974 M1975 L1976 L1977 N1978 F1979 K1980 D1981 D1982 K1983 S1984 E1985 C1986 P1989 E1990 E1991 I1992 R1993 L1996 I2009 E2010
LEU ASP GLU ASP
GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER K2053 K2054 S2055 S2056 T2057 L2058 Q2059 I2062 M2066 A2070 Q2071 V2074 I2075 E2076 D2077 L2080 V2081
M2084 L2087 R2090 Q2091 V2113 I2117 N2118 L2119 M2134 E2137 E2138 E2139 K2140 L2141 R2144 G2145 L2146 I2149 M2150 N2151 N2152 Q2157 H2158 M2167 T2170 V2171 M2172 E2173 V2174 M2175 V2176 N2177 V2178 L2179 G2180 G2181 G2182 E2183 S2184 K2185 E2186 I2187 K2191 M2192 V2193 A2194 N2195
L2200 C2201 Y2202 F2203 C2204 R2205 I2206 Q2211 K2212 A2213 M2214 Y2220 N2224 V2227 G2228 L2229 P2232 S2237 D2241 V2242 A2243 A2244 V2247 M2248 L2253 A2254 L2255 A2256 L2257 L2262 M2279 K2283 W2290 R2297 R2303 F2304 R2322 G2332 P2333 A2334 L2335 R2336
G2337 A2346 M2347 I2353 A2354 E2355 R2359 S2363 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 I2388 Y2392 I2396 D2397 L2398 L2399 C2400 R2401 M2406 I2409 K2413 G2414 E2415 A2416 I2417 L2423 R2424 S2425 L2426 I2427 P2428 L2429 G2430 D2431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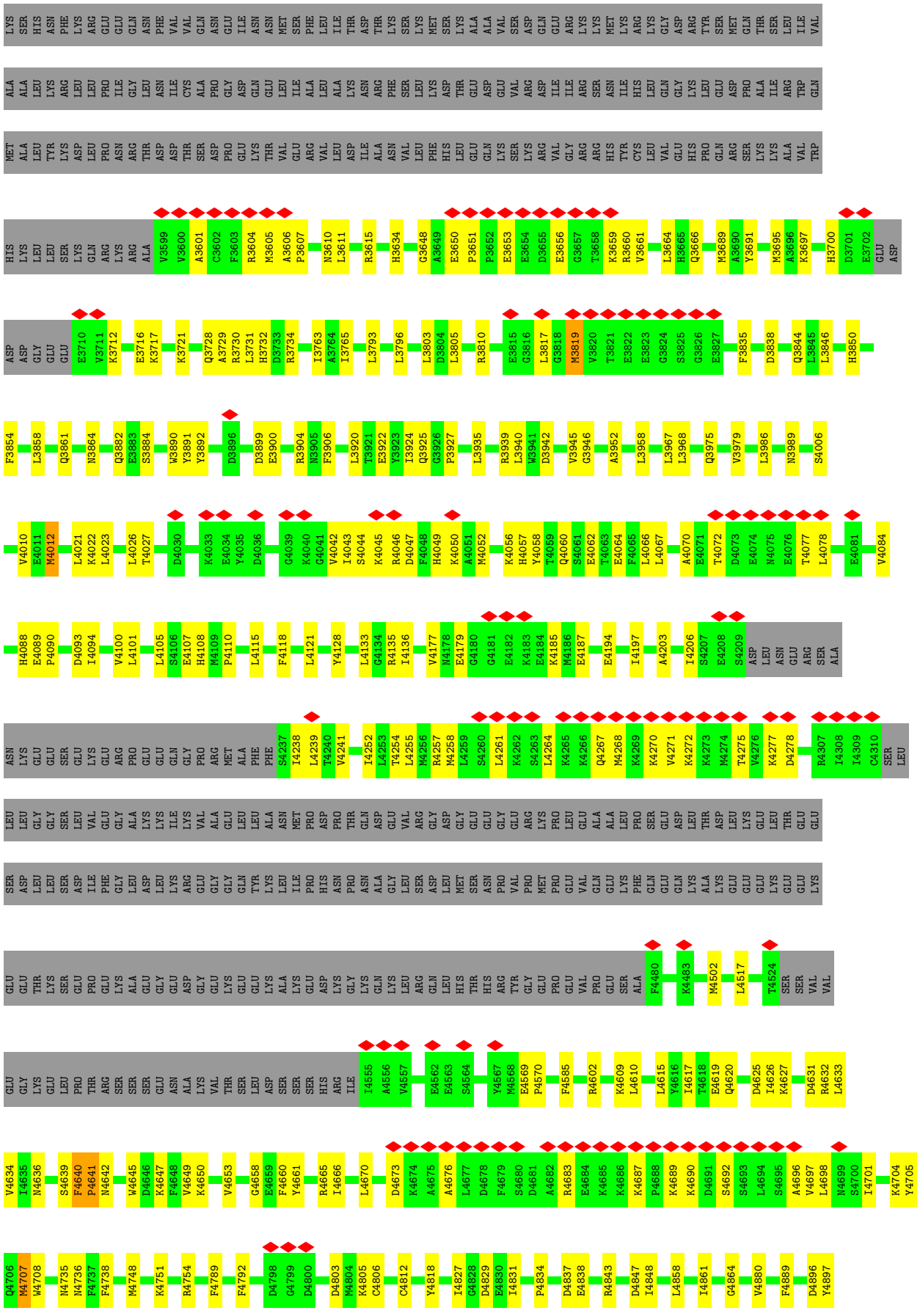
H2541 L2544 T2545 D2546 H2550 Y2553 R2554 L2555 S2556 K2557 G2558 C2559 S2560 L2561 R2566 E2570 I2576 L2580 R2581 P2582 S2583 M2584 M2585 Q2586 L2589 R2590 R2591 L2592 V2593 V2596 L2599 A2603 K2604 M2605 P2606 L2607 K2608 K2619 Y2620 Y2621 G2626 W2627 G2628 N2629 F2630
E2635 E2636 E2637 L2638 R2642 K2643 L2644 I2648 F2649 Q2654 K2655 K2656 Y2657 E2658 L2661 L2664 A2665 L2666 P2667 G2674 A2675 L2676 P2677 P2678 D2679 Y2680 M2681 E2682 S2683 N2684 Y2685 V2686 S2687 M2688 M2689 E2690 K2691 Q2692 S2693 S2694 M2695 D2696 S2697 E2698 G2699 N2700 F2701 N2702 P2703 Q2704 P2705 V2706 D2707 T2708
S2709 N2710 I2711 T2712 I2713 P2714 E2715 K2716 L2717 E2718 Y2719 F2720 I2721 Y2724 A2725 E2726 H2727 S2728 H2729 D2730 K2731 W2732 S2733 M2734 D2735 K2736 L2737 A2738 N2739 G2740 W2741 I2742 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769
I2770 Y2771 R2772 W2773 P2774 E2777 S2778 L2779 K2780 T2781 M2782 L2783 A2784 W2787 R2788 I2789 E2790 R2791 T2792 R2793 E2794 G2795 D2796 S2797 M2798 A2799 L2800 Y2801 N2802 ARG THR ARG ARG ILE SER GLN THR SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 A2825 I2826 D2827 M2828 S2829 N2830 V2831
T2832 L2833 S2834 R2835 D2836 L2837 H2838 A2839 M2840 A2841 E2842 M2843 M2844 A2845 E2846 N2847 Y2848 H2849 N2850 I2851 K2854 K2855 M2858 E2859 L2860 E2861 S2862 K2863 G2864 G2865 G2866 N2867 H2868 P2869 L2870 L2871 Y2874 D2875 T2876 L2877 E2881 K2882 A2883 K2884 D2885 R2886 E2887 K2888 A2889 Q2890 D2891 I2892 L2893 K2894 F2895 L2896
Q2897 I2898 Y2901 A2902 V2903 S2904 R2905 G2906 F2907 K2908 D2909 L2910 E2911 L2912 D2913 T2914 P2915 S2916 I2917 R2920 F2921 A2922 Y2923 L2926 Q2927 Q2928 R2931 Y2932 V2933 H2937 I2940 F2943 D2944 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 H2953 F2954 P2955 A2964 K2965 V2966 V2967 L2968 Y2974 F2975
K2976 N2977 H2978 R2979 L2980 Y2981 F2982 L2983 S2984 A2985 A2986 S2987 R2988 P2989 L2990 C2991 S2992 G2993 G2994 K3001 E3002 M3003 L3007 V3013 L3014 V3015 R3016 H3017 R3018 L3021 F3022 G3023 N3024 D3025 A3026 I3029 H3034 I3035 L3036 G3037 Q3038 T3039 L3040 D3041 A3042 R3043 T3044 V3045 M3046 K3047 L3050 V3053
K3054 L3057 R3058 L3061 A3064 L3068 E3069 K3070 T3071 M3072 E3073 N3074 L3075 K3076 Q3077 G3078 Q3079 F3080 T3081 HIS THR ARG ASN GLN PRO K3088 G3089 Y3090 T3091 Q3092 I3093 I3094 N3095 Y3096 T3097 A3100 L3101 L3102 P3103 M3104 S3107 E3110 H3111 Q3116 F3117 G3118 E3119 D3120 L3121 E3124 D3125
V3126 Q3127 C3130 Y3131 R3132 I3133 L3134 T3135 S3136 L3140 G3141 K3144 S3145 I3146 Y3147 V3148 E3149 R3150 Q3151 R3152 S3153 A3154 L3155 F3162 A3163 G3164 A3165 F3166 P3167 V3168 A3169 F3170 L3171 E3172 T3173 H3174 L3175 D3176 K3177 H3178 I3183 Y3184 K3187 S3188 S3189 R3190 E3191 R3192 T3199 N3200 V3201 V3204
N3207 I3208 L3211 E3212 K3213 L3214 M3215 E3216 E3217 I3218 V3219 E3220 L3221 R3227 Y3228 T3229 Q3230 M3231 P3232 H3233 V3234 M3235 E3236 V3237 I3238 L3239 L3242 Y3245 M3246 W3249 W3250 P3254 E3255 N3256 R3260 A3261 E3262 M3263 C3264 C3265 T3266 A3267 L3268 N3269 S3270 E3271 T3275 L3276 L3277 G3278 N3279
I3280 L3281 K3282 I3283 I3284 Y3285 M3286 N3287 L3288 G3289 I3290 D3291 E3292 M3296 K3297 R3298 L3299 A3300 V3301 Q3304 I3307 N3308 K3309 V3310 K3311 L3315 F3319 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 K3328 K3329 A3330 A3331 T3332 V3333 V3334 S3335 E3336 E3337 ASP HIS LEU LYS ALA GLU ALA ARG GLY ASP
MET SER GLU ALA GLU LEU LEU ILE LEU ASP GLU PHE THR THR LEU ALA ARG ASP LEU TYR ALA PHE TYR PRO LEU LEU ILE ARG PHE VAL ASP TYR ASN ARG ALA LYS TRP LEU LYS GLU PRO ASN PRO GLU ALA GLU GLU LEU PHE ARG MET VAL ALA GLU VAL PHE ILE TYR TRP SER

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G4904
N4917
F4921
L4922
M4923
Y4924
L4925
K4928
V4940
R4947
C4948
W4949
E4950
D4956
C4957
D4964
Q4965
L4966
M4967

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 14924 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 58 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 1200 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.660 | Depositor |
| Minimum map value | -0.004 | Depositor |
| Average map value | 0.017 | Depositor |
| Map value standard deviation | 0.035 | Depositor |
| Recommended contour level | 0.16 | Depositor |
| Map size (Å) | 426.752, 426.752, 426.752 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.8335, 0.8335, 0.8335 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | E | 0.31 | 0/834 | 0.53 | 0/1123 |
| 1 | F | 0.31 | 0/834 | 0.53 | 0/1123 |
| 1 | G | 0.31 | 0/834 | 0.53 | 0/1123 |
| 1 | H | 0.31 | 0/834 | 0.53 | 0/1123 |
| 2 | A | 0.28 | 0/34509 | 0.50 | 9/46612 (0.0%) |
| 2 | B | 0.28 | 0/34509 | 0.50 | 9/46612 (0.0%) |
| 2 | C | 0.28 | 0/34509 | 0.50 | 8/46612 (0.0%) |
| 2 | D | 0.28 | 0/34509 | 0.50 | 9/46612 (0.0%) |
| All | All | 0.28 | 0/141372 | 0.50 | 35/190940 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | A | 0 | 1 |
| 2 | B | 0 | 1 |
| 2 | C | 0 | 1 |
| 2 | D | 0 | 1 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (35) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 2605 | MET | CA-CB-CG | 7.43 | 125.92 | 113.30 |
| 2 | A | 2605 | MET | CA-CB-CG | 7.42 | 125.92 | 113.30 |
| 2 | C | 2605 | MET | CA-CB-CG | 7.41 | 125.89 | 113.30 |
| 2 | D | 2605 | MET | CA-CB-CG | 7.40 | 125.88 | 113.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 3262 | GLU | CA-CB-CG | 7.23 | 129.31 | 113.40 |
| 2 | B | 3262 | GLU | CA-CB-CG | 7.23 | 129.30 | 113.40 |
| 2 | D | 3262 | GLU | CA-CB-CG | 7.23 | 129.30 | 113.40 |
| 2 | C | 3262 | GLU | CA-CB-CG | 7.21 | 129.25 | 113.40 |
| 2 | C | 2605 | MET | CB-CG-SD | 6.72 | 132.57 | 112.40 |
| 2 | A | 2605 | MET | CB-CG-SD | 6.72 | 132.55 | 112.40 |
| 2 | D | 2605 | MET | CB-CG-SD | 6.72 | 132.55 | 112.40 |
| 2 | B | 2605 | MET | CB-CG-SD | 6.71 | 132.52 | 112.40 |
| 2 | C | 2689 | MET | CB-CG-SD | 6.11 | 130.72 | 112.40 |
| 2 | D | 2689 | MET | CB-CG-SD | 6.11 | 130.72 | 112.40 |
| 2 | A | 2689 | MET | CB-CG-SD | 6.10 | 130.71 | 112.40 |
| 2 | B | 2689 | MET | CB-CG-SD | 6.10 | 130.70 | 112.40 |
| 2 | C | 2134 | MET | CB-CG-SD | 6.00 | 130.41 | 112.40 |
| 2 | A | 2134 | MET | CB-CG-SD | 6.00 | 130.40 | 112.40 |
| 2 | B | 2134 | MET | CB-CG-SD | 5.99 | 130.37 | 112.40 |
| 2 | D | 2134 | MET | CB-CG-SD | 5.98 | 130.34 | 112.40 |
| 2 | B | 2990 | LEU | CA-CB-CG | 5.90 | 128.86 | 115.30 |
| 2 | D | 2990 | LEU | CA-CB-CG | 5.89 | 128.85 | 115.30 |
| 2 | A | 2990 | LEU | CA-CB-CG | 5.89 | 128.84 | 115.30 |
| 2 | C | 2990 | LEU | CA-CB-CG | 5.88 | 128.82 | 115.30 |
| 2 | B | 2896 | LEU | CA-CB-CG | 5.48 | 127.91 | 115.30 |
| 2 | D | 2896 | LEU | CA-CB-CG | 5.48 | 127.90 | 115.30 |
| 2 | A | 2896 | LEU | CA-CB-CG | 5.48 | 127.89 | 115.30 |
| 2 | C | 2798 | MET | CB-CG-SD | 5.46 | 128.78 | 112.40 |
| 2 | C | 2896 | LEU | CA-CB-CG | 5.45 | 127.84 | 115.30 |
| 2 | B | 2798 | MET | CB-CG-SD | 5.45 | 128.75 | 112.40 |
| 2 | A | 2798 | MET | CB-CG-SD | 5.45 | 128.75 | 112.40 |
| 2 | D | 2798 | MET | CB-CG-SD | 5.44 | 128.72 | 112.40 |
| 2 | D | 2798 | MET | CG-SD-CE | 5.02 | 108.24 | 100.20 |
| 2 | B | 2798 | MET | CG-SD-CE | 5.01 | 108.21 | 100.20 |
| 2 | A | 2798 | MET | CG-SD-CE | 5.00 | 108.20 | 100.20 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | A | 4640 | PHE | Peptide |
| 2 | B | 4640 | PHE | Peptide |
| 2 | C | 4640 | PHE | Peptide |
| 2 | D | 4640 | PHE | 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 | E | 818 | 0 | 821 | 19 | 0 |
| 1 | F | 818 | 0 | 821 | 22 | 0 |
| 1 | G | 818 | 0 | 821 | 18 | 0 |
| 1 | H | 818 | 0 | 821 | 18 | 0 |
| 2 | A | 33769 | 0 | 33450 | 886 | 0 |
| 2 | B | 33769 | 0 | 33450 | 877 | 0 |
| 2 | C | 33769 | 0 | 33450 | 879 | 0 |
| 2 | D | 33769 | 0 | 33450 | 875 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 62 | 0 | 24 | 3 | 0 |
| 4 | B | 62 | 0 | 24 | 3 | 0 |
| 4 | C | 62 | 0 | 24 | 3 | 0 |
| 4 | D | 62 | 0 | 24 | 3 | 0 |
| 5 | A | 23 | 0 | 0 | 2 | 0 |
| 5 | B | 23 | 0 | 0 | 2 | 0 |
| 5 | C | 23 | 0 | 0 | 2 | 0 |
| 5 | D | 23 | 0 | 0 | 2 | 0 |
| All | All | 138692 | 0 | 137180 | 3541 | 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 13.

All (3541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1031:ARG:HH21 | 2:B:1038:LEU:HD11 | 1.24 | 1.02 |
| 2:A:1031:ARG:HH21 | 2:A:1038:LEU:HD11 | 1.24 | 1.02 |
| 2:D:1031:ARG:HH21 | 2:D:1038:LEU:HD11 | 1.24 | 1.00 |
| 2:C:1031:ARG:HH21 | 2:C:1038:LEU:HD11 | 1.24 | 1.00 |
| 2:C:894:VAL:HG21 | 2:C:972:LEU:HD22 | 1.48 | 0.95 |
| 2:D:894:VAL:HG21 | 2:D:972:LEU:HD22 | 1.48 | 0.95 |
| 2:B:894:VAL:HG21 | 2:B:972:LEU:HD22 | 1.48 | 0.95 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:894:VAL:HG21 | 2:A:972:LEU:HD22 | 1.48 | 0.93 |
| 2:D:1968:PRO:HA | 2:D:3605:MET:HE1 | 1.52 | 0.89 |
| 2:A:4834:PRO:HB3 | 2:A:4843:ARG:HD3 | 1.57 | 0.87 |
| 2:B:1968:PRO:HA | 2:B:3605:MET:HE1 | 1.55 | 0.86 |
| 2:D:4834:PRO:HB3 | 2:D:4843:ARG:HD3 | 1.57 | 0.86 |
| 2:C:1968:PRO:HA | 2:C:3605:MET:HE1 | 1.56 | 0.86 |
| 2:B:4834:PRO:HB3 | 2:B:4843:ARG:HD3 | 1.57 | 0.85 |
| 2:B:1031:ARG:HH22 | 2:B:1042:THR:HG21 | 1.43 | 0.84 |
| 2:C:1031:ARG:HH22 | 2:C:1042:THR:HG21 | 1.42 | 0.84 |
| 2:C:4834:PRO:HB3 | 2:C:4843:ARG:HD3 | 1.57 | 0.84 |
| 2:A:999:LEU:HB3 | 2:A:1050:LEU:HD21 | 1.60 | 0.84 |
| 2:A:1031:ARG:HH22 | 2:A:1042:THR:HG21 | 1.42 | 0.84 |
| 2:B:999:LEU:HB3 | 2:B:1050:LEU:HD21 | 1.60 | 0.83 |
| 2:D:999:LEU:HB3 | 2:D:1050:LEU:HD21 | 1.60 | 0.83 |
| 2:C:999:LEU:HB3 | 2:C:1050:LEU:HD21 | 1.60 | 0.83 |
| 2:A:1968:PRO:HA | 2:A:3605:MET:HE1 | 1.58 | 0.82 |
| 2:A:1689:ILE:HA | 2:A:1703:TYR:HE1 | 1.44 | 0.82 |
| 2:B:2353:ILE:HG12 | 2:B:2359:ARG:HE | 1.45 | 0.82 |
| 2:D:2353:ILE:HG12 | 2:D:2359:ARG:HE | 1.45 | 0.82 |
| 2:C:1689:ILE:HA | 2:C:1703:TYR:HE1 | 1.43 | 0.81 |
| 2:C:2353:ILE:HG12 | 2:C:2359:ARG:HE | 1.45 | 0.81 |
| 2:D:1031:ARG:HH22 | 2:D:1042:THR:HG21 | 1.42 | 0.81 |
| 2:B:1689:ILE:HA | 2:B:1703:TYR:HE1 | 1.43 | 0.81 |
| 2:B:3227:ARG:HG2 | 2:B:3290:ILE:HD12 | 1.62 | 0.81 |
| 2:A:2353:ILE:HG12 | 2:A:2359:ARG:HE | 1.45 | 0.81 |
| 2:D:3227:ARG:HG2 | 2:D:3290:ILE:HD12 | 1.62 | 0.80 |
| 2:D:1689:ILE:HA | 2:D:1703:TYR:HE1 | 1.43 | 0.80 |
| 2:C:2711:ILE:O | 2:C:2780:LYS:NZ | 2.15 | 0.80 |
| 2:A:3227:ARG:HG2 | 2:A:3290:ILE:HD12 | 1.62 | 0.80 |
| 2:D:2711:ILE:O | 2:D:2780:LYS:NZ | 2.15 | 0.80 |
| 2:B:4640:PHE:CD2 | 2:B:4641:PRO:HD3 | 2.17 | 0.79 |
| 2:A:4640:PHE:CD2 | 2:A:4641:PRO:HD3 | 2.17 | 0.79 |
| 2:C:4640:PHE:CD2 | 2:C:4641:PRO:HD3 | 2.17 | 0.79 |
| 2:D:4640:PHE:CD2 | 2:D:4641:PRO:HD3 | 2.17 | 0.79 |
| 2:A:988:LEU:HB2 | 2:A:1055:ARG:HE | 1.48 | 0.79 |
| 2:D:988:LEU:HB2 | 2:D:1055:ARG:HE | 1.48 | 0.79 |
| 2:B:988:LEU:HB2 | 2:B:1055:ARG:HE | 1.48 | 0.79 |
| 2:C:3227:ARG:HG2 | 2:C:3290:ILE:HD12 | 1.62 | 0.79 |
| 2:B:2711:ILE:O | 2:B:2780:LYS:NZ | 2.15 | 0.79 |
| 2:A:1689:ILE:HD11 | 2:A:1706:LEU:HD13 | 1.65 | 0.78 |
| 2:B:1689:ILE:HD11 | 2:B:1706:LEU:HD13 | 1.65 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:2711:ILE:O | 2:A:2780:LYS:NZ | 2.15 | 0.78 |
| 2:A:4831:ILE:HG13 | 2:A:4843:ARG:HH21 | 1.48 | 0.78 |
| 2:A:1415:ASP:OD2 | 2:A:1559:ARG:NH2 | 2.17 | 0.78 |
| 2:D:1031:ARG:NH2 | 2:D:1038:LEU:HD11 | 1.99 | 0.78 |
| 2:B:4831:ILE:HG13 | 2:B:4843:ARG:HH21 | 1.48 | 0.78 |
| 2:D:4831:ILE:HG13 | 2:D:4843:ARG:HH21 | 1.48 | 0.78 |
| 2:D:1415:ASP:OD2 | 2:D:1559:ARG:NH2 | 2.17 | 0.77 |
| 2:C:1031:ARG:NH2 | 2:C:1038:LEU:HD11 | 1.99 | 0.77 |
| 2:D:1689:ILE:HD11 | 2:D:1706:LEU:HD13 | 1.65 | 0.77 |
| 2:C:1689:ILE:HD11 | 2:C:1706:LEU:HD13 | 1.65 | 0.77 |
| 2:C:1415:ASP:OD2 | 2:C:1559:ARG:NH2 | 2.17 | 0.77 |
| 2:C:4831:ILE:HG13 | 2:C:4843:ARG:HH21 | 1.49 | 0.77 |
| 2:D:3319:PHE:HB3 | 2:D:3323:MET:HE1 | 1.66 | 0.76 |
| 2:B:1031:ARG:NH2 | 2:B:1038:LEU:HD11 | 1.99 | 0.76 |
| 2:C:988:LEU:HB2 | 2:C:1055:ARG:HE | 1.48 | 0.76 |
| 2:A:3319:PHE:HB3 | 2:A:3323:MET:HE1 | 1.66 | 0.76 |
| 2:B:1415:ASP:OD2 | 2:B:1559:ARG:NH2 | 2.17 | 0.76 |
| 2:B:943:LEU:HA | 2:B:946:LEU:HD12 | 1.68 | 0.76 |
| 2:C:3319:PHE:HB3 | 2:C:3323:MET:HE1 | 1.66 | 0.76 |
| 2:A:943:LEU:HA | 2:A:946:LEU:HD12 | 1.68 | 0.75 |
| 2:A:866:PRO:HG2 | 2:A:1009:ARG:HD3 | 1.68 | 0.75 |
| 2:B:3319:PHE:HB3 | 2:B:3323:MET:HE1 | 1.66 | 0.75 |
| 2:D:866:PRO:HG2 | 2:D:1009:ARG:HD3 | 1.68 | 0.75 |
| 2:B:902:TRP:HB3 | 2:B:918:LEU:HD21 | 1.69 | 0.75 |
| 2:C:902:TRP:HB3 | 2:C:918:LEU:HD21 | 1.69 | 0.75 |
| 2:D:3803:LEU:HB2 | 2:D:3884:SER:HB3 | 1.69 | 0.75 |
| 2:A:1031:ARG:NH2 | 2:A:1038:LEU:HD11 | 1.99 | 0.74 |
| 2:A:3803:LEU:HB2 | 2:A:3884:SER:HB3 | 1.69 | 0.74 |
| 2:B:3945:VAL:HG23 | 2:B:4006:SER:HB3 | 1.70 | 0.74 |
| 2:C:2833:LEU:O | 2:C:2835:ARG:NH2 | 2.20 | 0.74 |
| 2:C:866:PRO:HG2 | 2:C:1009:ARG:HD3 | 1.68 | 0.74 |
| 2:B:2833:LEU:O | 2:B:2835:ARG:NH2 | 2.20 | 0.74 |
| 2:D:3945:VAL:HG23 | 2:D:4006:SER:HB3 | 1.70 | 0.74 |
| 2:A:2833:LEU:O | 2:A:2835:ARG:NH2 | 2.20 | 0.74 |
| 2:B:3803:LEU:HB2 | 2:B:3884:SER:HB3 | 1.69 | 0.74 |
| 2:D:943:LEU:HA | 2:D:946:LEU:HD12 | 1.68 | 0.74 |
| 2:B:866:PRO:HG2 | 2:B:1009:ARG:HD3 | 1.68 | 0.73 |
| 2:C:943:LEU:HA | 2:C:946:LEU:HD12 | 1.68 | 0.73 |
| 2:A:902:TRP:HB3 | 2:A:918:LEU:HD21 | 1.69 | 0.73 |
| 2:D:902:TRP:HB3 | 2:D:918:LEU:HD21 | 1.69 | 0.73 |
| 2:C:3803:LEU:HB2 | 2:C:3884:SER:HB3 | 1.69 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2833:LEU:O | 2:D:2835:ARG:NH2 | 2.20 | 0.73 |
| 2:B:4650:LYS:HG2 | 2:B:4670:LEU:HD22 | 1.71 | 0.73 |
| 2:A:3945:VAL:HG23 | 2:A:4006:SER:HB3 | 1.70 | 0.72 |
| 2:B:2241:ASP:OD1 | 2:B:2297:ARG:NH2 | 2.22 | 0.72 |
| 2:A:4650:LYS:HG2 | 2:A:4670:LEU:HD22 | 1.71 | 0.72 |
| 2:C:3945:VAL:HG23 | 2:C:4006:SER:HB3 | 1.70 | 0.72 |
| 2:C:2241:ASP:OD1 | 2:C:2297:ARG:NH2 | 2.23 | 0.71 |
| 1:H:19:LYS:NZ | 1:H:52:GLY:HA3 | 2.05 | 0.71 |
| 2:B:2627:TRP:HB2 | 2:B:2630:PHE:HB2 | 1.72 | 0.71 |
| 2:B:3250:TRP:O | 2:B:3256:ASN:ND2 | 2.21 | 0.71 |
| 2:C:2635:GLU:OE2 | 2:C:2680:TYR:OH | 2.08 | 0.71 |
| 2:C:4650:LYS:HG2 | 2:C:4670:LEU:HD22 | 1.71 | 0.71 |
| 2:B:2635:GLU:OE2 | 2:B:2680:TYR:OH | 2.08 | 0.71 |
| 2:C:4633:LEU:O | 2:C:4704:LYS:NZ | 2.24 | 0.71 |
| 2:D:4650:LYS:HG2 | 2:D:4670:LEU:HD22 | 1.71 | 0.71 |
| 1:G:19:LYS:NZ | 1:G:52:GLY:HA3 | 2.05 | 0.71 |
| 2:A:2241:ASP:OD1 | 2:A:2297:ARG:NH2 | 2.22 | 0.71 |
| 2:A:3260:ARG:NH1 | 2:A:3264:CYS:HA | 2.06 | 0.71 |
| 1:F:19:LYS:NZ | 1:F:52:GLY:HA3 | 2.05 | 0.71 |
| 2:D:114:LEU:HB2 | 2:D:117:HIS:CE1 | 2.26 | 0.71 |
| 2:B:4633:LEU:O | 2:B:4704:LYS:NZ | 2.24 | 0.71 |
| 2:D:2241:ASP:OD1 | 2:D:2297:ARG:NH2 | 2.23 | 0.71 |
| 1:E:19:LYS:NZ | 1:E:52:GLY:HA3 | 2.05 | 0.71 |
| 2:A:114:LEU:HB2 | 2:A:117:HIS:CE1 | 2.26 | 0.71 |
| 2:B:114:LEU:HB2 | 2:B:117:HIS:CE1 | 2.26 | 0.71 |
| 2:C:114:LEU:HB2 | 2:C:117:HIS:CE1 | 2.26 | 0.71 |
| 2:C:3172:GLU:HG3 | 2:C:3266:THR:HA | 1.73 | 0.71 |
| 2:D:2635:GLU:OE2 | 2:D:2680:TYR:OH | 2.08 | 0.70 |
| 2:A:1438:PRO:HG3 | 2:A:1500:ARG:HG2 | 1.72 | 0.70 |
| 2:A:2627:TRP:HB2 | 2:A:2630:PHE:HB2 | 1.72 | 0.70 |
| 2:A:2635:GLU:OE2 | 2:A:2680:TYR:OH | 2.08 | 0.70 |
| 2:A:4633:LEU:O | 2:A:4704:LYS:NZ | 2.24 | 0.70 |
| 2:B:2964:ALA:HA | 2:B:2968:LEU:HD12 | 1.74 | 0.70 |
| 2:B:3260:ARG:NH1 | 2:B:3264:CYS:HA | 2.06 | 0.70 |
| 2:D:3260:ARG:NH1 | 2:D:3264:CYS:HA | 2.06 | 0.70 |
| 2:A:2964:ALA:HA | 2:A:2968:LEU:HD12 | 1.74 | 0.70 |
| 2:A:3152:ARG:NH1 | 2:A:3236:GLU:OE2 | 2.25 | 0.70 |
| 2:B:1438:PRO:HG3 | 2:B:1500:ARG:HG2 | 1.72 | 0.70 |
| 2:A:3172:GLU:HG3 | 2:A:3266:THR:HA | 1.73 | 0.70 |
| 2:C:2627:TRP:HB2 | 2:C:2630:PHE:HB2 | 1.72 | 0.70 |
| 2:A:3250:TRP:O | 2:A:3256:ASN:ND2 | 2.21 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:1438:PRO:HG3 | 2:C:1500:ARG:HG2 | 1.72 | 0.70 |
| 2:D:1438:PRO:HG3 | 2:D:1500:ARG:HG2 | 1.72 | 0.70 |
| 2:D:4633:LEU:O | 2:D:4704:LYS:NZ | 2.24 | 0.70 |
| 2:B:3152:ARG:NH1 | 2:B:3236:GLU:OE2 | 2.25 | 0.70 |
| 2:C:3152:ARG:NH1 | 2:C:3236:GLU:OE2 | 2.25 | 0.70 |
| 2:D:1129:GLY:HA3 | 2:D:1145:TRP:HB3 | 1.74 | 0.70 |
| 2:B:1014:GLN:HB3 | 2:B:1027:ARG:HH21 | 1.57 | 0.69 |
| 2:C:2964:ALA:HA | 2:C:2968:LEU:HD12 | 1.74 | 0.69 |
| 2:C:1129:GLY:HA3 | 2:C:1145:TRP:HB3 | 1.74 | 0.69 |
| 2:B:1129:GLY:HA3 | 2:B:1145:TRP:HB3 | 1.74 | 0.69 |
| 2:C:1014:GLN:HB3 | 2:C:1027:ARG:HH21 | 1.57 | 0.69 |
| 2:C:2831:VAL:HB | 2:C:2894:LYS:HD3 | 1.73 | 0.69 |
| 2:C:3260:ARG:NH1 | 2:C:3264:CYS:HA | 2.06 | 0.69 |
| 2:D:3152:ARG:NH1 | 2:D:3236:GLU:OE2 | 2.25 | 0.69 |
| 2:D:3172:GLU:HG3 | 2:D:3266:THR:HA | 1.73 | 0.69 |
| 2:A:1129:GLY:HA3 | 2:A:1145:TRP:HB3 | 1.74 | 0.69 |
| 2:B:2831:VAL:HB | 2:B:2894:LYS:HD3 | 1.73 | 0.69 |
| 2:D:2831:VAL:HB | 2:D:2894:LYS:HD3 | 1.73 | 0.69 |
| 2:D:2964:ALA:HA | 2:D:2968:LEU:HD12 | 1.74 | 0.69 |
| 2:B:3172:GLU:HG3 | 2:B:3266:THR:HA | 1.73 | 0.69 |
| 2:B:932:ASN:HA | 2:B:935:MET:HE3 | 1.75 | 0.69 |
| 2:A:2831:VAL:HB | 2:A:2894:LYS:HD3 | 1.73 | 0.68 |
| 2:D:2627:TRP:HB2 | 2:D:2630:PHE:HB2 | 1.72 | 0.68 |
| 2:B:4690:LYS:NZ | 2:B:4692:SER:OG | 2.19 | 0.68 |
| 2:D:1014:GLN:HB3 | 2:D:1027:ARG:HH21 | 1.57 | 0.68 |
| 2:A:962:LYS:NZ | 2:A:964:MET:SD | 2.67 | 0.68 |
| 2:D:3250:TRP:O | 2:D:3256:ASN:ND2 | 2.21 | 0.68 |
| 2:A:1100:ARG:NH1 | 2:A:1234:GLU:O | 2.26 | 0.68 |
| 1:G:22:THR:N | 1:G:108:GLU:O | 2.27 | 0.68 |
| 2:A:1014:GLN:HB3 | 2:A:1027:ARG:HH21 | 1.57 | 0.68 |
| 2:D:962:LYS:NZ | 2:D:964:MET:SD | 2.67 | 0.68 |
| 2:B:908:ARG:HD2 | 2:B:916:PRO:HD2 | 1.76 | 0.68 |
| 2:D:2694:SER:O | 2:D:2702:ASN:N | 2.26 | 0.68 |
| 2:A:908:ARG:HD2 | 2:A:916:PRO:HD2 | 1.76 | 0.68 |
| 2:B:2599:LEU:HD12 | 2:B:2661:LEU:HD21 | 1.76 | 0.68 |
| 2:C:2599:LEU:HD12 | 2:C:2661:LEU:HD21 | 1.76 | 0.68 |
| 2:D:2424:ARG:HG2 | 2:D:2476:TYR:HE1 | 1.59 | 0.68 |
| 2:C:2424:ARG:HG2 | 2:C:2476:TYR:HE1 | 1.59 | 0.67 |
| 2:C:3227:ARG:HD3 | 2:C:3229:THR:H | 1.60 | 0.67 |
| 2:A:2424:ARG:HG2 | 2:A:2476:TYR:HE1 | 1.59 | 0.67 |
| 2:D:908:ARG:HD2 | 2:D:916:PRO:HD2 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2830:ASN:ND2 | 2:C:1549:SER:HB2 | 2.09 | 0.67 |
| 2:C:908:ARG:HD2 | 2:C:916:PRO:HD2 | 1.76 | 0.67 |
| 1:E:24:VAL:HG22 | 1:E:48:LYS:HG2 | 1.77 | 0.67 |
| 2:A:2599:LEU:HD12 | 2:A:2661:LEU:HD21 | 1.76 | 0.67 |
| 2:B:2424:ARG:HG2 | 2:B:2476:TYR:HE1 | 1.59 | 0.67 |
| 2:C:962:LYS:NZ | 2:C:964:MET:SD | 2.67 | 0.67 |
| 2:D:2599:LEU:HD12 | 2:D:2661:LEU:HD21 | 1.76 | 0.67 |
| 2:C:3284:ILE:HD12 | 2:C:3287:ASN:HD22 | 1.59 | 0.67 |
| 1:F:24:VAL:HG22 | 1:F:48:LYS:HG2 | 1.77 | 0.67 |
| 2:B:962:LYS:NZ | 2:B:964:MET:SD | 2.67 | 0.67 |
| 2:B:1100:ARG:NH1 | 2:B:1234:GLU:O | 2.26 | 0.67 |
| 1:E:22:THR:N | 1:E:108:GLU:O | 2.27 | 0.66 |
| 2:B:2694:SER:O | 2:B:2702:ASN:N | 2.26 | 0.66 |
| 2:D:3227:ARG:HD3 | 2:D:3229:THR:H | 1.60 | 0.66 |
| 1:H:24:VAL:HG22 | 1:H:48:LYS:HG2 | 1.77 | 0.66 |
| 2:A:2427:ILE:O | 2:A:2476:TYR:OH | 2.14 | 0.66 |
| 2:A:3284:ILE:HD12 | 2:A:3287:ASN:HD22 | 1.59 | 0.66 |
| 2:B:1286:THR:OG1 | 2:B:1550:PRO:O | 2.13 | 0.66 |
| 2:C:3250:TRP:O | 2:C:3256:ASN:ND2 | 2.21 | 0.66 |
| 2:D:3284:ILE:HD12 | 2:D:3287:ASN:HD22 | 1.59 | 0.66 |
| 1:H:22:THR:N | 1:H:108:GLU:O | 2.27 | 0.66 |
| 1:G:24:VAL:HG22 | 1:G:48:LYS:HG2 | 1.77 | 0.66 |
| 2:B:3284:ILE:HD12 | 2:B:3287:ASN:HD22 | 1.59 | 0.66 |
| 2:C:2830:ASN:ND2 | 2:D:1549:SER:HB2 | 2.10 | 0.66 |
| 2:A:2502:LEU:HG | 2:A:2512:MET:HE1 | 1.77 | 0.66 |
| 2:B:924:LEU:HD12 | 2:B:925:PRO:HD2 | 1.77 | 0.66 |
| 2:D:4047:ASP:HA | 2:D:4050:LYS:HE3 | 1.77 | 0.66 |
| 2:A:2139:GLU:HG3 | 2:A:2192:MET:HB3 | 1.78 | 0.66 |
| 2:A:2694:SER:O | 2:A:2702:ASN:N | 2.26 | 0.66 |
| 2:D:932:ASN:HA | 2:D:935:MET:HE3 | 1.76 | 0.66 |
| 2:A:3227:ARG:HD3 | 2:A:3229:THR:H | 1.60 | 0.66 |
| 2:D:1100:ARG:NH1 | 2:D:1234:GLU:O | 2.26 | 0.66 |
| 2:D:2139:GLU:HG3 | 2:D:2192:MET:HB3 | 1.78 | 0.66 |
| 2:D:4661:TYR:HB3 | 2:D:4665:ARG:HH21 | 1.60 | 0.66 |
| 1:F:22:THR:N | 1:F:108:GLU:O | 2.27 | 0.66 |
| 2:C:4661:TYR:HB3 | 2:C:4665:ARG:HH21 | 1.60 | 0.66 |
| 2:A:1286:THR:OG1 | 2:A:1550:PRO:O | 2.13 | 0.66 |
| 2:B:1017:THR:O | 2:B:1028:ARG:HA | 1.96 | 0.66 |
| 1:E:16:PHE:O | 1:E:18:LYS:NZ | 2.29 | 0.65 |
| 1:G:16:PHE:O | 1:G:18:LYS:NZ | 2.29 | 0.65 |
| 2:B:2139:GLU:HG3 | 2:B:2192:MET:HB3 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2427:ILE:O | 2:B:2476:TYR:OH | 2.14 | 0.65 |
| 2:C:2427:ILE:O | 2:C:2476:TYR:OH | 2.14 | 0.65 |
| 2:D:2427:ILE:O | 2:D:2476:TYR:OH | 2.14 | 0.65 |
| 1:G:79:PRO:HD3 | 1:G:97:THR:HG22 | 1.79 | 0.65 |
| 2:A:1017:THR:O | 2:A:1028:ARG:HA | 1.96 | 0.65 |
| 2:A:2179:LEU:O | 2:A:2183:GLU:HB2 | 1.97 | 0.65 |
| 2:B:2179:LEU:O | 2:B:2183:GLU:HB2 | 1.97 | 0.65 |
| 2:C:924:LEU:HD12 | 2:C:925:PRO:HD2 | 1.77 | 0.65 |
| 1:H:16:PHE:O | 1:H:18:LYS:NZ | 2.29 | 0.65 |
| 1:H:79:PRO:HD3 | 1:H:97:THR:HG22 | 1.79 | 0.65 |
| 2:B:4661:TYR:HB3 | 2:B:4665:ARG:HH21 | 1.60 | 0.65 |
| 2:C:1100:ARG:NH1 | 2:C:1234:GLU:O | 2.26 | 0.65 |
| 2:A:769:ARG:HG2 | 2:A:774:PRO:HA | 1.78 | 0.65 |
| 2:A:2436:ILE:HG22 | 2:A:2491:GLY:HA3 | 1.78 | 0.65 |
| 2:B:769:ARG:HG2 | 2:B:774:PRO:HA | 1.78 | 0.65 |
| 2:B:3227:ARG:HD3 | 2:B:3229:THR:H | 1.60 | 0.65 |
| 2:D:924:LEU:HD12 | 2:D:925:PRO:HD2 | 1.77 | 0.65 |
| 2:A:4661:TYR:HB3 | 2:A:4665:ARG:HH21 | 1.60 | 0.65 |
| 2:B:4047:ASP:HA | 2:B:4050:LYS:HE3 | 1.77 | 0.65 |
| 2:B:2943:PHE:O | 2:B:2947:SER:N | 2.29 | 0.65 |
| 2:C:1017:THR:O | 2:C:1028:ARG:HA | 1.96 | 0.65 |
| 1:E:79:PRO:HD3 | 1:E:97:THR:HG22 | 1.79 | 0.65 |
| 2:C:2139:GLU:HG3 | 2:C:2192:MET:HB3 | 1.78 | 0.65 |
| 2:C:2943:PHE:O | 2:C:2947:SER:N | 2.30 | 0.65 |
| 2:C:4047:ASP:HA | 2:C:4050:LYS:HE3 | 1.77 | 0.65 |
| 2:D:1017:THR:O | 2:D:1028:ARG:HA | 1.96 | 0.65 |
| 1:F:16:PHE:O | 1:F:18:LYS:NZ | 2.29 | 0.65 |
| 2:A:963:LYS:HD2 | 2:A:980:PRO:HA | 1.79 | 0.65 |
| 2:C:2157:GLN:O | 2:C:3615:ARG:NH2 | 2.30 | 0.65 |
| 2:C:2436:ILE:HG22 | 2:C:2491:GLY:HA3 | 1.78 | 0.65 |
| 2:D:1286:THR:OG1 | 2:D:1550:PRO:O | 2.13 | 0.65 |
| 2:A:2943:PHE:O | 2:A:2947:SER:N | 2.30 | 0.65 |
| 2:C:1431:ARG:NH1 | 2:C:1506:GLU:OE2 | 2.30 | 0.65 |
| 2:C:2694:SER:O | 2:C:2702:ASN:N | 2.26 | 0.65 |
| 2:C:2773:TRP:HB3 | 2:C:2774:PRO:HD3 | 1.79 | 0.65 |
| 2:B:2773:TRP:HB3 | 2:B:2774:PRO:HD3 | 1.79 | 0.65 |
| 1:F:79:PRO:HD3 | 1:F:97:THR:HG22 | 1.79 | 0.64 |
| 2:A:4047:ASP:HA | 2:A:4050:LYS:HE3 | 1.78 | 0.64 |
| 2:B:2157:GLN:O | 2:B:3615:ARG:NH2 | 2.30 | 0.64 |
| 2:A:924:LEU:HD12 | 2:A:925:PRO:HD2 | 1.77 | 0.64 |
| 2:D:2157:GLN:O | 2:D:3615:ARG:NH2 | 2.30 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2436:ILE:HG22 | 2:D:2491:GLY:HA3 | 1.78 | 0.64 |
| 2:A:1549:SER:HB2 | 2:D:2830:ASN:ND2 | 2.13 | 0.64 |
| 2:B:2436:ILE:HG22 | 2:B:2491:GLY:HA3 | 1.78 | 0.64 |
| 2:D:2455:ASP:OD2 | 2:D:2457:SER:OG | 2.15 | 0.64 |
| 2:A:2157:GLN:O | 2:A:3615:ARG:NH2 | 2.30 | 0.64 |
| 2:C:963:LYS:HD2 | 2:C:980:PRO:HA | 1.79 | 0.64 |
| 2:D:1431:ARG:NH1 | 2:D:1506:GLU:OE2 | 2.30 | 0.64 |
| 2:D:2179:LEU:O | 2:D:2183:GLU:HB2 | 1.97 | 0.64 |
| 2:B:963:LYS:HD2 | 2:B:980:PRO:HA | 1.79 | 0.64 |
| 2:C:769:ARG:HG2 | 2:C:774:PRO:HA | 1.78 | 0.64 |
| 1:H:41:ARG:NH2 | 1:H:103:GLU:OE1 | 2.31 | 0.64 |
| 2:B:1431:ARG:NH1 | 2:B:1506:GLU:OE2 | 2.30 | 0.64 |
| 1:E:41:ARG:NH2 | 1:E:103:GLU:OE1 | 2.31 | 0.64 |
| 2:C:2179:LEU:O | 2:C:2183:GLU:HB2 | 1.96 | 0.64 |
| 2:D:4690:LYS:NZ | 2:D:4692:SER:OG | 2.19 | 0.64 |
| 2:A:891:GLU:HB3 | 2:A:978:PRO:HB3 | 1.80 | 0.64 |
| 2:A:1685:LEU:HB3 | 2:A:1706:LEU:HD12 | 1.80 | 0.64 |
| 2:C:1029:ASN:ND2 | 2:C:1031:ARG:HB2 | 2.13 | 0.64 |
| 2:C:2642:ARG:HH12 | 2:C:2921:PHE:HA | 1.62 | 0.64 |
| 2:D:194:LEU:HD11 | 2:D:201:LEU:HB3 | 1.80 | 0.64 |
| 2:A:1431:ARG:NH1 | 2:A:1506:GLU:OE2 | 2.30 | 0.64 |
| 2:A:3044:THR:HA | 2:A:3047:LYS:HG2 | 1.80 | 0.64 |
| 2:A:4056:LYS:NZ | 2:B:4660:PHE:O | 2.31 | 0.64 |
| 2:B:912:LYS:NZ | 2:B:914:GLN:O | 2.26 | 0.64 |
| 2:C:520:ARG:NH1 | 2:C:521:GLU:HB3 | 2.13 | 0.64 |
| 2:D:1029:ASN:ND2 | 2:D:1031:ARG:HB2 | 2.13 | 0.64 |
| 2:A:1029:ASN:ND2 | 2:A:1031:ARG:HB2 | 2.13 | 0.63 |
| 2:D:891:GLU:HB3 | 2:D:978:PRO:HB3 | 1.80 | 0.63 |
| 2:D:924:LEU:HD23 | 2:D:929:ARG:HB2 | 1.80 | 0.63 |
| 2:A:3201:VAL:HA | 2:A:3204:VAL:HG12 | 1.80 | 0.63 |
| 2:B:924:LEU:HD23 | 2:B:929:ARG:HB2 | 1.79 | 0.63 |
| 2:B:1167:ASP:OD1 | 2:B:1169:ASN:ND2 | 2.30 | 0.63 |
| 2:C:3044:THR:HA | 2:C:3047:LYS:HG2 | 1.80 | 0.63 |
| 2:D:520:ARG:NH1 | 2:D:521:GLU:HB3 | 2.13 | 0.63 |
| 2:D:769:ARG:HG2 | 2:D:774:PRO:HA | 1.78 | 0.63 |
| 2:D:2642:ARG:HH12 | 2:D:2921:PHE:HA | 1.62 | 0.63 |
| 2:D:3044:THR:HA | 2:D:3047:LYS:HG2 | 1.80 | 0.63 |
| 2:C:320:GLU:OE1 | 2:C:320:GLU:N | 2.31 | 0.63 |
| 2:C:1522:ALA:HB3 | 2:C:1527:LEU:HD21 | 1.81 | 0.63 |
| 2:D:879:GLU:O | 2:D:882:ARG:NH1 | 2.32 | 0.63 |
| 2:D:963:LYS:HD2 | 2:D:980:PRO:HA | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2896:LEU:HD12 | 2:D:2901:TYR:HB2 | 1.81 | 0.63 |
| 2:A:320:GLU:OE1 | 2:A:320:GLU:N | 2.31 | 0.63 |
| 2:A:3605:MET:HG2 | 2:A:3606:ALA:H | 1.63 | 0.63 |
| 2:D:2773:TRP:HB3 | 2:D:2774:PRO:HD3 | 1.79 | 0.63 |
| 2:A:194:LEU:HD11 | 2:A:201:LEU:HB3 | 1.80 | 0.63 |
| 2:B:520:ARG:NH1 | 2:B:521:GLU:HB3 | 2.13 | 0.63 |
| 2:B:1029:ASN:ND2 | 2:B:1031:ARG:HB2 | 2.13 | 0.63 |
| 2:B:1685:LEU:HB3 | 2:B:1706:LEU:HD12 | 1.80 | 0.63 |
| 2:B:2642:ARG:HH12 | 2:B:2921:PHE:HA | 1.63 | 0.63 |
| 2:B:2896:LEU:HD12 | 2:B:2901:TYR:HB2 | 1.81 | 0.63 |
| 2:B:3201:VAL:HA | 2:B:3204:VAL:HG12 | 1.80 | 0.63 |
| 2:C:4045:LYS:HD3 | 2:C:4072:THR:HB | 1.80 | 0.63 |
| 2:C:4690:LYS:NZ | 2:C:4692:SER:OG | 2.19 | 0.63 |
| 1:F:41:ARG:NH2 | 1:F:103:GLU:OE1 | 2.31 | 0.63 |
| 2:A:879:GLU:O | 2:A:882:ARG:NH1 | 2.32 | 0.63 |
| 2:A:2773:TRP:HB3 | 2:A:2774:PRO:HD3 | 1.80 | 0.63 |
| 2:A:3242:LEU:O | 2:A:3246:MET:HG2 | 1.99 | 0.63 |
| 2:C:3325:LYS:HG3 | 2:C:3328:LYS:HZ2 | 1.64 | 0.63 |
| 2:D:3242:LEU:O | 2:D:3246:MET:HG2 | 1.99 | 0.63 |
| 2:A:1167:ASP:OD1 | 2:A:1169:ASN:ND2 | 2.30 | 0.63 |
| 2:A:2896:LEU:HD12 | 2:A:2901:TYR:HB2 | 1.81 | 0.63 |
| 2:B:891:GLU:HB3 | 2:B:978:PRO:HB3 | 1.80 | 0.63 |
| 2:B:4045:LYS:HD3 | 2:B:4072:THR:HB | 1.80 | 0.63 |
| 2:D:3325:LYS:HG3 | 2:D:3328:LYS:HZ2 | 1.64 | 0.63 |
| 1:G:41:ARG:NH2 | 1:G:103:GLU:OE1 | 2.31 | 0.63 |
| 2:B:1522:ALA:HB3 | 2:B:1527:LEU:HD21 | 1.81 | 0.63 |
| 2:C:924:LEU:HD23 | 2:C:929:ARG:HB2 | 1.79 | 0.63 |
| 2:C:2896:LEU:HD12 | 2:C:2901:TYR:HB2 | 1.81 | 0.63 |
| 2:C:3201:VAL:HA | 2:C:3204:VAL:HG12 | 1.80 | 0.63 |
| 2:D:2943:PHE:O | 2:D:2947:SER:N | 2.29 | 0.63 |
| 2:D:4045:LYS:HD3 | 2:D:4072:THR:HB | 1.80 | 0.63 |
| 2:A:2570:GLU:HG2 | 2:A:2605:MET:HG2 | 1.81 | 0.62 |
| 2:A:3040:LEU:O | 2:A:3111:HIS:NE2 | 2.33 | 0.62 |
| 2:C:3242:LEU:O | 2:C:3246:MET:HG2 | 1.98 | 0.62 |
| 2:D:694:ARG:NH1 | 2:D:718:VAL:O | 2.32 | 0.62 |
| 2:A:2642:ARG:HH12 | 2:A:2921:PHE:HA | 1.63 | 0.62 |
| 2:C:932:ASN:HA | 2:C:935:MET:HE3 | 1.79 | 0.62 |
| 2:C:2455:ASP:OD2 | 2:C:2457:SER:OG | 2.15 | 0.62 |
| 2:C:2570:GLU:HG2 | 2:C:2605:MET:HG2 | 1.81 | 0.62 |
| 2:A:2232:PRO:HD2 | 2:A:2379:ASP:HA | 1.82 | 0.62 |
| 2:A:2980:LEU:HG | 2:A:2990:LEU:HD23 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:4187:GLU:OE2 | 2:A:4947:ARG:NH2 | 2.33 | 0.62 |
| 2:B:965:LYS:HA | 2:B:977:LYS:HG3 | 1.82 | 0.62 |
| 2:B:2767:GLU:HA | 2:B:2770:ILE:HG12 | 1.81 | 0.62 |
| 2:B:3040:LEU:O | 2:B:3111:HIS:NE2 | 2.32 | 0.62 |
| 2:D:905:GLY:HA3 | 2:D:914:GLN:HB3 | 1.81 | 0.62 |
| 2:D:2232:PRO:HD2 | 2:D:2379:ASP:HA | 1.82 | 0.62 |
| 2:A:1980:LYS:O | 2:A:1983:LYS:NZ | 2.32 | 0.62 |
| 2:B:3044:THR:HA | 2:B:3047:LYS:HG2 | 1.80 | 0.62 |
| 2:C:194:LEU:HD11 | 2:C:201:LEU:HB3 | 1.80 | 0.62 |
| 2:C:1167:ASP:OD1 | 2:C:1169:ASN:ND2 | 2.30 | 0.62 |
| 4:C:5003:ATP:H5'2 | 5:C:5004:KVR:C17 | 2.29 | 0.62 |
| 2:D:1522:ALA:HB3 | 2:D:1527:LEU:HD21 | 1.81 | 0.62 |
| 2:A:520:ARG:NH1 | 2:A:521:GLU:HB3 | 2.13 | 0.62 |
| 2:A:4044:SER:HA | 2:A:4077:THR:HA | 1.80 | 0.62 |
| 2:B:320:GLU:OE1 | 2:B:320:GLU:N | 2.31 | 0.62 |
| 2:B:555:LEU:HD21 | 2:B:578:VAL:HG11 | 1.81 | 0.62 |
| 2:B:3242:LEU:O | 2:B:3246:MET:HG2 | 1.98 | 0.62 |
| 2:C:3040:LEU:O | 2:C:3111:HIS:NE2 | 2.33 | 0.62 |
| 2:D:320:GLU:OE1 | 2:D:320:GLU:N | 2.31 | 0.62 |
| 2:D:2980:LEU:HG | 2:D:2990:LEU:HD23 | 1.81 | 0.62 |
| 2:B:2980:LEU:HG | 2:B:2990:LEU:HD23 | 1.81 | 0.62 |
| 2:B:3605:MET:HG2 | 2:B:3606:ALA:H | 1.63 | 0.62 |
| 2:B:4027:THR:HG21 | 2:B:4084:VAL:HG11 | 1.82 | 0.62 |
| 2:B:4187:GLU:OE2 | 2:B:4947:ARG:NH2 | 2.33 | 0.62 |
| 2:D:1167:ASP:OD1 | 2:D:1169:ASN:ND2 | 2.30 | 0.62 |
| 2:D:3201:VAL:HA | 2:D:3204:VAL:HG12 | 1.80 | 0.62 |
| 2:A:3221:LEU:HD11 | 2:A:3234:VAL:HG21 | 1.82 | 0.62 |
| 4:A:5003:ATP:H5'2 | 5:A:5004:KVR:C17 | 2.29 | 0.62 |
| 2:B:1980:LYS:O | 2:B:1983:LYS:NZ | 2.33 | 0.62 |
| 2:C:694:ARG:NH1 | 2:C:718:VAL:O | 2.32 | 0.62 |
| 2:C:4044:SER:HA | 2:C:4077:THR:HA | 1.80 | 0.62 |
| 4:D:5003:ATP:H5'2 | 5:D:5004:KVR:C17 | 2.29 | 0.62 |
| 2:A:555:LEU:HD21 | 2:A:578:VAL:HG11 | 1.81 | 0.62 |
| 2:A:4027:THR:HG21 | 2:A:4084:VAL:HG11 | 1.82 | 0.62 |
| 2:B:274:LEU:HD11 | 2:B:412:GLU:HG2 | 1.82 | 0.62 |
| 2:B:3269:ASN:HD21 | 2:B:3271:GLU:HB3 | 1.65 | 0.62 |
| 2:C:1685:LEU:O | 2:C:1689:ILE:HG12 | 2.00 | 0.62 |
| 2:C:2767:GLU:HA | 2:C:2770:ILE:HG12 | 1.81 | 0.62 |
| 2:D:2570:GLU:HG2 | 2:D:2605:MET:HG2 | 1.81 | 0.62 |
| 2:A:965:LYS:HA | 2:A:977:LYS:HG3 | 1.82 | 0.62 |
| 2:A:2455:ASP:OD2 | 2:A:2457:SER:OG | 2.15 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:3141:GLY:O | 2:A:3152:ARG:NH1 | 2.33 | 0.62 |
| 2:A:3269:ASN:HD21 | 2:A:3271:GLU:HB3 | 1.65 | 0.62 |
| 2:B:194:LEU:HD11 | 2:B:201:LEU:HB3 | 1.80 | 0.62 |
| 2:B:1685:LEU:O | 2:B:1689:ILE:HG12 | 2.00 | 0.62 |
| 2:B:3141:GLY:O | 2:B:3152:ARG:NH1 | 2.33 | 0.62 |
| 2:C:1685:LEU:HB3 | 2:C:1706:LEU:HD12 | 1.80 | 0.62 |
| 2:C:1980:LYS:O | 2:C:1983:LYS:NZ | 2.32 | 0.62 |
| 2:D:274:LEU:HD11 | 2:D:412:GLU:HG2 | 1.82 | 0.62 |
| 2:D:555:LEU:HD21 | 2:D:578:VAL:HG11 | 1.81 | 0.62 |
| 2:D:2868:HIS:HB3 | 2:D:2871:LEU:HG | 1.82 | 0.62 |
| 2:D:3605:MET:HG2 | 2:D:3606:ALA:H | 1.63 | 0.62 |
| 2:D:4187:GLU:OE2 | 2:D:4947:ARG:NH2 | 2.33 | 0.62 |
| 2:A:924:LEU:HD23 | 2:A:929:ARG:HB2 | 1.80 | 0.62 |
| 2:A:1522:ALA:HB3 | 2:A:1527:LEU:HD21 | 1.81 | 0.62 |
| 2:A:2793:ARG:NH2 | 2:A:2796:ASP:OD2 | 2.33 | 0.62 |
| 2:C:965:LYS:HA | 2:C:977:LYS:HG3 | 1.82 | 0.62 |
| 2:C:4187:GLU:OE2 | 2:C:4947:ARG:NH2 | 2.33 | 0.62 |
| 2:D:1685:LEU:O | 2:D:1689:ILE:HG12 | 2.00 | 0.62 |
| 2:A:274:LEU:HD11 | 2:A:412:GLU:HG2 | 1.82 | 0.61 |
| 2:A:921:PHE:HB2 | 2:A:929:ARG:HD3 | 1.82 | 0.61 |
| 2:A:1685:LEU:O | 2:A:1689:ILE:HG12 | 2.00 | 0.61 |
| 2:B:2232:PRO:HD2 | 2:B:2379:ASP:HA | 1.82 | 0.61 |
| 2:C:905:GLY:HA3 | 2:C:914:GLN:HB3 | 1.81 | 0.61 |
| 2:C:1689:ILE:HA | 2:C:1703:TYR:CE1 | 2.32 | 0.61 |
| 2:B:2793:ARG:NH2 | 2:B:2796:ASP:OD2 | 2.33 | 0.61 |
| 2:B:4044:SER:HA | 2:B:4077:THR:HA | 1.80 | 0.61 |
| 2:C:891:GLU:HB3 | 2:C:978:PRO:HB3 | 1.80 | 0.61 |
| 2:C:3221:LEU:HD11 | 2:C:3234:VAL:HG21 | 1.81 | 0.61 |
| 2:D:2767:GLU:HA | 2:D:2770:ILE:HG12 | 1.81 | 0.61 |
| 2:D:4027:THR:HG21 | 2:D:4084:VAL:HG11 | 1.82 | 0.61 |
| 2:A:288:HIS:O | 2:A:290:ARG:NH1 | 2.33 | 0.61 |
| 2:A:932:ASN:HA | 2:A:935:MET:HE3 | 1.83 | 0.61 |
| 2:A:4045:LYS:HD3 | 2:A:4072:THR:HB | 1.80 | 0.61 |
| 2:B:905:GLY:HA3 | 2:B:914:GLN:HB3 | 1.81 | 0.61 |
| 2:C:2232:PRO:HD2 | 2:C:2379:ASP:HA | 1.81 | 0.61 |
| 2:C:2793:ARG:NH2 | 2:C:2796:ASP:OD2 | 2.33 | 0.61 |
| 2:A:905:GLY:HA3 | 2:A:914:GLN:HB3 | 1.81 | 0.61 |
| 2:B:921:PHE:HB2 | 2:B:929:ARG:HD3 | 1.82 | 0.61 |
| 2:C:175:VAL:HG11 | 2:C:181:LEU:HD21 | 1.82 | 0.61 |
| 2:C:3269:ASN:HD21 | 2:C:3271:GLU:HB3 | 1.65 | 0.61 |
| 2:C:3605:MET:HG2 | 2:C:3606:ALA:H | 1.63 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:4044:SER:HA | 2:D:4077:THR:HA | 1.80 | 0.61 |
| 2:A:3301:VAL:HA | 2:A:3304:GLN:HG2 | 1.83 | 0.61 |
| 2:B:2570:GLU:HG2 | 2:B:2605:MET:HG2 | 1.81 | 0.61 |
| 2:C:1286:THR:OG1 | 2:C:1550:PRO:O | 2.13 | 0.61 |
| 2:C:3141:GLY:O | 2:C:3152:ARG:NH1 | 2.33 | 0.61 |
| 2:D:2176:VAL:HG22 | 2:D:2220:TYR:CZ | 2.35 | 0.61 |
| 2:A:175:VAL:HG11 | 2:A:181:LEU:HD21 | 1.82 | 0.61 |
| 2:A:2868:HIS:HB3 | 2:A:2871:LEU:HG | 1.82 | 0.61 |
| 2:D:965:LYS:HA | 2:D:977:LYS:HG3 | 1.82 | 0.61 |
| 2:D:3040:LEU:O | 2:D:3111:HIS:NE2 | 2.33 | 0.61 |
| 4:B:5003:ATP:H5'2 | 5:B:5004:KVR:C17 | 2.29 | 0.61 |
| 2:C:555:LEU:HD21 | 2:C:578:VAL:HG11 | 1.81 | 0.61 |
| 2:A:4822:ARG:HH12 | 2:B:4829:ASP:N | 1.99 | 0.61 |
| 2:B:694:ARG:NH1 | 2:B:718:VAL:O | 2.32 | 0.61 |
| 2:C:912:LYS:NZ | 2:C:914:GLN:O | 2.26 | 0.61 |
| 2:D:3141:GLY:O | 2:D:3152:ARG:NH1 | 2.33 | 0.61 |
| 2:A:2176:VAL:HG22 | 2:A:2220:TYR:CZ | 2.35 | 0.61 |
| 2:A:2767:GLU:HA | 2:A:2770:ILE:HG12 | 1.81 | 0.61 |
| 2:A:4831:ILE:HG13 | 2:A:4843:ARG:NH2 | 2.16 | 0.61 |
| 2:B:3301:VAL:HA | 2:B:3304:GLN:HG2 | 1.83 | 0.61 |
| 2:B:4831:ILE:HG13 | 2:B:4843:ARG:NH2 | 2.16 | 0.61 |
| 2:C:274:LEU:HD11 | 2:C:412:GLU:HG2 | 1.82 | 0.61 |
| 2:C:879:GLU:O | 2:C:882:ARG:NH1 | 2.32 | 0.61 |
| 2:C:3018:ARG:HG2 | 2:C:3021:LEU:HD22 | 1.83 | 0.61 |
| 2:C:4027:THR:HG21 | 2:C:4084:VAL:HG11 | 1.82 | 0.61 |
| 2:D:1685:LEU:HB3 | 2:D:1706:LEU:HD12 | 1.80 | 0.61 |
| 2:A:1444:GLY:HA3 | 2:A:1487:MET:HA | 1.83 | 0.61 |
| 2:B:175:VAL:HG11 | 2:B:181:LEU:HD21 | 1.82 | 0.61 |
| 2:B:1031:ARG:HH22 | 2:B:1042:THR:CG2 | 2.13 | 0.61 |
| 2:C:2176:VAL:HG22 | 2:C:2220:TYR:CZ | 2.35 | 0.61 |
| 2:D:801:ARG:NH1 | 2:D:1615:GLN:O | 2.34 | 0.61 |
| 2:B:4056:LYS:NZ | 2:C:4660:PHE:O | 2.34 | 0.60 |
| 2:C:2724:TYR:OH | 2:C:2891:ASP:OD1 | 2.18 | 0.60 |
| 2:C:2868:HIS:HB3 | 2:C:2871:LEU:HG | 1.82 | 0.60 |
| 2:C:2980:LEU:HG | 2:C:2990:LEU:HD23 | 1.81 | 0.60 |
| 2:D:288:HIS:O | 2:D:290:ARG:NH1 | 2.33 | 0.60 |
| 2:D:3269:ASN:HD21 | 2:D:3271:GLU:HB3 | 1.65 | 0.60 |
| 2:B:1444:GLY:HA3 | 2:B:1487:MET:HA | 1.83 | 0.60 |
| 2:B:2176:VAL:HG22 | 2:B:2220:TYR:CZ | 2.35 | 0.60 |
| 2:C:515:ALA:HB2 | 2:C:523:GLY:HA3 | 1.84 | 0.60 |
| 2:C:921:PHE:HB2 | 2:C:929:ARG:HD3 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:2424:ARG:HG2 | 2:C:2476:TYR:CE1 | 2.36 | 0.60 |
| 2:C:4748:MET:HA | 2:C:4754:ARG:HH21 | 1.66 | 0.60 |
| 2:D:175:VAL:HG11 | 2:D:181:LEU:HD21 | 1.82 | 0.60 |
| 2:D:921:PHE:HB2 | 2:D:929:ARG:HD3 | 1.82 | 0.60 |
| 2:A:1031:ARG:HH22 | 2:A:1042:THR:CG2 | 2.13 | 0.60 |
| 2:B:3221:LEU:HD11 | 2:B:3234:VAL:HG21 | 1.82 | 0.60 |
| 2:C:2502:LEU:HG | 2:C:2512:MET:HE1 | 1.84 | 0.60 |
| 2:D:234:LEU:HD13 | 2:D:405:LEU:HD22 | 1.83 | 0.60 |
| 2:D:1980:LYS:O | 2:D:1983:LYS:NZ | 2.33 | 0.60 |
| 2:B:1689:ILE:HA | 2:B:1703:TYR:CE1 | 2.32 | 0.60 |
| 2:C:801:ARG:NH1 | 2:C:1615:GLN:O | 2.34 | 0.60 |
| 2:C:971:GLN:HE22 | 2:C:978:PRO:HD3 | 1.66 | 0.60 |
| 2:D:3221:LEU:HD11 | 2:D:3234:VAL:HG21 | 1.81 | 0.60 |
| 2:A:3018:ARG:HG2 | 2:A:3021:LEU:HD22 | 1.83 | 0.60 |
| 2:B:515:ALA:HB2 | 2:B:523:GLY:HA3 | 1.84 | 0.60 |
| 2:B:2455:ASP:OD2 | 2:B:2457:SER:OG | 2.15 | 0.60 |
| 2:D:3301:VAL:HA | 2:D:3304:GLN:HG2 | 1.83 | 0.60 |
| 2:A:3325:LYS:HG3 | 2:A:3328:LYS:HZ2 | 1.67 | 0.60 |
| 2:B:971:GLN:HE22 | 2:B:978:PRO:HD3 | 1.67 | 0.60 |
| 2:B:2717:LEU:HD23 | 2:B:2779:LEU:HD23 | 1.84 | 0.60 |
| 2:C:3301:VAL:HA | 2:C:3304:GLN:HG2 | 1.83 | 0.60 |
| 2:D:3018:ARG:HG2 | 2:D:3021:LEU:HD22 | 1.83 | 0.60 |
| 2:A:801:ARG:NH1 | 2:A:1615:GLN:O | 2.34 | 0.60 |
| 2:C:629:GLN:OE1 | 2:C:1669:ASN:ND2 | 2.29 | 0.60 |
| 2:D:1559:ARG:HD2 | 2:D:1565:PRO:HD3 | 1.84 | 0.60 |
| 2:A:2679:ASP:HA | 2:A:2920:ARG:HH21 | 1.67 | 0.60 |
| 2:A:4270:LYS:NZ | 2:A:4278:ASP:OD1 | 2.25 | 0.60 |
| 2:B:2424:ARG:HG2 | 2:B:2476:TYR:CE1 | 2.36 | 0.60 |
| 2:B:2868:HIS:HB3 | 2:B:2871:LEU:HG | 1.82 | 0.60 |
| 2:C:288:HIS:O | 2:C:290:ARG:NH1 | 2.33 | 0.60 |
| 2:C:894:VAL:CG2 | 2:C:972:LEU:HD22 | 2.29 | 0.60 |
| 2:C:3192:ARG:HD3 | 2:C:3199:THR:HA | 1.84 | 0.60 |
| 2:D:1444:GLY:HA3 | 2:D:1487:MET:HA | 1.83 | 0.60 |
| 2:A:2070:ALA:HA | 2:A:2075:ILE:HD11 | 1.83 | 0.60 |
| 2:A:2605:MET:HA | 2:A:2608:LYS:HE2 | 1.84 | 0.60 |
| 2:A:4690:LYS:NZ | 2:A:4692:SER:OG | 2.19 | 0.60 |
| 2:B:288:HIS:O | 2:B:290:ARG:NH1 | 2.33 | 0.60 |
| 2:B:2905:ARG:HH11 | 2:B:2906:GLY:H | 1.50 | 0.60 |
| 2:B:3018:ARG:HG2 | 2:B:3021:LEU:HD22 | 1.83 | 0.60 |
| 2:C:234:LEU:HD13 | 2:C:405:LEU:HD22 | 1.83 | 0.60 |
| 2:C:4831:ILE:HG13 | 2:C:4843:ARG:NH2 | 2.16 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:694:ARG:NH1 | 2:A:718:VAL:O | 2.32 | 0.59 |
| 2:A:2424:ARG:HG2 | 2:A:2476:TYR:CE1 | 2.36 | 0.59 |
| 2:B:879:GLU:O | 2:B:882:ARG:NH1 | 2.32 | 0.59 |
| 2:B:2920:ARG:HB2 | 2:B:2923:TYR:HB2 | 1.84 | 0.59 |
| 2:C:2920:ARG:HB2 | 2:C:2923:TYR:HB2 | 1.84 | 0.59 |
| 2:D:2793:ARG:NH2 | 2:D:2796:ASP:OD2 | 2.33 | 0.59 |
| 2:D:3192:ARG:HD3 | 2:D:3199:THR:HA | 1.84 | 0.59 |
| 2:A:912:LYS:NZ | 2:A:914:GLN:O | 2.26 | 0.59 |
| 2:B:3192:ARG:HD3 | 2:B:3199:THR:HA | 1.84 | 0.59 |
| 2:C:1031:ARG:HH22 | 2:C:1042:THR:CG2 | 2.13 | 0.59 |
| 2:D:307:SER:OG | 2:D:315:LEU:O | 2.20 | 0.59 |
| 2:D:1689:ILE:HA | 2:D:1703:TYR:CE1 | 2.32 | 0.59 |
| 2:D:2443:PRO:HD2 | 2:D:2512:MET:HE2 | 1.84 | 0.59 |
| 2:D:2679:ASP:HA | 2:D:2920:ARG:HH21 | 1.67 | 0.59 |
| 2:D:3689:MET:HE2 | 2:D:3689:MET:HA | 1.84 | 0.59 |
| 2:D:4748:MET:HA | 2:D:4754:ARG:HH21 | 1.66 | 0.59 |
| 2:A:307:SER:OG | 2:A:315:LEU:O | 2.20 | 0.59 |
| 2:B:234:LEU:HD13 | 2:B:405:LEU:HD22 | 1.83 | 0.59 |
| 2:B:4748:MET:HA | 2:B:4754:ARG:HH21 | 1.66 | 0.59 |
| 2:D:515:ALA:HB2 | 2:D:523:GLY:HA3 | 1.84 | 0.59 |
| 2:A:234:LEU:HD13 | 2:A:405:LEU:HD22 | 1.83 | 0.59 |
| 2:A:2905:ARG:HH11 | 2:A:2906:GLY:H | 1.50 | 0.59 |
| 2:A:2920:ARG:HB2 | 2:A:2923:TYR:HB2 | 1.84 | 0.59 |
| 2:C:2717:LEU:HD23 | 2:C:2779:LEU:HD23 | 1.84 | 0.59 |
| 2:D:2920:ARG:HB2 | 2:D:2923:TYR:HB2 | 1.84 | 0.59 |
| 2:A:515:ALA:HB2 | 2:A:523:GLY:HA3 | 1.84 | 0.59 |
| 2:A:1559:ARG:HD2 | 2:A:1565:PRO:HD3 | 1.84 | 0.59 |
| 2:B:2605:MET:HA | 2:B:2608:LYS:HE2 | 1.84 | 0.59 |
| 2:A:2717:LEU:HD23 | 2:A:2779:LEU:HD23 | 1.84 | 0.59 |
| 2:B:801:ARG:NH1 | 2:B:1615:GLN:O | 2.34 | 0.59 |
| 2:C:4056:LYS:NZ | 2:D:4660:PHE:O | 2.35 | 0.59 |
| 2:A:4748:MET:HA | 2:A:4754:ARG:HH21 | 1.66 | 0.59 |
| 2:B:2679:ASP:HA | 2:B:2920:ARG:HH21 | 1.67 | 0.59 |
| 2:C:2679:ASP:HA | 2:C:2920:ARG:HH21 | 1.67 | 0.59 |
| 2:D:2424:ARG:HG2 | 2:D:2476:TYR:CE1 | 2.36 | 0.59 |
| 2:A:4673:ASP:HB3 | 2:A:4676:ALA:HB3 | 1.83 | 0.59 |
| 2:C:1559:ARG:HD2 | 2:C:1565:PRO:HD3 | 1.84 | 0.59 |
| 2:C:2070:ALA:HA | 2:C:2075:ILE:HD11 | 1.84 | 0.59 |
| 2:D:2724:TYR:OH | 2:D:2891:ASP:OD1 | 2.18 | 0.59 |
| 2:D:3188:SER:OG | 2:D:3191:GLU:OE1 | 2.21 | 0.59 |
| 2:A:3192:ARG:HD3 | 2:A:3199:THR:HA | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2833:LEU:HB3 | 2:B:2838[B]:HIS:CE1 | 2.38 | 0.59 |
| 2:D:895:MET:HE3 | 2:D:978:PRO:HG2 | 1.85 | 0.59 |
| 2:D:2070:ALA:HA | 2:D:2075:ILE:HD11 | 1.84 | 0.59 |
| 2:D:2833:LEU:HB3 | 2:D:2838[B]:HIS:CE1 | 2.38 | 0.59 |
| 2:D:2905:ARG:HH11 | 2:D:2906:GLY:H | 1.50 | 0.59 |
| 2:D:3730:ARG:O | 2:D:3734:ARG:NH1 | 2.36 | 0.59 |
| 2:D:4673:ASP:HB3 | 2:D:4676:ALA:HB3 | 1.83 | 0.59 |
| 2:A:971:GLN:HE22 | 2:A:978:PRO:HD3 | 1.66 | 0.59 |
| 2:B:2070:ALA:HA | 2:B:2075:ILE:HD11 | 1.83 | 0.59 |
| 2:C:1444:GLY:HA3 | 2:C:1487:MET:HA | 1.83 | 0.59 |
| 2:C:2605:MET:HA | 2:C:2608:LYS:HE2 | 1.84 | 0.59 |
| 2:D:2605:MET:HA | 2:D:2608:LYS:HE2 | 1.84 | 0.59 |
| 2:B:804:LEU:HD13 | 2:B:832:LEU:HD21 | 1.85 | 0.58 |
| 2:B:2179:LEU:O | 2:B:2183:GLU:CB | 2.51 | 0.58 |
| 2:B:3188:SER:OG | 2:B:3191:GLU:OE1 | 2.21 | 0.58 |
| 2:C:2833:LEU:HB3 | 2:C:2838[B]:HIS:CE1 | 2.38 | 0.58 |
| 2:C:4673:ASP:HB3 | 2:C:4676:ALA:HB3 | 1.84 | 0.58 |
| 2:D:4831:ILE:HG13 | 2:D:4843:ARG:NH2 | 2.16 | 0.58 |
| 2:A:1788:LYS:NZ | 2:A:1838:ASP:OD2 | 2.36 | 0.58 |
| 2:A:3844:GLN:HG3 | 2:A:3922:GLU:HG3 | 1.86 | 0.58 |
| 2:B:1559:ARG:HD2 | 2:B:1565:PRO:HD3 | 1.84 | 0.58 |
| 2:B:2710:ASN:OD1 | 2:B:2711:ILE:HG13 | 2.03 | 0.58 |
| 2:D:894:VAL:CG2 | 2:D:972:LEU:HD22 | 2.29 | 0.58 |
| 2:A:2179:LEU:O | 2:A:2183:GLU:CB | 2.51 | 0.58 |
| 2:A:2621:TYR:OH | 2:A:2637:GLU:OE2 | 2.21 | 0.58 |
| 2:B:3325:LYS:HG3 | 2:B:3328:LYS:HZ2 | 1.68 | 0.58 |
| 2:B:4673:ASP:HB3 | 2:B:4676:ALA:HB3 | 1.83 | 0.58 |
| 2:C:3188:SER:OG | 2:C:3191:GLU:OE1 | 2.21 | 0.58 |
| 2:D:1031:ARG:HH22 | 2:D:1042:THR:CG2 | 2.13 | 0.58 |
| 2:D:2980:LEU:HD11 | 2:D:2989:PRO:HB2 | 1.85 | 0.58 |
| 2:D:4185:LYS:NZ | 2:D:4889:PHE:O | 2.33 | 0.58 |
| 2:B:629:GLN:OE1 | 2:B:1669:ASN:ND2 | 2.29 | 0.58 |
| 2:C:895:MET:HE3 | 2:C:978:PRO:HG2 | 1.85 | 0.58 |
| 2:C:2980:LEU:HD11 | 2:C:2989:PRO:HB2 | 1.85 | 0.58 |
| 2:D:218:SER:HB2 | 2:D:286:GLY:HA3 | 1.86 | 0.58 |
| 2:D:1051:ARG:HA | 2:D:1054:VAL:HG22 | 1.86 | 0.58 |
| 2:D:2179:LEU:O | 2:D:2183:GLU:CB | 2.51 | 0.58 |
| 2:D:2717:LEU:HD23 | 2:D:2779:LEU:HD23 | 1.84 | 0.58 |
| 2:A:804:LEU:HD13 | 2:A:832:LEU:HD21 | 1.85 | 0.58 |
| 2:B:894:VAL:CG2 | 2:B:972:LEU:HD22 | 2.29 | 0.58 |
| 2:C:2905:ARG:HH11 | 2:C:2906:GLY:H | 1.50 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:3730:ARG:O | 2:C:3734:ARG:NH1 | 2.36 | 0.58 |
| 2:D:3844:GLN:HG3 | 2:D:3922:GLU:HG3 | 1.86 | 0.58 |
| 2:A:2559:CYS:O | 2:A:2566:ARG:NH2 | 2.37 | 0.58 |
| 2:A:2833:LEU:HB3 | 2:A:2838[B]:HIS:CE1 | 2.38 | 0.58 |
| 2:B:1788:LYS:NZ | 2:B:1838:ASP:OD2 | 2.36 | 0.58 |
| 2:C:2179:LEU:O | 2:C:2183:GLU:CB | 2.51 | 0.58 |
| 2:C:2678:PRO:HA | 2:C:2921:PHE:HD2 | 1.69 | 0.58 |
| 2:C:3935:LEU:HD23 | 2:C:3940:LEU:HD22 | 1.85 | 0.58 |
| 2:D:2759:PRO:O | 2:D:2763:LEU:N | 2.36 | 0.58 |
| 1:H:19:LYS:HZ1 | 1:H:52:GLY:HA3 | 1.67 | 0.58 |
| 2:A:894:VAL:HA | 2:A:897:LYS:HD2 | 1.86 | 0.58 |
| 2:A:2759:PRO:O | 2:A:2763:LEU:N | 2.36 | 0.58 |
| 2:B:894:VAL:HA | 2:B:897:LYS:HD2 | 1.86 | 0.58 |
| 2:B:2502:LEU:HG | 2:B:2512:MET:HE1 | 1.85 | 0.58 |
| 2:B:2759:PRO:O | 2:B:2763:LEU:N | 2.36 | 0.58 |
| 2:C:3844:GLN:HG3 | 2:C:3922:GLU:HG3 | 1.86 | 0.58 |
| 2:D:661:LEU:O | 2:D:788:PHE:N | 2.37 | 0.58 |
| 2:D:971:GLN:HE22 | 2:D:978:PRO:HD3 | 1.66 | 0.58 |
| 2:D:1973:ILE:HA | 2:D:1976:LEU:HB2 | 1.86 | 0.58 |
| 2:D:3171:LEU:HB3 | 2:D:3211:LEU:HB2 | 1.86 | 0.58 |
| 2:D:3935:LEU:HD23 | 2:D:3940:LEU:HD22 | 1.85 | 0.58 |
| 2:A:1973:ILE:HA | 2:A:1976:LEU:HB2 | 1.86 | 0.58 |
| 2:B:2149:ILE:HG21 | 2:B:2167:MET:HE1 | 1.86 | 0.58 |
| 2:C:661:LEU:O | 2:C:788:PHE:N | 2.37 | 0.58 |
| 2:C:1788:LYS:NZ | 2:C:1838:ASP:OD2 | 2.36 | 0.58 |
| 2:A:218:SER:HB2 | 2:A:286:GLY:HA3 | 1.86 | 0.58 |
| 2:A:1051:ARG:HA | 2:A:1054:VAL:HG22 | 1.86 | 0.58 |
| 2:A:3188:SER:OG | 2:A:3191:GLU:OE1 | 2.21 | 0.58 |
| 2:B:3171:LEU:HB3 | 2:B:3211:LEU:HB2 | 1.86 | 0.58 |
| 2:B:3844:GLN:HG3 | 2:B:3922:GLU:HG3 | 1.86 | 0.58 |
| 2:C:307:SER:OG | 2:C:315:LEU:O | 2.20 | 0.58 |
| 2:C:2149:ILE:HG21 | 2:C:2167:MET:HE1 | 1.86 | 0.58 |
| 2:C:2710:ASN:OD1 | 2:C:2711:ILE:HG13 | 2.03 | 0.58 |
| 2:D:2710:ASN:OD1 | 2:D:2711:ILE:HG13 | 2.03 | 0.58 |
| 2:A:1689:ILE:HA | 2:A:1703:TYR:CE1 | 2.32 | 0.58 |
| 2:B:307:SER:OG | 2:B:315:LEU:O | 2.20 | 0.58 |
| 2:B:2559:CYS:O | 2:B:2566:ARG:NH2 | 2.37 | 0.58 |
| 2:C:2759:PRO:O | 2:C:2763:LEU:N | 2.36 | 0.58 |
| 2:A:2980:LEU:HD11 | 2:A:2989:PRO:HB2 | 1.85 | 0.57 |
| 2:B:2244:ALA:O | 2:B:2248:MET:HB2 | 2.04 | 0.57 |
| 2:C:894:VAL:HA | 2:C:897:LYS:HD2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:1051:ARG:HA | 2:C:1054:VAL:HG22 | 1.86 | 0.57 |
| 2:B:1717:ALA:HA | 2:B:1720:MET:HE2 | 1.86 | 0.57 |
| 2:C:3817:LEU:HD22 | 2:C:3819:MET:SD | 2.44 | 0.57 |
| 2:A:2710:ASN:OD1 | 2:A:2711:ILE:HG13 | 2.03 | 0.57 |
| 2:B:661:LEU:O | 2:B:788:PHE:N | 2.37 | 0.57 |
| 2:B:893:TRP:CE3 | 2:B:896:ASN:HB2 | 2.40 | 0.57 |
| 2:B:2678:PRO:HA | 2:B:2921:PHE:HD2 | 1.69 | 0.57 |
| 2:B:2980:LEU:HD11 | 2:B:2989:PRO:HB2 | 1.85 | 0.57 |
| 2:C:2436:ILE:HA | 2:C:2465:LYS:HE3 | 1.87 | 0.57 |
| 2:D:2546:ASP:O | 2:D:2550:HIS:ND1 | 2.37 | 0.57 |
| 2:A:2546:ASP:O | 2:A:2550:HIS:ND1 | 2.37 | 0.57 |
| 2:B:1004:HIS:NE2 | 2:B:1033:VAL:O | 2.25 | 0.57 |
| 2:B:2895:PHE:HA | 2:B:2898:ILE:HD12 | 1.87 | 0.57 |
| 2:B:3817:LEU:HD22 | 2:B:3819:MET:SD | 2.44 | 0.57 |
| 2:C:2244:ALA:O | 2:C:2248:MET:HB2 | 2.04 | 0.57 |
| 2:C:2546:ASP:O | 2:C:2550:HIS:ND1 | 2.37 | 0.57 |
| 2:C:2895:PHE:HA | 2:C:2898:ILE:HD12 | 1.87 | 0.57 |
| 2:D:912:LYS:NZ | 2:D:914:GLN:O | 2.26 | 0.57 |
| 2:D:3261:ALA:C | 2:D:3263:MET:H | 2.08 | 0.57 |
| 2:B:891:GLU:O | 2:B:894:VAL:HG22 | 2.05 | 0.57 |
| 2:B:916:PRO:HB3 | 2:B:923:LYS:NZ | 2.20 | 0.57 |
| 2:B:2546:ASP:O | 2:B:2550:HIS:ND1 | 2.37 | 0.57 |
| 2:C:893:TRP:CE3 | 2:C:896:ASN:HB2 | 2.40 | 0.57 |
| 2:A:893:TRP:CE3 | 2:A:896:ASN:HB2 | 2.40 | 0.57 |
| 2:A:2202:TYR:O | 2:A:2206:ILE:HG12 | 2.05 | 0.57 |
| 2:B:2436:ILE:HA | 2:B:2465:LYS:HE3 | 1.87 | 0.57 |
| 2:B:2541:HIS:HB3 | 2:B:2544:LEU:HB3 | 1.86 | 0.57 |
| 2:D:804:LEU:HD13 | 2:D:832:LEU:HD21 | 1.85 | 0.57 |
| 2:D:893:TRP:CE3 | 2:D:896:ASN:HB2 | 2.40 | 0.57 |
| 2:A:895:MET:HE3 | 2:A:978:PRO:HG2 | 1.86 | 0.57 |
| 2:A:3034:HIS:CE1 | 2:A:3038:GLN:HE22 | 2.23 | 0.57 |
| 2:B:218:SER:HB2 | 2:B:286:GLY:HA3 | 1.86 | 0.57 |
| 2:B:1051:ARG:HA | 2:B:1054:VAL:HG22 | 1.86 | 0.57 |
| 2:C:2202:TYR:O | 2:C:2206:ILE:HG12 | 2.05 | 0.57 |
| 2:D:1788:LYS:NZ | 2:D:1838:ASP:OD2 | 2.36 | 0.57 |
| 2:A:916:PRO:HB3 | 2:A:923:LYS:NZ | 2.20 | 0.57 |
| 2:A:2678:PRO:HA | 2:A:2921:PHE:HD2 | 1.69 | 0.57 |
| 2:B:2621:TYR:OH | 2:B:2637:GLU:OE2 | 2.21 | 0.57 |
| 2:C:2541:HIS:HB3 | 2:C:2544:LEU:HB3 | 1.86 | 0.57 |
| 2:C:2559:CYS:O | 2:C:2566:ARG:NH2 | 2.37 | 0.57 |
| 2:C:3171:LEU:HB3 | 2:C:3211:LEU:HB2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:894:VAL:HA | 2:D:897:LYS:HD2 | 1.86 | 0.57 |
| 2:A:661:LEU:O | 2:A:788:PHE:N | 2.37 | 0.57 |
| 2:A:3261:ALA:C | 2:A:3263:MET:H | 2.08 | 0.57 |
| 2:A:3817:LEU:HD22 | 2:A:3819:MET:SD | 2.44 | 0.57 |
| 2:C:218:SER:HB2 | 2:C:286:GLY:HA3 | 1.85 | 0.57 |
| 2:C:1004:HIS:NE2 | 2:C:1033:VAL:O | 2.25 | 0.57 |
| 2:C:3034:HIS:CE1 | 2:C:3038:GLN:HE22 | 2.23 | 0.57 |
| 2:D:2202:TYR:O | 2:D:2206:ILE:HG12 | 2.05 | 0.57 |
| 2:D:2678:PRO:HA | 2:D:2921:PHE:HD2 | 1.69 | 0.57 |
| 2:D:4948:CYS:SG | 2:D:4950:GLU:HG2 | 2.45 | 0.57 |
| 2:A:1074:ARG:NH1 | 2:A:1078:CYS:O | 2.38 | 0.57 |
| 2:A:4948:CYS:SG | 2:A:4950:GLU:HG2 | 2.45 | 0.57 |
| 2:B:162:ILE:HD11 | 2:B:181:LEU:HB3 | 1.87 | 0.57 |
| 2:C:804:LEU:HD13 | 2:C:832:LEU:HD21 | 1.85 | 0.57 |
| 2:D:1074:ARG:NH1 | 2:D:1078:CYS:O | 2.38 | 0.57 |
| 2:D:2149:ILE:HG21 | 2:D:2167:MET:HE1 | 1.87 | 0.57 |
| 2:D:2541:HIS:HB3 | 2:D:2544:LEU:HB3 | 1.86 | 0.57 |
| 2:D:2559:CYS:O | 2:D:2566:ARG:NH2 | 2.37 | 0.57 |
| 1:E:19:LYS:HZ1 | 1:E:52:GLY:HA3 | 1.68 | 0.56 |
| 2:B:1074:ARG:NH1 | 2:B:1078:CYS:O | 2.38 | 0.56 |
| 2:B:1973:ILE:HA | 2:B:1976:LEU:HB2 | 1.86 | 0.56 |
| 2:B:4948:CYS:SG | 2:B:4950:GLU:HG2 | 2.45 | 0.56 |
| 2:C:162:ILE:HD11 | 2:C:181:LEU:HB3 | 1.87 | 0.56 |
| 2:C:3174:HIS:ND1 | 2:C:3175:LEU:HG | 2.20 | 0.56 |
| 2:D:163:HIS:HB2 | 2:D:182:ILE:HG13 | 1.87 | 0.56 |
| 2:D:2895:PHE:HA | 2:D:2898:ILE:HD12 | 1.87 | 0.56 |
| 2:D:3043:ARG:NH2 | 2:D:3116:GLN:O | 2.38 | 0.56 |
| 2:D:3900:GLU:OE2 | 2:D:3904:ARG:NH2 | 2.38 | 0.56 |
| 2:A:894:VAL:CG2 | 2:A:972:LEU:HD22 | 2.29 | 0.56 |
| 2:A:3730:ARG:O | 2:A:3734:ARG:NH1 | 2.36 | 0.56 |
| 2:A:3935:LEU:HD23 | 2:A:3940:LEU:HD22 | 1.85 | 0.56 |
| 2:B:3043:ARG:NH2 | 2:B:3116:GLN:O | 2.38 | 0.56 |
| 2:B:3900:GLU:OE2 | 2:B:3904:ARG:NH2 | 2.38 | 0.56 |
| 2:B:3935:LEU:HD23 | 2:B:3940:LEU:HD22 | 1.85 | 0.56 |
| 2:C:891:GLU:O | 2:C:894:VAL:HG22 | 2.05 | 0.56 |
| 2:D:3817:LEU:HD22 | 2:D:3819:MET:SD | 2.44 | 0.56 |
| 2:A:2541:HIS:HB3 | 2:A:2544:LEU:HB3 | 1.86 | 0.56 |
| 2:A:2895:PHE:HA | 2:A:2898:ILE:HD12 | 1.87 | 0.56 |
| 2:A:3043:ARG:NH2 | 2:A:3116:GLN:O | 2.38 | 0.56 |
| 2:A:4185:LYS:NZ | 2:A:4889:PHE:O | 2.33 | 0.56 |
| 2:B:2724:TYR:OH | 2:B:2891:ASP:OD1 | 2.18 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:3174:HIS:ND1 | 2:B:3175:LEU:HG | 2.20 | 0.56 |
| 2:C:3900:GLU:OE2 | 2:C:3904:ARG:NH2 | 2.38 | 0.56 |
| 2:C:4948:CYS:SG | 2:C:4950:GLU:HG2 | 2.45 | 0.56 |
| 2:D:162:ILE:HD11 | 2:D:181:LEU:HB3 | 1.87 | 0.56 |
| 2:D:2436:ILE:HA | 2:D:2465:LYS:HE3 | 1.87 | 0.56 |
| 2:D:3174:HIS:ND1 | 2:D:3175:LEU:HG | 2.20 | 0.56 |
| 2:A:2149:ILE:HG21 | 2:A:2167:MET:HE1 | 1.88 | 0.56 |
| 2:B:3034:HIS:CE1 | 2:B:3038:GLN:HE22 | 2.23 | 0.56 |
| 2:C:1009:ARG:O | 2:C:1013:ARG:HG2 | 2.06 | 0.56 |
| 2:C:1973:ILE:HA | 2:C:1976:LEU:HB2 | 1.86 | 0.56 |
| 2:C:3214:LEU:HD13 | 2:C:3242:LEU:HD21 | 1.88 | 0.56 |
| 2:D:3034:HIS:CE1 | 2:D:3038:GLN:HE22 | 2.23 | 0.56 |
| 2:A:2080:LEU:O | 2:A:2084:MET:HG3 | 2.06 | 0.56 |
| 2:D:629:GLN:OE1 | 2:D:1669:ASN:ND2 | 2.29 | 0.56 |
| 2:A:891:GLU:O | 2:A:894:VAL:HG22 | 2.05 | 0.56 |
| 2:A:3607:PRO:HD2 | 2:A:3610:ASN:HB2 | 1.87 | 0.56 |
| 2:B:3214:LEU:HD13 | 2:B:3242:LEU:HD21 | 1.88 | 0.56 |
| 2:B:3730:ARG:O | 2:B:3734:ARG:NH1 | 2.36 | 0.56 |
| 2:C:163:HIS:HB2 | 2:C:182:ILE:HG13 | 1.87 | 0.56 |
| 2:C:1717:ALA:HA | 2:C:1720:MET:HE2 | 1.87 | 0.56 |
| 2:C:3261:ALA:C | 2:C:3263:MET:H | 2.08 | 0.56 |
| 2:A:2057:THR:HG22 | 2:A:2059:GLN:H | 1.71 | 0.56 |
| 2:A:2436:ILE:HA | 2:A:2465:LYS:HE3 | 1.87 | 0.56 |
| 2:A:4660:PHE:O | 2:D:4056:LYS:NZ | 2.39 | 0.56 |
| 2:B:1009:ARG:O | 2:B:1013:ARG:HG2 | 2.06 | 0.56 |
| 2:B:2202:TYR:O | 2:B:2206:ILE:HG12 | 2.05 | 0.56 |
| 2:B:2443:PRO:HD2 | 2:B:2512:MET:HE2 | 1.88 | 0.56 |
| 2:C:916:PRO:HB3 | 2:C:923:LYS:NZ | 2.20 | 0.56 |
| 2:C:3043:ARG:NH2 | 2:C:3116:GLN:O | 2.38 | 0.56 |
| 2:C:3325:LYS:HG3 | 2:C:3328:LYS:NZ | 2.20 | 0.56 |
| 2:D:2244:ALA:O | 2:D:2248:MET:HB2 | 2.04 | 0.56 |
| 2:D:2605:MET:SD | 2:D:2606:PRO:HD3 | 2.46 | 0.56 |
| 2:A:882:ARG:HD2 | 2:A:937:LEU:HD21 | 1.88 | 0.56 |
| 2:A:1766:PRO:HG3 | 2:A:1780:PRO:HB3 | 1.87 | 0.56 |
| 2:A:2279:MET:SD | 2:A:2283:LYS:HE2 | 2.46 | 0.56 |
| 2:A:3171:LEU:HB3 | 2:A:3211:LEU:HB2 | 1.86 | 0.56 |
| 2:B:2057:THR:HG22 | 2:B:2059:GLN:H | 1.71 | 0.56 |
| 2:B:3261:ALA:C | 2:B:3263:MET:H | 2.08 | 0.56 |
| 2:B:4185:LYS:NZ | 2:B:4889:PHE:O | 2.33 | 0.56 |
| 2:C:1074:ARG:NH1 | 2:C:1078:CYS:O | 2.38 | 0.56 |
| 2:C:3607:PRO:HD2 | 2:C:3610:ASN:HB2 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:891:GLU:O | 2:D:894:VAL:HG22 | 2.05 | 0.56 |
| 2:A:163:HIS:HB2 | 2:A:182:ILE:HG13 | 1.87 | 0.56 |
| 2:A:3689:MET:HA | 2:A:3689:MET:HE2 | 1.87 | 0.56 |
| 2:B:3325:LYS:HG3 | 2:B:3328:LYS:NZ | 2.20 | 0.56 |
| 2:C:1766:PRO:HG3 | 2:C:1780:PRO:HB3 | 1.87 | 0.56 |
| 2:C:2057:THR:HG22 | 2:C:2059:GLN:H | 1.71 | 0.56 |
| 2:D:363:ILE:HD11 | 2:D:403:ILE:HD13 | 1.88 | 0.56 |
| 2:D:916:PRO:HB3 | 2:D:923:LYS:NZ | 2.20 | 0.56 |
| 2:D:2057:THR:HG22 | 2:D:2059:GLN:H | 1.71 | 0.56 |
| 2:A:162:ILE:HD11 | 2:A:181:LEU:HB3 | 1.87 | 0.56 |
| 2:A:1502:ASN:OD1 | 2:A:1503:ASN:N | 2.39 | 0.56 |
| 2:A:2244:ALA:O | 2:A:2248:MET:HB2 | 2.04 | 0.56 |
| 2:D:2728:SER:HA | 2:D:2731:LYS:NZ | 2.21 | 0.56 |
| 2:D:4270:LYS:NZ | 2:D:4278:ASP:OD1 | 2.26 | 0.56 |
| 2:A:2605:MET:SD | 2:A:2606:PRO:HD3 | 2.46 | 0.55 |
| 2:A:3174:HIS:ND1 | 2:A:3175:LEU:HG | 2.20 | 0.55 |
| 2:B:363:ILE:HD11 | 2:B:403:ILE:HD13 | 1.88 | 0.55 |
| 2:B:4043:ILE:O | 2:B:4078:LEU:N | 2.31 | 0.55 |
| 2:C:2728:SER:HA | 2:C:2731:LYS:NZ | 2.21 | 0.55 |
| 2:D:46:LEU:HD23 | 2:D:137:ARG:HH21 | 1.72 | 0.55 |
| 2:D:1502:ASN:OD1 | 2:D:1503:ASN:N | 2.39 | 0.55 |
| 2:A:3148:VAL:HA | 2:A:3151:GLN:NE2 | 2.21 | 0.55 |
| 2:A:3298:ARG:HA | 2:A:3301:VAL:HG22 | 1.88 | 0.55 |
| 2:A:3892:TYR:OH | 2:A:3899:ASP:OD1 | 2.19 | 0.55 |
| 2:A:4837:ASP:OD2 | 2:A:4838:GLU:N | 2.39 | 0.55 |
| 2:B:882:ARG:HD2 | 2:B:937:LEU:HD21 | 1.88 | 0.55 |
| 2:B:2279:MET:SD | 2:B:2283:LYS:HE2 | 2.46 | 0.55 |
| 2:B:2605:MET:SD | 2:B:2606:PRO:HD3 | 2.46 | 0.55 |
| 2:B:3607:PRO:HD2 | 2:B:3610:ASN:HB2 | 1.87 | 0.55 |
| 2:A:46:LEU:HD23 | 2:A:137:ARG:HH21 | 1.71 | 0.55 |
| 2:A:2728:SER:HA | 2:A:2731:LYS:NZ | 2.21 | 0.55 |
| 2:A:4268:MET:O | 2:A:4272:LYS:HG2 | 2.07 | 0.55 |
| 2:B:1502:ASN:OD1 | 2:B:1503:ASN:N | 2.39 | 0.55 |
| 2:B:2581:ARG:HH11 | 2:B:2582:PRO:HD2 | 1.71 | 0.55 |
| 2:B:2728:SER:HA | 2:B:2731:LYS:NZ | 2.21 | 0.55 |
| 2:C:363:ILE:HD11 | 2:C:403:ILE:HD13 | 1.88 | 0.55 |
| 2:C:3281:LEU:O | 2:C:3284:ILE:HG22 | 2.07 | 0.55 |
| 2:C:4185:LYS:NZ | 2:C:4889:PHE:O | 2.33 | 0.55 |
| 1:F:22:THR:HG22 | 1:F:50:ARG:HG2 | 1.89 | 0.55 |
| 2:A:474:ASP:O | 2:A:478:ARG:HG2 | 2.07 | 0.55 |
| 2:A:3214:LEU:HD13 | 2:A:3242:LEU:HD21 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1766:PRO:HG3 | 2:B:1780:PRO:HB3 | 1.87 | 0.55 |
| 2:C:2279:MET:SD | 2:C:2283:LYS:HE2 | 2.46 | 0.55 |
| 2:C:2605:MET:SD | 2:C:2606:PRO:HD3 | 2.46 | 0.55 |
| 2:D:1009:ARG:O | 2:D:1013:ARG:HG2 | 2.06 | 0.55 |
| 2:D:3187:LYS:NZ | 2:D:3191:GLU:HB3 | 2.22 | 0.55 |
| 2:D:3214:LEU:HD13 | 2:D:3242:LEU:HD21 | 1.88 | 0.55 |
| 2:D:3325:LYS:HG3 | 2:D:3328:LYS:NZ | 2.20 | 0.55 |
| 2:A:363:ILE:HD11 | 2:A:403:ILE:HD13 | 1.88 | 0.55 |
| 2:A:1971:GLU:HA | 2:A:1974:ASN:HB2 | 1.88 | 0.55 |
| 2:A:3900:GLU:OE2 | 2:A:3904:ARG:NH2 | 2.38 | 0.55 |
| 2:B:163:HIS:HB2 | 2:B:182:ILE:HG13 | 1.87 | 0.55 |
| 2:B:2080:LEU:O | 2:B:2084:MET:HG3 | 2.06 | 0.55 |
| 2:C:882:ARG:HD2 | 2:C:937:LEU:HD21 | 1.88 | 0.55 |
| 2:C:2080:LEU:O | 2:C:2084:MET:HG3 | 2.06 | 0.55 |
| 2:C:3187:LYS:NZ | 2:C:3191:GLU:HB3 | 2.22 | 0.55 |
| 2:D:663:VAL:HA | 2:D:671:LYS:HZ3 | 1.72 | 0.55 |
| 1:F:19:LYS:HZ1 | 1:F:52:GLY:HA3 | 1.72 | 0.55 |
| 2:A:2426:LEU:HA | 2:B:143:LEU:HD21 | 1.88 | 0.55 |
| 2:A:3325:LYS:HG3 | 2:A:3328:LYS:NZ | 2.20 | 0.55 |
| 2:D:4043:ILE:O | 2:D:4078:LEU:N | 2.31 | 0.55 |
| 1:F:50:ARG:NH2 | 1:F:53:LYS:HE2 | 2.22 | 0.55 |
| 1:G:50:ARG:NH2 | 1:G:53:LYS:HE2 | 2.22 | 0.55 |
| 1:H:22:THR:HG22 | 1:H:50:ARG:HG2 | 1.89 | 0.55 |
| 2:A:1009:ARG:O | 2:A:1013:ARG:HG2 | 2.06 | 0.55 |
| 2:B:270:HIS:CE1 | 2:B:491:GLU:HG3 | 2.42 | 0.55 |
| 2:B:1006:VAL:HA | 2:B:1009:ARG:HG2 | 1.89 | 0.55 |
| 2:B:3281:LEU:O | 2:B:3284:ILE:HG22 | 2.07 | 0.55 |
| 2:B:4268:MET:O | 2:B:4272:LYS:HG2 | 2.07 | 0.55 |
| 2:C:280:LEU:HD12 | 2:C:294:PRO:HB2 | 1.89 | 0.55 |
| 2:D:280:LEU:HD12 | 2:D:294:PRO:HB2 | 1.89 | 0.55 |
| 2:D:882:ARG:HD2 | 2:D:937:LEU:HD21 | 1.88 | 0.55 |
| 2:D:1766:PRO:HG3 | 2:D:1780:PRO:HB3 | 1.87 | 0.55 |
| 2:D:2279:MET:SD | 2:D:2283:LYS:HE2 | 2.46 | 0.55 |
| 2:D:3249:TRP:HB3 | 2:D:3266:THR:HG21 | 1.89 | 0.55 |
| 2:D:3287:ASN:HA | 2:D:3290:ILE:HG12 | 1.89 | 0.55 |
| 1:H:50:ARG:NH2 | 1:H:53:LYS:HE2 | 2.22 | 0.55 |
| 2:A:270:HIS:CE1 | 2:A:491:GLU:HG3 | 2.42 | 0.55 |
| 2:A:1440:ASN:HB3 | 2:A:1546:GLN:HB3 | 1.89 | 0.55 |
| 2:A:1608:VAL:HA | 2:A:1618:LEU:O | 2.07 | 0.55 |
| 2:A:3150:ARG:NH2 | 2:A:3151:GLN:OE1 | 2.40 | 0.55 |
| 2:B:880:ARG:NH1 | 2:B:881:ILE:HB | 2.22 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:3150:ARG:NH2 | 2:D:3151:GLN:OE1 | 2.40 | 0.55 |
| 2:A:981:MET:N | 2:A:981:MET:SD | 2.80 | 0.55 |
| 2:A:2724:TYR:OH | 2:A:2891:ASP:OD1 | 2.18 | 0.55 |
| 2:C:2553:TYR:HE1 | 2:C:2557:LYS:HZ3 | 1.54 | 0.55 |
| 2:C:3150:ARG:NH2 | 2:C:3151:GLN:OE1 | 2.40 | 0.55 |
| 2:D:270:HIS:CE1 | 2:D:491:GLU:HG3 | 2.42 | 0.55 |
| 2:D:3236:GLU:HG3 | 2:D:3237:VAL:HG13 | 1.88 | 0.55 |
| 2:A:2581:ARG:HH11 | 2:A:2582:PRO:HD2 | 1.71 | 0.55 |
| 2:A:3187:LYS:NZ | 2:A:3191:GLU:HB3 | 2.22 | 0.55 |
| 2:B:3287:ASN:HA | 2:B:3290:ILE:HG12 | 1.89 | 0.55 |
| 2:C:2893:LEU:O | 2:C:2896:LEU:HB3 | 2.07 | 0.55 |
| 2:D:981:MET:N | 2:D:981:MET:SD | 2.80 | 0.55 |
| 2:D:2080:LEU:O | 2:D:2084:MET:HG3 | 2.06 | 0.55 |
| 2:D:3607:PRO:HD2 | 2:D:3610:ASN:HB2 | 1.87 | 0.55 |
| 2:A:4641:PRO:HB2 | 2:A:4647:LYS:HD2 | 1.90 | 0.54 |
| 2:B:1608:VAL:HA | 2:B:1618:LEU:O | 2.07 | 0.54 |
| 2:B:1971:GLU:HA | 2:B:1974:ASN:HB2 | 1.88 | 0.54 |
| 2:B:2893:LEU:O | 2:B:2896:LEU:HB3 | 2.08 | 0.54 |
| 2:B:3236:GLU:HG3 | 2:B:3237:VAL:HG13 | 1.88 | 0.54 |
| 2:B:3298:ARG:HA | 2:B:3301:VAL:HG22 | 1.88 | 0.54 |
| 2:C:1440:ASN:HB3 | 2:C:1546:GLN:HB3 | 1.89 | 0.54 |
| 2:C:3074:ASN:ND2 | 2:C:3094:ILE:HD11 | 2.22 | 0.54 |
| 2:C:3287:ASN:HA | 2:C:3290:ILE:HG12 | 1.89 | 0.54 |
| 2:D:880:ARG:NH1 | 2:D:881:ILE:HB | 2.22 | 0.54 |
| 2:D:1975:MET:HA | 2:D:1978:ASN:ND2 | 2.22 | 0.54 |
| 2:D:2502:LEU:HG | 2:D:2512:MET:HE1 | 1.89 | 0.54 |
| 2:A:189:GLU:OE2 | 2:D:2322:ARG:NH1 | 2.39 | 0.54 |
| 2:A:1975:MET:HA | 2:A:1978:ASN:ND2 | 2.22 | 0.54 |
| 2:A:2833:LEU:HB2 | 2:A:2894:LYS:NZ | 2.22 | 0.54 |
| 2:A:3281:LEU:O | 2:A:3284:ILE:HG22 | 2.07 | 0.54 |
| 2:B:3148:VAL:HA | 2:B:3151:GLN:NE2 | 2.21 | 0.54 |
| 2:B:4241:VAL:HG13 | 2:C:4626:ILE:HG12 | 1.88 | 0.54 |
| 2:C:1502:ASN:OD1 | 2:C:1503:ASN:N | 2.39 | 0.54 |
| 2:C:1608:VAL:HA | 2:C:1618:LEU:O | 2.07 | 0.54 |
| 2:C:1975:MET:HA | 2:C:1978:ASN:ND2 | 2.22 | 0.54 |
| 2:C:3148:VAL:HA | 2:C:3151:GLN:NE2 | 2.21 | 0.54 |
| 2:D:474:ASP:O | 2:D:478:ARG:HG2 | 2.07 | 0.54 |
| 2:D:1608:VAL:HA | 2:D:1618:LEU:O | 2.07 | 0.54 |
| 2:B:981:MET:SD | 2:B:981:MET:N | 2.80 | 0.54 |
| 2:B:2642:ARG:NE | 2:B:2682:GLU:OE1 | 2.40 | 0.54 |
| 2:B:3150:ARG:NH2 | 2:B:3151:GLN:OE1 | 2.40 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:3605:MET:HG2 | 2:B:3606:ALA:N | 2.22 | 0.54 |
| 2:C:441:LYS:HB3 | 2:C:444:THR:HG23 | 1.90 | 0.54 |
| 2:C:2642:ARG:NE | 2:C:2682:GLU:OE1 | 2.40 | 0.54 |
| 2:C:3298:ARG:HA | 2:C:3301:VAL:HG22 | 1.88 | 0.54 |
| 2:D:441:LYS:HB3 | 2:D:444:THR:HG23 | 1.90 | 0.54 |
| 2:D:1971:GLU:HA | 2:D:1974:ASN:HB2 | 1.88 | 0.54 |
| 2:D:3281:LEU:O | 2:D:3284:ILE:HG22 | 2.07 | 0.54 |
| 2:D:4837:ASP:OD2 | 2:D:4838:GLU:N | 2.40 | 0.54 |
| 1:E:50:ARG:NH2 | 1:E:53:LYS:HE2 | 2.22 | 0.54 |
| 2:A:629:GLN:OE1 | 2:A:1669:ASN:ND2 | 2.29 | 0.54 |
| 2:A:2893:LEU:O | 2:A:2896:LEU:HB3 | 2.08 | 0.54 |
| 2:A:4818:TYR:HA | 2:B:4848:ILE:HD11 | 1.90 | 0.54 |
| 2:B:280:LEU:HD12 | 2:B:294:PRO:HB2 | 1.89 | 0.54 |
| 2:B:3187:LYS:NZ | 2:B:3191:GLU:HB3 | 2.22 | 0.54 |
| 2:C:1006:VAL:HG22 | 2:C:1009:ARG:HE | 1.72 | 0.54 |
| 2:C:2406:MET:HA | 2:C:2409:ILE:HG22 | 1.90 | 0.54 |
| 2:C:2894:LYS:O | 2:C:2898:ILE:HG13 | 2.08 | 0.54 |
| 2:D:2247:VAL:HG21 | 2:D:2257:LEU:HD12 | 1.90 | 0.54 |
| 2:D:2894:LYS:O | 2:D:2898:ILE:HG13 | 2.07 | 0.54 |
| 2:A:280:LEU:HD12 | 2:A:294:PRO:HB2 | 1.89 | 0.54 |
| 2:A:3236:GLU:HG3 | 2:A:3237:VAL:HG13 | 1.89 | 0.54 |
| 2:A:4707:MET:HG3 | 2:D:4252:ILE:HG21 | 1.89 | 0.54 |
| 2:B:441:LYS:HB3 | 2:B:444:THR:HG23 | 1.90 | 0.54 |
| 2:B:1975:MET:HA | 2:B:1978:ASN:ND2 | 2.22 | 0.54 |
| 2:B:3074:ASN:ND2 | 2:B:3094:ILE:HD11 | 2.23 | 0.54 |
| 2:C:270:HIS:CE1 | 2:C:491:GLU:HG3 | 2.42 | 0.54 |
| 2:C:474:ASP:O | 2:C:478:ARG:HG2 | 2.07 | 0.54 |
| 2:C:880:ARG:NH1 | 2:C:881:ILE:HB | 2.22 | 0.54 |
| 2:D:2581:ARG:HH11 | 2:D:2582:PRO:HD2 | 1.71 | 0.54 |
| 2:D:2833:LEU:HB3 | 2:D:2838[A]:HIS:CE1 | 2.43 | 0.54 |
| 2:D:3148:VAL:HA | 2:D:3151:GLN:NE2 | 2.21 | 0.54 |
| 2:A:663:VAL:HA | 2:A:671:LYS:HZ3 | 1.73 | 0.54 |
| 2:A:880:ARG:NH1 | 2:A:881:ILE:HB | 2.22 | 0.54 |
| 2:A:1839:LEU:HD12 | 2:A:1842:ILE:HD11 | 1.90 | 0.54 |
| 2:A:1969:PRO:HD3 | 2:A:3605:MET:HE1 | 1.89 | 0.54 |
| 2:A:2247:VAL:HG21 | 2:A:2257:LEU:HD12 | 1.90 | 0.54 |
| 2:A:2642:ARG:NE | 2:A:2682:GLU:OE1 | 2.40 | 0.54 |
| 2:A:3074:ASN:ND2 | 2:A:3094:ILE:HD11 | 2.23 | 0.54 |
| 2:B:2172:MET:O | 2:B:2176:VAL:HG23 | 2.08 | 0.54 |
| 2:B:2406:MET:HA | 2:B:2409:ILE:HG22 | 1.90 | 0.54 |
| 2:B:3249:TRP:HB3 | 2:B:3266:THR:HG21 | 1.89 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:4045:LYS:HB3 | 2:B:4046:ARG:HH21 | 1.73 | 0.54 |
| 2:B:4837:ASP:OD2 | 2:B:4838:GLU:N | 2.40 | 0.54 |
| 2:C:28:ILE:O | 2:C:31:GLU:HG3 | 2.08 | 0.54 |
| 2:C:1074:ARG:HH11 | 2:C:1078:CYS:HB3 | 1.73 | 0.54 |
| 2:C:2833:LEU:HB3 | 2:C:2838[A]:HIS:CE1 | 2.43 | 0.54 |
| 2:C:4045:LYS:HB3 | 2:C:4046:ARG:HH21 | 1.73 | 0.54 |
| 2:C:4641:PRO:HB2 | 2:C:4647:LYS:HD2 | 1.89 | 0.54 |
| 2:D:2172:MET:O | 2:D:2176:VAL:HG23 | 2.08 | 0.54 |
| 2:D:4268:MET:O | 2:D:4272:LYS:HG2 | 2.07 | 0.54 |
| 2:A:23:GLN:HB3 | 2:A:34:LYS:HD2 | 1.90 | 0.54 |
| 2:A:1006:VAL:HA | 2:A:1009:ARG:HG2 | 1.89 | 0.54 |
| 2:B:2247:VAL:HG21 | 2:B:2257:LEU:HD12 | 1.90 | 0.54 |
| 2:C:46:LEU:HD23 | 2:C:137:ARG:HH21 | 1.72 | 0.54 |
| 2:C:2247:VAL:HG21 | 2:C:2257:LEU:HD12 | 1.90 | 0.54 |
| 2:C:2581:ARG:HH11 | 2:C:2582:PRO:HD2 | 1.71 | 0.54 |
| 2:C:4837:ASP:OD2 | 2:C:4838:GLU:N | 2.40 | 0.54 |
| 2:D:2406:MET:HA | 2:D:2409:ILE:HG22 | 1.90 | 0.54 |
| 2:A:3287:ASN:HA | 2:A:3290:ILE:HG12 | 1.89 | 0.54 |
| 2:B:28:ILE:O | 2:B:31:GLU:HG3 | 2.08 | 0.54 |
| 2:B:474:ASP:O | 2:B:478:ARG:HG2 | 2.07 | 0.54 |
| 2:B:663:VAL:HA | 2:B:671:LYS:HZ3 | 1.73 | 0.54 |
| 2:B:2981:TYR:O | 2:B:2984:SER:OG | 2.26 | 0.54 |
| 2:C:981:MET:N | 2:C:981:MET:SD | 2.80 | 0.54 |
| 2:C:2172:MET:O | 2:C:2176:VAL:HG23 | 2.08 | 0.54 |
| 2:C:3605:MET:HG2 | 2:C:3606:ALA:N | 2.22 | 0.54 |
| 2:D:2550:HIS:CD2 | 2:D:2591:ARG:HD2 | 2.43 | 0.54 |
| 2:D:3074:ASN:ND2 | 2:D:3094:ILE:HD11 | 2.22 | 0.54 |
| 2:D:4045:LYS:HB3 | 2:D:4046:ARG:HH21 | 1.73 | 0.54 |
| 1:E:22:THR:HG22 | 1:E:50:ARG:HG2 | 1.89 | 0.54 |
| 2:A:441:LYS:HB3 | 2:A:444:THR:HG23 | 1.90 | 0.54 |
| 2:A:1006:VAL:HG22 | 2:A:1009:ARG:HE | 1.73 | 0.54 |
| 2:A:2550:HIS:CD2 | 2:A:2591:ARG:HD2 | 2.43 | 0.54 |
| 2:A:3249:TRP:HB3 | 2:A:3266:THR:HG21 | 1.89 | 0.54 |
| 2:B:232:ASP:OD1 | 2:B:356:TYR:OH | 2.21 | 0.54 |
| 2:B:1440:ASN:HB3 | 2:B:1546:GLN:HB3 | 1.89 | 0.54 |
| 2:B:2833:LEU:HB2 | 2:B:2894:LYS:NZ | 2.22 | 0.54 |
| 2:B:2894:LYS:O | 2:B:2898:ILE:HG13 | 2.08 | 0.54 |
| 2:B:3227:ARG:HB3 | 2:B:3230:GLN:OE1 | 2.08 | 0.54 |
| 2:C:1971:GLU:HA | 2:C:1974:ASN:HB2 | 1.88 | 0.54 |
| 2:C:2833:LEU:HB2 | 2:C:2894:LYS:NZ | 2.22 | 0.54 |
| 2:C:3236:GLU:HG3 | 2:C:3237:VAL:HG13 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:4093:ASP:OD1 | 2:C:4094:ILE:N | 2.41 | 0.54 |
| 2:D:28:ILE:O | 2:D:31:GLU:HG3 | 2.08 | 0.54 |
| 2:D:1006:VAL:HG22 | 2:D:1009:ARG:HE | 1.72 | 0.54 |
| 2:D:3298:ARG:HA | 2:D:3301:VAL:HG22 | 1.88 | 0.54 |
| 2:D:4194:GLU:HG2 | 2:D:4645:TRP:HZ3 | 1.73 | 0.54 |
| 2:A:798:ILE:HD12 | 2:A:800:VAL:HG22 | 1.90 | 0.54 |
| 2:A:1074:ARG:HH11 | 2:A:1078:CYS:HB3 | 1.73 | 0.54 |
| 2:A:3605:MET:HG2 | 2:A:3606:ALA:N | 2.22 | 0.54 |
| 2:B:1006:VAL:HG22 | 2:B:1009:ARG:HE | 1.73 | 0.54 |
| 2:C:2443:PRO:HD2 | 2:C:2512:MET:HE2 | 1.90 | 0.54 |
| 2:D:2833:LEU:HB2 | 2:D:2894:LYS:NZ | 2.22 | 0.54 |
| 2:A:28:ILE:O | 2:A:31:GLU:HG3 | 2.08 | 0.53 |
| 2:A:76:ARG:HG2 | 2:D:3890:TRP:HB3 | 1.89 | 0.53 |
| 2:A:733:TRP:CE2 | 2:A:738:ALA:HB2 | 2.43 | 0.53 |
| 2:A:2172:MET:O | 2:A:2176:VAL:HG23 | 2.08 | 0.53 |
| 2:A:2521:CYS:HA | 2:A:2525:LEU:HD12 | 1.90 | 0.53 |
| 2:A:3217:GLU:O | 2:A:3221:LEU:HG | 2.08 | 0.53 |
| 2:B:798:ILE:HD12 | 2:B:800:VAL:HG22 | 1.90 | 0.53 |
| 2:B:1839:LEU:HD12 | 2:B:1842:ILE:HD11 | 1.90 | 0.53 |
| 2:B:2550:HIS:CD2 | 2:B:2591:ARG:HD2 | 2.43 | 0.53 |
| 2:B:2773:TRP:NE1 | 2:B:2777:GLU:OE2 | 2.42 | 0.53 |
| 2:C:2629:ASN:OD1 | 2:C:2630:PHE:N | 2.41 | 0.53 |
| 2:C:3249:TRP:HB3 | 2:C:3266:THR:HG21 | 1.89 | 0.53 |
| 2:D:3892:TYR:OH | 2:D:3899:ASP:OD1 | 2.19 | 0.53 |
| 2:D:4641:PRO:HB2 | 2:D:4647:LYS:HD2 | 1.90 | 0.53 |
| 1:G:19:LYS:HZ1 | 1:G:52:GLY:HA3 | 1.71 | 0.53 |
| 2:A:2406:MET:HA | 2:A:2409:ILE:HG22 | 1.90 | 0.53 |
| 2:A:2981:TYR:O | 2:A:2984:SER:OG | 2.26 | 0.53 |
| 2:B:3127:GLN:HB2 | 2:B:3183:ILE:HD12 | 1.90 | 0.53 |
| 2:B:4093:ASP:OD1 | 2:B:4094:ILE:N | 2.41 | 0.53 |
| 2:B:4641:PRO:HB2 | 2:B:4647:LYS:HD2 | 1.90 | 0.53 |
| 2:C:3227:ARG:HB3 | 2:C:3230:GLN:OE1 | 2.08 | 0.53 |
| 2:C:4052:MET:HE1 | 2:C:4066:LEU:HB2 | 1.90 | 0.53 |
| 2:D:23:GLN:HB3 | 2:D:34:LYS:HD2 | 1.90 | 0.53 |
| 2:D:798:ILE:HD12 | 2:D:800:VAL:HG22 | 1.90 | 0.53 |
| 2:D:2773:TRP:NE1 | 2:D:2777:GLU:OE2 | 2.42 | 0.53 |
| 2:D:2893:LEU:O | 2:D:2896:LEU:HB3 | 2.08 | 0.53 |
| 2:D:4093:ASP:OD1 | 2:D:4094:ILE:N | 2.41 | 0.53 |
| 2:A:2629:ASN:OD1 | 2:A:2630:PHE:N | 2.41 | 0.53 |
| 2:A:3292:GLU:HB2 | 2:A:3296:MET:HG2 | 1.90 | 0.53 |
| 2:A:4194:GLU:HG2 | 2:A:4645:TRP:HZ3 | 1.73 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2553:TYR:HE1 | 2:B:2557:LYS:HZ3 | 1.55 | 0.53 |
| 2:B:3217:GLU:O | 2:B:3221:LEU:HG | 2.08 | 0.53 |
| 2:B:3292:GLU:HB2 | 2:B:3296:MET:HG2 | 1.90 | 0.53 |
| 2:C:798:ILE:HD12 | 2:C:800:VAL:HG22 | 1.90 | 0.53 |
| 2:D:655:MET:HE2 | 2:D:1608:VAL:HG11 | 1.91 | 0.53 |
| 2:D:2642:ARG:NE | 2:D:2682:GLU:OE1 | 2.40 | 0.53 |
| 2:D:4023:LEU:HD12 | 2:D:4026:LEU:HD23 | 1.91 | 0.53 |
| 1:E:8:ILE:HA | 2:A:730:LEU:HD11 | 1.89 | 0.53 |
| 1:F:8:ILE:HA | 2:B:730:LEU:HD11 | 1.90 | 0.53 |
| 2:A:49:LEU:HD11 | 2:A:203:VAL:HB | 1.90 | 0.53 |
| 2:B:1299:ILE:HD11 | 2:B:1544:PHE:HB3 | 1.91 | 0.53 |
| 2:B:2521:CYS:HA | 2:B:2525:LEU:HD12 | 1.90 | 0.53 |
| 2:C:257:ARG:HH21 | 2:C:272:ARG:HG3 | 1.73 | 0.53 |
| 2:C:801:ARG:HG2 | 2:C:1618:LEU:HA | 1.89 | 0.53 |
| 2:C:2550:HIS:CD2 | 2:C:2591:ARG:HD2 | 2.43 | 0.53 |
| 2:C:4241:VAL:HG13 | 2:D:4626:ILE:HG12 | 1.89 | 0.53 |
| 2:D:2621:TYR:OH | 2:D:2637:GLU:OE2 | 2.21 | 0.53 |
| 2:D:2981:TYR:O | 2:D:2984:SER:OG | 2.26 | 0.53 |
| 1:G:8:ILE:HA | 2:C:730:LEU:HD11 | 1.89 | 0.53 |
| 2:A:1299:ILE:HD11 | 2:A:1544:PHE:HB3 | 1.91 | 0.53 |
| 2:A:2773:TRP:NE1 | 2:A:2777:GLU:OE2 | 2.42 | 0.53 |
| 2:A:4093:ASP:OD1 | 2:A:4094:ILE:N | 2.41 | 0.53 |
| 2:B:46:LEU:HD23 | 2:B:137:ARG:HH21 | 1.72 | 0.53 |
| 2:B:895:MET:HE3 | 2:B:978:PRO:HG2 | 1.89 | 0.53 |
| 2:B:1074:ARG:HH11 | 2:B:1078:CYS:HB3 | 1.73 | 0.53 |
| 2:B:2629:ASN:OD1 | 2:B:2630:PHE:N | 2.41 | 0.53 |
| 2:C:2200:LEU:HD13 | 2:C:2214:MET:HE1 | 1.90 | 0.53 |
| 2:C:3043:ARG:HG3 | 2:C:3047:LYS:NZ | 2.24 | 0.53 |
| 2:C:3127:GLN:HB2 | 2:C:3183:ILE:HD12 | 1.90 | 0.53 |
| 2:C:4268:MET:O | 2:C:4272:LYS:HG2 | 2.07 | 0.53 |
| 2:D:733:TRP:CE2 | 2:D:738:ALA:HB2 | 2.44 | 0.53 |
| 2:D:801:ARG:HG2 | 2:D:1618:LEU:HA | 1.90 | 0.53 |
| 2:D:967:PRO:O | 2:D:971:GLN:N | 2.40 | 0.53 |
| 2:D:1006:VAL:HA | 2:D:1009:ARG:HG2 | 1.89 | 0.53 |
| 2:D:2828:MET:SD | 2:D:2894:LYS:HB3 | 2.49 | 0.53 |
| 2:D:3043:ARG:HG3 | 2:D:3047:LYS:NZ | 2.24 | 0.53 |
| 2:D:3605:MET:HG2 | 2:D:3606:ALA:N | 2.22 | 0.53 |
| 2:A:2894:LYS:O | 2:A:2898:ILE:HG13 | 2.08 | 0.53 |
| 2:A:3043:ARG:HG3 | 2:A:3047:LYS:NZ | 2.24 | 0.53 |
| 2:B:257:ARG:HH21 | 2:B:272:ARG:HG3 | 1.73 | 0.53 |
| 2:B:2830:ASN:HD21 | 2:C:1549:SER:HB2 | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2833:LEU:HB3 | 2:B:2838[A]:HIS:CE1 | 2.43 | 0.53 |
| 2:B:4642:ASN:HD22 | 2:B:4705:TYR:HE2 | 1.57 | 0.53 |
| 2:C:4023:LEU:HD12 | 2:C:4026:LEU:HD23 | 1.91 | 0.53 |
| 2:D:2211:GLN:NE2 | 2:D:2248:MET:O | 2.35 | 0.53 |
| 2:D:2629:ASN:OD1 | 2:D:2630:PHE:N | 2.41 | 0.53 |
| 2:A:2828:MET:SD | 2:A:2894:LYS:HB3 | 2.48 | 0.53 |
| 2:B:658:ASN:ND2 | 2:B:833:LYS:HG2 | 2.24 | 0.53 |
| 2:B:893:TRP:CZ2 | 2:B:1049:SER:HB3 | 2.44 | 0.53 |
| 2:B:3117:PHE:HB3 | 2:B:3121:LEU:HD13 | 1.91 | 0.53 |
| 2:C:1299:ILE:HD11 | 2:C:1544:PHE:HB3 | 1.91 | 0.53 |
| 2:C:1969:PRO:HD3 | 2:C:3605:MET:HE1 | 1.91 | 0.53 |
| 2:D:1299:ILE:HD11 | 2:D:1544:PHE:HB3 | 1.91 | 0.53 |
| 2:A:66:THR:HG1 | 2:A:124:SER:HG | 1.57 | 0.53 |
| 2:A:670:TYR:O | 2:A:673:TRP:NE1 | 2.42 | 0.53 |
| 2:B:49:LEU:HD11 | 2:B:203:VAL:HB | 1.90 | 0.53 |
| 2:B:943:LEU:HD21 | 2:B:1064:LEU:HD21 | 1.90 | 0.53 |
| 2:B:2828:MET:SD | 2:B:2894:LYS:HB3 | 2.49 | 0.53 |
| 2:B:3043:ARG:HG3 | 2:B:3047:LYS:NZ | 2.24 | 0.53 |
| 2:C:232:ASP:OD1 | 2:C:356:TYR:OH | 2.22 | 0.53 |
| 2:C:893:TRP:CZ2 | 2:C:1049:SER:HB3 | 2.44 | 0.53 |
| 2:A:943:LEU:HD21 | 2:A:1064:LEU:HD21 | 1.90 | 0.53 |
| 2:C:670:TYR:O | 2:C:673:TRP:NE1 | 2.42 | 0.53 |
| 2:C:878:LEU:HA | 2:C:881:ILE:HG22 | 1.91 | 0.53 |
| 2:C:1839:LEU:HD12 | 2:C:1842:ILE:HD11 | 1.90 | 0.53 |
| 2:C:2445:ILE:HA | 2:C:2451:VAL:HA | 1.91 | 0.53 |
| 2:C:2773:TRP:NE1 | 2:C:2777:GLU:OE2 | 2.42 | 0.53 |
| 2:D:893:TRP:CZ2 | 2:D:1049:SER:HB3 | 2.44 | 0.53 |
| 2:D:3227:ARG:HB3 | 2:D:3230:GLN:OE1 | 2.08 | 0.53 |
| 2:A:801:ARG:HG2 | 2:A:1618:LEU:HA | 1.90 | 0.53 |
| 2:A:3117:PHE:HB3 | 2:A:3121:LEU:HD13 | 1.91 | 0.53 |
| 2:A:4642:ASN:HD22 | 2:A:4705:TYR:HE2 | 1.57 | 0.53 |
| 2:B:801:ARG:HG2 | 2:B:1618:LEU:HA | 1.90 | 0.53 |
| 2:B:992:GLN:O | 2:B:996:VAL:HG23 | 2.09 | 0.53 |
| 2:B:4042:VAL:HG12 | 2:B:4077:THR:HB | 1.91 | 0.53 |
| 2:C:1270:VAL:HG22 | 2:C:1285:VAL:HG22 | 1.91 | 0.53 |
| 2:C:2211:GLN:NE2 | 2:C:2248:MET:O | 2.35 | 0.53 |
| 2:C:3117:PHE:HB3 | 2:C:3121:LEU:HD13 | 1.91 | 0.53 |
| 2:C:3729:ALA:HA | 2:C:3732:HIS:CE1 | 2.44 | 0.53 |
| 2:C:4642:ASN:HD22 | 2:C:4705:TYR:HE2 | 1.57 | 0.53 |
| 2:D:670:TYR:O | 2:D:673:TRP:NE1 | 2.42 | 0.53 |
| 2:D:4052:MET:HE1 | 2:D:4066:LEU:HB2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:658:ASN:ND2 | 2:A:833:LYS:HG2 | 2.24 | 0.52 |
| 2:A:1004:HIS:NE2 | 2:A:1033:VAL:O | 2.25 | 0.52 |
| 2:A:2833:LEU:HB3 | 2:A:2838[A]:HIS:CE1 | 2.43 | 0.52 |
| 2:A:3712:LYS:O | 2:A:3717:LYS:NZ | 2.42 | 0.52 |
| 2:B:674:TYR:CE1 | 2:B:756:SER:HB2 | 2.45 | 0.52 |
| 2:B:1097:LYS:NZ | 2:B:1198:GLY:O | 2.42 | 0.52 |
| 2:B:2620:TYR:HB2 | 2:B:2627:TRP:CD1 | 2.44 | 0.52 |
| 2:B:2933:VAL:HG21 | 2:B:3007:LEU:HD11 | 1.91 | 0.52 |
| 2:B:2940:ILE:HA | 2:B:2943:PHE:HB3 | 1.92 | 0.52 |
| 2:B:4023:LEU:HD12 | 2:B:4026:LEU:HD23 | 1.91 | 0.52 |
| 2:C:23:GLN:HB3 | 2:C:34:LYS:HD2 | 1.90 | 0.52 |
| 2:C:2521:CYS:HA | 2:C:2525:LEU:HD12 | 1.90 | 0.52 |
| 2:D:878:LEU:HA | 2:D:881:ILE:HG22 | 1.91 | 0.52 |
| 2:D:992:GLN:O | 2:D:996:VAL:HG23 | 2.09 | 0.52 |
| 2:D:4617:ILE:HG23 | 2:D:4665:ARG:HH22 | 1.74 | 0.52 |
| 1:F:88:HIS:NE2 | 2:B:1776:TYR:OH | 2.33 | 0.52 |
| 1:G:22:THR:HG22 | 1:G:50:ARG:HG2 | 1.89 | 0.52 |
| 2:A:992:GLN:O | 2:A:996:VAL:HG23 | 2.09 | 0.52 |
| 2:A:1270:VAL:HG22 | 2:A:1285:VAL:HG22 | 1.91 | 0.52 |
| 2:A:1682:GLU:HG2 | 2:A:1683:PRO:HD3 | 1.92 | 0.52 |
| 2:A:2409:ILE:HD11 | 2:A:2417:ILE:HD13 | 1.91 | 0.52 |
| 2:A:2933:VAL:HG21 | 2:A:3007:LEU:HD11 | 1.91 | 0.52 |
| 2:A:3127:GLN:HB2 | 2:A:3183:ILE:HD12 | 1.91 | 0.52 |
| 2:A:4042:VAL:HG12 | 2:A:4077:THR:HB | 1.91 | 0.52 |
| 2:A:4045:LYS:HB3 | 2:A:4046:ARG:HH21 | 1.73 | 0.52 |
| 2:C:897:LYS:HB3 | 2:C:918:LEU:CD2 | 2.40 | 0.52 |
| 2:C:943:LEU:HD21 | 2:C:1064:LEU:HD21 | 1.90 | 0.52 |
| 2:C:1097:LYS:NZ | 2:C:1198:GLY:O | 2.42 | 0.52 |
| 2:C:4617:ILE:HG23 | 2:C:4665:ARG:HH22 | 1.74 | 0.52 |
| 2:D:1097:LYS:NZ | 2:D:1198:GLY:O | 2.42 | 0.52 |
| 2:D:3117:PHE:HB3 | 2:D:3121:LEU:HD13 | 1.91 | 0.52 |
| 2:A:674:TYR:CE1 | 2:A:756:SER:HB2 | 2.45 | 0.52 |
| 2:A:4043:ILE:O | 2:A:4078:LEU:N | 2.31 | 0.52 |
| 2:B:897:LYS:HD3 | 2:B:918:LEU:HG | 1.92 | 0.52 |
| 2:B:2409:ILE:HD11 | 2:B:2417:ILE:HD13 | 1.91 | 0.52 |
| 2:B:2826:ILE:HD13 | 2:B:2898:ILE:HD13 | 1.92 | 0.52 |
| 2:B:3050:LEU:HD23 | 2:B:3053:VAL:HG23 | 1.91 | 0.52 |
| 2:B:3729:ALA:HA | 2:B:3732:HIS:CE1 | 2.44 | 0.52 |
| 2:C:733:TRP:CE2 | 2:C:738:ALA:HB2 | 2.43 | 0.52 |
| 2:C:992:GLN:O | 2:C:996:VAL:HG23 | 2.10 | 0.52 |
| 2:C:1006:VAL:HA | 2:C:1009:ARG:HG2 | 1.89 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:2620:TYR:HB2 | 2:C:2627:TRP:CD1 | 2.44 | 0.52 |
| 2:D:1074:ARG:HH11 | 2:D:1078:CYS:HB3 | 1.73 | 0.52 |
| 2:D:1440:ASN:HB3 | 2:D:1546:GLN:HB3 | 1.89 | 0.52 |
| 2:D:2521:CYS:HA | 2:D:2525:LEU:HD12 | 1.90 | 0.52 |
| 2:D:3050:LEU:HD23 | 2:D:3053:VAL:HG23 | 1.91 | 0.52 |
| 2:A:188:SER:HB2 | 2:A:190:ARG:HH11 | 1.75 | 0.52 |
| 2:A:655:MET:HE2 | 2:A:1608:VAL:HG11 | 1.90 | 0.52 |
| 2:A:897:LYS:HD3 | 2:A:918:LEU:HG | 1.92 | 0.52 |
| 2:A:2940:ILE:HA | 2:A:2943:PHE:HB3 | 1.92 | 0.52 |
| 2:A:3227:ARG:HB3 | 2:A:3230:GLN:OE1 | 2.08 | 0.52 |
| 2:A:4023:LEU:HD12 | 2:A:4026:LEU:HD23 | 1.91 | 0.52 |
| 2:B:878:LEU:HA | 2:B:881:ILE:HG22 | 1.91 | 0.52 |
| 2:B:4194:GLU:HG2 | 2:B:4645:TRP:HZ3 | 1.73 | 0.52 |
| 2:C:2791:ARG:NH2 | 2:C:2795:GLY:O | 2.42 | 0.52 |
| 2:D:658:ASN:HD21 | 2:D:833:LYS:HG2 | 1.75 | 0.52 |
| 2:D:897:LYS:HD3 | 2:D:918:LEU:HG | 1.92 | 0.52 |
| 2:D:4197:ILE:HG12 | 2:D:4923:MET:HE2 | 1.92 | 0.52 |
| 2:A:257:ARG:HH21 | 2:A:272:ARG:HG3 | 1.73 | 0.52 |
| 2:A:1097:LYS:NZ | 2:A:1198:GLY:O | 2.42 | 0.52 |
| 2:A:1722:ASN:O | 2:A:1919:ARG:NH2 | 2.43 | 0.52 |
| 2:A:3013:VAL:O | 2:A:3018:ARG:NH2 | 2.43 | 0.52 |
| 2:B:733:TRP:CE2 | 2:B:738:ALA:HB2 | 2.43 | 0.52 |
| 2:B:1682:GLU:HG2 | 2:B:1683:PRO:HD3 | 1.92 | 0.52 |
| 2:B:2788:ARG:HH22 | 2:B:2908:LYS:HE2 | 1.75 | 0.52 |
| 2:C:821:PRO:HB2 | 2:C:823:TYR:CE1 | 2.45 | 0.52 |
| 2:C:2826:ILE:HD13 | 2:C:2898:ILE:HD13 | 1.91 | 0.52 |
| 2:C:2828:MET:SD | 2:C:2894:LYS:HB3 | 2.49 | 0.52 |
| 2:D:3292:GLU:HB2 | 2:D:3296:MET:HG2 | 1.90 | 0.52 |
| 2:D:4275:THR:HG22 | 2:D:4278:ASP:H | 1.74 | 0.52 |
| 2:A:541:ILE:HD11 | 2:A:574:VAL:HG13 | 1.92 | 0.52 |
| 2:B:658:ASN:HD21 | 2:B:833:LYS:HG2 | 1.75 | 0.52 |
| 2:C:663:VAL:HA | 2:C:671:LYS:HZ3 | 1.74 | 0.52 |
| 2:C:1682:GLU:HG2 | 2:C:1683:PRO:HD3 | 1.92 | 0.52 |
| 2:D:1682:GLU:HG2 | 2:D:1683:PRO:HD3 | 1.92 | 0.52 |
| 2:D:2445:ILE:HA | 2:D:2451:VAL:HA | 1.91 | 0.52 |
| 2:D:2940:ILE:HA | 2:D:2943:PHE:HB3 | 1.92 | 0.52 |
| 2:D:3127:GLN:HB2 | 2:D:3183:ILE:HD12 | 1.90 | 0.52 |
| 2:D:4642:ASN:HD22 | 2:D:4705:TYR:HE2 | 1.57 | 0.52 |
| 2:A:3140:LEU:O | 2:A:3152:ARG:NH2 | 2.43 | 0.52 |
| 2:A:3729:ALA:HA | 2:A:3732:HIS:CE1 | 2.44 | 0.52 |
| 2:B:1722:ASN:O | 2:B:1919:ARG:NH2 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:3013:VAL:O | 2:B:3018:ARG:NH2 | 2.43 | 0.52 |
| 2:C:2830:ASN:HD21 | 2:D:1549:SER:HB2 | 1.72 | 0.52 |
| 2:C:2981:TYR:O | 2:C:2984:SER:OG | 2.26 | 0.52 |
| 2:C:3217:GLU:O | 2:C:3221:LEU:HG | 2.08 | 0.52 |
| 2:C:3292:GLU:HB2 | 2:C:3296:MET:HG2 | 1.90 | 0.52 |
| 2:C:4275:THR:HG22 | 2:C:4278:ASP:H | 1.74 | 0.52 |
| 2:D:2788:ARG:HH22 | 2:D:2908:LYS:HE2 | 1.75 | 0.52 |
| 2:A:881:ILE:HG23 | 2:A:885:LEU:HD13 | 1.92 | 0.52 |
| 2:A:916:PRO:HB3 | 2:A:923:LYS:HZ2 | 1.75 | 0.52 |
| 2:A:2212:LYS:HG2 | 2:A:2253:LEU:HD21 | 1.92 | 0.52 |
| 2:A:2620:TYR:HB2 | 2:A:2627:TRP:CD1 | 2.44 | 0.52 |
| 2:A:3050:LEU:HD23 | 2:A:3053:VAL:HG23 | 1.91 | 0.52 |
| 2:B:23:GLN:HB3 | 2:B:34:LYS:HD2 | 1.90 | 0.52 |
| 2:B:670:TYR:O | 2:B:673:TRP:NE1 | 2.42 | 0.52 |
| 2:B:897:LYS:HB3 | 2:B:918:LEU:CD2 | 2.40 | 0.52 |
| 2:B:3689:MET:HE2 | 2:B:3689:MET:HA | 1.91 | 0.52 |
| 2:B:4617:ILE:HG23 | 2:B:4665:ARG:HH22 | 1.74 | 0.52 |
| 2:C:674:TYR:CE1 | 2:C:756:SER:HB2 | 2.45 | 0.52 |
| 2:C:1722:ASN:O | 2:C:1919:ARG:NH2 | 2.43 | 0.52 |
| 2:C:2087:LEU:O | 2:C:2091:GLN:HG2 | 2.10 | 0.52 |
| 2:C:3282:LYS:HA | 2:C:3285:TYR:CD2 | 2.45 | 0.52 |
| 2:C:4610:LEU:HD21 | 2:C:4670:LEU:HD21 | 1.92 | 0.52 |
| 2:D:821:PRO:HB2 | 2:D:823:TYR:CE1 | 2.45 | 0.52 |
| 2:D:897:LYS:HB3 | 2:D:918:LEU:CD2 | 2.40 | 0.52 |
| 2:D:1839:LEU:HD12 | 2:D:1842:ILE:HD11 | 1.90 | 0.52 |
| 2:D:2212:LYS:HG2 | 2:D:2253:LEU:HD21 | 1.92 | 0.52 |
| 2:A:3282:LYS:HA | 2:A:3285:TYR:CD2 | 2.45 | 0.52 |
| 2:A:3882:GLN:NE2 | 2:A:3946:GLY:HA3 | 2.25 | 0.52 |
| 2:A:3890:TRP:HB3 | 2:B:76:ARG:HG2 | 1.92 | 0.52 |
| 2:B:188:SER:HB2 | 2:B:190:ARG:HH11 | 1.75 | 0.52 |
| 2:B:541:ILE:HD11 | 2:B:574:VAL:HG13 | 1.92 | 0.52 |
| 2:B:1270:VAL:HG22 | 2:B:1285:VAL:HG22 | 1.91 | 0.52 |
| 2:B:3140:LEU:O | 2:B:3152:ARG:NH2 | 2.43 | 0.52 |
| 2:B:3282:LYS:HA | 2:B:3285:TYR:CD2 | 2.45 | 0.52 |
| 2:C:49:LEU:HD11 | 2:C:203:VAL:HB | 1.90 | 0.52 |
| 2:C:677:LEU:HD11 | 2:C:800:VAL:HB | 1.92 | 0.52 |
| 2:C:3140:LEU:O | 2:C:3152:ARG:NH2 | 2.43 | 0.52 |
| 2:C:3689:MET:HE2 | 2:C:3689:MET:HA | 1.91 | 0.52 |
| 2:D:257:ARG:HH21 | 2:D:272:ARG:HG3 | 1.73 | 0.52 |
| 2:D:674:TYR:CE1 | 2:D:756:SER:HB2 | 2.45 | 0.52 |
| 2:D:677:LEU:HD11 | 2:D:800:VAL:HB | 1.92 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:881:ILE:HG23 | 2:D:885:LEU:HD13 | 1.92 | 0.52 |
| 2:D:2620:TYR:HB2 | 2:D:2627:TRP:CD1 | 2.45 | 0.52 |
| 2:D:3013:VAL:O | 2:D:3018:ARG:NH2 | 2.43 | 0.52 |
| 2:D:3140:LEU:O | 2:D:3152:ARG:NH2 | 2.43 | 0.52 |
| 2:A:3101:LEU:HA | 2:A:3104:MET:HG2 | 1.92 | 0.52 |
| 2:B:4610:LEU:HD21 | 2:B:4670:LEU:HD21 | 1.92 | 0.52 |
| 2:C:1689:ILE:HD13 | 2:C:1703:TYR:CE1 | 2.45 | 0.52 |
| 2:C:3050:LEU:HD23 | 2:C:3053:VAL:HG23 | 1.91 | 0.52 |
| 2:D:232:ASP:OD2 | 2:D:233:VAL:N | 2.43 | 0.52 |
| 2:D:1270:VAL:HG22 | 2:D:1285:VAL:HG22 | 1.91 | 0.52 |
| 2:D:2087:LEU:O | 2:D:2091:GLN:HG2 | 2.10 | 0.52 |
| 2:D:2933:VAL:HG21 | 2:D:3007:LEU:HD11 | 1.91 | 0.52 |
| 2:D:4042:VAL:HG12 | 2:D:4077:THR:HB | 1.91 | 0.52 |
| 1:H:8:ILE:HA | 2:D:730:LEU:HD11 | 1.91 | 0.51 |
| 2:A:878:LEU:HA | 2:A:881:ILE:HG22 | 1.91 | 0.51 |
| 2:A:4241:VAL:HG13 | 2:B:4626:ILE:HG12 | 1.92 | 0.51 |
| 2:B:1689:ILE:HD13 | 2:B:1703:TYR:CE1 | 2.46 | 0.51 |
| 2:B:4275:THR:HG22 | 2:B:4278:ASP:H | 1.74 | 0.51 |
| 2:C:3882:GLN:NE2 | 2:C:3946:GLY:HA3 | 2.25 | 0.51 |
| 2:D:188:SER:HB2 | 2:D:190:ARG:HH11 | 1.75 | 0.51 |
| 2:D:514:PHE:HD2 | 2:D:526:TRP:HB2 | 1.76 | 0.51 |
| 2:D:943:LEU:HD21 | 2:D:1064:LEU:HD21 | 1.90 | 0.51 |
| 2:D:1722:ASN:O | 2:D:1919:ARG:NH2 | 2.43 | 0.51 |
| 2:A:514:PHE:HD2 | 2:A:526:TRP:HB2 | 1.75 | 0.51 |
| 2:A:2445:ILE:HA | 2:A:2451:VAL:HA | 1.91 | 0.51 |
| 2:A:2826:ILE:HD13 | 2:A:2898:ILE:HD13 | 1.91 | 0.51 |
| 2:B:2851:ILE:HG22 | 2:B:2855:LYS:NZ | 2.25 | 0.51 |
| 2:B:3712:LYS:O | 2:B:3717:LYS:NZ | 2.42 | 0.51 |
| 2:B:3892:TYR:OH | 2:B:3899:ASP:OD1 | 2.19 | 0.51 |
| 2:C:514:PHE:CD2 | 2:C:526:TRP:HB2 | 2.45 | 0.51 |
| 2:C:658:ASN:ND2 | 2:C:833:LYS:HG2 | 2.24 | 0.51 |
| 2:C:881:ILE:HG23 | 2:C:885:LEU:HD13 | 1.92 | 0.51 |
| 2:C:2851:ILE:HG22 | 2:C:2855:LYS:NZ | 2.25 | 0.51 |
| 2:D:658:ASN:ND2 | 2:D:833:LYS:HG2 | 2.24 | 0.51 |
| 2:D:2409:ILE:HD11 | 2:D:2417:ILE:HD13 | 1.91 | 0.51 |
| 2:D:2826:ILE:HD13 | 2:D:2898:ILE:HD13 | 1.91 | 0.51 |
| 2:D:2851:ILE:HG22 | 2:D:2855:LYS:NZ | 2.25 | 0.51 |
| 2:D:3729:ALA:HA | 2:D:3732:HIS:CE1 | 2.44 | 0.51 |
| 2:A:2851:ILE:HG22 | 2:A:2855:LYS:NZ | 2.25 | 0.51 |
| 2:B:821:PRO:HB2 | 2:B:823:TYR:CE1 | 2.45 | 0.51 |
| 2:B:881:ILE:HG23 | 2:B:885:LEU:HD13 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1944:TYR:O | 2:B:1948:MET:HG2 | 2.11 | 0.51 |
| 2:C:3013:VAL:O | 2:C:3018:ARG:NH2 | 2.43 | 0.51 |
| 2:D:49:LEU:HD11 | 2:D:203:VAL:HB | 1.90 | 0.51 |
| 2:D:3217:GLU:O | 2:D:3221:LEU:HG | 2.08 | 0.51 |
| 1:G:88:HIS:NE2 | 2:C:1776:TYR:OH | 2.33 | 0.51 |
| 2:A:143:LEU:HD13 | 2:A:207:PHE:HE2 | 1.76 | 0.51 |
| 2:A:677:LEU:HD11 | 2:A:800:VAL:HB | 1.92 | 0.51 |
| 2:A:893:TRP:CZ2 | 2:A:1049:SER:HB3 | 2.44 | 0.51 |
| 2:A:1944:TYR:O | 2:A:1948:MET:HG2 | 2.11 | 0.51 |
| 2:A:2553:TYR:HE1 | 2:A:2557:LYS:HZ3 | 1.58 | 0.51 |
| 2:A:2788:ARG:HH22 | 2:A:2908:LYS:HE2 | 1.75 | 0.51 |
| 2:A:3097:THR:HA | 2:A:3101:LEU:HB3 | 1.92 | 0.51 |
| 2:B:232:ASP:OD2 | 2:B:233:VAL:N | 2.43 | 0.51 |
| 2:B:514:PHE:CD2 | 2:B:526:TRP:HB2 | 2.45 | 0.51 |
| 2:B:677:LEU:HD11 | 2:B:800:VAL:HB | 1.92 | 0.51 |
| 2:C:658:ASN:HD21 | 2:C:833:LYS:HG2 | 1.75 | 0.51 |
| 2:C:2409:ILE:HD11 | 2:C:2417:ILE:HD13 | 1.91 | 0.51 |
| 2:C:2788:ARG:HH22 | 2:C:2908:LYS:HE2 | 1.75 | 0.51 |
| 2:C:3712:LYS:O | 2:C:3717:LYS:NZ | 2.42 | 0.51 |
| 2:C:4194:GLU:HG2 | 2:C:4645:TRP:HZ3 | 1.73 | 0.51 |
| 2:D:232:ASP:OD1 | 2:D:356:TYR:OH | 2.21 | 0.51 |
| 2:D:514:PHE:CD2 | 2:D:526:TRP:HB2 | 2.46 | 0.51 |
| 2:A:658:ASN:HD21 | 2:A:833:LYS:HG2 | 1.75 | 0.51 |
| 2:A:4896:ASP:OD1 | 2:A:4897:TYR:N | 2.44 | 0.51 |
| 2:B:2445:ILE:HA | 2:B:2451:VAL:HA | 1.91 | 0.51 |
| 2:B:4896:ASP:OD1 | 2:B:4897:TYR:N | 2.44 | 0.51 |
| 2:C:162:ILE:O | 2:C:163:HIS:ND1 | 2.43 | 0.51 |
| 2:C:897:LYS:HD3 | 2:C:918:LEU:HG | 1.92 | 0.51 |
| 2:C:1034:PRO:HG2 | 2:C:1037:LEU:HD12 | 1.92 | 0.51 |
| 2:C:2621:TYR:OH | 2:C:2637:GLU:OE2 | 2.21 | 0.51 |
| 2:C:2940:ILE:HA | 2:C:2943:PHE:HB3 | 1.92 | 0.51 |
| 2:D:541:ILE:HD11 | 2:D:574:VAL:HG13 | 1.92 | 0.51 |
| 2:D:1944:TYR:O | 2:D:1948:MET:HG2 | 2.10 | 0.51 |
| 2:D:2695:MET:HG2 | 2:D:2700:ASN:O | 2.11 | 0.51 |
| 2:A:173:GLU:HG2 | 2:D:3939:ARG:NH1 | 2.25 | 0.51 |
| 2:A:1689:ILE:HD13 | 2:A:1703:TYR:CE1 | 2.46 | 0.51 |
| 2:B:162:ILE:O | 2:B:163:HIS:ND1 | 2.43 | 0.51 |
| 2:B:3805:LEU:HD21 | 2:B:3891:TYR:HB2 | 1.92 | 0.51 |
| 2:B:4052:MET:HE1 | 2:B:4066:LEU:HB2 | 1.91 | 0.51 |
| 2:C:188:SER:HB2 | 2:C:190:ARG:HH11 | 1.75 | 0.51 |
| 2:C:1989:PRO:HD2 | 2:C:1992:ILE:HD12 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:4042:VAL:HG12 | 2:C:4077:THR:HB | 1.91 | 0.51 |
| 1:E:88:HIS:NE2 | 2:A:1776:TYR:OH | 2.36 | 0.51 |
| 2:A:232:ASP:OD2 | 2:A:233:VAL:N | 2.43 | 0.51 |
| 2:A:821:PRO:HB2 | 2:A:823:TYR:CE1 | 2.45 | 0.51 |
| 2:A:1016:TRP:CE3 | 2:A:1029:ASN:HB2 | 2.46 | 0.51 |
| 2:A:2087:LEU:O | 2:A:2091:GLN:HG2 | 2.10 | 0.51 |
| 2:A:2778:SER:HA | 2:A:2848:TYR:OH | 2.11 | 0.51 |
| 2:A:4610:LEU:HD21 | 2:A:4670:LEU:HD21 | 1.92 | 0.51 |
| 2:A:4617:ILE:HG23 | 2:A:4665:ARG:HH22 | 1.74 | 0.51 |
| 2:B:1969:PRO:HD3 | 2:B:3605:MET:HE1 | 1.92 | 0.51 |
| 2:C:1016:TRP:CE3 | 2:C:1029:ASN:HB2 | 2.46 | 0.51 |
| 2:C:1944:TYR:O | 2:C:1948:MET:HG2 | 2.10 | 0.51 |
| 2:D:749:LEU:HD22 | 2:D:755:ILE:HD11 | 1.93 | 0.51 |
| 2:D:1004:HIS:NE2 | 2:D:1033:VAL:O | 2.25 | 0.51 |
| 2:D:1989:PRO:O | 2:D:1993:ARG:HG3 | 2.11 | 0.51 |
| 2:D:3101:LEU:HA | 2:D:3104:MET:HG2 | 1.92 | 0.51 |
| 2:D:4896:ASP:OD1 | 2:D:4897:TYR:N | 2.44 | 0.51 |
| 2:A:1989:PRO:O | 2:A:1993:ARG:HG3 | 2.11 | 0.51 |
| 2:A:3068:LEU:HD12 | 2:A:3133:ILE:HG12 | 1.93 | 0.51 |
| 2:A:3805:LEU:HD21 | 2:A:3891:TYR:HB2 | 1.92 | 0.51 |
| 2:B:2212:LYS:HG2 | 2:B:2253:LEU:HD21 | 1.92 | 0.51 |
| 2:C:541:ILE:HD11 | 2:C:574:VAL:HG13 | 1.92 | 0.51 |
| 2:C:966:LEU:H | 2:C:977:LYS:HD2 | 1.75 | 0.51 |
| 2:C:3069:GLU:O | 2:C:3072:MET:HB2 | 2.11 | 0.51 |
| 2:D:893:TRP:CE2 | 2:D:1049:SER:HB3 | 2.46 | 0.51 |
| 2:A:4275:THR:HG22 | 2:A:4278:ASP:H | 1.74 | 0.51 |
| 2:B:28:ILE:HD11 | 2:B:201:LEU:HD21 | 1.93 | 0.51 |
| 2:B:3068:LEU:HD12 | 2:B:3133:ILE:HG12 | 1.93 | 0.51 |
| 2:C:232:ASP:OD2 | 2:C:233:VAL:N | 2.43 | 0.51 |
| 2:C:514:PHE:HD2 | 2:C:526:TRP:HB2 | 1.75 | 0.51 |
| 2:C:749:LEU:HD22 | 2:C:755:ILE:HD11 | 1.93 | 0.51 |
| 2:C:2933:VAL:HG21 | 2:C:3007:LEU:HD11 | 1.91 | 0.51 |
| 2:C:3892:TYR:OH | 2:C:3899:ASP:OD1 | 2.19 | 0.51 |
| 2:D:3069:GLU:O | 2:D:3072:MET:HB2 | 2.11 | 0.51 |
| 2:D:4610:LEU:HD21 | 2:D:4670:LEU:HD21 | 1.92 | 0.51 |
| 2:A:514:PHE:CD2 | 2:A:526:TRP:HB2 | 2.45 | 0.51 |
| 2:A:893:TRP:CE2 | 2:A:1049:SER:HB3 | 2.46 | 0.51 |
| 2:A:1435:GLY:CA | 2:D:2831:VAL:HG22 | 2.41 | 0.51 |
| 2:A:3068:LEU:O | 2:A:3071:THR:OG1 | 2.25 | 0.51 |
| 2:A:3697:LYS:HA | 2:A:3700:HIS:CD2 | 2.46 | 0.51 |
| 2:B:514:PHE:HD2 | 2:B:526:TRP:HB2 | 1.75 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:658:ASN:ND2 | 2:B:831:LYS:O | 2.44 | 0.51 |
| 2:B:967:PRO:O | 2:B:971:GLN:N | 2.40 | 0.51 |
| 2:B:2087:LEU:O | 2:B:2091:GLN:HG2 | 2.10 | 0.51 |
| 2:B:3097:THR:HA | 2:B:3101:LEU:HB3 | 1.92 | 0.51 |
| 2:C:1989:PRO:O | 2:C:1993:ARG:HG3 | 2.11 | 0.51 |
| 2:C:3846:LEU:HB3 | 2:C:3854:PHE:CE2 | 2.46 | 0.51 |
| 2:D:28:ILE:HD11 | 2:D:201:LEU:HD21 | 1.93 | 0.51 |
| 2:D:2591:ARG:HG2 | 2:D:2695:MET:HE1 | 1.93 | 0.51 |
| 2:D:3068:LEU:O | 2:D:3071:THR:OG1 | 2.25 | 0.51 |
| 2:D:3882:GLN:NE2 | 2:D:3946:GLY:HA3 | 2.25 | 0.51 |
| 2:A:162:ILE:O | 2:A:163:HIS:ND1 | 2.43 | 0.50 |
| 2:A:967:PRO:O | 2:A:971:GLN:N | 2.40 | 0.50 |
| 2:A:2322:ARG:NH1 | 2:B:189:GLU:OE2 | 2.44 | 0.50 |
| 2:A:2695:MET:HG2 | 2:A:2700:ASN:O | 2.11 | 0.50 |
| 2:A:3069:GLU:O | 2:A:3072:MET:HB2 | 2.11 | 0.50 |
| 2:B:749:LEU:HD22 | 2:B:755:ILE:HD11 | 1.93 | 0.50 |
| 2:D:658:ASN:ND2 | 2:D:831:LYS:O | 2.44 | 0.50 |
| 2:D:3282:LYS:HA | 2:D:3285:TYR:CD2 | 2.45 | 0.50 |
| 2:D:3712:LYS:O | 2:D:3717:LYS:NZ | 2.42 | 0.50 |
| 2:A:28:ILE:HD11 | 2:A:201:LEU:HD21 | 1.93 | 0.50 |
| 2:A:749:LEU:HD22 | 2:A:755:ILE:HD11 | 1.93 | 0.50 |
| 2:A:897:LYS:HB3 | 2:A:918:LEU:CD2 | 2.40 | 0.50 |
| 2:A:966:LEU:H | 2:A:977:LYS:HD2 | 1.76 | 0.50 |
| 2:A:1034:PRO:HG2 | 2:A:1037:LEU:HD12 | 1.92 | 0.50 |
| 2:A:1575:HIS:O | 2:A:1576:LYS:NZ | 2.40 | 0.50 |
| 2:A:1608:VAL:HG12 | 2:A:1619:VAL:HG22 | 1.94 | 0.50 |
| 2:A:3846:LEU:HB3 | 2:A:3854:PHE:CE2 | 2.47 | 0.50 |
| 2:B:143:LEU:HD13 | 2:B:207:PHE:HE2 | 1.76 | 0.50 |
| 2:B:893:TRP:CE2 | 2:B:1049:SER:HB3 | 2.46 | 0.50 |
| 2:B:1016:TRP:CE3 | 2:B:1029:ASN:HB2 | 2.46 | 0.50 |
| 2:C:28:ILE:HD11 | 2:C:201:LEU:HD21 | 1.93 | 0.50 |
| 2:C:658:ASN:ND2 | 2:C:831:LYS:O | 2.44 | 0.50 |
| 2:C:2695:MET:HG2 | 2:C:2700:ASN:O | 2.11 | 0.50 |
| 2:C:4751:LYS:HG3 | 2:C:4754:ARG:NH1 | 2.27 | 0.50 |
| 2:D:728:ASP:OD2 | 2:D:731:HIS:HB2 | 2.12 | 0.50 |
| 2:D:1016:TRP:CD1 | 2:D:1027:ARG:HB3 | 2.46 | 0.50 |
| 2:D:1016:TRP:CE3 | 2:D:1029:ASN:HB2 | 2.46 | 0.50 |
| 2:D:1564:MET:HG3 | 2:D:1565:PRO:HD2 | 1.93 | 0.50 |
| 2:D:1689:ILE:HD13 | 2:D:1703:TYR:CE1 | 2.45 | 0.50 |
| 2:D:2214:MET:HE2 | 2:D:2242:VAL:CG1 | 2.41 | 0.50 |
| 2:A:625:VAL:HG23 | 2:A:628:ASN:HB2 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:1564:MET:HG3 | 2:A:1565:PRO:HD2 | 1.93 | 0.50 |
| 2:A:2603:ALA:C | 2:A:2606:PRO:HD2 | 2.32 | 0.50 |
| 2:A:2791:ARG:NH2 | 2:A:2795:GLY:O | 2.42 | 0.50 |
| 2:B:981:MET:HG2 | 2:B:986:ILE:HD11 | 1.93 | 0.50 |
| 2:B:1034:PRO:HG2 | 2:B:1037:LEU:HD12 | 1.92 | 0.50 |
| 2:B:3101:LEU:HA | 2:B:3104:MET:HG2 | 1.92 | 0.50 |
| 2:B:4028:SER:O | 2:B:4033:LYS:NZ | 2.39 | 0.50 |
| 2:C:893:TRP:CE2 | 2:C:1049:SER:HB3 | 2.46 | 0.50 |
| 2:C:1016:TRP:CD1 | 2:C:1027:ARG:HB3 | 2.46 | 0.50 |
| 2:C:3068:LEU:O | 2:C:3071:THR:OG1 | 2.25 | 0.50 |
| 2:C:4177:VAL:HG11 | 2:C:4880:VAL:HA | 1.94 | 0.50 |
| 2:D:162:ILE:O | 2:D:163:HIS:ND1 | 2.43 | 0.50 |
| 2:D:966:LEU:H | 2:D:977:LYS:HD2 | 1.75 | 0.50 |
| 2:D:2759:PRO:HD2 | 2:D:2762:LEU:HD22 | 1.94 | 0.50 |
| 2:D:3097:THR:HA | 2:D:3101:LEU:HB3 | 1.92 | 0.50 |
| 2:B:1016:TRP:CD1 | 2:B:1027:ARG:HB3 | 2.46 | 0.50 |
| 2:B:3846:LEU:HB3 | 2:B:3854:PHE:CE2 | 2.47 | 0.50 |
| 2:D:3697:LYS:HA | 2:D:3700:HIS:CD2 | 2.47 | 0.50 |
| 2:D:4254:THR:HA | 2:D:4257:ARG:HE | 1.77 | 0.50 |
| 2:D:4751:LYS:HG3 | 2:D:4754:ARG:NH1 | 2.27 | 0.50 |
| 2:B:2778:SER:HA | 2:B:2848:TYR:OH | 2.11 | 0.50 |
| 2:B:3697:LYS:HA | 2:B:3700:HIS:CD2 | 2.46 | 0.50 |
| 2:C:2212:LYS:HG2 | 2:C:2253:LEU:HD21 | 1.92 | 0.50 |
| 2:C:2791:ARG:NH1 | 2:C:2901:TYR:OH | 2.45 | 0.50 |
| 2:C:3805:LEU:HD21 | 2:C:3891:TYR:HB2 | 1.92 | 0.50 |
| 2:D:897:LYS:HB3 | 2:D:918:LEU:HD23 | 1.93 | 0.50 |
| 2:D:1989:PRO:HD2 | 2:D:1992:ILE:HD12 | 1.92 | 0.50 |
| 2:A:942:THR:HG21 | 2:A:1002:ASN:HD22 | 1.77 | 0.50 |
| 2:A:981:MET:HG2 | 2:A:986:ILE:HD11 | 1.93 | 0.50 |
| 2:A:1019:GLY:O | 2:A:1030:PRO:HB3 | 2.12 | 0.50 |
| 2:B:625:VAL:HG23 | 2:B:628:ASN:HB2 | 1.94 | 0.50 |
| 2:B:1564:MET:HG3 | 2:B:1565:PRO:HD2 | 1.93 | 0.50 |
| 2:B:1989:PRO:O | 2:B:1993:ARG:HG3 | 2.11 | 0.50 |
| 2:C:728:ASP:OD2 | 2:C:731:HIS:HB2 | 2.12 | 0.50 |
| 2:C:897:LYS:HB3 | 2:C:918:LEU:HD23 | 1.94 | 0.50 |
| 2:C:1287:GLN:NE2 | 2:C:1295:SER:OG | 2.45 | 0.50 |
| 2:C:2591:ARG:HG2 | 2:C:2695:MET:HE1 | 1.93 | 0.50 |
| 2:C:3101:LEU:HA | 2:C:3104:MET:HG2 | 1.92 | 0.50 |
| 2:D:143:LEU:HD13 | 2:D:207:PHE:HE2 | 1.76 | 0.50 |
| 2:D:1034:PRO:HG2 | 2:D:1037:LEU:HD12 | 1.92 | 0.50 |
| 2:D:1287:GLN:NE2 | 2:D:1295:SER:OG | 2.45 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:1552:VAL:HG12 | 2:D:1553:PHE:HD1 | 1.77 | 0.50 |
| 2:D:2791:ARG:NH1 | 2:D:2901:TYR:OH | 2.45 | 0.50 |
| 1:G:19:LYS:HZ3 | 1:G:52:GLY:HA3 | 1.76 | 0.50 |
| 2:B:1989:PRO:HD2 | 2:B:1992:ILE:HD12 | 1.92 | 0.50 |
| 2:B:3882:GLN:NE2 | 2:B:3946:GLY:HA3 | 2.25 | 0.50 |
| 2:C:1029:ASN:C | 2:C:1031:ARG:H | 2.15 | 0.50 |
| 2:C:3097:THR:HA | 2:C:3101:LEU:HB3 | 1.92 | 0.50 |
| 2:D:1019:GLY:O | 2:D:1030:PRO:HB3 | 2.12 | 0.50 |
| 2:D:2603:ALA:C | 2:D:2606:PRO:HD2 | 2.32 | 0.50 |
| 2:D:3284:ILE:HA | 2:D:3287:ASN:HD22 | 1.76 | 0.50 |
| 2:D:3989:ASN:HB3 | 2:D:4108:HIS:CD2 | 2.47 | 0.50 |
| 2:A:897:LYS:CB | 2:A:918:LEU:HD23 | 2.42 | 0.50 |
| 2:A:2791:ARG:NH1 | 2:A:2901:TYR:OH | 2.45 | 0.50 |
| 2:A:4252:ILE:HG21 | 2:B:4707:MET:HG3 | 1.94 | 0.50 |
| 2:B:942:THR:HG21 | 2:B:1002:ASN:HD22 | 1.77 | 0.50 |
| 2:B:2603:ALA:C | 2:B:2606:PRO:HD2 | 2.32 | 0.50 |
| 2:B:2706:VAL:HG23 | 2:B:2847:ASN:HD21 | 1.77 | 0.50 |
| 2:B:2791:ARG:NH1 | 2:B:2901:TYR:OH | 2.45 | 0.50 |
| 2:B:3034:HIS:CE1 | 2:B:3107:SER:HB2 | 2.47 | 0.50 |
| 2:B:3069:GLU:O | 2:B:3072:MET:HB2 | 2.11 | 0.50 |
| 2:B:3284:ILE:HA | 2:B:3287:ASN:HD22 | 1.76 | 0.50 |
| 2:B:3989:ASN:HB3 | 2:B:4108:HIS:CD2 | 2.47 | 0.50 |
| 2:C:143:LEU:HD13 | 2:C:207:PHE:HE2 | 1.76 | 0.50 |
| 2:C:2478:ILE:HG21 | 2:C:2484:LEU:HD13 | 1.94 | 0.50 |
| 2:D:1717:ALA:HA | 2:D:1720:MET:HE2 | 1.93 | 0.50 |
| 2:D:4177:VAL:HG11 | 2:D:4880:VAL:HA | 1.94 | 0.50 |
| 2:A:271:ALA:O | 2:A:301:THR:OG1 | 2.30 | 0.50 |
| 2:A:1989:PRO:HD2 | 2:A:1992:ILE:HD12 | 1.92 | 0.50 |
| 2:A:2200:LEU:HD13 | 2:A:2214:MET:HE1 | 1.93 | 0.50 |
| 2:B:537:LEU:O | 2:B:541:ILE:HG12 | 2.12 | 0.50 |
| 2:B:1608:VAL:HG12 | 2:B:1619:VAL:HG22 | 1.94 | 0.50 |
| 2:B:1954:SER:HB3 | 2:B:1957:LEU:HB2 | 1.94 | 0.50 |
| 2:B:2478:ILE:HG21 | 2:B:2484:LEU:HD13 | 1.94 | 0.50 |
| 2:B:2591:ARG:HG2 | 2:B:2695:MET:HE1 | 1.93 | 0.50 |
| 2:B:2791:ARG:NH2 | 2:B:2795:GLY:O | 2.42 | 0.50 |
| 2:C:537:LEU:O | 2:C:541:ILE:HG12 | 2.12 | 0.50 |
| 2:C:2759:PRO:HD2 | 2:C:2762:LEU:HD22 | 1.94 | 0.50 |
| 2:C:2766:LYS:HA | 2:C:2766:LYS:HE2 | 1.94 | 0.50 |
| 2:D:897:LYS:CB | 2:D:918:LEU:HD23 | 2.42 | 0.50 |
| 2:D:981:MET:HG2 | 2:D:986:ILE:HD11 | 1.93 | 0.50 |
| 2:D:1608:VAL:HG12 | 2:D:1619:VAL:HG22 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2766:LYS:HE2 | 2:D:2766:LYS:HA | 1.94 | 0.50 |
| 2:A:1018:TYR:CE1 | 2:A:1030:PRO:HA | 2.47 | 0.49 |
| 2:A:1975:MET:HA | 2:A:1978:ASN:HD22 | 1.77 | 0.49 |
| 2:A:3284:ILE:HA | 2:A:3287:ASN:HD22 | 1.76 | 0.49 |
| 2:B:514:PHE:CE2 | 2:B:522:ALA:HB1 | 2.47 | 0.49 |
| 2:B:953:SER:OG | 2:B:1063:ASN:OD1 | 2.30 | 0.49 |
| 2:B:1011:ARG:O | 2:B:1014:GLN:HB2 | 2.12 | 0.49 |
| 2:C:1018:TYR:CE1 | 2:C:1030:PRO:HA | 2.47 | 0.49 |
| 2:C:3697:LYS:HA | 2:C:3700:HIS:CD2 | 2.46 | 0.49 |
| 2:D:953:SER:OG | 2:D:1063:ASN:OD1 | 2.30 | 0.49 |
| 2:D:1011:ARG:O | 2:D:1014:GLN:HB2 | 2.12 | 0.49 |
| 2:A:4689:LYS:HE3 | 2:A:4696:ALA:HB2 | 1.94 | 0.49 |
| 2:B:271:ALA:O | 2:B:301:THR:OG1 | 2.30 | 0.49 |
| 2:B:897:LYS:CB | 2:B:918:LEU:HD23 | 2.42 | 0.49 |
| 2:B:1975:MET:HA | 2:B:1978:ASN:HD22 | 1.77 | 0.49 |
| 2:B:2759:PRO:HD2 | 2:B:2762:LEU:HD22 | 1.94 | 0.49 |
| 2:C:942:THR:HG21 | 2:C:1002:ASN:HD22 | 1.77 | 0.49 |
| 2:C:2603:ALA:C | 2:C:2606:PRO:HD2 | 2.32 | 0.49 |
| 2:C:2706:VAL:HG23 | 2:C:2847:ASN:HD21 | 1.77 | 0.49 |
| 2:D:2778:SER:HA | 2:D:2848:TYR:OH | 2.11 | 0.49 |
| 2:D:4689:LYS:HE3 | 2:D:4696:ALA:HB2 | 1.94 | 0.49 |
| 2:A:537:LEU:O | 2:A:541:ILE:HG12 | 2.12 | 0.49 |
| 2:A:728:ASP:OD2 | 2:A:731:HIS:HB2 | 2.12 | 0.49 |
| 2:A:1011:ARG:O | 2:A:1014:GLN:HB2 | 2.12 | 0.49 |
| 2:A:1287:GLN:NE2 | 2:A:1295:SER:OG | 2.45 | 0.49 |
| 2:A:1717:ALA:HA | 2:A:1720:MET:HE2 | 1.94 | 0.49 |
| 2:A:2211:GLN:NE2 | 2:A:2248:MET:O | 2.35 | 0.49 |
| 2:A:2478:ILE:HG21 | 2:A:2484:LEU:HD13 | 1.94 | 0.49 |
| 2:A:2704:GLN:HA | 2:A:2854:LYS:HE2 | 1.94 | 0.49 |
| 2:A:3989:ASN:HB3 | 2:A:4108:HIS:CD2 | 2.47 | 0.49 |
| 2:B:2447:LYS:HD2 | 2:B:2864:GLY:HA3 | 1.95 | 0.49 |
| 2:B:2591:ARG:HH22 | 2:B:2875:ASP:HB3 | 1.78 | 0.49 |
| 2:B:2766:LYS:HE2 | 2:B:2766:LYS:HA | 1.94 | 0.49 |
| 2:C:981:MET:HG2 | 2:C:986:ILE:HD11 | 1.93 | 0.49 |
| 2:C:1011:ARG:O | 2:C:1014:GLN:HB2 | 2.12 | 0.49 |
| 2:C:1552:VAL:HG12 | 2:C:1553:PHE:HD1 | 1.77 | 0.49 |
| 2:C:1681:ASP:HB3 | 2:C:1683:PRO:HD2 | 1.94 | 0.49 |
| 2:C:2778:SER:HA | 2:C:2848:TYR:OH | 2.11 | 0.49 |
| 2:C:3068:LEU:HD12 | 2:C:3133:ILE:HG12 | 1.93 | 0.49 |
| 2:C:3989:ASN:HB3 | 2:C:4108:HIS:CD2 | 2.47 | 0.49 |
| 2:C:4697:VAL:O | 2:C:4701:ILE:HG12 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:4896:ASP:OD1 | 2:C:4897:TYR:N | 2.44 | 0.49 |
| 2:D:1415:ASP:HB3 | 2:D:1561:LYS:HD2 | 1.94 | 0.49 |
| 2:D:2791:ARG:HD3 | 2:D:2901:TYR:CE1 | 2.47 | 0.49 |
| 1:E:8:ILE:HG23 | 2:A:748:LEU:HB2 | 1.94 | 0.49 |
| 2:A:514:PHE:CE2 | 2:A:522:ALA:HB1 | 2.47 | 0.49 |
| 2:A:658:ASN:ND2 | 2:A:831:LYS:O | 2.44 | 0.49 |
| 2:A:2591:ARG:HG2 | 2:A:2695:MET:HE1 | 1.94 | 0.49 |
| 2:A:2759:PRO:HD2 | 2:A:2762:LEU:HD22 | 1.94 | 0.49 |
| 2:A:3089:GLY:O | 2:A:3093:ILE:HG12 | 2.13 | 0.49 |
| 2:A:4052:MET:HE1 | 2:A:4066:LEU:HB2 | 1.93 | 0.49 |
| 2:A:4254:THR:HA | 2:A:4257:ARG:HE | 1.77 | 0.49 |
| 2:B:1019:GLY:O | 2:B:1030:PRO:HB3 | 2.12 | 0.49 |
| 2:B:1029:ASN:C | 2:B:1031:ARG:H | 2.15 | 0.49 |
| 2:B:2695:MET:HG2 | 2:B:2700:ASN:O | 2.11 | 0.49 |
| 2:B:2704:GLN:HA | 2:B:2854:LYS:HE2 | 1.95 | 0.49 |
| 2:B:3089:GLY:O | 2:B:3093:ILE:HG12 | 2.13 | 0.49 |
| 2:B:4751:LYS:HG3 | 2:B:4754:ARG:NH1 | 2.27 | 0.49 |
| 2:C:1019:GLY:O | 2:C:1030:PRO:HB3 | 2.12 | 0.49 |
| 2:C:1564:MET:HG3 | 2:C:1565:PRO:HD2 | 1.93 | 0.49 |
| 2:C:2591:ARG:HH22 | 2:C:2875:ASP:HB3 | 1.78 | 0.49 |
| 2:C:2704:GLN:HA | 2:C:2854:LYS:HE2 | 1.94 | 0.49 |
| 2:D:4517:LEU:HD21 | 2:D:4736:ASN:HB3 | 1.95 | 0.49 |
| 2:A:953:SER:OG | 2:A:1063:ASN:OD1 | 2.30 | 0.49 |
| 2:A:3304:GLN:HA | 2:A:3307:ILE:HG12 | 1.94 | 0.49 |
| 2:A:4089:GLU:HB2 | 2:A:4090:PRO:HD3 | 1.95 | 0.49 |
| 2:B:966:LEU:H | 2:B:977:LYS:HD2 | 1.76 | 0.49 |
| 2:B:1018:TYR:CE1 | 2:B:1030:PRO:HA | 2.47 | 0.49 |
| 2:B:4517:LEU:HD21 | 2:B:4736:ASN:HB3 | 1.95 | 0.49 |
| 2:C:4254:THR:HA | 2:C:4257:ARG:HE | 1.77 | 0.49 |
| 2:C:4270:LYS:NZ | 2:C:4278:ASP:OD1 | 2.26 | 0.49 |
| 2:D:1018:TYR:CE1 | 2:D:1030:PRO:HA | 2.47 | 0.49 |
| 2:D:2868:HIS:CE1 | 2:D:2870:LEU:HB2 | 2.48 | 0.49 |
| 2:D:3075:LEU:HD12 | 2:D:3076:LYS:HD2 | 1.95 | 0.49 |
| 2:D:3805:LEU:HD21 | 2:D:3891:TYR:HB2 | 1.92 | 0.49 |
| 2:D:4089:GLU:HB2 | 2:D:4090:PRO:HD3 | 1.95 | 0.49 |
| 1:F:19:LYS:HZ3 | 1:F:52:GLY:HA3 | 1.76 | 0.49 |
| 2:A:232:ASP:OD1 | 2:A:356:TYR:OH | 2.22 | 0.49 |
| 2:A:1016:TRP:CD1 | 2:A:1027:ARG:HB3 | 2.47 | 0.49 |
| 2:A:2833:LEU:HB2 | 2:A:2894:LYS:HZ1 | 1.78 | 0.49 |
| 2:A:4751:LYS:HG3 | 2:A:4754:ARG:NH1 | 2.27 | 0.49 |
| 2:B:2214:MET:HE2 | 2:B:2242:VAL:CG1 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2488:LEU:HA | 2:B:2492:PHE:HB2 | 1.95 | 0.49 |
| 2:B:4689:LYS:HE3 | 2:B:4696:ALA:HB2 | 1.94 | 0.49 |
| 2:C:271:ALA:O | 2:C:301:THR:OG1 | 2.30 | 0.49 |
| 2:C:2791:ARG:HD3 | 2:C:2901:TYR:CE1 | 2.47 | 0.49 |
| 2:C:3284:ILE:HA | 2:C:3287:ASN:HD22 | 1.76 | 0.49 |
| 2:D:1975:MET:HA | 2:D:1978:ASN:HD22 | 1.77 | 0.49 |
| 2:D:2591:ARG:HH22 | 2:D:2875:ASP:HB3 | 1.78 | 0.49 |
| 2:D:3068:LEU:HD12 | 2:D:3133:ILE:HG12 | 1.93 | 0.49 |
| 2:D:3846:LEU:HB3 | 2:D:3854:PHE:CE2 | 2.47 | 0.49 |
| 2:A:897:LYS:HB3 | 2:A:918:LEU:HD23 | 1.94 | 0.49 |
| 2:A:907:VAL:HB | 2:A:912:LYS:HE2 | 1.94 | 0.49 |
| 2:A:3861:GLN:HB3 | 2:A:3864:ASN:HD22 | 1.78 | 0.49 |
| 2:B:728:ASP:OD2 | 2:B:731:HIS:HB2 | 2.12 | 0.49 |
| 2:B:1118:SER:HB3 | 2:B:1204:VAL:HG11 | 1.95 | 0.49 |
| 2:B:2158:HIS:CE1 | 2:B:3615:ARG:HH12 | 2.31 | 0.49 |
| 2:B:3036:LEU:O | 2:B:3040:LEU:HG | 2.13 | 0.49 |
| 2:C:514:PHE:CE2 | 2:C:522:ALA:HB1 | 2.47 | 0.49 |
| 2:C:1954:SER:HB3 | 2:C:1957:LEU:HB2 | 1.94 | 0.49 |
| 2:C:2674:GLY:HA2 | 2:C:2978:HIS:CE1 | 2.48 | 0.49 |
| 2:C:2714:PRO:HG2 | 2:C:2717:LEU:HD13 | 1.95 | 0.49 |
| 2:C:3036:LEU:O | 2:C:3040:LEU:HG | 2.13 | 0.49 |
| 2:C:3986:LEU:HD12 | 2:C:4101:LEU:HD12 | 1.94 | 0.49 |
| 2:D:537:LEU:O | 2:D:541:ILE:HG12 | 2.12 | 0.49 |
| 2:D:1029:ASN:C | 2:D:1031:ARG:H | 2.15 | 0.49 |
| 2:D:2704:GLN:HA | 2:D:2854:LYS:HE2 | 1.94 | 0.49 |
| 2:D:3089:GLY:O | 2:D:3093:ILE:HG12 | 2.13 | 0.49 |
| 2:D:4858:LEU:HA | 2:D:4861:ILE:HD12 | 1.94 | 0.49 |
| 2:A:1118:SER:HB3 | 2:A:1204:VAL:HG11 | 1.95 | 0.49 |
| 2:A:2119:LEU:HB2 | 2:A:2152:ASN:ND2 | 2.28 | 0.49 |
| 2:A:2591:ARG:HH22 | 2:A:2875:ASP:HB3 | 1.78 | 0.49 |
| 2:A:2706:VAL:HG23 | 2:A:2847:ASN:HD21 | 1.77 | 0.49 |
| 2:A:3034:HIS:CE1 | 2:A:3107:SER:HB2 | 2.47 | 0.49 |
| 2:B:3239:LEU:HD23 | 2:B:3242:LEU:HD12 | 1.95 | 0.49 |
| 2:B:3304:GLN:HA | 2:B:3307:ILE:HG12 | 1.94 | 0.49 |
| 2:B:4697:VAL:O | 2:B:4701:ILE:HG12 | 2.12 | 0.49 |
| 2:C:897:LYS:CB | 2:C:918:LEU:HD23 | 2.42 | 0.49 |
| 2:C:2894:LYS:NZ | 2:C:2897:GLN:OE1 | 2.46 | 0.49 |
| 2:C:3034:HIS:CE1 | 2:C:3107:SER:HB2 | 2.47 | 0.49 |
| 2:C:4089:GLU:HB2 | 2:C:4090:PRO:HD3 | 1.95 | 0.49 |
| 2:D:312:LYS:HE2 | 2:D:394:HIS:HA | 1.95 | 0.49 |
| 2:D:942:THR:HG21 | 2:D:1002:ASN:HD22 | 1.77 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:1074:ARG:HH12 | 2:D:1209:VAL:HG11 | 1.78 | 0.49 |
| 2:D:1681:ASP:HB3 | 2:D:1683:PRO:HD2 | 1.94 | 0.49 |
| 2:D:1954:SER:HB3 | 2:D:1957:LEU:HB2 | 1.94 | 0.49 |
| 2:D:2488:LEU:HA | 2:D:2492:PHE:HB2 | 1.95 | 0.49 |
| 2:D:3861:GLN:HB3 | 2:D:3864:ASN:HD22 | 1.78 | 0.49 |
| 2:A:931:TYR:OH | 4:A:5003:ATP:H2' | 2.13 | 0.49 |
| 2:A:1029:ASN:C | 2:A:1031:ARG:H | 2.15 | 0.49 |
| 2:A:2488:LEU:HA | 2:A:2492:PHE:HB2 | 1.95 | 0.49 |
| 2:A:3986:LEU:HD12 | 2:A:4101:LEU:HD12 | 1.94 | 0.49 |
| 2:A:4177:VAL:HG11 | 2:A:4880:VAL:HA | 1.94 | 0.49 |
| 2:B:258:ARG:NH1 | 2:B:316:LEU:O | 2.46 | 0.49 |
| 2:B:312:LYS:HE2 | 2:B:394:HIS:HA | 1.94 | 0.49 |
| 2:B:1552:VAL:HG12 | 2:B:1553:PHE:HD1 | 1.77 | 0.49 |
| 2:B:2211:GLN:NE2 | 2:B:2248:MET:O | 2.35 | 0.49 |
| 2:B:2791:ARG:HD3 | 2:B:2901:TYR:CE1 | 2.47 | 0.49 |
| 2:B:2894:LYS:NZ | 2:B:2897:GLN:OE1 | 2.46 | 0.49 |
| 2:B:4089:GLU:HB2 | 2:B:4090:PRO:HD3 | 1.95 | 0.49 |
| 2:B:4858:LEU:HA | 2:B:4861:ILE:HD12 | 1.95 | 0.49 |
| 2:C:907:VAL:HB | 2:C:912:LYS:HE2 | 1.95 | 0.49 |
| 2:C:953:SER:OG | 2:C:1061:GLY:O | 2.31 | 0.49 |
| 2:C:2716:LYS:HG3 | 2:C:2717:LEU:HD12 | 1.95 | 0.49 |
| 2:C:4043:ILE:O | 2:C:4078:LEU:N | 2.31 | 0.49 |
| 2:C:4517:LEU:HD21 | 2:C:4736:ASN:HB3 | 1.95 | 0.49 |
| 2:D:514:PHE:CE2 | 2:D:522:ALA:HB1 | 2.47 | 0.49 |
| 2:D:625:VAL:HG23 | 2:D:628:ASN:HB2 | 1.93 | 0.49 |
| 2:D:953:SER:OG | 2:D:1061:GLY:O | 2.31 | 0.49 |
| 2:D:1074:ARG:HD2 | 2:D:1078:CYS:HB3 | 1.95 | 0.49 |
| 2:D:2119:LEU:HB2 | 2:D:2152:ASN:ND2 | 2.28 | 0.49 |
| 2:D:2674:GLY:HA2 | 2:D:2978:HIS:CE1 | 2.48 | 0.49 |
| 2:D:4697:VAL:O | 2:D:4701:ILE:HG12 | 2.12 | 0.49 |
| 2:A:1552:VAL:HG12 | 2:A:1553:PHE:HD1 | 1.77 | 0.49 |
| 2:B:411:GLU:OE2 | 2:B:485:ARG:NE | 2.46 | 0.49 |
| 2:B:456:LEU:HD11 | 2:B:533:LEU:HG | 1.95 | 0.49 |
| 2:B:2200:LEU:HD13 | 2:B:2214:MET:HE1 | 1.93 | 0.49 |
| 2:C:967:PRO:O | 2:C:971:GLN:N | 2.40 | 0.49 |
| 2:C:1415:ASP:HB3 | 2:C:1561:LYS:HD2 | 1.94 | 0.49 |
| 2:C:1608:VAL:HG12 | 2:C:1619:VAL:HG22 | 1.94 | 0.49 |
| 2:C:3089:GLY:O | 2:C:3093:ILE:HG12 | 2.13 | 0.49 |
| 2:D:2478:ILE:HG21 | 2:D:2484:LEU:HD13 | 1.94 | 0.49 |
| 2:D:3034:HIS:CE1 | 2:D:3107:SER:HB2 | 2.47 | 0.49 |
| 2:A:953:SER:OG | 2:A:1061:GLY:O | 2.31 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:1415:ASP:HB3 | 2:A:1561:LYS:HD2 | 1.94 | 0.48 |
| 2:A:1954:SER:HB3 | 2:A:1957:LEU:HB2 | 1.94 | 0.48 |
| 2:A:2447:LYS:HD2 | 2:A:2864:GLY:HA3 | 1.95 | 0.48 |
| 2:A:2710:ASN:OD1 | 2:A:2711:ILE:N | 2.46 | 0.48 |
| 2:A:3075:LEU:HD12 | 2:A:3076:LYS:HD2 | 1.95 | 0.48 |
| 2:A:4238:ILE:HG23 | 2:A:4239:LEU:HD12 | 1.95 | 0.48 |
| 2:B:897:LYS:HB3 | 2:B:918:LEU:HD23 | 1.94 | 0.48 |
| 2:B:1287:GLN:NE2 | 2:B:1295:SER:OG | 2.45 | 0.48 |
| 2:B:2674:GLY:HA2 | 2:B:2978:HIS:CE1 | 2.48 | 0.48 |
| 2:B:4177:VAL:HG11 | 2:B:4880:VAL:HA | 1.94 | 0.48 |
| 2:B:4254:THR:HA | 2:B:4257:ARG:HE | 1.77 | 0.48 |
| 2:C:456:LEU:HD11 | 2:C:533:LEU:HG | 1.95 | 0.48 |
| 2:C:3075:LEU:HD12 | 2:C:3076:LYS:HD2 | 1.95 | 0.48 |
| 2:D:411:GLU:OE2 | 2:D:485:ARG:NE | 2.46 | 0.48 |
| 2:D:931:TYR:OH | 4:D:5003:ATP:H2' | 2.13 | 0.48 |
| 2:D:2716:LYS:HG3 | 2:D:2717:LEU:HD12 | 1.95 | 0.48 |
| 2:D:3986:LEU:HD12 | 2:D:4101:LEU:HD12 | 1.94 | 0.48 |
| 2:A:3235:MET:HA | 2:A:3239:LEU:HD12 | 1.96 | 0.48 |
| 2:A:4697:VAL:O | 2:A:4701:ILE:HG12 | 2.12 | 0.48 |
| 2:B:227:TYR:CG | 2:B:352:SER:HB2 | 2.49 | 0.48 |
| 2:B:2716:LYS:HG3 | 2:B:2717:LEU:HD12 | 1.95 | 0.48 |
| 2:B:3920:LEU:HD22 | 2:B:3935:LEU:HD21 | 1.95 | 0.48 |
| 2:B:4010:VAL:HG11 | 2:B:4118:PHE:HZ | 1.78 | 0.48 |
| 2:C:2488:LEU:HA | 2:C:2492:PHE:HB2 | 1.95 | 0.48 |
| 2:C:2868:HIS:CE1 | 2:C:2870:LEU:HB2 | 2.48 | 0.48 |
| 2:D:1031:ARG:HE | 2:D:1038:LEU:HD11 | 1.78 | 0.48 |
| 2:D:2754:GLN:HE22 | 2:D:2757:MET:HG2 | 1.78 | 0.48 |
| 2:D:2791:ARG:HD3 | 2:D:2901:TYR:CZ | 2.48 | 0.48 |
| 2:A:1972:GLN:HA | 2:A:1975:MET:SD | 2.53 | 0.48 |
| 2:A:2716:LYS:HG3 | 2:A:2717:LEU:HD12 | 1.95 | 0.48 |
| 2:A:4010:VAL:HG11 | 2:A:4118:PHE:HZ | 1.78 | 0.48 |
| 2:B:1074:ARG:HD2 | 2:B:1078:CYS:HB3 | 1.95 | 0.48 |
| 2:B:1972:GLN:HA | 2:B:1975:MET:SD | 2.53 | 0.48 |
| 2:B:2714:PRO:HG2 | 2:B:2717:LEU:HD13 | 1.95 | 0.48 |
| 2:B:3001:LYS:HZ1 | 2:B:3044:THR:H | 1.61 | 0.48 |
| 2:B:3861:GLN:HB3 | 2:B:3864:ASN:HD22 | 1.78 | 0.48 |
| 2:C:1074:ARG:HD2 | 2:C:1078:CYS:HB3 | 1.95 | 0.48 |
| 2:C:3304:GLN:HA | 2:C:3307:ILE:HG12 | 1.94 | 0.48 |
| 2:C:4625:ASP:OD1 | 2:C:4625:ASP:N | 2.46 | 0.48 |
| 2:D:1031:ARG:NH2 | 2:D:1042:THR:HG21 | 2.21 | 0.48 |
| 2:A:1074:ARG:HH12 | 2:A:1209:VAL:HG11 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:2158:HIS:CE1 | 2:A:3615:ARG:HH12 | 2.31 | 0.48 |
| 2:A:2766:LYS:HE2 | 2:A:2766:LYS:HA | 1.94 | 0.48 |
| 2:A:3239:LEU:HD23 | 2:A:3242:LEU:HD12 | 1.95 | 0.48 |
| 2:A:4626:ILE:HG12 | 2:D:4241:VAL:HG13 | 1.95 | 0.48 |
| 2:B:66:THR:HG1 | 2:B:124:SER:HG | 1.60 | 0.48 |
| 2:B:1074:ARG:HH12 | 2:B:1209:VAL:HG11 | 1.78 | 0.48 |
| 2:B:1939:ASN:ND2 | 2:B:1989:PRO:HG2 | 2.28 | 0.48 |
| 2:C:1043:LYS:HB2 | 2:C:1043:LYS:HE2 | 1.54 | 0.48 |
| 2:C:3239:LEU:HD23 | 2:C:3242:LEU:HD12 | 1.95 | 0.48 |
| 2:D:227:TYR:CG | 2:D:352:SER:HB2 | 2.49 | 0.48 |
| 2:D:2561:LEU:O | 2:D:2566:ARG:NH1 | 2.46 | 0.48 |
| 2:D:2714:PRO:HG2 | 2:D:2717:LEU:HD13 | 1.95 | 0.48 |
| 2:D:3152:ARG:HA | 2:D:3155:LEU:HD12 | 1.96 | 0.48 |
| 2:D:4238:ILE:HG23 | 2:D:4239:LEU:HD12 | 1.95 | 0.48 |
| 2:A:1681:ASP:HB3 | 2:A:1683:PRO:HD2 | 1.94 | 0.48 |
| 2:A:2214:MET:HE2 | 2:A:2242:VAL:CG1 | 2.42 | 0.48 |
| 2:A:2791:ARG:HD3 | 2:A:2901:TYR:CZ | 2.48 | 0.48 |
| 2:A:4517:LEU:HD21 | 2:A:4736:ASN:HB3 | 1.95 | 0.48 |
| 2:A:4689:LYS:HD2 | 2:A:4690:LYS:H | 1.78 | 0.48 |
| 2:B:2976:LYS:HG3 | 2:B:2979:ARG:NH2 | 2.29 | 0.48 |
| 2:B:3235:MET:HA | 2:B:3239:LEU:HD12 | 1.96 | 0.48 |
| 2:B:3986:LEU:HD12 | 2:B:4101:LEU:HD12 | 1.94 | 0.48 |
| 2:B:4921:PHE:HE2 | 2:B:4940:VAL:HG11 | 1.78 | 0.48 |
| 2:C:227:TYR:CG | 2:C:352:SER:HB2 | 2.49 | 0.48 |
| 2:C:375:GLN:HG2 | 2:C:377:VAL:HG23 | 1.96 | 0.48 |
| 2:C:625:VAL:HG23 | 2:C:628:ASN:HB2 | 1.94 | 0.48 |
| 2:C:2071:GLN:CD | 2:C:3648:GLY:HA3 | 2.34 | 0.48 |
| 2:C:2158:HIS:CE1 | 2:C:3615:ARG:HH12 | 2.31 | 0.48 |
| 2:C:2561:LEU:O | 2:C:2566:ARG:NH1 | 2.46 | 0.48 |
| 2:C:2710:ASN:OD1 | 2:C:2711:ILE:N | 2.47 | 0.48 |
| 2:D:271:ALA:O | 2:D:301:THR:OG1 | 2.30 | 0.48 |
| 2:D:2158:HIS:CE1 | 2:D:3615:ARG:HH12 | 2.31 | 0.48 |
| 2:D:2976:LYS:HG3 | 2:D:2979:ARG:NH2 | 2.28 | 0.48 |
| 2:A:288:HIS:CE1 | 2:A:349:MET:HG3 | 2.49 | 0.48 |
| 2:A:2976:LYS:HG3 | 2:A:2979:ARG:NH2 | 2.28 | 0.48 |
| 2:A:4257:ARG:O | 2:A:4261:LEU:HG | 2.14 | 0.48 |
| 2:A:4863:GLN:HG2 | 2:B:4860:ALA:HB2 | 1.96 | 0.48 |
| 2:B:907:VAL:HB | 2:B:912:LYS:HE2 | 1.94 | 0.48 |
| 2:B:953:SER:OG | 2:B:1061:GLY:O | 2.31 | 0.48 |
| 2:B:1628:MET:HB3 | 2:B:1628:MET:HE2 | 1.75 | 0.48 |
| 2:C:118:ALA:HA | 2:C:161:THR:HA | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:2791:ARG:HD3 | 2:C:2901:TYR:CZ | 2.48 | 0.48 |
| 2:C:4010:VAL:HG11 | 2:C:4118:PHE:HZ | 1.78 | 0.48 |
| 2:C:4689:LYS:HE3 | 2:C:4696:ALA:HB2 | 1.94 | 0.48 |
| 2:D:118:ALA:HA | 2:D:161:THR:HA | 1.95 | 0.48 |
| 2:D:894:VAL:HG23 | 2:D:895:MET:HE2 | 1.96 | 0.48 |
| 2:D:2447:LYS:HD2 | 2:D:2864:GLY:HA3 | 1.95 | 0.48 |
| 2:A:1936:LEU:HD11 | 2:A:1976:LEU:HD22 | 1.96 | 0.48 |
| 2:A:2754:GLN:HE22 | 2:A:2757:MET:HG2 | 1.78 | 0.48 |
| 2:A:2798:MET:HA | 2:A:2798:MET:HE3 | 1.95 | 0.48 |
| 2:A:3920:LEU:HD22 | 2:A:3935:LEU:HD21 | 1.95 | 0.48 |
| 2:A:4658:GLY:HA2 | 2:A:4666:ILE:HD12 | 1.95 | 0.48 |
| 2:A:4858:LEU:HA | 2:A:4861:ILE:HD12 | 1.95 | 0.48 |
| 2:B:288:HIS:CE1 | 2:B:349:MET:HG3 | 2.49 | 0.48 |
| 2:B:375:GLN:HG2 | 2:B:377:VAL:HG23 | 1.96 | 0.48 |
| 2:B:2502:LEU:HD13 | 2:B:2507:LEU:HD13 | 1.96 | 0.48 |
| 2:B:2710:ASN:OD1 | 2:B:2711:ILE:N | 2.46 | 0.48 |
| 2:B:2791:ARG:HD3 | 2:B:2901:TYR:CZ | 2.48 | 0.48 |
| 2:B:4257:ARG:O | 2:B:4261:LEU:HG | 2.14 | 0.48 |
| 4:B:5003:ATP:H5'1 | 4:B:5003:ATP:H8 | 1.79 | 0.48 |
| 2:C:288:HIS:CE1 | 2:C:349:MET:HG3 | 2.49 | 0.48 |
| 2:C:1967:SER:O | 2:C:1972:GLN:NE2 | 2.40 | 0.48 |
| 2:C:2888:LYS:HA | 2:C:2891:ASP:OD2 | 2.14 | 0.48 |
| 2:D:907:VAL:HB | 2:D:912:LYS:HE2 | 1.94 | 0.48 |
| 2:D:1118:SER:HB3 | 2:D:1204:VAL:HG11 | 1.95 | 0.48 |
| 2:D:3235:MET:HA | 2:D:3239:LEU:HD12 | 1.96 | 0.48 |
| 2:D:3321:PRO:HA | 2:D:3324:GLU:HG3 | 1.96 | 0.48 |
| 2:A:2077:ASP:O | 2:A:2081:VAL:HG23 | 2.14 | 0.48 |
| 2:A:2674:GLY:HA2 | 2:A:2978:HIS:CE1 | 2.48 | 0.48 |
| 2:A:4107:GLU:OE2 | 2:A:4135:ARG:NE | 2.47 | 0.48 |
| 4:A:5003:ATP:H8 | 4:A:5003:ATP:H5'1 | 1.79 | 0.48 |
| 2:B:1415:ASP:HB3 | 2:B:1561:LYS:HD2 | 1.94 | 0.48 |
| 2:B:2561:LEU:O | 2:B:2566:ARG:NH1 | 2.46 | 0.48 |
| 2:C:1575:HIS:O | 2:C:1576:LYS:NZ | 2.40 | 0.48 |
| 2:C:2077:ASP:O | 2:C:2081:VAL:HG23 | 2.14 | 0.48 |
| 2:C:2976:LYS:HG3 | 2:C:2979:ARG:NH2 | 2.29 | 0.48 |
| 2:C:3221:LEU:HD22 | 2:C:3231:MET:SD | 2.54 | 0.48 |
| 2:C:3861:GLN:HB3 | 2:C:3864:ASN:HD22 | 1.78 | 0.48 |
| 2:C:4238:ILE:HG23 | 2:C:4239:LEU:HD12 | 1.95 | 0.48 |
| 2:C:4620:GLN:OE1 | 2:C:4632:ARG:NH1 | 2.47 | 0.48 |
| 2:D:2074:VAL:HG23 | 2:D:3660:ARG:HG2 | 1.96 | 0.48 |
| 2:D:2710:ASN:OD1 | 2:D:2711:ILE:N | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2894:LYS:NZ | 2:D:2897:GLN:OE1 | 2.46 | 0.48 |
| 2:D:3036:LEU:O | 2:D:3040:LEU:HG | 2.13 | 0.48 |
| 2:D:3304:GLN:HA | 2:D:3307:ILE:HG12 | 1.94 | 0.48 |
| 1:E:27:TYR:HA | 1:E:101:ASP:O | 2.14 | 0.48 |
| 2:A:312:LYS:HE2 | 2:A:394:HIS:HA | 1.94 | 0.48 |
| 2:A:375:GLN:HG2 | 2:A:377:VAL:HG23 | 1.96 | 0.48 |
| 2:A:2502:LEU:HD13 | 2:A:2507:LEU:HD13 | 1.96 | 0.48 |
| 2:A:2894:LYS:NZ | 2:A:2897:GLN:OE1 | 2.46 | 0.48 |
| 2:A:3001:LYS:HE2 | 2:A:3045:VAL:HG23 | 1.96 | 0.48 |
| 2:B:1681:ASP:HB3 | 2:B:1683:PRO:HD2 | 1.94 | 0.48 |
| 2:B:2119:LEU:HB2 | 2:B:2152:ASN:ND2 | 2.28 | 0.48 |
| 2:B:2688:MET:HB3 | 2:B:2689:MET:HE1 | 1.95 | 0.48 |
| 2:B:4238:ILE:HG23 | 2:B:4239:LEU:HD12 | 1.95 | 0.48 |
| 2:B:4658:GLY:HA2 | 2:B:4666:ILE:HD12 | 1.95 | 0.48 |
| 2:C:312:LYS:HE2 | 2:C:394:HIS:HA | 1.94 | 0.48 |
| 2:C:931:TYR:OH | 4:C:5003:ATP:H2' | 2.13 | 0.48 |
| 2:C:1031:ARG:HE | 2:C:1038:LEU:HD11 | 1.78 | 0.48 |
| 2:C:3920:LEU:HD22 | 2:C:3935:LEU:HD21 | 1.95 | 0.48 |
| 2:C:4107:GLU:OE2 | 2:C:4135:ARG:NE | 2.47 | 0.48 |
| 2:C:4197:ILE:HG12 | 2:C:4923:MET:HE2 | 1.96 | 0.48 |
| 2:D:219:SER:H | 2:D:349:MET:HE3 | 1.78 | 0.48 |
| 2:D:717:GLY:N | 2:D:720:ASP:OD2 | 2.42 | 0.48 |
| 2:D:1936:LEU:HD11 | 2:D:1976:LEU:HD22 | 1.96 | 0.48 |
| 2:D:1939:ASN:ND2 | 2:D:1989:PRO:HG2 | 2.28 | 0.48 |
| 2:D:2888:LYS:HA | 2:D:2891:ASP:OD2 | 2.14 | 0.48 |
| 2:D:3277:LEU:O | 2:D:3281:LEU:HG | 2.14 | 0.48 |
| 2:D:3920:LEU:HD22 | 2:D:3935:LEU:HD21 | 1.95 | 0.48 |
| 2:D:4631:ASP:OD1 | 2:D:4708:TRP:NE1 | 2.42 | 0.48 |
| 2:A:258:ARG:NH1 | 2:A:316:LEU:O | 2.46 | 0.48 |
| 2:A:2074:VAL:HG23 | 2:A:3660:ARG:HG2 | 1.96 | 0.48 |
| 2:A:2868:HIS:CE1 | 2:A:2870:LEU:HB2 | 2.48 | 0.48 |
| 2:A:3152:ARG:HA | 2:A:3155:LEU:HD12 | 1.96 | 0.48 |
| 2:A:4620:GLN:OE1 | 2:A:4632:ARG:NH1 | 2.47 | 0.48 |
| 2:B:3075:LEU:HD12 | 2:B:3076:LYS:HD2 | 1.95 | 0.48 |
| 2:B:3221:LEU:HD22 | 2:B:3231:MET:SD | 2.54 | 0.48 |
| 2:B:4620:GLN:OE1 | 2:B:4632:ARG:NH1 | 2.47 | 0.48 |
| 2:C:953:SER:OG | 2:C:1063:ASN:OD1 | 2.30 | 0.48 |
| 2:C:4257:ARG:O | 2:C:4261:LEU:HG | 2.14 | 0.48 |
| 2:D:456:LEU:HD11 | 2:D:533:LEU:HG | 1.95 | 0.48 |
| 2:D:872:ILE:O | 2:D:941:LYS:NZ | 2.47 | 0.48 |
| 2:D:2077:ASP:O | 2:D:2081:VAL:HG23 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2943:PHE:HD2 | 2:D:3021:LEU:HD23 | 1.78 | 0.48 |
| 2:A:1074:ARG:HD2 | 2:A:1078:CYS:HB3 | 1.95 | 0.47 |
| 2:A:2071:GLN:CD | 2:A:3648:GLY:HA3 | 2.34 | 0.47 |
| 2:A:2561:LEU:O | 2:A:2566:ARG:NH1 | 2.46 | 0.47 |
| 2:A:2590:ARG:HG2 | 2:A:2691:LYS:HE3 | 1.96 | 0.47 |
| 2:A:2791:ARG:HD3 | 2:A:2901:TYR:CE1 | 2.47 | 0.47 |
| 2:A:3016:ARG:HG2 | 2:A:3017:HIS:CD2 | 2.49 | 0.47 |
| 2:A:3036:LEU:O | 2:A:3040:LEU:HG | 2.13 | 0.47 |
| 2:A:3221:LEU:HD22 | 2:A:3231:MET:SD | 2.54 | 0.47 |
| 2:A:4848:ILE:HD11 | 2:D:4818:TYR:HA | 1.96 | 0.47 |
| 2:B:1936:LEU:HD11 | 2:B:1976:LEU:HD22 | 1.96 | 0.47 |
| 2:B:2071:GLN:CD | 2:B:3648:GLY:HA3 | 2.34 | 0.47 |
| 2:B:2550:HIS:HD2 | 2:B:2591:ARG:HD2 | 1.79 | 0.47 |
| 2:B:2758:LYS:HE2 | 2:B:2762:LEU:O | 2.14 | 0.47 |
| 2:B:3187:LYS:O | 2:B:3191:GLU:HB2 | 2.14 | 0.47 |
| 2:B:4689:LYS:HD2 | 2:B:4690:LYS:H | 1.78 | 0.47 |
| 2:C:1074:ARG:HH12 | 2:C:1209:VAL:HG11 | 1.78 | 0.47 |
| 2:C:1118:SER:HB3 | 2:C:1204:VAL:HG11 | 1.95 | 0.47 |
| 2:C:1939:ASN:ND2 | 2:C:1989:PRO:HG2 | 2.28 | 0.47 |
| 2:C:1972:GLN:HA | 2:C:1975:MET:SD | 2.53 | 0.47 |
| 2:C:1975:MET:HA | 2:C:1978:ASN:HD22 | 1.77 | 0.47 |
| 2:C:2074:VAL:HG23 | 2:C:3660:ARG:HG2 | 1.96 | 0.47 |
| 2:C:2214:MET:HE2 | 2:C:2242:VAL:CG1 | 2.43 | 0.47 |
| 2:C:2550:HIS:HD2 | 2:C:2591:ARG:HD2 | 1.79 | 0.47 |
| 2:C:2754:GLN:HE22 | 2:C:2757:MET:HG2 | 1.78 | 0.47 |
| 2:C:3235:MET:HA | 2:C:3239:LEU:HD12 | 1.96 | 0.47 |
| 2:C:4858:LEU:HA | 2:C:4861:ILE:HD12 | 1.95 | 0.47 |
| 2:D:1575:HIS:O | 2:D:1576:LYS:NZ | 2.40 | 0.47 |
| 2:D:4107:GLU:OE2 | 2:D:4135:ARG:NE | 2.47 | 0.47 |
| 2:D:4658:GLY:HA2 | 2:D:4666:ILE:HD12 | 1.95 | 0.47 |
| 2:A:118:ALA:HA | 2:A:161:THR:HA | 1.95 | 0.47 |
| 2:A:456:LEU:HD11 | 2:A:533:LEU:HG | 1.95 | 0.47 |
| 2:A:1939:ASN:ND2 | 2:A:1989:PRO:HG2 | 2.28 | 0.47 |
| 2:A:3712:LYS:HB2 | 2:A:3712:LYS:HE3 | 1.69 | 0.47 |
| 2:B:2077:ASP:O | 2:B:2081:VAL:HG23 | 2.14 | 0.47 |
| 2:B:3016:ARG:HG2 | 2:B:3017:HIS:CD2 | 2.49 | 0.47 |
| 2:C:655:MET:HE2 | 2:C:1608:VAL:HG11 | 1.95 | 0.47 |
| 2:C:2758:LYS:HE2 | 2:C:2762:LEU:O | 2.14 | 0.47 |
| 2:C:3321:PRO:HA | 2:C:3324:GLU:HG3 | 1.96 | 0.47 |
| 2:D:1967:SER:HB3 | 2:D:1971:GLU:OE1 | 2.14 | 0.47 |
| 2:D:1972:GLN:HA | 2:D:1975:MET:SD | 2.53 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2502:LEU:HD13 | 2:D:2507:LEU:HD13 | 1.96 | 0.47 |
| 2:D:2706:VAL:HG23 | 2:D:2847:ASN:HD21 | 1.77 | 0.47 |
| 2:D:2791:ARG:NH2 | 2:D:2795:GLY:O | 2.42 | 0.47 |
| 2:D:3924:ILE:HG21 | 2:D:3935:LEU:HD22 | 1.96 | 0.47 |
| 2:D:4179:GLU:HG2 | 2:D:4179:GLU:O | 2.15 | 0.47 |
| 1:G:27:TYR:HA | 1:G:101:ASP:O | 2.14 | 0.47 |
| 2:A:227:TYR:CG | 2:A:352:SER:HB2 | 2.49 | 0.47 |
| 2:A:2943:PHE:HD2 | 2:A:3021:LEU:HD23 | 1.79 | 0.47 |
| 2:A:4179:GLU:HG2 | 2:A:4179:GLU:O | 2.15 | 0.47 |
| 2:B:931:TYR:OH | 4:B:5003:ATP:H2' | 2.13 | 0.47 |
| 2:B:2888:LYS:HA | 2:B:2891:ASP:OD2 | 2.14 | 0.47 |
| 2:B:3002:GLU:OE2 | 2:B:3045:VAL:HA | 2.14 | 0.47 |
| 2:C:2502:LEU:HD13 | 2:C:2507:LEU:HD13 | 1.96 | 0.47 |
| 2:C:2664:LEU:O | 2:C:2667:PRO:HD2 | 2.15 | 0.47 |
| 2:D:2071:GLN:CD | 2:D:3648:GLY:HA3 | 2.34 | 0.47 |
| 2:D:3260:ARG:HH11 | 2:D:3264:CYS:HA | 1.79 | 0.47 |
| 2:D:4620:GLN:OE1 | 2:D:4632:ARG:NH1 | 2.47 | 0.47 |
| 1:E:23:CYS:SG | 1:E:51:ILE:HD11 | 2.55 | 0.47 |
| 1:F:27:TYR:HA | 1:F:101:ASP:O | 2.14 | 0.47 |
| 2:A:1031:ARG:HE | 2:A:1038:LEU:HD11 | 1.78 | 0.47 |
| 2:A:2664:LEU:O | 2:A:2667:PRO:HD2 | 2.15 | 0.47 |
| 2:A:2714:PRO:HG2 | 2:A:2717:LEU:HD13 | 1.95 | 0.47 |
| 2:A:3277:LEU:O | 2:A:3281:LEU:HG | 2.14 | 0.47 |
| 2:B:1967:SER:O | 2:B:1972:GLN:NE2 | 2.40 | 0.47 |
| 2:B:2664:LEU:O | 2:B:2667:PRO:HD2 | 2.15 | 0.47 |
| 2:B:2868:HIS:CE1 | 2:B:2870:LEU:HB2 | 2.48 | 0.47 |
| 2:B:2943:PHE:HD2 | 2:B:3021:LEU:HD23 | 1.78 | 0.47 |
| 2:B:3277:LEU:O | 2:B:3281:LEU:HG | 2.14 | 0.47 |
| 2:B:3321:PRO:HA | 2:B:3324:GLU:HG3 | 1.96 | 0.47 |
| 2:C:2119:LEU:HB2 | 2:C:2152:ASN:ND2 | 2.28 | 0.47 |
| 2:C:2447:LYS:HD2 | 2:C:2864:GLY:HA3 | 1.95 | 0.47 |
| 1:H:27:TYR:HA | 1:H:101:ASP:O | 2.14 | 0.47 |
| 2:A:1914:CYS:HB3 | 2:A:2090:ARG:HH21 | 1.80 | 0.47 |
| 2:A:2888:LYS:HA | 2:A:2891:ASP:OD2 | 2.14 | 0.47 |
| 2:B:1967:SER:HB3 | 2:B:1971:GLU:OE1 | 2.14 | 0.47 |
| 2:B:2590:ARG:HG2 | 2:B:2691:LYS:HE3 | 1.97 | 0.47 |
| 2:B:3025:ASP:O | 2:B:3029:ILE:HD12 | 2.15 | 0.47 |
| 2:C:3016:ARG:HG2 | 2:C:3017:HIS:CD2 | 2.49 | 0.47 |
| 2:C:3171:LEU:HB2 | 2:C:3245:TYR:CZ | 2.50 | 0.47 |
| 2:D:3239:LEU:HD23 | 2:D:3242:LEU:HD12 | 1.95 | 0.47 |
| 2:A:872:ILE:O | 2:A:941:LYS:NZ | 2.47 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:2758:LYS:HE2 | 2:A:2762:LEU:O | 2.14 | 0.47 |
| 2:A:3187:LYS:O | 2:A:3191:GLU:HB2 | 2.14 | 0.47 |
| 2:A:4921:PHE:HE2 | 2:A:4940:VAL:HG11 | 1.79 | 0.47 |
| 2:B:66:THR:HG22 | 2:B:217:ILE:HG13 | 1.97 | 0.47 |
| 2:B:118:ALA:HA | 2:B:161:THR:HA | 1.95 | 0.47 |
| 2:B:902:TRP:CB | 2:B:918:LEU:HD21 | 2.42 | 0.47 |
| 2:B:1914:CYS:HB3 | 2:B:2090:ARG:HH21 | 1.80 | 0.47 |
| 2:B:4118:PHE:HA | 2:B:4121:LEU:HD12 | 1.97 | 0.47 |
| 2:C:258:ARG:NH1 | 2:C:316:LEU:O | 2.46 | 0.47 |
| 2:C:1967:SER:HB3 | 2:C:1971:GLU:OE1 | 2.14 | 0.47 |
| 2:C:3043:ARG:HG3 | 2:C:3047:LYS:HZ2 | 1.79 | 0.47 |
| 2:C:3924:ILE:HG21 | 2:C:3935:LEU:HD22 | 1.96 | 0.47 |
| 2:C:4658:GLY:HA2 | 2:C:4666:ILE:HD12 | 1.95 | 0.47 |
| 2:D:258:ARG:NH1 | 2:D:316:LEU:O | 2.46 | 0.47 |
| 2:D:3016:ARG:HG2 | 2:D:3017:HIS:CD2 | 2.49 | 0.47 |
| 2:D:3187:LYS:O | 2:D:3191:GLU:HB2 | 2.14 | 0.47 |
| 2:D:4010:VAL:HG11 | 2:D:4118:PHE:HZ | 1.78 | 0.47 |
| 2:D:4569:GLU:HB3 | 2:D:4570:PRO:HD3 | 1.97 | 0.47 |
| 1:F:23:CYS:SG | 1:F:51:ILE:HD11 | 2.55 | 0.47 |
| 2:A:1967:SER:HB3 | 2:A:1971:GLU:OE1 | 2.14 | 0.47 |
| 2:A:4867:ILE:HG12 | 2:B:4864:GLY:HA2 | 1.97 | 0.47 |
| 2:B:28:ILE:HG22 | 2:B:29:HIS:HD2 | 1.80 | 0.47 |
| 2:B:1001:GLU:OE2 | 2:B:1035:TYR:HB3 | 2.14 | 0.47 |
| 2:B:1031:ARG:HE | 2:B:1038:LEU:HD11 | 1.78 | 0.47 |
| 2:B:1199:ASP:OD1 | 2:B:1199:ASP:N | 2.45 | 0.47 |
| 2:B:1575:HIS:O | 2:B:1576:LYS:NZ | 2.40 | 0.47 |
| 2:B:1957:LEU:HG | 2:B:1961:LYS:HB3 | 1.97 | 0.47 |
| 2:B:2754:GLN:HE22 | 2:B:2757:MET:HG2 | 1.78 | 0.47 |
| 2:B:3171:LEU:HB2 | 2:B:3245:TYR:CZ | 2.50 | 0.47 |
| 2:B:4107:GLU:OE2 | 2:B:4135:ARG:NE | 2.47 | 0.47 |
| 2:C:307:SER:HB3 | 2:C:327:THR:HG22 | 1.97 | 0.47 |
| 2:C:1936:LEU:HD11 | 2:C:1976:LEU:HD22 | 1.96 | 0.47 |
| 2:C:2943:PHE:HD2 | 2:C:3021:LEU:HD23 | 1.78 | 0.47 |
| 2:C:3002:GLU:OE2 | 2:C:3045:VAL:HA | 2.14 | 0.47 |
| 2:C:3140:LEU:HB3 | 2:C:3155:LEU:HD13 | 1.97 | 0.47 |
| 2:C:3187:LYS:O | 2:C:3191:GLU:HB2 | 2.14 | 0.47 |
| 2:C:3277:LEU:O | 2:C:3281:LEU:HG | 2.14 | 0.47 |
| 4:C:5003:ATP:H8 | 4:C:5003:ATP:H5'1 | 1.79 | 0.47 |
| 2:D:375:GLN:HG2 | 2:D:377:VAL:HG23 | 1.96 | 0.47 |
| 2:D:1969:PRO:HD3 | 2:D:3605:MET:HE1 | 1.97 | 0.47 |
| 2:D:2664:LEU:O | 2:D:2667:PRO:HD2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2788:ARG:HH12 | 2:D:2908:LYS:HG2 | 1.80 | 0.47 |
| 2:D:2928:GLN:HA | 2:D:2931:ARG:HE | 1.80 | 0.47 |
| 2:D:3001:LYS:HE2 | 2:D:3045:VAL:HG23 | 1.96 | 0.47 |
| 2:D:3001:LYS:NZ | 2:D:3044:THR:H | 2.13 | 0.47 |
| 2:D:3002:GLU:OE2 | 2:D:3045:VAL:HA | 2.14 | 0.47 |
| 2:D:3221:LEU:HD22 | 2:D:3231:MET:SD | 2.54 | 0.47 |
| 2:D:4921:PHE:HE2 | 2:D:4940:VAL:HG11 | 1.78 | 0.47 |
| 1:G:23:CYS:SG | 1:G:51:ILE:HD11 | 2.55 | 0.47 |
| 2:A:808:HIS:O | 2:A:1616:GLY:HA2 | 2.15 | 0.47 |
| 2:A:902:TRP:CB | 2:A:918:LEU:HD21 | 2.42 | 0.47 |
| 2:A:2441:GLN:OE1 | 2:A:2454:PRO:HG3 | 2.14 | 0.47 |
| 2:A:3321:PRO:HA | 2:A:3324:GLU:HG3 | 1.96 | 0.47 |
| 2:A:3653:GLU:HB2 | 2:A:3660:ARG:HH22 | 1.80 | 0.47 |
| 2:A:4569:GLU:HB3 | 2:A:4570:PRO:HD3 | 1.97 | 0.47 |
| 2:B:810:GLU:HB2 | 2:B:1614:ARG:HE | 1.80 | 0.47 |
| 2:B:4502:MET:SD | 2:B:4585:PHE:HB3 | 2.55 | 0.47 |
| 2:C:703:TYR:HD2 | 2:C:858:THR:HG22 | 1.80 | 0.47 |
| 2:C:872:ILE:O | 2:C:941:LYS:NZ | 2.48 | 0.47 |
| 2:C:877:HIS:O | 2:C:880:ARG:HD3 | 2.15 | 0.47 |
| 2:C:2974:TYR:CZ | 2:C:2982:PHE:HZ | 2.33 | 0.47 |
| 2:C:3001:LYS:HE2 | 2:C:3045:VAL:HG23 | 1.96 | 0.47 |
| 2:C:3152:ARG:HA | 2:C:3155:LEU:HD12 | 1.96 | 0.47 |
| 2:D:66:THR:HG22 | 2:D:217:ILE:HG13 | 1.97 | 0.47 |
| 2:D:1161:VAL:HG21 | 2:D:1225:LYS:HE2 | 1.97 | 0.47 |
| 2:D:2441:GLN:OE1 | 2:D:2454:PRO:HG3 | 2.14 | 0.47 |
| 2:D:3171:LEU:HB2 | 2:D:3245:TYR:CZ | 2.50 | 0.47 |
| 4:D:5003:ATP:H8 | 4:D:5003:ATP:H5'1 | 1.79 | 0.47 |
| 2:A:143:LEU:HD21 | 2:D:2426:LEU:HA | 1.97 | 0.47 |
| 2:A:1161:VAL:HG21 | 2:A:1225:LYS:HE2 | 1.97 | 0.47 |
| 2:A:1957:LEU:HG | 2:A:1961:LYS:HB3 | 1.97 | 0.47 |
| 2:A:2332:GLY:N | 2:A:2336:ARG:HH12 | 2.13 | 0.47 |
| 2:A:3171:LEU:HB2 | 2:A:3245:TYR:CZ | 2.50 | 0.47 |
| 2:A:3260:ARG:O | 2:A:3260:ARG:HD3 | 2.15 | 0.47 |
| 2:A:4502:MET:SD | 2:A:4585:PHE:HB3 | 2.55 | 0.47 |
| 2:B:717:GLY:N | 2:B:720:ASP:OD2 | 2.42 | 0.47 |
| 2:B:2074:VAL:HG23 | 2:B:3660:ARG:HG2 | 1.96 | 0.47 |
| 2:B:2229:LEU:HD13 | 2:B:2297:ARG:HB2 | 1.97 | 0.47 |
| 2:B:2884:LYS:HA | 2:B:2887:GLU:OE2 | 2.15 | 0.47 |
| 2:C:66:THR:HG22 | 2:C:217:ILE:HG13 | 1.97 | 0.47 |
| 2:C:890:HIS:O | 2:C:894:VAL:HG13 | 2.15 | 0.47 |
| 2:C:2688:MET:HB3 | 2:C:2689:MET:HE1 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:2705:PRO:HG3 | 2:C:2851:ILE:HG12 | 1.97 | 0.47 |
| 2:C:4569:GLU:HB3 | 2:C:4570:PRO:HD3 | 1.97 | 0.47 |
| 2:C:4921:PHE:HE2 | 2:C:4940:VAL:HG11 | 1.78 | 0.47 |
| 2:D:1001:GLU:OE2 | 2:D:1035:TYR:HB3 | 2.14 | 0.47 |
| 2:D:1986:CYS:O | 2:D:1993:ARG:NH2 | 2.48 | 0.47 |
| 2:D:2590:ARG:HG2 | 2:D:2691:LYS:HE3 | 1.96 | 0.47 |
| 2:A:307:SER:HB3 | 2:A:327:THR:HG22 | 1.97 | 0.47 |
| 2:A:794:PHE:CG | 2:A:798:ILE:HD13 | 2.51 | 0.47 |
| 2:A:2596:VAL:O | 2:A:2599:LEU:HD22 | 2.15 | 0.47 |
| 2:A:2928:GLN:HA | 2:A:2931:ARG:HE | 1.80 | 0.47 |
| 2:A:3261:ALA:C | 2:A:3262:GLU:OE1 | 2.54 | 0.47 |
| 2:A:4197:ILE:HG12 | 2:A:4923:MET:HE2 | 1.97 | 0.47 |
| 2:B:3140:LEU:HB3 | 2:B:3155:LEU:HD13 | 1.97 | 0.47 |
| 2:B:3152:ARG:HA | 2:B:3155:LEU:HD12 | 1.96 | 0.47 |
| 2:C:28:ILE:HG22 | 2:C:29:HIS:HD2 | 1.80 | 0.47 |
| 2:C:2596:VAL:O | 2:C:2599:LEU:HD22 | 2.15 | 0.47 |
| 2:C:3025:ASP:O | 2:C:3029:ILE:HD12 | 2.15 | 0.47 |
| 2:C:4502:MET:SD | 2:C:4585:PHE:HB3 | 2.55 | 0.47 |
| 2:D:877:HIS:O | 2:D:880:ARG:HD3 | 2.15 | 0.47 |
| 2:D:890:HIS:O | 2:D:894:VAL:HG13 | 2.15 | 0.47 |
| 2:D:2596:VAL:O | 2:D:2599:LEU:HD22 | 2.15 | 0.47 |
| 2:D:2974:TYR:CZ | 2:D:2982:PHE:HZ | 2.33 | 0.47 |
| 2:D:4617:ILE:HG23 | 2:D:4665:ARG:NH2 | 2.30 | 0.47 |
| 2:A:28:ILE:HG22 | 2:A:29:HIS:HD2 | 1.80 | 0.46 |
| 2:A:606:ARG:HH22 | 2:A:1634:GLU:HG2 | 1.80 | 0.46 |
| 2:A:703:TYR:HD2 | 2:A:858:THR:HG22 | 1.80 | 0.46 |
| 2:A:877:HIS:O | 2:A:880:ARG:HD3 | 2.15 | 0.46 |
| 2:A:2009:ILE:HD12 | 2:A:3634:HIS:CD2 | 2.50 | 0.46 |
| 2:A:2229:LEU:HD13 | 2:A:2297:ARG:HB2 | 1.97 | 0.46 |
| 2:A:2788:ARG:HH12 | 2:A:2908:LYS:HG2 | 1.80 | 0.46 |
| 2:A:3002:GLU:OE2 | 2:A:3045:VAL:HA | 2.14 | 0.46 |
| 2:B:872:ILE:O | 2:B:941:LYS:NZ | 2.47 | 0.46 |
| 2:B:2141:LEU:O | 2:B:2144:ARG:HD3 | 2.15 | 0.46 |
| 2:B:2178:VAL:HG21 | 2:B:2192:MET:SD | 2.55 | 0.46 |
| 2:C:1001:GLU:OE2 | 2:C:1035:TYR:HB3 | 2.14 | 0.46 |
| 2:D:288:HIS:CE1 | 2:D:349:MET:HG3 | 2.49 | 0.46 |
| 2:D:1199:ASP:OD1 | 2:D:1199:ASP:N | 2.45 | 0.46 |
| 2:D:2884:LYS:HA | 2:D:2887:GLU:OE2 | 2.15 | 0.46 |
| 2:D:4118:PHE:HA | 2:D:4121:LEU:HD12 | 1.97 | 0.46 |
| 2:A:1945:ASN:O | 2:A:1949:GLN:NE2 | 2.42 | 0.46 |
| 2:A:3227:ARG:NH1 | 2:A:3228:TYR:HB3 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:824:GLU:HA | 2:B:1020:ILE:HD12 | 1.97 | 0.46 |
| 2:B:1161:VAL:HG21 | 2:B:1225:LYS:HE2 | 1.97 | 0.46 |
| 2:B:2596:VAL:O | 2:B:2599:LEU:HD22 | 2.15 | 0.46 |
| 2:B:2788:ARG:HH12 | 2:B:2908:LYS:HG2 | 1.80 | 0.46 |
| 2:B:3227:ARG:NH1 | 2:B:3228:TYR:HB3 | 2.30 | 0.46 |
| 2:B:4179:GLU:O | 2:B:4179:GLU:HG2 | 2.15 | 0.46 |
| 2:C:606:ARG:HH22 | 2:C:1634:GLU:HG2 | 1.80 | 0.46 |
| 2:C:810:GLU:HB2 | 2:C:1614:ARG:HE | 1.80 | 0.46 |
| 2:C:2009:ILE:HD12 | 2:C:3634:HIS:CD2 | 2.50 | 0.46 |
| 2:C:3001:LYS:NZ | 2:C:3044:THR:H | 2.13 | 0.46 |
| 2:D:606:ARG:HH22 | 2:D:1634:GLU:HG2 | 1.80 | 0.46 |
| 2:D:2170:THR:O | 2:D:2174:VAL:HG23 | 2.16 | 0.46 |
| 2:D:2681:MET:SD | 2:D:2914:THR:HA | 2.55 | 0.46 |
| 2:D:4257:ARG:O | 2:D:4261:LEU:HG | 2.14 | 0.46 |
| 2:A:890:HIS:O | 2:A:894:VAL:HG13 | 2.15 | 0.46 |
| 2:A:2550:HIS:HD2 | 2:A:2591:ARG:HD2 | 1.79 | 0.46 |
| 2:B:2441:GLN:OE1 | 2:B:2454:PRO:HG3 | 2.14 | 0.46 |
| 2:B:4197:ILE:HG12 | 2:B:4923:MET:HE2 | 1.97 | 0.46 |
| 2:C:267:VAL:HG22 | 2:C:272:ARG:HH12 | 1.81 | 0.46 |
| 2:C:1161:VAL:HG21 | 2:C:1225:LYS:HE2 | 1.97 | 0.46 |
| 2:C:1957:LEU:HG | 2:C:1961:LYS:HB3 | 1.97 | 0.46 |
| 2:C:1986:CYS:O | 2:C:1993:ARG:NH2 | 2.48 | 0.46 |
| 2:C:2178:VAL:HG21 | 2:C:2192:MET:SD | 2.55 | 0.46 |
| 2:C:2229:LEU:HD13 | 2:C:2297:ARG:HB2 | 1.97 | 0.46 |
| 2:C:2681:MET:SD | 2:C:2914:THR:HA | 2.56 | 0.46 |
| 2:C:2788:ARG:HH12 | 2:C:2908:LYS:HG2 | 1.80 | 0.46 |
| 2:C:3653:GLU:HB2 | 2:C:3660:ARG:HH22 | 1.80 | 0.46 |
| 2:C:4617:ILE:HG23 | 2:C:4665:ARG:NH2 | 2.30 | 0.46 |
| 2:C:4822:ARG:HH12 | 2:D:4829:ASP:N | 2.13 | 0.46 |
| 2:D:1914:CYS:HB3 | 2:D:2090:ARG:HH21 | 1.80 | 0.46 |
| 2:D:2059:GLN:HG3 | 2:D:2091:GLN:HB3 | 1.98 | 0.46 |
| 2:D:2758:LYS:HE2 | 2:D:2762:LEU:O | 2.14 | 0.46 |
| 2:D:4689:LYS:HD2 | 2:D:4690:LYS:H | 1.78 | 0.46 |
| 1:H:23:CYS:SG | 1:H:51:ILE:HD11 | 2.55 | 0.46 |
| 2:A:66:THR:HG22 | 2:A:217:ILE:HG13 | 1.97 | 0.46 |
| 2:A:810:GLU:HB2 | 2:A:1614:ARG:HE | 1.80 | 0.46 |
| 2:A:1001:GLU:OE2 | 2:A:1035:TYR:HB3 | 2.14 | 0.46 |
| 2:A:3001:LYS:NZ | 2:A:3044:THR:H | 2.13 | 0.46 |
| 2:A:4118:PHE:HA | 2:A:4121:LEU:HD12 | 1.97 | 0.46 |
| 2:B:606:ARG:HH22 | 2:B:1634:GLU:HG2 | 1.80 | 0.46 |
| 2:B:1489:CYS:O | 2:B:1492:GLU:HG3 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2113:VAL:O | 2:B:2117:ILE:HG13 | 2.15 | 0.46 |
| 2:B:2170:THR:O | 2:B:2174:VAL:HG23 | 2.16 | 0.46 |
| 2:B:2332:GLY:N | 2:B:2336:ARG:HH12 | 2.13 | 0.46 |
| 2:B:3001:LYS:HE2 | 2:B:3045:VAL:HG23 | 1.96 | 0.46 |
| 2:B:3653:GLU:HB2 | 2:B:3660:ARG:HH22 | 1.80 | 0.46 |
| 2:C:1914:CYS:HB3 | 2:C:2090:ARG:HH21 | 1.80 | 0.46 |
| 2:C:2141:LEU:O | 2:C:2144:ARG:HD3 | 2.15 | 0.46 |
| 2:C:2441:GLN:OE1 | 2:C:2454:PRO:HG3 | 2.15 | 0.46 |
| 2:C:3134:LEU:HB2 | 2:C:3162:PHE:CE2 | 2.51 | 0.46 |
| 2:D:2760:TYR:CE2 | 2:D:2768:LYS:HE3 | 2.51 | 0.46 |
| 2:D:4264:LEU:HA | 2:D:4267:GLN:OE1 | 2.16 | 0.46 |
| 1:H:19:LYS:HZ3 | 1:H:52:GLY:HA3 | 1.80 | 0.46 |
| 2:A:1489:CYS:O | 2:A:1492:GLU:HG3 | 2.15 | 0.46 |
| 2:A:2884:LYS:HA | 2:A:2887:GLU:OE2 | 2.15 | 0.46 |
| 2:B:20:VAL:HB | 2:B:214:VAL:HG13 | 1.97 | 0.46 |
| 2:B:890:HIS:O | 2:B:894:VAL:HG13 | 2.15 | 0.46 |
| 2:B:2974:TYR:CZ | 2:B:2982:PHE:HZ | 2.33 | 0.46 |
| 2:B:3924:ILE:HG21 | 2:B:3935:LEU:HD22 | 1.96 | 0.46 |
| 2:C:66:THR:HG1 | 2:C:124:SER:HG | 1.58 | 0.46 |
| 2:C:794:PHE:CG | 2:C:798:ILE:HD13 | 2.50 | 0.46 |
| 2:C:2590:ARG:HG2 | 2:C:2691:LYS:HE3 | 1.97 | 0.46 |
| 2:C:2884:LYS:HA | 2:C:2887:GLU:OE2 | 2.15 | 0.46 |
| 2:C:2928:GLN:HA | 2:C:2931:ARG:HE | 1.80 | 0.46 |
| 2:D:20:VAL:HB | 2:D:214:VAL:HG13 | 1.97 | 0.46 |
| 2:D:810:GLU:HB2 | 2:D:1614:ARG:HE | 1.80 | 0.46 |
| 2:D:1819:VAL:HG13 | 2:D:1905:GLN:NE2 | 2.31 | 0.46 |
| 2:D:2229:LEU:HD13 | 2:D:2297:ARG:HB2 | 1.97 | 0.46 |
| 2:D:2553:TYR:HE1 | 2:D:2557:LYS:HZ1 | 1.63 | 0.46 |
| 1:E:19:LYS:HZ3 | 1:E:52:GLY:HA3 | 1.79 | 0.46 |
| 1:H:88:HIS:NE2 | 2:D:1776:TYR:OH | 2.37 | 0.46 |
| 2:A:1016:TRP:CG | 2:A:1027:ARG:HB3 | 2.51 | 0.46 |
| 2:A:1549:SER:HB2 | 2:D:2830:ASN:HD21 | 1.79 | 0.46 |
| 2:A:2113:VAL:O | 2:A:2117:ILE:HG13 | 2.16 | 0.46 |
| 2:A:2898:ILE:O | 2:B:1498:GLN:NE2 | 2.49 | 0.46 |
| 2:A:2974:TYR:CZ | 2:A:2982:PHE:HZ | 2.33 | 0.46 |
| 2:A:3140:LEU:HB3 | 2:A:3155:LEU:HD13 | 1.97 | 0.46 |
| 2:B:546:LYS:O | 2:B:550:GLN:HG2 | 2.16 | 0.46 |
| 2:B:703:TYR:HD2 | 2:B:858:THR:HG22 | 1.80 | 0.46 |
| 2:B:2009:ILE:HD12 | 2:B:3634:HIS:CD2 | 2.50 | 0.46 |
| 2:B:3134:LEU:HB2 | 2:B:3162:PHE:CE2 | 2.51 | 0.46 |
| 2:B:3261:ALA:C | 2:B:3262:GLU:OE1 | 2.54 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:824:GLU:HA | 2:C:1020:ILE:HD12 | 1.97 | 0.46 |
| 2:C:1016:TRP:CG | 2:C:1027:ARG:HB3 | 2.51 | 0.46 |
| 2:C:3261:ALA:C | 2:C:3262:GLU:OE1 | 2.54 | 0.46 |
| 2:C:3275:THR:O | 2:C:3279:ASN:ND2 | 2.49 | 0.46 |
| 2:C:4118:PHE:HA | 2:C:4121:LEU:HD12 | 1.96 | 0.46 |
| 2:C:4252:ILE:HG21 | 2:D:4707:MET:HG3 | 1.96 | 0.46 |
| 2:D:2550:HIS:HD2 | 2:D:2591:ARG:HD2 | 1.79 | 0.46 |
| 2:D:3025:ASP:O | 2:D:3029:ILE:HD12 | 2.15 | 0.46 |
| 2:D:3275:THR:O | 2:D:3279:ASN:ND2 | 2.49 | 0.46 |
| 2:D:4502:MET:SD | 2:D:4585:PHE:HB3 | 2.55 | 0.46 |
| 2:A:546:LYS:O | 2:A:550:GLN:HG2 | 2.16 | 0.46 |
| 2:A:717:GLY:N | 2:A:720:ASP:OD2 | 2.42 | 0.46 |
| 2:A:824:GLU:HA | 2:A:1020:ILE:HD12 | 1.97 | 0.46 |
| 2:A:2141:LEU:O | 2:A:2144:ARG:HD3 | 2.15 | 0.46 |
| 2:A:2204:CYS:SG | 2:A:2214:MET:HG2 | 2.56 | 0.46 |
| 2:A:2681:MET:SD | 2:A:2914:THR:HA | 2.56 | 0.46 |
| 2:A:3025:ASP:O | 2:A:3029:ILE:HD12 | 2.15 | 0.46 |
| 2:A:4264:LEU:HA | 2:A:4267:GLN:OE1 | 2.16 | 0.46 |
| 2:B:438:LYS:HD3 | 2:B:438:LYS:HA | 1.70 | 0.46 |
| 2:B:1016:TRP:CG | 2:B:1027:ARG:HB3 | 2.51 | 0.46 |
| 2:B:2705:PRO:HG3 | 2:B:2851:ILE:HG12 | 1.97 | 0.46 |
| 2:B:3650:GLU:OE1 | 2:B:3659:LYS:NZ | 2.49 | 0.46 |
| 2:B:4569:GLU:HB3 | 2:B:4570:PRO:HD3 | 1.97 | 0.46 |
| 2:C:411:GLU:OE2 | 2:C:485:ARG:NE | 2.46 | 0.46 |
| 2:C:902:TRP:HB3 | 2:C:918:LEU:CD2 | 2.44 | 0.46 |
| 2:C:4179:GLU:O | 2:C:4179:GLU:HG2 | 2.15 | 0.46 |
| 2:D:28:ILE:HG22 | 2:D:29:HIS:HD2 | 1.80 | 0.46 |
| 2:D:2332:GLY:N | 2:D:2336:ARG:HH12 | 2.13 | 0.46 |
| 2:D:3260:ARG:O | 2:D:3260:ARG:HD3 | 2.15 | 0.46 |
| 2:A:483:LYS:HE2 | 2:A:483:LYS:HB2 | 1.80 | 0.46 |
| 2:B:808:HIS:O | 2:B:1616:GLY:HA2 | 2.15 | 0.46 |
| 2:B:877:HIS:O | 2:B:880:ARG:HD3 | 2.15 | 0.46 |
| 2:B:880:ARG:HH11 | 2:B:881:ILE:HB | 1.81 | 0.46 |
| 2:B:886:ALA:HB1 | 2:B:929:ARG:HH12 | 1.81 | 0.46 |
| 2:B:1415:ASP:N | 2:B:1415:ASP:OD1 | 2.49 | 0.46 |
| 2:B:4203:ALA:HA | 2:B:4206:ILE:HG12 | 1.98 | 0.46 |
| 2:C:20:VAL:HB | 2:C:214:VAL:HG13 | 1.97 | 0.46 |
| 2:C:2431:ASP:O | 2:C:2435:VAL:HG23 | 2.16 | 0.46 |
| 2:C:2760:TYR:CE2 | 2:C:2768:LYS:HE3 | 2.51 | 0.46 |
| 2:C:3601:ALA:HA | 2:C:3604:ARG:HH11 | 1.81 | 0.46 |
| 2:C:4203:ALA:HA | 2:C:4206:ILE:HG12 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:4639:SER:O | 2:C:4642:ASN:HB2 | 2.16 | 0.46 |
| 2:D:703:TYR:HD2 | 2:D:858:THR:HG22 | 1.80 | 0.46 |
| 2:D:794:PHE:CG | 2:D:798:ILE:HD13 | 2.50 | 0.46 |
| 2:D:808:HIS:O | 2:D:1616:GLY:HA2 | 2.15 | 0.46 |
| 2:D:2009:ILE:HD12 | 2:D:3634:HIS:CD2 | 2.50 | 0.46 |
| 2:D:2431:ASP:O | 2:D:2435:VAL:HG23 | 2.16 | 0.46 |
| 2:A:267:VAL:HG22 | 2:A:272:ARG:HH12 | 1.81 | 0.46 |
| 2:A:1649:GLU:HG2 | 2:A:1650:LEU:N | 2.31 | 0.46 |
| 2:A:1819:VAL:HG13 | 2:A:1905:GLN:NE2 | 2.31 | 0.46 |
| 2:A:2178:VAL:HG21 | 2:A:2192:MET:SD | 2.55 | 0.46 |
| 2:A:2705:PRO:HG3 | 2:A:2851:ILE:HG12 | 1.97 | 0.46 |
| 2:A:3275:THR:O | 2:A:3279:ASN:ND2 | 2.49 | 0.46 |
| 2:B:2431:ASP:O | 2:B:2435:VAL:HG23 | 2.16 | 0.46 |
| 2:B:2681:MET:SD | 2:B:2914:THR:HA | 2.56 | 0.46 |
| 2:B:3260:ARG:O | 2:B:3260:ARG:HD3 | 2.15 | 0.46 |
| 2:C:886:ALA:HB1 | 2:C:929:ARG:HH12 | 1.81 | 0.46 |
| 2:C:1489:CYS:O | 2:C:1492:GLU:HG3 | 2.15 | 0.46 |
| 2:C:1819:VAL:HG13 | 2:C:1905:GLN:NE2 | 2.31 | 0.46 |
| 2:C:2332:GLY:N | 2:C:2336:ARG:HH12 | 2.13 | 0.46 |
| 2:C:2581:ARG:HD3 | 2:C:2583:SER:H | 1.81 | 0.46 |
| 2:C:4689:LYS:HD2 | 2:C:4690:LYS:H | 1.79 | 0.46 |
| 2:D:1649:GLU:HG2 | 2:D:1650:LEU:N | 2.31 | 0.46 |
| 2:D:3601:ALA:HA | 2:D:3604:ARG:HH11 | 1.81 | 0.46 |
| 2:D:4639:SER:O | 2:D:4642:ASN:HB2 | 2.16 | 0.46 |
| 2:A:1415:ASP:N | 2:A:1415:ASP:OD1 | 2.49 | 0.46 |
| 2:A:2059:GLN:HG3 | 2:A:2091:GLN:HB3 | 1.98 | 0.46 |
| 2:A:2290:TRP:CZ2 | 2:A:2388:ILE:HG12 | 2.51 | 0.46 |
| 2:A:2431:ASP:O | 2:A:2435:VAL:HG23 | 2.16 | 0.46 |
| 2:A:2620:TYR:HB2 | 2:A:2627:TRP:HD1 | 1.81 | 0.46 |
| 2:A:3227:ARG:HH11 | 2:A:3228:TYR:HB3 | 1.81 | 0.46 |
| 2:B:794:PHE:CG | 2:B:798:ILE:HD13 | 2.50 | 0.46 |
| 2:B:889:ILE:HA | 2:B:892:LEU:HD12 | 1.98 | 0.46 |
| 2:B:2928:GLN:HA | 2:B:2931:ARG:HE | 1.80 | 0.46 |
| 2:B:4264:LEU:HA | 2:B:4267:GLN:OE1 | 2.16 | 0.46 |
| 2:C:808:HIS:O | 2:C:1616:GLY:HA2 | 2.15 | 0.46 |
| 2:C:4022:LYS:NZ | 2:C:4057:HIS:O | 2.35 | 0.46 |
| 2:D:267:VAL:HG22 | 2:D:272:ARG:HH12 | 1.81 | 0.46 |
| 2:D:889:ILE:HA | 2:D:892:LEU:HD12 | 1.98 | 0.46 |
| 2:D:1016:TRP:CG | 2:D:1027:ARG:HB3 | 2.51 | 0.46 |
| 2:D:2141:LEU:O | 2:D:2144:ARG:HD3 | 2.15 | 0.46 |
| 2:D:2620:TYR:HB2 | 2:D:2627:TRP:HD1 | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:3227:ARG:NH1 | 2:D:3228:TYR:HB3 | 2.30 | 0.46 |
| 2:A:20:VAL:HB | 2:A:214:VAL:HG13 | 1.97 | 0.45 |
| 2:A:888:ASN:ND2 | 2:A:1060:TYR:OH | 2.23 | 0.45 |
| 2:B:2191:LYS:O | 2:B:2195:ASN:ND2 | 2.50 | 0.45 |
| 2:B:2581:ARG:HD3 | 2:B:2583:SER:H | 1.81 | 0.45 |
| 2:B:2745:GLU:HA | 2:B:2755:PRO:HB3 | 1.98 | 0.45 |
| 2:B:4631:ASP:OD1 | 2:B:4708:TRP:NE1 | 2.42 | 0.45 |
| 2:C:902:TRP:CB | 2:C:918:LEU:HD21 | 2.42 | 0.45 |
| 2:C:1649:GLU:HG2 | 2:C:1650:LEU:N | 2.31 | 0.45 |
| 2:C:2191:LYS:O | 2:C:2195:ASN:ND2 | 2.49 | 0.45 |
| 2:C:3227:ARG:NH1 | 2:C:3228:TYR:HB3 | 2.31 | 0.45 |
| 2:D:66:THR:HG1 | 2:D:124:SER:HG | 1.57 | 0.45 |
| 2:D:438:LYS:HD3 | 2:D:438:LYS:HA | 1.69 | 0.45 |
| 2:D:2413:LYS:HZ2 | 2:D:2415:GLU:HB3 | 1.81 | 0.45 |
| 2:D:2705:PRO:HG3 | 2:D:2851:ILE:HG12 | 1.97 | 0.45 |
| 2:D:3261:ALA:C | 2:D:3262:GLU:OE1 | 2.54 | 0.45 |
| 2:A:1031:ARG:CZ | 2:A:1031:ARG:HB3 | 2.44 | 0.45 |
| 2:A:2170:THR:O | 2:A:2174:VAL:HG23 | 2.16 | 0.45 |
| 2:A:2745:GLU:HA | 2:A:2755:PRO:HB3 | 1.98 | 0.45 |
| 2:A:3924:ILE:HG21 | 2:A:3935:LEU:HD22 | 1.96 | 0.45 |
| 2:A:4617:ILE:HG23 | 2:A:4665:ARG:NH2 | 2.30 | 0.45 |
| 2:B:1986:CYS:O | 2:B:1993:ARG:NH2 | 2.48 | 0.45 |
| 2:B:2204:CYS:SG | 2:B:2214:MET:HG2 | 2.56 | 0.45 |
| 2:B:2496:LEU:HD23 | 2:B:2520:LEU:HD13 | 1.99 | 0.45 |
| 2:B:2576:ILE:O | 2:B:2580:LEU:HG | 2.17 | 0.45 |
| 2:B:2760:TYR:CE2 | 2:B:2768:LYS:HE3 | 2.51 | 0.45 |
| 2:B:3275:THR:O | 2:B:3279:ASN:ND2 | 2.49 | 0.45 |
| 2:B:3601:ALA:HA | 2:B:3604:ARG:HH11 | 1.81 | 0.45 |
| 2:C:717:GLY:N | 2:C:720:ASP:OD2 | 2.42 | 0.45 |
| 2:C:964:MET:HE1 | 2:C:982:ASP:HA | 1.99 | 0.45 |
| 2:C:1031:ARG:CZ | 2:C:1031:ARG:HB3 | 2.44 | 0.45 |
| 2:C:2498:ALA:O | 2:C:2502:LEU:HD23 | 2.16 | 0.45 |
| 2:C:3054:LYS:O | 2:C:3057:LEU:HG | 2.16 | 0.45 |
| 2:D:2178:VAL:HG21 | 2:D:2192:MET:SD | 2.56 | 0.45 |
| 2:D:2589:LEU:O | 2:D:2593:VAL:HG13 | 2.17 | 0.45 |
| 2:D:3134:LEU:HB2 | 2:D:3162:PHE:CE2 | 2.51 | 0.45 |
| 2:D:3227:ARG:HH11 | 2:D:3228:TYR:HB3 | 1.81 | 0.45 |
| 2:D:3653:GLU:HB2 | 2:D:3660:ARG:HH22 | 1.80 | 0.45 |
| 2:A:411:GLU:OE2 | 2:A:485:ARG:NE | 2.46 | 0.45 |
| 2:A:447:LEU:HG | 2:A:449:ILE:HG12 | 1.98 | 0.45 |
| 2:A:3134:LEU:HB2 | 2:A:3162:PHE:CE2 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:3656:GLU:OE1 | 2:A:3656:GLU:N | 2.50 | 0.45 |
| 2:B:267:VAL:HG22 | 2:B:272:ARG:HH12 | 1.81 | 0.45 |
| 2:B:307:SER:HB3 | 2:B:327:THR:HG22 | 1.97 | 0.45 |
| 2:B:1031:ARG:HH21 | 2:B:1038:LEU:CD1 | 2.11 | 0.45 |
| 2:B:2290:TRP:CZ2 | 2:B:2388:ILE:HG12 | 2.52 | 0.45 |
| 2:B:2620:TYR:HB2 | 2:B:2627:TRP:HD1 | 1.81 | 0.45 |
| 2:B:4252:ILE:HG21 | 2:C:4707:MET:HG3 | 1.97 | 0.45 |
| 2:B:4639:SER:O | 2:B:4642:ASN:HB2 | 2.16 | 0.45 |
| 2:C:29:HIS:CE1 | 2:C:31:GLU:HG2 | 2.52 | 0.45 |
| 2:C:447:LEU:HG | 2:C:449:ILE:HG12 | 1.98 | 0.45 |
| 2:C:916:PRO:HB3 | 2:C:923:LYS:HZ2 | 1.80 | 0.45 |
| 2:C:2113:VAL:O | 2:C:2117:ILE:HG13 | 2.16 | 0.45 |
| 2:C:3260:ARG:O | 2:C:3260:ARG:HD3 | 2.15 | 0.45 |
| 2:C:4631:ASP:OD1 | 2:C:4708:TRP:NE1 | 2.42 | 0.45 |
| 2:D:546:LYS:O | 2:D:550:GLN:HG2 | 2.16 | 0.45 |
| 2:D:1489:CYS:O | 2:D:1492:GLU:HG3 | 2.15 | 0.45 |
| 2:D:1898:LEU:HD13 | 2:D:1902:VAL:HG12 | 1.99 | 0.45 |
| 2:D:2204:CYS:SG | 2:D:2214:MET:HG2 | 2.56 | 0.45 |
| 2:D:2290:TRP:CZ2 | 2:D:2388:ILE:HG12 | 2.52 | 0.45 |
| 2:D:2581:ARG:HG2 | 2:D:2582:PRO:HD2 | 1.99 | 0.45 |
| 2:A:892:LEU:HD21 | 2:A:980:PRO:HD3 | 1.99 | 0.45 |
| 2:A:2498:ALA:O | 2:A:2502:LEU:HD23 | 2.16 | 0.45 |
| 2:A:2581:ARG:HB3 | 2:A:2584:MET:HE2 | 1.98 | 0.45 |
| 2:B:2059:GLN:HG3 | 2:B:2091:GLN:HB3 | 1.98 | 0.45 |
| 2:C:546:LYS:O | 2:C:550:GLN:HG2 | 2.16 | 0.45 |
| 2:C:880:ARG:HH11 | 2:C:881:ILE:HB | 1.81 | 0.45 |
| 2:C:889:ILE:HA | 2:C:892:LEU:HD12 | 1.98 | 0.45 |
| 2:C:2576:ILE:O | 2:C:2580:LEU:HG | 2.17 | 0.45 |
| 2:C:2745:GLU:HA | 2:C:2755:PRO:HB3 | 1.98 | 0.45 |
| 2:C:3054:LYS:O | 2:C:3058:ARG:HG3 | 2.17 | 0.45 |
| 2:D:826:VAL:HG21 | 2:D:832:LEU:HB2 | 1.98 | 0.45 |
| 2:D:2496:LEU:HD23 | 2:D:2520:LEU:HD13 | 1.99 | 0.45 |
| 2:D:2576:ILE:O | 2:D:2580:LEU:HG | 2.17 | 0.45 |
| 2:D:3311:LYS:O | 2:D:3315:LEU:N | 2.49 | 0.45 |
| 2:D:3321:PRO:O | 2:D:3324:GLU:HG3 | 2.17 | 0.45 |
| 2:A:29:HIS:CE1 | 2:A:31:GLU:HG2 | 2.52 | 0.45 |
| 2:A:911:ASN:OD1 | 2:A:912:LYS:N | 2.50 | 0.45 |
| 2:A:2496:LEU:HD23 | 2:A:2520:LEU:HD13 | 1.99 | 0.45 |
| 2:A:2581:ARG:HG2 | 2:A:2582:PRO:HD2 | 1.99 | 0.45 |
| 2:A:2642:ARG:HA | 2:A:2676:LEU:HD11 | 1.99 | 0.45 |
| 2:A:2760:TYR:CE2 | 2:A:2768:LYS:HE3 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:2840:MET:HA | 2:A:2843:MET:HG2 | 1.99 | 0.45 |
| 2:B:624:ALA:HB2 | 2:B:1667:LEU:HD12 | 1.99 | 0.45 |
| 2:B:911:ASN:OD1 | 2:B:912:LYS:N | 2.50 | 0.45 |
| 2:B:2581:ARG:HG2 | 2:B:2582:PRO:HD2 | 1.99 | 0.45 |
| 2:B:3054:LYS:O | 2:B:3057:LEU:HG | 2.16 | 0.45 |
| 2:B:3068:LEU:O | 2:B:3071:THR:OG1 | 2.25 | 0.45 |
| 2:B:3074:ASN:O | 2:B:3077:GLN:HG3 | 2.17 | 0.45 |
| 2:B:3656:GLU:N | 2:B:3656:GLU:OE1 | 2.50 | 0.45 |
| 2:C:131:CYS:SG | 2:C:150:GLN:HB2 | 2.57 | 0.45 |
| 2:C:892:LEU:HD21 | 2:C:980:PRO:HD3 | 1.99 | 0.45 |
| 2:C:1031:ARG:NH2 | 2:C:1042:THR:HG21 | 2.21 | 0.45 |
| 2:C:1170:GLU:HG2 | 2:C:1172:THR:HG23 | 1.99 | 0.45 |
| 2:C:1945:ASN:O | 2:C:1949:GLN:NE2 | 2.42 | 0.45 |
| 2:C:2170:THR:O | 2:C:2174:VAL:HG23 | 2.16 | 0.45 |
| 2:C:2589:LEU:O | 2:C:2593:VAL:HG13 | 2.17 | 0.45 |
| 2:D:29:HIS:CE1 | 2:D:31:GLU:HG2 | 2.52 | 0.45 |
| 2:D:964:MET:HE1 | 2:D:982:ASP:HA | 1.97 | 0.45 |
| 2:D:2113:VAL:O | 2:D:2117:ILE:HG13 | 2.16 | 0.45 |
| 2:D:3728:GLN:HG2 | 2:D:3765:ILE:HA | 1.98 | 0.45 |
| 2:A:1273:ILE:HB | 2:A:1282:CYS:HB2 | 1.99 | 0.45 |
| 2:A:1986:CYS:O | 2:A:1993:ARG:NH2 | 2.48 | 0.45 |
| 2:A:4639:SER:O | 2:A:4642:ASN:HB2 | 2.16 | 0.45 |
| 2:B:131:CYS:SG | 2:B:150:GLN:HB2 | 2.57 | 0.45 |
| 2:B:2642:ARG:HA | 2:B:2676:LEU:HD11 | 1.99 | 0.45 |
| 2:B:3653:GLU:OE1 | 2:B:3660:ARG:NH1 | 2.50 | 0.45 |
| 2:C:2620:TYR:HB2 | 2:C:2627:TRP:HD1 | 1.82 | 0.45 |
| 2:C:3227:ARG:HH11 | 2:C:3228:TYR:HB3 | 1.82 | 0.45 |
| 2:C:4602:ARG:NH1 | 2:C:4627:LYS:HG3 | 2.32 | 0.45 |
| 2:D:3054:LYS:O | 2:D:3057:LEU:HG | 2.16 | 0.45 |
| 2:D:3140:LEU:HB3 | 2:D:3155:LEU:HD13 | 1.97 | 0.45 |
| 2:A:2191:LYS:O | 2:A:2195:ASN:ND2 | 2.49 | 0.45 |
| 2:A:2926:LEU:C | 2:A:3003:MET:HE1 | 2.37 | 0.45 |
| 2:A:3653:GLU:OE1 | 2:A:3660:ARG:NH1 | 2.50 | 0.45 |
| 2:A:4203:ALA:HA | 2:A:4206:ILE:HG12 | 1.98 | 0.45 |
| 2:B:1649:GLU:HG2 | 2:B:1650:LEU:N | 2.31 | 0.45 |
| 2:B:2589:LEU:O | 2:B:2593:VAL:HG13 | 2.16 | 0.45 |
| 2:B:3001:LYS:NZ | 2:B:3044:THR:H | 2.13 | 0.45 |
| 2:B:3260:ARG:HH11 | 2:B:3264:CYS:HA | 1.79 | 0.45 |
| 2:B:3321:PRO:O | 2:B:3324:GLU:HG3 | 2.17 | 0.45 |
| 2:B:4100:VAL:HG22 | 2:B:4133:LEU:HD13 | 1.99 | 0.45 |
| 2:C:911:ASN:OD1 | 2:C:912:LYS:N | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:1031:ARG:HH22 | 2:C:1042:THR:CB | 2.30 | 0.45 |
| 2:C:2496:LEU:HD23 | 2:C:2520:LEU:HD13 | 1.99 | 0.45 |
| 2:C:2581:ARG:HG2 | 2:C:2582:PRO:HD2 | 1.99 | 0.45 |
| 2:C:2788:ARG:HH22 | 2:C:2908:LYS:CE | 2.30 | 0.45 |
| 2:D:892:LEU:HD21 | 2:D:980:PRO:HD3 | 1.99 | 0.45 |
| 2:D:902:TRP:HB3 | 2:D:918:LEU:CD2 | 2.44 | 0.45 |
| 2:D:1957:LEU:HG | 2:D:1961:LYS:HB3 | 1.97 | 0.45 |
| 2:D:4735:ASN:HB3 | 2:D:4738:PHE:CD2 | 2.52 | 0.45 |
| 1:F:12:ASP:HB2 | 1:F:14:ARG:HH12 | 1.81 | 0.45 |
| 1:G:12:ASP:HB2 | 1:G:14:ARG:HH12 | 1.81 | 0.45 |
| 2:A:624:ALA:HB2 | 2:A:1667:LEU:HD12 | 1.99 | 0.45 |
| 2:A:889:ILE:HA | 2:A:892:LEU:HD12 | 1.98 | 0.45 |
| 2:A:2303:ARG:HH11 | 2:A:2304:PHE:HA | 1.82 | 0.45 |
| 2:B:826:VAL:HG21 | 2:B:832:LEU:HB2 | 1.98 | 0.45 |
| 2:B:892:LEU:HD21 | 2:B:980:PRO:HD3 | 1.99 | 0.45 |
| 2:B:1031:ARG:CZ | 2:B:1031:ARG:HB3 | 2.44 | 0.45 |
| 2:B:1044:LYS:HD3 | 2:B:1044:LYS:HA | 1.77 | 0.45 |
| 2:B:2788:ARG:HH22 | 2:B:2908:LYS:CE | 2.30 | 0.45 |
| 2:B:2840:MET:HA | 2:B:2843:MET:HG2 | 1.99 | 0.45 |
| 2:B:4617:ILE:HG23 | 2:B:4665:ARG:NH2 | 2.30 | 0.45 |
| 2:C:826:VAL:HG21 | 2:C:832:LEU:HB2 | 1.98 | 0.45 |
| 2:D:131:CYS:SG | 2:D:150:GLN:HB2 | 2.57 | 0.45 |
| 2:D:911:ASN:OD1 | 2:D:912:LYS:N | 2.50 | 0.45 |
| 2:D:2498:ALA:O | 2:D:2502:LEU:HD23 | 2.16 | 0.45 |
| 2:D:3653:GLU:OE1 | 2:D:3660:ARG:NH1 | 2.50 | 0.45 |
| 2:D:4602:ARG:NH1 | 2:D:4627:LYS:HG3 | 2.32 | 0.45 |
| 2:D:4636:ASN:HB2 | 2:D:4704:LYS:HZ1 | 1.82 | 0.45 |
| 1:E:12:ASP:HB2 | 1:E:14:ARG:HH12 | 1.81 | 0.45 |
| 2:A:131:CYS:SG | 2:A:150:GLN:HB2 | 2.57 | 0.45 |
| 2:A:677:LEU:HD12 | 2:A:801:ARG:O | 2.17 | 0.45 |
| 2:A:1963:LYS:HE2 | 2:A:1963:LYS:HB2 | 1.77 | 0.45 |
| 2:A:2788:ARG:HH22 | 2:A:2908:LYS:CE | 2.30 | 0.45 |
| 2:A:3763:ILE:HD11 | 2:A:3838:ASP:O | 2.17 | 0.45 |
| 2:B:29:HIS:CE1 | 2:B:31:GLU:HG2 | 2.52 | 0.45 |
| 2:B:1031:ARG:HH22 | 2:B:1042:THR:CB | 2.30 | 0.45 |
| 2:B:3227:ARG:HH11 | 2:B:3228:TYR:HB3 | 1.81 | 0.45 |
| 2:C:1415:ASP:OD1 | 2:C:1415:ASP:N | 2.49 | 0.45 |
| 2:C:2204:CYS:SG | 2:C:2214:MET:HG2 | 2.56 | 0.45 |
| 2:D:307:SER:HB3 | 2:D:327:THR:HG22 | 1.97 | 0.45 |
| 2:D:902:TRP:CB | 2:D:918:LEU:HD21 | 2.42 | 0.45 |
| 2:D:1226:TYR:HD1 | 2:D:1229:ILE:HD11 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:1273:ILE:HB | 2:D:1282:CYS:HB2 | 1.99 | 0.45 |
| 2:D:2642:ARG:HA | 2:D:2676:LEU:HD11 | 1.99 | 0.45 |
| 2:A:1226:TYR:HD1 | 2:A:1229:ILE:HD11 | 1.82 | 0.45 |
| 2:A:2761:LYS:HA | 2:A:2761:LYS:HD3 | 1.83 | 0.45 |
| 2:A:3207:ASN:OD1 | 2:A:3208:ILE:N | 2.50 | 0.45 |
| 2:A:3601:ALA:HA | 2:A:3604:ARG:HH11 | 1.81 | 0.45 |
| 2:A:4100:VAL:HG22 | 2:A:4133:LEU:HD13 | 1.99 | 0.45 |
| 2:A:4625:ASP:OD1 | 2:A:4625:ASP:N | 2.46 | 0.45 |
| 2:B:447:LEU:HG | 2:B:449:ILE:HG12 | 1.98 | 0.45 |
| 2:B:1819:VAL:HG13 | 2:B:1905:GLN:NE2 | 2.31 | 0.45 |
| 2:B:2322:ARG:NH1 | 2:C:189:GLU:OE2 | 2.50 | 0.45 |
| 2:B:2498:ALA:O | 2:B:2502:LEU:HD23 | 2.16 | 0.45 |
| 2:B:3728:GLN:HG2 | 2:B:3765:ILE:HA | 1.98 | 0.45 |
| 2:B:4084:VAL:O | 2:B:4088:HIS:HB3 | 2.17 | 0.45 |
| 2:C:2290:TRP:CZ2 | 2:C:2388:ILE:HG12 | 2.52 | 0.45 |
| 2:C:3763:ILE:HD11 | 2:C:3838:ASP:O | 2.17 | 0.45 |
| 2:D:916:PRO:HB3 | 2:D:923:LYS:HZ2 | 1.81 | 0.45 |
| 2:D:1598:ARG:NH2 | 2:D:1601:ASN:OD1 | 2.47 | 0.45 |
| 2:D:4100:VAL:HG22 | 2:D:4133:LEU:HD13 | 1.99 | 0.45 |
| 2:D:4203:ALA:HA | 2:D:4206:ILE:HG12 | 1.98 | 0.45 |
| 2:A:1839:LEU:HA | 2:A:1842:ILE:HG12 | 1.99 | 0.44 |
| 2:A:1967:SER:O | 2:A:1972:GLN:NE2 | 2.40 | 0.44 |
| 2:A:2576:ILE:O | 2:A:2580:LEU:HG | 2.17 | 0.44 |
| 2:A:2688:MET:HB3 | 2:A:2689:MET:HE1 | 1.99 | 0.44 |
| 2:A:4602:ARG:NH1 | 2:A:4627:LYS:HG3 | 2.32 | 0.44 |
| 2:B:1273:ILE:HB | 2:B:1282:CYS:HB2 | 1.99 | 0.44 |
| 2:B:1839:LEU:HA | 2:B:1842:ILE:HG12 | 1.99 | 0.44 |
| 2:B:3166:PHE:CD1 | 2:B:3167:PRO:HD2 | 2.53 | 0.44 |
| 2:B:3763:ILE:HD11 | 2:B:3838:ASP:O | 2.17 | 0.44 |
| 2:B:4602:ARG:NH1 | 2:B:4627:LYS:HG3 | 2.32 | 0.44 |
| 2:C:624:ALA:HB2 | 2:C:1667:LEU:HD12 | 1.99 | 0.44 |
| 2:C:1168:MET:HE3 | 2:C:1197:VAL:HG22 | 1.99 | 0.44 |
| 2:C:1199:ASP:OD1 | 2:C:1199:ASP:N | 2.45 | 0.44 |
| 2:C:1727:VAL:HG11 | 2:C:1926:VAL:HG21 | 1.99 | 0.44 |
| 2:C:2798:MET:SD | 2:D:1498:GLN:HG3 | 2.58 | 0.44 |
| 2:C:3311:LYS:O | 2:C:3315:LEU:N | 2.49 | 0.44 |
| 2:C:3321:PRO:O | 2:C:3324:GLU:HG3 | 2.17 | 0.44 |
| 2:C:3656:GLU:OE1 | 2:C:3656:GLU:N | 2.50 | 0.44 |
| 2:C:4264:LEU:HA | 2:C:4267:GLN:OE1 | 2.16 | 0.44 |
| 2:D:447:LEU:HG | 2:D:449:ILE:HG12 | 1.98 | 0.44 |
| 2:D:2586:GLN:HE22 | 2:D:2590:ARG:NH2 | 2.15 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:880:ARG:HH11 | 2:A:881:ILE:HB | 1.81 | 0.44 |
| 2:A:1727:VAL:HG11 | 2:A:1926:VAL:HG21 | 1.99 | 0.44 |
| 2:A:3054:LYS:O | 2:A:3058:ARG:HG3 | 2.17 | 0.44 |
| 2:B:4735:ASN:HB3 | 2:B:4738:PHE:CD2 | 2.52 | 0.44 |
| 2:C:1018:TYR:CD1 | 2:C:1030:PRO:HA | 2.52 | 0.44 |
| 2:C:4100:VAL:HG22 | 2:C:4133:LEU:HD13 | 1.99 | 0.44 |
| 2:D:677:LEU:HD12 | 2:D:801:ARG:O | 2.17 | 0.44 |
| 2:D:824:GLU:HA | 2:D:1020:ILE:HD12 | 1.97 | 0.44 |
| 2:D:3216:GLU:HA | 2:D:3219:VAL:HG22 | 2.00 | 0.44 |
| 2:D:3656:GLU:OE1 | 2:D:3656:GLU:N | 2.50 | 0.44 |
| 2:D:3763:ILE:HD11 | 2:D:3838:ASP:O | 2.17 | 0.44 |
| 2:A:1170:GLU:HG2 | 2:A:1172:THR:HG23 | 1.99 | 0.44 |
| 2:A:1898:LEU:HD13 | 2:A:1902:VAL:HG12 | 1.98 | 0.44 |
| 2:A:1971:GLU:HA | 2:A:1974:ASN:HD22 | 1.82 | 0.44 |
| 2:A:2434:GLY:O | 2:A:2438:ILE:HG13 | 2.18 | 0.44 |
| 2:A:2586:GLN:HE22 | 2:A:2590:ARG:NH2 | 2.15 | 0.44 |
| 2:A:3054:LYS:O | 2:A:3057:LEU:HG | 2.16 | 0.44 |
| 2:A:3288:LEU:HD22 | 2:A:3332:THR:HG21 | 2.00 | 0.44 |
| 2:A:3321:PRO:O | 2:A:3324:GLU:HG3 | 2.17 | 0.44 |
| 2:B:954:ASP:OD2 | 2:B:957:ALA:N | 2.51 | 0.44 |
| 2:B:1991:GLU:HG2 | 2:B:1992:ILE:N | 2.32 | 0.44 |
| 2:B:3729:ALA:HA | 2:B:3732:HIS:ND1 | 2.32 | 0.44 |
| 2:B:4277:LYS:HD2 | 2:B:4277:LYS:HA | 1.73 | 0.44 |
| 2:C:34:LYS:H | 2:C:53:SER:HB3 | 1.82 | 0.44 |
| 2:C:849:ASP:OD1 | 2:C:1214:ARG:NE | 2.51 | 0.44 |
| 2:C:1226:TYR:HD1 | 2:C:1229:ILE:HD11 | 1.82 | 0.44 |
| 2:C:1839:LEU:HA | 2:C:1842:ILE:HG12 | 1.99 | 0.44 |
| 2:D:624:ALA:HB2 | 2:D:1667:LEU:HD12 | 1.99 | 0.44 |
| 2:D:1931:ASP:OD1 | 2:D:1932:PHE:N | 2.51 | 0.44 |
| 2:D:3054:LYS:O | 2:D:3058:ARG:HG3 | 2.17 | 0.44 |
| 2:D:3074:ASN:O | 2:D:3077:GLN:HG3 | 2.17 | 0.44 |
| 2:A:2379:ASP:OD1 | 2:A:2380:ASP:N | 2.51 | 0.44 |
| 2:A:3729:ALA:HA | 2:A:3732:HIS:ND1 | 2.32 | 0.44 |
| 2:A:4631:ASP:OD1 | 2:A:4708:TRP:NE1 | 2.42 | 0.44 |
| 2:A:4735:ASN:HB3 | 2:A:4738:PHE:CD2 | 2.52 | 0.44 |
| 2:B:677:LEU:HD12 | 2:B:801:ARG:O | 2.17 | 0.44 |
| 2:B:987:LYS:HZ3 | 2:B:989:THR:HA | 1.82 | 0.44 |
| 2:B:1170:GLU:HG2 | 2:B:1172:THR:HG23 | 1.99 | 0.44 |
| 2:B:2303:ARG:HH11 | 2:B:2304:PHE:HA | 1.82 | 0.44 |
| 2:B:3300:ALA:O | 2:B:3304:GLN:HG2 | 2.18 | 0.44 |
| 2:C:555:LEU:HD12 | 2:C:588:ILE:HD11 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:674:TYR:HE1 | 2:C:756:SER:HB2 | 1.83 | 0.44 |
| 2:C:894:VAL:HG23 | 2:C:895:MET:HE2 | 1.99 | 0.44 |
| 2:C:1931:ASP:OD1 | 2:C:1932:PHE:N | 2.51 | 0.44 |
| 2:C:2726:GLU:HG2 | 2:C:2760:TYR:CD2 | 2.52 | 0.44 |
| 2:C:2736:LYS:HD3 | 2:C:2736:LYS:HA | 1.82 | 0.44 |
| 2:C:3650:GLU:OE1 | 2:C:3659:LYS:NZ | 2.49 | 0.44 |
| 2:C:3695:MET:HB3 | 2:C:3731:LEU:HD11 | 2.00 | 0.44 |
| 2:C:3728:GLN:HG2 | 2:C:3765:ILE:HA | 1.98 | 0.44 |
| 2:C:4084:VAL:O | 2:C:4088:HIS:HB3 | 2.17 | 0.44 |
| 2:D:1415:ASP:N | 2:D:1415:ASP:OD1 | 2.49 | 0.44 |
| 2:D:1727:VAL:HG11 | 2:D:1926:VAL:HG21 | 1.99 | 0.44 |
| 2:D:2726:GLU:HG2 | 2:D:2760:TYR:CD2 | 2.52 | 0.44 |
| 2:D:2788:ARG:HH22 | 2:D:2908:LYS:CE | 2.30 | 0.44 |
| 2:D:3288:LEU:HD22 | 2:D:3332:THR:HG21 | 2.00 | 0.44 |
| 2:A:28:ILE:HG22 | 2:A:29:HIS:CD2 | 2.53 | 0.44 |
| 2:A:1598:ARG:NH2 | 2:A:1601:ASN:OD1 | 2.47 | 0.44 |
| 2:A:3216:GLU:HA | 2:A:3219:VAL:HG22 | 2.00 | 0.44 |
| 2:A:3997:LYS:HD3 | 2:A:4109:MET:HE1 | 1.99 | 0.44 |
| 2:B:28:ILE:HG22 | 2:B:29:HIS:CD2 | 2.53 | 0.44 |
| 2:B:3043:ARG:HH21 | 2:B:3117:PHE:HD1 | 1.66 | 0.44 |
| 2:B:3054:LYS:O | 2:B:3058:ARG:HG3 | 2.17 | 0.44 |
| 2:B:3695:MET:HB3 | 2:B:3731:LEU:HD11 | 2.00 | 0.44 |
| 2:B:3952:ALA:HB1 | 2:B:4012:MET:HE3 | 2.00 | 0.44 |
| 2:C:1971:GLU:HA | 2:C:1974:ASN:HD22 | 1.82 | 0.44 |
| 2:C:1991:GLU:HG2 | 2:C:1992:ILE:N | 2.32 | 0.44 |
| 2:C:2586:GLN:HE22 | 2:C:2590:ARG:NH2 | 2.15 | 0.44 |
| 2:C:4956:ASP:OD1 | 2:C:4957:CYS:N | 2.50 | 0.44 |
| 2:D:1031:ARG:HH22 | 2:D:1042:THR:CB | 2.30 | 0.44 |
| 2:D:1692:LYS:HB3 | 2:D:1692:LYS:HE3 | 1.86 | 0.44 |
| 2:D:2200:LEU:HD13 | 2:D:2214:MET:HE1 | 1.98 | 0.44 |
| 2:D:2840:MET:HA | 2:D:2843:MET:HG2 | 1.99 | 0.44 |
| 2:D:3712:LYS:HE3 | 2:D:3712:LYS:HB2 | 1.69 | 0.44 |
| 2:D:4084:VAL:O | 2:D:4088:HIS:HB3 | 2.17 | 0.44 |
| 2:A:2392:TYR:O | 2:A:2396:ILE:HD12 | 2.18 | 0.44 |
| 2:A:2589:LEU:O | 2:A:2593:VAL:HG13 | 2.17 | 0.44 |
| 2:A:3016:ARG:HA | 2:A:3096:TYR:CZ | 2.53 | 0.44 |
| 2:A:3074:ASN:O | 2:A:3077:GLN:HG3 | 2.17 | 0.44 |
| 2:B:555:LEU:HD12 | 2:B:588:ILE:HD11 | 2.00 | 0.44 |
| 2:B:674:TYR:OH | 2:B:676:GLU:OE1 | 2.31 | 0.44 |
| 2:B:2443:PRO:HG3 | 2:B:2454:PRO:HD2 | 1.99 | 0.44 |
| 2:B:2729:HIS:CG | 2:B:2763:LEU:HD22 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:1898:LEU:HD13 | 2:C:1902:VAL:HG12 | 1.99 | 0.44 |
| 2:C:2642:ARG:HA | 2:C:2676:LEU:HD11 | 1.99 | 0.44 |
| 2:C:2681:MET:HE1 | 2:C:2917:ILE:HA | 2.00 | 0.44 |
| 2:C:3061:LEU:HD23 | 2:C:3061:LEU:HA | 1.84 | 0.44 |
| 2:C:3216:GLU:HA | 2:C:3219:VAL:HG22 | 2.00 | 0.44 |
| 2:C:4270:LYS:HE3 | 2:C:4270:LYS:HB3 | 1.84 | 0.44 |
| 2:D:674:TYR:OH | 2:D:676:GLU:OE1 | 2.31 | 0.44 |
| 2:D:2194:ALA:HA | 2:D:2237:SER:HB3 | 2.00 | 0.44 |
| 2:D:2676:LEU:HD23 | 2:D:2676:LEU:HA | 1.83 | 0.44 |
| 2:D:2745:GLU:HA | 2:D:2755:PRO:HB3 | 1.98 | 0.44 |
| 2:D:4924:TYR:CZ | 2:D:4928:LYS:HD2 | 2.53 | 0.44 |
| 1:G:67:MET:SD | 1:G:73:ALA:HB3 | 2.58 | 0.44 |
| 1:H:67:MET:SD | 1:H:73:ALA:HB3 | 2.58 | 0.44 |
| 2:A:555:LEU:HD12 | 2:A:588:ILE:HD11 | 2.00 | 0.44 |
| 2:A:2179:LEU:HD13 | 2:A:2224:ASN:HD22 | 1.83 | 0.44 |
| 2:A:2905:ARG:NH1 | 2:A:2906:GLY:H | 2.15 | 0.44 |
| 2:A:3300:ALA:O | 2:A:3304:GLN:HG2 | 2.18 | 0.44 |
| 2:A:4956:ASP:OD1 | 2:A:4957:CYS:N | 2.50 | 0.44 |
| 2:B:36:CYS:SG | 2:B:65:CYS:HB3 | 2.58 | 0.44 |
| 2:B:964:MET:HE1 | 2:B:982:ASP:HA | 2.00 | 0.44 |
| 2:B:1007:TRP:CZ2 | 2:B:1011:ARG:HD3 | 2.53 | 0.44 |
| 2:B:1748:LEU:HD23 | 2:B:1748:LEU:HA | 1.84 | 0.44 |
| 2:B:1971:GLU:HA | 2:B:1974:ASN:HD22 | 1.82 | 0.44 |
| 2:B:2831:VAL:HG22 | 2:C:1435:GLY:CA | 2.47 | 0.44 |
| 2:B:3261:ALA:C | 2:B:3263:MET:N | 2.71 | 0.44 |
| 2:C:954:ASP:OD2 | 2:C:957:ALA:N | 2.51 | 0.44 |
| 2:C:2379:ASP:OD1 | 2:C:2380:ASP:N | 2.51 | 0.44 |
| 2:C:2833:LEU:HB2 | 2:C:2894:LYS:HZ1 | 1.81 | 0.44 |
| 2:C:3246:MET:O | 2:C:3250:TRP:HB2 | 2.17 | 0.44 |
| 2:C:3288:LEU:HD22 | 2:C:3332:THR:HG21 | 2.00 | 0.44 |
| 2:C:3300:ALA:O | 2:C:3304:GLN:HG2 | 2.18 | 0.44 |
| 2:C:4735:ASN:HB3 | 2:C:4738:PHE:CD2 | 2.52 | 0.44 |
| 2:D:456:LEU:HD23 | 2:D:456:LEU:HA | 1.84 | 0.44 |
| 2:D:1967:SER:O | 2:D:1972:GLN:NE2 | 2.40 | 0.44 |
| 2:D:2443:PRO:HG3 | 2:D:2454:PRO:HD2 | 1.99 | 0.44 |
| 2:D:3691:TYR:O | 2:D:3695:MET:HG3 | 2.18 | 0.44 |
| 1:H:12:ASP:HB2 | 1:H:14:ARG:HH12 | 1.81 | 0.44 |
| 2:A:849:ASP:OD1 | 2:A:1214:ARG:NE | 2.51 | 0.44 |
| 2:A:4924:TYR:CZ | 2:A:4928:LYS:HD2 | 2.53 | 0.44 |
| 2:B:849:ASP:OD1 | 2:B:1214:ARG:NE | 2.51 | 0.44 |
| 2:B:1018:TYR:CD1 | 2:B:1030:PRO:HA | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1929:SER:O | 2:B:1933:VAL:HG12 | 2.18 | 0.44 |
| 2:B:3102:LEU:HB2 | 2:B:3103:PRO:HD3 | 2.00 | 0.44 |
| 2:B:4060:GLN:O | 2:B:4064:GLU:OE1 | 2.36 | 0.44 |
| 2:B:4818:TYR:HA | 2:C:4848:ILE:HD11 | 1.99 | 0.44 |
| 2:C:36:CYS:SG | 2:C:65:CYS:HB3 | 2.58 | 0.44 |
| 2:C:1979:PHE:HZ | 2:C:1996:LEU:HB3 | 1.83 | 0.44 |
| 2:C:2666:LEU:HD13 | 2:C:2966:VAL:HA | 2.00 | 0.44 |
| 2:C:2729:HIS:CG | 2:C:2763:LEU:HD22 | 2.53 | 0.44 |
| 2:C:3074:ASN:O | 2:C:3077:GLN:HG3 | 2.17 | 0.44 |
| 2:C:3653:GLU:OE1 | 2:C:3660:ARG:NH1 | 2.50 | 0.44 |
| 2:D:674:TYR:HE1 | 2:D:756:SER:HB2 | 1.83 | 0.44 |
| 2:D:1829:LEU:HD12 | 2:D:1829:LEU:HA | 1.88 | 0.44 |
| 2:D:1945:ASN:O | 2:D:1949:GLN:NE2 | 2.42 | 0.44 |
| 2:D:2581:ARG:HD3 | 2:D:2583:SER:H | 1.81 | 0.44 |
| 2:D:3952:ALA:HB1 | 2:D:4012:MET:HE3 | 2.00 | 0.44 |
| 2:A:886:ALA:HB1 | 2:A:929:ARG:HH12 | 1.81 | 0.44 |
| 2:A:1014:GLN:HB3 | 2:A:1027:ARG:NH2 | 2.31 | 0.44 |
| 2:A:1018:TYR:CD1 | 2:A:1030:PRO:HA | 2.52 | 0.44 |
| 2:A:1473:LYS:NZ | 2:A:1475:LYS:HB2 | 2.33 | 0.44 |
| 2:A:2443:PRO:HG3 | 2:A:2454:PRO:HD2 | 1.99 | 0.44 |
| 2:A:2729:HIS:CG | 2:A:2763:LEU:HD22 | 2.53 | 0.44 |
| 2:A:3728:GLN:HG2 | 2:A:3765:ILE:HA | 1.98 | 0.44 |
| 2:B:1168:MET:HE3 | 2:B:1197:VAL:HG22 | 2.00 | 0.44 |
| 2:B:2379:ASP:OD1 | 2:B:2380:ASP:N | 2.51 | 0.44 |
| 2:B:2434:GLY:O | 2:B:2438:ILE:HG13 | 2.18 | 0.44 |
| 2:B:2726:GLU:HG2 | 2:B:2760:TYR:CD2 | 2.52 | 0.44 |
| 2:B:3216:GLU:HA | 2:B:3219:VAL:HG22 | 2.00 | 0.44 |
| 2:C:2059:GLN:HG3 | 2:C:2091:GLN:HB3 | 1.98 | 0.44 |
| 2:C:2434:GLY:O | 2:C:2438:ILE:HG13 | 2.17 | 0.44 |
| 2:C:2831:VAL:HB | 2:C:2894:LYS:CD | 2.46 | 0.44 |
| 2:C:2840:MET:HA | 2:C:2843:MET:HG2 | 1.99 | 0.44 |
| 2:C:3260:ARG:HH11 | 2:C:3264:CYS:HA | 1.79 | 0.44 |
| 2:C:3952:ALA:HB1 | 2:C:4012:MET:HE3 | 2.00 | 0.44 |
| 2:D:1007:TRP:CZ2 | 2:D:1011:ARG:HD3 | 2.53 | 0.44 |
| 2:D:1473:LYS:NZ | 2:D:1475:LYS:HB2 | 2.33 | 0.44 |
| 2:D:2179:LEU:HD13 | 2:D:2224:ASN:HD22 | 1.83 | 0.44 |
| 2:D:2379:ASP:OD1 | 2:D:2380:ASP:N | 2.51 | 0.44 |
| 2:D:2392:TYR:O | 2:D:2396:ILE:HD12 | 2.18 | 0.44 |
| 2:D:2729:HIS:CG | 2:D:2763:LEU:HD22 | 2.53 | 0.44 |
| 2:D:3246:MET:O | 2:D:3250:TRP:HB2 | 2.17 | 0.44 |
| 2:D:3300:ALA:O | 2:D:3304:GLN:HG2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:1031:ARG:HH22 | 2:A:1042:THR:CB | 2.30 | 0.43 |
| 2:A:1929:SER:O | 2:A:1933:VAL:HG12 | 2.18 | 0.43 |
| 2:A:1931:ASP:OD1 | 2:A:1932:PHE:N | 2.51 | 0.43 |
| 2:A:2726:GLU:HG2 | 2:A:2760:TYR:CD2 | 2.52 | 0.43 |
| 2:A:3166:PHE:CD1 | 2:A:3167:PRO:HD2 | 2.53 | 0.43 |
| 2:B:1014:GLN:HB3 | 2:B:1027:ARG:NH2 | 2.30 | 0.43 |
| 2:B:1598:ARG:NH2 | 2:B:1601:ASN:OD1 | 2.47 | 0.43 |
| 2:B:1727:VAL:HG11 | 2:B:1926:VAL:HG21 | 1.99 | 0.43 |
| 2:B:2392:TYR:O | 2:B:2396:ILE:HD12 | 2.18 | 0.43 |
| 2:B:3712:LYS:HE3 | 2:B:3712:LYS:HB2 | 1.70 | 0.43 |
| 2:C:2194:ALA:HA | 2:C:2237:SER:HB3 | 2.00 | 0.43 |
| 2:C:3261:ALA:C | 2:C:3263:MET:N | 2.71 | 0.43 |
| 2:D:36:CYS:SG | 2:D:65:CYS:HB3 | 2.58 | 0.43 |
| 2:D:1043:LYS:HB2 | 2:D:1043:LYS:HE2 | 1.54 | 0.43 |
| 2:D:1170:GLU:HG2 | 2:D:1172:THR:HG23 | 1.99 | 0.43 |
| 2:D:1971:GLU:HA | 2:D:1974:ASN:HD22 | 1.82 | 0.43 |
| 2:D:3061:LEU:HD23 | 2:D:3061:LEU:HA | 1.84 | 0.43 |
| 2:D:3729:ALA:HA | 2:D:3732:HIS:ND1 | 2.32 | 0.43 |
| 2:A:826:VAL:HG21 | 2:A:832:LEU:HB2 | 1.98 | 0.43 |
| 2:A:1007:TRP:CZ2 | 2:A:1011:ARG:HD3 | 2.53 | 0.43 |
| 2:A:2194:ALA:HA | 2:A:2237:SER:HB3 | 2.00 | 0.43 |
| 2:A:2581:ARG:HD3 | 2:A:2583:SER:H | 1.81 | 0.43 |
| 2:A:3043:ARG:HH21 | 2:A:3117:PHE:HD1 | 1.66 | 0.43 |
| 2:A:4806:CYS:HA | 2:A:4812:CYS:HB2 | 2.00 | 0.43 |
| 2:B:1226:TYR:HD1 | 2:B:1229:ILE:HD11 | 1.82 | 0.43 |
| 2:B:1473:LYS:NZ | 2:B:1475:LYS:HB2 | 2.33 | 0.43 |
| 2:B:3235:MET:O | 2:B:3299:LEU:HD21 | 2.19 | 0.43 |
| 2:B:3246:MET:O | 2:B:3250:TRP:HB2 | 2.17 | 0.43 |
| 2:B:3288:LEU:HD22 | 2:B:3332:THR:HG21 | 2.00 | 0.43 |
| 2:B:4956:ASP:OD1 | 2:B:4957:CYS:N | 2.50 | 0.43 |
| 2:C:677:LEU:HD12 | 2:C:801:ARG:O | 2.17 | 0.43 |
| 2:C:1273:ILE:HB | 2:C:1282:CYS:HB2 | 1.99 | 0.43 |
| 2:C:2443:PRO:HG3 | 2:C:2454:PRO:HD2 | 1.99 | 0.43 |
| 2:C:2504:THR:OG1 | 2:C:2507:LEU:HB2 | 2.18 | 0.43 |
| 2:C:3102:LEU:HB2 | 2:C:3103:PRO:HD3 | 2.00 | 0.43 |
| 2:C:3729:ALA:HA | 2:C:3732:HIS:ND1 | 2.32 | 0.43 |
| 2:C:4277:LYS:HD2 | 2:C:4277:LYS:HA | 1.73 | 0.43 |
| 2:C:4818:TYR:HA | 2:D:4848:ILE:HD11 | 1.99 | 0.43 |
| 2:D:1979:PHE:HZ | 2:D:1996:LEU:HB3 | 1.83 | 0.43 |
| 2:D:4022:LYS:NZ | 2:D:4057:HIS:O | 2.35 | 0.43 |
| 2:A:3246:MET:O | 2:A:3250:TRP:HB2 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:3260:ARG:HH11 | 2:A:3264:CYS:HA | 1.79 | 0.43 |
| 2:A:3695:MET:HB3 | 2:A:3731:LEU:HD11 | 2.00 | 0.43 |
| 2:A:4270:LYS:HE3 | 2:A:4270:LYS:HB3 | 1.83 | 0.43 |
| 2:B:1963:LYS:HB2 | 2:B:1963:LYS:HE2 | 1.77 | 0.43 |
| 2:B:1979:PHE:HZ | 2:B:1996:LEU:HB3 | 1.83 | 0.43 |
| 2:C:1473:LYS:NZ | 2:C:1475:LYS:HB2 | 2.33 | 0.43 |
| 2:C:4060:GLN:O | 2:C:4064:GLU:OE1 | 2.36 | 0.43 |
| 2:D:555:LEU:HD12 | 2:D:588:ILE:HD11 | 2.00 | 0.43 |
| 2:D:880:ARG:HH11 | 2:D:881:ILE:HB | 1.81 | 0.43 |
| 2:D:3001:LYS:HD2 | 2:D:3041:ASP:OD2 | 2.18 | 0.43 |
| 2:D:3043:ARG:HG3 | 2:D:3047:LYS:HZ2 | 1.83 | 0.43 |
| 2:D:3069:GLU:HG3 | 2:D:3132:ARG:HH11 | 1.83 | 0.43 |
| 2:D:3166:PHE:CD1 | 2:D:3167:PRO:HD2 | 2.53 | 0.43 |
| 2:D:4060:GLN:O | 2:D:4064:GLU:OE1 | 2.36 | 0.43 |
| 2:B:1042:THR:HG23 | 5:B:5004:KVR:C15 | 2.49 | 0.43 |
| 2:B:2504:THR:OG1 | 2:B:2507:LEU:HB2 | 2.19 | 0.43 |
| 2:B:2586:GLN:HE22 | 2:B:2590:ARG:NH2 | 2.15 | 0.43 |
| 2:C:1091:GLU:HB3 | 2:C:1094:TYR:HD2 | 1.84 | 0.43 |
| 2:C:2511:ASP:HA | 2:C:2514:LEU:HD12 | 2.01 | 0.43 |
| 2:D:28:ILE:HG22 | 2:D:29:HIS:CD2 | 2.53 | 0.43 |
| 2:D:291:TRP:O | 2:D:343:ARG:NH1 | 2.52 | 0.43 |
| 2:D:886:ALA:HB1 | 2:D:929:ARG:HH12 | 1.81 | 0.43 |
| 2:D:1018:TYR:CD1 | 2:D:1030:PRO:HA | 2.52 | 0.43 |
| 2:D:1716:THR:O | 2:D:1720:MET:HG3 | 2.18 | 0.43 |
| 2:D:1968:PRO:O | 2:D:1972:GLN:HG3 | 2.19 | 0.43 |
| 2:D:1991:GLU:HG2 | 2:D:1992:ILE:N | 2.32 | 0.43 |
| 2:D:2581:ARG:HB3 | 2:D:2584:MET:HE2 | 2.00 | 0.43 |
| 2:D:4267:GLN:O | 2:D:4271:VAL:HG23 | 2.19 | 0.43 |
| 2:D:4956:ASP:OD1 | 2:D:4957:CYS:N | 2.50 | 0.43 |
| 2:A:1716:THR:O | 2:A:1720:MET:HG3 | 2.18 | 0.43 |
| 2:A:2423:LEU:HD23 | 2:A:2426:LEU:HD12 | 2.01 | 0.43 |
| 2:A:2429:LEU:HD21 | 2:A:2483:PHE:CE1 | 2.54 | 0.43 |
| 2:A:2782:MET:HG2 | 2:A:2787:TRP:CE3 | 2.54 | 0.43 |
| 2:A:4136:ILE:HG22 | 2:A:4917:ASN:HB3 | 2.01 | 0.43 |
| 2:A:4848:ILE:HD11 | 2:D:4818:TYR:HD1 | 1.83 | 0.43 |
| 2:B:34:LYS:H | 2:B:53:SER:HB3 | 1.82 | 0.43 |
| 2:B:257:ARG:NH2 | 2:B:272:ARG:HG3 | 2.33 | 0.43 |
| 2:B:674:TYR:HE1 | 2:B:756:SER:HB2 | 1.83 | 0.43 |
| 2:B:2511:ASP:HA | 2:B:2514:LEU:HD12 | 2.00 | 0.43 |
| 2:B:2666:LEU:HD13 | 2:B:2966:VAL:HA | 2.00 | 0.43 |
| 2:B:3069:GLU:HG3 | 2:B:3132:ARG:HH11 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:3207:ASN:OD1 | 2:B:3208:ILE:N | 2.50 | 0.43 |
| 2:B:4924:TYR:CZ | 2:B:4928:LYS:HD2 | 2.53 | 0.43 |
| 2:C:987:LYS:HZ3 | 2:C:989:THR:HA | 1.84 | 0.43 |
| 2:C:2429:LEU:HD21 | 2:C:2483:PHE:CE1 | 2.54 | 0.43 |
| 2:C:3166:PHE:CD1 | 2:C:3167:PRO:HD2 | 2.53 | 0.43 |
| 2:C:3691:TYR:O | 2:C:3695:MET:HG3 | 2.18 | 0.43 |
| 2:D:849:ASP:OD1 | 2:D:1214:ARG:NE | 2.51 | 0.43 |
| 2:D:987:LYS:HZ3 | 2:D:989:THR:HA | 1.84 | 0.43 |
| 2:D:1042:THR:HG23 | 5:D:5004:KVR:C15 | 2.49 | 0.43 |
| 2:D:2146:LEU:O | 2:D:2150:MET:HG2 | 2.18 | 0.43 |
| 2:D:3235:MET:O | 2:D:3299:LEU:HD21 | 2.19 | 0.43 |
| 2:D:3650:GLU:HB2 | 2:D:3651:PRO:HD3 | 2.01 | 0.43 |
| 2:D:3695:MET:HB3 | 2:D:3731:LEU:HD11 | 2.00 | 0.43 |
| 1:F:67:MET:SD | 1:F:73:ALA:HB3 | 2.58 | 0.43 |
| 2:A:34:LYS:H | 2:A:53:SER:HB3 | 1.82 | 0.43 |
| 2:A:538:ALA:O | 2:A:542:ARG:HB2 | 2.19 | 0.43 |
| 2:A:902:TRP:HZ2 | 2:A:915:HIS:ND1 | 2.17 | 0.43 |
| 2:A:3217:GLU:O | 2:A:3220:GLU:HG3 | 2.19 | 0.43 |
| 2:A:3288:LEU:HA | 2:A:3292:GLU:OE1 | 2.19 | 0.43 |
| 2:B:456:LEU:HD23 | 2:B:456:LEU:HA | 1.84 | 0.43 |
| 2:B:902:TRP:HZ2 | 2:B:915:HIS:ND1 | 2.17 | 0.43 |
| 2:B:1689:ILE:HD13 | 2:B:1703:TYR:CD1 | 2.54 | 0.43 |
| 2:B:1898:LEU:HD13 | 2:B:1902:VAL:HG12 | 1.99 | 0.43 |
| 2:B:1945:ASN:O | 2:B:1949:GLN:NE2 | 2.42 | 0.43 |
| 2:B:2790:GLU:O | 2:B:2901:TYR:HA | 2.19 | 0.43 |
| 2:B:3217:GLU:O | 2:B:3220:GLU:HG3 | 2.19 | 0.43 |
| 2:C:694:ARG:HD3 | 2:C:733:TRP:HB2 | 2.01 | 0.43 |
| 2:C:1716:THR:O | 2:C:1720:MET:HG3 | 2.18 | 0.43 |
| 2:C:1929:SER:O | 2:C:1933:VAL:HG12 | 2.18 | 0.43 |
| 2:C:2322:ARG:NH1 | 2:D:189:GLU:OE2 | 2.52 | 0.43 |
| 2:C:2423:LEU:HD23 | 2:C:2426:LEU:HD12 | 2.01 | 0.43 |
| 2:C:2782:MET:HG2 | 2:C:2787:TRP:CE3 | 2.54 | 0.43 |
| 2:D:34:LYS:H | 2:D:53:SER:HB3 | 1.82 | 0.43 |
| 2:D:1839:LEU:HA | 2:D:1842:ILE:HG12 | 1.99 | 0.43 |
| 2:D:2191:LYS:O | 2:D:2195:ASN:ND2 | 2.50 | 0.43 |
| 2:D:2688:MET:HB3 | 2:D:2689:MET:HE1 | 2.00 | 0.43 |
| 2:D:2926:LEU:C | 2:D:3003:MET:HE1 | 2.39 | 0.43 |
| 2:D:4806:CYS:HA | 2:D:4812:CYS:HB2 | 2.00 | 0.43 |
| 2:A:1043:LYS:HE2 | 2:A:1043:LYS:HB2 | 1.55 | 0.43 |
| 2:A:2443:PRO:HD2 | 2:A:2512:MET:HE2 | 1.99 | 0.43 |
| 2:A:2504:THR:OG1 | 2:A:2507:LEU:HB2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:3001:LYS:HD2 | 2:A:3041:ASP:OD2 | 2.18 | 0.43 |
| 2:A:3235:MET:O | 2:A:3299:LEU:HD21 | 2.19 | 0.43 |
| 2:A:3691:TYR:O | 2:A:3695:MET:HG3 | 2.18 | 0.43 |
| 2:A:3952:ALA:HB1 | 2:A:4012:MET:HE3 | 2.01 | 0.43 |
| 2:A:4615:LEU:HA | 2:A:4619:GLU:OE2 | 2.19 | 0.43 |
| 2:B:1043:LYS:HB2 | 2:B:1043:LYS:HE2 | 1.54 | 0.43 |
| 2:B:2179:LEU:HD13 | 2:B:2224:ASN:HD22 | 1.83 | 0.43 |
| 2:B:2194:ALA:HA | 2:B:2237:SER:HB3 | 2.00 | 0.43 |
| 2:B:2423:LEU:HD23 | 2:B:2426:LEU:HD12 | 2.01 | 0.43 |
| 2:B:2782:MET:HG2 | 2:B:2787:TRP:CE3 | 2.54 | 0.43 |
| 2:B:3679:LYS:HE2 | 2:B:3679:LYS:HB2 | 1.88 | 0.43 |
| 2:B:3942:ASP:HA | 2:B:3945:VAL:HG12 | 2.01 | 0.43 |
| 2:C:893:TRP:NE1 | 2:C:1049:SER:HB3 | 2.34 | 0.43 |
| 2:C:1042:THR:HG23 | 5:C:5004:KVR:C15 | 2.49 | 0.43 |
| 2:C:1044:LYS:HD3 | 2:C:1044:LYS:HA | 1.77 | 0.43 |
| 2:C:1628:MET:HB3 | 2:C:1628:MET:HE2 | 1.72 | 0.43 |
| 2:C:1968:PRO:O | 2:C:1972:GLN:HG3 | 2.19 | 0.43 |
| 2:C:2790:GLU:O | 2:C:2901:TYR:HA | 2.19 | 0.43 |
| 2:C:2894:LYS:HE2 | 2:C:2894:LYS:HB2 | 1.81 | 0.43 |
| 2:C:3712:LYS:HB3 | 2:C:3716:GLU:HG3 | 2.01 | 0.43 |
| 2:C:3997:LYS:HD3 | 2:C:4109:MET:HE1 | 2.00 | 0.43 |
| 2:C:4924:TYR:CZ | 2:C:4928:LYS:HD2 | 2.53 | 0.43 |
| 2:D:672:LYS:HB3 | 2:D:819:TYR:HA | 2.01 | 0.43 |
| 2:D:2303:ARG:HH11 | 2:D:2304:PHE:HA | 1.82 | 0.43 |
| 2:D:2397:ASP:O | 2:D:2401:ARG:HG3 | 2.19 | 0.43 |
| 2:D:2429:LEU:HD21 | 2:D:2483:PHE:CE1 | 2.54 | 0.43 |
| 2:D:2434:GLY:O | 2:D:2438:ILE:HG13 | 2.18 | 0.43 |
| 2:D:2666:LEU:HD13 | 2:D:2966:VAL:HA | 2.00 | 0.43 |
| 2:D:2782:MET:HG2 | 2:D:2787:TRP:CE3 | 2.54 | 0.43 |
| 2:A:36:CYS:SG | 2:A:65:CYS:HB3 | 2.58 | 0.43 |
| 2:A:291:TRP:O | 2:A:343:ARG:NH1 | 2.52 | 0.43 |
| 2:A:306:LEU:HA | 2:A:316:LEU:HD23 | 2.01 | 0.43 |
| 2:A:980:PRO:HB2 | 2:A:981:MET:SD | 2.59 | 0.43 |
| 2:A:2413:LYS:NZ | 2:A:2415:GLU:OE1 | 2.52 | 0.43 |
| 2:A:2666:LEU:HD13 | 2:A:2966:VAL:HA | 2.00 | 0.43 |
| 2:A:3198:PRO:O | 2:A:3199:THR:OG1 | 2.35 | 0.43 |
| 2:A:3650:GLU:HB2 | 2:A:3651:PRO:HD3 | 2.01 | 0.43 |
| 2:A:4084:VAL:O | 2:A:4088:HIS:HB3 | 2.17 | 0.43 |
| 2:A:4631:ASP:O | 2:A:4634:VAL:HG12 | 2.19 | 0.43 |
| 2:B:291:TRP:O | 2:B:343:ARG:NH1 | 2.52 | 0.43 |
| 2:B:2334:ALA:HB2 | 2:B:2346:ALA:HB2 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:3288:LEU:HA | 2:B:3292:GLU:OE1 | 2.19 | 0.43 |
| 2:B:3691:TYR:O | 2:B:3695:MET:HG3 | 2.18 | 0.43 |
| 2:B:4615:LEU:HA | 2:B:4619:GLU:OE2 | 2.19 | 0.43 |
| 2:C:363:ILE:HD13 | 2:C:372:LEU:HD23 | 2.01 | 0.43 |
| 2:C:1007:TRP:CZ2 | 2:C:1011:ARG:HD3 | 2.53 | 0.43 |
| 2:C:1014:GLN:HB3 | 2:C:1027:ARG:NH2 | 2.31 | 0.43 |
| 2:C:2146:LEU:O | 2:C:2150:MET:HG2 | 2.18 | 0.43 |
| 2:C:2182:GLY:HA2 | 2:C:2185:LYS:HE2 | 2.00 | 0.43 |
| 2:C:4021:LEU:HD22 | 2:C:4128:TYR:CE2 | 2.54 | 0.43 |
| 2:C:4136:ILE:HG22 | 2:C:4917:ASN:HB3 | 2.01 | 0.43 |
| 2:C:4615:LEU:HA | 2:C:4619:GLU:OE2 | 2.19 | 0.43 |
| 2:D:306:LEU:HA | 2:D:316:LEU:HD23 | 2.01 | 0.43 |
| 2:D:902:TRP:HZ2 | 2:D:915:HIS:ND1 | 2.17 | 0.43 |
| 2:D:954:ASP:OD2 | 2:D:957:ALA:N | 2.51 | 0.43 |
| 2:D:1014:GLN:HB3 | 2:D:1027:ARG:NH2 | 2.31 | 0.43 |
| 2:D:1689:ILE:HD13 | 2:D:1703:TYR:CD1 | 2.54 | 0.43 |
| 2:D:3016:ARG:HA | 2:D:3096:TYR:CZ | 2.53 | 0.43 |
| 2:D:3288:LEU:HA | 2:D:3292:GLU:OE1 | 2.19 | 0.43 |
| 1:E:67:MET:SD | 1:E:73:ALA:HB3 | 2.58 | 0.43 |
| 2:A:141:ASP:HA | 2:D:2337:GLY:O | 2.19 | 0.43 |
| 2:A:718:VAL:HG23 | 2:A:793:SER:HB3 | 2.01 | 0.43 |
| 2:A:1991:GLU:HG2 | 2:A:1992:ILE:N | 2.32 | 0.43 |
| 2:A:2790:GLU:O | 2:A:2901:TYR:HA | 2.19 | 0.43 |
| 2:A:2894:LYS:HE2 | 2:A:2894:LYS:HB2 | 1.81 | 0.43 |
| 2:A:4021:LEU:HD22 | 2:A:4128:TYR:CE2 | 2.54 | 0.43 |
| 2:A:4052:MET:HE1 | 2:A:4063:THR:HA | 2.01 | 0.43 |
| 2:A:4060:GLN:O | 2:A:4064:GLU:OE1 | 2.36 | 0.43 |
| 2:B:718:VAL:HG23 | 2:B:793:SER:HB3 | 2.01 | 0.43 |
| 2:B:811:PHE:CE2 | 2:B:821:PRO:HB3 | 2.54 | 0.43 |
| 2:B:1091:GLU:HB3 | 2:B:1094:TYR:HD2 | 1.84 | 0.43 |
| 2:B:1931:ASP:OD1 | 2:B:1932:PHE:N | 2.51 | 0.43 |
| 2:B:2182:GLY:HA2 | 2:B:2185:LYS:HE2 | 2.00 | 0.43 |
| 2:B:2727:HIS:O | 2:B:2731:LYS:HG3 | 2.19 | 0.43 |
| 2:B:4021:LEU:HD22 | 2:B:4128:TYR:CE2 | 2.54 | 0.43 |
| 2:C:2303:ARG:HH11 | 2:C:2304:PHE:HA | 1.82 | 0.43 |
| 2:C:2397:ASP:O | 2:C:2401:ARG:HG3 | 2.19 | 0.43 |
| 2:C:3207:ASN:OD1 | 2:C:3208:ILE:N | 2.50 | 0.43 |
| 2:C:4070:ALA:HB1 | 2:C:4078:LEU:CD1 | 2.49 | 0.43 |
| 2:D:811:PHE:CE2 | 2:D:821:PRO:HB3 | 2.54 | 0.43 |
| 2:D:893:TRP:NE1 | 2:D:1049:SER:HB3 | 2.34 | 0.43 |
| 2:D:2894:LYS:HE2 | 2:D:2894:LYS:HB2 | 1.81 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:3254:PRO:HD2 | 2:D:3268:LEU:O | 2.19 | 0.43 |
| 2:D:4070:ALA:HB1 | 2:D:4078:LEU:CD1 | 2.49 | 0.43 |
| 1:E:19:LYS:HD3 | 1:E:19:LYS:HA | 1.81 | 0.43 |
| 2:A:551:PHE:HE2 | 2:A:558:LEU:HD22 | 1.84 | 0.43 |
| 2:A:811:PHE:CE2 | 2:A:821:PRO:HB3 | 2.54 | 0.43 |
| 2:A:1689:ILE:HD13 | 2:A:1703:TYR:CD1 | 2.54 | 0.43 |
| 2:A:1968:PRO:O | 2:A:1972:GLN:HG3 | 2.19 | 0.43 |
| 2:A:2658:GLU:OE1 | 2:A:2661:LEU:N | 2.34 | 0.43 |
| 2:A:4735:ASN:HB3 | 2:A:4738:PHE:HD2 | 1.84 | 0.43 |
| 2:B:694:ARG:HD3 | 2:B:733:TRP:HB2 | 2.01 | 0.43 |
| 2:B:893:TRP:NE1 | 2:B:1049:SER:HB3 | 2.34 | 0.43 |
| 2:B:1716:THR:O | 2:B:1720:MET:HG3 | 2.18 | 0.43 |
| 2:B:1968:PRO:O | 2:B:1972:GLN:HG3 | 2.19 | 0.43 |
| 2:B:4058:TYR:HD1 | 2:B:4062:GLU:HB3 | 1.84 | 0.43 |
| 2:C:28:ILE:HG22 | 2:C:29:HIS:CD2 | 2.53 | 0.43 |
| 2:C:902:TRP:HZ2 | 2:C:915:HIS:ND1 | 2.17 | 0.43 |
| 2:C:2179:LEU:HD13 | 2:C:2224:ASN:HD22 | 1.83 | 0.43 |
| 2:C:2334:ALA:HB2 | 2:C:2346:ALA:HB2 | 2.01 | 0.43 |
| 2:C:3001:LYS:HD2 | 2:C:3041:ASP:OD2 | 2.18 | 0.43 |
| 2:C:3288:LEU:HA | 2:C:3292:GLU:OE1 | 2.19 | 0.43 |
| 2:C:4735:ASN:HB3 | 2:C:4738:PHE:HD2 | 1.84 | 0.43 |
| 2:D:133:LEU:HD23 | 2:D:133:LEU:HA | 1.88 | 0.43 |
| 2:D:694:ARG:HD3 | 2:D:733:TRP:HB2 | 2.01 | 0.43 |
| 2:D:980:PRO:HB2 | 2:D:981:MET:SD | 2.59 | 0.43 |
| 2:D:1031:ARG:CZ | 2:D:1031:ARG:HB3 | 2.44 | 0.43 |
| 2:D:1429:SER:OG | 2:D:1556:GLU:HB2 | 2.19 | 0.43 |
| 2:D:2182:GLY:HA2 | 2:D:2185:LYS:HE2 | 2.00 | 0.43 |
| 2:D:2843:MET:O | 2:D:2846:GLU:HG2 | 2.19 | 0.43 |
| 2:D:3712:LYS:HB3 | 2:D:3716:GLU:HG3 | 2.01 | 0.43 |
| 2:D:4615:LEU:HA | 2:D:4619:GLU:OE2 | 2.19 | 0.43 |
| 2:D:4687:LYS:HD3 | 2:D:4687:LYS:HA | 1.88 | 0.43 |
| 2:A:143:LEU:HD13 | 2:A:207:PHE:CE2 | 2.54 | 0.42 |
| 2:A:874:LEU:HD12 | 2:A:875:PRO:HD2 | 2.01 | 0.42 |
| 2:A:986:ILE:HG22 | 2:A:1055:ARG:HD2 | 2.01 | 0.42 |
| 2:A:1757:LEU:HD23 | 2:A:1757:LEU:HA | 1.86 | 0.42 |
| 2:A:1986:CYS:HA | 2:A:1987:PRO:HD3 | 1.91 | 0.42 |
| 2:A:3214:LEU:HD23 | 2:A:3214:LEU:HA | 1.90 | 0.42 |
| 2:B:2134:MET:HE3 | 2:B:2134:MET:HA | 2.00 | 0.42 |
| 2:B:3016:ARG:HA | 2:B:3096:TYR:CZ | 2.53 | 0.42 |
| 2:C:794:PHE:HB2 | 2:C:798:ILE:HG21 | 2.01 | 0.42 |
| 2:C:811:PHE:HE2 | 2:C:821:PRO:HB3 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:1429:SER:OG | 2:C:1556:GLU:HB2 | 2.19 | 0.42 |
| 2:C:2581:ARG:HB3 | 2:C:2584:MET:HE2 | 2.01 | 0.42 |
| 2:C:3016:ARG:HA | 2:C:3096:TYR:CZ | 2.53 | 0.42 |
| 2:C:3942:ASP:HA | 2:C:3945:VAL:HG12 | 2.01 | 0.42 |
| 2:C:3958:LEU:HB2 | 2:C:3968:LEU:HD13 | 2.01 | 0.42 |
| 2:C:4631:ASP:O | 2:C:4634:VAL:HG12 | 2.19 | 0.42 |
| 2:D:2504:THR:OG1 | 2:D:2507:LEU:HB2 | 2.19 | 0.42 |
| 2:D:3217:GLU:O | 2:D:3220:GLU:HG3 | 2.19 | 0.42 |
| 2:A:986:ILE:CG2 | 2:A:1055:ARG:HD2 | 2.50 | 0.42 |
| 2:A:3261:ALA:C | 2:A:3263:MET:N | 2.71 | 0.42 |
| 2:A:3650:GLU:OE1 | 2:A:3659:LYS:NZ | 2.49 | 0.42 |
| 2:A:4070:ALA:HB1 | 2:A:4078:LEU:CD1 | 2.49 | 0.42 |
| 2:B:143:LEU:HD13 | 2:B:207:PHE:CE2 | 2.54 | 0.42 |
| 2:B:672:LYS:HB3 | 2:B:819:TYR:HA | 2.01 | 0.42 |
| 2:B:2146:LEU:O | 2:B:2150:MET:HG2 | 2.18 | 0.42 |
| 2:B:2798:MET:SD | 2:C:1498:GLN:HG3 | 2.59 | 0.42 |
| 2:B:3124:GLU:C | 2:B:3126:VAL:H | 2.23 | 0.42 |
| 2:C:986:ILE:HG22 | 2:C:1055:ARG:HD2 | 2.01 | 0.42 |
| 2:C:1689:ILE:HD13 | 2:C:1703:TYR:CD1 | 2.54 | 0.42 |
| 2:C:3043:ARG:HH21 | 2:C:3117:PHE:HD1 | 1.65 | 0.42 |
| 2:C:3069:GLU:HG3 | 2:C:3132:ARG:HH11 | 1.83 | 0.42 |
| 2:C:3650:GLU:HB2 | 2:C:3651:PRO:HD3 | 2.01 | 0.42 |
| 2:D:986:ILE:HG22 | 2:D:1055:ARG:HD2 | 2.01 | 0.42 |
| 2:D:1608:VAL:HG12 | 2:D:1619:VAL:HA | 2.01 | 0.42 |
| 2:D:1678:SER:HB2 | 2:D:1768:PHE:CZ | 2.55 | 0.42 |
| 2:D:2423:LEU:HD23 | 2:D:2426:LEU:HD12 | 2.01 | 0.42 |
| 2:D:3043:ARG:HH21 | 2:D:3117:PHE:HD1 | 1.66 | 0.42 |
| 2:A:257:ARG:NH2 | 2:A:272:ARG:HG3 | 2.33 | 0.42 |
| 2:A:505:LEU:HB3 | 2:A:530:LEU:HD21 | 2.01 | 0.42 |
| 2:A:674:TYR:HE1 | 2:A:756:SER:HB2 | 1.83 | 0.42 |
| 2:A:935:MET:HE3 | 2:A:935:MET:HB3 | 1.80 | 0.42 |
| 2:A:988:LEU:HB2 | 2:A:1055:ARG:NE | 2.26 | 0.42 |
| 2:A:1678:SER:HB2 | 2:A:1768:PHE:CZ | 2.55 | 0.42 |
| 2:A:2397:ASP:O | 2:A:2401:ARG:HG3 | 2.19 | 0.42 |
| 2:A:2827:ASP:OD1 | 2:B:1434:PRO:HB2 | 2.19 | 0.42 |
| 2:A:2885:ASP:O | 2:A:2888:LYS:HG2 | 2.19 | 0.42 |
| 2:A:3254:PRO:HD2 | 2:A:3268:LEU:O | 2.19 | 0.42 |
| 2:A:3958:LEU:HB2 | 2:A:3968:LEU:HD13 | 2.02 | 0.42 |
| 2:B:538:ALA:O | 2:B:542:ARG:HB2 | 2.19 | 0.42 |
| 2:B:794:PHE:HB2 | 2:B:798:ILE:HG21 | 2.02 | 0.42 |
| 2:B:962:LYS:HZ2 | 2:B:982:ASP:H | 1.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:980:PRO:HB2 | 2:B:981:MET:SD | 2.59 | 0.42 |
| 2:B:1026:ASN:HB3 | 2:B:1028:ARG:HG2 | 2.02 | 0.42 |
| 2:B:1429:SER:OG | 2:B:1556:GLU:HB2 | 2.19 | 0.42 |
| 2:B:2413:LYS:NZ | 2:B:2415:GLU:OE1 | 2.52 | 0.42 |
| 2:B:2429:LEU:HD21 | 2:B:2483:PHE:CE1 | 2.54 | 0.42 |
| 2:B:2681:MET:HE1 | 2:B:2917:ILE:HA | 2.02 | 0.42 |
| 2:B:2843:MET:O | 2:B:2846:GLU:HG2 | 2.19 | 0.42 |
| 2:B:2844:MET:O | 2:B:2848:TYR:HD2 | 2.02 | 0.42 |
| 2:B:3001:LYS:HD2 | 2:B:3041:ASP:OD2 | 2.18 | 0.42 |
| 2:C:521:GLU:HG2 | 2:C:522:ALA:N | 2.34 | 0.42 |
| 2:C:980:PRO:HB2 | 2:C:981:MET:SD | 2.59 | 0.42 |
| 2:C:1608:VAL:HG12 | 2:C:1619:VAL:HA | 2.01 | 0.42 |
| 2:C:2413:LYS:NZ | 2:C:2415:GLU:OE1 | 2.52 | 0.42 |
| 2:C:2926:LEU:C | 2:C:3003:MET:HE1 | 2.40 | 0.42 |
| 2:C:3217:GLU:O | 2:C:3220:GLU:HG3 | 2.19 | 0.42 |
| 2:C:4267:GLN:O | 2:C:4271:VAL:HG23 | 2.19 | 0.42 |
| 2:D:1091:GLU:HB3 | 2:D:1094:TYR:HD2 | 1.84 | 0.42 |
| 2:D:1929:SER:O | 2:D:1933:VAL:HG12 | 2.18 | 0.42 |
| 2:D:2413:LYS:NZ | 2:D:2415:GLU:OE1 | 2.52 | 0.42 |
| 2:D:2727:HIS:O | 2:D:2731:LYS:HG3 | 2.19 | 0.42 |
| 2:D:3102:LEU:HB2 | 2:D:3103:PRO:HD3 | 2.00 | 0.42 |
| 2:D:3650:GLU:OE1 | 2:D:3659:LYS:NZ | 2.49 | 0.42 |
| 2:A:1608:VAL:HG12 | 2:A:1619:VAL:HA | 2.01 | 0.42 |
| 2:A:1748:LEU:HD23 | 2:A:1748:LEU:HA | 1.83 | 0.42 |
| 2:A:2137:GLU:HG2 | 2:A:2138:GLU:N | 2.35 | 0.42 |
| 2:A:2146:LEU:O | 2:A:2150:MET:HG2 | 2.18 | 0.42 |
| 2:A:2187:ILE:HG13 | 2:A:2227:VAL:HG13 | 2.01 | 0.42 |
| 2:B:306:LEU:HA | 2:B:316:LEU:HD23 | 2.01 | 0.42 |
| 2:B:363:ILE:HD13 | 2:B:372:LEU:HD23 | 2.01 | 0.42 |
| 2:B:811:PHE:HE2 | 2:B:821:PRO:HB3 | 1.84 | 0.42 |
| 2:B:1608:VAL:HG12 | 2:B:1619:VAL:HA | 2.01 | 0.42 |
| 2:B:1678:SER:HB2 | 2:B:1768:PHE:CZ | 2.55 | 0.42 |
| 2:B:3712:LYS:HB3 | 2:B:3716:GLU:HG3 | 2.01 | 0.42 |
| 2:B:4070:ALA:HB1 | 2:B:4078:LEU:CD1 | 2.49 | 0.42 |
| 2:C:133:LEU:HD23 | 2:C:133:LEU:HA | 1.88 | 0.42 |
| 2:C:811:PHE:CE2 | 2:C:821:PRO:HB3 | 2.54 | 0.42 |
| 2:C:1026:ASN:HB3 | 2:C:1028:ARG:HG2 | 2.02 | 0.42 |
| 2:C:1943:ARG:O | 2:C:1947:VAL:HG23 | 2.20 | 0.42 |
| 2:C:2392:TYR:O | 2:C:2396:ILE:HD12 | 2.18 | 0.42 |
| 2:C:2905:ARG:NH1 | 2:C:2906:GLY:H | 2.15 | 0.42 |
| 2:D:538:ALA:O | 2:D:542:ARG:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:2511:ASP:HA | 2:D:2514:LEU:HD12 | 2.01 | 0.42 |
| 2:D:2885:ASP:O | 2:D:2888:LYS:HG2 | 2.19 | 0.42 |
| 2:D:2937:HIS:HA | 2:D:3014:LEU:HD13 | 2.01 | 0.42 |
| 2:D:3213:LYS:O | 2:D:3216:GLU:HG3 | 2.20 | 0.42 |
| 2:D:3958:LEU:HB2 | 2:D:3968:LEU:HD13 | 2.01 | 0.42 |
| 2:D:4021:LEU:HD22 | 2:D:4128:TYR:CE2 | 2.54 | 0.42 |
| 2:D:4631:ASP:O | 2:D:4634:VAL:HG12 | 2.19 | 0.42 |
| 2:A:363:ILE:HD13 | 2:A:372:LEU:HD23 | 2.01 | 0.42 |
| 2:A:1011:ARG:HA | 2:A:1014:GLN:CD | 2.40 | 0.42 |
| 2:A:1042:THR:HG23 | 5:A:5004:KVR:C15 | 2.49 | 0.42 |
| 2:A:2182:GLY:HA2 | 2:A:2185:LYS:HE2 | 2.00 | 0.42 |
| 2:A:2844:MET:O | 2:A:2848:TYR:HD2 | 2.02 | 0.42 |
| 2:A:2910:LEU:HD12 | 2:A:2911:GLU:N | 2.35 | 0.42 |
| 2:A:3069:GLU:HG3 | 2:A:3132:ARG:HH11 | 1.83 | 0.42 |
| 2:A:3712:LYS:HB3 | 2:A:3716:GLU:HG3 | 2.01 | 0.42 |
| 2:B:874:LEU:HD12 | 2:B:875:PRO:HD2 | 2.01 | 0.42 |
| 2:B:2397:ASP:O | 2:B:2401:ARG:HG3 | 2.19 | 0.42 |
| 2:C:291:TRP:O | 2:C:343:ARG:NH1 | 2.52 | 0.42 |
| 2:C:2760:TYR:CE1 | 2:C:2768:LYS:HG2 | 2.55 | 0.42 |
| 2:D:961:VAL:HG13 | 2:D:961:VAL:O | 2.19 | 0.42 |
| 2:D:986:ILE:CG2 | 2:D:1055:ARG:HD2 | 2.50 | 0.42 |
| 2:D:1013:ARG:NE | 2:D:1013:ARG:HA | 2.35 | 0.42 |
| 2:D:1963:LYS:HB2 | 2:D:1963:LYS:HE2 | 1.77 | 0.42 |
| 2:D:2721:ILE:HD11 | 2:D:2779:LEU:HD22 | 2.02 | 0.42 |
| 2:D:2760:TYR:CE1 | 2:D:2768:LYS:HG2 | 2.55 | 0.42 |
| 2:D:2831:VAL:HB | 2:D:2894:LYS:CD | 2.46 | 0.42 |
| 2:D:3018:ARG:HA | 2:D:3021:LEU:HD13 | 2.01 | 0.42 |
| 2:D:3296:MET:HA | 2:D:3299:LEU:HD12 | 2.01 | 0.42 |
| 2:D:3942:ASP:HA | 2:D:3945:VAL:HG12 | 2.01 | 0.42 |
| 2:D:4803:ASP:OD2 | 2:D:4805:LYS:HE2 | 2.20 | 0.42 |
| 2:A:811:PHE:HE2 | 2:A:821:PRO:HB3 | 1.84 | 0.42 |
| 2:A:1013:ARG:NE | 2:A:1013:ARG:HA | 2.35 | 0.42 |
| 2:A:1979:PHE:HZ | 2:A:1996:LEU:HB3 | 1.83 | 0.42 |
| 2:A:2843:MET:O | 2:A:2846:GLU:HG2 | 2.19 | 0.42 |
| 2:A:3942:ASP:HA | 2:A:3945:VAL:HG12 | 2.01 | 0.42 |
| 2:A:4105:LEU:HB3 | 2:A:4115:LEU:HD21 | 2.02 | 0.42 |
| 2:A:4267:GLN:O | 2:A:4271:VAL:HG23 | 2.18 | 0.42 |
| 2:A:4649:VAL:O | 2:A:4653:VAL:HG23 | 2.20 | 0.42 |
| 2:B:551:PHE:HE2 | 2:B:558:LEU:HD22 | 1.84 | 0.42 |
| 2:B:1932:PHE:CE1 | 2:B:1996:LEU:HB2 | 2.54 | 0.42 |
| 2:B:1943:ARG:O | 2:B:1947:VAL:HG23 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2187:ILE:HG13 | 2:B:2227:VAL:HG13 | 2.01 | 0.42 |
| 2:B:2914:THR:N | 2:B:2915:PRO:HD2 | 2.35 | 0.42 |
| 2:B:2937:HIS:HA | 2:B:3014:LEU:HD13 | 2.01 | 0.42 |
| 2:B:3018:ARG:HA | 2:B:3021:LEU:HD13 | 2.01 | 0.42 |
| 2:B:3650:GLU:HB2 | 2:B:3651:PRO:HD3 | 2.01 | 0.42 |
| 2:B:4631:ASP:O | 2:B:4634:VAL:HG12 | 2.19 | 0.42 |
| 2:B:4822:ARG:HH12 | 2:C:4829:ASP:N | 2.17 | 0.42 |
| 2:C:1932:PHE:CE1 | 2:C:1996:LEU:HB2 | 2.54 | 0.42 |
| 2:C:2910:LEU:HD12 | 2:C:2911:GLU:N | 2.35 | 0.42 |
| 2:C:3235:MET:O | 2:C:3299:LEU:HD21 | 2.19 | 0.42 |
| 2:D:811:PHE:HE2 | 2:D:821:PRO:HB3 | 1.84 | 0.42 |
| 2:D:1031:ARG:HH21 | 2:D:1038:LEU:CD1 | 2.11 | 0.42 |
| 2:D:1053:ALA:O | 2:D:1057:LEU:HG | 2.20 | 0.42 |
| 2:D:4049:HIS:HB2 | 2:D:4067:LEU:HD21 | 2.02 | 0.42 |
| 1:F:53:LYS:HE3 | 1:F:53:LYS:HB3 | 1.88 | 0.42 |
| 2:A:694:ARG:HD3 | 2:A:733:TRP:HB2 | 2.01 | 0.42 |
| 2:A:1932:PHE:CE1 | 2:A:1996:LEU:HB2 | 2.54 | 0.42 |
| 2:A:2334:ALA:HB2 | 2:A:2346:ALA:HB2 | 2.01 | 0.42 |
| 2:A:2727:HIS:O | 2:A:2731:LYS:HG3 | 2.19 | 0.42 |
| 2:A:3124:GLU:C | 2:A:3126:VAL:H | 2.23 | 0.42 |
| 2:B:133:LEU:HD23 | 2:B:133:LEU:HA | 1.88 | 0.42 |
| 2:B:521:GLU:HG2 | 2:B:522:ALA:N | 2.34 | 0.42 |
| 2:B:986:ILE:HG22 | 2:B:1055:ARG:HD2 | 2.02 | 0.42 |
| 2:B:3043:ARG:HG3 | 2:B:3047:LYS:HZ2 | 1.85 | 0.42 |
| 2:B:3254:PRO:HD2 | 2:B:3268:LEU:O | 2.19 | 0.42 |
| 2:B:3296:MET:HA | 2:B:3299:LEU:HD12 | 2.01 | 0.42 |
| 2:B:4136:ILE:HG22 | 2:B:4917:ASN:HB3 | 2.01 | 0.42 |
| 2:B:4267:GLN:O | 2:B:4271:VAL:HG23 | 2.19 | 0.42 |
| 2:B:4649:VAL:O | 2:B:4653:VAL:HG23 | 2.20 | 0.42 |
| 2:C:505:LEU:HD23 | 2:C:505:LEU:HA | 1.88 | 0.42 |
| 2:C:680:ASP:O | 2:C:751:THR:HG23 | 2.20 | 0.42 |
| 2:C:1678:SER:HB2 | 2:C:1768:PHE:CZ | 2.55 | 0.42 |
| 2:C:2095:ILE:HD12 | 2:C:2095:ILE:HA | 1.93 | 0.42 |
| 2:C:2399:LEU:HD12 | 2:C:2427:ILE:HD11 | 2.02 | 0.42 |
| 2:C:2885:ASP:O | 2:C:2888:LYS:HG2 | 2.19 | 0.42 |
| 2:C:2914:THR:N | 2:C:2915:PRO:HD2 | 2.35 | 0.42 |
| 2:C:3213:LYS:O | 2:C:3216:GLU:HG3 | 2.20 | 0.42 |
| 2:C:4649:VAL:O | 2:C:4653:VAL:HG23 | 2.20 | 0.42 |
| 2:C:4803:ASP:OD2 | 2:C:4805:LYS:HE2 | 2.20 | 0.42 |
| 2:C:4806:CYS:HA | 2:C:4812:CYS:HB2 | 2.00 | 0.42 |
| 2:D:143:LEU:HD13 | 2:D:207:PHE:CE2 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:505:LEU:HB3 | 2:D:530:LEU:HD21 | 2.01 | 0.42 |
| 2:D:874:LEU:HD12 | 2:D:875:PRO:HD2 | 2.01 | 0.42 |
| 2:D:3124:GLU:C | 2:D:3126:VAL:H | 2.23 | 0.42 |
| 2:D:3611:LEU:HD23 | 2:D:3611:LEU:HA | 1.90 | 0.42 |
| 2:A:794:PHE:HB2 | 2:A:798:ILE:HG21 | 2.02 | 0.42 |
| 2:A:894:VAL:HG23 | 2:A:895:MET:HE2 | 2.02 | 0.42 |
| 2:A:954:ASP:OD2 | 2:A:957:ALA:N | 2.51 | 0.42 |
| 2:A:1053:ALA:O | 2:A:1057:LEU:HG | 2.20 | 0.42 |
| 2:A:1091:GLU:HB3 | 2:A:1094:TYR:HD2 | 1.84 | 0.42 |
| 2:A:1181:ILE:HG21 | 2:A:1189:GLU:HB3 | 2.02 | 0.42 |
| 2:A:2511:ASP:HA | 2:A:2514:LEU:HD12 | 2.01 | 0.42 |
| 2:A:3102:LEU:HB2 | 2:A:3103:PRO:HD3 | 2.00 | 0.42 |
| 2:A:3311:LYS:O | 2:A:3315:LEU:N | 2.49 | 0.42 |
| 2:B:219:SER:H | 2:B:349:MET:HE3 | 1.84 | 0.42 |
| 2:B:269:VAL:O | 2:B:269:VAL:HG12 | 2.20 | 0.42 |
| 2:B:2137:GLU:HG2 | 2:B:2138:GLU:N | 2.35 | 0.42 |
| 2:B:2760:TYR:CE1 | 2:B:2768:LYS:HG2 | 2.55 | 0.42 |
| 2:B:2841:ALA:HB2 | 2:B:2893:LEU:HD12 | 2.02 | 0.42 |
| 2:B:2885:ASP:O | 2:B:2888:LYS:HG2 | 2.19 | 0.42 |
| 2:B:3890:TRP:HB3 | 2:C:76:ARG:HG2 | 2.02 | 0.42 |
| 2:B:3958:LEU:HB2 | 2:B:3968:LEU:HD13 | 2.01 | 0.42 |
| 2:C:143:LEU:HD13 | 2:C:207:PHE:CE2 | 2.55 | 0.42 |
| 2:C:306:LEU:HA | 2:C:316:LEU:HD23 | 2.01 | 0.42 |
| 2:C:874:LEU:HD12 | 2:C:875:PRO:HD2 | 2.01 | 0.42 |
| 2:C:1031:ARG:HH21 | 2:C:1038:LEU:CD1 | 2.11 | 0.42 |
| 2:C:2841:ALA:HB2 | 2:C:2893:LEU:HD12 | 2.02 | 0.42 |
| 2:C:4058:TYR:HD1 | 2:C:4062:GLU:HB3 | 1.84 | 0.42 |
| 2:D:2399:LEU:HD12 | 2:D:2427:ILE:HD11 | 2.02 | 0.42 |
| 2:D:2910:LEU:HD12 | 2:D:2911:GLU:N | 2.35 | 0.42 |
| 2:D:3207:ASN:OD1 | 2:D:3208:ILE:N | 2.50 | 0.42 |
| 2:D:4058:TYR:HD1 | 2:D:4062:GLU:HB3 | 1.84 | 0.42 |
| 2:A:890:HIS:CE1 | 2:A:924:LEU:HD22 | 2.55 | 0.42 |
| 2:A:1040:ASP:HA | 2:A:1043:LYS:HE2 | 2.02 | 0.42 |
| 2:A:1435:GLY:HA2 | 2:D:2831:VAL:HG22 | 2.01 | 0.42 |
| 2:A:1900:GLU:HG2 | 2:A:2080:LEU:HD23 | 2.02 | 0.42 |
| 2:A:2841:ALA:HB2 | 2:A:2893:LEU:HD12 | 2.02 | 0.42 |
| 2:A:2914:THR:N | 2:A:2915:PRO:HD2 | 2.35 | 0.42 |
| 2:A:3679:LYS:HE2 | 2:A:3679:LYS:HB2 | 1.88 | 0.42 |
| 2:B:986:ILE:CG2 | 2:B:1055:ARG:HD2 | 2.50 | 0.42 |
| 2:B:1900:GLU:HG2 | 2:B:2080:LEU:HD23 | 2.02 | 0.42 |
| 2:B:2761:LYS:HA | 2:B:2761:LYS:HD3 | 1.83 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:3997:LYS:HD3 | 2:B:4109:MET:HE1 | 2.02 | 0.42 |
| 2:C:505:LEU:HB3 | 2:C:530:LEU:HD21 | 2.01 | 0.42 |
| 2:C:538:ALA:O | 2:C:542:ARG:HB2 | 2.19 | 0.42 |
| 2:C:674:TYR:OH | 2:C:676:GLU:OE1 | 2.31 | 0.42 |
| 2:C:694:ARG:HD2 | 2:C:718:VAL:O | 2.20 | 0.42 |
| 2:C:2187:ILE:HG13 | 2:C:2227:VAL:HG13 | 2.01 | 0.42 |
| 2:C:2721:ILE:HD11 | 2:C:2779:LEU:HD22 | 2.02 | 0.42 |
| 2:C:3254:PRO:HD2 | 2:C:3268:LEU:O | 2.19 | 0.42 |
| 2:D:363:ILE:HD13 | 2:D:372:LEU:HD23 | 2.01 | 0.42 |
| 2:D:902:TRP:CG | 2:D:918:LEU:HD21 | 2.55 | 0.42 |
| 2:D:981:MET:SD | 2:D:1059:GLY:HA3 | 2.60 | 0.42 |
| 2:D:1011:ARG:HA | 2:D:1014:GLN:CD | 2.40 | 0.42 |
| 2:D:1040:ASP:HA | 2:D:1043:LYS:HE2 | 2.02 | 0.42 |
| 2:D:1628:MET:HB3 | 2:D:1628:MET:HE2 | 1.72 | 0.42 |
| 2:D:1943:ARG:O | 2:D:1947:VAL:HG23 | 2.20 | 0.42 |
| 2:D:2736:LYS:HA | 2:D:2736:LYS:HD3 | 1.82 | 0.42 |
| 2:D:2841:ALA:HB2 | 2:D:2893:LEU:HD12 | 2.02 | 0.42 |
| 1:F:19:LYS:HA | 1:F:19:LYS:HD3 | 1.81 | 0.42 |
| 2:A:521:GLU:HG2 | 2:A:522:ALA:N | 2.34 | 0.42 |
| 2:A:961:VAL:HG13 | 2:A:961:VAL:O | 2.19 | 0.42 |
| 2:A:1026:ASN:HB3 | 2:A:1028:ARG:HG2 | 2.02 | 0.42 |
| 2:A:2721:ILE:HD11 | 2:A:2779:LEU:HD22 | 2.02 | 0.42 |
| 2:A:2937:HIS:HA | 2:A:3014:LEU:HD13 | 2.01 | 0.42 |
| 2:A:3213:LYS:O | 2:A:3216:GLU:HG3 | 2.20 | 0.42 |
| 2:A:3260:ARG:HH12 | 2:A:3265:CYS:H | 1.68 | 0.42 |
| 2:A:3850:HIS:HE1 | 2:A:3925:GLN:OE1 | 2.03 | 0.42 |
| 2:B:1031:ARG:NH2 | 2:B:1042:THR:HG21 | 2.22 | 0.42 |
| 2:B:1825:PHE:CZ | 2:B:1842:ILE:HD12 | 2.55 | 0.42 |
| 2:B:3213:LYS:O | 2:B:3216:GLU:HG3 | 2.20 | 0.42 |
| 2:B:4806:CYS:HA | 2:B:4812:CYS:HB2 | 2.00 | 0.42 |
| 2:C:2257:LEU:HD21 | 2:C:2262:LEU:HG | 2.02 | 0.42 |
| 2:C:3018:ARG:HA | 2:C:3021:LEU:HD13 | 2.01 | 0.42 |
| 2:D:249:SER:HA | 2:D:272:ARG:HD2 | 2.02 | 0.42 |
| 2:D:257:ARG:NH2 | 2:D:272:ARG:HG3 | 2.33 | 0.42 |
| 2:D:718:VAL:HG23 | 2:D:793:SER:HB3 | 2.01 | 0.42 |
| 2:D:962:LYS:HZ2 | 2:D:982:ASP:H | 1.68 | 0.42 |
| 2:D:1019:GLY:HA3 | 2:D:1028:ARG:HB3 | 2.02 | 0.42 |
| 2:D:3144:LYS:HE3 | 2:D:3233:HIS:NE2 | 2.35 | 0.42 |
| 2:D:3178:HIS:HB2 | 2:D:3265:CYS:HA | 2.02 | 0.42 |
| 2:A:981:MET:SD | 2:A:1059:GLY:HA3 | 2.60 | 0.41 |
| 2:A:1031:ARG:NH2 | 2:A:1042:THR:HG21 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:1777:GLN:O | 2:A:1778:TYR:HB2 | 2.20 | 0.41 |
| 2:B:555:LEU:HD11 | 2:B:578:VAL:HG11 | 2.02 | 0.41 |
| 2:B:694:ARG:HD2 | 2:B:718:VAL:O | 2.20 | 0.41 |
| 2:B:961:VAL:O | 2:B:961:VAL:HG13 | 2.19 | 0.41 |
| 2:B:2910:LEU:HD12 | 2:B:2911:GLU:N | 2.35 | 0.41 |
| 2:B:3850:HIS:HE1 | 2:B:3925:GLN:OE1 | 2.03 | 0.41 |
| 2:C:672:LYS:NZ | 2:C:818:GLY:HA3 | 2.35 | 0.41 |
| 2:C:718:VAL:HG23 | 2:C:793:SER:HB3 | 2.01 | 0.41 |
| 2:C:2844:MET:O | 2:C:2848:TYR:HD2 | 2.02 | 0.41 |
| 2:C:3124:GLU:C | 2:C:3126:VAL:H | 2.23 | 0.41 |
| 2:C:3661:VAL:HG23 | 2:C:3666:GLN:HG2 | 2.02 | 0.41 |
| 2:C:3732:HIS:O | 2:C:3776:LYS:NZ | 2.49 | 0.41 |
| 2:C:3850:HIS:HE1 | 2:C:3925:GLN:OE1 | 2.03 | 0.41 |
| 2:C:4049:HIS:HB2 | 2:C:4067:LEU:HD21 | 2.02 | 0.41 |
| 2:D:657:PRO:HB2 | 2:D:659:ILE:HG12 | 2.02 | 0.41 |
| 2:D:794:PHE:HB2 | 2:D:798:ILE:HG21 | 2.02 | 0.41 |
| 2:D:2644:LEU:O | 2:D:2648:ILE:HG13 | 2.20 | 0.41 |
| 2:D:3166:PHE:CG | 2:D:3167:PRO:HD2 | 2.55 | 0.41 |
| 2:D:4277:LYS:HA | 2:D:4277:LYS:HD2 | 1.73 | 0.41 |
| 2:D:4649:VAL:O | 2:D:4653:VAL:HG23 | 2.20 | 0.41 |
| 2:A:520:ARG:HH11 | 2:A:521:GLU:HB3 | 1.85 | 0.41 |
| 2:A:672:LYS:HB3 | 2:A:819:TYR:HA | 2.01 | 0.41 |
| 2:A:756:SER:OG | 2:A:769:ARG:HB2 | 2.20 | 0.41 |
| 2:A:902:TRP:CG | 2:A:918:LEU:HD21 | 2.55 | 0.41 |
| 2:A:1429:SER:OG | 2:A:1556:GLU:HB2 | 2.19 | 0.41 |
| 2:A:3018:ARG:HA | 2:A:3021:LEU:HD13 | 2.01 | 0.41 |
| 2:A:3061:LEU:HD23 | 2:A:3061:LEU:HA | 1.84 | 0.41 |
| 2:A:3144:LYS:HE3 | 2:A:3233:HIS:NE2 | 2.35 | 0.41 |
| 2:A:3296:MET:HA | 2:A:3299:LEU:HD12 | 2.00 | 0.41 |
| 2:B:2257:LEU:HD21 | 2:B:2262:LEU:HG | 2.02 | 0.41 |
| 2:B:3233:HIS:O | 2:B:3236:GLU:HG2 | 2.21 | 0.41 |
| 2:B:4105:LEU:HB3 | 2:B:4115:LEU:HD21 | 2.02 | 0.41 |
| 2:C:657:PRO:HB2 | 2:C:659:ILE:HG12 | 2.02 | 0.41 |
| 2:C:890:HIS:CE1 | 2:C:924:LEU:HD22 | 2.55 | 0.41 |
| 2:C:1011:ARG:HA | 2:C:1014:GLN:CD | 2.40 | 0.41 |
| 2:C:1029:ASN:OD1 | 2:C:1030:PRO:HD2 | 2.21 | 0.41 |
| 2:C:1282:CYS:SG | 2:C:1556:GLU:HG2 | 2.61 | 0.41 |
| 2:C:3023:GLY:N | 2:C:3025:ASP:OD1 | 2.53 | 0.41 |
| 2:C:3145:SER:O | 2:C:3148:VAL:HG12 | 2.20 | 0.41 |
| 2:C:3296:MET:HA | 2:C:3299:LEU:HD12 | 2.01 | 0.41 |
| 2:C:4255:LEU:O | 2:C:4258:MET:HG3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:551:PHE:HE2 | 2:D:558:LEU:HD22 | 1.84 | 0.41 |
| 2:D:1026:ASN:HB3 | 2:D:1028:ARG:HG2 | 2.02 | 0.41 |
| 2:D:1029:ASN:OD1 | 2:D:1030:PRO:HD2 | 2.21 | 0.41 |
| 2:D:1181:ILE:HG21 | 2:D:1189:GLU:HB3 | 2.02 | 0.41 |
| 2:D:2137:GLU:HG2 | 2:D:2138:GLU:N | 2.35 | 0.41 |
| 2:D:2433:VAL:HG13 | 2:D:2490:VAL:HG21 | 2.03 | 0.41 |
| 2:A:893:TRP:NE1 | 2:A:1049:SER:HB3 | 2.34 | 0.41 |
| 2:A:1282:CYS:SG | 2:A:1556:GLU:HG2 | 2.61 | 0.41 |
| 2:A:2222:LEU:HD23 | 2:A:2222:LEU:HA | 1.94 | 0.41 |
| 2:A:2767:GLU:HG3 | 2:A:2771:TYR:CE2 | 2.55 | 0.41 |
| 2:A:3023:GLY:N | 2:A:3025:ASP:OD1 | 2.53 | 0.41 |
| 2:A:3793:LEU:HD23 | 2:A:3793:LEU:HA | 1.93 | 0.41 |
| 2:B:890:HIS:CE1 | 2:B:924:LEU:HD22 | 2.55 | 0.41 |
| 2:B:916:PRO:HB3 | 2:B:923:LYS:HZ2 | 1.83 | 0.41 |
| 2:B:1011:ARG:HA | 2:B:1014:GLN:CD | 2.40 | 0.41 |
| 2:B:1181:ILE:HG21 | 2:B:1189:GLU:HB3 | 2.02 | 0.41 |
| 2:B:2831:VAL:HB | 2:B:2894:LYS:CD | 2.46 | 0.41 |
| 2:B:2905:ARG:NH1 | 2:B:2906:GLY:H | 2.15 | 0.41 |
| 2:B:4735:ASN:HB3 | 2:B:4738:PHE:HD2 | 1.84 | 0.41 |
| 2:C:257:ARG:NH2 | 2:C:272:ARG:HG3 | 2.33 | 0.41 |
| 2:C:672:LYS:HB3 | 2:C:819:TYR:HA | 2.01 | 0.41 |
| 2:C:961:VAL:O | 2:C:961:VAL:HG13 | 2.19 | 0.41 |
| 2:C:986:ILE:CG2 | 2:C:1055:ARG:HD2 | 2.50 | 0.41 |
| 2:C:1019:GLY:HA3 | 2:C:1028:ARG:HB3 | 2.02 | 0.41 |
| 2:C:1053:ALA:O | 2:C:1057:LEU:HG | 2.20 | 0.41 |
| 2:C:2593:VAL:HG12 | 2:C:2644:LEU:HB2 | 2.02 | 0.41 |
| 2:C:2649:PHE:CE2 | 2:C:2932:TYR:HE2 | 2.38 | 0.41 |
| 2:C:2727:HIS:O | 2:C:2731:LYS:HG3 | 2.19 | 0.41 |
| 2:C:2767:GLU:HG3 | 2:C:2771:TYR:CE2 | 2.55 | 0.41 |
| 2:C:3278:GLY:O | 2:C:3282:LYS:HG2 | 2.21 | 0.41 |
| 2:C:3712:LYS:HE3 | 2:C:3712:LYS:HB2 | 1.70 | 0.41 |
| 2:D:1932:PHE:CE1 | 2:D:1996:LEU:HB2 | 2.54 | 0.41 |
| 2:D:2062:ILE:O | 2:D:2066:MET:HG2 | 2.20 | 0.41 |
| 2:D:2694:SER:HA | 2:D:2704:GLN:HE22 | 1.85 | 0.41 |
| 2:D:2849:HIS:NE2 | 2:D:2877:LEU:HD11 | 2.36 | 0.41 |
| 2:D:2905:ARG:NH1 | 2:D:2906:GLY:H | 2.15 | 0.41 |
| 2:D:3237:VAL:HG23 | 2:D:3238:ILE:HG13 | 2.02 | 0.41 |
| 2:D:4110:PRO:HG3 | 2:D:4966:LEU:HD12 | 2.02 | 0.41 |
| 1:F:8:ILE:HG23 | 2:B:748:LEU:HB2 | 2.02 | 0.41 |
| 2:A:249:SER:HA | 2:A:272:ARG:HD2 | 2.03 | 0.41 |
| 2:A:680:ASP:O | 2:A:751:THR:HG23 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:1610:ARG:HD3 | 2:A:1617:TRP:CE2 | 2.56 | 0.41 |
| 2:A:2409:ILE:HG12 | 2:A:2420:ARG:NH2 | 2.36 | 0.41 |
| 2:A:2429:LEU:HD21 | 2:A:2483:PHE:CZ | 2.56 | 0.41 |
| 2:A:2478:ILE:HB | 2:A:2531:CYS:SG | 2.60 | 0.41 |
| 2:A:2649:PHE:CE2 | 2:A:2932:TYR:HE2 | 2.38 | 0.41 |
| 2:A:2681:MET:HE1 | 2:A:2917:ILE:HA | 2.02 | 0.41 |
| 2:A:2760:TYR:CE1 | 2:A:2768:LYS:HG2 | 2.55 | 0.41 |
| 2:A:2849:HIS:NE2 | 2:A:2877:LEU:HD11 | 2.35 | 0.41 |
| 2:A:2927:GLN:HG3 | 2:A:2931:ARG:NE | 2.35 | 0.41 |
| 2:A:3130:CYS:HA | 2:A:3133:ILE:HD12 | 2.02 | 0.41 |
| 2:A:3664:LEU:HD21 | 2:A:3731:LEU:HD23 | 2.02 | 0.41 |
| 2:A:4803:ASP:OD2 | 2:A:4805:LYS:HE2 | 2.20 | 0.41 |
| 2:B:1100:ARG:HH12 | 2:B:1234:GLU:C | 2.21 | 0.41 |
| 2:B:1703:TYR:HD2 | 2:B:1820:PRO:CB | 2.34 | 0.41 |
| 2:B:2409:ILE:HG12 | 2:B:2420:ARG:NH2 | 2.36 | 0.41 |
| 2:B:2721:ILE:HD11 | 2:B:2779:LEU:HD22 | 2.02 | 0.41 |
| 2:B:3130:CYS:HA | 2:B:3133:ILE:HD12 | 2.02 | 0.41 |
| 2:B:3145:SER:O | 2:B:3148:VAL:HG12 | 2.20 | 0.41 |
| 2:B:3237:VAL:HG23 | 2:B:3238:ILE:HG13 | 2.02 | 0.41 |
| 2:B:3260:ARG:HH12 | 2:B:3265:CYS:H | 1.68 | 0.41 |
| 2:B:4636:ASN:HB2 | 2:B:4704:LYS:HZ1 | 1.85 | 0.41 |
| 2:C:756:SER:OG | 2:C:769:ARG:HB2 | 2.20 | 0.41 |
| 2:C:1703:TYR:HD2 | 2:C:1820:PRO:CB | 2.34 | 0.41 |
| 2:C:2488:LEU:HG | 2:C:2544:LEU:HD11 | 2.03 | 0.41 |
| 2:C:2644:LEU:O | 2:C:2648:ILE:HG13 | 2.20 | 0.41 |
| 2:C:2658:GLU:OE1 | 2:C:2661:LEU:N | 2.34 | 0.41 |
| 2:C:3166:PHE:CG | 2:C:3167:PRO:HD2 | 2.55 | 0.41 |
| 2:C:3237:VAL:HG23 | 2:C:3238:ILE:HG13 | 2.02 | 0.41 |
| 2:D:555:LEU:HD11 | 2:D:578:VAL:HG11 | 2.02 | 0.41 |
| 2:D:680:ASP:O | 2:D:751:THR:HG23 | 2.20 | 0.41 |
| 2:D:1255:LEU:HG | 2:D:1451:HIS:HB3 | 2.03 | 0.41 |
| 2:D:1825:PHE:CZ | 2:D:1842:ILE:HD12 | 2.55 | 0.41 |
| 2:D:2914:THR:N | 2:D:2915:PRO:HD2 | 2.35 | 0.41 |
| 2:D:4136:ILE:HG22 | 2:D:4917:ASN:HB3 | 2.01 | 0.41 |
| 2:D:4270:LYS:HE3 | 2:D:4270:LYS:HB3 | 1.84 | 0.41 |
| 1:F:12:ASP:OD1 | 1:F:13:GLY:N | 2.54 | 0.41 |
| 2:A:269:VAL:O | 2:A:269:VAL:HG12 | 2.20 | 0.41 |
| 2:A:1559:ARG:HB3 | 2:A:1565:PRO:HB3 | 2.03 | 0.41 |
| 2:A:2255:LEU:O | 2:A:3810:ARG:HD3 | 2.21 | 0.41 |
| 2:A:2426:LEU:HA | 2:B:143:LEU:CD2 | 2.50 | 0.41 |
| 2:A:3233:HIS:O | 2:A:3236:GLU:HG2 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:3732:HIS:O | 2:A:3776:LYS:NZ | 2.49 | 0.41 |
| 2:A:4255:LEU:O | 2:A:4258:MET:HG3 | 2.20 | 0.41 |
| 2:A:4609:LYS:HD2 | 2:A:4615:LEU:HD13 | 2.02 | 0.41 |
| 2:B:680:ASP:O | 2:B:751:THR:HG23 | 2.20 | 0.41 |
| 2:B:902:TRP:CG | 2:B:918:LEU:HD21 | 2.55 | 0.41 |
| 2:B:1053:ALA:O | 2:B:1057:LEU:HG | 2.20 | 0.41 |
| 2:B:1425:THR:HG22 | 2:B:1563:VAL:HG13 | 2.02 | 0.41 |
| 2:B:2429:LEU:HD21 | 2:B:2483:PHE:CZ | 2.56 | 0.41 |
| 2:B:2990:LEU:HD12 | 2:B:2990:LEU:O | 2.21 | 0.41 |
| 2:B:3278:GLY:O | 2:B:3282:LYS:HG2 | 2.21 | 0.41 |
| 2:B:3661:VAL:HG23 | 2:B:3666:GLN:HG2 | 2.02 | 0.41 |
| 2:C:962:LYS:HZ2 | 2:C:982:ASP:H | 1.68 | 0.41 |
| 2:C:2062:ILE:O | 2:C:2066:MET:HG2 | 2.21 | 0.41 |
| 2:C:2255:LEU:O | 2:C:3810:ARG:HD3 | 2.21 | 0.41 |
| 2:D:1610:ARG:HD3 | 2:D:1617:TRP:CE2 | 2.56 | 0.41 |
| 2:D:1703:TYR:HD2 | 2:D:1820:PRO:CB | 2.33 | 0.41 |
| 2:D:2257:LEU:HD21 | 2:D:2262:LEU:HG | 2.02 | 0.41 |
| 2:D:2334:ALA:HB2 | 2:D:2346:ALA:HB2 | 2.01 | 0.41 |
| 2:D:2790:GLU:O | 2:D:2901:TYR:HA | 2.19 | 0.41 |
| 2:D:3145:SER:O | 2:D:3148:VAL:HG12 | 2.20 | 0.41 |
| 2:D:3261:ALA:C | 2:D:3263:MET:N | 2.71 | 0.41 |
| 2:D:3906:PHE:HB3 | 2:D:3967:LEU:HD11 | 2.03 | 0.41 |
| 2:D:4255:LEU:O | 2:D:4258:MET:HG3 | 2.20 | 0.41 |
| 2:D:4625:ASP:OD1 | 2:D:4625:ASP:N | 2.46 | 0.41 |
| 2:D:4735:ASN:HB3 | 2:D:4738:PHE:HD2 | 1.84 | 0.41 |
| 2:D:4843:ARG:NH1 | 2:D:4847:ASP:OD2 | 2.54 | 0.41 |
| 1:G:28:THR:O | 1:G:30:MET:HG3 | 2.21 | 0.41 |
| 2:A:21:VAL:HG23 | 2:A:215:ALA:HB3 | 2.03 | 0.41 |
| 2:A:657:PRO:HB2 | 2:A:659:ILE:HG12 | 2.02 | 0.41 |
| 2:A:902:TRP:HB3 | 2:A:918:LEU:CD2 | 2.44 | 0.41 |
| 2:A:1703:TYR:HD2 | 2:A:1820:PRO:CB | 2.34 | 0.41 |
| 2:A:2062:ILE:O | 2:A:2066:MET:HG2 | 2.21 | 0.41 |
| 2:A:2433:VAL:HG13 | 2:A:2490:VAL:HG21 | 2.02 | 0.41 |
| 2:A:2694:SER:HA | 2:A:2704:GLN:HE22 | 1.85 | 0.41 |
| 2:A:3661:VAL:HG23 | 2:A:3666:GLN:HG2 | 2.02 | 0.41 |
| 2:A:3975:GLN:O | 2:A:3979:VAL:HG23 | 2.20 | 0.41 |
| 2:B:324:VAL:O | 2:B:328:ALA:HB2 | 2.21 | 0.41 |
| 2:B:505:LEU:HB3 | 2:B:530:LEU:HD21 | 2.01 | 0.41 |
| 2:B:1971:GLU:HA | 2:B:1974:ASN:ND2 | 2.36 | 0.41 |
| 2:B:2062:ILE:O | 2:B:2066:MET:HG2 | 2.20 | 0.41 |
| 2:B:2413:LYS:HZ2 | 2:B:2415:GLU:HB3 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2478:ILE:HB | 2:B:2531:CYS:SG | 2.60 | 0.41 |
| 2:B:2591:ARG:HG2 | 2:B:2691:LYS:HZ3 | 1.86 | 0.41 |
| 2:B:2593:VAL:HG12 | 2:B:2644:LEU:HB2 | 2.02 | 0.41 |
| 2:B:2891:ASP:OD1 | 2:B:2892:ILE:N | 2.54 | 0.41 |
| 2:B:3178:HIS:HB2 | 2:B:3265:CYS:HA | 2.02 | 0.41 |
| 2:B:3271:GLU:O | 2:B:3275:THR:HG23 | 2.21 | 0.41 |
| 2:B:4609:LYS:HD2 | 2:B:4615:LEU:HD13 | 2.02 | 0.41 |
| 2:B:4803:ASP:OD2 | 2:B:4805:LYS:HE2 | 2.20 | 0.41 |
| 2:C:436:LEU:HG | 2:C:445:VAL:HG11 | 2.03 | 0.41 |
| 2:C:981:MET:SD | 2:C:1059:GLY:HA3 | 2.60 | 0.41 |
| 2:C:1598:ARG:NH2 | 2:C:1601:ASN:OD1 | 2.47 | 0.41 |
| 2:C:1730:THR:HG22 | 2:C:1731:GLU:N | 2.36 | 0.41 |
| 2:C:1900:GLU:HG2 | 2:C:2080:LEU:HD23 | 2.02 | 0.41 |
| 2:C:2694:SER:HA | 2:C:2704:GLN:HE22 | 1.85 | 0.41 |
| 2:C:2843:MET:O | 2:C:2846:GLU:HG2 | 2.19 | 0.41 |
| 2:C:2937:HIS:HA | 2:C:3014:LEU:HD13 | 2.01 | 0.41 |
| 2:C:3319:PHE:O | 2:C:3322:LEU:N | 2.54 | 0.41 |
| 2:C:3975:GLN:O | 2:C:3979:VAL:HG23 | 2.20 | 0.41 |
| 2:C:4751:LYS:HG3 | 2:C:4754:ARG:HH12 | 1.86 | 0.41 |
| 2:D:1914:CYS:SG | 2:D:2091:GLN:NE2 | 2.89 | 0.41 |
| 2:D:2488:LEU:HG | 2:D:2544:LEU:HD11 | 2.03 | 0.41 |
| 2:D:2681:MET:HE1 | 2:D:2917:ILE:HA | 2.02 | 0.41 |
| 2:D:3319:PHE:O | 2:D:3322:LEU:N | 2.54 | 0.41 |
| 2:D:4105:LEU:HB3 | 2:D:4115:LEU:HD21 | 2.02 | 0.41 |
| 1:H:28:THR:O | 1:H:30:MET:HG3 | 2.21 | 0.41 |
| 2:A:964:MET:HE1 | 2:A:982:ASP:HA | 2.02 | 0.41 |
| 2:A:1825:PHE:CZ | 2:A:1842:ILE:HD12 | 2.55 | 0.41 |
| 2:A:1971:GLU:HA | 2:A:1974:ASN:ND2 | 2.36 | 0.41 |
| 2:A:4687:LYS:HD3 | 2:A:4687:LYS:HA | 1.87 | 0.41 |
| 2:B:125:TYR:CE1 | 2:B:417:ARG:HG2 | 2.56 | 0.41 |
| 2:B:678:MET:SD | 2:B:801:ARG:NH2 | 2.93 | 0.41 |
| 2:B:1019:GLY:HA3 | 2:B:1028:ARG:HB3 | 2.02 | 0.41 |
| 2:B:1282:CYS:SG | 2:B:1556:GLU:HG2 | 2.61 | 0.41 |
| 2:B:1559:ARG:HB3 | 2:B:1565:PRO:HB3 | 2.03 | 0.41 |
| 2:B:1610:ARG:HD3 | 2:B:1617:TRP:CE2 | 2.56 | 0.41 |
| 2:B:1730:THR:HG22 | 2:B:1731:GLU:N | 2.36 | 0.41 |
| 2:B:1829:LEU:HD12 | 2:B:1829:LEU:HA | 1.88 | 0.41 |
| 2:B:3780:TYR:HE1 | 2:B:3784:LYS:HZ2 | 1.69 | 0.41 |
| 2:C:902:TRP:CG | 2:C:918:LEU:HD21 | 2.55 | 0.41 |
| 2:C:983:LEU:HD12 | 2:C:983:LEU:HA | 1.94 | 0.41 |
| 2:C:2433:VAL:HG13 | 2:C:2490:VAL:HG21 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:3178:HIS:HB2 | 2:C:3265:CYS:HA | 2.02 | 0.41 |
| 2:C:3184:TYR:HB3 | 2:C:3192:ARG:NH2 | 2.36 | 0.41 |
| 2:C:3271:GLU:O | 2:C:3275:THR:HG23 | 2.21 | 0.41 |
| 2:C:3664:LEU:HD21 | 2:C:3731:LEU:HD23 | 2.02 | 0.41 |
| 2:C:4843:ARG:NH1 | 2:C:4847:ASP:OD2 | 2.54 | 0.41 |
| 2:C:4867:ILE:HG12 | 2:D:4864:GLY:HA2 | 2.03 | 0.41 |
| 2:D:678:MET:SD | 2:D:801:ARG:NH2 | 2.93 | 0.41 |
| 2:D:919:VAL:HG12 | 2:D:920:GLU:N | 2.36 | 0.41 |
| 2:D:1282:CYS:SG | 2:D:1556:GLU:HG2 | 2.61 | 0.41 |
| 2:D:1425:THR:HG22 | 2:D:1563:VAL:HG13 | 2.02 | 0.41 |
| 2:D:3023:GLY:N | 2:D:3025:ASP:OD1 | 2.53 | 0.41 |
| 2:D:3260:ARG:HH12 | 2:D:3265:CYS:H | 1.68 | 0.41 |
| 1:F:67:MET:HE3 | 1:F:104:LEU:HB2 | 2.03 | 0.41 |
| 2:A:42:PHE:HZ | 2:A:459:LEU:HG | 1.86 | 0.41 |
| 2:A:281:ARG:NH1 | 2:A:345:GLU:OE2 | 2.54 | 0.41 |
| 2:A:678:MET:SD | 2:A:801:ARG:NH2 | 2.93 | 0.41 |
| 2:A:1029:ASN:OD1 | 2:A:1030:PRO:HD2 | 2.21 | 0.41 |
| 2:A:1943:ARG:O | 2:A:1947:VAL:HG23 | 2.20 | 0.41 |
| 2:A:2445:ILE:HG22 | 2:A:2451:VAL:HG12 | 2.03 | 0.41 |
| 2:A:2591:ARG:HG2 | 2:A:2691:LYS:HZ3 | 1.85 | 0.41 |
| 2:A:2593:VAL:HG12 | 2:A:2644:LEU:HB2 | 2.02 | 0.41 |
| 2:A:2638:LEU:HD23 | 2:A:2638:LEU:HA | 1.93 | 0.41 |
| 2:A:3100:ALA:C | 2:A:3103:PRO:HD2 | 2.41 | 0.41 |
| 2:A:3169:ALA:HB1 | 2:A:3245:TYR:OH | 2.21 | 0.41 |
| 2:A:4049:HIS:HB2 | 2:A:4067:LEU:HD21 | 2.02 | 0.41 |
| 2:A:4898:PHE:O | 2:A:4904:GLY:HA3 | 2.21 | 0.41 |
| 2:B:657:PRO:HB2 | 2:B:659:ILE:HG12 | 2.02 | 0.41 |
| 2:B:1604:LEU:HD23 | 2:B:1604:LEU:HA | 1.92 | 0.41 |
| 2:B:2445:ILE:HG22 | 2:B:2451:VAL:HG12 | 2.03 | 0.41 |
| 2:B:2649:PHE:CE2 | 2:B:2932:TYR:HE2 | 2.38 | 0.41 |
| 2:B:2767:GLU:HG3 | 2:B:2771:TYR:CE2 | 2.56 | 0.41 |
| 2:B:2930:ILE:HD12 | 2:B:3003:MET:HE3 | 2.03 | 0.41 |
| 2:B:3023:GLY:N | 2:B:3025:ASP:OD1 | 2.53 | 0.41 |
| 2:B:3184:TYR:HB3 | 2:B:3192:ARG:NH2 | 2.36 | 0.41 |
| 2:B:3285:TYR:O | 2:B:3329:LYS:NZ | 2.54 | 0.41 |
| 2:B:3664:LEU:HD21 | 2:B:3731:LEU:HD23 | 2.02 | 0.41 |
| 2:B:3689:MET:HA | 2:B:3689:MET:CE | 2.51 | 0.41 |
| 2:B:4270:LYS:NZ | 2:B:4278:ASP:OD1 | 2.25 | 0.41 |
| 2:C:1013:ARG:NE | 2:C:1013:ARG:HA | 2.35 | 0.41 |
| 2:C:1777:GLN:O | 2:C:1778:TYR:HB2 | 2.20 | 0.41 |
| 2:C:1825:PHE:CZ | 2:C:1842:ILE:HD12 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:2429:LEU:HD21 | 2:C:2483:PHE:CZ | 2.56 | 0.41 |
| 2:C:2478:ILE:HB | 2:C:2531:CYS:SG | 2.60 | 0.41 |
| 2:C:2990:LEU:O | 2:C:2990:LEU:HD12 | 2.21 | 0.41 |
| 2:C:3144:LYS:HE3 | 2:C:3233:HIS:NE2 | 2.35 | 0.41 |
| 2:C:4609:LYS:HD2 | 2:C:4615:LEU:HD13 | 2.02 | 0.41 |
| 2:D:614:LEU:HD22 | 2:D:632:ILE:HG12 | 2.03 | 0.41 |
| 2:D:672:LYS:NZ | 2:D:818:GLY:HA3 | 2.35 | 0.41 |
| 2:D:1730:THR:HG22 | 2:D:1731:GLU:H | 1.86 | 0.41 |
| 2:D:1900:GLU:HG2 | 2:D:2080:LEU:HD23 | 2.02 | 0.41 |
| 2:D:2478:ILE:HB | 2:D:2531:CYS:SG | 2.61 | 0.41 |
| 2:D:2593:VAL:HG12 | 2:D:2644:LEU:HB2 | 2.02 | 0.41 |
| 2:D:3100:ALA:C | 2:D:3103:PRO:HD2 | 2.41 | 0.41 |
| 2:D:3793:LEU:HD23 | 2:D:3793:LEU:HA | 1.93 | 0.41 |
| 1:E:28:THR:O | 1:E:30:MET:HG3 | 2.21 | 0.41 |
| 2:A:76:ARG:NH2 | 2:D:3891:TYR:HA | 2.36 | 0.41 |
| 2:A:125:TYR:CE1 | 2:A:417:ARG:HG2 | 2.56 | 0.41 |
| 2:A:324:VAL:O | 2:A:328:ALA:HB2 | 2.21 | 0.41 |
| 2:A:742:SER:HA | 2:A:746:GLN:NE2 | 2.36 | 0.41 |
| 2:A:987:LYS:HZ3 | 2:A:989:THR:HA | 1.86 | 0.41 |
| 2:A:1031:ARG:HH21 | 2:A:1038:LEU:CD1 | 2.11 | 0.41 |
| 2:A:1100:ARG:HG2 | 2:A:1167:ASP:OD1 | 2.21 | 0.41 |
| 2:A:1255:LEU:HG | 2:A:1451:HIS:HB3 | 2.03 | 0.41 |
| 2:A:1268:ILE:HG21 | 2:A:1302:TYR:HE1 | 1.86 | 0.41 |
| 2:A:1726:ILE:HD11 | 2:A:2165:LEU:HD21 | 2.03 | 0.41 |
| 2:A:1730:THR:HG22 | 2:A:1731:GLU:H | 1.86 | 0.41 |
| 2:A:2257:LEU:HD21 | 2:A:2262:LEU:HG | 2.02 | 0.41 |
| 2:A:2891:ASP:OD1 | 2:A:2892:ILE:N | 2.54 | 0.41 |
| 2:A:3072:MET:SD | 2:A:3136:SER:HA | 2.61 | 0.41 |
| 2:A:3166:PHE:CG | 2:A:3167:PRO:HD2 | 2.55 | 0.41 |
| 2:A:3237:VAL:HG23 | 2:A:3238:ILE:HG13 | 2.02 | 0.41 |
| 2:A:3319:PHE:O | 2:A:3322:LEU:N | 2.54 | 0.41 |
| 2:A:3717:LYS:O | 2:A:3721:LYS:HG3 | 2.21 | 0.41 |
| 2:A:4110:PRO:HG3 | 2:A:4966:LEU:HD12 | 2.02 | 0.41 |
| 2:A:4789:PHE:HB3 | 2:A:4792:PHE:HD2 | 1.86 | 0.41 |
| 2:A:4943:MET:HE2 | 2:A:4951:PHE:HB3 | 2.03 | 0.41 |
| 2:B:281:ARG:NH1 | 2:B:345:GLU:OE2 | 2.54 | 0.41 |
| 2:B:981:MET:SD | 2:B:1059:GLY:HA3 | 2.60 | 0.41 |
| 2:B:1011:ARG:HG3 | 2:B:1014:GLN:NE2 | 2.36 | 0.41 |
| 2:B:1013:ARG:HA | 2:B:1013:ARG:NE | 2.35 | 0.41 |
| 2:B:2255:LEU:O | 2:B:3810:ARG:HD3 | 2.21 | 0.41 |
| 2:B:2399:LEU:HD12 | 2:B:2427:ILE:HD11 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2433:VAL:HG13 | 2:B:2490:VAL:HG21 | 2.02 | 0.41 |
| 2:B:2827:ASP:O | 2:B:2831:VAL:HG23 | 2.21 | 0.41 |
| 2:B:4049:HIS:HB2 | 2:B:4067:LEU:HD21 | 2.02 | 0.41 |
| 2:B:4093:ASP:OD1 | 2:B:4094:ILE:HG13 | 2.21 | 0.41 |
| 2:B:4255:LEU:O | 2:B:4258:MET:HG3 | 2.20 | 0.41 |
| 2:B:4898:PHE:O | 2:B:4904:GLY:HA3 | 2.21 | 0.41 |
| 2:C:249:SER:HA | 2:C:272:ARG:HD2 | 2.03 | 0.41 |
| 2:C:551:PHE:HE2 | 2:C:558:LEU:HD22 | 1.84 | 0.41 |
| 2:C:742:SER:HA | 2:C:746:GLN:NE2 | 2.36 | 0.41 |
| 2:C:869:THR:OG1 | 2:C:941:LYS:HB3 | 2.21 | 0.41 |
| 2:C:906:PRO:HB2 | 2:C:907:VAL:HG23 | 2.03 | 0.41 |
| 2:C:1685:LEU:HD22 | 2:C:1706:LEU:HB2 | 2.03 | 0.41 |
| 2:C:2555:LEU:O | 2:C:2561:LEU:HD11 | 2.21 | 0.41 |
| 2:C:2591:ARG:HG2 | 2:C:2691:LYS:HZ3 | 1.86 | 0.41 |
| 2:C:2676:LEU:HD23 | 2:C:2676:LEU:HA | 1.83 | 0.41 |
| 2:C:2831:VAL:HG22 | 2:D:1435:GLY:CA | 2.50 | 0.41 |
| 2:C:2849:HIS:NE2 | 2:C:2877:LEU:HD11 | 2.36 | 0.41 |
| 2:C:2933:VAL:HG22 | 2:C:2963:PHE:HZ | 1.86 | 0.41 |
| 2:C:3285:TYR:O | 2:C:3329:LYS:NZ | 2.54 | 0.41 |
| 2:C:3689:MET:HA | 2:C:3689:MET:CE | 2.51 | 0.41 |
| 2:C:4105:LEU:HB3 | 2:C:4115:LEU:HD21 | 2.02 | 0.41 |
| 2:C:4110:PRO:HG3 | 2:C:4966:LEU:HD12 | 2.02 | 0.41 |
| 2:D:269:VAL:HG12 | 2:D:269:VAL:O | 2.20 | 0.41 |
| 2:D:694:ARG:HD2 | 2:D:718:VAL:O | 2.20 | 0.41 |
| 2:D:742:SER:HA | 2:D:746:GLN:NE2 | 2.36 | 0.41 |
| 2:D:756:SER:OG | 2:D:769:ARG:HB2 | 2.20 | 0.41 |
| 2:D:890:HIS:CE1 | 2:D:924:LEU:HD22 | 2.55 | 0.41 |
| 2:D:1268:ILE:HG21 | 2:D:1302:TYR:HE1 | 1.86 | 0.41 |
| 2:D:1446:ILE:HG12 | 2:D:1542:ALA:HB2 | 2.02 | 0.41 |
| 2:D:2255:LEU:O | 2:D:3810:ARG:HD3 | 2.21 | 0.41 |
| 2:D:2767:GLU:HG3 | 2:D:2771:TYR:CE2 | 2.55 | 0.41 |
| 2:D:2844:MET:O | 2:D:2848:TYR:HD2 | 2.02 | 0.41 |
| 2:D:3661:VAL:HG23 | 2:D:3666:GLN:HG2 | 2.02 | 0.41 |
| 2:D:3850:HIS:HE1 | 2:D:3925:GLN:OE1 | 2.03 | 0.41 |
| 2:D:3858:LEU:HD23 | 2:D:3858:LEU:HA | 1.94 | 0.41 |
| 1:G:12:ASP:OD1 | 1:G:13:GLY:N | 2.54 | 0.41 |
| 1:H:12:ASP:OD1 | 1:H:13:GLY:N | 2.54 | 0.41 |
| 2:A:1011:ARG:HG3 | 2:A:1014:GLN:NE2 | 2.36 | 0.41 |
| 2:A:1446:ILE:HG12 | 2:A:1542:ALA:HB2 | 2.02 | 0.41 |
| 2:A:2644:LEU:O | 2:A:2648:ILE:HG13 | 2.20 | 0.41 |
| 2:A:2782:MET:HG2 | 2:A:2787:TRP:HE3 | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:2990:LEU:HD12 | 2:A:2990:LEU:O | 2.21 | 0.41 |
| 2:A:3041:ASP:HA | 2:A:3117:PHE:HE2 | 1.86 | 0.41 |
| 2:A:3178:HIS:HB2 | 2:A:3265:CYS:HA | 2.02 | 0.41 |
| 2:A:3669:LEU:HD23 | 2:A:3669:LEU:HA | 1.95 | 0.41 |
| 2:A:3689:MET:HA | 2:A:3689:MET:CE | 2.51 | 0.41 |
| 2:B:436:LEU:HG | 2:B:445:VAL:HG11 | 2.03 | 0.41 |
| 2:B:614:LEU:HD22 | 2:B:632:ILE:HG12 | 2.03 | 0.41 |
| 2:B:1029:ASN:OD1 | 2:B:1030:PRO:HD2 | 2.20 | 0.41 |
| 2:B:1446:ILE:HG12 | 2:B:1542:ALA:HB2 | 2.02 | 0.41 |
| 2:B:1726:ILE:HD11 | 2:B:2165:LEU:HD21 | 2.03 | 0.41 |
| 2:B:2644:LEU:O | 2:B:2648:ILE:HG13 | 2.21 | 0.41 |
| 2:B:2694:SER:HA | 2:B:2704:GLN:HE22 | 1.85 | 0.41 |
| 2:B:2927:GLN:HG3 | 2:B:2931:ARG:NE | 2.35 | 0.41 |
| 2:B:3072:MET:SD | 2:B:3136:SER:HA | 2.61 | 0.41 |
| 2:B:3100:ALA:C | 2:B:3103:PRO:HD2 | 2.41 | 0.41 |
| 2:B:4789:PHE:HB3 | 2:B:4792:PHE:HD2 | 1.86 | 0.41 |
| 2:C:269:VAL:HG12 | 2:C:269:VAL:O | 2.20 | 0.41 |
| 2:C:483:LYS:HE2 | 2:C:483:LYS:HB2 | 1.80 | 0.41 |
| 2:C:678:MET:SD | 2:C:801:ARG:NH2 | 2.93 | 0.41 |
| 2:C:1181:ILE:HG21 | 2:C:1189:GLU:HB3 | 2.02 | 0.41 |
| 2:C:1425:THR:HG22 | 2:C:1563:VAL:HG13 | 2.02 | 0.41 |
| 2:C:1576:LYS:HA | 2:C:1576:LYS:HD3 | 1.95 | 0.41 |
| 2:C:2134:MET:HA | 2:C:2134:MET:HE3 | 2.02 | 0.41 |
| 2:C:2445:ILE:HG22 | 2:C:2451:VAL:HG12 | 2.03 | 0.41 |
| 2:C:2782:MET:HG2 | 2:C:2787:TRP:HE3 | 1.86 | 0.41 |
| 2:C:3169:ALA:HB1 | 2:C:3245:TYR:OH | 2.21 | 0.41 |
| 2:C:3235:MET:SD | 2:C:3235:MET:N | 2.93 | 0.41 |
| 2:C:3717:LYS:O | 2:C:3721:LYS:HG3 | 2.21 | 0.41 |
| 2:C:3986:LEU:HD23 | 2:C:3986:LEU:HA | 1.83 | 0.41 |
| 2:C:4789:PHE:HB3 | 2:C:4792:PHE:HD2 | 1.86 | 0.41 |
| 2:C:4898:PHE:O | 2:C:4904:GLY:HA3 | 2.21 | 0.41 |
| 2:D:281:ARG:NH1 | 2:D:345:GLU:OE2 | 2.54 | 0.41 |
| 2:D:1777:GLN:O | 2:D:1778:TYR:HB2 | 2.20 | 0.41 |
| 2:D:2429:LEU:HD21 | 2:D:2483:PHE:CZ | 2.56 | 0.41 |
| 2:D:2658:GLU:OE1 | 2:D:2661:LEU:N | 2.34 | 0.41 |
| 2:D:2827:ASP:O | 2:D:2831:VAL:HG23 | 2.21 | 0.41 |
| 2:D:3072:MET:SD | 2:D:3136:SER:HA | 2.61 | 0.41 |
| 2:D:4827:ILE:O | 2:D:4831:ILE:HG12 | 2.21 | 0.41 |
| 2:A:694:ARG:HD2 | 2:A:718:VAL:O | 2.20 | 0.40 |
| 2:A:906:PRO:HB2 | 2:A:907:VAL:HG23 | 2.03 | 0.40 |
| 2:A:1011:ARG:CB | 2:A:1032:LEU:HD21 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:1425:THR:HG22 | 2:A:1563:VAL:HG13 | 2.02 | 0.40 |
| 2:A:1730:THR:HG22 | 2:A:1731:GLU:N | 2.36 | 0.40 |
| 2:A:1929:SER:HG | 2:A:3620:PHE:HD2 | 1.65 | 0.40 |
| 2:A:2420:ARG:HD3 | 2:A:2424:ARG:NE | 2.37 | 0.40 |
| 2:A:4058:TYR:HD1 | 2:A:4062:GLU:HB3 | 1.84 | 0.40 |
| 2:B:249:SER:HA | 2:B:272:ARG:HD2 | 2.03 | 0.40 |
| 2:B:897:LYS:HB3 | 2:B:902:TRP:HB3 | 2.03 | 0.40 |
| 2:B:916:PRO:HB3 | 2:B:923:LYS:HZ3 | 1.85 | 0.40 |
| 2:B:919:VAL:HG12 | 2:B:920:GLU:N | 2.36 | 0.40 |
| 2:B:3975:GLN:O | 2:B:3979:VAL:HG23 | 2.20 | 0.40 |
| 2:B:4753:LEU:HD12 | 2:B:4753:LEU:HA | 1.91 | 0.40 |
| 2:C:1559:ARG:HB3 | 2:C:1565:PRO:HB3 | 2.03 | 0.40 |
| 2:C:1914:CYS:SG | 2:C:2091:GLN:NE2 | 2.89 | 0.40 |
| 2:C:2137:GLU:HG2 | 2:C:2138:GLU:N | 2.35 | 0.40 |
| 2:C:2409:ILE:HG12 | 2:C:2420:ARG:NH2 | 2.36 | 0.40 |
| 2:C:2891:ASP:OD1 | 2:C:2892:ILE:N | 2.54 | 0.40 |
| 2:C:3150:ARG:NH2 | 2:C:3151:GLN:HB3 | 2.36 | 0.40 |
| 2:C:3260:ARG:HH12 | 2:C:3265:CYS:H | 1.68 | 0.40 |
| 2:C:4563:GLU:HG2 | 2:C:4566:GLY:H | 1.86 | 0.40 |
| 2:D:21:VAL:HG23 | 2:D:215:ALA:HB3 | 2.03 | 0.40 |
| 2:D:324:VAL:O | 2:D:328:ALA:HB2 | 2.21 | 0.40 |
| 2:D:520:ARG:HH11 | 2:D:521:GLU:HB3 | 1.85 | 0.40 |
| 2:D:521:GLU:HG2 | 2:D:522:ALA:N | 2.34 | 0.40 |
| 2:D:1100:ARG:HG2 | 2:D:1167:ASP:OD1 | 2.21 | 0.40 |
| 2:D:2187:ILE:HG13 | 2:D:2227:VAL:HG13 | 2.01 | 0.40 |
| 2:D:2798:MET:HA | 2:D:2798:MET:CE | 2.51 | 0.40 |
| 2:D:2927:GLN:HG3 | 2:D:2931:ARG:NE | 2.35 | 0.40 |
| 2:D:2990:LEU:HD12 | 2:D:2990:LEU:O | 2.21 | 0.40 |
| 2:D:3130:CYS:HA | 2:D:3133:ILE:HD12 | 2.02 | 0.40 |
| 2:D:3172:GLU:O | 2:D:3176:ASP:N | 2.54 | 0.40 |
| 2:D:3271:GLU:O | 2:D:3275:THR:HG23 | 2.21 | 0.40 |
| 2:D:3664:LEU:HD21 | 2:D:3731:LEU:HD23 | 2.02 | 0.40 |
| 2:D:4609:LYS:HD2 | 2:D:4615:LEU:HD13 | 2.02 | 0.40 |
| 2:D:4751:LYS:HG3 | 2:D:4754:ARG:HH12 | 1.86 | 0.40 |
| 2:D:4789:PHE:HB3 | 2:D:4792:PHE:HD2 | 1.86 | 0.40 |
| 2:A:674:TYR:OH | 2:A:676:GLU:OE1 | 2.31 | 0.40 |
| 2:A:889:ILE:HA | 2:A:892:LEU:HB2 | 2.04 | 0.40 |
| 2:A:2399:LEU:HD12 | 2:A:2427:ILE:HD11 | 2.02 | 0.40 |
| 2:A:2488:LEU:HD23 | 2:A:2544:LEU:HD21 | 2.03 | 0.40 |
| 2:A:2555:LEU:O | 2:A:2561:LEU:HD11 | 2.21 | 0.40 |
| 2:A:2736:LYS:HA | 2:A:2736:LYS:HD3 | 1.82 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:A:2827:ASP:O | 2:A:2831:VAL:HG23 | 2.21 | 0.40 |
| 2:A:3145:SER:O | 2:A:3148:VAL:HG12 | 2.20 | 0.40 |
| 2:A:3184:TYR:HB3 | 2:A:3192:ARG:NH2 | 2.36 | 0.40 |
| 2:A:3796:LEU:HD22 | 2:A:3835:PHE:HZ | 1.86 | 0.40 |
| 2:A:4827:ILE:O | 2:A:4831:ILE:HG12 | 2.21 | 0.40 |
| 2:B:742:SER:HA | 2:B:746:GLN:NE2 | 2.36 | 0.40 |
| 2:B:756:SER:OG | 2:B:769:ARG:HB2 | 2.20 | 0.40 |
| 2:B:2849:HIS:NE2 | 2:B:2877:LEU:HD11 | 2.36 | 0.40 |
| 2:B:3150:ARG:NH2 | 2:B:3151:GLN:HB3 | 2.36 | 0.40 |
| 2:B:3166:PHE:CG | 2:B:3167:PRO:HD2 | 2.55 | 0.40 |
| 2:B:3172:GLU:O | 2:B:3176:ASP:N | 2.54 | 0.40 |
| 2:B:3796:LEU:HD22 | 2:B:3835:PHE:HZ | 1.86 | 0.40 |
| 2:C:614:LEU:HD22 | 2:C:632:ILE:HG12 | 2.02 | 0.40 |
| 2:C:1011:ARG:HG3 | 2:C:1014:GLN:NE2 | 2.36 | 0.40 |
| 2:C:1029:ASN:HD21 | 2:C:1031:ARG:HB2 | 1.86 | 0.40 |
| 2:C:1255:LEU:HG | 2:C:1451:HIS:HB3 | 2.03 | 0.40 |
| 2:C:1730:THR:HG22 | 2:C:1731:GLU:H | 1.86 | 0.40 |
| 2:C:1921:ARG:O | 2:C:1925:ILE:HG13 | 2.21 | 0.40 |
| 2:C:3130:CYS:HA | 2:C:3133:ILE:HD12 | 2.02 | 0.40 |
| 2:C:3233:HIS:O | 2:C:3236:GLU:HG2 | 2.20 | 0.40 |
| 2:C:3288:LEU:HB2 | 2:C:3329:LYS:NZ | 2.36 | 0.40 |
| 2:C:4093:ASP:OD1 | 2:C:4094:ILE:HG13 | 2.21 | 0.40 |
| 2:D:2891:ASP:OD1 | 2:D:2892:ILE:N | 2.54 | 0.40 |
| 2:D:3107:SER:HA | 2:D:3110:GLU:HG2 | 2.03 | 0.40 |
| 2:D:3184:TYR:HB3 | 2:D:3192:ARG:NH2 | 2.36 | 0.40 |
| 2:D:3278:GLY:O | 2:D:3282:LYS:HG2 | 2.21 | 0.40 |
| 2:D:3796:LEU:HD22 | 2:D:3835:PHE:HZ | 1.85 | 0.40 |
| 2:D:4698:LEU:HD23 | 2:D:4698:LEU:HA | 1.95 | 0.40 |
| 2:D:4925:LEU:HD12 | 2:D:4925:LEU:HA | 1.89 | 0.40 |
| 2:A:505:LEU:HA | 2:A:505:LEU:HD23 | 1.88 | 0.40 |
| 2:A:555:LEU:HD11 | 2:A:578:VAL:HG11 | 2.02 | 0.40 |
| 2:A:1921:ARG:O | 2:A:1925:ILE:HG13 | 2.21 | 0.40 |
| 2:A:3906:PHE:HB3 | 2:A:3967:LEU:HD11 | 2.03 | 0.40 |
| 2:B:21:VAL:HG23 | 2:B:215:ALA:HB3 | 2.03 | 0.40 |
| 2:B:623:VAL:HA | 2:B:2131:SER:O | 2.22 | 0.40 |
| 2:B:644:LEU:HD13 | 2:B:1630:LEU:HD21 | 2.03 | 0.40 |
| 2:B:655:MET:SD | 2:B:836:HIS:HA | 2.61 | 0.40 |
| 2:B:1040:ASP:HA | 2:B:1043:LYS:HE2 | 2.02 | 0.40 |
| 2:B:1685:LEU:HD22 | 2:B:1706:LEU:HB2 | 2.03 | 0.40 |
| 2:B:1777:GLN:O | 2:B:1778:TYR:HB2 | 2.20 | 0.40 |
| 2:B:1921:ARG:O | 2:B:1925:ILE:HG13 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:2666:LEU:HB3 | 2:B:2667:PRO:HD3 | 2.04 | 0.40 |
| 2:B:3144:LYS:HE3 | 2:B:3233:HIS:NE2 | 2.35 | 0.40 |
| 2:B:3208:ILE:HA | 2:B:3209:PRO:HD3 | 1.96 | 0.40 |
| 2:B:3235:MET:SD | 2:B:3235:MET:N | 2.93 | 0.40 |
| 2:B:4625:ASP:OD1 | 2:B:4625:ASP:N | 2.46 | 0.40 |
| 2:C:258:ARG:HH12 | 2:C:317:MET:HA | 1.87 | 0.40 |
| 2:C:644:LEU:HD13 | 2:C:1630:LEU:HD21 | 2.04 | 0.40 |
| 2:C:888:ASN:ND2 | 2:C:1060:TYR:OH | 2.23 | 0.40 |
| 2:C:897:LYS:HB3 | 2:C:902:TRP:HB3 | 2.03 | 0.40 |
| 2:C:1610:ARG:HD3 | 2:C:1617:TRP:CE2 | 2.56 | 0.40 |
| 2:C:1914:CYS:O | 2:C:1918:VAL:HG23 | 2.21 | 0.40 |
| 2:C:1971:GLU:HA | 2:C:1974:ASN:ND2 | 2.36 | 0.40 |
| 2:C:1986:CYS:HA | 2:C:1987:PRO:HD3 | 1.91 | 0.40 |
| 2:C:2666:LEU:HB3 | 2:C:2667:PRO:HD3 | 2.04 | 0.40 |
| 2:C:3890:TRP:HB3 | 2:D:76:ARG:HG2 | 2.03 | 0.40 |
| 2:C:3906:PHE:HB3 | 2:C:3967:LEU:HD11 | 2.03 | 0.40 |
| 2:C:4841:ILE:HD12 | 2:C:4841:ILE:HA | 1.98 | 0.40 |
| 2:D:644:LEU:HD13 | 2:D:1630:LEU:HD21 | 2.03 | 0.40 |
| 2:D:889:ILE:HA | 2:D:892:LEU:HB2 | 2.04 | 0.40 |
| 2:D:1100:ARG:HB3 | 2:D:1236:TYR:CD1 | 2.57 | 0.40 |
| 2:D:2555:LEU:O | 2:D:2561:LEU:HD11 | 2.21 | 0.40 |
| 2:D:3169:ALA:HB1 | 2:D:3245:TYR:OH | 2.21 | 0.40 |
| 2:D:4898:PHE:O | 2:D:4904:GLY:HA3 | 2.21 | 0.40 |
| 2:A:614:LEU:HD22 | 2:A:632:ILE:HG12 | 2.02 | 0.40 |
| 2:A:1019:GLY:HA3 | 2:A:1028:ARG:HB3 | 2.02 | 0.40 |
| 2:A:1100:ARG:HB3 | 2:A:1236:TYR:CD1 | 2.57 | 0.40 |
| 2:A:1255:LEU:HD12 | 2:A:1255:LEU:HA | 1.91 | 0.40 |
| 2:A:2429:LEU:HA | 2:A:2476:TYR:HE2 | 1.87 | 0.40 |
| 2:A:2933:VAL:HG22 | 2:A:2963:PHE:HZ | 1.86 | 0.40 |
| 2:A:2943:PHE:HD1 | 2:A:2954:PHE:CE2 | 2.39 | 0.40 |
| 2:A:3271:GLU:O | 2:A:3275:THR:HG23 | 2.20 | 0.40 |
| 2:A:3288:LEU:HB2 | 2:A:3329:LYS:NZ | 2.36 | 0.40 |
| 2:B:42:PHE:HZ | 2:B:459:LEU:HG | 1.86 | 0.40 |
| 2:B:869:THR:OG1 | 2:B:941:LYS:HB3 | 2.21 | 0.40 |
| 2:B:1730:THR:HG22 | 2:B:1731:GLU:H | 1.86 | 0.40 |
| 2:B:1956:ALA:O | 2:B:1960:ARG:HG3 | 2.22 | 0.40 |
| 2:B:2200:LEU:HD23 | 2:B:2200:LEU:HA | 1.93 | 0.40 |
| 2:B:2748:SER:HB3 | 2:B:2751:SER:HB3 | 2.03 | 0.40 |
| 2:B:2798:MET:HA | 2:B:2798:MET:CE | 2.52 | 0.40 |
| 2:B:2833:LEU:HB2 | 2:B:2894:LYS:HZ3 | 1.85 | 0.40 |
| 2:B:3041:ASP:HA | 2:B:3117:PHE:HE2 | 1.86 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:3159:LEU:HG | 2:B:3241:MET:HB3 | 2.04 | 0.40 |
| 2:B:3319:PHE:O | 2:B:3322:LEU:N | 2.54 | 0.40 |
| 2:C:324:VAL:O | 2:C:328:ALA:HB2 | 2.21 | 0.40 |
| 2:C:555:LEU:HD11 | 2:C:578:VAL:HG11 | 2.02 | 0.40 |
| 2:C:686:VAL:HG13 | 2:C:687:THR:HG23 | 2.04 | 0.40 |
| 2:C:1100:ARG:HG2 | 2:C:1167:ASP:OD1 | 2.21 | 0.40 |
| 2:C:1268:ILE:HG21 | 2:C:1302:TYR:HE1 | 1.86 | 0.40 |
| 2:C:2488:LEU:HD23 | 2:C:2544:LEU:HD21 | 2.03 | 0.40 |
| 2:C:2827:ASP:O | 2:C:2831:VAL:HG23 | 2.21 | 0.40 |
| 2:D:42:PHE:HZ | 2:D:459:LEU:HG | 1.86 | 0.40 |
| 2:D:983:LEU:HD12 | 2:D:983:LEU:HA | 1.94 | 0.40 |
| 2:D:1168:MET:HE3 | 2:D:1197:VAL:HG22 | 2.03 | 0.40 |
| 2:D:1730:THR:HG22 | 2:D:1731:GLU:N | 2.36 | 0.40 |
| 2:D:1914:CYS:O | 2:D:1918:VAL:HG23 | 2.21 | 0.40 |
| 2:D:1956:ALA:O | 2:D:1960:ARG:HG3 | 2.22 | 0.40 |
| 2:D:1971:GLU:HA | 2:D:1974:ASN:ND2 | 2.36 | 0.40 |
| 2:D:2134:MET:HE3 | 2:D:2134:MET:HA | 2.04 | 0.40 |
| 2:D:2638:LEU:HD23 | 2:D:2638:LEU:HA | 1.93 | 0.40 |
| 2:D:3717:LYS:O | 2:D:3721:LYS:HG3 | 2.21 | 0.40 |
| 1:F:88:HIS:HD2 | 1:F:89:PRO:HD2 | 1.87 | 0.40 |
| 2:A:1719:LEU:HD21 | 2:A:1830:ILE:HD12 | 2.04 | 0.40 |
| 2:A:2095:ILE:HD12 | 2:A:2095:ILE:HA | 1.93 | 0.40 |
| 2:A:2488:LEU:HG | 2:A:2544:LEU:HD11 | 2.03 | 0.40 |
| 2:A:2518:ARG:O | 2:A:2522:THR:OG1 | 2.36 | 0.40 |
| 2:A:3172:GLU:O | 2:A:3176:ASP:N | 2.54 | 0.40 |
| 2:A:4563:GLU:HG2 | 2:A:4566:GLY:H | 1.86 | 0.40 |
| 2:A:4843:ARG:NH1 | 2:A:4847:ASP:OD2 | 2.54 | 0.40 |
| 2:B:672:LYS:NZ | 2:B:818:GLY:HA3 | 2.35 | 0.40 |
| 2:B:988:LEU:HB2 | 2:B:1055:ARG:NE | 2.26 | 0.40 |
| 2:B:1100:ARG:HG2 | 2:B:1167:ASP:OD1 | 2.21 | 0.40 |
| 2:B:2581:ARG:HB3 | 2:B:2584:MET:HE2 | 2.03 | 0.40 |
| 2:B:2933:VAL:HG22 | 2:B:2963:PHE:HZ | 1.86 | 0.40 |
| 2:B:3068:LEU:O | 2:B:3072:MET:HG2 | 2.22 | 0.40 |
| 2:B:3169:ALA:HB1 | 2:B:3245:TYR:OH | 2.21 | 0.40 |
| 2:B:4563:GLU:HG2 | 2:B:4566:GLY:H | 1.86 | 0.40 |
| 2:B:4751:LYS:HG3 | 2:B:4754:ARG:HH12 | 1.86 | 0.40 |
| 2:C:281:ARG:NH1 | 2:C:345:GLU:OE2 | 2.54 | 0.40 |
| 2:C:1011:ARG:CB | 2:C:1032:LEU:HD21 | 2.51 | 0.40 |
| 2:C:1040:ASP:HA | 2:C:1043:LYS:HE2 | 2.02 | 0.40 |
| 2:C:1940:GLN:NE2 | 2:C:1964:GLU:OE2 | 2.55 | 0.40 |
| 2:C:3100:ALA:C | 2:C:3103:PRO:HD2 | 2.42 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:3172:GLU:O | 2:C:3176:ASP:N | 2.55 | 0.40 |
| 2:C:4827:ILE:O | 2:C:4831:ILE:HG12 | 2.21 | 0.40 |
| 2:D:387:ILE:HD11 | 2:D:389:ARG:CZ | 2.52 | 0.40 |
| 2:D:1011:ARG:HG3 | 2:D:1014:GLN:NE2 | 2.36 | 0.40 |
| 2:D:2619:LYS:O | 2:D:2626:GLY:HA2 | 2.22 | 0.40 |
| 2:D:2649:PHE:CE2 | 2:D:2932:TYR:HE2 | 2.38 | 0.40 |
| 2:D:3689:MET:HA | 2:D:3689:MET:CE | 2.51 | 0.40 |
| 2:D:3975:GLN:O | 2:D:3979:VAL:HG23 | 2.20 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | E | 105/108 (97%) | 103 (98%) | 2 (2%) | 0 | 100 | 100 |
| 1 | F | 105/108 (97%) | 103 (98%) | 2 (2%) | 0 | 100 | 100 |
| 1 | G | 105/108 (97%) | 103 (98%) | 2 (2%) | 0 | 100 | 100 |
| 1 | H | 105/108 (97%) | 103 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | A | 4198/4967 (84%) | 4061 (97%) | 132 (3%) | 5 (0%) | 51 | 84 |
| 2 | B | 4198/4967 (84%) | 4061 (97%) | 132 (3%) | 5 (0%) | 51 | 84 |
| 2 | C | 4198/4967 (84%) | 4061 (97%) | 132 (3%) | 5 (0%) | 51 | 84 |
| 2 | D | 4198/4967 (84%) | 4060 (97%) | 133 (3%) | 5 (0%) | 51 | 84 |
| All | All | 17212/20300 (85%) | 16655 (97%) | 537 (3%) | 20 (0%) | 54 | 84 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 3927 | PRO |
| 2 | A | 4641 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 3927 | PRO |
| 2 | B | 4641 | PRO |
| 2 | C | 3927 | PRO |
| 2 | C | 4641 | PRO |
| 2 | D | 3927 | PRO |
| 2 | D | 4641 | PRO |
| 2 | A | 3262 | GLU |
| 2 | B | 3262 | GLU |
| 2 | C | 3262 | GLU |
| 2 | D | 3262 | GLU |
| 2 | A | 3292 | GLU |
| 2 | B | 3292 | GLU |
| 2 | C | 3292 | GLU |
| 2 | D | 3292 | GLU |
| 2 | A | 1836 | ASN |
| 2 | B | 1836 | ASN |
| 2 | C | 1836 | ASN |
| 2 | D | 1836 | ASN |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | E | 88/89 (99%) | 87 (99%) | 1 (1%) | 73 | 88 |
| 1 | F | 88/89 (99%) | 87 (99%) | 1 (1%) | 73 | 88 |
| 1 | G | 88/89 (99%) | 87 (99%) | 1 (1%) | 73 | 88 |
| 1 | H | 88/89 (99%) | 87 (99%) | 1 (1%) | 73 | 88 |
| 2 | A | 3708/4358 (85%) | 3667 (99%) | 41 (1%) | 73 | 88 |
| 2 | B | 3708/4358 (85%) | 3667 (99%) | 41 (1%) | 73 | 88 |
| 2 | C | 3708/4358 (85%) | 3667 (99%) | 41 (1%) | 73 | 88 |
| 2 | D | 3708/4358 (85%) | 3667 (99%) | 41 (1%) | 73 | 88 |
| All | All | 15184/17788 (85%) | 15016 (99%) | 168 (1%) | 74 | 88 |

All (168) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 19 | LYS |
| 1 | F | 19 | LYS |
| 1 | G | 19 | LYS |
| 1 | H | 19 | LYS |
| 2 | A | 325 | LYS |
| 2 | A | 344 | LYS |
| 2 | A | 520 | ARG |
| 2 | A | 880 | ARG |
| 2 | A | 891 | GLU |
| 2 | A | 893 | TRP |
| 2 | A | 894 | VAL |
| 2 | A | 917 | CYS |
| 2 | A | 931 | TYR |
| 2 | A | 935 | MET |
| 2 | A | 944 | LEU |
| 2 | A | 1011 | ARG |
| 2 | A | 1017 | THR |
| 2 | A | 1021 | GLN |
| 2 | A | 1043 | LYS |
| 2 | A | 1044 | LYS |
| 2 | A | 1046 | ASN |
| 2 | A | 1048 | ASP |
| 2 | A | 1049 | SER |
| 2 | A | 1050 | LEU |
| 2 | A | 2134 | MET |
| 2 | A | 2144 | ARG |
| 2 | A | 2303 | ARG |
| 2 | A | 2347 | MET |
| 2 | A | 2581 | ARG |
| 2 | A | 2585 | MET |
| 2 | A | 2605 | MET |
| 2 | A | 2656 | LYS |
| 2 | A | 2689 | MET |
| 2 | A | 2798 | MET |
| 2 | A | 2830 | ASN |
| 2 | A | 2884 | LYS |
| 2 | A | 2931 | ARG |
| 2 | A | 3088 | LYS |
| 2 | A | 3150 | ARG |
| 2 | A | 3227 | ARG |
| 2 | A | 3262 | GLU |
| 2 | A | 3819 | MET |
| 2 | A | 4012 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 4683 | ARG |
| 2 | A | 4707 | MET |
| 2 | B | 325 | LYS |
| 2 | B | 344 | LYS |
| 2 | B | 520 | ARG |
| 2 | B | 880 | ARG |
| 2 | B | 891 | GLU |
| 2 | B | 893 | TRP |
| 2 | B | 894 | VAL |
| 2 | B | 917 | CYS |
| 2 | B | 931 | TYR |
| 2 | B | 935 | MET |
| 2 | B | 944 | LEU |
| 2 | B | 1011 | ARG |
| 2 | B | 1017 | THR |
| 2 | B | 1021 | GLN |
| 2 | B | 1043 | LYS |
| 2 | B | 1044 | LYS |
| 2 | B | 1046 | ASN |
| 2 | B | 1048 | ASP |
| 2 | B | 1049 | SER |
| 2 | B | 1050 | LEU |
| 2 | B | 2134 | MET |
| 2 | B | 2144 | ARG |
| 2 | B | 2303 | ARG |
| 2 | B | 2347 | MET |
| 2 | B | 2581 | ARG |
| 2 | B | 2585 | MET |
| 2 | B | 2605 | MET |
| 2 | B | 2656 | LYS |
| 2 | B | 2689 | MET |
| 2 | B | 2798 | MET |
| 2 | B | 2830 | ASN |
| 2 | B | 2884 | LYS |
| 2 | B | 2931 | ARG |
| 2 | B | 3088 | LYS |
| 2 | B | 3150 | ARG |
| 2 | B | 3227 | ARG |
| 2 | B | 3262 | GLU |
| 2 | B | 3819 | MET |
| 2 | B | 4012 | MET |
| 2 | B | 4683 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 4707 | MET |
| 2 | C | 325 | LYS |
| 2 | C | 344 | LYS |
| 2 | C | 520 | ARG |
| 2 | C | 880 | ARG |
| 2 | C | 891 | GLU |
| 2 | C | 893 | TRP |
| 2 | C | 894 | VAL |
| 2 | C | 917 | CYS |
| 2 | C | 931 | TYR |
| 2 | C | 935 | MET |
| 2 | C | 944 | LEU |
| 2 | C | 1011 | ARG |
| 2 | C | 1017 | THR |
| 2 | C | 1021 | GLN |
| 2 | C | 1043 | LYS |
| 2 | C | 1044 | LYS |
| 2 | C | 1046 | ASN |
| 2 | C | 1048 | ASP |
| 2 | C | 1049 | SER |
| 2 | C | 1050 | LEU |
| 2 | C | 2134 | MET |
| 2 | C | 2144 | ARG |
| 2 | C | 2303 | ARG |
| 2 | C | 2347 | MET |
| 2 | C | 2581 | ARG |
| 2 | C | 2585 | MET |
| 2 | C | 2605 | MET |
| 2 | C | 2656 | LYS |
| 2 | C | 2689 | MET |
| 2 | C | 2798 | MET |
| 2 | C | 2830 | ASN |
| 2 | C | 2884 | LYS |
| 2 | C | 2931 | ARG |
| 2 | C | 3088 | LYS |
| 2 | C | 3150 | ARG |
| 2 | C | 3227 | ARG |
| 2 | C | 3262 | GLU |
| 2 | C | 3819 | MET |
| 2 | C | 4012 | MET |
| 2 | C | 4683 | ARG |
| 2 | C | 4707 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 325 | LYS |
| 2 | D | 344 | LYS |
| 2 | D | 520 | ARG |
| 2 | D | 880 | ARG |
| 2 | D | 891 | GLU |
| 2 | D | 893 | TRP |
| 2 | D | 894 | VAL |
| 2 | D | 917 | CYS |
| 2 | D | 931 | TYR |
| 2 | D | 935 | MET |
| 2 | D | 944 | LEU |
| 2 | D | 1011 | ARG |
| 2 | D | 1017 | THR |
| 2 | D | 1021 | GLN |
| 2 | D | 1043 | LYS |
| 2 | D | 1044 | LYS |
| 2 | D | 1046 | ASN |
| 2 | D | 1048 | ASP |
| 2 | D | 1049 | SER |
| 2 | D | 1050 | LEU |
| 2 | D | 2134 | MET |
| 2 | D | 2144 | ARG |
| 2 | D | 2303 | ARG |
| 2 | D | 2347 | MET |
| 2 | D | 2581 | ARG |
| 2 | D | 2585 | MET |
| 2 | D | 2605 | MET |
| 2 | D | 2656 | LYS |
| 2 | D | 2689 | MET |
| 2 | D | 2798 | MET |
| 2 | D | 2830 | ASN |
| 2 | D | 2884 | LYS |
| 2 | D | 2931 | ARG |
| 2 | D | 3088 | LYS |
| 2 | D | 3150 | ARG |
| 2 | D | 3227 | ARG |
| 2 | D | 3262 | GLU |
| 2 | D | 3819 | MET |
| 2 | D | 4012 | MET |
| 2 | D | 4683 | ARG |
| 2 | D | 4707 | MET |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 29 | HIS |
| 2 | A | 117 | HIS |
| 2 | A | 890 | HIS |
| 2 | A | 1014 | GLN |
| 2 | A | 1046 | ASN |
| 2 | A | 1974 | ASN |
| 2 | A | 1978 | ASN |
| 2 | A | 2830 | ASN |
| 2 | A | 2847 | ASN |
| 2 | A | 3034 | HIS |
| 2 | A | 3287 | ASN |
| 2 | A | 3850 | HIS |
| 2 | A | 3882 | GLN |
| 2 | B | 29 | HIS |
| 2 | B | 117 | HIS |
| 2 | B | 890 | HIS |
| 2 | B | 1014 | GLN |
| 2 | B | 1046 | ASN |
| 2 | B | 1974 | ASN |
| 2 | B | 1978 | ASN |
| 2 | B | 2830 | ASN |
| 2 | B | 2847 | ASN |
| 2 | B | 3034 | HIS |
| 2 | B | 3287 | ASN |
| 2 | B | 3850 | HIS |
| 2 | C | 29 | HIS |
| 2 | C | 117 | HIS |
| 2 | C | 890 | HIS |
| 2 | C | 1046 | ASN |
| 2 | C | 1974 | ASN |
| 2 | C | 1978 | ASN |
| 2 | C | 2830 | ASN |
| 2 | C | 2847 | ASN |
| 2 | C | 3034 | HIS |
| 2 | C | 3287 | ASN |
| 2 | C | 3850 | HIS |
| 2 | D | 29 | HIS |
| 2 | D | 117 | HIS |
| 2 | D | 890 | HIS |
| 2 | D | 1014 | GLN |
| 2 | D | 1046 | ASN |
| 2 | D | 1974 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | D | 1978 | ASN |
| 2 | D | 2830 | ASN |
| 2 | D | 2847 | ASN |
| 2 | D | 3034 | HIS |
| 2 | D | 3287 | ASN |
| 2 | D | 3850 | HIS |
| 2 | D | 3882 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 4 | ATP | D | 5002 | - | 26,33,33 | 0.61 | 0 | 31,52,52 | 0.82 | 2 (6%) |
| 4 | ATP | C | 5003 | - | 26,33,33 | 0.66 | 0 | 31,52,52 | 0.77 | 1 (3%) |
| 5 | KVR | C | 5004 | - | 24,25,25 | 0.50 | 0 | 32,34,34 | 0.83 | 2 (6%) |
| 4 | ATP | D | 5003 | - | 26,33,33 | 0.67 | 0 | 31,52,52 | 0.77 | 1 (3%) |
| 4 | ATP | C | 5002 | - | 26,33,33 | 0.61 | 0 | 31,52,52 | 0.81 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 4 | ATP | B | 5002 | - | 26,33,33 | 0.61 | 0 | 31,52,52 | 0.81 | 2 (6%) |
| 4 | ATP | A | 5002 | - | 26,33,33 | 0.61 | 0 | 31,52,52 | 0.82 | 2 (6%) |
| 4 | ATP | A | 5003 | - | 26,33,33 | 0.67 | 0 | 31,52,52 | 0.77 | 1 (3%) |
| 5 | KVR | D | 5004 | - | 24,25,25 | 0.49 | 0 | 32,34,34 | 0.83 | 2 (6%) |
| 5 | KVR | A | 5004 | - | 24,25,25 | 0.49 | 0 | 32,34,34 | 0.83 | 2 (6%) |
| 5 | KVR | B | 5004 | - | 24,25,25 | 0.48 | 0 | 32,34,34 | 0.83 | 2 (6%) |
| 4 | ATP | B | 5003 | - | 26,33,33 | 0.67 | 0 | 31,52,52 | 0.77 | 1 (3%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | ATP | D | 5002 | - | - | 5/18/38/38 | 0/3/3/3 |
| 4 | ATP | C | 5003 | - | - | 6/18/38/38 | 0/3/3/3 |
| 5 | KVR | C | 5004 | - | - | 6/10/20/20 | 0/2/3/3 |
| 4 | ATP | D | 5003 | - | - | 6/18/38/38 | 0/3/3/3 |
| 4 | ATP | C | 5002 | - | - | 5/18/38/38 | 0/3/3/3 |
| 4 | ATP | B | 5002 | - | - | 5/18/38/38 | 0/3/3/3 |
| 4 | ATP | A | 5002 | - | - | 5/18/38/38 | 0/3/3/3 |
| 4 | ATP | A | 5003 | - | - | 6/18/38/38 | 0/3/3/3 |
| 5 | KVR | D | 5004 | - | - | 6/10/20/20 | 0/2/3/3 |
| 5 | KVR | A | 5004 | - | - | 6/10/20/20 | 0/2/3/3 |
| 5 | KVR | B | 5004 | - | - | 6/10/20/20 | 0/2/3/3 |
| 4 | ATP | B | 5003 | - | - | 6/18/38/38 | 0/3/3/3 |

There are no bond length outliers.

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | C | 5004 | KVR | C10-S09-C06 | 3.24 | 107.30 | 102.71 |
| 5 | D | 5004 | KVR | C10-S09-C06 | 3.23 | 107.28 | 102.71 |
| 5 | A | 5004 | KVR | C10-S09-C06 | 3.22 | 107.28 | 102.71 |
| 5 | B | 5004 | KVR | C10-S09-C06 | 3.18 | 107.21 | 102.71 |
| 4 | A | 5002 | ATP | C5-C6-N6 | 2.30 | 123.84 | 120.35 |
| 4 | D | 5002 | ATP | C5-C6-N6 | 2.29 | 123.83 | 120.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | C | 5002 | ATP | C5-C6-N6 | 2.29 | 123.83 | 120.35 |
| 4 | C | 5003 | ATP | C5-C6-N6 | 2.28 | 123.81 | 120.35 |
| 4 | B | 5003 | ATP | C5-C6-N6 | 2.28 | 123.81 | 120.35 |
| 4 | B | 5002 | ATP | C5-C6-N6 | 2.27 | 123.80 | 120.35 |
| 4 | D | 5003 | ATP | C5-C6-N6 | 2.26 | 123.78 | 120.35 |
| 4 | A | 5003 | ATP | C5-C6-N6 | 2.25 | 123.77 | 120.35 |
| 5 | B | 5004 | KVR | C14-N12-C11 | 2.15 | 114.54 | 111.06 |
| 5 | D | 5004 | KVR | C14-N12-C11 | 2.11 | 114.49 | 111.06 |
| 5 | C | 5004 | KVR | C14-N12-C11 | 2.11 | 114.48 | 111.06 |
| 5 | A | 5004 | KVR | C14-N12-C11 | 2.11 | 114.47 | 111.06 |
| 4 | B | 5002 | ATP | PB-O3B-PG | 2.07 | 139.92 | 132.83 |
| 4 | A | 5002 | ATP | PB-O3B-PG | 2.07 | 139.92 | 132.83 |
| 4 | D | 5002 | ATP | PB-O3B-PG | 2.07 | 139.91 | 132.83 |
| 4 | C | 5002 | ATP | PB-O3B-PG | 2.06 | 139.90 | 132.83 |

There are no chirality outliers.

All (68) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | A | 5002 | ATP | C5'-O5'-PA-O2A |
| 4 | A | 5002 | ATP | C5'-O5'-PA-O3A |
| 4 | A | 5003 | ATP | C5'-O5'-PA-O1A |
| 4 | A | 5003 | ATP | C5'-O5'-PA-O2A |
| 4 | A | 5003 | ATP | O4'-C4'-C5'-O5' |
| 4 | B | 5002 | ATP | C5'-O5'-PA-O2A |
| 4 | B | 5002 | ATP | C5'-O5'-PA-O3A |
| 4 | B | 5003 | ATP | C5'-O5'-PA-O1A |
| 4 | B | 5003 | ATP | C5'-O5'-PA-O2A |
| 4 | B | 5003 | ATP | O4'-C4'-C5'-O5' |
| 4 | C | 5002 | ATP | C5'-O5'-PA-O2A |
| 4 | C | 5002 | ATP | C5'-O5'-PA-O3A |
| 4 | C | 5003 | ATP | C5'-O5'-PA-O1A |
| 4 | C | 5003 | ATP | C5'-O5'-PA-O2A |
| 4 | C | 5003 | ATP | O4'-C4'-C5'-O5' |
| 4 | D | 5002 | ATP | C5'-O5'-PA-O2A |
| 4 | D | 5002 | ATP | C5'-O5'-PA-O3A |
| 4 | D | 5003 | ATP | C5'-O5'-PA-O1A |
| 4 | D | 5003 | ATP | C5'-O5'-PA-O2A |
| 4 | D | 5003 | ATP | O4'-C4'-C5'-O5' |
| 5 | A | 5004 | KVR | C04-C03-O02-C01 |
| 5 | A | 5004 | KVR | C08-C03-O02-C01 |
| 5 | B | 5004 | KVR | C04-C03-O02-C01 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | B | 5004 | KVR | C08-C03-O02-C01 |
| 5 | C | 5004 | KVR | C04-C03-O02-C01 |
| 5 | C | 5004 | KVR | C08-C03-O02-C01 |
| 5 | D | 5004 | KVR | C04-C03-O02-C01 |
| 5 | D | 5004 | KVR | C08-C03-O02-C01 |
| 4 | A | 5002 | ATP | C3'-C4'-C5'-O5' |
| 4 | B | 5002 | ATP | C3'-C4'-C5'-O5' |
| 4 | C | 5002 | ATP | C3'-C4'-C5'-O5' |
| 4 | D | 5002 | ATP | C3'-C4'-C5'-O5' |
| 5 | A | 5004 | KVR | C19-C18-C21-O23 |
| 5 | C | 5004 | KVR | C19-C18-C21-O23 |
| 5 | D | 5004 | KVR | C19-C18-C21-O23 |
| 5 | B | 5004 | KVR | C19-C18-C21-O23 |
| 5 | A | 5004 | KVR | C17-C18-C21-O23 |
| 5 | B | 5004 | KVR | C17-C18-C21-O23 |
| 5 | C | 5004 | KVR | C17-C18-C21-O23 |
| 5 | D | 5004 | KVR | C17-C18-C21-O23 |
| 5 | A | 5004 | KVR | C19-C18-C21-O22 |
| 5 | B | 5004 | KVR | C19-C18-C21-O22 |
| 5 | C | 5004 | KVR | C19-C18-C21-O22 |
| 5 | D | 5004 | KVR | C19-C18-C21-O22 |
| 5 | A | 5004 | KVR | C17-C18-C21-O22 |
| 5 | D | 5004 | KVR | C17-C18-C21-O22 |
| 5 | B | 5004 | KVR | C17-C18-C21-O22 |
| 5 | C | 5004 | KVR | C17-C18-C21-O22 |
| 4 | A | 5002 | ATP | O4'-C4'-C5'-O5' |
| 4 | B | 5002 | ATP | O4'-C4'-C5'-O5' |
| 4 | C | 5002 | ATP | O4'-C4'-C5'-O5' |
| 4 | D | 5002 | ATP | O4'-C4'-C5'-O5' |
| 4 | A | 5003 | ATP | C5'-O5'-PA-O3A |
| 4 | B | 5003 | ATP | C5'-O5'-PA-O3A |
| 4 | C | 5003 | ATP | C5'-O5'-PA-O3A |
| 4 | D | 5003 | ATP | C5'-O5'-PA-O3A |
| 4 | A | 5002 | ATP | C5'-O5'-PA-O1A |
| 4 | B | 5002 | ATP | C5'-O5'-PA-O1A |
| 4 | C | 5002 | ATP | C5'-O5'-PA-O1A |
| 4 | D | 5002 | ATP | C5'-O5'-PA-O1A |
| 4 | A | 5003 | ATP | C3'-C4'-C5'-O5' |
| 4 | B | 5003 | ATP | C3'-C4'-C5'-O5' |
| 4 | C | 5003 | ATP | C3'-C4'-C5'-O5' |
| 4 | D | 5003 | ATP | C3'-C4'-C5'-O5' |
| 4 | A | 5003 | ATP | PA-O3A-PB-O2B |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | B | 5003 | ATP | PA-O3A-PB-O2B |
| 4 | C | 5003 | ATP | PA-O3A-PB-O2B |
| 4 | D | 5003 | ATP | PA-O3A-PB-O2B |

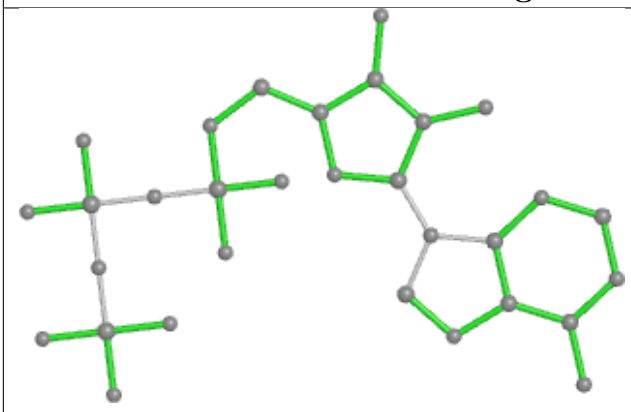
There are no ring outliers.

8 monomers are involved in 16 short contacts:

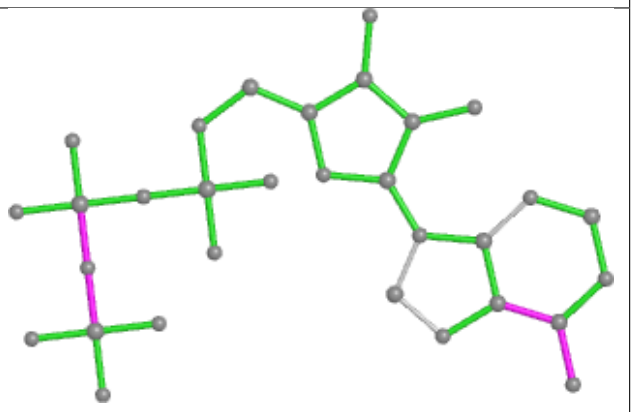
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | C | 5003 | ATP | 3 | 0 |
| 5 | C | 5004 | KVR | 2 | 0 |
| 4 | D | 5003 | ATP | 3 | 0 |
| 4 | A | 5003 | ATP | 3 | 0 |
| 5 | D | 5004 | KVR | 2 | 0 |
| 5 | A | 5004 | KVR | 2 | 0 |
| 5 | B | 5004 | KVR | 2 | 0 |
| 4 | B | 5003 | ATP | 3 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

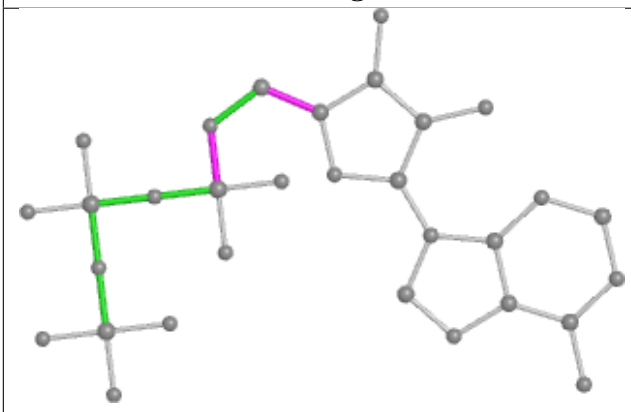
**Ligand ATP D 5002**



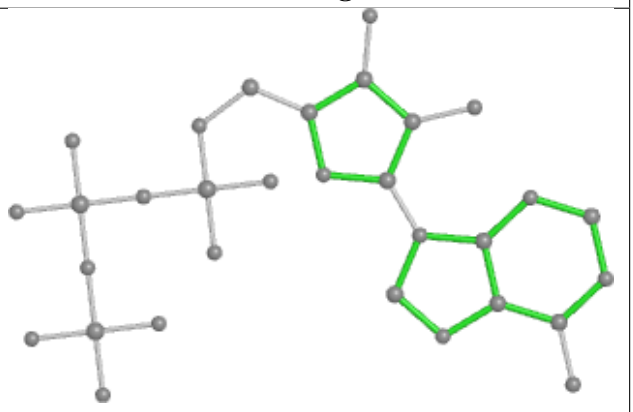
Bond lengths



Bond angles

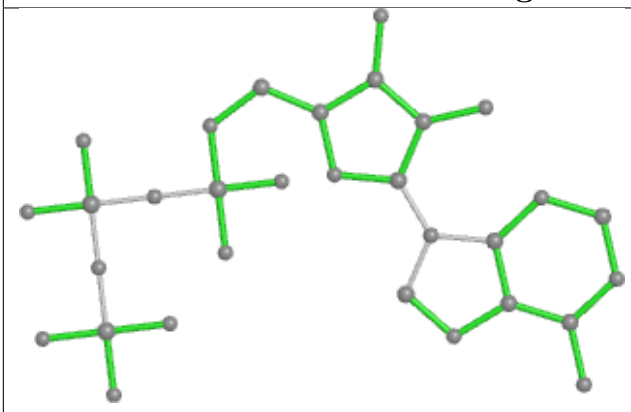


Torsions

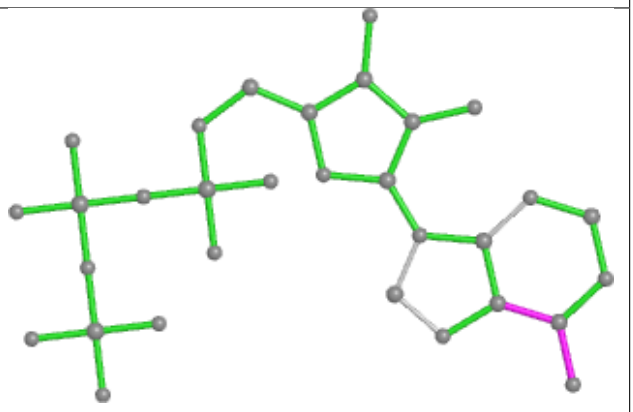


Rings

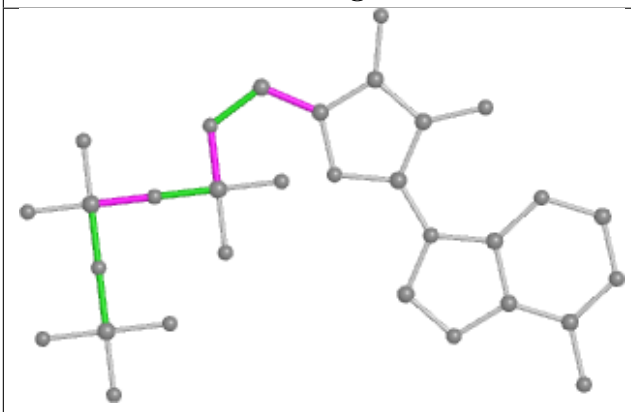
## Ligand ATP C 5003



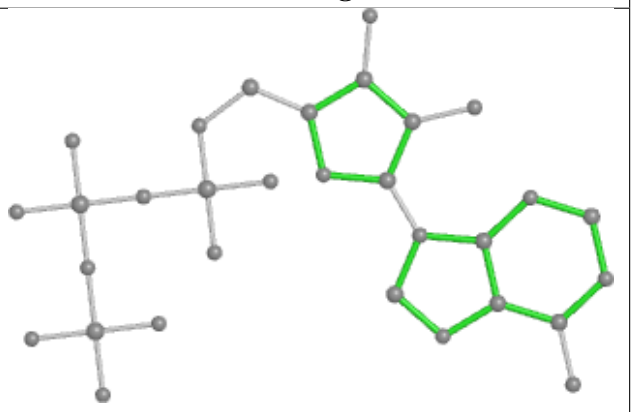
Bond lengths



Bond angles

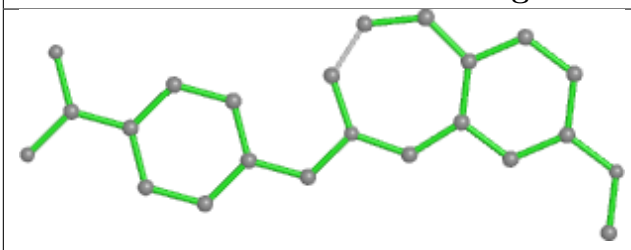


Torsions

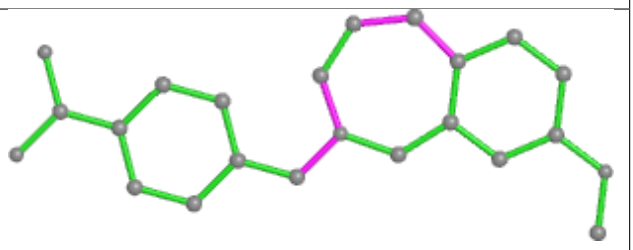


Rings

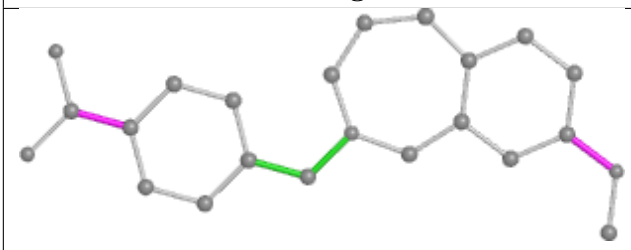
## Ligand KVR C 5004



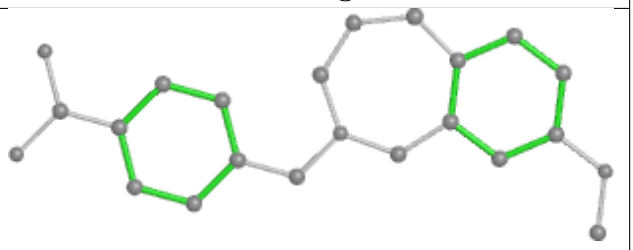
Bond lengths



Bond angles

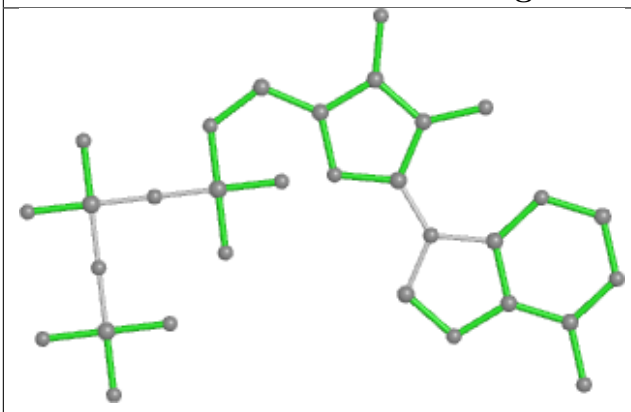


Torsions

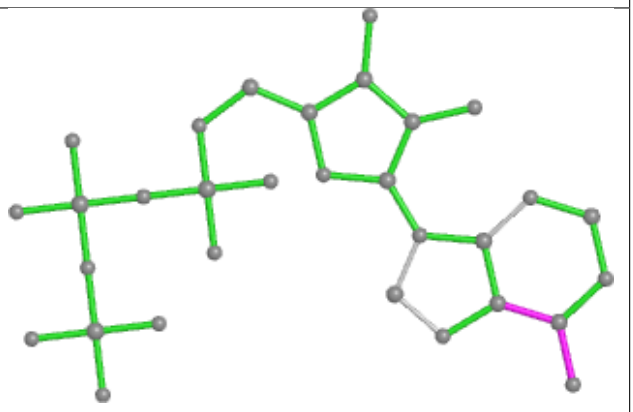


Rings

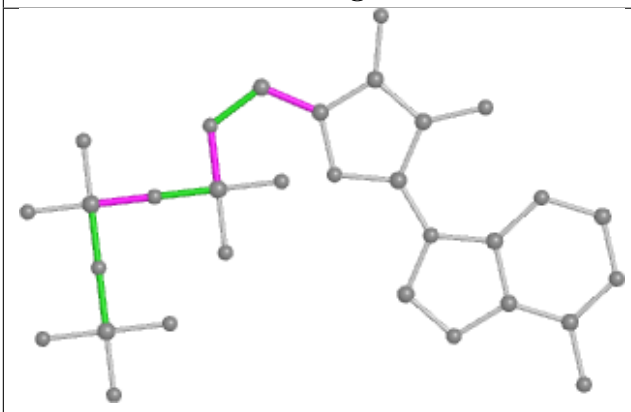
**Ligand ATP D 5003**



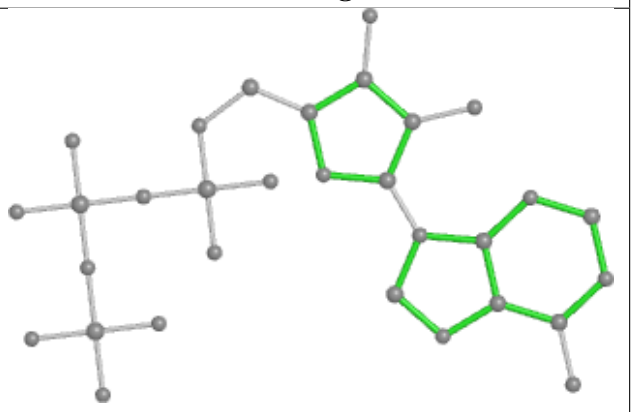
Bond lengths



Bond angles

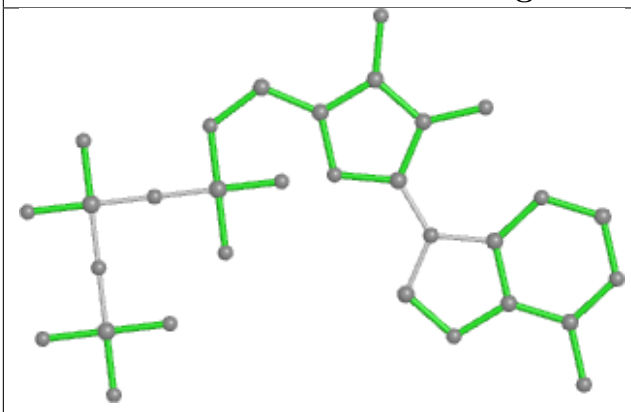


Torsions

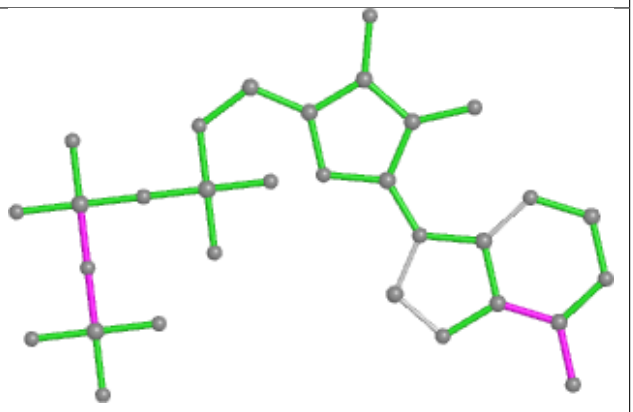


Rings

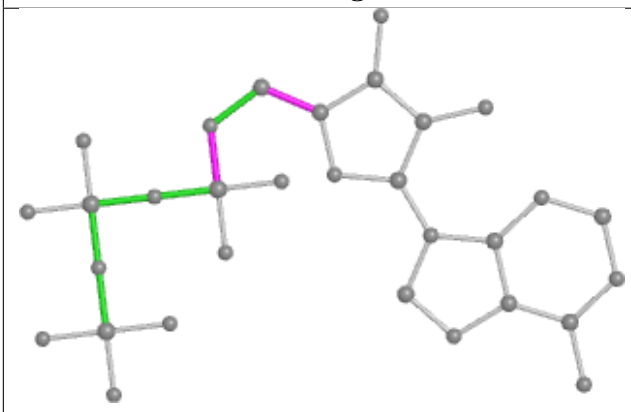
**Ligand ATP C 5002**



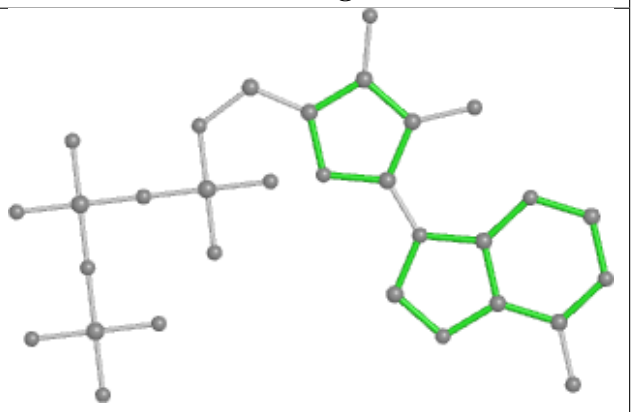
Bond lengths



Bond angles

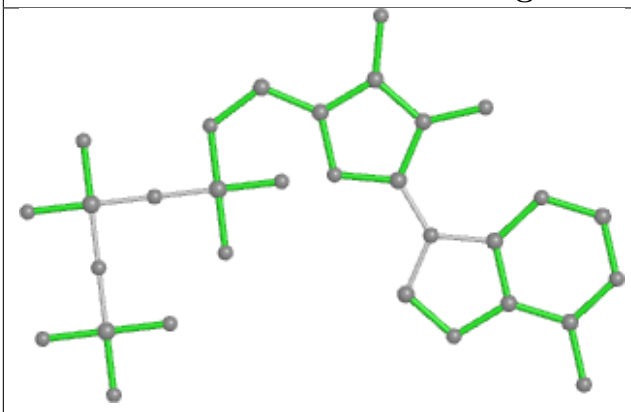


Torsions

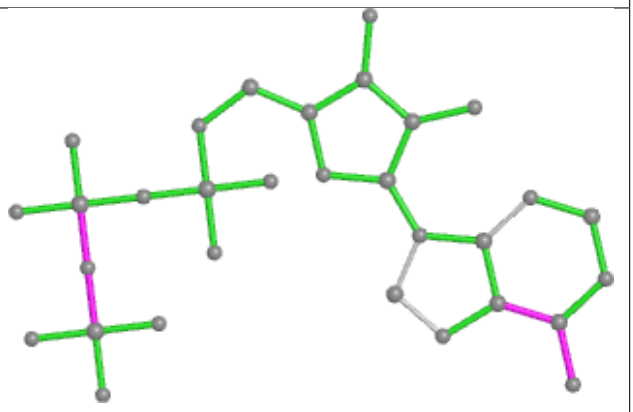


Rings

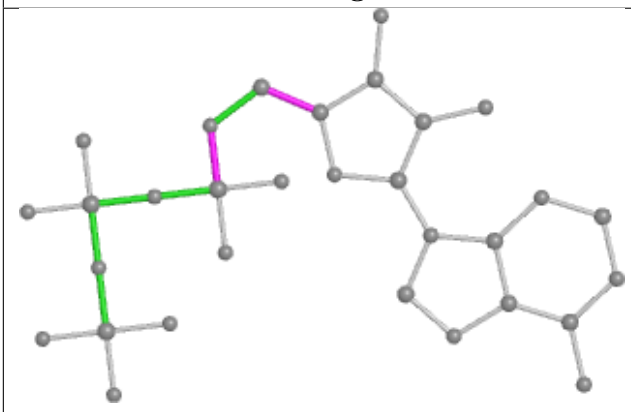
**Ligand ATP B 5002**



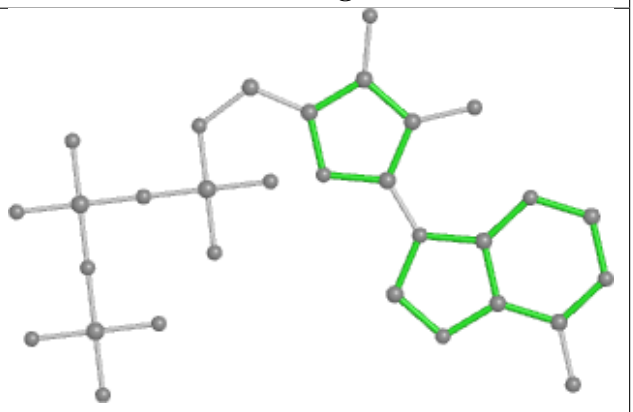
Bond lengths



Bond angles

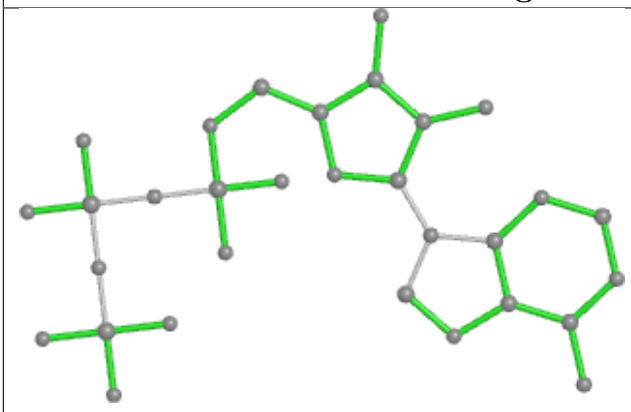


Torsions

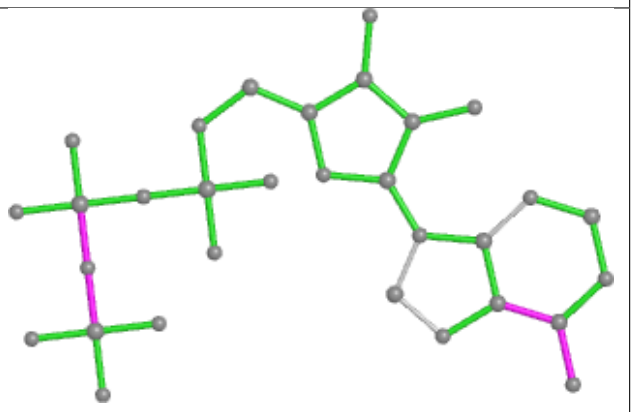


Rings

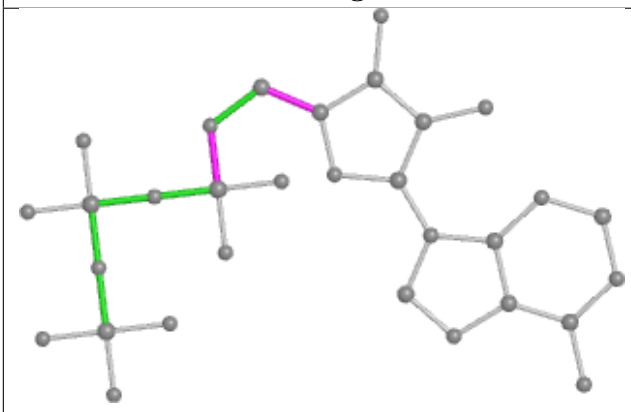
**Ligand ATP A 5002**



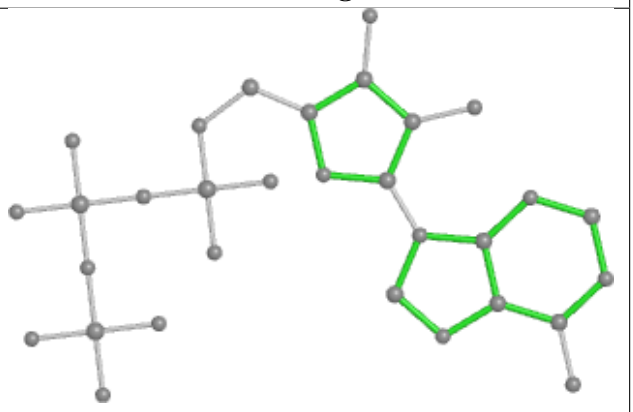
Bond lengths



Bond angles

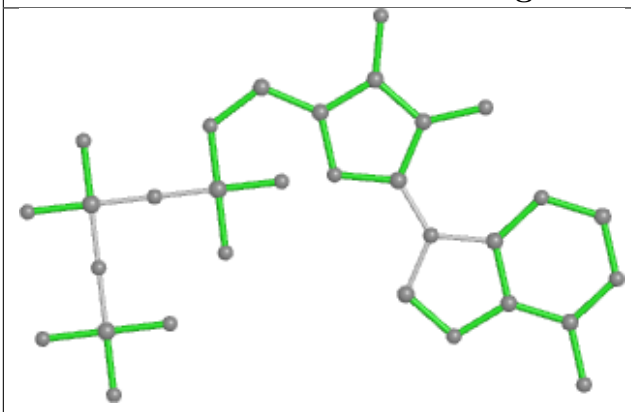


Torsions

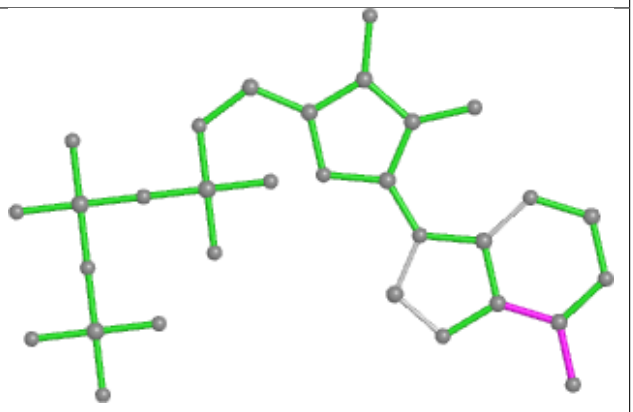


Rings

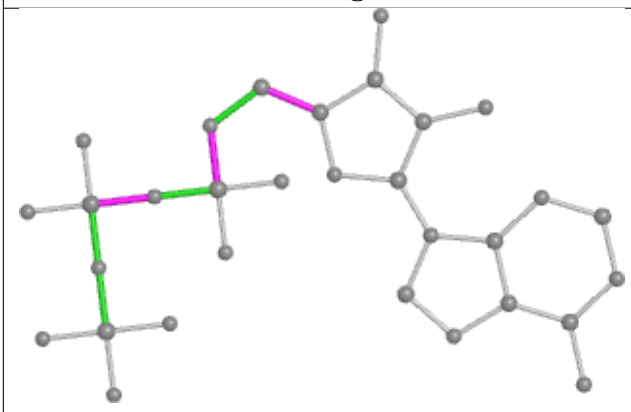
## Ligand ATP A 5003



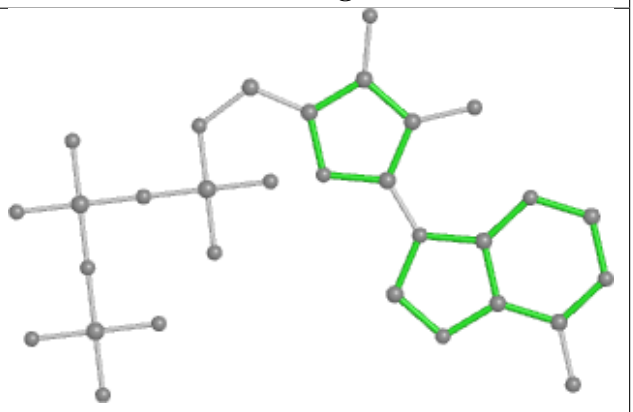
Bond lengths



Bond angles

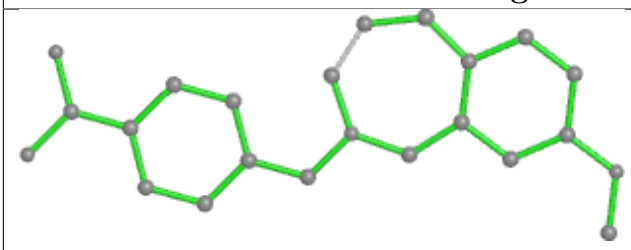


Torsions

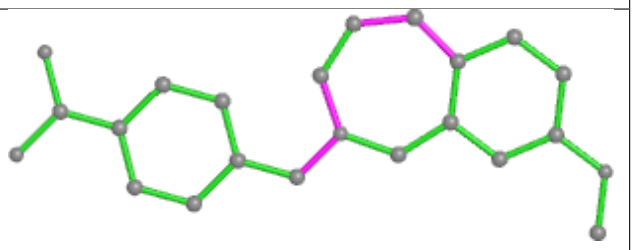


Rings

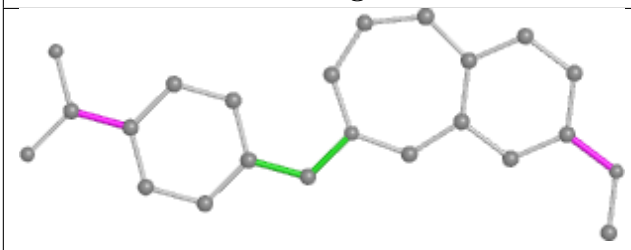
## Ligand KVR D 5004



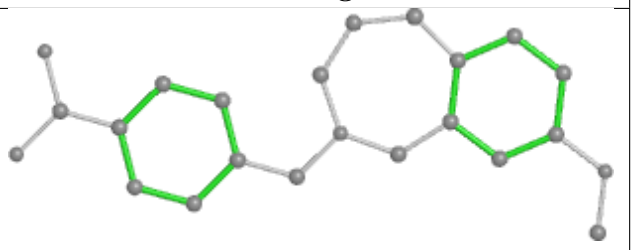
Bond lengths



Bond angles

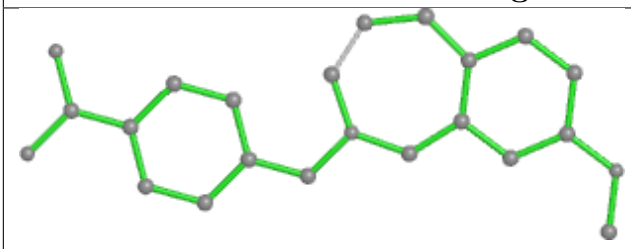


Torsions

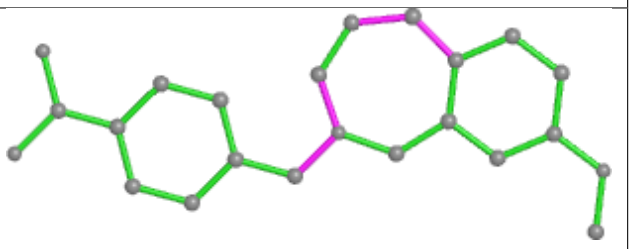


Rings

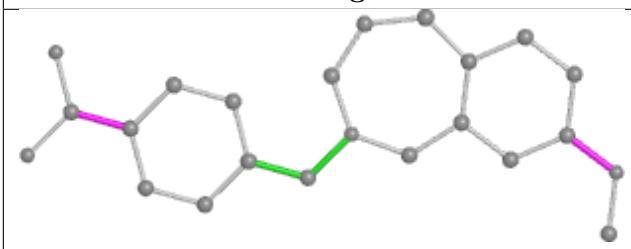
**Ligand KVR A 5004**



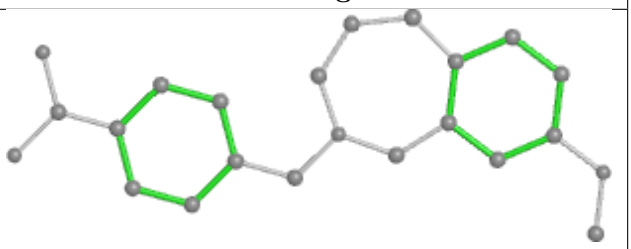
Bond lengths



Bond angles

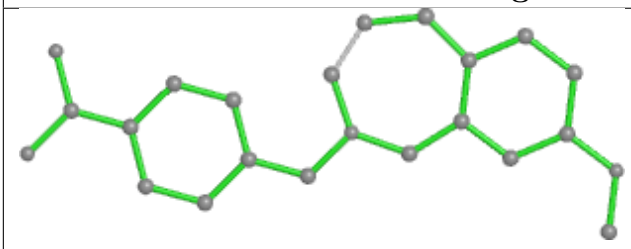


Torsions

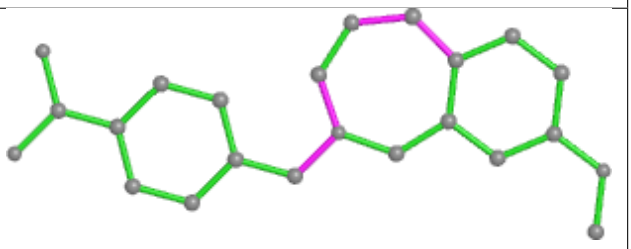


Rings

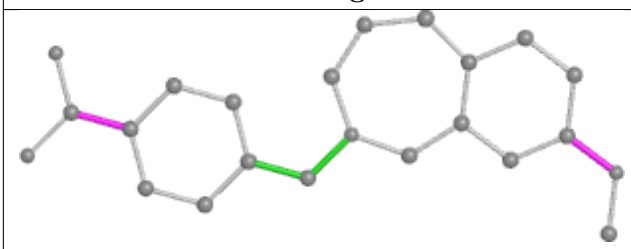
**Ligand KVR B 5004**



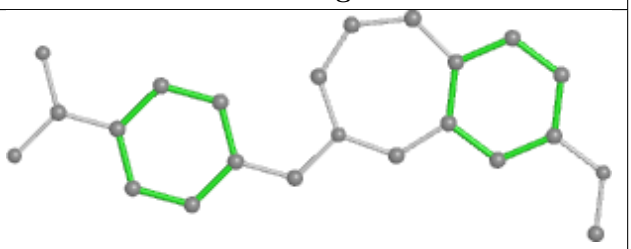
Bond lengths



Bond angles

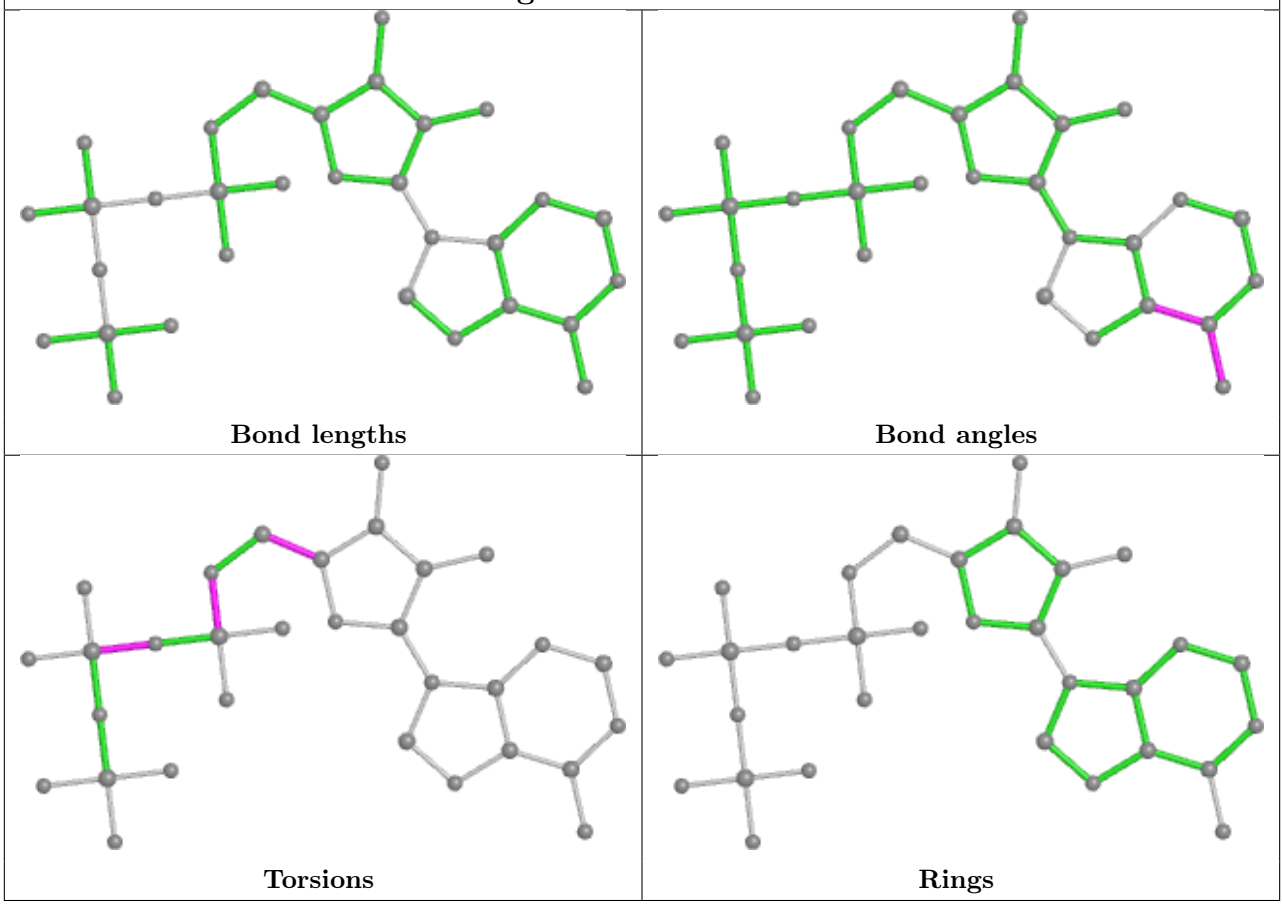


Torsions



Rings

**Ligand ATP B 5003**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

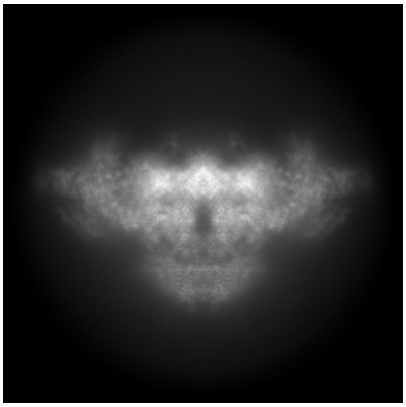
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42761. These allow visual inspection of the internal detail of the map and identification of artifacts.

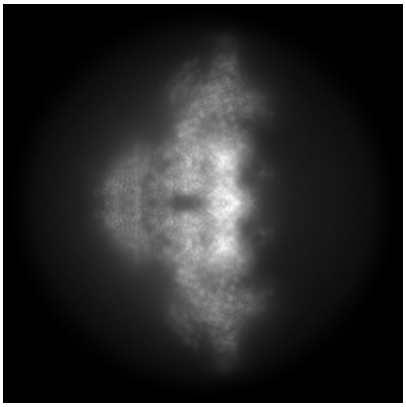
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

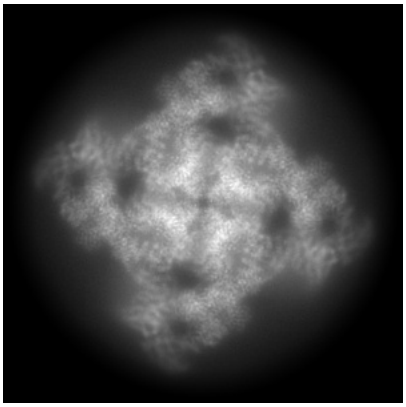
### 6.1.1 Primary map



X



Y

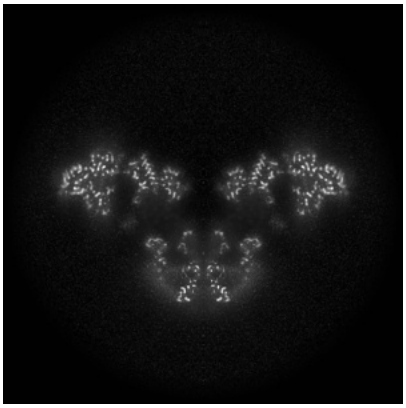


Z

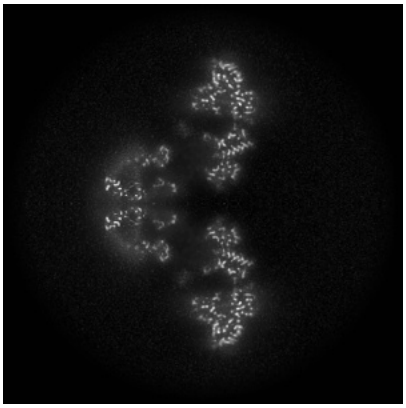
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

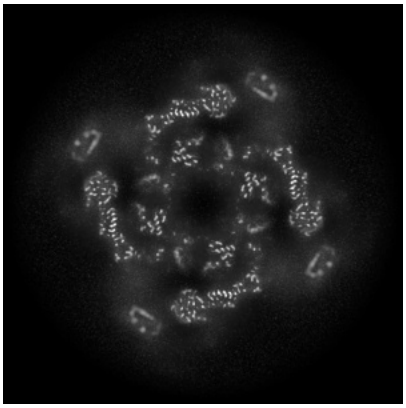
### 6.2.1 Primary map



X Index: 256



Y Index: 256

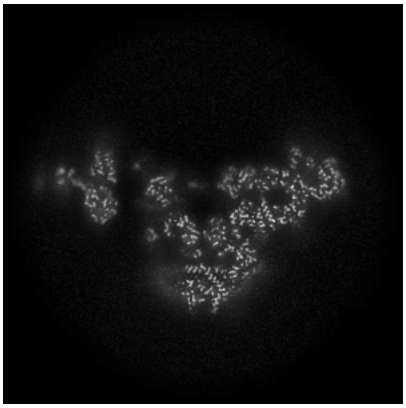


Z Index: 256

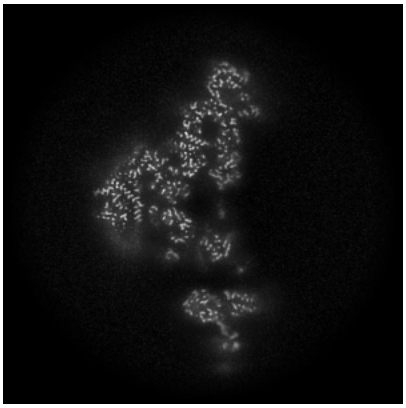
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

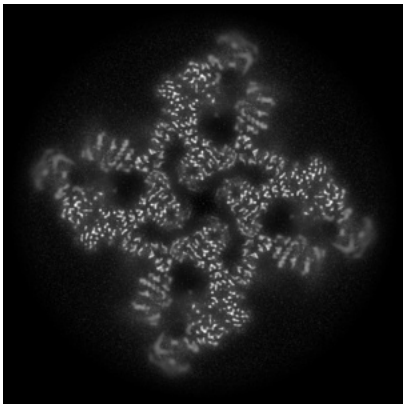
### 6.3.1 Primary map



X Index: 238



Y Index: 274

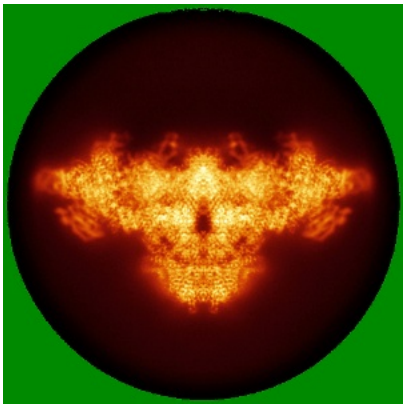


Z Index: 282

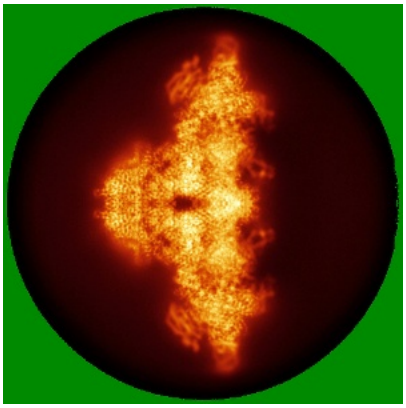
The images above show the largest variance slices of the map in three orthogonal directions.

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

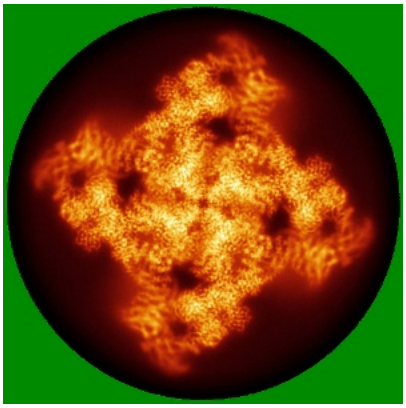
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

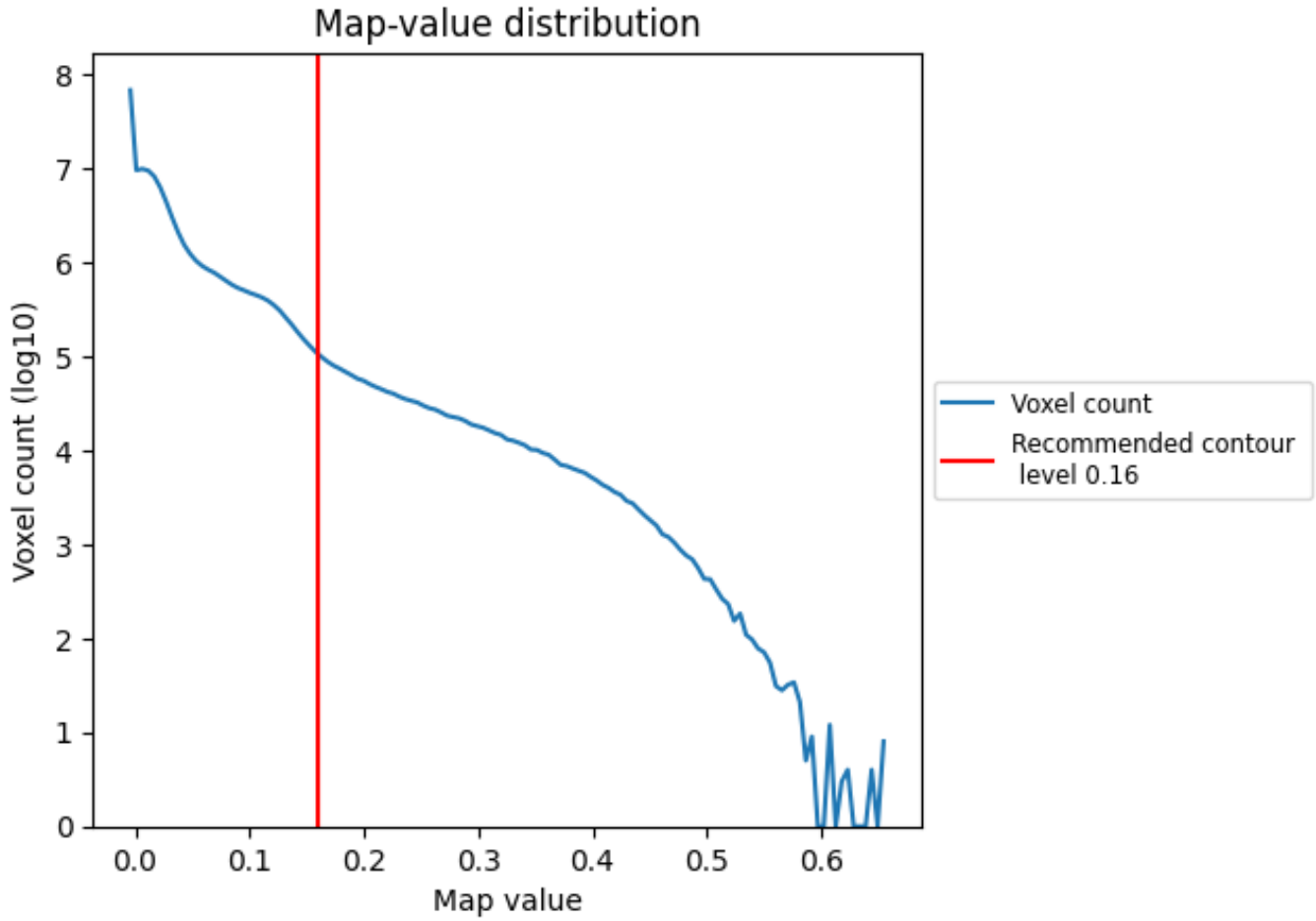
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

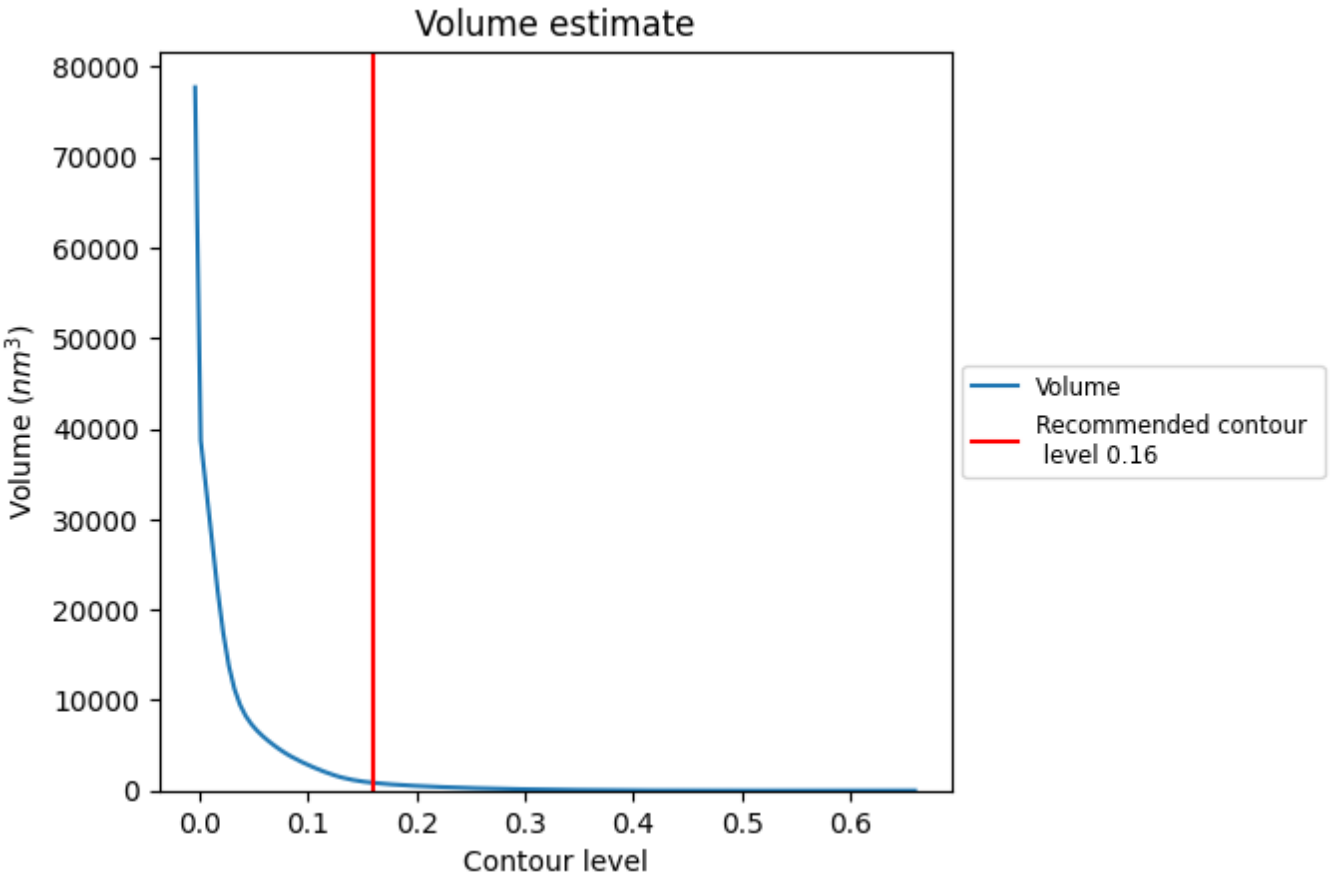
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

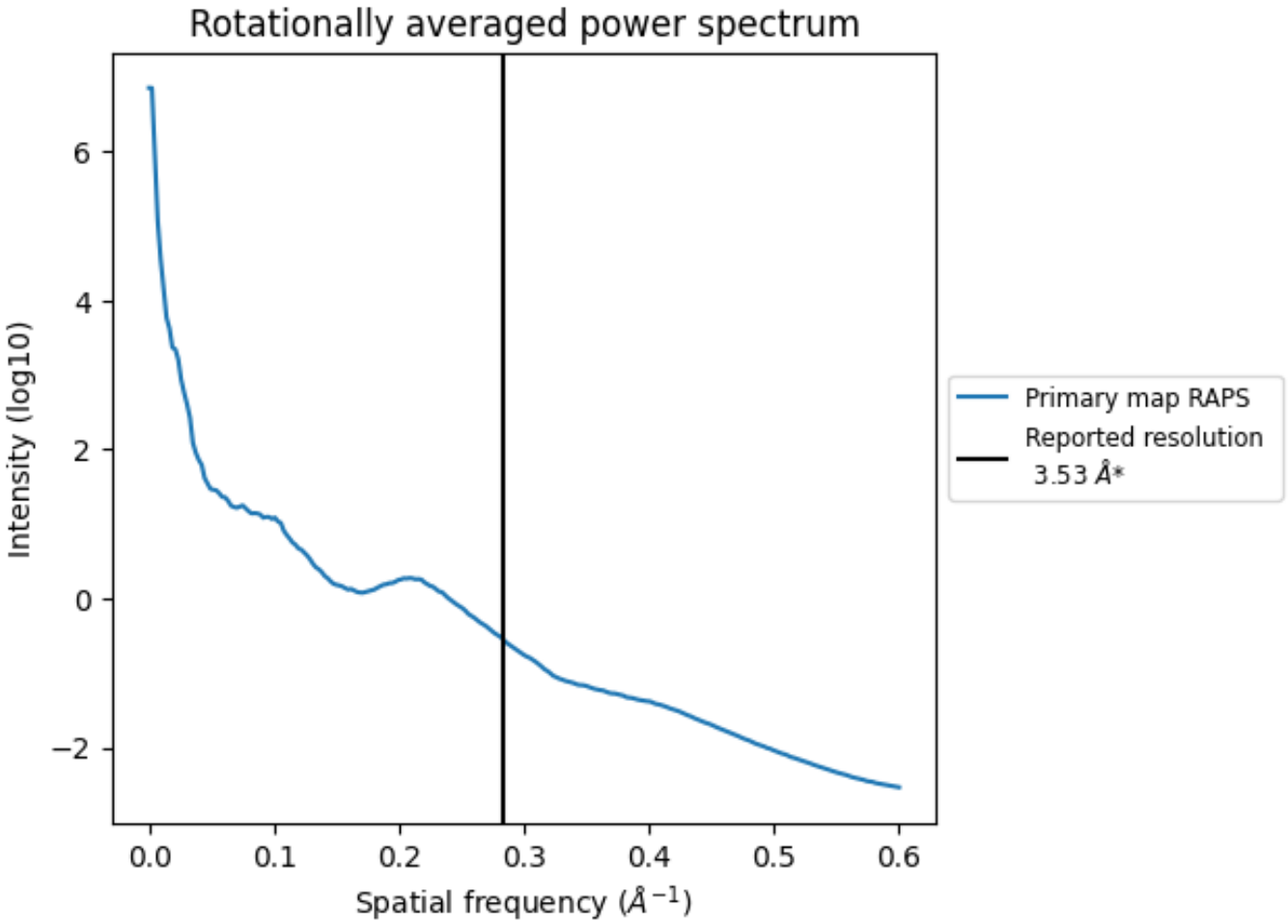
## 7.2 Volume estimate




The volume at the recommended contour level is 858 $nm^3$; this corresponds to an approximate mass of 775 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.283 $Å^{-1}$

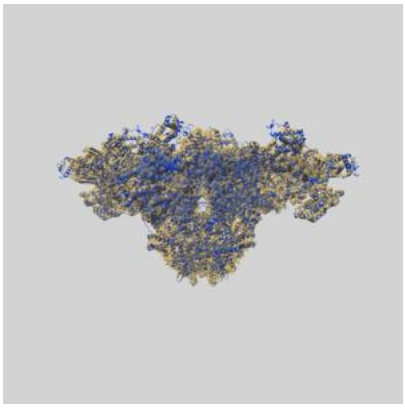
# 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

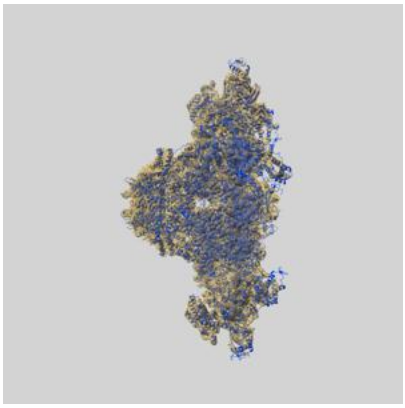
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42761 and PDB model 8UXE. Per-residue inclusion information can be found in section 3 on page 6.

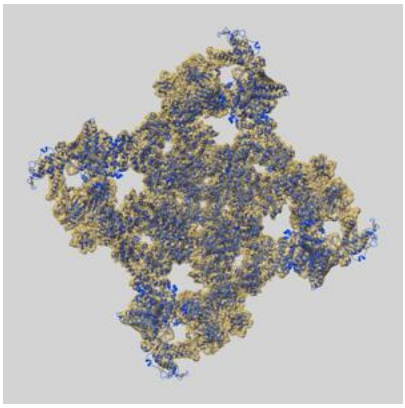
## 9.1 Map-model overlay



X



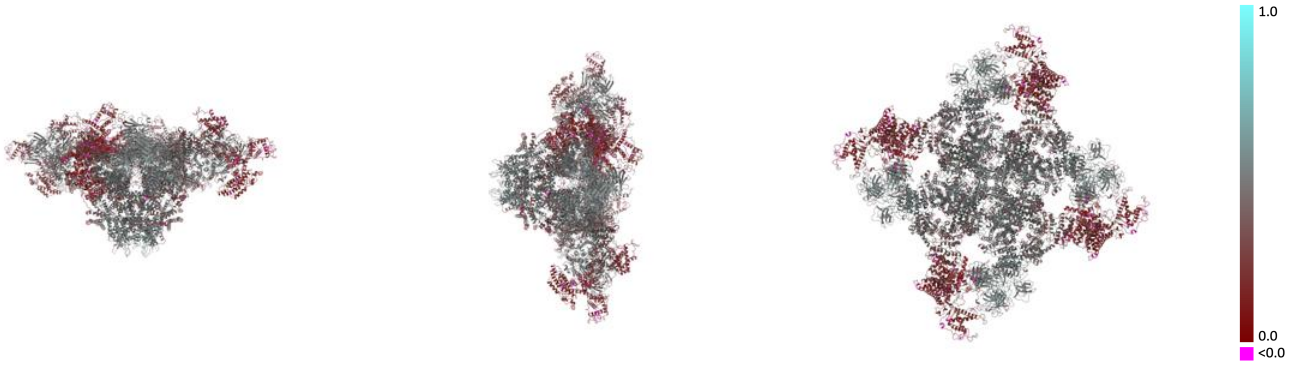
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

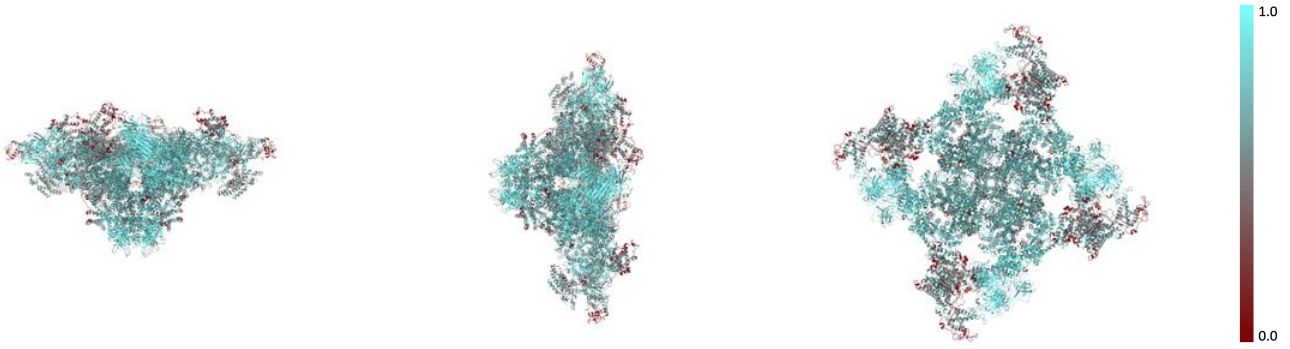
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

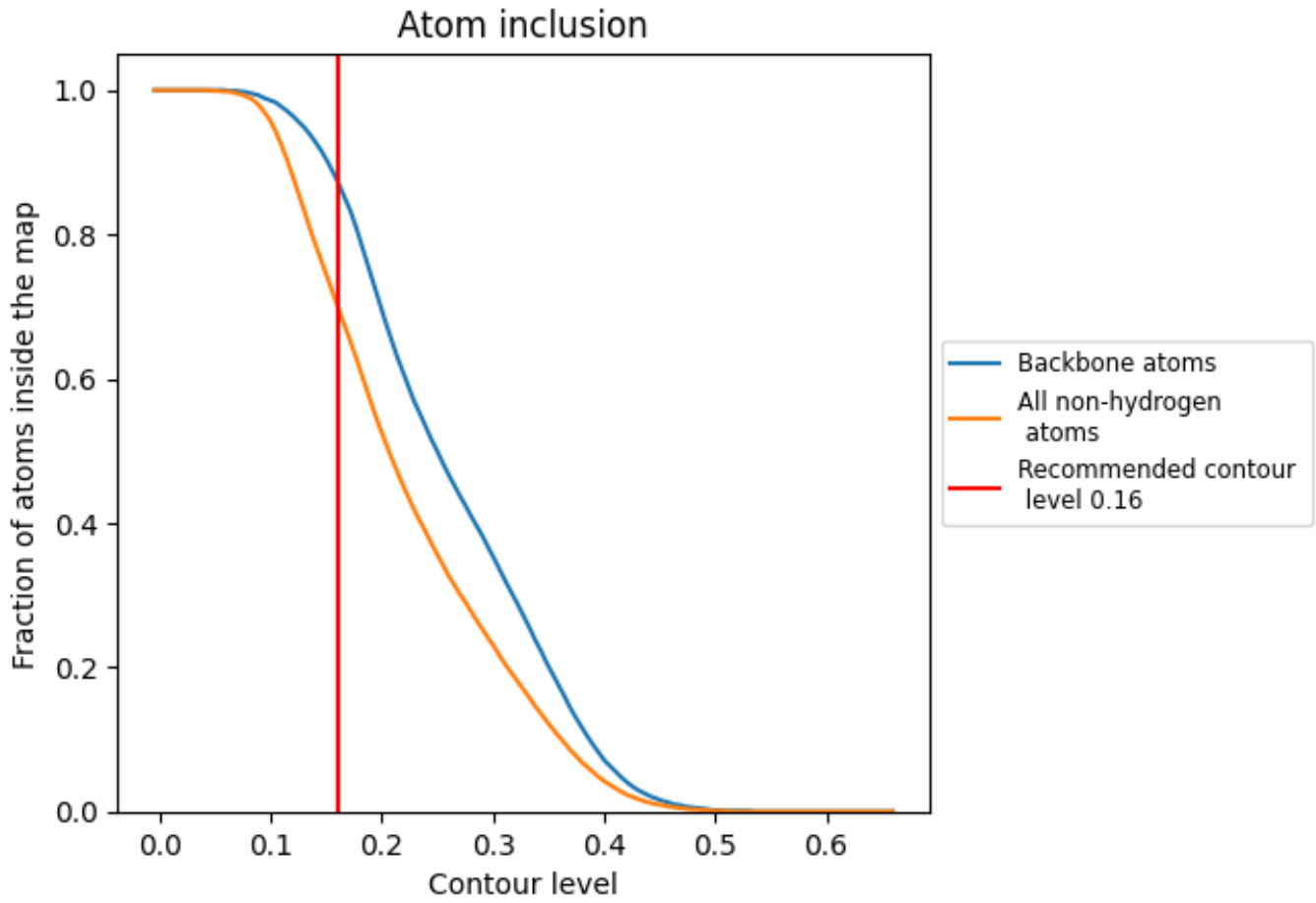
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

## 9.4 Atom inclusion (i)




At the recommended contour level, 88% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7020 | 0.3910 |
| A | 0.6990 | 0.3870 |
| B | 0.7000 | 0.3900 |
| C | 0.7000 | 0.3900 |
| D | 0.7000 | 0.3900 |
| E | 0.8190 | 0.4810 |
| F | 0.8090 | 0.4800 |
| G | 0.8180 | 0.4790 |
| H | 0.8230 | 0.4800 |