# Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:12 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 3HMJ |
| Title | : | Saccharomyces cerevisiae FAS type I |
| Authors | : | Johansson, P.; Mulinacci, B.; Koestler, C.; Vollrath, R.; Oesterhelt, D.; Grininger, M. |
| Deposited on | : | 2009-05-29 |
| Resolution | : | 4.00 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

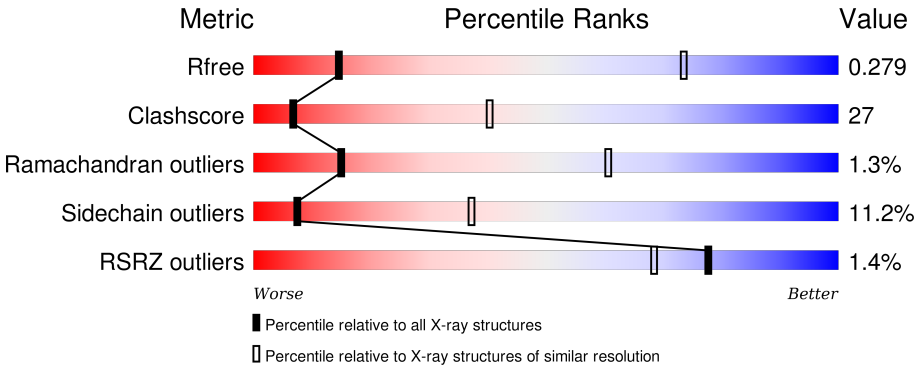
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026982 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20026982 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 1010 (4.42-3.56) |
| Clashscore | 102246 | 1052 (4.40-3.60) |
| Ramachandran outliers | 100387 | 1005 (4.40-3.60) |
| Sidechain outliers | 100360 | 1013 (4.42-3.58) |
| RSRZ outliers | 91569 | 1013 (4.42-3.56) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1887 | 2% 55% 32% 5% 7% |
| 1 | B | 1887 | 2% 55% 32% 5% 7% |
| 1 | C | 1887 | 3% 54% 33% 5% 7% |
| 2 | G | 2051 | 51% 40% 8% |
| 2 | H | 2051 | 51% 40% 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | I | 2051 | 51% 40% 8% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 3 | CER | C | 2748 | - | - | - | X |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 88830 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

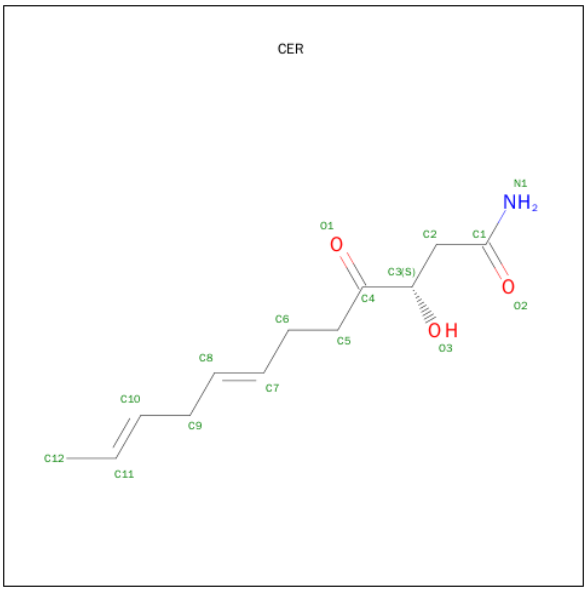
- Molecule 1 is a protein called Fatty acid synthase subunit alpha.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1750 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13572 | 8594 | 2292 | 2637 | 49 | | | |
| 1 | B | 1750 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13572 | 8594 | 2292 | 2637 | 49 | | | |
| 1 | C | 1750 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13572 | 8594 | 2292 | 2637 | 49 | | | |

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

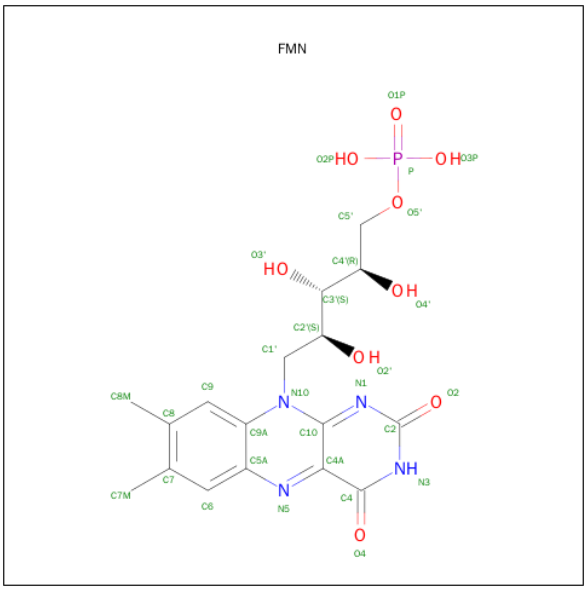
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | G | 2033 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 15995 | 10253 | 2660 | 3026 | 56 | | | |
| 2 | H | 2033 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 15995 | 10253 | 2660 | 3026 | 56 | | | |
| 2 | I | 2033 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 15995 | 10253 | 2660 | 3026 | 56 | | | |

- Molecule 3 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: CER) (formula: $C_{12}H_{19}NO_3$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total C N O<br>12 8 1 3 | 0 | 0 |
| 3 | B | 1 | Total C N O<br>12 8 1 3 | 0 | 0 |
| 3 | C | 1 | Total C N O<br>12 8 1 3 | 0 | 0 |

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | G | 1 | Total C N O P<br>31 17 4 9 1 | 0 | 0 |

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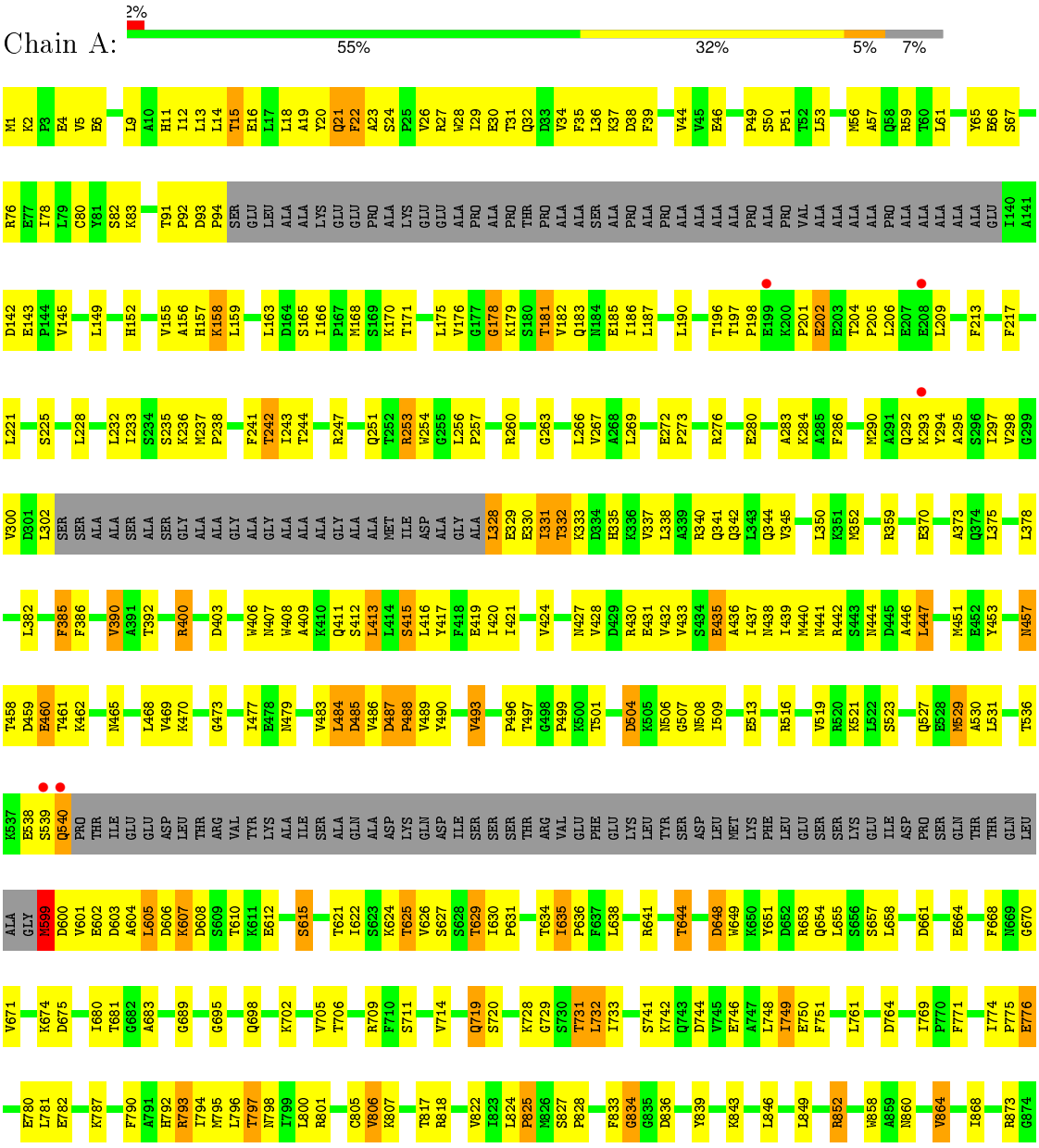
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 4 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |
| 4 | I | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | | |

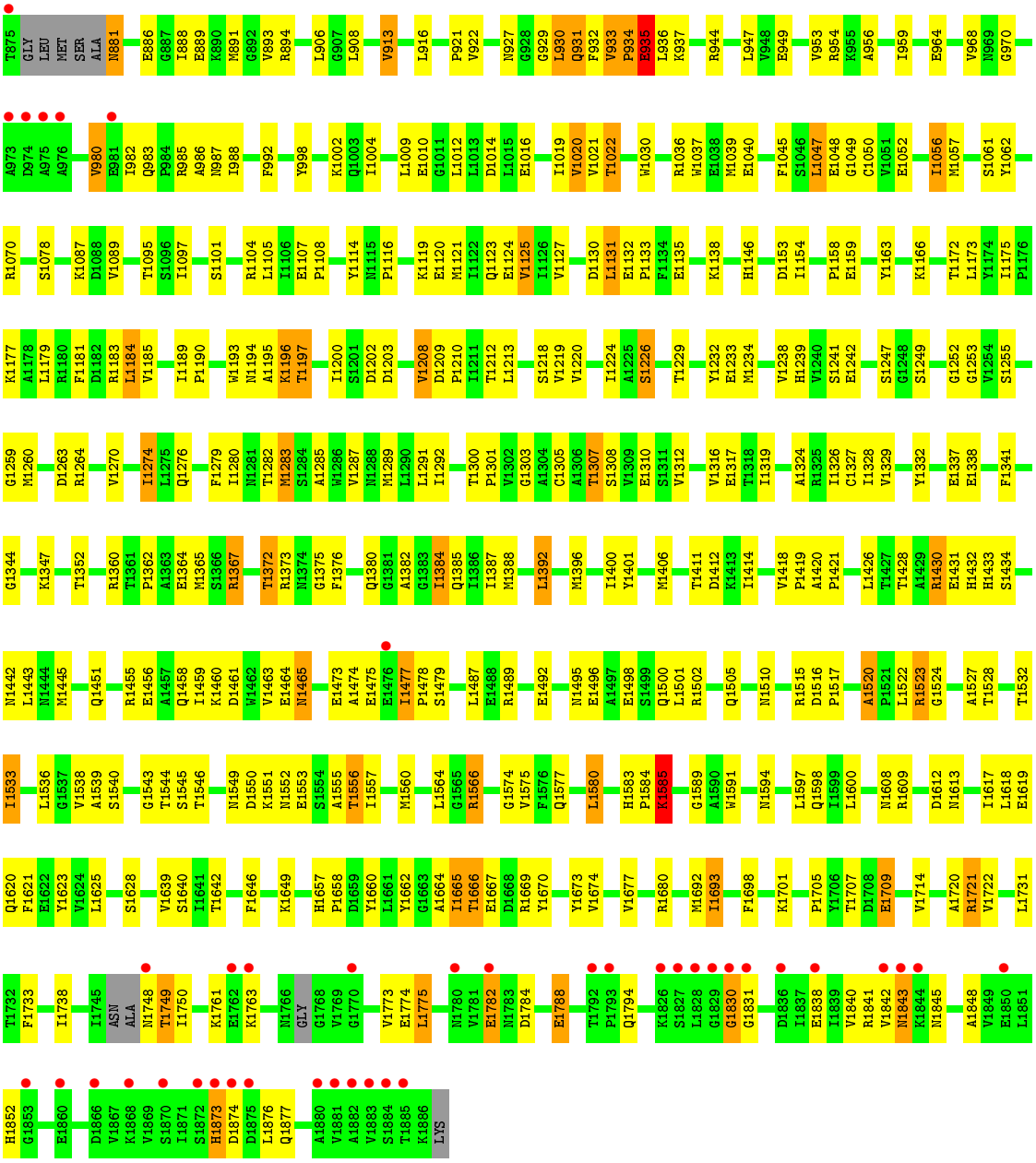
# 3 Residue-property plots (i)

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

- Molecule 1: Fatty acid synthase subunit alpha

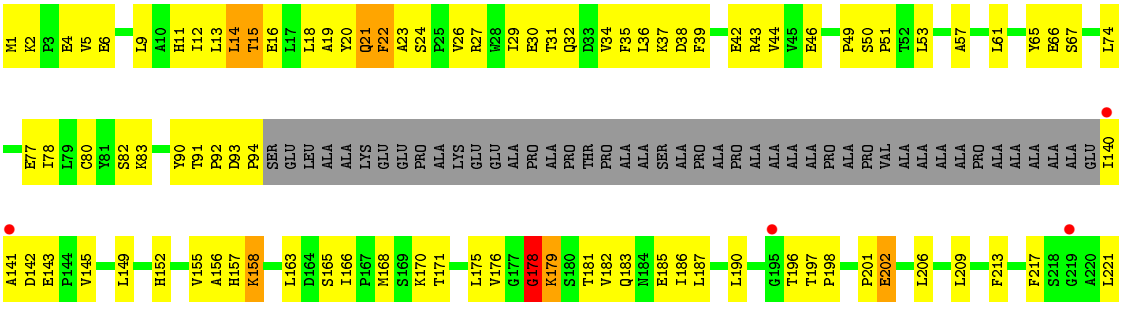
Chain A:

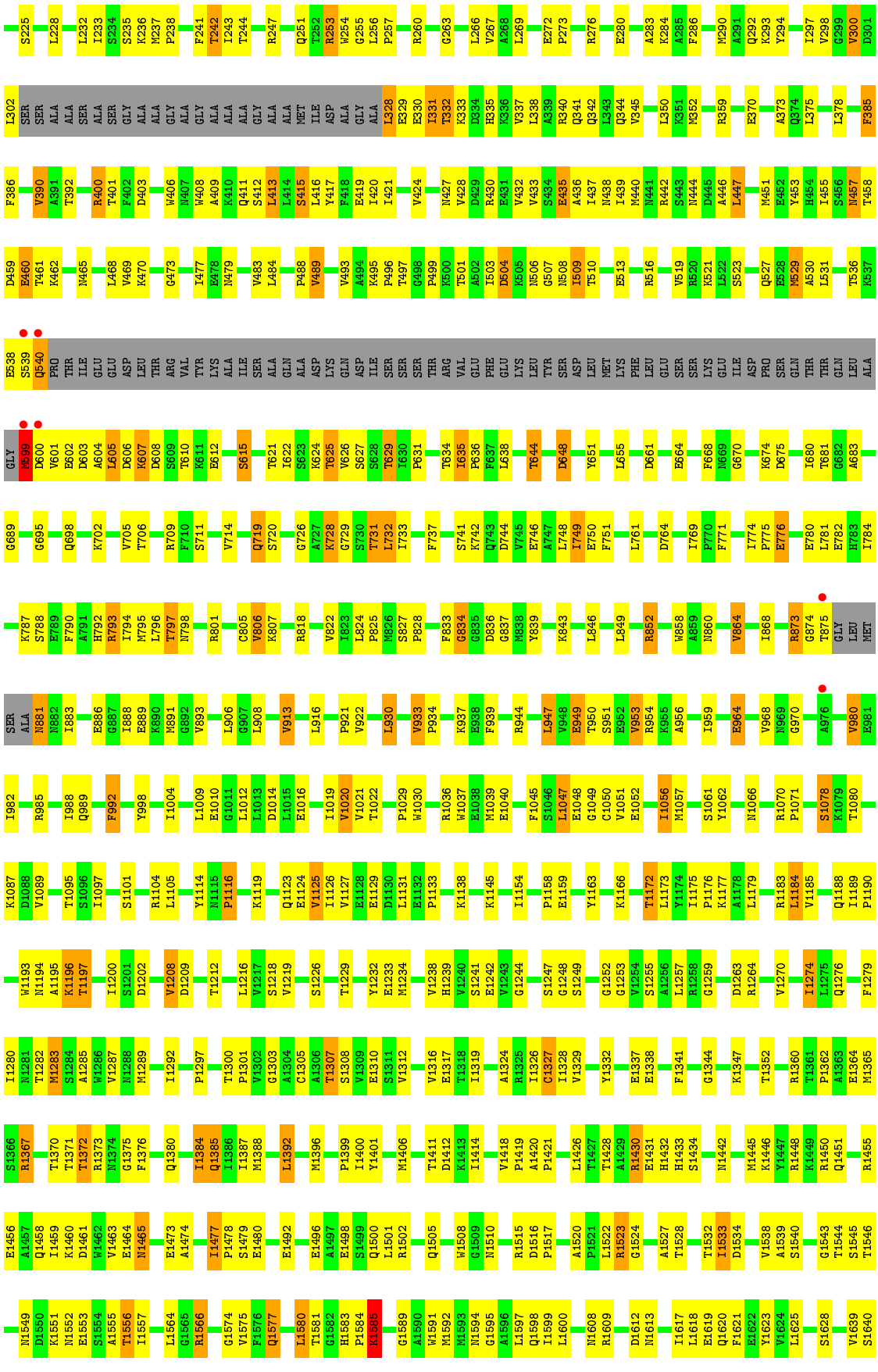


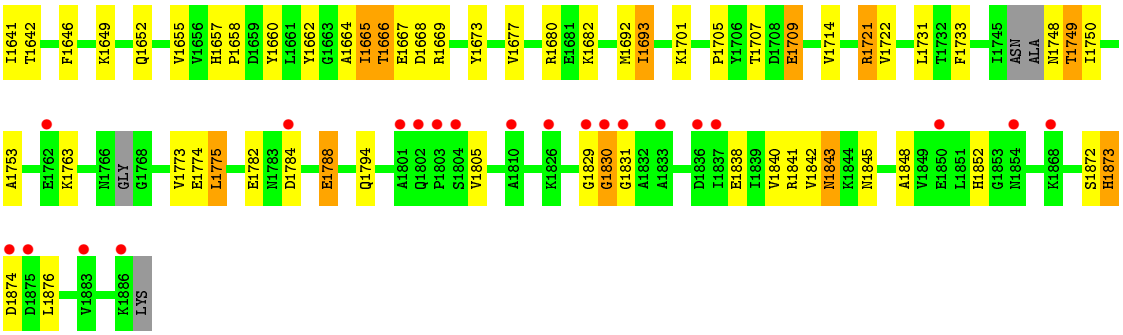


• Molecule 1: Fatty acid synthase subunit alpha

Chain B:


S225 L228 L232 I233 S234 S235 K236 M237 P238 F241 T242 I243 T244 R247 Q251 T252 R253 W254 G255 L256 P257 R260 G263 L266 V267 A268 L269 E272 P273 R276 E280 A283 K284 A285 F286 M290 A291 Q292 K293 Y294 I297 V298 G299 V300 D301
L302 SER SER ALA ALA SER ALA ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA ALA MET ILE ASP ALA GLY ALA L328 E329 E330 I331 T332 K333 D334 H335 K336 V337 L338 A339 R340 Q341 Q342 L343 Q344 V345 L350 K351 M352 R359 E370 A373 Q374 L375 L378 F385
F386 V390 A391 T392 R400 T401 F402 D403 W406 N407 W408 A409 K410 Q411 S412 L413 L414 S415 L416 Y417 F418 E419 I420 I421 V424 N427 V428 D429 R430 E431 V432 V433 S434 E435 A436 I437 N438 I439 M440 N441 R442 S443 N444 D445 A446 L447 M451 E452 Y453 H454 I455 S456 N457 T458
D459 E460 T461 K462 N465 L468 V469 K470 G473 I477 E478 N479 V483 L484 P488 V489 V493 A494 K495 P496 T497 G498 P499 K500 T501 A502 I503 D504 K505 N506 G507 N508 I509 T510 E513 R516 V519 R520 K521 L522 S523 Q527 E528 M529 A530 L531 T536 K537
E538 S539 Q540 PRO THR ILE GLU GLU ASP LEU THR ARG VAL TYR LYS ALA ILE SER ALA GLN ALA ASP LYS GLN ASP ILE SER SER THR ARG VAL GLU PHE GLU LYS LEU TYR SER ASP LEU MET LYS PHE LEU GLU SER SER LYS GLU ILE ASP PRO SER GLN THR THR GLN LEU ALA
GLY M599 D600 V601 E602 D603 A604 L605 D606 K607 D608 S609 T610 K611 E612 S615 T621 I622 S623 K624 T625 V626 S627 S628 T629 I630 P631 T634 I635 P636 F637 L638 T644 D648 Y651 L655 D661 E664 F668 N669 G670 K674 D675 I680 T681 G682 A683
G689 G695 Q698 K702 V705 T706 R709 F710 S711 V714 Q719 S720 G726 A727 K728 G729 S730 T731 L732 I733 F737 S741 K742 Q743 D744 V745 E746 A747 L748 I749 E750 F751 L761 D764 I769 P770 F771 I774 P775 E776 E780 L781 E782 H783 I784
K787 S788 E789 F790 A791 H792 R793 I794 M795 L796 T797 N798 R801 C805 V806 K807 R818 V822 I823 L824 P825 M826 S827 P828 F833 G834 G835 D836 G837 M838 Y839 K843 L846 L849 R852 W858 A859 N860 V864 I868 R873 G874 T875 GLY LEU MET
SER ALA N881 N882 I883 E886 G887 I888 E889 K890 M891 G892 V893 L906 G907 L908 V913 L916 P921 V922 L930 V933 P934 K937 E938 F939 R944 I947 V948 E949 T950 S951 E952 Y953 R954 K955 A956 I959 E964 V968 N969 G970 A976 V980 E981
I982 R985 I988 Q989 F992 Y998 I1004 L1009 E1010 G1011 L1012 L1013 D1014 L1015 E1016 I1019 V1020 V1021 T1022 P1029 W1030 R1036 W1037 E1038 M1039 E1040 F1045 S1046 L1047 E1048 G1049 C1050 V1051 E1052 I1056 M1057 S1061 Y1062 N1066 R1070 P1071 S1078 K1079 T1080
K1087 D1088 V1089 T1095 S1096 I1097 S1101 R1104 L1105 Y1114 N1115 P1116 K1119 Q1123 E1124 V1125 I1126 V1127 E1128 E1129 D1130 L1131 E1132 P1133 K1138 K1145 I1154 P1158 E1159 Y1163 K1166 T1172 L1173 Y1174 I1175 P1176 K1177 A1178 L1179 R1183 L1184 V1185 Q1188 I1189 P1190
W1193 N1194 A1195 K1196 T1197 I1200 S1201 D1202 Y1208 D1209 T1212 L1216 Y1217 S1218 V1219 S1226 T1229 Y1232 E1233 M1234 V1238 H1239 Y1240 S1241 E1242 Y1243 G1244 S1247 G1248 S1249 G1252 G1253 Y1254 S1255 A1256 L1257 R1258 G1259 D1263 R1264 V1270 I1274 L1275 Q1276 F1279
I1280 N1281 T1282 M1283 S1284 A1285 W1286 Y1287 N1288 M1289 I1292 P1297 T1300 P1301 Y1302 G1303 A1304 C1305 A1306 T1307 S1308 V1309 E1310 S1311 V1312 V1316 E1317 T1318 I1319 A1324 R1325 I1326 C1327 I1328 V1329 Y1332 E1337 E1338 F1341 G1344 K1347 T1352 R1360 T1361 P1362 A1363 E1364 M1365
S1366 R1367 T1370 T1371 T1372 R1373 N1374 G1375 F1376 Q1380 I1384 Q1385 I1386 I1387 M1388 L1392 M1396 P1399 I1400 Y1401 M1406 T1411 D1412 K1413 I1414 Y1418 P1419 A1420 P1421 L1426 T1427 T1428 A1429 R1430 E1431 H1432 H1433 S1434 N1442 M1445 K1446 Y1447 R1448 K1449 R1450 Q1451 R1455
E1456 A1457 Q1458 I1459 K1460 D1461 W1462 V1463 E1464 N1465 E1473 A1474 I1477 P1478 S1479 E1480 E1492 E1496 A1497 E1498 S1499 Q1500 L1501 R1502 Q1505 W1508 G1509 N1510 R1515 D1516 P1517 A1520 P1521 L1522 R1523 G1524 A1527 T1528 T1532 I1533 D1534 V1538 A1539 S1540 G1543 T1544 T1546
N1549 D1550 K1551 N1552 E1553 S1554 A1555 T1556 I1557 L1564 G1565 R1566 G1574 V1575 F1576 Q1577 L1580 T1581 G1582 H1583 P1584 K1585 G1589 A1590 W1591 M1592 M1593 M1594 G1595 A1596 L1597 Q1598 I1599 L1600 N1608 R1609 D1612 M1613 I1617 L1618 E1619 Q1620 F1621 E1622 Y1623 V1624 L1625 S1628 V1639 S1640

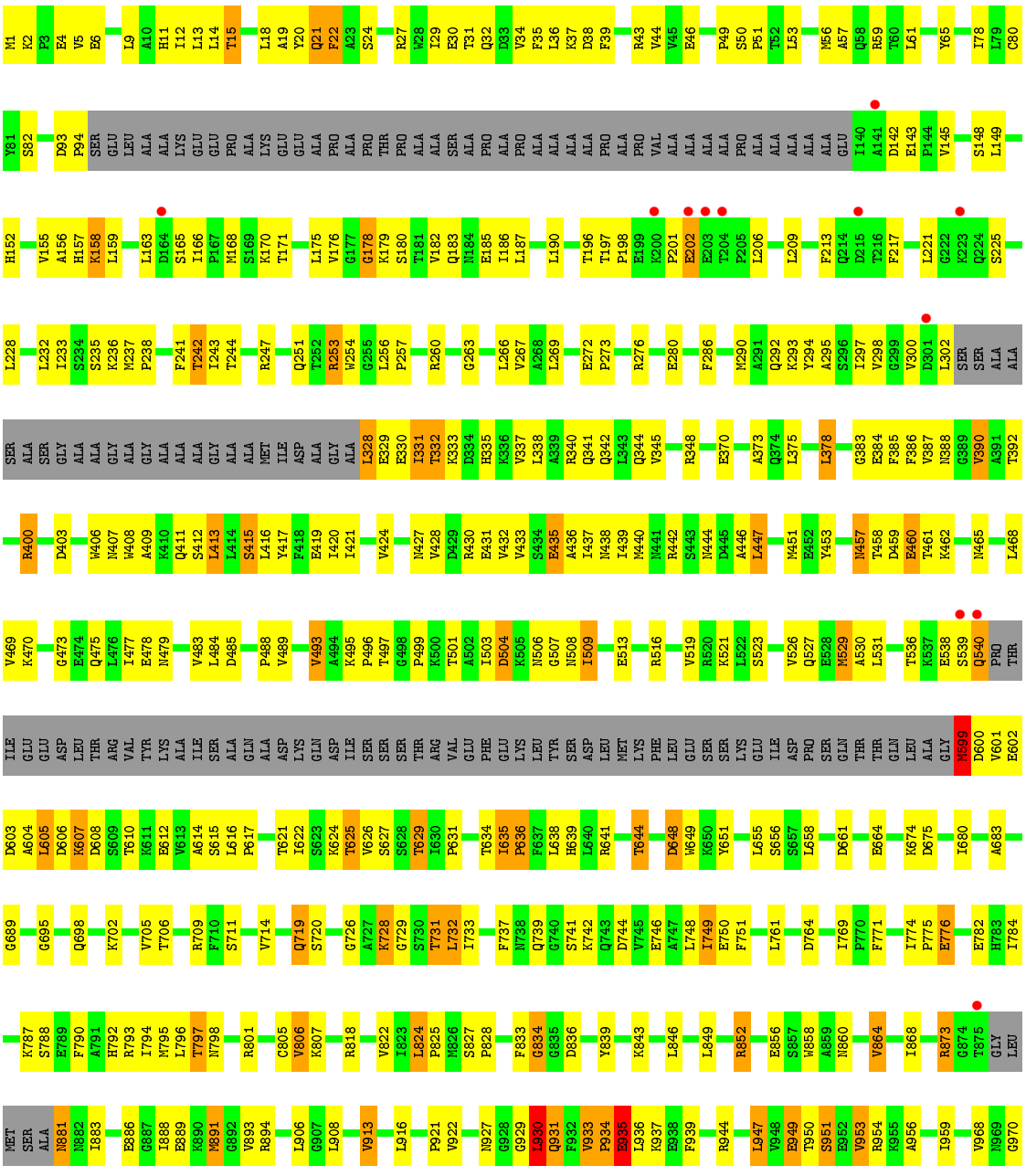


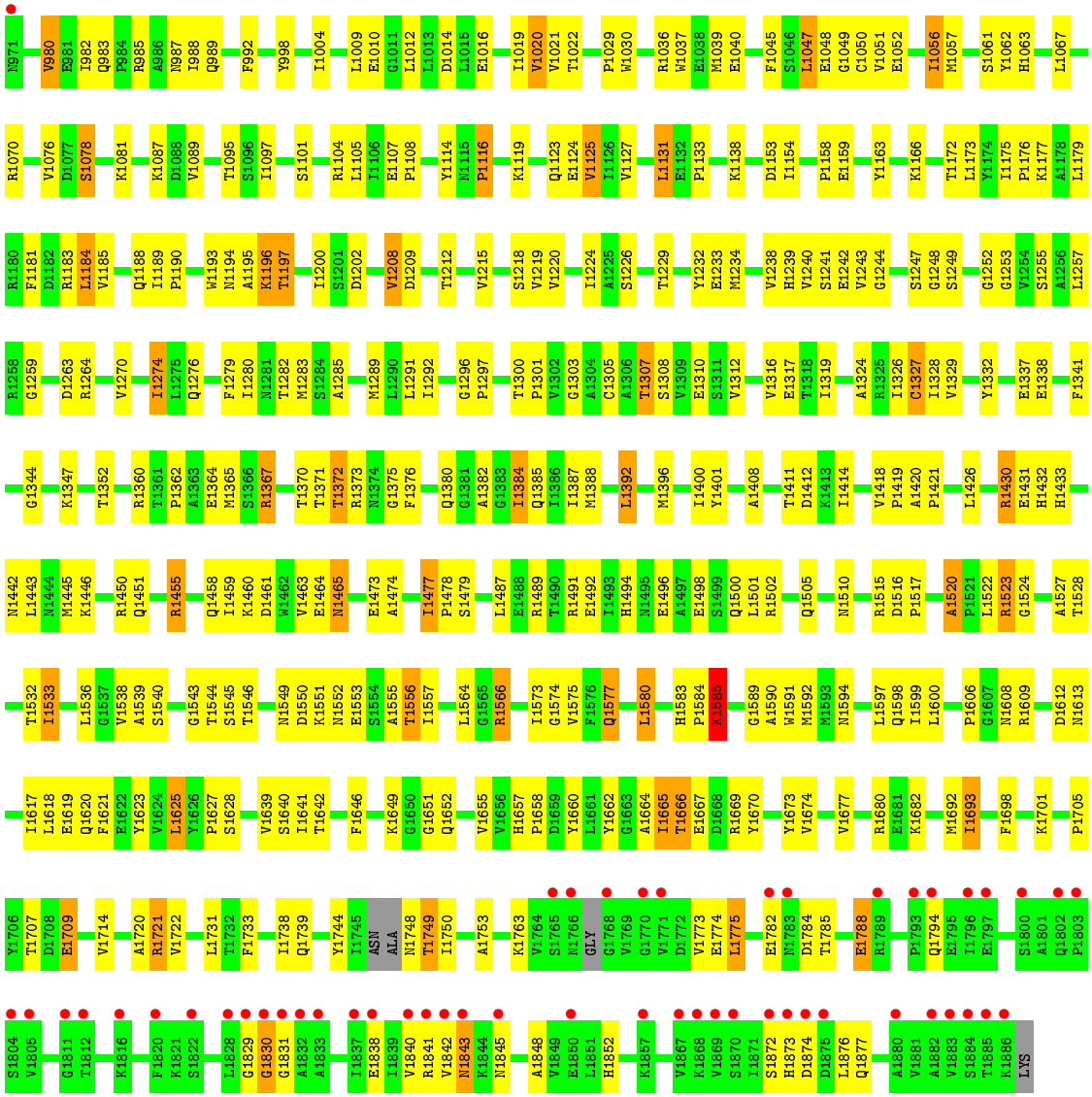




• Molecule 1: Fatty acid synthase subunit alpha

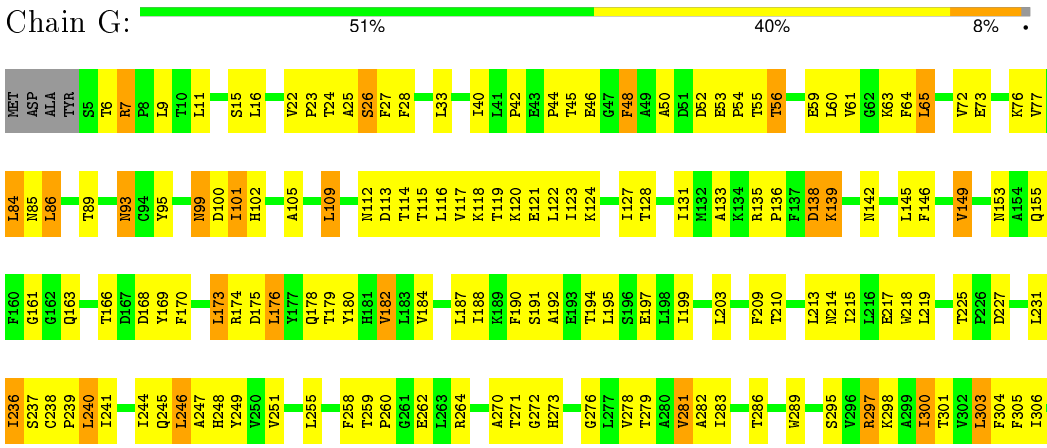
Chain C:

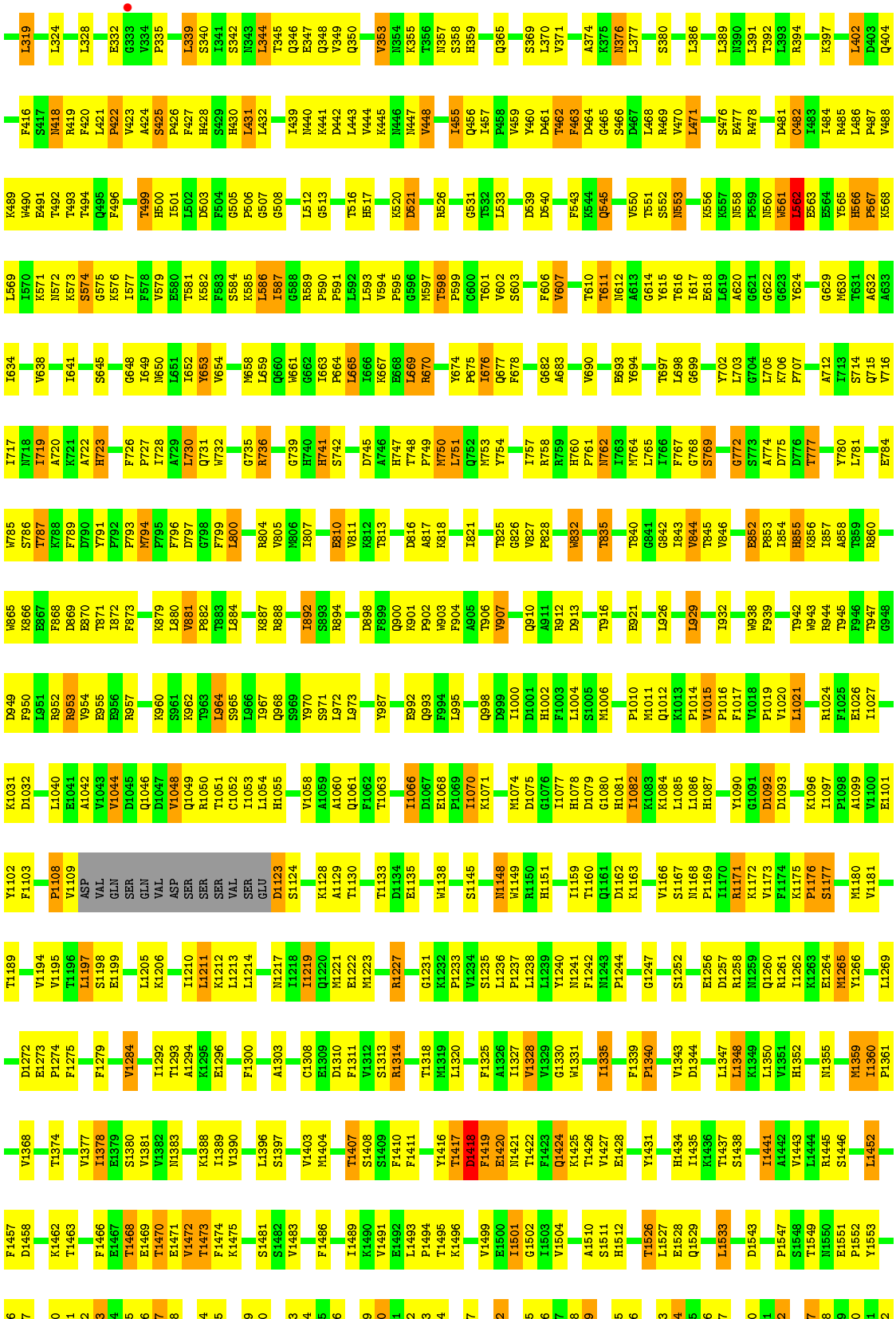



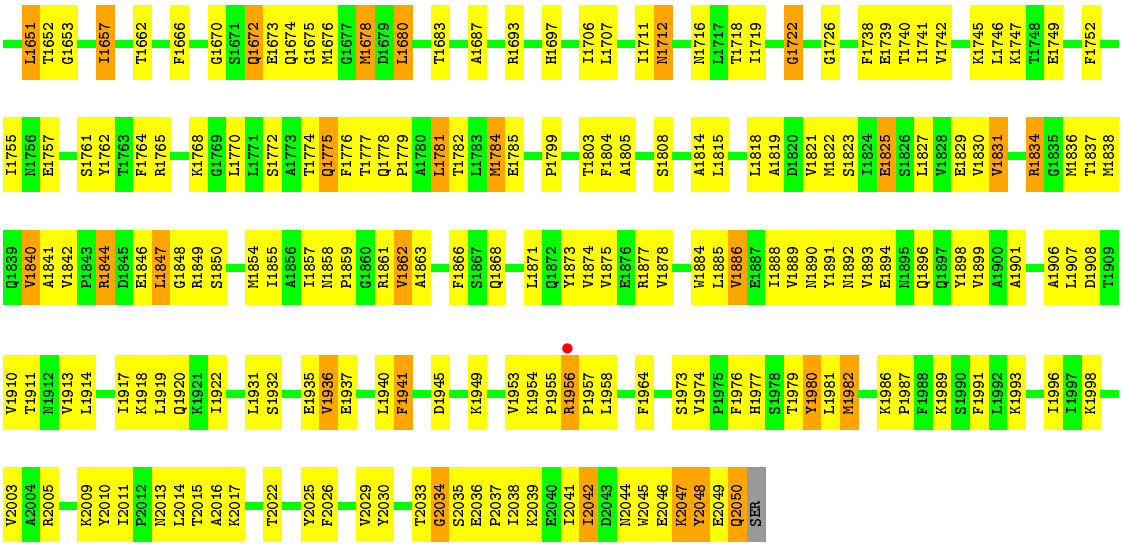


• Molecule 2: Fatty acid synthase subunit beta

Chain G:

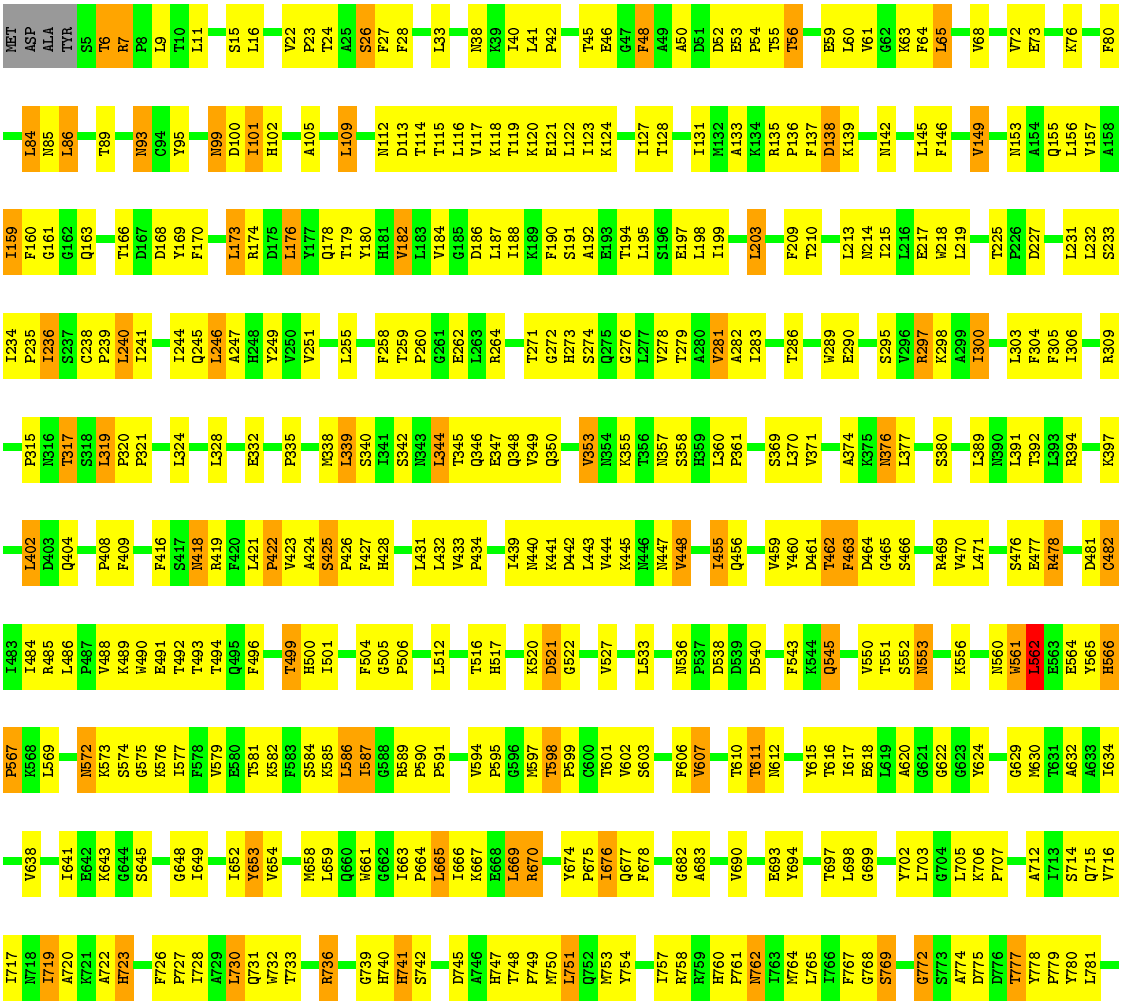


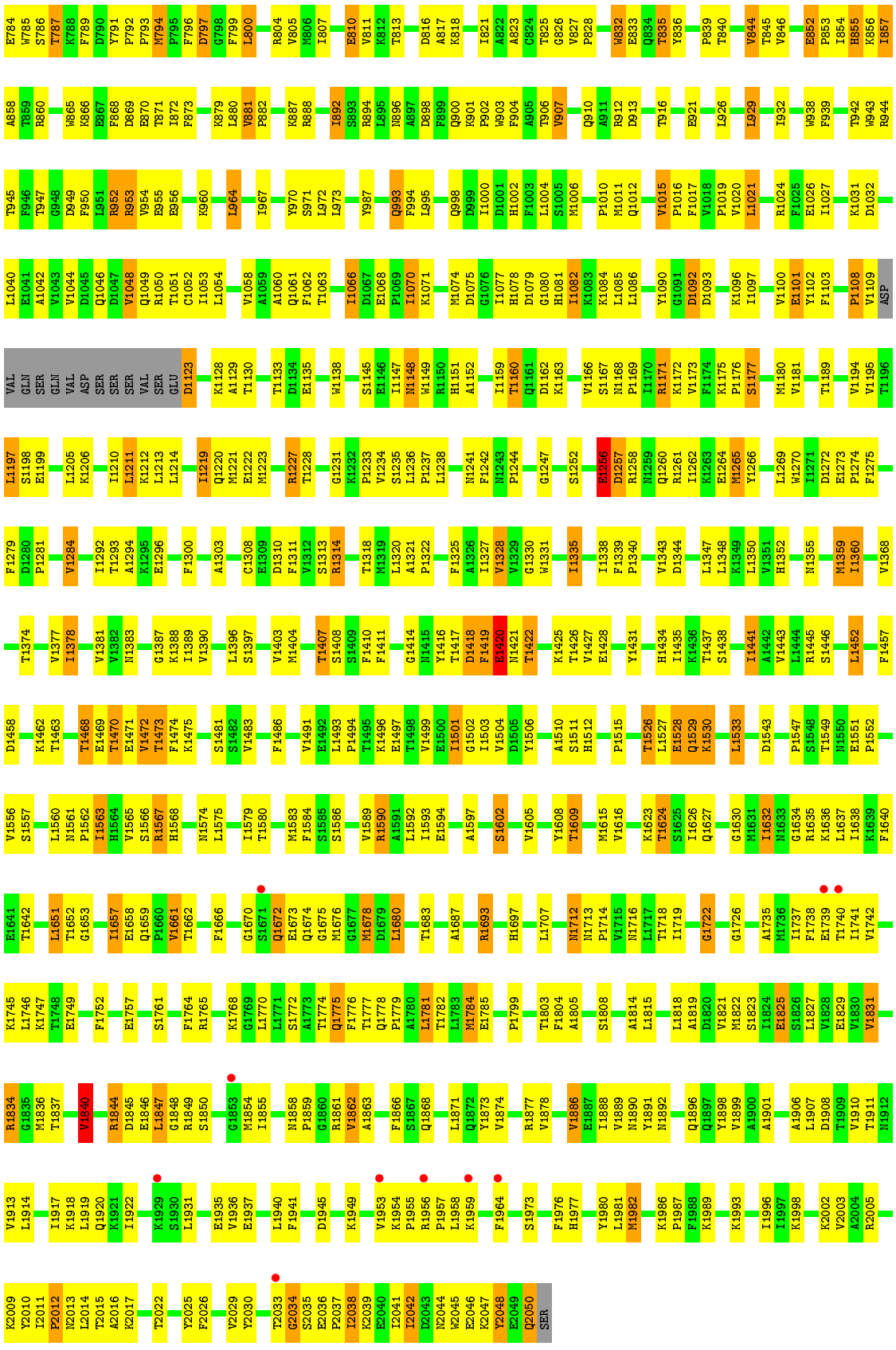




• Molecule 2: Fatty acid synthase subunit beta

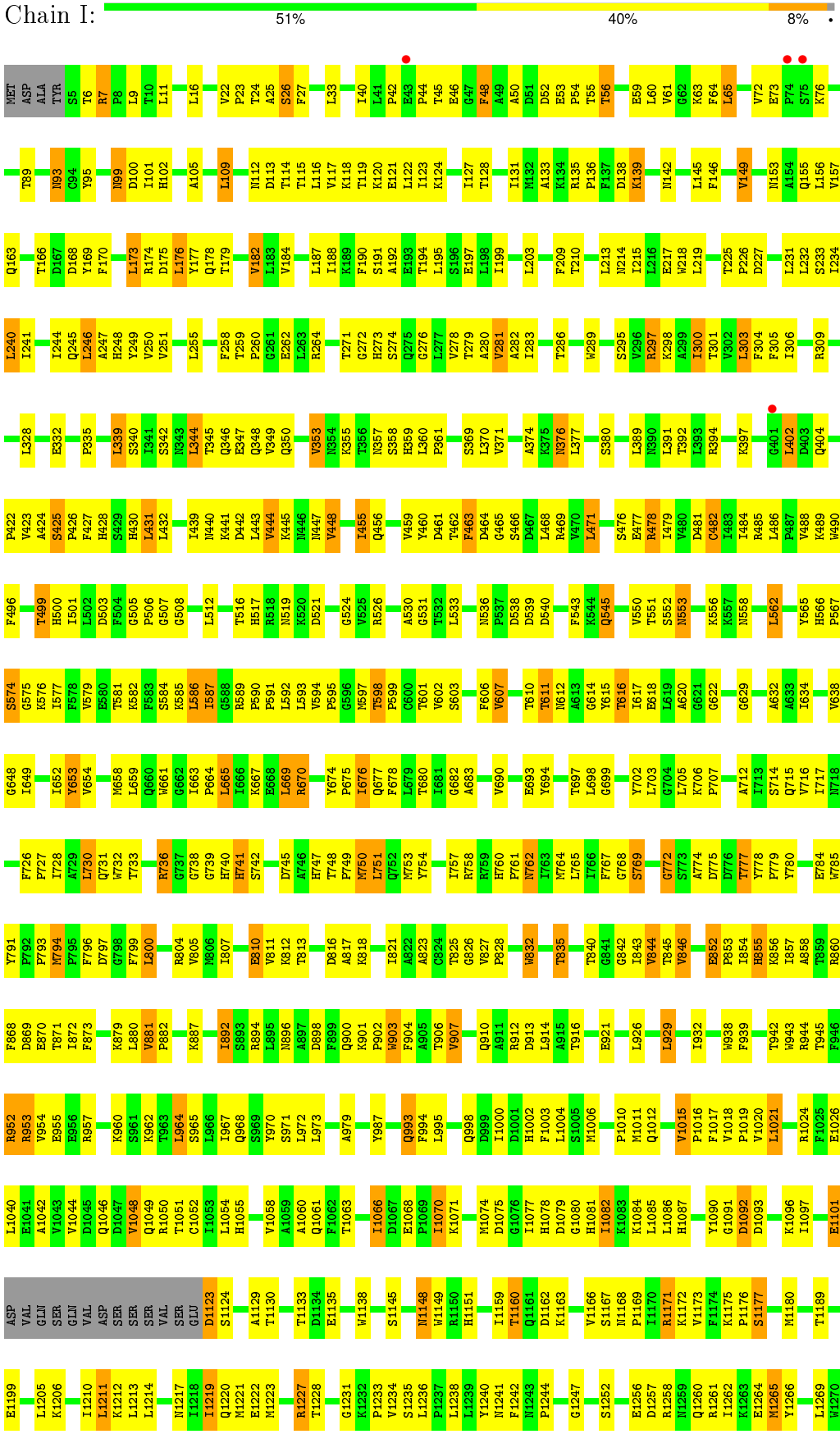
Chain H:

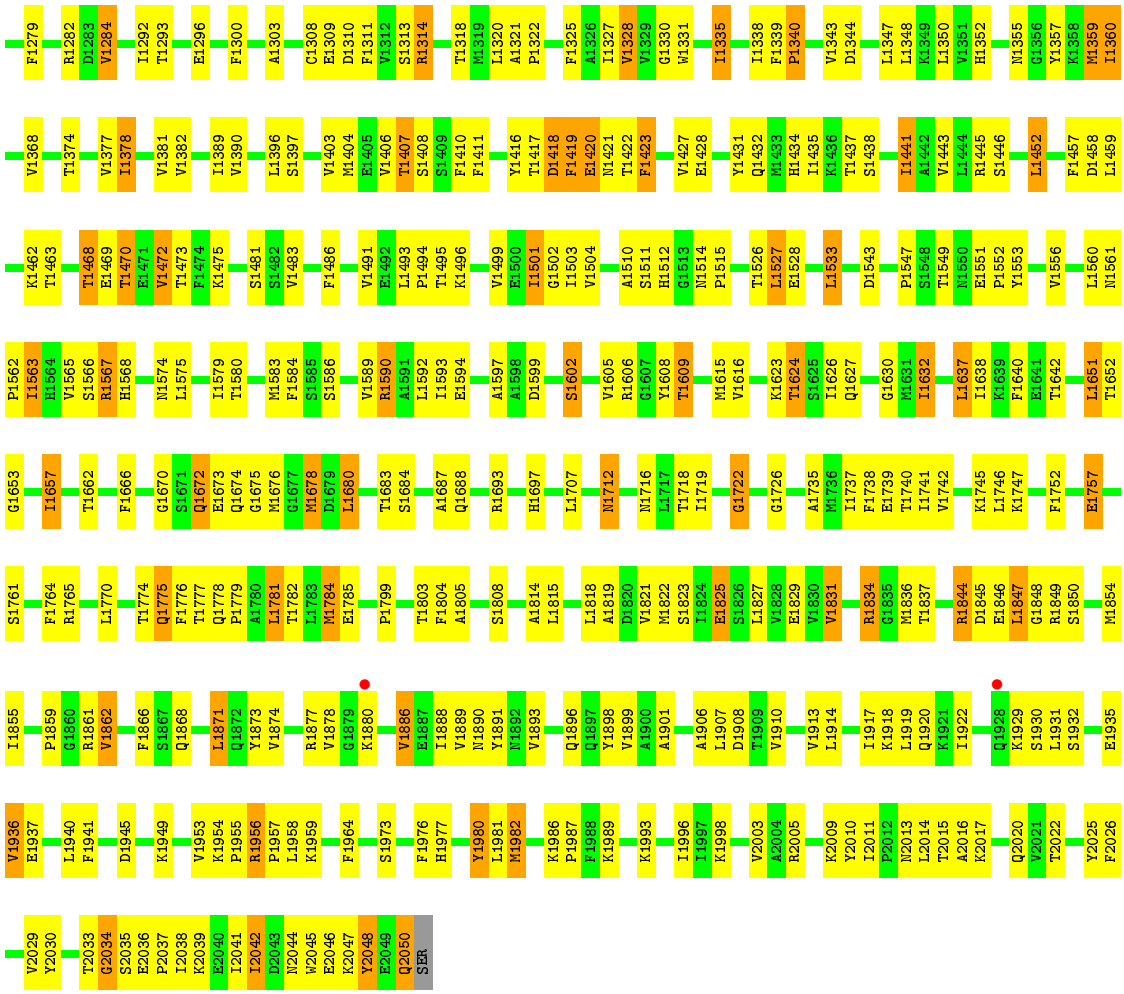





• Molecule 2: Fatty acid synthase subunit beta

Chain I:




F1279 R1282 D1283 V1284 I1292 T1293 E1296 F1300 A1303 C1308 E1309 D1310 F1311 V1312 S1313 R1314 T1318 M1319 L1320 A1321 P1322 F1325 A1326 I1327 V1328 V1329 G1330 W1331 I1335 I1338 F1339 P1340 V1343 D1344 L1347 L1348 K1349 L1350 V1351 H1352 N1355 G1356 Y1357 K1358 M1359 I1360
V1368 T1374 V1377 I1378 V1381 V1382 I1389 V1390 L1396 S1397 V1403 M1404 E1405 V1406 T1407 S1408 S1409 F1410 F1411 Y1416 T1417 D1418 F1419 E1420 N1421 T1422 F1423 V1427 E1428 Y1431 Q1432 M1433 H1434 I1435 K1436 T1437 S1438 I1441 A1442 V1443 L1444 R1445 S1446 L1452 F1457 D1458 L1459
K1462 T1463 T1468 E1469 T1470 E1471 V1472 T1473 F1474 K1475 S1481 S1482 V1483 F1486 V1491 E1492 L1493 P1494 T1495 K1496 V1499 E1500 I1501 G1502 I1503 V1504 A1510 S1511 H1512 G1513 N1514 P1515 T1526 L1527 E1528 L1533 D1543 P1547 S1548 T1549 N1550 E1551 P1552 Y1553 V1556 L1560 N1561
P1562 I1563 H1564 V1565 S1566 R1567 H1568 N1574 L1575 I1579 T1580 M1583 F1584 S1585 S1586 V1589 R1590 A1591 L1592 I1593 E1594 A1597 A1598 D1599 S1602 V1605 R1606 G1607 Y1608 T1609 M1615 V1616 K1623 T1624 S1625 I1626 Q1627 G1630 M1631 I1632 L1637 I1638 K1639 F1640 E1641 T1642 L1651 T1652
G1653 I1657 T1662 F1666 G1670 S1671 Q1672 E1673 Q1674 G1675 M1676 G1677 M1678 D1679 L1680 T1683 S1684 A1687 Q1688 R1693 H1697 L1707 N1712 N1716 L1717 T1718 I1719 G1722 G1726 A1735 M1736 I1737 F1738 E1739 T1740 I1741 V1742 K1745 L1746 K1747 F1752 E1757
S1761 F1764 R1765 L1770 T1774 Q1775 F1776 T1777 Q1778 P1779 A1780 L1781 T1782 L1783 M1784 E1785 P1799 T1803 F1804 A1805 S1808 A1814 L1815 L1818 A1819 D1820 V1821 M1822 S1823 I1824 E1825 S1826 L1827 V1828 E1829 V1830 V1831 R1834 G1835 M1836 T1837 R1844 D1845 E1846 L1847 G1848 R1849 S1850 M1854
I1855 P1859 G1860 R1861 V1862 F1866 S1867 Q1868 L1871 Q1872 Y1873 V1874 R1877 V1878 G1879 K1880 V1886 E1887 I1888 V1889 N1890 Y1891 N1892 V1893 Q1896 Q1897 Y1898 V1899 A1900 A1901 A1906 L1907 D1908 T1909 V1910 V1913 L1914 I1917 K1918 L1919 Q1920 K1921 I1922 Q1928 K1929 S1930 L1931 S1932 E1935
V1936 E1937 L1940 F1941 D1945 K1949 V1953 K1954 P1955 R1956 P1957 L1958 K1959 F1964 S1973 F1976 H1977 Y1980 L1981 M1982 K1986 P1987 F1988 K1989 K1993 I1996 I1997 K1998 V2003 A2004 R2005 K2009 Y2010 I2011 P2012 N2013 L2014 T2015 A2016 K2017 Q2020 V2021 T2022 Y2025 F2026
V2029 Y2030 T2033 G2034 S2035 E2036 P2037 I2038 K2039 E2040 I2041 I2042 D2043 N2044 W2045 E2046 K2047 Y2048 E2049 Q2050 SER

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 43 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 231.88Å 231.88Å 756.78Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 4.00<br>20.00 – 4.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.3 (20.00-4.00)<br>97.3 (20.00-4.00) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.71 (at 3.94Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.266 , 0.267<br>0.275 , 0.279 | Depositor<br>DCC |
| $R_{free}$ test set | 8521 reflections (5.34%) | DCC |
| Wilson B-factor (Å$^2$) | 130.2 | Xtriage |
| Anisotropy | 0.319 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.23 , 75.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.36$, $< L^2 > = 0.19$ | Xtriage |
| Outliers | 0 of 168120 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 88830 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 168.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, CER

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.43 | 5/13822 (0.0%) | 0.59 | 6/18682 (0.0%) |
| 1 | B | 0.43 | 3/13822 (0.0%) | 0.61 | 9/18682 (0.0%) |
| 1 | C | 0.43 | 4/13822 (0.0%) | 0.59 | 4/18682 (0.0%) |
| 2 | G | 0.41 | 7/16360 (0.0%) | 0.58 | 6/22198 (0.0%) |
| 2 | H | 0.40 | 7/16360 (0.0%) | 0.57 | 3/22198 (0.0%) |
| 2 | I | 0.40 | 5/16360 (0.0%) | 0.58 | 10/22198 (0.0%) |
| All | All | 0.42 | 31/90546 (0.0%) | 0.59 | 38/122640 (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 | G | 0 | 1 |
| 2 | H | 0 | 2 |
| 2 | I | 0 | 1 |
| All | All | 0 | 4 |

All (31) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 992 | PHE | C-N | 13.35 | 1.59 | 1.34 |
| 1 | C | 992 | PHE | C-N | 13.18 | 1.59 | 1.34 |
| 2 | I | 842 | GLY | C-N | 11.12 | 1.59 | 1.34 |
| 2 | G | 315 | PRO | C-N | 10.45 | 1.58 | 1.34 |
| 1 | C | 485 | ASP | C-N | 9.61 | 1.56 | 1.34 |
| 2 | H | 1256 | GLU | C-N | 9.35 | 1.55 | 1.34 |
| 2 | H | 138 | ASP | C-N | 9.07 | 1.54 | 1.34 |
| 2 | H | 1840 | VAL | C-N | 8.47 | 1.53 | 1.34 |
| 2 | G | 1657 | ILE | C-N | 8.15 | 1.52 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | I | 315 | PRO | C-N | 7.84 | 1.52 | 1.34 |
| 1 | A | 668 | PHE | C-N | 7.73 | 1.51 | 1.34 |
| 2 | I | 1980 | TYR | C-N | 7.70 | 1.51 | 1.34 |
| 1 | A | 181 | THR | C-N | 7.05 | 1.50 | 1.34 |
| 2 | G | 422 | PRO | C-N | 6.97 | 1.50 | 1.34 |
| 2 | I | 1018 | VAL | C-N | -6.57 | 1.21 | 1.34 |
| 2 | G | 1256 | GLU | C-N | 6.43 | 1.48 | 1.34 |
| 1 | C | 1520 | ALA | C-N | -6.36 | 1.22 | 1.34 |
| 2 | I | 903 | TRP | C-N | 6.33 | 1.48 | 1.34 |
| 2 | H | 1053 | ILE | C-N | 6.30 | 1.48 | 1.34 |
| 2 | H | 422 | PRO | C-N | 6.29 | 1.48 | 1.34 |
| 2 | G | 842 | GLY | C-N | 6.06 | 1.48 | 1.34 |
| 2 | H | 137 | PHE | C-N | 5.95 | 1.47 | 1.34 |
| 1 | A | 1520 | ALA | C-N | 5.79 | 1.45 | 1.34 |
| 2 | H | 1982 | MET | C-N | 5.67 | 1.47 | 1.34 |
| 1 | B | 181 | THR | C-N | -5.65 | 1.21 | 1.34 |
| 2 | G | 1529 | GLN | C-N | -5.50 | 1.21 | 1.34 |
| 2 | G | 1980 | TYR | C-N | 5.38 | 1.46 | 1.34 |
| 1 | C | 636 | PRO | C-N | -5.29 | 1.21 | 1.34 |
| 1 | B | 668 | PHE | C-N | 5.29 | 1.46 | 1.34 |
| 1 | B | 1430 | ARG | C-N | -5.19 | 1.22 | 1.34 |
| 1 | A | 1181 | PHE | C-N | 5.13 | 1.45 | 1.34 |

All (38) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 1116 | PRO | O-C-N | -11.67 | 104.02 | 122.70 |
| 2 | I | 1982 | MET | O-C-N | -9.44 | 107.59 | 122.70 |
| 2 | G | 842 | GLY | O-C-N | -8.86 | 108.52 | 122.70 |
| 2 | G | 1053 | ILE | O-C-N | -8.58 | 108.97 | 122.70 |
| 1 | B | 992 | PHE | O-C-N | 8.47 | 137.19 | 121.10 |
| 2 | I | 422 | PRO | O-C-N | -8.30 | 109.42 | 122.70 |
| 1 | B | 992 | PHE | C-N-CD | 8.15 | 145.52 | 128.40 |
| 2 | I | 1982 | MET | C-N-CA | 8.08 | 141.89 | 121.70 |
| 1 | B | 1116 | PRO | CA-C-N | 8.00 | 134.79 | 117.20 |
| 2 | I | 1657 | ILE | O-C-N | -7.47 | 110.75 | 122.70 |
| 1 | C | 1520 | ALA | O-C-N | 7.43 | 135.22 | 121.10 |
| 1 | A | 1430 | ARG | O-C-N | -7.40 | 110.85 | 122.70 |
| 1 | B | 1116 | PRO | C-N-CA | 7.29 | 139.94 | 121.70 |
| 1 | B | 599 | MET | N-CA-C | -6.93 | 92.27 | 111.00 |
| 1 | C | 599 | MET | N-CA-C | -6.92 | 92.32 | 111.00 |
| 1 | A | 599 | MET | N-CA-C | -6.90 | 92.37 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 992 | PHE | C-N-CD | 6.65 | 142.37 | 128.40 |
| 2 | I | 422 | PRO | CA-C-N | 6.52 | 131.55 | 117.20 |
| 2 | H | 1840 | VAL | O-C-N | -6.51 | 112.29 | 122.70 |
| 2 | I | 1982 | MET | CA-C-N | 6.50 | 131.50 | 117.20 |
| 1 | C | 1116 | PRO | O-C-N | -6.36 | 112.52 | 122.70 |
| 1 | B | 992 | PHE | CA-C-N | -6.11 | 100.00 | 117.10 |
| 2 | G | 1053 | ILE | CA-C-N | 6.05 | 130.50 | 117.20 |
| 1 | A | 992 | PHE | O-C-N | 5.97 | 132.45 | 121.10 |
| 2 | I | 315 | PRO | O-C-N | -5.75 | 113.50 | 122.70 |
| 1 | B | 540 | GLN | N-CA-C | -5.65 | 95.74 | 111.00 |
| 1 | A | 540 | GLN | N-CA-C | -5.64 | 95.77 | 111.00 |
| 1 | C | 540 | GLN | N-CA-C | -5.63 | 95.80 | 111.00 |
| 1 | B | 178 | GLY | O-C-N | 5.57 | 131.61 | 122.70 |
| 2 | I | 422 | PRO | C-N-CA | 5.52 | 135.50 | 121.70 |
| 2 | G | 138 | ASP | O-C-N | -5.44 | 113.99 | 122.70 |
| 1 | A | 1520 | ALA | O-C-N | 5.44 | 131.44 | 121.10 |
| 2 | H | 1256 | GLU | CA-C-N | -5.39 | 105.35 | 117.20 |
| 2 | I | 1657 | ILE | CA-C-N | 5.34 | 128.95 | 117.20 |
| 2 | G | 842 | GLY | CA-C-N | 5.30 | 128.86 | 117.20 |
| 2 | H | 138 | ASP | O-C-N | -5.08 | 114.56 | 122.70 |
| 2 | G | 138 | ASP | C-N-CA | 5.05 | 134.32 | 121.70 |
| 2 | I | 1657 | ILE | C-N-CA | 5.03 | 134.27 | 121.70 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | G | 1108 | PRO | Peptide |
| 2 | H | 1108 | PRO | Peptide |
| 2 | H | 1256 | GLU | Mainchain |
| 2 | I | 1108 | PRO | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 13572 | 0 | 13489 | 663 | 15 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | B | 13572 | 0 | 13490 | 618 | 6 |
| 1 | C | 13572 | 0 | 13490 | 638 | 22 |
| 2 | G | 15995 | 0 | 15978 | 1026 | 32 |
| 2 | H | 15995 | 0 | 15978 | 1023 | 7 |
| 2 | I | 15995 | 0 | 15977 | 983 | 26 |
| 3 | A | 12 | 0 | 10 | 3 | 0 |
| 3 | B | 12 | 0 | 10 | 4 | 0 |
| 3 | C | 12 | 0 | 10 | 4 | 0 |
| 4 | G | 31 | 0 | 19 | 7 | 0 |
| 4 | H | 31 | 0 | 19 | 6 | 0 |
| 4 | I | 31 | 0 | 19 | 8 | 0 |
| All | All | 88830 | 0 | 88489 | 4773 | 54 |

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 27.

All (4773) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1749:THR:CB | 1:A:1874:ASP:HB3 | 1.53 | 1.37 |
| 1:B:1749:THR:CB | 1:B:1874:ASP:HB3 | 1.56 | 1.34 |
| 1:B:1749:THR:CB | 1:B:1873:HIS:O | 1.75 | 1.32 |
| 1:A:1464:GLU:HG3 | 1:A:1773:VAL:CG1 | 1.58 | 1.32 |
| 1:C:1749:THR:CB | 1:C:1874:ASP:HB3 | 1.62 | 1.29 |
| 1:A:1464:GLU:CG | 1:A:1773:VAL:HG12 | 1.65 | 1.26 |
| 1:A:1749:THR:CB | 1:A:1873:HIS:O | 1.88 | 1.21 |
| 1:C:1749:THR:CB | 1:C:1874:ASP:CA | 2.20 | 1.19 |
| 2:H:1956:ARG:HB2 | 2:H:1957:PRO:HD3 | 1.24 | 1.18 |
| 1:C:1749:THR:CB | 1:C:1874:ASP:CB | 2.22 | 1.16 |
| 2:G:28:PHE:CE2 | 2:H:7:ARG:HD2 | 1.80 | 1.16 |
| 1:C:1464:GLU:CG | 1:C:1773:VAL:HG12 | 1.75 | 1.16 |
| 2:G:1859:PRO:HG3 | 2:G:1871:LEU:HD12 | 1.29 | 1.15 |
| 2:H:1834:ARG:HH11 | 2:H:1834:ARG:HG2 | 1.06 | 1.15 |
| 1:C:1501:LEU:CD1 | 1:C:1775:LEU:HD21 | 1.75 | 1.15 |
| 1:C:1460:LYS:NZ | 1:C:1774:GLU:OE2 | 1.80 | 1.15 |
| 1:C:1464:GLU:HG3 | 1:C:1773:VAL:CG1 | 1.77 | 1.14 |
| 2:H:490:TRP:HE1 | 2:H:516:THR:HG22 | 1.12 | 1.14 |
| 1:C:1498:GLU:HG3 | 1:C:1876:LEU:HD13 | 1.19 | 1.14 |
| 2:H:499:THR:HB | 2:H:500:HIS:HD2 | 1.10 | 1.12 |
| 2:I:490:TRP:HE1 | 2:I:516:THR:HG22 | 1.10 | 1.12 |
| 2:G:1956:ARG:HB2 | 2:G:1957:PRO:HD3 | 1.23 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:131:ILE:HD12 | 2:G:182:VAL:HB | 1.18 | 1.12 |
| 2:H:131:ILE:HD12 | 2:H:182:VAL:CB | 1.79 | 1.11 |
| 2:I:601:THR:HG21 | 2:I:618:GLU:O | 1.50 | 1.11 |
| 2:I:1956:ARG:HB2 | 2:I:1957:PRO:HD3 | 1.23 | 1.11 |
| 1:A:253:ARG:HG3 | 1:A:254:TRP:HD1 | 1.15 | 1.10 |
| 2:H:601:THR:HG21 | 2:H:618:GLU:O | 1.50 | 1.10 |
| 1:A:1721:ARG:HG2 | 1:A:1721:ARG:HH11 | 1.16 | 1.10 |
| 2:G:601:THR:HG21 | 2:G:618:GLU:O | 1.52 | 1.10 |
| 1:B:1464:GLU:HG3 | 1:B:1773:VAL:HG12 | 1.31 | 1.09 |
| 2:G:499:THR:HB | 2:G:500:HIS:HD2 | 1.08 | 1.09 |
| 2:H:131:ILE:CB | 2:H:182:VAL:HG11 | 1.82 | 1.09 |
| 2:I:297:ARG:HD3 | 2:I:447:ASN:HD21 | 1.15 | 1.09 |
| 2:G:131:ILE:HB | 2:G:182:VAL:HG11 | 1.31 | 1.09 |
| 2:I:499:THR:HB | 2:I:500:HIS:HD2 | 1.07 | 1.08 |
| 2:G:490:TRP:HE1 | 2:G:516:THR:HG22 | 1.12 | 1.08 |
| 1:B:1749:THR:CB | 1:B:1874:ASP:CB | 2.32 | 1.08 |
| 1:B:1460:LYS:NZ | 1:B:1774:GLU:OE2 | 1.85 | 1.08 |
| 1:A:1749:THR:CB | 1:A:1874:ASP:CB | 2.31 | 1.08 |
| 1:C:852:ARG:HG2 | 1:C:852:ARG:HH11 | 1.14 | 1.08 |
| 1:C:1498:GLU:CG | 1:C:1876:LEU:HD13 | 1.84 | 1.07 |
| 2:H:131:ILE:HG21 | 2:H:182:VAL:HG12 | 1.35 | 1.07 |
| 2:H:128:THR:HA | 2:H:182:VAL:HG21 | 1.31 | 1.07 |
| 2:I:1227:ARG:HG3 | 2:I:1227:ARG:HH11 | 1.18 | 1.07 |
| 2:G:297:ARG:HD3 | 2:G:447:ASN:HD21 | 1.17 | 1.06 |
| 2:G:28:PHE:CZ | 2:H:7:ARG:HD2 | 1.91 | 1.06 |
| 2:I:1834:ARG:HG2 | 2:I:1834:ARG:HH11 | 1.16 | 1.06 |
| 1:C:1367:ARG:NH1 | 1:C:1372:THR:HB | 1.71 | 1.06 |
| 2:G:903:TRP:O | 2:G:906:THR:HG22 | 1.57 | 1.05 |
| 1:C:1721:ARG:HG2 | 1:C:1721:ARG:HH11 | 1.19 | 1.05 |
| 2:G:1834:ARG:HG2 | 2:G:1834:ARG:HH11 | 1.16 | 1.05 |
| 2:I:7:ARG:HH21 | 2:I:27:PHE:HB3 | 1.20 | 1.05 |
| 1:B:253:ARG:HG3 | 1:B:254:TRP:HD1 | 1.17 | 1.04 |
| 1:C:253:ARG:HG3 | 1:C:254:TRP:HD1 | 1.15 | 1.04 |
| 1:A:1367:ARG:NH1 | 1:A:1372:THR:HB | 1.72 | 1.04 |
| 2:I:1739:GLU:HB2 | 2:I:1987:PRO:HB3 | 1.40 | 1.04 |
| 2:G:932:ILE:HD11 | 2:G:1042:ALA:HB2 | 1.36 | 1.04 |
| 1:B:1367:ARG:NH1 | 1:B:1372:THR:HB | 1.73 | 1.04 |
| 2:H:1227:ARG:HG3 | 2:H:1227:ARG:HH11 | 1.19 | 1.03 |
| 2:H:297:ARG:HD3 | 2:H:447:ASN:HD21 | 1.16 | 1.03 |
| 2:G:1227:ARG:HH11 | 2:G:1227:ARG:HG3 | 1.18 | 1.03 |
| 1:B:1721:ARG:HH11 | 1:B:1721:ARG:HG2 | 1.21 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1722:VAL:HG11 | 1:B:1731:LEU:HB3 | 1.37 | 1.03 |
| 1:C:1722:VAL:HG11 | 1:C:1731:LEU:HB3 | 1.37 | 1.02 |
| 2:G:7:ARG:HH21 | 2:G:27:PHE:HB3 | 1.22 | 1.02 |
| 2:H:7:ARG:HH21 | 2:H:27:PHE:HB3 | 1.22 | 1.02 |
| 1:B:599:MET:HB2 | 1:B:624:LYS:HD2 | 1.42 | 1.02 |
| 1:C:1498:GLU:HG3 | 1:C:1876:LEU:CD1 | 1.84 | 1.02 |
| 1:B:852:ARG:HG2 | 1:B:852:ARG:HH11 | 1.20 | 1.02 |
| 1:A:852:ARG:HH11 | 1:A:852:ARG:HG2 | 1.23 | 1.02 |
| 1:C:1501:LEU:HD12 | 1:C:1775:LEU:HD21 | 1.38 | 1.02 |
| 2:H:1739:GLU:HB2 | 2:H:1987:PRO:HB3 | 1.42 | 1.02 |
| 2:H:1859:PRO:HG3 | 2:H:1871:LEU:HD12 | 1.37 | 1.01 |
| 2:I:1859:PRO:HG3 | 2:I:1871:LEU:HD12 | 1.41 | 1.01 |
| 2:H:131:ILE:HB | 2:H:182:VAL:CG1 | 1.89 | 1.01 |
| 1:C:1219:VAL:HA | 1:C:1384:ILE:HD11 | 1.40 | 1.01 |
| 2:H:131:ILE:CD1 | 2:H:182:VAL:HB | 1.91 | 1.00 |
| 1:C:1014:ASP:H | 1:C:1510:ASN:HD21 | 1.03 | 1.00 |
| 2:H:903:TRP:O | 2:H:906:THR:HG22 | 1.59 | 1.00 |
| 2:I:741:HIS:NE2 | 2:I:855:HIS:CE1 | 2.30 | 1.00 |
| 1:A:1722:VAL:HG11 | 1:A:1731:LEU:HB3 | 1.40 | 1.00 |
| 1:A:599:MET:HB2 | 1:A:624:LYS:HD2 | 1.43 | 0.99 |
| 2:H:1567:ARG:HG3 | 2:H:1567:ARG:HH11 | 1.27 | 0.99 |
| 1:C:1749:THR:CB | 1:C:1874:ASP:HA | 1.90 | 0.99 |
| 1:C:599:MET:HB2 | 1:C:624:LYS:HD2 | 1.43 | 0.99 |
| 1:C:253:ARG:HG3 | 1:C:254:TRP:CD1 | 1.98 | 0.99 |
| 2:G:499:THR:HB | 2:G:500:HIS:CD2 | 1.97 | 0.98 |
| 2:I:892:ILE:HD11 | 2:I:903:TRP:CE2 | 1.98 | 0.98 |
| 1:A:253:ARG:HG3 | 1:A:254:TRP:CD1 | 1.98 | 0.98 |
| 1:B:1219:VAL:HA | 1:B:1384:ILE:HD11 | 1.45 | 0.98 |
| 1:C:1460:LYS:HE3 | 1:C:1774:GLU:CD | 1.83 | 0.98 |
| 2:H:1803:THR:HG22 | 2:H:2009:LYS:HA | 1.45 | 0.98 |
| 2:H:762:ASN:H | 2:H:762:ASN:HD22 | 1.03 | 0.98 |
| 2:H:131:ILE:HB | 2:H:182:VAL:HG11 | 1.00 | 0.98 |
| 2:I:499:THR:HB | 2:I:500:HIS:CD2 | 1.97 | 0.98 |
| 2:I:903:TRP:O | 2:I:906:THR:HG22 | 1.63 | 0.98 |
| 2:G:1844:ARG:HG2 | 2:G:1844:ARG:HH11 | 1.26 | 0.97 |
| 1:A:400:ARG:HG2 | 1:A:400:ARG:HH11 | 1.28 | 0.97 |
| 2:G:892:ILE:HD11 | 2:G:903:TRP:CE2 | 1.98 | 0.97 |
| 1:A:400:ARG:CG | 1:A:400:ARG:HH11 | 1.76 | 0.97 |
| 2:H:499:THR:HB | 2:H:500:HIS:CD2 | 1.99 | 0.97 |
| 2:H:1172:LYS:HE3 | 2:H:1574:ASN:OD1 | 1.64 | 0.97 |
| 1:B:198:PRO:HG3 | 1:B:209:LEU:HD21 | 1.47 | 0.97 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:253:ARG:HG3 | 1:B:254:TRP:CD1 | 1.99 | 0.96 |
| 2:I:490:TRP:NE1 | 2:I:516:THR:HG22 | 1.79 | 0.96 |
| 2:I:762:ASN:HD22 | 2:I:762:ASN:H | 1.08 | 0.96 |
| 2:H:594:VAL:HB | 2:H:617:ILE:HG13 | 1.44 | 0.96 |
| 1:A:1014:ASP:H | 1:A:1510:ASN:HD21 | 1.10 | 0.96 |
| 2:H:490:TRP:NE1 | 2:H:516:THR:HG22 | 1.81 | 0.96 |
| 2:H:131:ILE:HD12 | 2:H:182:VAL:HB | 0.96 | 0.96 |
| 1:A:12:ILE:HD11 | 2:G:2041:ILE:HD12 | 1.47 | 0.95 |
| 2:G:490:TRP:NE1 | 2:G:516:THR:HG22 | 1.81 | 0.95 |
| 2:H:892:ILE:HD11 | 2:H:903:TRP:CE2 | 2.01 | 0.95 |
| 2:H:1567:ARG:HH11 | 2:H:1567:ARG:CG | 1.79 | 0.95 |
| 1:C:198:PRO:HG3 | 1:C:209:LEU:HD21 | 1.48 | 0.95 |
| 2:G:1803:THR:HG22 | 2:G:2009:LYS:HA | 1.48 | 0.95 |
| 1:B:1460:LYS:CE | 1:B:1773:VAL:O | 2.15 | 0.95 |
| 2:I:594:VAL:HB | 2:I:617:ILE:HG13 | 1.46 | 0.95 |
| 2:I:1567:ARG:HH11 | 2:I:1567:ARG:HG3 | 1.29 | 0.95 |
| 2:I:1567:ARG:HH11 | 2:I:1567:ARG:CG | 1.79 | 0.95 |
| 2:H:1199:GLU:OE2 | 2:H:1567:ARG:NH1 | 2.00 | 0.95 |
| 2:G:1741:ILE:HD12 | 2:G:1986:LYS:HD2 | 1.47 | 0.95 |
| 2:G:1878:VAL:HG11 | 2:G:1910:VAL:HG22 | 1.48 | 0.95 |
| 2:I:741:HIS:CE1 | 2:I:855:HIS:CE1 | 2.55 | 0.95 |
| 1:A:198:PRO:HG3 | 1:A:209:LEU:HD21 | 1.47 | 0.95 |
| 2:G:1567:ARG:CG | 2:G:1567:ARG:HH11 | 1.80 | 0.95 |
| 1:B:1464:GLU:HG3 | 1:B:1773:VAL:CG1 | 1.95 | 0.95 |
| 2:H:741:HIS:HE1 | 2:H:845:THR:CG2 | 1.80 | 0.95 |
| 1:A:444:ASN:HB2 | 1:A:447:LEU:H | 1.31 | 0.95 |
| 2:H:835:THR:HG21 | 2:H:855:HIS:CD2 | 1.99 | 0.94 |
| 2:G:1739:GLU:HB2 | 2:G:1987:PRO:HB3 | 1.43 | 0.94 |
| 2:G:1589:VAL:HA | 2:G:1592:LEU:HD12 | 1.49 | 0.94 |
| 1:B:1460:LYS:HE3 | 1:B:1773:VAL:O | 1.68 | 0.94 |
| 2:H:55:THR:HG22 | 2:H:56:THR:HG22 | 1.48 | 0.94 |
| 1:B:444:ASN:HB2 | 1:B:447:LEU:H | 1.31 | 0.94 |
| 1:C:1498:GLU:OE2 | 1:C:1876:LEU:HA | 1.65 | 0.94 |
| 2:I:1741:ILE:HD12 | 2:I:1986:LYS:HD2 | 1.49 | 0.94 |
| 1:C:400:ARG:HG2 | 1:C:400:ARG:HH11 | 1.33 | 0.94 |
| 2:I:1878:VAL:HG11 | 2:I:1910:VAL:HG22 | 1.50 | 0.94 |
| 1:C:2:LYS:HD2 | 2:I:2050:GLN:HB3 | 1.50 | 0.94 |
| 2:H:1314:ARG:HH11 | 2:H:1314:ARG:HG3 | 1.31 | 0.94 |
| 2:G:942:THR:HB | 2:G:1012:GLN:HG2 | 1.50 | 0.93 |
| 2:G:762:ASN:H | 2:G:762:ASN:HD22 | 1.03 | 0.93 |
| 1:A:1219:VAL:HA | 1:A:1384:ILE:HD11 | 1.45 | 0.93 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:529:MET:HE3 | 1:B:529:MET:HA | 1.47 | 0.93 |
| 2:I:741:HIS:HE1 | 2:I:845:THR:CG2 | 1.81 | 0.93 |
| 1:A:1501:LEU:CD1 | 1:A:1775:LEU:HD21 | 1.98 | 0.93 |
| 2:H:652:ILE:H | 2:H:658:MET:HE3 | 1.30 | 0.93 |
| 2:H:1845:ASP:HB2 | 2:H:1849:ARG:H | 1.34 | 0.93 |
| 1:B:400:ARG:HH11 | 1:B:400:ARG:CG | 1.81 | 0.93 |
| 2:H:1589:VAL:HA | 2:H:1592:LEU:HD12 | 1.49 | 0.93 |
| 2:G:565:TYR:CZ | 2:G:758:ARG:HD2 | 2.04 | 0.93 |
| 2:I:1314:ARG:HG3 | 2:I:1314:ARG:HH11 | 1.32 | 0.93 |
| 1:A:12:ILE:HD11 | 2:G:2041:ILE:CD1 | 1.99 | 0.93 |
| 2:I:56:THR:HG23 | 2:I:59:GLU:HG3 | 1.49 | 0.93 |
| 1:C:1501:LEU:HD11 | 1:C:1775:LEU:CD2 | 1.99 | 0.93 |
| 2:G:1567:ARG:HG3 | 2:G:1567:ARG:HH11 | 1.30 | 0.93 |
| 2:G:128:THR:HA | 2:G:182:VAL:HG21 | 1.51 | 0.92 |
| 1:C:1523:ARG:HH11 | 1:C:1523:ARG:HG3 | 1.32 | 0.92 |
| 1:A:1523:ARG:HG3 | 1:A:1523:ARG:HH11 | 1.33 | 0.92 |
| 1:C:1501:LEU:CD1 | 1:C:1775:LEU:CD2 | 2.47 | 0.92 |
| 2:I:741:HIS:CE1 | 2:I:845:THR:CG2 | 2.52 | 0.92 |
| 2:G:55:THR:HG21 | 2:G:113:ASP:HB2 | 1.52 | 0.92 |
| 1:A:1460:LYS:CE | 1:A:1773:VAL:O | 2.17 | 0.92 |
| 2:G:741:HIS:NE2 | 2:G:855:HIS:CE1 | 2.38 | 0.92 |
| 1:A:152:HIS:CD2 | 1:A:163:LEU:HB2 | 2.05 | 0.92 |
| 1:B:1749:THR:CB | 1:B:1873:HIS:C | 2.37 | 0.92 |
| 2:G:1844:ARG:CG | 2:G:1844:ARG:HH11 | 1.82 | 0.92 |
| 2:I:55:THR:HG22 | 2:I:56:THR:HG22 | 1.51 | 0.91 |
| 2:I:667:LYS:HD2 | 2:I:697:THR:HG22 | 1.51 | 0.91 |
| 2:I:741:HIS:CE1 | 2:I:845:THR:HG22 | 2.04 | 0.91 |
| 1:A:1721:ARG:CG | 1:A:1721:ARG:HH11 | 1.84 | 0.91 |
| 1:C:400:ARG:HH11 | 1:C:400:ARG:CG | 1.81 | 0.91 |
| 2:G:1314:ARG:HH11 | 2:G:1314:ARG:HG3 | 1.32 | 0.91 |
| 2:G:56:THR:HG23 | 2:G:59:GLU:HG3 | 1.50 | 0.91 |
| 2:G:741:HIS:CE1 | 2:G:855:HIS:CE1 | 2.57 | 0.91 |
| 1:C:152:HIS:CD2 | 1:C:163:LEU:HB2 | 2.05 | 0.91 |
| 2:I:1803:THR:HG22 | 2:I:2009:LYS:HA | 1.51 | 0.91 |
| 2:I:707:PRO:HG3 | 2:I:716:VAL:HG21 | 1.52 | 0.91 |
| 1:A:1693:ILE:HD11 | 2:G:998:GLN:HB2 | 1.51 | 0.91 |
| 1:C:1464:GLU:HG3 | 1:C:1773:VAL:HG12 | 0.91 | 0.91 |
| 1:B:1523:ARG:HH11 | 1:B:1523:ARG:HG3 | 1.36 | 0.91 |
| 1:C:793:ARG:HA | 1:C:797:THR:HG23 | 1.52 | 0.90 |
| 2:H:1741:ILE:HD12 | 2:H:1986:LYS:HD2 | 1.54 | 0.90 |
| 2:I:942:THR:HB | 2:I:1012:GLN:HG2 | 1.52 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:707:PRO:HG3 | 2:H:716:VAL:HG21 | 1.54 | 0.90 |
| 1:C:1498:GLU:HG3 | 1:C:1876:LEU:HB3 | 1.53 | 0.90 |
| 2:I:1441:ILE:HD11 | 2:I:1445:ARG:CZ | 2.02 | 0.90 |
| 2:I:652:ILE:H | 2:I:658:MET:HE3 | 1.36 | 0.90 |
| 1:C:1498:GLU:CG | 1:C:1876:LEU:HB3 | 2.02 | 0.90 |
| 2:G:55:THR:HG22 | 2:G:56:THR:HG22 | 1.52 | 0.90 |
| 2:H:565:TYR:CZ | 2:H:758:ARG:HD2 | 2.06 | 0.90 |
| 2:G:131:ILE:HD12 | 2:G:182:VAL:CB | 2.01 | 0.89 |
| 1:B:1456:GLU:OE1 | 1:B:1775:LEU:HD23 | 1.71 | 0.89 |
| 2:G:1847:LEU:H | 2:G:1847:LEU:HD12 | 1.37 | 0.89 |
| 1:C:1431:GLU:HG3 | 1:C:1433:HIS:CE1 | 2.07 | 0.89 |
| 1:C:444:ASN:HB2 | 1:C:447:LEU:H | 1.33 | 0.89 |
| 2:G:594:VAL:HB | 2:G:617:ILE:HG13 | 1.52 | 0.89 |
| 1:B:1721:ARG:HH11 | 1:B:1721:ARG:CG | 1.85 | 0.89 |
| 2:I:1589:VAL:HA | 2:I:1592:LEU:HD12 | 1.51 | 0.89 |
| 1:B:793:ARG:HA | 1:B:797:THR:HG23 | 1.54 | 0.89 |
| 1:A:253:ARG:HE | 1:A:254:TRP:HE1 | 1.21 | 0.89 |
| 2:G:1441:ILE:HD11 | 2:G:1445:ARG:CZ | 2.02 | 0.89 |
| 2:H:55:THR:HG21 | 2:H:113:ASP:HB2 | 1.53 | 0.89 |
| 2:H:1847:LEU:H | 2:H:1847:LEU:HD12 | 1.37 | 0.89 |
| 2:H:56:THR:HG23 | 2:H:59:GLU:HG3 | 1.54 | 0.89 |
| 1:A:529:MET:HA | 1:A:529:MET:HE3 | 1.53 | 0.89 |
| 1:B:1749:THR:CB | 1:B:1874:ASP:CA | 2.51 | 0.88 |
| 1:A:1474:ALA:HA | 1:A:1478:PRO:HG2 | 1.54 | 0.88 |
| 2:G:667:LYS:HD2 | 2:G:697:THR:HG22 | 1.55 | 0.88 |
| 1:A:1501:LEU:HD11 | 1:A:1775:LEU:CD2 | 2.01 | 0.88 |
| 2:H:667:LYS:HD2 | 2:H:697:THR:HG22 | 1.55 | 0.88 |
| 1:A:1367:ARG:HH12 | 1:A:1372:THR:HB | 1.35 | 0.88 |
| 1:A:403:ASP:HB2 | 1:A:1613:ASN:HD21 | 1.38 | 0.88 |
| 2:I:55:THR:HG21 | 2:I:113:ASP:HB2 | 1.53 | 0.88 |
| 1:B:31:THR:HG23 | 2:H:2011:ILE:HG21 | 1.56 | 0.88 |
| 2:H:942:THR:HB | 2:H:1012:GLN:HG2 | 1.54 | 0.88 |
| 1:B:1464:GLU:CG | 1:B:1773:VAL:HG12 | 2.01 | 0.88 |
| 1:B:1367:ARG:HH12 | 1:B:1372:THR:HB | 1.38 | 0.88 |
| 1:B:152:HIS:CD2 | 1:B:163:LEU:HB2 | 2.09 | 0.88 |
| 2:I:1227:ARG:CG | 2:I:1227:ARG:HH11 | 1.87 | 0.88 |
| 1:C:1721:ARG:CG | 1:C:1721:ARG:HH11 | 1.87 | 0.87 |
| 2:I:131:ILE:HD12 | 2:I:182:VAL:HB | 1.55 | 0.87 |
| 2:G:707:PRO:HG3 | 2:G:716:VAL:HG21 | 1.56 | 0.87 |
| 2:H:1441:ILE:HD11 | 2:H:1445:ARG:CZ | 2.04 | 0.87 |
| 1:B:1501:LEU:HD11 | 1:B:1775:LEU:HD21 | 1.56 | 0.87 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1422:THR:CG2 | 2:G:1474:PHE:HB2 | 2.05 | 0.87 |
| 1:A:793:ARG:HA | 1:A:797:THR:HG23 | 1.53 | 0.87 |
| 1:C:59:ARG:HH11 | 2:I:1896:GLN:NE2 | 1.71 | 0.87 |
| 2:I:369:SER:OG | 2:I:380:SER:HB3 | 1.74 | 0.87 |
| 2:I:298:LYS:HG2 | 2:I:448:VAL:HG22 | 1.56 | 0.87 |
| 1:C:1498:GLU:OE2 | 1:C:1876:LEU:CA | 2.12 | 0.87 |
| 2:H:131:ILE:CG2 | 2:H:182:VAL:HG12 | 2.04 | 0.87 |
| 1:C:529:MET:HA | 1:C:529:MET:HE3 | 1.57 | 0.87 |
| 2:I:1845:ASP:HB2 | 2:I:1849:ARG:H | 1.38 | 0.87 |
| 2:I:932:ILE:HD11 | 2:I:1042:ALA:HB2 | 1.57 | 0.87 |
| 1:B:260:ARG:HH12 | 1:B:300:VAL:HG21 | 1.38 | 0.87 |
| 1:C:253:ARG:HE | 1:C:254:TRP:HE1 | 1.21 | 0.87 |
| 1:A:1119:LYS:HD3 | 1:A:1121:MET:HE2 | 1.55 | 0.87 |
| 1:B:893:VAL:HG11 | 1:B:930:LEU:HD23 | 1.55 | 0.87 |
| 1:A:340:ARG:NH1 | 1:A:344:GLN:HG2 | 1.88 | 0.87 |
| 2:H:741:HIS:HE1 | 2:H:845:THR:HG22 | 1.38 | 0.86 |
| 2:H:1422:THR:CG2 | 2:H:1474:PHE:HB2 | 2.04 | 0.86 |
| 1:C:1474:ALA:HA | 1:C:1478:PRO:HG2 | 1.57 | 0.86 |
| 2:I:1739:GLU:HB3 | 2:I:1746:LEU:HD11 | 1.58 | 0.86 |
| 2:H:1878:VAL:HG11 | 2:H:1910:VAL:HG22 | 1.55 | 0.86 |
| 1:B:1474:ALA:HA | 1:B:1478:PRO:HG2 | 1.58 | 0.86 |
| 2:G:741:HIS:HE1 | 2:G:845:THR:CG2 | 1.88 | 0.86 |
| 2:H:1533:LEU:HD13 | 2:H:1630:GLY:HA2 | 1.55 | 0.86 |
| 2:H:1739:GLU:HB3 | 2:H:1746:LEU:HD11 | 1.56 | 0.85 |
| 1:B:400:ARG:HH11 | 1:B:400:ARG:HG2 | 1.41 | 0.85 |
| 2:G:741:HIS:CE1 | 2:G:845:THR:CG2 | 2.59 | 0.85 |
| 2:I:1533:LEU:HD13 | 2:I:1630:GLY:HA2 | 1.59 | 0.85 |
| 2:I:1422:THR:HG23 | 2:I:1422:THR:O | 1.77 | 0.85 |
| 1:A:1749:THR:CB | 1:A:1874:ASP:CA | 2.55 | 0.85 |
| 2:H:774:ALA:HB1 | 2:H:1081:HIS:HD2 | 1.41 | 0.85 |
| 2:I:1847:LEU:HD12 | 2:I:1847:LEU:H | 1.40 | 0.85 |
| 2:G:28:PHE:HE2 | 2:H:7:ARG:HD2 | 1.36 | 0.85 |
| 2:H:1844:ARG:HH11 | 2:H:1844:ARG:CG | 1.89 | 0.85 |
| 1:B:340:ARG:NH1 | 1:B:344:GLN:HG2 | 1.91 | 0.85 |
| 2:G:28:PHE:CZ | 2:H:7:ARG:CD | 2.59 | 0.85 |
| 1:A:1119:LYS:HD3 | 1:A:1121:MET:CE | 2.07 | 0.85 |
| 2:H:1844:ARG:HH11 | 2:H:1844:ARG:HG2 | 1.41 | 0.85 |
| 2:H:297:ARG:HD3 | 2:H:447:ASN:ND2 | 1.91 | 0.84 |
| 2:H:932:ILE:HD11 | 2:H:1042:ALA:HB2 | 1.58 | 0.84 |
| 2:H:777:THR:CG2 | 2:H:1081:HIS:NE2 | 2.41 | 0.84 |
| 2:G:369:SER:OG | 2:G:380:SER:HB3 | 1.75 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:131:ILE:HG21 | 2:G:182:VAL:HG12 | 1.57 | 0.84 |
| 2:I:297:ARG:HD3 | 2:I:447:ASN:ND2 | 1.92 | 0.84 |
| 1:C:340:ARG:NH1 | 1:C:344:GLN:HG2 | 1.91 | 0.84 |
| 2:G:1054:LEU:HB2 | 4:G:3051:FMN:HM72 | 1.60 | 0.84 |
| 2:H:2038:ILE:HG22 | 2:H:2042:ILE:HD11 | 1.60 | 0.84 |
| 2:H:369:SER:OG | 2:H:380:SER:HB3 | 1.78 | 0.84 |
| 2:G:652:ILE:H | 2:G:658:MET:HE3 | 1.42 | 0.84 |
| 1:C:852:ARG:HG2 | 1:C:852:ARG:NH1 | 1.93 | 0.84 |
| 2:I:774:ALA:HB2 | 2:I:1077:ILE:HA | 1.58 | 0.84 |
| 2:I:995:LEU:HD23 | 2:I:1000:ILE:HD13 | 1.60 | 0.84 |
| 1:C:1303:GLY:HA2 | 1:C:1649:LYS:HE2 | 1.58 | 0.84 |
| 1:B:11:HIS:ND1 | 2:H:1998:LYS:HA | 1.93 | 0.84 |
| 2:H:741:HIS:CE1 | 2:H:845:THR:HG22 | 2.12 | 0.84 |
| 1:C:31:THR:HG23 | 2:I:2011:ILE:HG21 | 1.59 | 0.84 |
| 2:G:1425:LYS:HG2 | 2:G:1471:GLU:HG3 | 1.58 | 0.83 |
| 2:G:1533:LEU:HD13 | 2:G:1630:GLY:HA2 | 1.60 | 0.83 |
| 1:A:980:VAL:HG23 | 2:G:968:GLN:OE1 | 1.78 | 0.83 |
| 2:G:774:ALA:HB2 | 2:G:1077:ILE:HA | 1.61 | 0.83 |
| 1:B:253:ARG:HE | 1:B:254:TRP:HE1 | 1.21 | 0.83 |
| 2:G:1227:ARG:HH11 | 2:G:1227:ARG:CG | 1.89 | 0.83 |
| 2:I:774:ALA:HB1 | 2:I:1081:HIS:HD2 | 1.43 | 0.83 |
| 2:H:1227:ARG:HH11 | 2:H:1227:ARG:CG | 1.90 | 0.83 |
| 2:H:741:HIS:CE1 | 2:H:845:THR:CG2 | 2.60 | 0.83 |
| 2:H:1672:GLN:HG2 | 2:H:1777:THR:HG23 | 1.59 | 0.83 |
| 2:I:1844:ARG:HH11 | 2:I:1844:ARG:HG2 | 1.43 | 0.83 |
| 2:G:1293:THR:HG23 | 2:G:1296:GLU:H | 1.44 | 0.83 |
| 2:I:598:THR:HG22 | 2:I:622:GLY:HA3 | 1.61 | 0.83 |
| 1:B:403:ASP:HB2 | 1:B:1613:ASN:HD21 | 1.44 | 0.82 |
| 2:G:297:ARG:HD3 | 2:G:447:ASN:ND2 | 1.94 | 0.82 |
| 1:A:20:TYR:CG | 2:G:2033:THR:OG1 | 2.32 | 0.82 |
| 2:G:777:THR:CG2 | 2:G:1081:HIS:NE2 | 2.41 | 0.82 |
| 2:H:85:ASN:HD22 | 2:H:135:ARG:HH11 | 1.26 | 0.82 |
| 2:G:131:ILE:CB | 2:G:182:VAL:HG11 | 2.07 | 0.82 |
| 1:C:1367:ARG:HH12 | 1:C:1372:THR:HB | 1.37 | 0.82 |
| 2:G:1739:GLU:HB3 | 2:G:1746:LEU:HD11 | 1.60 | 0.82 |
| 2:I:1672:GLN:HG2 | 2:I:1777:THR:HG23 | 1.61 | 0.82 |
| 2:G:298:LYS:HG2 | 2:G:448:VAL:HG22 | 1.61 | 0.82 |
| 1:A:1249:SER:HB3 | 1:A:1280:ILE:HG23 | 1.62 | 0.82 |
| 2:H:995:LEU:HD23 | 2:H:1000:ILE:HD13 | 1.58 | 0.82 |
| 1:B:1014:ASP:H | 1:B:1510:ASN:HD21 | 1.28 | 0.82 |
| 1:A:36:LEU:HD22 | 1:A:61:LEU:HD21 | 1.60 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:2038:ILE:HG22 | 2:I:2042:ILE:HD11 | 1.61 | 0.82 |
| 2:I:1931:LEU:HB3 | 2:I:1935:GLU:HG2 | 1.62 | 0.82 |
| 1:B:12:ILE:HD11 | 2:H:2041:ILE:CD1 | 2.10 | 0.82 |
| 1:A:335:HIS:HE1 | 1:B:335:HIS:CE1 | 1.98 | 0.82 |
| 2:G:1847:LEU:HD13 | 2:G:1849:ARG:HD2 | 1.62 | 0.81 |
| 1:C:333:LYS:O | 1:C:337:VAL:HG23 | 1.80 | 0.81 |
| 2:G:995:LEU:HD23 | 2:G:1000:ILE:HD13 | 1.60 | 0.81 |
| 2:I:128:THR:HA | 2:I:182:VAL:HG21 | 1.62 | 0.81 |
| 1:A:1464:GLU:HG3 | 1:A:1773:VAL:HG12 | 0.85 | 0.81 |
| 1:A:1501:LEU:HD11 | 1:A:1775:LEU:HD21 | 1.61 | 0.81 |
| 2:I:1844:ARG:CG | 2:I:1844:ARG:HH11 | 1.93 | 0.81 |
| 2:H:543:PHE:HB2 | 2:H:545:GLN:HE22 | 1.45 | 0.81 |
| 2:H:1159:ILE:HG12 | 2:H:1168:ASN:HA | 1.61 | 0.81 |
| 2:I:1054:LEU:HB2 | 4:I:3051:FMN:C7M | 2.11 | 0.81 |
| 2:I:777:THR:CG2 | 2:I:1081:HIS:NE2 | 2.43 | 0.81 |
| 2:I:345:THR:HG22 | 2:I:347:GLU:H | 1.46 | 0.81 |
| 2:G:543:PHE:HB2 | 2:G:545:GLN:HE22 | 1.46 | 0.81 |
| 1:B:1249:SER:HB3 | 1:B:1280:ILE:HG23 | 1.62 | 0.81 |
| 2:G:1931:LEU:HB3 | 2:G:1935:GLU:HG2 | 1.61 | 0.81 |
| 1:A:1460:LYS:HE2 | 1:A:1773:VAL:O | 1.80 | 0.81 |
| 1:C:59:ARG:HH11 | 2:I:1896:GLN:HE22 | 1.25 | 0.81 |
| 2:H:1149:TRP:HA | 2:H:1242:PHE:CE1 | 2.15 | 0.81 |
| 1:B:93:ASP:HB3 | 1:B:94:PRO:HD2 | 1.62 | 0.81 |
| 1:B:881:ASN:HA | 1:B:944:ARG:NH2 | 1.96 | 0.81 |
| 2:G:2038:ILE:HG22 | 2:G:2042:ILE:HD11 | 1.60 | 0.81 |
| 1:A:1203:ASP:HB3 | 1:B:179:LYS:NZ | 1.95 | 0.81 |
| 1:A:335:HIS:CE1 | 1:C:335:HIS:HE1 | 1.98 | 0.81 |
| 2:I:345:THR:HB | 2:I:348:GLN:H | 1.46 | 0.81 |
| 2:I:1159:ILE:HG12 | 2:I:1168:ASN:HA | 1.63 | 0.81 |
| 1:A:93:ASP:HB3 | 1:A:94:PRO:HD2 | 1.63 | 0.81 |
| 1:A:400:ARG:HG2 | 1:A:400:ARG:NH1 | 1.91 | 0.80 |
| 2:I:1693:ARG:HD2 | 2:I:1825:GLU:OE2 | 1.80 | 0.80 |
| 1:A:333:LYS:O | 1:A:337:VAL:HG23 | 1.82 | 0.80 |
| 1:A:1552:ASN:O | 1:A:1556:THR:HG22 | 1.80 | 0.80 |
| 2:G:1693:ARG:HD2 | 2:G:1825:GLU:OE2 | 1.81 | 0.80 |
| 2:I:584:SER:HB3 | 2:I:591:PRO:HG3 | 1.63 | 0.80 |
| 2:H:298:LYS:HG2 | 2:H:448:VAL:HG22 | 1.63 | 0.80 |
| 2:H:1931:LEU:HB3 | 2:H:1935:GLU:HG2 | 1.62 | 0.80 |
| 1:B:1030:TRP:CD1 | 1:B:1580:LEU:HD22 | 2.17 | 0.80 |
| 1:A:20:TYR:CE1 | 2:G:2035:SER:HB2 | 2.17 | 0.80 |
| 1:A:340:ARG:HH12 | 1:A:344:GLN:HG2 | 1.45 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:259:THR:HG22 | 2:I:262:GLU:HG3 | 1.63 | 0.80 |
| 2:G:1672:GLN:HG2 | 2:G:1777:THR:HG23 | 1.61 | 0.80 |
| 2:H:1159:ILE:HG12 | 2:H:1169:PRO:HD3 | 1.63 | 0.80 |
| 1:B:36:LEU:HD22 | 1:B:61:LEU:HD21 | 1.64 | 0.80 |
| 1:B:24:SER:CB | 2:H:2014:LEU:HD12 | 2.11 | 0.80 |
| 2:H:1847:LEU:HD13 | 2:H:1849:ARG:HD2 | 1.63 | 0.80 |
| 2:G:741:HIS:CE1 | 2:G:845:THR:HG22 | 2.17 | 0.80 |
| 2:I:192:ALA:HA | 2:I:215:ILE:HD12 | 1.64 | 0.80 |
| 1:C:1460:LYS:CE | 1:C:1774:GLU:OE2 | 2.29 | 0.80 |
| 1:C:1249:SER:HB3 | 1:C:1280:ILE:HG23 | 1.63 | 0.80 |
| 2:I:1242:PHE:HE2 | 2:I:1244:PRO:HG3 | 1.46 | 0.80 |
| 2:H:598:THR:HG22 | 2:H:622:GLY:HA3 | 1.64 | 0.79 |
| 1:A:1501:LEU:HD12 | 1:A:1775:LEU:HD21 | 1.63 | 0.79 |
| 2:H:907:VAL:HG21 | 2:H:921:GLU:HG2 | 1.64 | 0.79 |
| 2:I:455:ILE:HD11 | 2:I:469:ARG:HD3 | 1.63 | 0.79 |
| 1:A:484:LEU:O | 1:A:485:ASP:HB2 | 1.82 | 0.79 |
| 1:C:1460:LYS:CE | 1:C:1774:GLU:CD | 2.50 | 0.79 |
| 2:I:1293:THR:HG23 | 2:I:1296:GLU:H | 1.47 | 0.79 |
| 2:H:1199:GLU:OE2 | 2:H:1567:ARG:CZ | 2.31 | 0.79 |
| 2:I:55:THR:CG2 | 2:I:113:ASP:HB2 | 2.12 | 0.79 |
| 1:C:1501:LEU:HD11 | 1:C:1775:LEU:HD21 | 1.55 | 0.79 |
| 2:I:1310:ASP:OD2 | 2:I:1602:SER:HB3 | 1.82 | 0.79 |
| 1:A:31:THR:HG23 | 2:G:2011:ILE:HG21 | 1.64 | 0.79 |
| 2:H:774:ALA:HB2 | 2:H:1077:ILE:HA | 1.64 | 0.79 |
| 2:H:1636:LYS:N | 2:H:1657:ILE:O | 2.14 | 0.79 |
| 2:H:455:ILE:HD11 | 2:H:469:ARG:HD3 | 1.63 | 0.79 |
| 2:I:543:PHE:HB2 | 2:I:545:GLN:HE22 | 1.46 | 0.79 |
| 2:I:238:CYS:HB2 | 2:I:239:PRO:HD3 | 1.64 | 0.79 |
| 2:G:634:ILE:HD11 | 2:G:649:ILE:HD11 | 1.63 | 0.79 |
| 2:I:907:VAL:HG21 | 2:I:921:GLU:HG2 | 1.65 | 0.79 |
| 2:G:1314:ARG:CG | 2:G:1314:ARG:HH11 | 1.95 | 0.79 |
| 1:B:260:ARG:NH1 | 1:B:300:VAL:HG21 | 1.97 | 0.79 |
| 2:G:774:ALA:HB1 | 2:G:1081:HIS:HD2 | 1.47 | 0.79 |
| 1:C:403:ASP:HB2 | 1:C:1613:ASN:HD21 | 1.46 | 0.79 |
| 2:G:55:THR:CG2 | 2:G:113:ASP:HB2 | 2.13 | 0.79 |
| 2:I:1847:LEU:HD13 | 2:I:1849:ARG:HD2 | 1.64 | 0.79 |
| 2:H:757:ILE:HG21 | 2:H:765:LEU:HD13 | 1.64 | 0.79 |
| 1:B:1303:GLY:HA2 | 1:B:1649:LYS:HE2 | 1.63 | 0.79 |
| 2:H:105:ALA:HB1 | 2:H:119:THR:HG23 | 1.65 | 0.79 |
| 1:B:1722:VAL:CG1 | 1:B:1731:LEU:HB3 | 2.13 | 0.78 |
| 1:C:1523:ARG:HH11 | 1:C:1523:ARG:CG | 1.96 | 0.78 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1149:TRP:HA | 2:I:1242:PHE:CE1 | 2.19 | 0.78 |
| 2:G:85:ASN:HD22 | 2:G:135:ARG:HH11 | 1.28 | 0.78 |
| 2:H:1567:ARG:NH1 | 2:H:1567:ARG:HG3 | 1.98 | 0.78 |
| 1:C:328:LEU:O | 1:C:331:ILE:HG22 | 1.84 | 0.78 |
| 2:H:960:LYS:HA | 2:H:960:LYS:HE2 | 1.65 | 0.78 |
| 2:I:85:ASN:HD22 | 2:I:135:ARG:HH11 | 1.28 | 0.78 |
| 2:H:345:THR:HB | 2:H:348:GLN:H | 1.48 | 0.78 |
| 2:H:131:ILE:CB | 2:H:182:VAL:CG1 | 2.53 | 0.78 |
| 2:G:7:ARG:NH2 | 2:G:27:PHE:HB3 | 1.99 | 0.78 |
| 1:B:12:ILE:HD11 | 2:H:2041:ILE:HD12 | 1.63 | 0.78 |
| 2:I:741:HIS:HE1 | 2:I:845:THR:HG22 | 1.41 | 0.78 |
| 1:A:328:LEU:O | 1:A:331:ILE:HG22 | 1.84 | 0.78 |
| 1:B:333:LYS:O | 1:B:337:VAL:HG23 | 1.81 | 0.78 |
| 1:C:1014:ASP:N | 1:C:1510:ASN:HD21 | 1.82 | 0.78 |
| 2:I:1770:LEU:HD23 | 2:I:1776:PHE:CE2 | 2.19 | 0.78 |
| 2:I:138:ASP:O | 2:I:139:LYS:HG3 | 1.83 | 0.78 |
| 1:B:198:PRO:HG3 | 1:B:209:LEU:CD2 | 2.13 | 0.78 |
| 2:H:55:THR:CG2 | 2:H:113:ASP:HB2 | 2.13 | 0.78 |
| 1:B:24:SER:O | 2:H:1977:HIS:HD2 | 1.67 | 0.78 |
| 1:A:2:LYS:HD2 | 2:G:2050:GLN:HB3 | 1.66 | 0.78 |
| 1:C:1498:GLU:CG | 1:C:1876:LEU:CD1 | 2.51 | 0.78 |
| 2:I:7:ARG:NH2 | 2:I:27:PHE:HB3 | 1.97 | 0.78 |
| 2:I:634:ILE:HD11 | 2:I:649:ILE:HD11 | 1.66 | 0.78 |
| 2:G:1227:ARG:HD2 | 2:G:1565:VAL:HG11 | 1.66 | 0.77 |
| 2:H:1693:ARG:HD2 | 2:H:1825:GLU:OE2 | 1.83 | 0.77 |
| 2:G:1770:LEU:HD23 | 2:G:1776:PHE:CE2 | 2.20 | 0.77 |
| 1:A:335:HIS:CE1 | 1:C:335:HIS:CE1 | 2.72 | 0.77 |
| 2:H:1293:THR:HG23 | 2:H:1296:GLU:H | 1.49 | 0.77 |
| 1:C:1463:VAL:HG11 | 1:C:1877:GLN:HE22 | 1.48 | 0.77 |
| 2:G:455:ILE:HD11 | 2:G:469:ARG:HD3 | 1.66 | 0.77 |
| 1:C:1665:ILE:HG13 | 1:C:1669:ARG:HD3 | 1.66 | 0.77 |
| 2:G:28:PHE:HZ | 2:H:7:ARG:CD | 1.97 | 0.77 |
| 2:H:131:ILE:CG2 | 2:H:182:VAL:CG1 | 2.63 | 0.77 |
| 2:I:741:HIS:CE1 | 2:I:855:HIS:NE2 | 2.52 | 0.77 |
| 2:G:355:LYS:O | 2:G:358:SER:HB3 | 1.84 | 0.77 |
| 1:A:1523:ARG:CG | 1:A:1523:ARG:HH11 | 1.97 | 0.77 |
| 2:H:1310:ASP:OD2 | 2:H:1602:SER:HB3 | 1.82 | 0.77 |
| 1:A:24:SER:HB3 | 2:G:2014:LEU:HD12 | 1.64 | 0.77 |
| 2:I:1314:ARG:CG | 2:I:1314:ARG:HH11 | 1.98 | 0.77 |
| 2:I:1423:PHE:H | 2:I:1423:PHE:HD1 | 1.30 | 0.77 |
| 1:B:1239:HIS:HD2 | 1:B:1241:SER:OG | 1.67 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:598:THR:HG22 | 2:G:622:GLY:HA3 | 1.67 | 0.77 |
| 2:G:1284:VAL:HG13 | 2:G:1377:VAL:HG22 | 1.65 | 0.77 |
| 1:C:1030:TRP:CD1 | 1:C:1580:LEU:HD22 | 2.20 | 0.77 |
| 2:G:345:THR:HG22 | 2:G:347:GLU:H | 1.47 | 0.77 |
| 1:C:1693:ILE:HD11 | 2:I:998:GLN:HB2 | 1.67 | 0.77 |
| 1:B:29:ILE:HG13 | 2:H:1891:TYR:O | 1.85 | 0.77 |
| 1:C:93:ASP:HB3 | 1:C:94:PRO:HD2 | 1.65 | 0.77 |
| 1:C:12:ILE:HD11 | 2:I:2041:ILE:HD12 | 1.67 | 0.77 |
| 1:C:340:ARG:HH12 | 1:C:344:GLN:HG2 | 1.49 | 0.77 |
| 1:C:1030:TRP:NE1 | 1:C:1580:LEU:HD22 | 2.00 | 0.77 |
| 2:G:907:VAL:HG21 | 2:G:921:GLU:HG2 | 1.65 | 0.77 |
| 2:H:1834:ARG:NH1 | 2:H:1834:ARG:HG2 | 1.86 | 0.76 |
| 2:I:1956:ARG:CB | 2:I:1957:PRO:HD3 | 2.09 | 0.76 |
| 2:I:1834:ARG:NH1 | 2:I:1834:ARG:HG2 | 1.93 | 0.76 |
| 2:I:1567:ARG:HG3 | 2:I:1567:ARG:NH1 | 2.00 | 0.76 |
| 1:A:1665:ILE:HG13 | 1:A:1669:ARG:HD3 | 1.66 | 0.76 |
| 1:B:1030:TRP:NE1 | 1:B:1580:LEU:HD22 | 2.00 | 0.76 |
| 1:A:1030:TRP:NE1 | 1:A:1580:LEU:HD22 | 1.99 | 0.76 |
| 1:A:198:PRO:HG3 | 1:A:209:LEU:CD2 | 2.14 | 0.76 |
| 1:C:198:PRO:HG3 | 1:C:209:LEU:CD2 | 2.15 | 0.76 |
| 2:G:1678:MET:HE3 | 2:G:1707:LEU:HD22 | 1.66 | 0.76 |
| 2:H:762:ASN:N | 2:H:762:ASN:HD22 | 1.82 | 0.76 |
| 1:C:400:ARG:HG2 | 1:C:400:ARG:NH1 | 1.94 | 0.76 |
| 2:G:146:PHE:HA | 2:G:149:VAL:CG1 | 2.15 | 0.76 |
| 2:G:345:THR:HB | 2:G:348:GLN:H | 1.50 | 0.76 |
| 2:I:355:LYS:O | 2:I:358:SER:HB3 | 1.85 | 0.76 |
| 2:H:598:THR:OG1 | 2:H:599:PRO:HD3 | 1.86 | 0.76 |
| 1:A:1030:TRP:CD1 | 1:A:1580:LEU:HD22 | 2.21 | 0.76 |
| 2:I:2015:THR:HG22 | 2:I:2017:LYS:H | 1.51 | 0.76 |
| 2:G:964:LEU:H | 2:G:964:LEU:HD23 | 1.50 | 0.76 |
| 2:G:1149:TRP:HA | 2:G:1242:PHE:CE1 | 2.20 | 0.76 |
| 2:H:1956:ARG:HB2 | 2:H:1957:PRO:CD | 2.12 | 0.76 |
| 1:C:1722:VAL:CG1 | 1:C:1731:LEU:HB3 | 2.14 | 0.76 |
| 2:H:1638:ILE:HD12 | 2:H:1657:ILE:HG13 | 1.67 | 0.76 |
| 1:C:24:SER:O | 2:I:1977:HIS:HD2 | 1.68 | 0.76 |
| 1:C:1239:HIS:HD2 | 1:C:1241:SER:OG | 1.68 | 0.76 |
| 2:H:584:SER:HB3 | 2:H:591:PRO:HG3 | 1.67 | 0.76 |
| 2:H:1314:ARG:HH11 | 2:H:1314:ARG:CG | 1.97 | 0.75 |
| 2:I:707:PRO:CG | 2:I:716:VAL:HG21 | 2.15 | 0.75 |
| 1:B:1501:LEU:CD1 | 1:B:1775:LEU:HD21 | 2.16 | 0.75 |
| 1:A:988:ILE:HD13 | 1:A:1048:GLU:CB | 2.15 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:317:THR:HG21 | 2:I:1309:GLU:HG3 | 1.67 | 0.75 |
| 2:G:2015:THR:HG22 | 2:G:2017:LYS:H | 1.51 | 0.75 |
| 1:B:1523:ARG:HH11 | 1:B:1523:ARG:CG | 1.98 | 0.75 |
| 1:B:340:ARG:HH12 | 1:B:344:GLN:HG2 | 1.48 | 0.75 |
| 2:I:1054:LEU:HB2 | 4:I:3051:FMN:HM72 | 1.66 | 0.75 |
| 2:H:192:ALA:HA | 2:H:215:ILE:HD12 | 1.68 | 0.75 |
| 2:H:7:ARG:NH2 | 2:H:27:PHE:HB3 | 1.99 | 0.75 |
| 2:G:1956:ARG:HB2 | 2:G:1957:PRO:CD | 2.11 | 0.75 |
| 2:I:856:LYS:HG2 | 2:I:1054:LEU:HD12 | 1.68 | 0.75 |
| 2:G:1159:ILE:HG12 | 2:G:1168:ASN:HA | 1.67 | 0.75 |
| 1:B:1665:ILE:HG13 | 1:B:1669:ARG:HD3 | 1.66 | 0.75 |
| 1:A:1460:LYS:HE3 | 1:A:1773:VAL:O | 1.86 | 0.75 |
| 2:H:355:LYS:O | 2:H:358:SER:HB3 | 1.85 | 0.75 |
| 2:G:960:LYS:HA | 2:G:960:LYS:HE2 | 1.67 | 0.75 |
| 2:H:84:LEU:HD13 | 2:H:133:ALA:HB2 | 1.69 | 0.75 |
| 1:B:328:LEU:O | 1:B:331:ILE:HG22 | 1.86 | 0.75 |
| 2:H:259:THR:HG22 | 2:H:262:GLU:HG3 | 1.68 | 0.75 |
| 2:H:1770:LEU:HD23 | 2:H:1776:PHE:CE2 | 2.22 | 0.75 |
| 1:B:1460:LYS:HE2 | 1:B:1773:VAL:O | 1.86 | 0.75 |
| 1:A:1498:GLU:HB2 | 1:A:1876:LEU:HD13 | 1.67 | 0.75 |
| 2:H:2015:THR:HG22 | 2:H:2017:LYS:H | 1.51 | 0.75 |
| 1:B:1208:VAL:HG13 | 1:B:1212:THR:HB | 1.68 | 0.75 |
| 2:H:579:VAL:HG23 | 2:H:1078:HIS:CD2 | 2.21 | 0.75 |
| 2:H:741:HIS:CB | 2:H:853:PRO:HB2 | 2.16 | 0.75 |
| 2:H:455:ILE:HD11 | 2:H:469:ARG:CD | 2.17 | 0.75 |
| 2:G:192:ALA:HA | 2:G:215:ILE:HD12 | 1.67 | 0.75 |
| 2:G:572:ASN:HB3 | 2:G:576:LYS:H | 1.52 | 0.75 |
| 2:I:960:LYS:HA | 2:I:960:LYS:HE2 | 1.67 | 0.75 |
| 1:A:1303:GLY:HA2 | 1:A:1649:LYS:HE2 | 1.68 | 0.75 |
| 1:A:1310:GLU:OE1 | 1:A:1649:LYS:HE3 | 1.86 | 0.75 |
| 2:I:1956:ARG:HB2 | 2:I:1957:PRO:CD | 2.11 | 0.75 |
| 2:I:757:ILE:HG21 | 2:I:765:LEU:HD13 | 1.69 | 0.75 |
| 2:I:572:ASN:HB3 | 2:I:576:LYS:H | 1.52 | 0.75 |
| 2:I:1129:ALA:HB2 | 2:I:1138:TRP:CZ3 | 2.22 | 0.75 |
| 2:H:1834:ARG:CG | 2:H:1834:ARG:HH11 | 1.92 | 0.74 |
| 2:I:1159:ILE:HG12 | 2:I:1169:PRO:HD3 | 1.67 | 0.74 |
| 2:H:943:TRP:CH2 | 2:H:1016:PRO:HG3 | 2.22 | 0.74 |
| 2:I:1284:VAL:HG13 | 2:I:1377:VAL:HG22 | 1.69 | 0.74 |
| 1:B:1552:ASN:O | 1:B:1556:THR:HG22 | 1.88 | 0.74 |
| 1:A:427:ASN:HD21 | 1:A:610:THR:H | 1.33 | 0.74 |
| 2:H:1678:MET:HE3 | 2:H:1707:LEU:HD22 | 1.67 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:20:TYR:CD2 | 2:G:2033:THR:OG1 | 2.40 | 0.74 |
| 2:H:1672:GLN:HA | 2:H:1676:MET:HE1 | 1.68 | 0.74 |
| 2:H:1242:PHE:HE2 | 2:H:1244:PRO:HG3 | 1.51 | 0.74 |
| 2:I:943:TRP:CH2 | 2:I:1016:PRO:HG3 | 2.21 | 0.74 |
| 2:H:1784:MET:HG3 | 2:H:1785:GLU:N | 2.03 | 0.74 |
| 2:H:1956:ARG:CB | 2:H:1957:PRO:HD3 | 2.11 | 0.74 |
| 2:I:131:ILE:HB | 2:I:182:VAL:HG11 | 1.69 | 0.74 |
| 2:H:1672:GLN:HA | 2:H:1676:MET:CE | 2.18 | 0.74 |
| 1:A:335:HIS:CE1 | 1:B:335:HIS:CE1 | 2.74 | 0.74 |
| 1:B:335:HIS:HE1 | 1:C:335:HIS:CE1 | 2.06 | 0.74 |
| 1:C:749:ILE:HD13 | 1:C:806:VAL:HG12 | 1.70 | 0.74 |
| 2:I:105:ALA:HB1 | 2:I:119:THR:HG23 | 1.67 | 0.74 |
| 2:H:1129:ALA:HB2 | 2:H:1138:TRP:CZ3 | 2.21 | 0.74 |
| 1:A:1239:HIS:HD2 | 1:A:1241:SER:OG | 1.69 | 0.74 |
| 1:A:1749:THR:CB | 1:A:1873:HIS:C | 2.56 | 0.74 |
| 2:I:2035:SER:HB3 | 2:I:2038:ILE:HG13 | 1.69 | 0.74 |
| 2:I:835:THR:HG21 | 2:I:855:HIS:CD2 | 2.23 | 0.74 |
| 2:G:1310:ASP:OD2 | 2:G:1602:SER:HB3 | 1.88 | 0.74 |
| 1:C:1552:ASN:O | 1:C:1556:THR:HG22 | 1.88 | 0.74 |
| 2:I:741:HIS:CE1 | 2:I:845:THR:HG21 | 2.22 | 0.74 |
| 2:G:705:LEU:HD12 | 2:G:716:VAL:HG13 | 1.70 | 0.74 |
| 1:B:1551:LYS:HD2 | 1:B:1617:ILE:HG21 | 1.70 | 0.74 |
| 1:A:1456:GLU:OE1 | 1:A:1775:LEU:HD23 | 1.87 | 0.74 |
| 2:G:757:ILE:HG21 | 2:G:765:LEU:HD13 | 1.67 | 0.74 |
| 2:I:1889:VAL:HG13 | 2:I:1977:HIS:HB2 | 1.69 | 0.74 |
| 1:B:18:LEU:HD21 | 2:H:1815:LEU:HD12 | 1.70 | 0.74 |
| 2:H:7:ARG:NH1 | 2:H:24:THR:HG23 | 2.03 | 0.73 |
| 1:B:833:PHE:HA | 1:B:937:LYS:HD2 | 1.69 | 0.73 |
| 2:H:1194:VAL:HG22 | 2:H:1212:LYS:HB3 | 1.70 | 0.73 |
| 1:A:44:VAL:CG1 | 1:A:78:ILE:HG12 | 2.18 | 0.73 |
| 2:H:1004:LEU:HD21 | 2:H:1020:VAL:HG23 | 1.70 | 0.73 |
| 2:H:705:LEU:HD12 | 2:H:716:VAL:HG13 | 1.70 | 0.73 |
| 2:G:1159:ILE:HG12 | 2:G:1169:PRO:HD3 | 1.71 | 0.73 |
| 1:A:982:ILE:HD11 | 2:G:965:SER:HB2 | 1.69 | 0.73 |
| 1:C:36:LEU:HD22 | 1:C:61:LEU:HD21 | 1.68 | 0.73 |
| 2:H:1680:LEU:HD13 | 2:H:1687:ALA:HB2 | 1.71 | 0.73 |
| 2:I:1784:MET:HG3 | 2:I:1785:GLU:N | 2.02 | 0.73 |
| 1:C:888:ILE:HD11 | 1:C:930:LEU:HD21 | 1.71 | 0.73 |
| 2:G:7:ARG:NH1 | 2:G:24:THR:HG23 | 2.03 | 0.73 |
| 2:I:455:ILE:HD11 | 2:I:469:ARG:CD | 2.19 | 0.73 |
| 2:G:105:ALA:HB1 | 2:G:119:THR:HG23 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:7:ARG:NH1 | 2:I:24:THR:HG23 | 2.03 | 0.73 |
| 1:C:1431:GLU:CG | 1:C:1433:HIS:CE1 | 2.72 | 0.73 |
| 2:G:777:THR:HG22 | 2:G:1081:HIS:NE2 | 2.03 | 0.73 |
| 1:B:749:ILE:HD13 | 1:B:806:VAL:HG12 | 1.70 | 0.73 |
| 2:G:259:THR:HG22 | 2:G:262:GLU:HG3 | 1.68 | 0.73 |
| 2:H:1422:THR:HG21 | 2:H:1474:PHE:HB2 | 1.70 | 0.73 |
| 2:H:345:THR:HG22 | 2:H:347:GLU:H | 1.51 | 0.73 |
| 2:H:1300:PHE:CA | 2:H:1556:VAL:HG11 | 2.19 | 0.73 |
| 2:G:194:THR:HG23 | 2:G:300:ILE:HD11 | 1.70 | 0.73 |
| 1:A:1551:LYS:HD2 | 1:A:1617:ILE:HG21 | 1.70 | 0.73 |
| 1:C:260:ARG:HH12 | 1:C:300:VAL:HG21 | 1.52 | 0.73 |
| 2:G:562:LEU:HG | 2:G:793:PRO:HG2 | 1.71 | 0.73 |
| 2:G:652:ILE:H | 2:G:658:MET:CE | 2.01 | 0.73 |
| 2:H:194:THR:HG23 | 2:H:300:ILE:HD11 | 1.71 | 0.73 |
| 2:H:1355:ASN:HA | 2:H:1407:THR:O | 1.88 | 0.73 |
| 2:H:1331:TRP:CZ2 | 2:H:1335:ILE:HG13 | 2.23 | 0.73 |
| 2:H:7:ARG:HH21 | 2:H:27:PHE:CB | 2.01 | 0.73 |
| 2:H:146:PHE:HA | 2:H:149:VAL:CG1 | 2.18 | 0.73 |
| 2:H:1300:PHE:HA | 2:H:1556:VAL:HG11 | 1.70 | 0.73 |
| 2:I:707:PRO:HG3 | 2:I:716:VAL:CG2 | 2.18 | 0.72 |
| 2:H:579:VAL:HG23 | 2:H:1078:HIS:NE2 | 2.03 | 0.72 |
| 2:H:1284:VAL:HG13 | 2:H:1377:VAL:HG22 | 1.71 | 0.72 |
| 1:B:44:VAL:CG1 | 1:B:78:ILE:HG12 | 2.18 | 0.72 |
| 2:G:762:ASN:N | 2:G:762:ASN:HD22 | 1.82 | 0.72 |
| 2:I:579:VAL:HG23 | 2:I:1078:HIS:CD2 | 2.24 | 0.72 |
| 2:H:128:THR:HA | 2:H:182:VAL:CG2 | 2.16 | 0.72 |
| 2:I:1672:GLN:HA | 2:I:1676:MET:HE1 | 1.70 | 0.72 |
| 2:G:1889:VAL:HG13 | 2:G:1977:HIS:HB2 | 1.72 | 0.72 |
| 2:H:634:ILE:HD11 | 2:H:649:ILE:HD11 | 1.71 | 0.72 |
| 1:A:655:LEU:HD22 | 1:A:916:LEU:HD11 | 1.71 | 0.72 |
| 1:A:1045:PHE:HB3 | 1:A:1049:GLY:HA3 | 1.71 | 0.72 |
| 1:C:1551:LYS:HD2 | 1:C:1617:ILE:HG21 | 1.70 | 0.72 |
| 1:C:1208:VAL:HG13 | 1:C:1212:THR:HB | 1.71 | 0.72 |
| 1:A:1722:VAL:CG1 | 1:A:1731:LEU:HB3 | 2.19 | 0.72 |
| 1:C:473:GLY:O | 1:C:477:ILE:HG13 | 1.88 | 0.72 |
| 2:I:191:SER:HA | 2:I:194:THR:HG22 | 1.71 | 0.72 |
| 2:I:194:THR:HG23 | 2:I:300:ILE:HD11 | 1.70 | 0.72 |
| 1:A:24:SER:CB | 2:G:2014:LEU:HD12 | 2.19 | 0.72 |
| 2:H:109:LEU:HD11 | 2:H:116:LEU:HD23 | 1.72 | 0.72 |
| 1:C:427:ASN:HD21 | 1:C:610:THR:H | 1.38 | 0.72 |
| 2:I:7:ARG:HH21 | 2:I:27:PHE:CB | 1.99 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:254:TRP:CZ3 | 1:B:302:LEU:HD13 | 2.24 | 0.72 |
| 2:I:777:THR:HG22 | 2:I:1081:HIS:NE2 | 2.04 | 0.72 |
| 2:I:1672:GLN:HA | 2:I:1676:MET:CE | 2.20 | 0.72 |
| 1:A:1208:VAL:HG13 | 1:A:1212:THR:HB | 1.70 | 0.72 |
| 1:B:1668:ASP:OD2 | 1:B:1805:VAL:HB | 1.90 | 0.72 |
| 2:I:259:THR:HG22 | 2:I:262:GLU:CG | 2.20 | 0.72 |
| 1:B:24:SER:HB3 | 2:H:2014:LEU:HD12 | 1.69 | 0.72 |
| 2:H:455:ILE:CD1 | 2:H:469:ARG:HD3 | 2.20 | 0.72 |
| 2:H:455:ILE:CG1 | 2:H:469:ARG:HD3 | 2.20 | 0.72 |
| 2:G:584:SER:HB3 | 2:G:591:PRO:HG3 | 1.70 | 0.72 |
| 2:G:598:THR:OG1 | 2:G:599:PRO:HD3 | 1.89 | 0.72 |
| 1:B:473:GLY:O | 1:B:477:ILE:HG13 | 1.89 | 0.72 |
| 2:H:572:ASN:HB3 | 2:H:576:LYS:H | 1.54 | 0.72 |
| 2:G:1680:LEU:HD13 | 2:G:1687:ALA:HB2 | 1.71 | 0.72 |
| 2:G:131:ILE:CD1 | 2:G:182:VAL:HB | 2.09 | 0.72 |
| 2:H:777:THR:HG22 | 2:H:1081:HIS:NE2 | 2.04 | 0.72 |
| 2:G:741:HIS:CE1 | 2:G:845:THR:HG21 | 2.24 | 0.72 |
| 2:G:741:HIS:CE1 | 2:G:855:HIS:NE2 | 2.58 | 0.72 |
| 2:I:1086:LEU:HG | 2:I:1092:ASP:HA | 1.72 | 0.72 |
| 2:G:751:LEU:HD23 | 2:G:791:TYR:CE2 | 2.25 | 0.72 |
| 2:I:84:LEU:HD13 | 2:I:133:ALA:HB2 | 1.71 | 0.72 |
| 2:I:2036:GLU:HB2 | 2:I:2037:PRO:HD3 | 1.72 | 0.71 |
| 2:G:1567:ARG:HG3 | 2:G:1567:ARG:NH1 | 2.02 | 0.71 |
| 2:G:161:GLY:H | 2:G:505:GLY:HA3 | 1.54 | 0.71 |
| 1:B:1232:TYR:CZ | 1:B:1701:LYS:HD2 | 2.26 | 0.71 |
| 2:H:741:HIS:NE2 | 2:H:855:HIS:CE1 | 2.58 | 0.71 |
| 1:A:1501:LEU:CD1 | 1:A:1775:LEU:CD2 | 2.62 | 0.71 |
| 2:H:652:ILE:H | 2:H:658:MET:CE | 2.03 | 0.71 |
| 1:C:59:ARG:NH1 | 2:I:1896:GLN:NE2 | 2.38 | 0.71 |
| 2:I:1673:GLU:H | 2:I:1676:MET:HE3 | 1.55 | 0.71 |
| 1:B:888:ILE:HD12 | 1:B:939:PHE:HE2 | 1.55 | 0.71 |
| 2:H:1227:ARG:HD2 | 2:H:1565:VAL:HG11 | 1.71 | 0.71 |
| 2:G:762:ASN:H | 2:G:762:ASN:ND2 | 1.85 | 0.71 |
| 2:I:1670:GLY:H | 2:I:1672:GLN:HE21 | 1.38 | 0.71 |
| 1:B:1030:TRP:NE1 | 1:B:1580:LEU:CD2 | 2.54 | 0.71 |
| 2:G:1638:ILE:HD12 | 2:G:1657:ILE:HD12 | 1.71 | 0.71 |
| 2:G:2036:GLU:HB2 | 2:G:2037:PRO:HD3 | 1.73 | 0.71 |
| 2:I:455:ILE:CG1 | 2:I:469:ARG:HD3 | 2.21 | 0.71 |
| 1:A:982:ILE:HD11 | 2:G:965:SER:CB | 2.21 | 0.71 |
| 2:H:1819:ALA:HA | 2:H:2005:ARG:HH11 | 1.55 | 0.71 |
| 2:G:50:ALA:HB3 | 2:G:53:GLU:HG3 | 1.72 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:733:ILE:HD13 | 1:A:761:LEU:HD11 | 1.71 | 0.71 |
| 1:B:2:LYS:HD2 | 2:H:2050:GLN:HB3 | 1.72 | 0.71 |
| 1:A:983:GLN:NE2 | 2:G:962:LYS:HD2 | 2.05 | 0.71 |
| 2:I:1331:TRP:CZ2 | 2:I:1335:ILE:HG13 | 2.25 | 0.71 |
| 1:C:733:ILE:HD13 | 1:C:761:LEU:HD11 | 1.72 | 0.71 |
| 2:H:1054:LEU:HB2 | 4:H:3051:FMN:C7M | 2.21 | 0.71 |
| 2:I:732:TRP:CG | 2:I:750:MET:CE | 2.73 | 0.71 |
| 1:C:1219:VAL:HG22 | 1:C:1384:ILE:HD12 | 1.73 | 0.71 |
| 2:G:1199:GLU:OE2 | 2:G:1567:ARG:NH1 | 2.23 | 0.71 |
| 2:G:1672:GLN:HA | 2:G:1676:MET:HE1 | 1.72 | 0.71 |
| 1:A:1208:VAL:CG1 | 1:A:1212:THR:HB | 2.21 | 0.71 |
| 2:G:949:ASP:HB3 | 2:G:1006:MET:HE2 | 1.71 | 0.71 |
| 2:I:1058:VAL:O | 2:I:1061:GLN:HG2 | 1.90 | 0.71 |
| 2:G:238:CYS:HB2 | 2:G:239:PRO:HD3 | 1.71 | 0.71 |
| 2:H:238:CYS:HB2 | 2:H:239:PRO:HD3 | 1.71 | 0.71 |
| 2:G:1917:ILE:HG23 | 2:G:1922:ILE:HB | 1.72 | 0.71 |
| 2:G:109:LEU:HD11 | 2:G:116:LEU:HD23 | 1.71 | 0.71 |
| 1:C:1498:GLU:CB | 1:C:1876:LEU:HD13 | 2.21 | 0.71 |
| 2:G:707:PRO:CG | 2:G:716:VAL:HG21 | 2.20 | 0.71 |
| 1:B:18:LEU:HD21 | 2:H:1815:LEU:CD1 | 2.20 | 0.71 |
| 1:B:655:LEU:HD22 | 1:B:916:LEU:HD11 | 1.72 | 0.71 |
| 2:H:964:LEU:HD23 | 2:H:964:LEU:H | 1.56 | 0.71 |
| 1:C:1498:GLU:HG3 | 1:C:1876:LEU:CB | 2.09 | 0.70 |
| 1:C:59:ARG:NH1 | 2:I:1896:GLN:HE22 | 1.88 | 0.70 |
| 2:I:1242:PHE:CE2 | 2:I:1244:PRO:HG3 | 2.26 | 0.70 |
| 2:I:751:LEU:HD23 | 2:I:791:TYR:CE2 | 2.25 | 0.70 |
| 1:C:459:ASP:HB3 | 1:C:462:LYS:HG3 | 1.73 | 0.70 |
| 1:B:1721:ARG:NH1 | 1:B:1721:ARG:HG2 | 2.00 | 0.70 |
| 2:H:707:PRO:CG | 2:H:716:VAL:HG21 | 2.21 | 0.70 |
| 1:A:1119:LYS:HE2 | 1:A:1341:PHE:CD1 | 2.27 | 0.70 |
| 2:H:562:LEU:O | 2:H:566:HIS:HB2 | 1.90 | 0.70 |
| 1:B:1460:LYS:HZ1 | 1:B:1774:GLU:CD | 1.92 | 0.70 |
| 1:C:12:ILE:HD11 | 2:I:2041:ILE:CD1 | 2.21 | 0.70 |
| 2:G:1672:GLN:HA | 2:G:1676:MET:CE | 2.21 | 0.70 |
| 1:A:1:MET:CE | 1:A:6:GLU:HA | 2.21 | 0.70 |
| 1:C:631:PRO:HB2 | 1:C:634:THR:OG1 | 1.91 | 0.70 |
| 2:I:964:LEU:H | 2:I:964:LEU:HD23 | 1.56 | 0.70 |
| 2:G:650:ASN:HD21 | 4:G:3051:FMN:HN3 | 1.40 | 0.70 |
| 2:I:732:TRP:CG | 2:I:750:MET:HE1 | 2.26 | 0.70 |
| 2:I:1680:LEU:HD13 | 2:I:1687:ALA:HB2 | 1.72 | 0.70 |
| 1:C:881:ASN:HA | 1:C:944:ARG:NH2 | 2.06 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1501:LEU:HD11 | 1:B:1775:LEU:CD2 | 2.22 | 0.70 |
| 2:G:123:ILE:HD11 | 2:G:533:LEU:CD2 | 2.21 | 0.70 |
| 2:I:455:ILE:CD1 | 2:I:469:ARG:HD3 | 2.20 | 0.70 |
| 1:B:1208:VAL:CG1 | 1:B:1212:THR:HB | 2.20 | 0.70 |
| 2:I:748:THR:HB | 2:I:749:PRO:HD3 | 1.74 | 0.70 |
| 1:B:90:TYR:HE2 | 2:H:1659:GLN:OE1 | 1.73 | 0.70 |
| 2:G:579:VAL:HG23 | 2:G:1078:HIS:CD2 | 2.27 | 0.70 |
| 2:G:1956:ARG:CB | 2:G:1957:PRO:HD3 | 2.10 | 0.70 |
| 2:I:146:PHE:HA | 2:I:149:VAL:CG1 | 2.20 | 0.70 |
| 2:G:707:PRO:HG3 | 2:G:716:VAL:CG2 | 2.22 | 0.70 |
| 2:G:732:TRP:CG | 2:G:750:MET:HE1 | 2.27 | 0.70 |
| 1:B:459:ASP:HB3 | 1:B:462:LYS:HG3 | 1.73 | 0.70 |
| 2:G:1242:PHE:HE2 | 2:G:1244:PRO:HG3 | 1.55 | 0.70 |
| 1:B:1:MET:CE | 1:B:6:GLU:HA | 2.21 | 0.70 |
| 1:A:1312:VAL:HG22 | 1:A:1329:VAL:HG11 | 1.73 | 0.70 |
| 1:B:968:VAL:HG23 | 2:H:1515:PRO:HG3 | 1.74 | 0.70 |
| 1:C:260:ARG:NH1 | 1:C:300:VAL:HG21 | 2.06 | 0.70 |
| 2:I:1264:GLU:HA | 2:I:1275:PHE:CE1 | 2.27 | 0.70 |
| 2:G:1355:ASN:HA | 2:G:1407:THR:O | 1.92 | 0.70 |
| 2:H:234:ILE:HG13 | 2:H:235:PRO:HD3 | 1.73 | 0.70 |
| 2:H:741:HIS:CE1 | 2:H:845:THR:HG21 | 2.26 | 0.70 |
| 2:G:455:ILE:HD11 | 2:G:469:ARG:CD | 2.22 | 0.70 |
| 1:C:655:LEU:HD22 | 1:C:916:LEU:HD11 | 1.74 | 0.70 |
| 1:A:12:ILE:HA | 1:A:15:THR:CG2 | 2.21 | 0.70 |
| 2:H:2036:GLU:HB2 | 2:H:2037:PRO:HD3 | 1.72 | 0.70 |
| 2:G:1673:GLU:H | 2:G:1676:MET:HE3 | 1.57 | 0.70 |
| 2:G:1331:TRP:CZ2 | 2:G:1335:ILE:HG13 | 2.26 | 0.70 |
| 2:H:499:THR:CB | 2:H:500:HIS:HD2 | 1.99 | 0.69 |
| 2:G:7:ARG:HH21 | 2:G:27:PHE:CB | 2.01 | 0.69 |
| 2:H:835:THR:HB | 2:H:845:THR:HG23 | 1.73 | 0.69 |
| 2:H:1673:GLU:H | 2:H:1676:MET:HE3 | 1.57 | 0.69 |
| 2:I:926:LEU:HD13 | 2:I:947:THR:HG22 | 1.73 | 0.69 |
| 1:A:1232:TYR:CZ | 1:A:1701:LYS:HD2 | 2.27 | 0.69 |
| 2:I:1862:VAL:HG11 | 2:I:1866:PHE:CD1 | 2.26 | 0.69 |
| 2:G:1422:THR:HG21 | 2:G:1474:PHE:HB2 | 1.72 | 0.69 |
| 2:H:1670:GLY:H | 2:H:1672:GLN:HE21 | 1.40 | 0.69 |
| 2:G:1194:VAL:HG22 | 2:G:1212:LYS:HB3 | 1.74 | 0.69 |
| 1:B:427:ASN:HD21 | 1:B:610:THR:H | 1.40 | 0.69 |
| 2:G:1054:LEU:HB2 | 4:G:3051:FMN:C7M | 2.22 | 0.69 |
| 1:C:852:ARG:CG | 1:C:852:ARG:HH11 | 2.00 | 0.69 |
| 1:C:12:ILE:HA | 1:C:15:THR:CG2 | 2.22 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:652:ILE:H | 2:I:658:MET:CE | 2.04 | 0.69 |
| 2:H:567:PRO:HG3 | 2:H:781:LEU:CD1 | 2.22 | 0.69 |
| 2:H:1195:VAL:CG1 | 2:H:1211:LEU:HB3 | 2.23 | 0.69 |
| 2:H:1381:VAL:HG13 | 2:H:1390:VAL:HG22 | 1.74 | 0.69 |
| 1:A:749:ILE:HD13 | 1:A:806:VAL:HG12 | 1.72 | 0.69 |
| 1:A:254:TRP:CZ3 | 1:A:292:GLN:HG3 | 2.26 | 0.69 |
| 1:B:254:TRP:CZ3 | 1:B:292:GLN:HG3 | 2.27 | 0.69 |
| 2:I:1770:LEU:HD23 | 2:I:1776:PHE:HE2 | 1.55 | 0.69 |
| 2:G:964:LEU:CD2 | 2:G:964:LEU:H | 2.05 | 0.69 |
| 2:I:1678:MET:HE3 | 2:I:1707:LEU:HD22 | 1.75 | 0.69 |
| 2:G:84:LEU:HD13 | 2:G:133:ALA:HB2 | 1.75 | 0.69 |
| 2:G:856:LYS:HG2 | 2:G:1054:LEU:HD12 | 1.73 | 0.69 |
| 2:H:1889:VAL:HG13 | 2:H:1977:HIS:CB | 2.22 | 0.69 |
| 1:C:1208:VAL:CG1 | 1:C:1212:THR:HB | 2.23 | 0.69 |
| 2:H:1917:ILE:HG23 | 2:H:1922:ILE:HB | 1.74 | 0.69 |
| 1:A:1721:ARG:NH1 | 1:A:1721:ARG:HG2 | 1.97 | 0.69 |
| 2:G:191:SER:HA | 2:G:194:THR:HG22 | 1.74 | 0.69 |
| 1:A:749:ILE:HD11 | 1:A:805:CYS:HB3 | 1.75 | 0.69 |
| 1:B:1376:PHE:HB3 | 1:B:1544:THR:HG22 | 1.74 | 0.69 |
| 2:I:109:LEU:HD11 | 2:I:116:LEU:HD23 | 1.73 | 0.69 |
| 2:I:1194:VAL:HG22 | 2:I:1212:LYS:HB3 | 1.75 | 0.69 |
| 1:A:1693:ILE:CD1 | 2:G:998:GLN:HB2 | 2.23 | 0.69 |
| 2:I:652:ILE:N | 2:I:658:MET:HE3 | 2.08 | 0.69 |
| 2:G:1670:GLY:H | 2:G:1672:GLN:HE21 | 1.39 | 0.69 |
| 2:H:1889:VAL:HG13 | 2:H:1977:HIS:HB2 | 1.72 | 0.69 |
| 1:A:479:ASN:O | 1:A:483:VAL:HG23 | 1.91 | 0.69 |
| 2:H:751:LEU:HD23 | 2:H:791:TYR:CE2 | 2.27 | 0.69 |
| 2:H:2022:THR:HG23 | 2:H:2025:TYR:H | 1.58 | 0.69 |
| 2:G:1172:LYS:HE3 | 2:G:1574:ASN:OD1 | 1.92 | 0.69 |
| 2:H:663:ILE:HB | 2:H:664:PRO:HD3 | 1.75 | 0.69 |
| 2:I:1739:GLU:CB | 2:I:1987:PRO:HB3 | 2.20 | 0.69 |
| 2:H:1739:GLU:CB | 2:H:1987:PRO:HB3 | 2.21 | 0.69 |
| 2:H:1172:LYS:CE | 2:H:1574:ASN:OD1 | 2.40 | 0.69 |
| 2:G:1496:LYS:HE2 | 2:G:1693:ARG:HH21 | 1.57 | 0.69 |
| 2:I:768:GLY:HA3 | 2:I:800:LEU:HD21 | 1.74 | 0.69 |
| 1:C:1838:GLU:OE1 | 1:C:1852:HIS:HE1 | 1.76 | 0.69 |
| 2:I:663:ILE:HB | 2:I:664:PRO:HD3 | 1.75 | 0.69 |
| 1:A:631:PRO:HB2 | 1:A:634:THR:OG1 | 1.92 | 0.69 |
| 2:G:1264:GLU:HA | 2:G:1275:PHE:CE1 | 2.28 | 0.69 |
| 2:H:305:PHE:CE1 | 2:H:442:ASP:HB3 | 2.28 | 0.69 |
| 2:I:499:THR:CB | 2:I:500:HIS:HD2 | 1.95 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1219:VAL:HA | 1:C:1384:ILE:CD1 | 2.20 | 0.69 |
| 2:H:652:ILE:N | 2:H:658:MET:HE3 | 2.05 | 0.69 |
| 1:C:1431:GLU:OE2 | 1:C:1433:HIS:HE1 | 1.76 | 0.69 |
| 2:H:54:PRO:HG3 | 2:H:63:LYS:HG3 | 1.72 | 0.69 |
| 1:A:1376:PHE:HB3 | 1:A:1544:THR:HG22 | 1.74 | 0.69 |
| 2:G:663:ILE:HB | 2:G:664:PRO:HD3 | 1.74 | 0.69 |
| 2:I:1917:ILE:HG23 | 2:I:1922:ILE:HB | 1.74 | 0.69 |
| 1:C:1021:VAL:HG11 | 1:C:1597:LEU:HD11 | 1.74 | 0.69 |
| 1:A:257:PRO:HD2 | 1:A:260:ARG:HB2 | 1.75 | 0.69 |
| 2:H:259:THR:HG22 | 2:H:262:GLU:CG | 2.22 | 0.68 |
| 1:A:1838:GLU:OE1 | 1:A:1852:HIS:HE1 | 1.75 | 0.68 |
| 2:I:234:ILE:HG13 | 2:I:235:PRO:HD3 | 1.73 | 0.68 |
| 1:A:1203:ASP:HB3 | 1:B:179:LYS:HZ3 | 1.58 | 0.68 |
| 2:G:1058:VAL:O | 2:G:1061:GLN:HG2 | 1.93 | 0.68 |
| 2:G:2035:SER:HB3 | 2:G:2038:ILE:HG13 | 1.74 | 0.68 |
| 1:A:1431:GLU:HG3 | 1:A:1433:HIS:CE1 | 2.28 | 0.68 |
| 2:H:1101:GLU:HB3 | 2:H:1147:ILE:HG22 | 1.76 | 0.68 |
| 2:H:161:GLY:H | 2:H:505:GLY:HA3 | 1.59 | 0.68 |
| 1:C:1045:PHE:HB3 | 1:C:1049:GLY:HA3 | 1.74 | 0.68 |
| 2:I:1227:ARG:NH1 | 2:I:1227:ARG:HG3 | 2.00 | 0.68 |
| 2:G:1834:ARG:NH1 | 2:G:1834:ARG:HG2 | 1.93 | 0.68 |
| 2:I:598:THR:CG2 | 2:I:622:GLY:HA3 | 2.23 | 0.68 |
| 1:C:1376:PHE:HB3 | 1:C:1544:THR:HG22 | 1.74 | 0.68 |
| 1:B:400:ARG:HG2 | 1:B:400:ARG:NH1 | 2.00 | 0.68 |
| 2:I:187:LEU:HA | 2:I:190:PHE:HB3 | 1.76 | 0.68 |
| 2:I:161:GLY:H | 2:I:505:GLY:HA3 | 1.56 | 0.68 |
| 1:A:888:ILE:HD11 | 1:A:930:LEU:HD21 | 1.75 | 0.68 |
| 1:C:985:ARG:NH1 | 2:I:953:ARG:CZ | 2.57 | 0.68 |
| 1:B:1312:VAL:HG22 | 1:B:1329:VAL:HG11 | 1.73 | 0.68 |
| 1:C:1014:ASP:H | 1:C:1510:ASN:ND2 | 1.84 | 0.68 |
| 2:I:594:VAL:HG21 | 2:I:610:THR:HG21 | 1.75 | 0.68 |
| 2:G:259:THR:HG22 | 2:G:262:GLU:CG | 2.22 | 0.68 |
| 1:B:90:TYR:CE2 | 2:H:1659:GLN:OE1 | 2.47 | 0.68 |
| 2:G:732:TRP:CG | 2:G:750:MET:CE | 2.76 | 0.68 |
| 2:G:54:PRO:HG3 | 2:G:63:LYS:HG3 | 1.76 | 0.68 |
| 2:G:1784:MET:HG3 | 2:G:1785:GLU:N | 2.07 | 0.68 |
| 2:I:1638:ILE:HD12 | 2:I:1657:ILE:HD12 | 1.75 | 0.68 |
| 2:H:648:GLY:HA3 | 2:H:678:PHE:CE2 | 2.29 | 0.68 |
| 1:A:1474:ALA:HA | 1:A:1478:PRO:CG | 2.24 | 0.68 |
| 1:C:987:ASN:HD22 | 2:I:957:ARG:HD2 | 1.58 | 0.68 |
| 1:C:1460:LYS:HE3 | 1:C:1774:GLU:OE1 | 1.92 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:332:THR:HG22 | 1:B:331:ILE:HD11 | 1.76 | 0.68 |
| 2:G:455:ILE:CG1 | 2:G:469:ARG:HD3 | 2.23 | 0.68 |
| 2:H:187:LEU:HA | 2:H:190:PHE:HB3 | 1.75 | 0.68 |
| 1:A:504:ASP:HB3 | 1:A:508:ASN:H | 1.56 | 0.68 |
| 2:I:305:PHE:CE1 | 2:I:442:ASP:HB3 | 2.28 | 0.68 |
| 1:B:1219:VAL:HG22 | 1:B:1384:ILE:HD12 | 1.75 | 0.68 |
| 2:H:641:ILE:HG12 | 2:H:645:SER:HB2 | 1.76 | 0.68 |
| 1:C:1310:GLU:OE1 | 1:C:1649:LYS:HE3 | 1.93 | 0.68 |
| 2:G:455:ILE:CD1 | 2:G:469:ARG:HD3 | 2.24 | 0.68 |
| 2:G:1176:PRO:O | 2:G:1177:SER:HB3 | 1.93 | 0.68 |
| 1:B:1838:GLU:OE1 | 1:B:1852:HIS:HE1 | 1.76 | 0.68 |
| 1:A:1056:ILE:HD13 | 1:A:1193:TRP:HD1 | 1.59 | 0.68 |
| 2:H:1058:VAL:O | 2:H:1061:GLN:HG2 | 1.94 | 0.68 |
| 2:H:1054:LEU:HB2 | 4:H:3051:FMN:HM72 | 1.76 | 0.67 |
| 1:C:254:TRP:CZ3 | 1:C:292:GLN:HG3 | 2.29 | 0.67 |
| 2:H:707:PRO:HG3 | 2:H:716:VAL:CG2 | 2.24 | 0.67 |
| 1:C:1303:GLY:H | 1:C:1307:THR:HG22 | 1.60 | 0.67 |
| 1:A:1303:GLY:H | 1:A:1307:THR:HG22 | 1.59 | 0.67 |
| 2:G:187:LEU:HA | 2:G:190:PHE:HB3 | 1.74 | 0.67 |
| 2:G:1475:LYS:CG | 2:G:1481:SER:HB2 | 2.24 | 0.67 |
| 1:A:1594:ASN:O | 1:A:1598:GLN:HG3 | 1.94 | 0.67 |
| 1:B:183:GLN:HE21 | 1:B:202:GLU:HG2 | 1.59 | 0.67 |
| 1:C:44:VAL:CG1 | 1:C:78:ILE:HG12 | 2.24 | 0.67 |
| 2:H:191:SER:HA | 2:H:194:THR:HG22 | 1.77 | 0.67 |
| 1:C:1455:ARG:HH11 | 1:C:1458:GLN:HE21 | 1.42 | 0.67 |
| 2:G:1889:VAL:HG13 | 2:G:1977:HIS:CB | 2.24 | 0.67 |
| 2:I:579:VAL:HG23 | 2:I:1078:HIS:NE2 | 2.10 | 0.67 |
| 2:H:50:ALA:HB3 | 2:H:53:GLU:HG3 | 1.76 | 0.67 |
| 2:G:163:GLN:HG2 | 2:G:423:VAL:HG12 | 1.77 | 0.67 |
| 1:C:1232:TYR:CZ | 1:C:1701:LYS:HD2 | 2.29 | 0.67 |
| 2:I:598:THR:OG1 | 2:I:599:PRO:HD3 | 1.94 | 0.67 |
| 2:G:1129:ALA:HB2 | 2:G:1138:TRP:CZ3 | 2.30 | 0.67 |
| 1:C:504:ASP:HB3 | 1:C:508:ASN:H | 1.60 | 0.67 |
| 1:C:1523:ARG:CG | 1:C:1523:ARG:NH1 | 2.57 | 0.67 |
| 2:I:910:GLN:HE21 | 2:I:912:ARG:HH21 | 1.40 | 0.67 |
| 1:B:1303:GLY:H | 1:B:1307:THR:HG22 | 1.59 | 0.67 |
| 2:G:910:GLN:HE21 | 2:G:912:ARG:HH21 | 1.42 | 0.67 |
| 2:I:904:PHE:HB2 | 2:I:1017:PHE:CD1 | 2.28 | 0.67 |
| 2:H:902:PRO:HG2 | 2:H:929:LEU:HD21 | 1.74 | 0.67 |
| 1:C:409:ALA:HB2 | 1:C:442:ARG:HD2 | 1.76 | 0.67 |
| 2:G:768:GLY:HA3 | 2:G:800:LEU:HD21 | 1.76 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1056:ILE:HD13 | 1:C:1193:TRP:HD1 | 1.60 | 0.67 |
| 1:A:459:ASP:HB3 | 1:A:462:LYS:HG3 | 1.76 | 0.67 |
| 2:G:1741:ILE:HG12 | 2:G:1746:LEU:HD13 | 1.77 | 0.67 |
| 1:B:1039:MET:O | 1:B:1609:ARG:NH2 | 2.27 | 0.67 |
| 1:A:1360:ARG:HH11 | 1:A:1364:GLU:HG2 | 1.60 | 0.67 |
| 1:B:1310:GLU:OE1 | 1:B:1649:LYS:HE3 | 1.94 | 0.67 |
| 2:I:1675:GLY:O | 2:I:1678:MET:HB2 | 1.94 | 0.67 |
| 2:H:594:VAL:HG21 | 2:H:610:THR:HG21 | 1.77 | 0.67 |
| 1:A:328:LEU:O | 1:A:328:LEU:HD22 | 1.94 | 0.67 |
| 2:H:545:GLN:HE21 | 2:H:545:GLN:H | 1.41 | 0.67 |
| 1:C:746:GLU:O | 1:C:750:GLU:HG3 | 1.95 | 0.67 |
| 2:I:54:PRO:HG3 | 2:I:63:LYS:HG3 | 1.75 | 0.67 |
| 2:H:768:GLY:HA3 | 2:H:800:LEU:HD21 | 1.77 | 0.67 |
| 2:H:315:PRO:O | 2:I:1314:ARG:NH2 | 2.28 | 0.67 |
| 2:I:703:LEU:HD21 | 2:I:705:LEU:HD21 | 1.76 | 0.67 |
| 2:H:1242:PHE:CE2 | 2:H:1244:PRO:HG3 | 2.30 | 0.67 |
| 2:G:1676:MET:HE1 | 2:G:1781:LEU:HD21 | 1.76 | 0.67 |
| 2:G:1770:LEU:HD23 | 2:G:1776:PHE:HE2 | 1.58 | 0.67 |
| 2:H:1086:LEU:HG | 2:H:1092:ASP:HA | 1.77 | 0.67 |
| 2:H:1264:GLU:HA | 2:H:1275:PHE:CE1 | 2.29 | 0.67 |
| 2:G:1004:LEU:HD21 | 2:G:1020:VAL:HG23 | 1.77 | 0.67 |
| 2:I:1889:VAL:HG13 | 2:I:1977:HIS:CB | 2.24 | 0.67 |
| 2:I:949:ASP:HB3 | 2:I:1006:MET:HE2 | 1.77 | 0.67 |
| 2:G:353:VAL:HG23 | 2:G:357:ASN:ND2 | 2.10 | 0.67 |
| 2:H:1256:GLU:O | 2:H:1257:ASP:HB2 | 1.93 | 0.67 |
| 2:I:1227:ARG:HD2 | 2:I:1565:VAL:HG11 | 1.77 | 0.66 |
| 1:C:257:PRO:HD2 | 1:C:260:ARG:HB2 | 1.76 | 0.66 |
| 2:H:1862:VAL:HG11 | 2:H:1866:PHE:CD1 | 2.30 | 0.66 |
| 2:H:1159:ILE:CG1 | 2:H:1169:PRO:HD3 | 2.24 | 0.66 |
| 1:A:1030:TRP:NE1 | 1:A:1580:LEU:CD2 | 2.57 | 0.66 |
| 1:C:888:ILE:HD12 | 1:C:939:PHE:HE2 | 1.60 | 0.66 |
| 2:G:670:ARG:HD3 | 2:G:699:GLY:O | 1.95 | 0.66 |
| 2:I:50:ALA:HB3 | 2:I:53:GLU:HG3 | 1.76 | 0.66 |
| 2:I:163:GLN:HG2 | 2:I:423:VAL:HG12 | 1.76 | 0.66 |
| 2:I:1739:GLU:O | 2:I:1987:PRO:HG3 | 1.95 | 0.66 |
| 2:H:670:ARG:HD3 | 2:H:699:GLY:O | 1.95 | 0.66 |
| 1:B:335:HIS:CE1 | 1:C:335:HIS:CE1 | 2.82 | 0.66 |
| 1:B:328:LEU:O | 1:B:328:LEU:HD22 | 1.95 | 0.66 |
| 1:C:328:LEU:HD22 | 1:C:328:LEU:O | 1.95 | 0.66 |
| 1:A:1662:TYR:O | 1:A:1665:ILE:HG22 | 1.95 | 0.66 |
| 2:I:1920:GLN:HG2 | 2:I:1922:ILE:HD11 | 1.75 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:473:GLY:O | 1:A:477:ILE:HG13 | 1.95 | 0.66 |
| 1:C:1430:ARG:O | 1:C:1430:ARG:HG2 | 1.94 | 0.66 |
| 1:C:294:TYR:CE1 | 1:C:298:VAL:HG21 | 2.29 | 0.66 |
| 2:I:762:ASN:ND2 | 2:I:762:ASN:H | 1.88 | 0.66 |
| 2:H:910:GLN:HE21 | 2:H:912:ARG:HH21 | 1.43 | 0.66 |
| 1:C:1030:TRP:NE1 | 1:C:1580:LEU:CD2 | 2.58 | 0.66 |
| 1:B:27:ARG:HB2 | 2:H:2016:ALA:HB2 | 1.76 | 0.66 |
| 2:I:750:MET:HG3 | 2:I:796:PHE:HZ | 1.60 | 0.66 |
| 1:C:460:GLU:HG2 | 1:C:470:LYS:HD3 | 1.77 | 0.66 |
| 1:B:1045:PHE:HB3 | 1:B:1049:GLY:HA3 | 1.76 | 0.66 |
| 1:C:507:GLY:N | 1:C:954:ARG:HG2 | 2.11 | 0.66 |
| 1:A:183:GLN:HE21 | 1:A:202:GLU:HG2 | 1.59 | 0.66 |
| 2:I:705:LEU:HD12 | 2:I:716:VAL:HG13 | 1.75 | 0.66 |
| 1:B:12:ILE:HA | 1:B:15:THR:CG2 | 2.25 | 0.66 |
| 1:A:864:VAL:HG22 | 1:A:921:PRO:HB3 | 1.78 | 0.66 |
| 2:G:1862:VAL:HG11 | 2:G:1866:PHE:CD1 | 2.30 | 0.66 |
| 2:H:835:THR:HG21 | 2:H:855:HIS:HD2 | 1.59 | 0.66 |
| 2:H:741:HIS:CE1 | 2:H:855:HIS:CE1 | 2.84 | 0.66 |
| 2:G:560:ASN:O | 2:G:561:TRP:C | 2.34 | 0.66 |
| 2:H:826:GLY:HA3 | 2:H:1061:GLN:HB3 | 1.75 | 0.66 |
| 2:G:1300:PHE:HA | 2:G:1556:VAL:HG11 | 1.77 | 0.66 |
| 2:G:61:VAL:O | 2:G:65:LEU:HB2 | 1.96 | 0.66 |
| 1:C:934:PRO:O | 1:C:935:GLU:C | 2.34 | 0.66 |
| 1:B:504:ASP:HB3 | 1:B:508:ASN:H | 1.60 | 0.66 |
| 1:B:1749:THR:CB | 1:B:1874:ASP:N | 2.58 | 0.66 |
| 2:H:1986:LYS:N | 2:H:1987:PRO:HD2 | 2.11 | 0.66 |
| 2:H:1173:VAL:HG21 | 2:H:1221:MET:HE1 | 1.77 | 0.66 |
| 1:A:988:ILE:HD13 | 1:A:1048:GLU:HB3 | 1.76 | 0.66 |
| 2:G:579:VAL:HG23 | 2:G:1078:HIS:NE2 | 2.10 | 0.66 |
| 2:H:1741:ILE:HG12 | 2:H:1746:LEU:HD13 | 1.76 | 0.66 |
| 1:C:1431:GLU:OE2 | 1:C:1433:HIS:CE1 | 2.48 | 0.66 |
| 2:G:1920:GLN:HG2 | 2:G:1922:ILE:HD11 | 1.78 | 0.66 |
| 1:B:1540:SER:HA | 1:B:1575:VAL:HG22 | 1.78 | 0.66 |
| 1:A:836:ASP:HB3 | 1:A:839:TYR:HB3 | 1.76 | 0.66 |
| 2:H:904:PHE:HB2 | 2:H:1017:PHE:CD1 | 2.30 | 0.66 |
| 2:H:61:VAL:O | 2:H:65:LEU:HB2 | 1.96 | 0.66 |
| 1:B:497:THR:OG1 | 1:B:513:GLU:HG2 | 1.95 | 0.66 |
| 2:H:131:ILE:HG21 | 2:H:182:VAL:CG1 | 2.18 | 0.66 |
| 2:I:1173:VAL:HG21 | 2:I:1221:MET:HE1 | 1.77 | 0.66 |
| 2:G:1808:SER:H | 2:G:2013:ASN:ND2 | 1.93 | 0.66 |
| 1:B:733:ILE:HD13 | 1:B:761:LEU:HD11 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1195:VAL:CG1 | 2:I:1211:LEU:HB3 | 2.25 | 0.66 |
| 2:G:1457:PHE:CZ | 2:G:1501:ILE:HD11 | 2.30 | 0.66 |
| 1:A:254:TRP:CH2 | 1:A:292:GLN:HG3 | 2.31 | 0.66 |
| 1:C:295:ALA:HB2 | 1:C:302:LEU:HD11 | 1.77 | 0.66 |
| 1:B:1219:VAL:HA | 1:B:1384:ILE:CD1 | 2.24 | 0.66 |
| 2:H:1770:LEU:HD23 | 2:H:1776:PHE:HE2 | 1.59 | 0.66 |
| 2:H:560:ASN:O | 2:H:561:TRP:C | 2.33 | 0.66 |
| 2:I:1808:SER:H | 2:I:2013:ASN:ND2 | 1.94 | 0.66 |
| 2:I:1381:VAL:HG13 | 2:I:1390:VAL:HG22 | 1.78 | 0.66 |
| 2:G:843:ILE:HD11 | 2:G:1055:HIS:HB3 | 1.78 | 0.66 |
| 2:I:1819:ALA:HA | 2:I:2005:ARG:HH11 | 1.61 | 0.66 |
| 2:G:904:PHE:HB2 | 2:G:1017:PHE:CD1 | 2.30 | 0.66 |
| 1:C:1360:ARG:HH11 | 1:C:1364:GLU:HG2 | 1.60 | 0.66 |
| 1:B:501:THR:N | 1:B:886:GLU:OE1 | 2.21 | 0.66 |
| 2:G:1352:HIS:CD2 | 2:G:1410:PHE:CE2 | 2.84 | 0.66 |
| 2:G:33:LEU:HD11 | 2:G:80:PHE:HD2 | 1.61 | 0.66 |
| 1:B:529:MET:CG | 1:B:638:LEU:HG | 2.26 | 0.65 |
| 2:H:2035:SER:HB3 | 2:H:2038:ILE:HG13 | 1.78 | 0.65 |
| 2:G:652:ILE:N | 2:G:658:MET:HE3 | 2.11 | 0.65 |
| 1:C:1317:GLU:HA | 1:C:1317:GLU:OE1 | 1.96 | 0.65 |
| 1:C:1:MET:CE | 1:C:6:GLU:HA | 2.25 | 0.65 |
| 2:G:1976:PHE:HA | 2:G:1981:LEU:HD22 | 1.78 | 0.65 |
| 1:A:497:THR:OG1 | 1:A:513:GLU:HG2 | 1.96 | 0.65 |
| 2:G:1986:LYS:N | 2:G:1987:PRO:HD2 | 2.12 | 0.65 |
| 1:C:330:GLU:HA | 1:C:333:LYS:HD2 | 1.79 | 0.65 |
| 2:G:1352:HIS:HE1 | 2:G:1583:MET:HE1 | 1.60 | 0.65 |
| 1:B:836:ASP:HB3 | 1:B:839:TYR:HB3 | 1.79 | 0.65 |
| 2:I:1782:THR:HG22 | 2:I:1827:LEU:HD21 | 1.78 | 0.65 |
| 1:C:836:ASP:HB3 | 1:C:839:TYR:HB3 | 1.77 | 0.65 |
| 2:H:1325:PHE:CZ | 2:H:1328:VAL:HG11 | 2.32 | 0.65 |
| 2:H:732:TRP:CG | 2:H:750:MET:CE | 2.79 | 0.65 |
| 1:C:1312:VAL:HG22 | 1:C:1329:VAL:HG11 | 1.78 | 0.65 |
| 2:G:597:MET:HA | 4:G:3051:FMN:N5 | 2.10 | 0.65 |
| 1:A:27:ARG:HB2 | 2:G:2016:ALA:HB2 | 1.77 | 0.65 |
| 1:A:934:PRO:O | 1:A:935:GLU:C | 2.35 | 0.65 |
| 1:A:331:ILE:HD11 | 1:C:332:THR:HG22 | 1.79 | 0.65 |
| 1:A:27:ARG:HD2 | 1:A:30:GLU:OE2 | 1.97 | 0.65 |
| 2:G:259:THR:HG23 | 2:G:262:GLU:H | 1.62 | 0.65 |
| 2:I:251:VAL:O | 2:I:255:LEU:HB2 | 1.96 | 0.65 |
| 1:B:460:GLU:HG2 | 1:B:470:LYS:HD3 | 1.78 | 0.65 |
| 1:C:32:GLN:HA | 1:C:35:PHE:CE2 | 2.31 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1719:ILE:O | 2:H:1761:SER:HB2 | 1.97 | 0.65 |
| 1:B:1317:GLU:OE1 | 1:B:1317:GLU:HA | 1.96 | 0.65 |
| 2:G:234:ILE:HG13 | 2:G:235:PRO:HD3 | 1.77 | 0.65 |
| 2:G:902:PRO:HG2 | 2:G:929:LEU:HD21 | 1.79 | 0.65 |
| 2:G:1086:LEU:HG | 2:G:1092:ASP:HA | 1.77 | 0.65 |
| 1:B:257:PRO:HD2 | 1:B:260:ARG:HB2 | 1.78 | 0.65 |
| 1:B:749:ILE:HD11 | 1:B:805:CYS:HB3 | 1.77 | 0.65 |
| 2:G:736:ARG:NH1 | 2:G:769:SER:O | 2.29 | 0.65 |
| 2:G:131:ILE:HG21 | 2:G:182:VAL:CG1 | 2.26 | 0.65 |
| 1:A:1219:VAL:HG22 | 1:A:1384:ILE:HD12 | 1.77 | 0.65 |
| 1:A:331:ILE:CD1 | 1:C:332:THR:HG22 | 2.26 | 0.65 |
| 2:I:545:GLN:HE21 | 2:I:545:GLN:H | 1.42 | 0.65 |
| 2:G:1381:VAL:HG13 | 2:G:1390:VAL:HG22 | 1.77 | 0.65 |
| 2:G:1740:THR:HG22 | 2:G:1742:VAL:HG23 | 1.78 | 0.65 |
| 1:C:435:GLU:O | 1:C:439:ILE:HG13 | 1.96 | 0.65 |
| 1:A:968:VAL:O | 2:G:1512:HIS:HB2 | 1.97 | 0.65 |
| 2:H:667:LYS:HB2 | 2:H:698:LEU:HD23 | 1.79 | 0.65 |
| 2:G:826:GLY:HA3 | 2:G:1061:GLN:HB3 | 1.77 | 0.65 |
| 2:H:748:THR:HB | 2:H:749:PRO:HD3 | 1.78 | 0.65 |
| 2:H:949:ASP:HB3 | 2:H:1006:MET:HE2 | 1.79 | 0.65 |
| 1:B:294:TYR:CE1 | 1:B:298:VAL:HG21 | 2.32 | 0.65 |
| 1:C:497:THR:OG1 | 1:C:513:GLU:HG2 | 1.97 | 0.65 |
| 1:A:1219:VAL:HA | 1:A:1384:ILE:CD1 | 2.23 | 0.65 |
| 1:A:529:MET:CG | 1:A:638:LEU:HG | 2.27 | 0.65 |
| 1:A:340:ARG:HH12 | 1:A:344:GLN:CG | 2.09 | 0.65 |
| 2:G:1242:PHE:CE2 | 2:G:1244:PRO:HG3 | 2.31 | 0.65 |
| 2:G:259:THR:CG2 | 2:G:262:GLU:H | 2.10 | 0.65 |
| 2:H:567:PRO:HG3 | 2:H:781:LEU:HD12 | 1.77 | 0.65 |
| 2:G:1418:ASP:O | 2:G:1420:GLU:N | 2.30 | 0.65 |
| 1:C:11:HIS:ND1 | 2:I:1998:LYS:HA | 2.12 | 0.65 |
| 2:I:1176:PRO:O | 2:I:1177:SER:HB3 | 1.95 | 0.65 |
| 1:A:294:TYR:CE1 | 1:A:298:VAL:HG21 | 2.32 | 0.65 |
| 1:C:1292:ILE:CD1 | 1:C:1328:ILE:HD11 | 2.27 | 0.65 |
| 2:I:490:TRP:HE1 | 2:I:516:THR:CG2 | 2.00 | 0.64 |
| 1:B:254:TRP:CH2 | 1:B:292:GLN:HG3 | 2.32 | 0.64 |
| 2:H:741:HIS:HB3 | 2:H:853:PRO:HB2 | 1.77 | 0.64 |
| 2:H:1195:VAL:HG13 | 2:H:1211:LEU:HB3 | 1.80 | 0.64 |
| 2:G:1841:ALA:O | 2:G:1842:VAL:HG23 | 1.97 | 0.64 |
| 2:I:1475:LYS:CG | 2:I:1481:SER:HB2 | 2.27 | 0.64 |
| 1:C:1721:ARG:CG | 1:C:1721:ARG:NH1 | 2.56 | 0.64 |
| 1:B:599:MET:HB2 | 1:B:624:LYS:CD | 2.24 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1859:PRO:O | 2:H:1862:VAL:HG13 | 1.98 | 0.64 |
| 2:G:1906:ALA:O | 2:G:1910:VAL:HG23 | 1.97 | 0.64 |
| 2:I:719:ILE:O | 2:I:722:ALA:HB3 | 1.97 | 0.64 |
| 2:G:353:VAL:HG23 | 2:G:357:ASN:HD22 | 1.61 | 0.64 |
| 2:I:1355:ASN:HA | 2:I:1407:THR:O | 1.97 | 0.64 |
| 1:C:749:ILE:HD11 | 1:C:805:CYS:HB3 | 1.78 | 0.64 |
| 1:A:893:VAL:HG11 | 1:A:930:LEU:HD23 | 1.80 | 0.64 |
| 2:H:1635:ARG:HG2 | 2:H:1658:GLU:CD | 2.18 | 0.64 |
| 2:H:115:THR:HB | 2:H:118:LYS:HB2 | 1.80 | 0.64 |
| 1:B:864:VAL:HG22 | 1:B:921:PRO:HB3 | 1.77 | 0.64 |
| 1:A:421:ILE:CG1 | 1:A:469:VAL:HG21 | 2.28 | 0.64 |
| 2:H:1906:ALA:O | 2:H:1910:VAL:HG23 | 1.98 | 0.64 |
| 2:H:259:THR:HG23 | 2:H:262:GLU:H | 1.63 | 0.64 |
| 2:I:1265:MET:HE1 | 2:I:1562:PRO:HG2 | 1.78 | 0.64 |
| 2:G:138:ASP:O | 2:G:139:LYS:HG3 | 1.97 | 0.64 |
| 2:H:1352:HIS:CD2 | 2:H:1410:PHE:CE2 | 2.85 | 0.64 |
| 1:C:604:ALA:HB3 | 1:C:612:GLU:HG2 | 1.80 | 0.64 |
| 2:G:490:TRP:HE1 | 2:G:516:THR:CG2 | 1.99 | 0.64 |
| 2:H:658:MET:HA | 2:H:661:TRP:NE1 | 2.13 | 0.64 |
| 2:H:1823:SER:OG | 2:H:1825:GLU:HG2 | 1.96 | 0.64 |
| 2:H:259:THR:CG2 | 2:H:262:GLU:H | 2.10 | 0.64 |
| 1:A:1039:MET:O | 1:A:1609:ARG:NH2 | 2.30 | 0.64 |
| 1:B:746:GLU:O | 1:B:750:GLU:HG3 | 1.97 | 0.64 |
| 2:G:1359:MET:HE3 | 2:G:1404:MET:HB3 | 1.79 | 0.64 |
| 2:I:826:GLY:HA3 | 2:I:1061:GLN:HB3 | 1.78 | 0.64 |
| 1:B:504:ASP:HB2 | 1:B:508:ASN:HB2 | 1.79 | 0.64 |
| 2:G:1840:VAL:O | 2:G:1840:VAL:CG1 | 2.44 | 0.64 |
| 1:C:1540:SER:HA | 1:C:1575:VAL:HG22 | 1.79 | 0.64 |
| 2:G:1195:VAL:CG1 | 2:G:1211:LEU:HB3 | 2.27 | 0.64 |
| 2:I:61:VAL:O | 2:I:65:LEU:HB2 | 1.96 | 0.64 |
| 2:G:1103:PHE:O | 2:G:1247:GLY:HA3 | 1.97 | 0.64 |
| 1:C:1594:ASN:O | 1:C:1598:GLN:HG3 | 1.97 | 0.64 |
| 1:C:1460:LYS:NZ | 1:C:1774:GLU:CD | 2.51 | 0.64 |
| 2:G:499:THR:CB | 2:G:500:HIS:HD2 | 1.97 | 0.64 |
| 2:I:7:ARG:HE | 2:I:27:PHE:HB2 | 1.62 | 0.64 |
| 1:A:504:ASP:HB2 | 1:A:508:ASN:HB2 | 1.78 | 0.64 |
| 2:H:1808:SER:H | 2:H:2013:ASN:HD21 | 1.46 | 0.64 |
| 1:A:746:GLU:O | 1:A:750:GLU:HG3 | 1.97 | 0.64 |
| 1:A:1022:THR:HG22 | 1:A:1226:SER:HB2 | 1.80 | 0.64 |
| 1:C:833:PHE:HA | 1:C:937:LYS:HD2 | 1.78 | 0.64 |
| 2:I:1457:PHE:CZ | 2:I:1501:ILE:HD11 | 2.33 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:648:GLY:HA3 | 2:I:678:PHE:CE2 | 2.32 | 0.64 |
| 1:B:852:ARG:NH1 | 1:B:852:ARG:HG2 | 1.98 | 0.64 |
| 2:G:1739:GLU:CB | 2:G:1987:PRO:HB3 | 2.23 | 0.64 |
| 2:I:1676:MET:HE1 | 2:I:1781:LEU:HD21 | 1.79 | 0.64 |
| 1:B:330:GLU:HA | 1:B:333:LYS:HD2 | 1.80 | 0.64 |
| 2:I:2022:THR:HG23 | 2:I:2025:TYR:H | 1.63 | 0.64 |
| 2:H:1457:PHE:CZ | 2:H:1501:ILE:HD11 | 2.32 | 0.64 |
| 2:G:1838:MET:O | 2:G:1974:VAL:HG21 | 1.98 | 0.64 |
| 1:C:1194:ASN:HB3 | 1:C:1197:THR:CG2 | 2.27 | 0.64 |
| 2:H:232:LEU:HD23 | 2:H:232:LEU:O | 1.98 | 0.64 |
| 2:I:892:ILE:HD11 | 2:I:903:TRP:NE1 | 2.12 | 0.64 |
| 2:H:1676:MET:HE1 | 2:H:1781:LEU:HD21 | 1.80 | 0.64 |
| 2:G:545:GLN:H | 2:G:545:GLN:HE21 | 1.46 | 0.64 |
| 2:I:964:LEU:CD2 | 2:I:964:LEU:H | 2.11 | 0.64 |
| 2:H:1205:LEU:O | 2:H:1206:LYS:HG3 | 1.97 | 0.64 |
| 1:A:1317:GLU:OE1 | 1:A:1317:GLU:HA | 1.96 | 0.64 |
| 1:B:421:ILE:CG1 | 1:B:469:VAL:HG21 | 2.27 | 0.64 |
| 2:I:670:ARG:HD3 | 2:I:699:GLY:O | 1.98 | 0.64 |
| 2:H:703:LEU:HD21 | 2:H:705:LEU:HD21 | 1.79 | 0.64 |
| 1:B:1474:ALA:HA | 1:B:1478:PRO:CG | 2.27 | 0.64 |
| 2:H:163:GLN:HG2 | 2:H:423:VAL:HG12 | 1.79 | 0.64 |
| 2:G:305:PHE:CE1 | 2:G:442:ASP:HB3 | 2.32 | 0.64 |
| 2:G:648:GLY:HA3 | 2:G:678:PHE:CE2 | 2.33 | 0.63 |
| 2:H:1176:PRO:O | 2:H:1177:SER:HB3 | 1.97 | 0.63 |
| 2:I:641:ILE:HG12 | 2:I:645:SER:HB2 | 1.79 | 0.63 |
| 1:A:152:HIS:HD2 | 1:A:163:LEU:HB2 | 1.61 | 0.63 |
| 1:C:1474:ALA:HA | 1:C:1478:PRO:CG | 2.27 | 0.63 |
| 1:C:24:SER:CB | 2:I:2014:LEU:HD12 | 2.27 | 0.63 |
| 2:H:964:LEU:CD2 | 2:H:964:LEU:H | 2.09 | 0.63 |
| 1:C:934:PRO:O | 1:C:936:LEU:N | 2.30 | 0.63 |
| 2:H:1266:TYR:CB | 2:H:1347:LEU:HD23 | 2.28 | 0.63 |
| 1:A:1021:VAL:HG11 | 1:A:1597:LEU:HD11 | 1.79 | 0.63 |
| 2:H:1227:ARG:CG | 2:H:1227:ARG:NH1 | 2.57 | 0.63 |
| 1:A:504:ASP:CB | 1:A:508:ASN:H | 2.10 | 0.63 |
| 1:C:504:ASP:HB2 | 1:C:508:ASN:HB2 | 1.80 | 0.63 |
| 2:I:1378:ILE:HD11 | 2:I:1381:VAL:CG2 | 2.28 | 0.63 |
| 2:H:1808:SER:H | 2:H:2013:ASN:ND2 | 1.95 | 0.63 |
| 1:C:989:GLN:NE2 | 2:I:993:GLN:OE1 | 2.32 | 0.63 |
| 2:I:1279:PHE:HB2 | 2:I:1340:PRO:HG3 | 1.79 | 0.63 |
| 2:I:1266:TYR:CB | 2:I:1347:LEU:HD23 | 2.28 | 0.63 |
| 2:I:902:PRO:HG2 | 2:I:929:LEU:HD21 | 1.79 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1205:LEU:O | 2:G:1206:LYS:HG3 | 1.98 | 0.63 |
| 1:C:436:ALA:O | 1:C:440:MET:HG3 | 1.98 | 0.63 |
| 1:B:438:ASN:HD21 | 1:B:698:GLN:HE21 | 1.46 | 0.63 |
| 2:G:2022:THR:HG23 | 2:G:2025:TYR:H | 1.63 | 0.63 |
| 1:C:1721:ARG:HG2 | 1:C:1721:ARG:NH1 | 2.00 | 0.63 |
| 2:G:7:ARG:HE | 2:G:27:PHE:HB2 | 1.63 | 0.63 |
| 2:G:259:THR:OG1 | 2:G:260:PRO:HD2 | 1.97 | 0.63 |
| 2:H:353:VAL:HG23 | 2:H:357:ASN:ND2 | 2.13 | 0.63 |
| 1:A:956:ALA:O | 1:A:959:ILE:HG22 | 1.98 | 0.63 |
| 1:A:1461:ASP:O | 1:A:1465:ASN:HB2 | 1.99 | 0.63 |
| 2:G:745:ASP:HA | 2:G:832:TRP:HH2 | 1.64 | 0.63 |
| 1:A:1292:ILE:CD1 | 1:A:1328:ILE:HD11 | 2.28 | 0.63 |
| 2:I:1976:PHE:HA | 2:I:1981:LEU:HD22 | 1.81 | 0.63 |
| 1:B:992:PHE:CE2 | 1:B:1399:PRO:HG3 | 2.34 | 0.63 |
| 2:I:1890:ASN:HB2 | 2:I:1899:VAL:HB | 1.81 | 0.63 |
| 1:A:852:ARG:NH1 | 1:A:852:ARG:HG2 | 2.00 | 0.63 |
| 1:C:599:MET:HB2 | 1:C:624:LYS:CD | 2.25 | 0.63 |
| 2:G:835:THR:HG21 | 2:G:855:HIS:CD2 | 2.33 | 0.63 |
| 1:B:881:ASN:HA | 1:B:944:ARG:HH21 | 1.63 | 0.63 |
| 2:I:1159:ILE:CG1 | 2:I:1169:PRO:HD3 | 2.28 | 0.63 |
| 1:A:824:LEU:HD12 | 1:A:846:LEU:HB3 | 1.80 | 0.63 |
| 2:H:1740:THR:HG22 | 2:H:1742:VAL:HG23 | 1.79 | 0.63 |
| 1:C:680:ILE:HG13 | 1:C:769:ILE:HB | 1.80 | 0.63 |
| 2:G:1266:TYR:CB | 2:G:1347:LEU:HD23 | 2.29 | 0.63 |
| 2:G:1859:PRO:O | 2:G:1862:VAL:HG13 | 1.99 | 0.63 |
| 2:I:159:ILE:HD11 | 2:I:512:LEU:HG | 1.80 | 0.63 |
| 2:H:598:THR:CG2 | 2:H:622:GLY:HA3 | 2.28 | 0.63 |
| 2:I:1195:VAL:HG13 | 2:I:1211:LEU:HB3 | 1.79 | 0.63 |
| 1:B:421:ILE:HG13 | 1:B:469:VAL:HG21 | 1.81 | 0.63 |
| 2:G:1738:PHE:CE1 | 2:G:1837:THR:HG23 | 2.34 | 0.63 |
| 2:H:601:THR:CG2 | 2:H:618:GLU:O | 2.38 | 0.63 |
| 2:I:1741:ILE:HG12 | 2:I:1746:LEU:HD13 | 1.80 | 0.63 |
| 1:B:1721:ARG:CG | 1:B:1721:ARG:NH1 | 2.55 | 0.63 |
| 2:I:1859:PRO:O | 2:I:1862:VAL:HG13 | 1.98 | 0.63 |
| 2:H:835:THR:HG22 | 2:H:845:THR:N | 2.14 | 0.63 |
| 1:B:444:ASN:HB3 | 1:B:446:ALA:H | 1.63 | 0.63 |
| 1:A:330:GLU:HA | 1:A:333:LYS:HD2 | 1.80 | 0.63 |
| 1:A:484:LEU:O | 1:A:485:ASP:CB | 2.47 | 0.63 |
| 1:B:1:MET:HE3 | 1:B:5:VAL:HG12 | 1.81 | 0.63 |
| 2:G:115:THR:HB | 2:G:118:LYS:HB2 | 1.80 | 0.63 |
| 2:H:1475:LYS:CG | 2:H:1481:SER:HB2 | 2.29 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:251:VAL:O | 2:G:255:LEU:HB2 | 1.99 | 0.63 |
| 1:A:436:ALA:O | 1:A:440:MET:HG3 | 1.99 | 0.63 |
| 2:I:241:ILE:HG23 | 2:I:506:PRO:HG3 | 1.81 | 0.63 |
| 1:A:1194:ASN:HB3 | 1:A:1197:THR:CG2 | 2.28 | 0.63 |
| 1:A:233:ILE:HD13 | 1:A:237:MET:HE2 | 1.81 | 0.63 |
| 2:H:892:ILE:HD11 | 2:H:903:TRP:NE1 | 2.14 | 0.63 |
| 1:B:27:ARG:HH21 | 2:H:2015:THR:HA | 1.64 | 0.63 |
| 2:G:748:THR:HB | 2:G:749:PRO:HD3 | 1.78 | 0.63 |
| 2:I:1194:VAL:HG12 | 2:I:1194:VAL:O | 1.99 | 0.63 |
| 1:C:864:VAL:HG22 | 1:C:921:PRO:HB3 | 1.79 | 0.63 |
| 2:G:1360:ILE:HG23 | 2:G:1403:VAL:O | 1.99 | 0.63 |
| 2:G:490:TRP:O | 2:G:494:THR:HG22 | 1.99 | 0.63 |
| 2:I:259:THR:OG1 | 2:I:260:PRO:HD2 | 1.98 | 0.63 |
| 2:I:259:THR:HG23 | 2:I:262:GLU:H | 1.64 | 0.63 |
| 1:C:742:LYS:HD3 | 1:C:746:GLU:OE2 | 1.98 | 0.63 |
| 1:A:460:GLU:HG2 | 1:A:470:LYS:HD3 | 1.79 | 0.63 |
| 2:I:115:THR:HB | 2:I:118:LYS:HB2 | 1.80 | 0.63 |
| 2:G:1227:ARG:HG3 | 2:G:1227:ARG:NH1 | 2.00 | 0.62 |
| 2:H:1874:VAL:O | 2:H:1878:VAL:HG12 | 1.98 | 0.62 |
| 2:H:33:LEU:HD11 | 2:H:80:PHE:HD2 | 1.63 | 0.62 |
| 1:C:956:ALA:O | 1:C:959:ILE:HG22 | 1.98 | 0.62 |
| 1:B:1056:ILE:HD13 | 1:B:1193:TRP:HD1 | 1.64 | 0.62 |
| 1:C:1753:ALA:HB2 | 1:C:1872:SER:OG | 1.98 | 0.62 |
| 1:A:411:GLN:HE22 | 1:A:1628:SER:H | 1.47 | 0.62 |
| 1:A:13:LEU:HB2 | 2:G:2026:PHE:CE1 | 2.34 | 0.62 |
| 1:B:529:MET:HG3 | 1:B:638:LEU:HG | 1.80 | 0.62 |
| 2:H:1931:LEU:HD22 | 2:H:1935:GLU:HG2 | 1.81 | 0.62 |
| 2:G:85:ASN:ND2 | 2:G:135:ARG:HH11 | 1.97 | 0.62 |
| 2:G:1173:VAL:HG21 | 2:G:1221:MET:HE1 | 1.80 | 0.62 |
| 2:G:943:TRP:CH2 | 2:G:1016:PRO:HG3 | 2.34 | 0.62 |
| 2:G:1378:ILE:HD11 | 2:G:1381:VAL:CG2 | 2.29 | 0.62 |
| 2:H:1374:THR:HG23 | 2:H:1396:LEU:HD12 | 1.81 | 0.62 |
| 2:H:251:VAL:O | 2:H:255:LEU:HB2 | 1.99 | 0.62 |
| 1:A:158:LYS:HD3 | 1:A:185:GLU:HB3 | 1.81 | 0.62 |
| 2:H:856:LYS:HG2 | 2:H:1054:LEU:HD12 | 1.81 | 0.62 |
| 1:C:254:TRP:CH2 | 1:C:292:GLN:HG3 | 2.34 | 0.62 |
| 2:G:726:PHE:O | 2:G:762:ASN:HB2 | 1.98 | 0.62 |
| 2:I:1624:THR:HB | 2:I:1642:THR:HG23 | 1.81 | 0.62 |
| 1:C:529:MET:CG | 1:C:638:LEU:HG | 2.30 | 0.62 |
| 2:H:750:MET:HG3 | 2:H:796:PHE:HZ | 1.64 | 0.62 |
| 2:I:1472:VAL:HG22 | 2:I:1483:VAL:HG22 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:324:LEU:HD12 | 2:I:328:LEU:HG | 1.82 | 0.62 |
| 1:A:1259:GLY:HA2 | 1:A:1263:ASP:HB2 | 1.81 | 0.62 |
| 2:I:1906:ALA:O | 2:I:1910:VAL:HG23 | 2.00 | 0.62 |
| 2:H:871:THR:HB | 2:H:872:ILE:HD12 | 1.80 | 0.62 |
| 2:H:1472:VAL:HG22 | 2:H:1483:VAL:HG22 | 1.79 | 0.62 |
| 2:I:1868:GLN:HG3 | 2:I:1898:TYR:OH | 1.99 | 0.62 |
| 2:H:601:THR:O | 2:H:601:THR:HG22 | 2.00 | 0.62 |
| 2:G:1102:TYR:HB3 | 2:G:1244:PRO:HA | 1.80 | 0.62 |
| 1:B:507:GLY:N | 1:B:954:ARG:HG2 | 2.15 | 0.62 |
| 1:A:1292:ILE:HD11 | 1:A:1328:ILE:HD11 | 1.81 | 0.62 |
| 2:G:1782:THR:HG22 | 2:G:1827:LEU:HD21 | 1.81 | 0.62 |
| 1:A:1455:ARG:HH11 | 1:A:1458:GLN:HE21 | 1.46 | 0.62 |
| 1:B:1584:PRO:HG3 | 1:B:1591:TRP:CZ3 | 2.35 | 0.62 |
| 1:C:1039:MET:O | 1:C:1609:ARG:NH2 | 2.31 | 0.62 |
| 2:G:1819:ALA:HA | 2:G:2005:ARG:HH11 | 1.65 | 0.62 |
| 2:H:1168:ASN:ND2 | 2:H:1171:ARG:HB2 | 2.14 | 0.62 |
| 2:I:1740:THR:HG22 | 2:I:1742:VAL:HG23 | 1.79 | 0.62 |
| 1:B:1455:ARG:HH11 | 1:B:1458:GLN:HE21 | 1.47 | 0.62 |
| 1:C:822:VAL:HG12 | 1:C:824:LEU:HD22 | 1.82 | 0.62 |
| 2:I:846:VAL:HG13 | 2:I:865:TRP:NE1 | 2.15 | 0.62 |
| 2:I:464:ASP:HB3 | 2:I:466:SER:HB3 | 1.80 | 0.62 |
| 2:H:131:ILE:HD12 | 2:H:182:VAL:CG1 | 2.29 | 0.62 |
| 2:I:259:THR:CG2 | 2:I:262:GLU:H | 2.11 | 0.62 |
| 2:I:184:VAL:HG13 | 2:I:187:LEU:HD21 | 1.80 | 0.62 |
| 2:G:241:ILE:HG23 | 2:G:506:PRO:HG3 | 1.80 | 0.62 |
| 1:A:749:ILE:CD1 | 1:A:805:CYS:HB3 | 2.29 | 0.62 |
| 2:G:871:THR:HB | 2:G:872:ILE:HD12 | 1.82 | 0.62 |
| 2:G:1908:ASP:HB2 | 2:G:1958:LEU:HD21 | 1.81 | 0.62 |
| 1:C:233:ILE:HD13 | 1:C:237:MET:CE | 2.30 | 0.62 |
| 1:A:1540:SER:HA | 1:A:1575:VAL:HG22 | 1.81 | 0.62 |
| 2:G:159:ILE:HD11 | 2:G:512:LEU:HG | 1.80 | 0.62 |
| 1:C:444:ASN:HB3 | 1:C:446:ALA:H | 1.65 | 0.62 |
| 2:G:641:ILE:HG12 | 2:G:645:SER:HB2 | 1.80 | 0.62 |
| 2:I:1805:ALA:HB2 | 2:I:2011:ILE:HB | 1.82 | 0.62 |
| 2:H:85:ASN:ND2 | 2:H:135:ARG:HH11 | 1.96 | 0.62 |
| 2:G:1300:PHE:CA | 2:G:1556:VAL:HG11 | 2.29 | 0.62 |
| 2:H:490:TRP:O | 2:H:494:THR:HG22 | 2.00 | 0.62 |
| 1:A:20:TYR:HE1 | 2:G:2035:SER:HB2 | 1.60 | 0.62 |
| 1:A:1523:ARG:CG | 1:A:1523:ARG:NH1 | 2.57 | 0.62 |
| 1:B:27:ARG:HD2 | 1:B:30:GLU:OE2 | 2.00 | 0.62 |
| 2:G:750:MET:HG3 | 2:G:796:PHE:HZ | 1.65 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:501:THR:N | 1:C:886:GLU:OE1 | 2.21 | 0.62 |
| 2:G:1931:LEU:HD22 | 2:G:1935:GLU:HG2 | 1.82 | 0.62 |
| 2:H:1149:TRP:CD1 | 2:H:1213:LEU:HD12 | 2.34 | 0.62 |
| 2:I:1823:SER:OG | 2:I:1825:GLU:HG2 | 2.00 | 0.62 |
| 2:I:1086:LEU:HD12 | 2:I:1090:TYR:HB2 | 1.82 | 0.62 |
| 2:I:745:ASP:HA | 2:I:832:TRP:HH2 | 1.65 | 0.62 |
| 1:A:1326:ILE:HG12 | 1:A:1388:MET:HG3 | 1.82 | 0.62 |
| 2:G:1719:ILE:O | 2:G:1761:SER:HB2 | 2.00 | 0.62 |
| 2:H:159:ILE:HD11 | 2:H:512:LEU:HG | 1.82 | 0.61 |
| 2:H:100:ASP:OD2 | 2:H:102:HIS:HD2 | 1.82 | 0.61 |
| 2:G:1199:GLU:OE2 | 2:G:1567:ARG:CZ | 2.46 | 0.61 |
| 2:H:1675:GLY:O | 2:H:1678:MET:HB2 | 1.99 | 0.61 |
| 1:C:233:ILE:HD13 | 1:C:237:MET:HE2 | 1.80 | 0.61 |
| 2:G:719:ILE:O | 2:G:722:ALA:HB3 | 2.00 | 0.61 |
| 1:C:509:ILE:HG12 | 1:C:951:SER:HB2 | 1.82 | 0.61 |
| 1:C:1057:MET:SD | 1:C:1097:ILE:HG23 | 2.40 | 0.61 |
| 2:H:7:ARG:HE | 2:H:27:PHE:HB2 | 1.64 | 0.61 |
| 1:A:934:PRO:O | 1:A:936:LEU:N | 2.33 | 0.61 |
| 2:H:353:VAL:HG23 | 2:H:357:ASN:HD22 | 1.65 | 0.61 |
| 1:B:631:PRO:HB2 | 1:B:634:THR:OG1 | 2.00 | 0.61 |
| 1:B:1292:ILE:CD1 | 1:B:1328:ILE:HD11 | 2.30 | 0.61 |
| 1:C:1498:GLU:HB2 | 1:C:1876:LEU:HD13 | 1.82 | 0.61 |
| 2:H:856:LYS:NZ | 2:H:1052:CYS:SG | 2.70 | 0.61 |
| 1:B:340:ARG:HH12 | 1:B:344:GLN:CG | 2.13 | 0.61 |
| 2:I:1054:LEU:HB2 | 4:I:3051:FMN:HM71 | 1.82 | 0.61 |
| 2:H:589:ARG:HB3 | 2:H:590:PRO:HD2 | 1.82 | 0.61 |
| 1:B:158:LYS:HD3 | 1:B:185:GLU:HB3 | 1.82 | 0.61 |
| 1:B:824:LEU:HD12 | 1:B:846:LEU:HB3 | 1.82 | 0.61 |
| 2:H:1528:GLU:O | 2:H:1530:LYS:N | 2.30 | 0.61 |
| 2:I:860:ARG:HB3 | 2:I:898:ASP:HB3 | 1.81 | 0.61 |
| 1:A:1721:ARG:NH1 | 1:A:1721:ARG:CG | 2.52 | 0.61 |
| 1:C:20:TYR:CE1 | 2:I:2035:SER:HB2 | 2.35 | 0.61 |
| 2:G:1739:GLU:O | 2:G:1987:PRO:HG3 | 2.00 | 0.61 |
| 2:H:835:THR:HG21 | 2:H:855:HIS:NE2 | 2.14 | 0.61 |
| 2:H:1378:ILE:HD11 | 2:H:1381:VAL:CG2 | 2.31 | 0.61 |
| 2:I:1808:SER:H | 2:I:2013:ASN:HD21 | 1.47 | 0.61 |
| 2:I:100:ASP:OD2 | 2:I:102:HIS:HD2 | 1.83 | 0.61 |
| 1:B:1555:ALA:HA | 1:B:1621:PHE:CE1 | 2.36 | 0.61 |
| 1:C:20:TYR:CG | 2:I:2033:THR:OG1 | 2.53 | 0.61 |
| 2:I:56:THR:HG23 | 2:I:59:GLU:CG | 2.28 | 0.61 |
| 1:B:20:TYR:CE1 | 2:H:2035:SER:HB2 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:24:SER:O | 2:G:1977:HIS:HD2 | 1.84 | 0.61 |
| 2:H:1086:LEU:HD12 | 2:H:1090:TYR:HB2 | 1.83 | 0.61 |
| 1:C:1292:ILE:HD11 | 1:C:1328:ILE:HD11 | 1.81 | 0.61 |
| 2:H:33:LEU:HD11 | 2:H:80:PHE:CD2 | 2.35 | 0.61 |
| 1:B:644:THR:HG23 | 1:B:648:ASP:H | 1.65 | 0.61 |
| 2:H:174:ARG:NH2 | 2:H:225:THR:OG1 | 2.33 | 0.61 |
| 2:G:324:LEU:HD12 | 2:G:328:LEU:HG | 1.81 | 0.61 |
| 2:H:1419:PHE:O | 2:H:1421:ASN:N | 2.33 | 0.61 |
| 2:H:1279:PHE:HB2 | 2:H:1340:PRO:HG3 | 1.81 | 0.61 |
| 2:H:603:SER:O | 2:H:607:VAL:HG12 | 2.00 | 0.61 |
| 1:B:24:SER:O | 2:H:1977:HIS:CD2 | 2.53 | 0.61 |
| 1:B:1693:ILE:HD11 | 2:H:998:GLN:HB2 | 1.83 | 0.61 |
| 1:A:705:VAL:HG23 | 1:A:732:LEU:HD21 | 1.82 | 0.61 |
| 1:B:1431:GLU:HG3 | 1:B:1433:HIS:CE1 | 2.36 | 0.61 |
| 1:C:24:SER:HB3 | 2:I:2014:LEU:HD12 | 1.82 | 0.61 |
| 2:I:1352:HIS:HE1 | 2:I:1583:MET:HE1 | 1.65 | 0.61 |
| 2:I:663:ILE:HG13 | 2:I:694:TYR:HE1 | 1.66 | 0.61 |
| 1:A:822:VAL:HG12 | 1:A:824:LEU:HD22 | 1.82 | 0.61 |
| 1:C:824:LEU:HD12 | 1:C:846:LEU:HB3 | 1.82 | 0.61 |
| 1:A:644:THR:HG23 | 1:A:648:ASP:H | 1.65 | 0.61 |
| 1:B:1194:ASN:HB3 | 1:B:1197:THR:CG2 | 2.30 | 0.61 |
| 2:I:1325:PHE:CZ | 2:I:1328:VAL:HG11 | 2.36 | 0.61 |
| 1:B:1052:GLU:O | 1:B:1056:ILE:HG23 | 2.01 | 0.61 |
| 1:B:1594:ASN:O | 1:B:1598:GLN:HG3 | 2.00 | 0.61 |
| 2:G:601:THR:O | 2:G:601:THR:HG22 | 2.01 | 0.61 |
| 1:A:599:MET:HB2 | 1:A:624:LYS:CD | 2.25 | 0.61 |
| 1:A:11:HIS:ND1 | 2:G:1998:LYS:HA | 2.15 | 0.61 |
| 2:H:260:PRO:HD3 | 2:H:289:TRP:CE2 | 2.36 | 0.61 |
| 2:G:1976:PHE:HB3 | 2:G:1981:LEU:HD21 | 1.82 | 0.61 |
| 1:B:1292:ILE:HD11 | 1:B:1328:ILE:HD11 | 1.82 | 0.61 |
| 1:B:1360:ARG:HH11 | 1:B:1364:GLU:HG2 | 1.66 | 0.61 |
| 2:G:1123:ASP:N | 2:G:1123:ASP:OD1 | 2.34 | 0.61 |
| 1:C:1501:LEU:HD11 | 1:C:1775:LEU:HD23 | 1.79 | 0.61 |
| 2:G:856:LYS:NZ | 2:G:1052:CYS:SG | 2.69 | 0.61 |
| 2:H:1805:ALA:HB2 | 2:H:2011:ILE:HB | 1.83 | 0.61 |
| 2:I:1219:ILE:HD11 | 2:I:1242:PHE:HB2 | 1.83 | 0.61 |
| 1:A:1:MET:HE3 | 1:A:5:VAL:HG12 | 1.82 | 0.61 |
| 2:H:184:VAL:HG13 | 2:H:187:LEU:HD21 | 1.83 | 0.61 |
| 2:G:1472:VAL:HG22 | 2:G:1483:VAL:HG22 | 1.83 | 0.61 |
| 1:C:504:ASP:CB | 1:C:508:ASN:H | 2.14 | 0.60 |
| 2:G:1417:THR:C | 2:G:1419:PHE:H | 2.04 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:846:VAL:HG13 | 2:H:865:TRP:NE1 | 2.16 | 0.60 |
| 2:I:565:TYR:CZ | 2:I:758:ARG:HD2 | 2.35 | 0.60 |
| 1:C:2:LYS:CD | 2:I:2050:GLN:HB3 | 2.30 | 0.60 |
| 1:A:32:GLN:HA | 1:A:35:PHE:CE2 | 2.35 | 0.60 |
| 2:I:856:LYS:NZ | 2:I:1052:CYS:SG | 2.70 | 0.60 |
| 2:G:33:LEU:HD11 | 2:G:80:PHE:CD2 | 2.35 | 0.60 |
| 2:I:1300:PHE:HA | 2:I:1556:VAL:HG11 | 1.84 | 0.60 |
| 2:I:33:LEU:HD11 | 2:I:80:PHE:CD2 | 2.36 | 0.60 |
| 2:G:174:ARG:NH2 | 2:G:225:THR:OG1 | 2.34 | 0.60 |
| 1:B:233:ILE:HD13 | 1:B:237:MET:HE2 | 1.82 | 0.60 |
| 2:G:1844:ARG:NH1 | 2:G:1844:ARG:CG | 2.49 | 0.60 |
| 2:G:607:VAL:HA | 2:G:617:ILE:HD13 | 1.82 | 0.60 |
| 2:G:1808:SER:H | 2:G:2013:ASN:HD21 | 1.47 | 0.60 |
| 2:G:747:HIS:HE1 | 2:G:780:TYR:OH | 1.84 | 0.60 |
| 2:I:1908:ASP:HB2 | 2:I:1958:LEU:HD21 | 1.83 | 0.60 |
| 2:I:1198:SER:HB3 | 2:I:1205:LEU:HD21 | 1.82 | 0.60 |
| 1:A:232:LEU:HD22 | 1:A:269:LEU:HA | 1.83 | 0.60 |
| 1:A:20:TYR:OH | 2:G:2035:SER:HB2 | 2.01 | 0.60 |
| 2:I:674:TYR:HB3 | 2:I:676:ILE:HG22 | 1.84 | 0.60 |
| 1:B:400:ARG:HH11 | 1:B:400:ARG:HG3 | 1.64 | 0.60 |
| 2:H:1219:ILE:HD11 | 2:H:1242:PHE:HB2 | 1.83 | 0.60 |
| 2:I:1352:HIS:CD2 | 2:I:1410:PHE:CE2 | 2.90 | 0.60 |
| 2:H:1198:SER:HB3 | 2:H:1205:LEU:HD21 | 1.83 | 0.60 |
| 2:G:846:VAL:HG13 | 2:G:865:TRP:NE1 | 2.16 | 0.60 |
| 1:A:1842:VAL:O | 1:A:1845:ASN:HB2 | 2.02 | 0.60 |
| 2:I:1360:ILE:HG23 | 2:I:1403:VAL:O | 2.01 | 0.60 |
| 2:H:324:LEU:HD12 | 2:H:328:LEU:HG | 1.84 | 0.60 |
| 2:G:499:THR:CB | 2:G:500:HIS:CD2 | 2.80 | 0.60 |
| 2:I:667:LYS:HB2 | 2:I:698:LEU:HD23 | 1.82 | 0.60 |
| 1:B:1523:ARG:NH1 | 1:B:1523:ARG:CG | 2.59 | 0.60 |
| 2:G:61:VAL:HG21 | 2:G:95:TYR:HE1 | 1.67 | 0.60 |
| 2:I:1205:LEU:O | 2:I:1206:LYS:HG3 | 2.00 | 0.60 |
| 2:G:926:LEU:HD13 | 2:G:947:THR:HG22 | 1.84 | 0.60 |
| 2:I:817:ALA:O | 2:I:821:ILE:HG13 | 2.01 | 0.60 |
| 2:H:745:ASP:HA | 2:H:832:TRP:HH2 | 1.66 | 0.60 |
| 2:I:1123:ASP:OD1 | 2:I:1123:ASP:N | 2.35 | 0.60 |
| 2:G:1325:PHE:CZ | 2:G:1328:VAL:HG11 | 2.37 | 0.60 |
| 1:B:509:ILE:HG12 | 1:B:951:SER:HB2 | 1.82 | 0.60 |
| 1:C:221:LEU:O | 1:C:225:SER:HB3 | 2.02 | 0.60 |
| 2:H:1624:THR:HB | 2:H:1642:THR:HG23 | 1.82 | 0.60 |
| 2:G:561:TRP:O | 2:G:562:LEU:C | 2.39 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1976:PHE:HB3 | 2:I:1981:LEU:HD21 | 1.83 | 0.60 |
| 1:C:644:THR:HG23 | 1:C:648:ASP:H | 1.65 | 0.60 |
| 2:I:589:ARG:HB3 | 2:I:590:PRO:HD2 | 1.83 | 0.60 |
| 2:G:1822:MET:HE2 | 2:G:1996:ILE:HG12 | 1.84 | 0.60 |
| 2:G:816:ASP:HB3 | 2:G:1048:VAL:HG21 | 1.83 | 0.60 |
| 1:A:529:MET:HG3 | 1:A:638:LEU:HG | 1.84 | 0.60 |
| 2:G:184:VAL:HG13 | 2:G:187:LEU:HD21 | 1.84 | 0.60 |
| 1:B:513:GLU:OE2 | 1:B:873:ARG:NH1 | 2.33 | 0.60 |
| 1:A:1194:ASN:O | 1:A:1197:THR:HG23 | 2.02 | 0.60 |
| 2:I:33:LEU:HD11 | 2:I:80:PHE:HD2 | 1.65 | 0.60 |
| 2:G:271:THR:OG1 | 2:G:460:TYR:HB2 | 2.01 | 0.60 |
| 2:I:1986:LYS:N | 2:I:1987:PRO:HD2 | 2.16 | 0.60 |
| 2:H:1739:GLU:O | 2:H:1987:PRO:HG3 | 2.02 | 0.60 |
| 2:H:1149:TRP:CD1 | 2:H:1213:LEU:CD1 | 2.85 | 0.60 |
| 1:C:1062:TYR:CD2 | 1:C:1693:ILE:HG23 | 2.36 | 0.60 |
| 1:A:233:ILE:HD13 | 1:A:237:MET:CE | 2.32 | 0.60 |
| 2:G:892:ILE:HD11 | 2:G:903:TRP:NE1 | 2.17 | 0.60 |
| 2:H:719:ILE:O | 2:H:722:ALA:HB3 | 2.02 | 0.60 |
| 1:C:529:MET:HG3 | 1:C:638:LEU:HG | 1.82 | 0.60 |
| 2:G:732:TRP:CD2 | 2:G:750:MET:CE | 2.85 | 0.60 |
| 1:B:1657:HIS:ND1 | 1:B:1658:PRO:HD2 | 2.17 | 0.60 |
| 1:B:604:ALA:HB3 | 1:B:612:GLU:HG2 | 1.82 | 0.60 |
| 2:I:601:THR:HG22 | 2:I:601:THR:O | 2.02 | 0.60 |
| 2:I:1989:LYS:O | 2:I:1993:LYS:HG3 | 2.02 | 0.60 |
| 2:I:741:HIS:CB | 2:I:853:PRO:HB2 | 2.32 | 0.60 |
| 2:I:1874:VAL:O | 2:I:1878:VAL:HG12 | 2.02 | 0.60 |
| 1:C:1662:TYR:O | 1:C:1665:ILE:HG22 | 2.01 | 0.60 |
| 1:B:1057:MET:SD | 1:B:1097:ILE:HG23 | 2.42 | 0.60 |
| 2:H:1093:ASP:HB3 | 2:H:1096:LYS:HG3 | 1.84 | 0.60 |
| 1:B:1021:VAL:HG11 | 1:B:1597:LEU:HD11 | 1.83 | 0.60 |
| 1:C:1842:VAL:O | 1:C:1845:ASN:HB2 | 2.02 | 0.60 |
| 2:G:598:THR:CG2 | 2:G:622:GLY:HA3 | 2.30 | 0.59 |
| 1:A:1119:LYS:HE2 | 1:A:1341:PHE:CG | 2.37 | 0.59 |
| 2:G:1425:LYS:HG2 | 2:G:1471:GLU:CG | 2.30 | 0.59 |
| 2:H:1494:PRO:HB2 | 2:H:1823:SER:HB2 | 1.84 | 0.59 |
| 2:I:732:TRP:CD2 | 2:I:750:MET:CE | 2.84 | 0.59 |
| 2:G:1417:THR:HG22 | 2:G:1419:PHE:CE2 | 2.37 | 0.59 |
| 1:B:1189:ILE:HD12 | 1:B:1380:GLN:HG3 | 1.82 | 0.59 |
| 2:G:100:ASP:OD2 | 2:G:102:HIS:HD2 | 1.85 | 0.59 |
| 1:C:1585:LYS:HB3 | 3:C:2748:CER:H52 | 1.84 | 0.59 |
| 1:C:1461:ASP:O | 1:C:1465:ASN:HB2 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:163:GLN:CG | 2:I:423:VAL:HG12 | 2.32 | 0.59 |
| 2:I:1378:ILE:HD11 | 2:I:1381:VAL:HG21 | 1.84 | 0.59 |
| 1:B:1062:TYR:CD2 | 1:B:1693:ILE:HG23 | 2.36 | 0.59 |
| 1:B:1184:LEU:HB2 | 1:B:1352:THR:HG21 | 1.83 | 0.59 |
| 1:A:1475:GLU:CG | 1:A:1761:LYS:O | 2.50 | 0.59 |
| 1:A:67:SER:OG | 2:I:359:HIS:HE1 | 1.85 | 0.59 |
| 1:B:80:CYS:SG | 1:B:82:SER:HB3 | 2.42 | 0.59 |
| 2:H:813:THR:HB | 2:H:818:LYS:HE3 | 1.84 | 0.59 |
| 1:A:37:LYS:HB2 | 1:A:65:TYR:HE1 | 1.67 | 0.59 |
| 1:B:1460:LYS:NZ | 1:B:1774:GLU:CD | 2.51 | 0.59 |
| 2:H:1314:ARG:NH1 | 2:H:1314:ARG:CG | 2.62 | 0.59 |
| 2:G:594:VAL:HG21 | 2:G:610:THR:HG21 | 1.84 | 0.59 |
| 1:C:705:VAL:HG23 | 1:C:732:LEU:HD21 | 1.83 | 0.59 |
| 1:B:32:GLN:HA | 1:B:35:PHE:CE2 | 2.38 | 0.59 |
| 1:B:680:ILE:HG13 | 1:B:769:ILE:HB | 1.83 | 0.59 |
| 2:I:1575:LEU:HD13 | 2:I:1579:ILE:HD12 | 1.84 | 0.59 |
| 1:A:435:GLU:O | 1:A:439:ILE:HG13 | 2.03 | 0.59 |
| 2:G:2038:ILE:O | 2:G:2042:ILE:HG12 | 2.02 | 0.59 |
| 2:I:658:MET:HA | 2:I:661:TRP:NE1 | 2.17 | 0.59 |
| 2:G:754:TYR:CD2 | 2:G:794:MET:HG3 | 2.38 | 0.59 |
| 2:H:241:ILE:HG23 | 2:H:506:PRO:HG3 | 1.83 | 0.59 |
| 1:B:1259:GLY:HA2 | 1:B:1263:ASP:HB2 | 1.84 | 0.59 |
| 1:A:1584:PRO:HG3 | 1:A:1591:TRP:CZ3 | 2.37 | 0.59 |
| 2:H:409:PHE:HB3 | 2:H:833:GLU:OE1 | 2.02 | 0.59 |
| 1:B:221:LEU:O | 1:B:225:SER:HB3 | 2.02 | 0.59 |
| 2:H:1223:MET:HE3 | 2:H:1238:LEU:HD12 | 1.84 | 0.59 |
| 1:C:421:ILE:CG1 | 1:C:469:VAL:HG21 | 2.32 | 0.59 |
| 2:H:860:ARG:HB3 | 2:H:898:ASP:HB3 | 1.83 | 0.59 |
| 1:C:56:MET:HG3 | 2:I:1893:VAL:CG2 | 2.32 | 0.59 |
| 1:A:1749:THR:CB | 1:A:1874:ASP:HA | 2.31 | 0.59 |
| 2:G:443:LEU:HD22 | 2:G:448:VAL:HG11 | 1.84 | 0.59 |
| 2:I:1149:TRP:CD1 | 2:I:1213:LEU:HD12 | 2.37 | 0.59 |
| 2:G:1805:ALA:HB2 | 2:G:2011:ILE:HB | 1.84 | 0.59 |
| 2:I:85:ASN:ND2 | 2:I:135:ARG:HH11 | 1.99 | 0.59 |
| 1:C:1194:ASN:O | 1:C:1197:THR:HG23 | 2.02 | 0.59 |
| 1:B:233:ILE:HD13 | 1:B:237:MET:CE | 2.32 | 0.59 |
| 1:B:956:ALA:O | 1:B:959:ILE:HG22 | 2.02 | 0.59 |
| 1:C:1492:GLU:O | 1:C:1496:GLU:HG3 | 2.01 | 0.59 |
| 1:B:1842:VAL:O | 1:B:1845:ASN:HB2 | 2.02 | 0.59 |
| 1:A:1432:HIS:CE1 | 1:A:1434:SER:OG | 2.55 | 0.59 |
| 2:I:402:LEU:HD13 | 2:I:402:LEU:O | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:932:ILE:HD11 | 2:G:1042:ALA:CB | 2.24 | 0.59 |
| 2:G:603:SER:O | 2:G:607:VAL:HG12 | 2.03 | 0.59 |
| 2:I:1422:THR:CG2 | 2:I:1422:THR:O | 2.49 | 0.59 |
| 1:B:504:ASP:CB | 1:B:508:ASN:H | 2.15 | 0.59 |
| 2:G:1195:VAL:HG13 | 2:G:1211:LEU:HB3 | 1.84 | 0.59 |
| 2:H:817:ALA:O | 2:H:821:ILE:HG13 | 2.02 | 0.59 |
| 1:C:1584:PRO:HG3 | 1:C:1591:TRP:CZ3 | 2.38 | 0.59 |
| 2:H:726:PHE:O | 2:H:762:ASN:HB2 | 2.03 | 0.59 |
| 2:I:1496:LYS:HE2 | 2:I:1693:ARG:HH21 | 1.67 | 0.59 |
| 2:I:1086:LEU:HD12 | 2:I:1090:TYR:CB | 2.33 | 0.59 |
| 1:C:733:ILE:HD12 | 1:C:761:LEU:HD21 | 1.85 | 0.59 |
| 2:H:663:ILE:HG13 | 2:H:694:TYR:HE1 | 1.66 | 0.59 |
| 1:A:516:ARG:NH2 | 1:A:889:GLU:OE1 | 2.35 | 0.59 |
| 2:G:1417:THR:O | 2:G:1419:PHE:N | 2.30 | 0.59 |
| 1:A:417:TYR:OH | 1:A:458:THR:HG22 | 2.02 | 0.59 |
| 1:B:1585:LYS:HB3 | 3:B:2748:CER:H52 | 1.85 | 0.59 |
| 2:I:99:ASN:HA | 2:I:550:VAL:CG2 | 2.32 | 0.59 |
| 2:G:131:ILE:CG2 | 2:G:182:VAL:CG1 | 2.80 | 0.59 |
| 2:H:455:ILE:HG13 | 2:H:469:ARG:HD3 | 1.83 | 0.59 |
| 2:G:1417:THR:HG22 | 2:G:1419:PHE:CD2 | 2.37 | 0.59 |
| 2:H:197:GLU:HA | 2:H:197:GLU:OE1 | 2.02 | 0.59 |
| 1:A:409:ALA:HB2 | 1:A:442:ARG:HD2 | 1.84 | 0.59 |
| 2:H:2038:ILE:O | 2:H:2042:ILE:HG12 | 2.03 | 0.59 |
| 2:G:1086:LEU:HD12 | 2:G:1090:TYR:HB2 | 1.84 | 0.59 |
| 1:C:1555:ALA:HA | 1:C:1621:PHE:CE1 | 2.38 | 0.59 |
| 1:A:50:SER:HB2 | 1:A:51:PRO:HD3 | 1.85 | 0.59 |
| 2:G:402:LEU:HD13 | 2:G:402:LEU:O | 2.03 | 0.59 |
| 1:A:1002:LYS:NZ | 1:A:1782:GLU:HG2 | 2.17 | 0.59 |
| 2:I:490:TRP:O | 2:I:494:THR:HG22 | 2.03 | 0.59 |
| 1:B:1474:ALA:O | 1:B:1478:PRO:HD2 | 2.03 | 0.59 |
| 2:G:1293:THR:CG2 | 2:G:1296:GLU:H | 2.14 | 0.59 |
| 1:A:440:MET:HB3 | 1:A:483:VAL:HG21 | 1.85 | 0.59 |
| 2:H:259:THR:OG1 | 2:H:260:PRO:HD2 | 2.03 | 0.59 |
| 1:B:417:TYR:OH | 1:B:458:THR:HG22 | 2.03 | 0.59 |
| 2:G:1374:THR:HG23 | 2:G:1396:LEU:HD12 | 1.85 | 0.59 |
| 2:I:353:VAL:HG23 | 2:I:357:ASN:ND2 | 2.18 | 0.59 |
| 2:G:1210:ILE:HB | 2:G:1222:GLU:HB3 | 1.85 | 0.59 |
| 2:H:1130:THR:H | 2:H:1133:THR:HG23 | 1.68 | 0.59 |
| 2:I:174:ARG:NH2 | 2:I:225:THR:OG1 | 2.36 | 0.59 |
| 2:G:1198:SER:HB3 | 2:G:1205:LEU:HD21 | 1.85 | 0.58 |
| 1:A:1585:LYS:HB3 | 3:A:2748:CER:H52 | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:488:PRO:HG3 | 1:C:728:LYS:HG3 | 1.83 | 0.58 |
| 1:B:1234:MET:HG2 | 1:B:1326:ILE:HD12 | 1.85 | 0.58 |
| 1:A:1524:GLY:O | 1:A:1528:THR:HG23 | 2.03 | 0.58 |
| 2:G:1279:PHE:HB2 | 2:G:1340:PRO:HG3 | 1.85 | 0.58 |
| 2:H:273:HIS:HB3 | 2:H:512:LEU:HD22 | 1.85 | 0.58 |
| 2:I:455:ILE:HG13 | 2:I:469:ARG:HD3 | 1.85 | 0.58 |
| 2:G:1378:ILE:HD11 | 2:G:1381:VAL:HG21 | 1.85 | 0.58 |
| 2:I:499:THR:CB | 2:I:500:HIS:CD2 | 2.79 | 0.58 |
| 2:I:907:VAL:O | 2:I:910:GLN:HB3 | 2.03 | 0.58 |
| 2:G:1149:TRP:CD1 | 2:G:1213:LEU:HD12 | 2.38 | 0.58 |
| 1:C:749:ILE:CD1 | 1:C:805:CYS:HB3 | 2.32 | 0.58 |
| 1:A:421:ILE:HG12 | 1:A:469:VAL:HG21 | 1.85 | 0.58 |
| 1:B:1392:LEU:HD22 | 1:B:1396:MET:HG3 | 1.84 | 0.58 |
| 2:I:1822:MET:CE | 2:I:1996:ILE:HG12 | 2.34 | 0.58 |
| 1:C:1657:HIS:ND1 | 1:C:1658:PRO:HD2 | 2.17 | 0.58 |
| 2:H:1010:PRO:O | 2:H:1011:MET:HB2 | 2.03 | 0.58 |
| 2:H:665:LEU:O | 2:H:669:LEU:HB2 | 2.04 | 0.58 |
| 1:C:80:CYS:SG | 1:C:82:SER:HB3 | 2.42 | 0.58 |
| 1:A:531:LEU:HD21 | 1:A:629:THR:HG22 | 1.85 | 0.58 |
| 2:G:28:PHE:CZ | 2:H:7:ARG:NE | 2.70 | 0.58 |
| 2:I:601:THR:CG2 | 2:I:618:GLU:O | 2.39 | 0.58 |
| 2:I:1227:ARG:NH1 | 2:I:1227:ARG:CG | 2.55 | 0.58 |
| 1:A:1463:VAL:HG11 | 1:A:1877:GLN:HE22 | 1.68 | 0.58 |
| 1:B:37:LYS:HB2 | 1:B:65:TYR:HE1 | 1.69 | 0.58 |
| 2:I:1374:THR:HG23 | 2:I:1396:LEU:HD12 | 1.83 | 0.58 |
| 2:G:166:THR:HG22 | 2:G:168:ASP:N | 2.19 | 0.58 |
| 1:A:444:ASN:HB3 | 1:A:446:ALA:H | 1.66 | 0.58 |
| 2:I:127:ILE:O | 2:I:131:ILE:HG13 | 2.03 | 0.58 |
| 1:C:24:SER:O | 2:I:1977:HIS:CD2 | 2.54 | 0.58 |
| 1:A:260:ARG:HH12 | 1:A:300:VAL:HG21 | 1.68 | 0.58 |
| 1:B:409:ALA:HB2 | 1:B:442:ARG:HD2 | 1.86 | 0.58 |
| 2:H:1360:ILE:HG23 | 2:H:1403:VAL:O | 2.04 | 0.58 |
| 2:I:736:ARG:NH1 | 2:I:769:SER:O | 2.36 | 0.58 |
| 2:H:1103:PHE:O | 2:H:1247:GLY:HA3 | 2.03 | 0.58 |
| 1:C:1233:GLU:OE2 | 1:C:1680:ARG:NH2 | 2.36 | 0.58 |
| 2:H:499:THR:CB | 2:H:500:HIS:CD2 | 2.81 | 0.58 |
| 2:H:762:ASN:H | 2:H:762:ASN:ND2 | 1.85 | 0.58 |
| 2:G:1823:SER:OG | 2:G:1825:GLU:HG2 | 2.03 | 0.58 |
| 2:G:1597:ALA:HB1 | 2:G:1638:ILE:CD1 | 2.33 | 0.58 |
| 2:I:1269:LEU:O | 2:I:1560:LEU:HD23 | 2.03 | 0.58 |
| 2:H:271:THR:OG1 | 2:H:460:TYR:HB2 | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1009:LEU:HA | 1:C:1445:MET:HE2 | 1.85 | 0.58 |
| 2:G:807:ILE:CG2 | 2:G:1066:ILE:HA | 2.34 | 0.58 |
| 1:C:232:LEU:HD22 | 1:C:269:LEU:HA | 1.83 | 0.58 |
| 1:B:436:ALA:O | 1:B:440:MET:HG3 | 2.04 | 0.58 |
| 2:G:131:ILE:CG2 | 2:G:182:VAL:HG12 | 2.33 | 0.58 |
| 2:I:707:PRO:HG2 | 2:I:730:LEU:HD13 | 1.85 | 0.58 |
| 1:C:340:ARG:HH12 | 1:C:344:GLN:CG | 2.13 | 0.58 |
| 1:C:1665:ILE:HD11 | 1:C:1669:ARG:HG2 | 1.85 | 0.58 |
| 2:G:907:VAL:O | 2:G:910:GLN:HB3 | 2.02 | 0.58 |
| 1:C:421:ILE:HG13 | 1:C:469:VAL:HG21 | 1.84 | 0.58 |
| 1:C:232:LEU:HD13 | 1:C:272:GLU:HB2 | 1.85 | 0.58 |
| 1:B:1461:ASP:O | 1:B:1465:ASN:HB2 | 2.03 | 0.58 |
| 1:A:986:ALA:HB2 | 1:A:1047:LEU:HD13 | 1.85 | 0.58 |
| 2:G:1223:MET:HE3 | 2:G:1238:LEU:HD12 | 1.85 | 0.58 |
| 2:H:490:TRP:CH2 | 2:H:512:LEU:HD21 | 2.39 | 0.58 |
| 2:G:565:TYR:OH | 2:G:758:ARG:HD2 | 2.02 | 0.58 |
| 2:I:942:THR:HG21 | 2:I:1012:GLN:HA | 1.85 | 0.58 |
| 2:H:543:PHE:CB | 2:H:545:GLN:HE22 | 2.17 | 0.58 |
| 1:B:29:ILE:HG13 | 2:H:1891:TYR:C | 2.23 | 0.58 |
| 2:G:1159:ILE:CG1 | 2:G:1169:PRO:HD3 | 2.33 | 0.58 |
| 2:G:260:PRO:HD3 | 2:G:289:TRP:CE2 | 2.38 | 0.58 |
| 2:G:674:TYR:HB3 | 2:G:676:ILE:HG22 | 1.85 | 0.58 |
| 2:I:1719:ILE:O | 2:I:1761:SER:HB2 | 2.01 | 0.58 |
| 1:A:1600:LEU:HD13 | 1:A:1657:HIS:HA | 1.85 | 0.58 |
| 1:C:419:GLU:HG2 | 1:C:424:VAL:HB | 1.86 | 0.58 |
| 1:C:968:VAL:O | 2:I:1512:HIS:HB2 | 2.04 | 0.58 |
| 1:B:198:PRO:CG | 1:B:209:LEU:HD21 | 2.26 | 0.58 |
| 2:G:638:VAL:HA | 2:G:641:ILE:HG22 | 1.86 | 0.58 |
| 2:H:163:GLN:CG | 2:H:423:VAL:HG12 | 2.32 | 0.58 |
| 2:I:1822:MET:HE2 | 2:I:1996:ILE:HG12 | 1.86 | 0.58 |
| 1:B:286:PHE:O | 1:B:290:MET:HG2 | 2.03 | 0.58 |
| 1:C:1020:VAL:HG13 | 1:C:1400:ILE:HG23 | 1.84 | 0.58 |
| 2:G:273:HIS:HB3 | 2:G:512:LEU:HD22 | 1.86 | 0.58 |
| 1:A:20:TYR:CZ | 2:G:2035:SER:HB2 | 2.39 | 0.58 |
| 1:A:198:PRO:CG | 1:A:209:LEU:HD21 | 2.28 | 0.58 |
| 2:G:611:THR:CG2 | 2:G:641:ILE:HG13 | 2.34 | 0.58 |
| 1:B:1473:GLU:O | 1:B:1478:PRO:HD3 | 2.04 | 0.58 |
| 1:C:27:ARG:HH21 | 2:I:2015:THR:HA | 1.68 | 0.58 |
| 1:B:1662:TYR:O | 1:B:1665:ILE:HG22 | 2.04 | 0.58 |
| 1:B:749:ILE:CD1 | 1:B:805:CYS:HB3 | 2.33 | 0.58 |
| 2:G:232:LEU:HD23 | 2:G:232:LEU:O | 2.03 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1359:MET:HA | 2:G:1359:MET:HE3 | 1.86 | 0.58 |
| 1:B:232:LEU:HD22 | 1:B:269:LEU:HA | 1.85 | 0.58 |
| 1:C:1247:SER:HB2 | 1:C:1332:TYR:HE2 | 1.68 | 0.58 |
| 2:H:1210:ILE:HB | 2:H:1222:GLU:HB3 | 1.85 | 0.58 |
| 2:G:860:ARG:HB3 | 2:G:898:ASP:HB3 | 1.85 | 0.58 |
| 1:A:987:ASN:HD22 | 2:G:957:ARG:HD2 | 1.68 | 0.58 |
| 2:G:817:ALA:O | 2:G:821:ILE:HG13 | 2.04 | 0.58 |
| 2:G:146:PHE:HA | 2:G:149:VAL:HG12 | 1.86 | 0.57 |
| 2:G:7:ARG:NH1 | 2:G:24:THR:HA | 2.19 | 0.57 |
| 1:C:1219:VAL:CA | 1:C:1384:ILE:HD11 | 2.27 | 0.57 |
| 2:G:56:THR:HG23 | 2:G:59:GLU:CG | 2.29 | 0.57 |
| 1:A:1062:TYR:CD2 | 1:A:1693:ILE:HG23 | 2.39 | 0.57 |
| 1:A:329:GLU:O | 1:A:333:LYS:HG3 | 2.04 | 0.57 |
| 2:I:239:PRO:HG3 | 2:I:304:PHE:HA | 1.86 | 0.57 |
| 1:A:1419:PRO:HB3 | 1:A:1646:PHE:CZ | 2.39 | 0.57 |
| 1:C:433:VAL:O | 1:C:437:ILE:HG13 | 2.04 | 0.57 |
| 2:I:376:ASN:HD22 | 2:I:377:LEU:N | 2.02 | 0.57 |
| 1:B:419:GLU:HG2 | 1:B:424:VAL:HB | 1.86 | 0.57 |
| 2:G:376:ASN:HD22 | 2:G:377:LEU:N | 2.02 | 0.57 |
| 1:B:1247:SER:HB2 | 1:B:1332:TYR:HE2 | 1.69 | 0.57 |
| 1:A:1189:ILE:HD12 | 1:A:1380:GLN:HG3 | 1.86 | 0.57 |
| 1:A:1464:GLU:CD | 1:A:1773:VAL:HG12 | 2.23 | 0.57 |
| 2:I:726:PHE:O | 2:I:762:ASN:HB2 | 2.04 | 0.57 |
| 1:A:11:HIS:O | 1:A:15:THR:HG22 | 2.04 | 0.57 |
| 2:H:722:ALA:HB1 | 2:H:723:HIS:CE1 | 2.38 | 0.57 |
| 1:C:1431:GLU:CD | 1:C:1433:HIS:HE1 | 2.08 | 0.57 |
| 2:G:658:MET:HA | 2:G:661:TRP:NE1 | 2.19 | 0.57 |
| 1:A:1203:ASP:HB3 | 1:B:179:LYS:HZ1 | 1.68 | 0.57 |
| 2:G:1149:TRP:CD1 | 2:G:1213:LEU:CD1 | 2.87 | 0.57 |
| 2:H:1331:TRP:CE2 | 2:H:1335:ILE:HG13 | 2.38 | 0.57 |
| 1:A:1056:ILE:CD1 | 1:A:1193:TRP:HD1 | 2.17 | 0.57 |
| 1:C:1052:GLU:O | 1:C:1056:ILE:HG23 | 2.04 | 0.57 |
| 1:B:232:LEU:HD13 | 1:B:272:GLU:HB2 | 1.87 | 0.57 |
| 1:B:1496:GLU:O | 1:B:1500:GLN:HG3 | 2.03 | 0.57 |
| 1:A:1247:SER:HB2 | 1:A:1332:TYR:HE2 | 1.66 | 0.57 |
| 2:G:942:THR:HG21 | 2:G:1012:GLN:HA | 1.86 | 0.57 |
| 2:G:826:GLY:O | 2:G:827:VAL:HG23 | 2.03 | 0.57 |
| 1:C:1056:ILE:CD1 | 1:C:1193:TRP:HD1 | 2.16 | 0.57 |
| 1:A:1538:VAL:HB | 1:A:1639:VAL:HG22 | 1.86 | 0.57 |
| 1:B:1125:VAL:HG21 | 1:B:1175:ILE:HD12 | 1.86 | 0.57 |
| 1:B:50:SER:HB2 | 1:B:51:PRO:HD3 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1022:THR:HG22 | 1:B:1226:SER:HB2 | 1.87 | 0.57 |
| 2:H:124:LYS:HG2 | 2:H:179:THR:HA | 1.86 | 0.57 |
| 2:H:601:THR:HG22 | 2:H:620:ALA:H | 1.69 | 0.57 |
| 2:I:145:LEU:O | 2:I:149:VAL:HG12 | 2.03 | 0.57 |
| 2:H:1567:ARG:HH12 | 2:H:1568:HIS:HB3 | 1.70 | 0.57 |
| 2:H:907:VAL:O | 2:H:910:GLN:HB3 | 2.03 | 0.57 |
| 2:G:163:GLN:CG | 2:G:423:VAL:HG12 | 2.33 | 0.57 |
| 2:H:1086:LEU:HD12 | 2:H:1090:TYR:CB | 2.34 | 0.57 |
| 2:H:732:TRP:CG | 2:H:750:MET:HE3 | 2.39 | 0.57 |
| 1:B:413:LEU:HD13 | 1:B:451:MET:HG2 | 1.85 | 0.57 |
| 2:H:1908:ASP:HB2 | 2:H:1958:LEU:HD21 | 1.86 | 0.57 |
| 1:C:183:GLN:HE21 | 1:C:202:GLU:HG2 | 1.69 | 0.57 |
| 2:H:1231:GLY:O | 2:H:1233:PRO:HD3 | 2.04 | 0.57 |
| 2:I:654:VAL:HG23 | 2:I:683:ALA:HB1 | 1.87 | 0.57 |
| 1:B:705:VAL:HG23 | 1:B:732:LEU:HD21 | 1.85 | 0.57 |
| 2:G:932:ILE:CD1 | 2:G:1042:ALA:HB2 | 2.24 | 0.57 |
| 1:C:198:PRO:CG | 1:C:209:LEU:HD21 | 2.28 | 0.57 |
| 2:G:562:LEU:O | 2:G:566:HIS:HB2 | 2.05 | 0.57 |
| 1:A:232:LEU:HD13 | 1:A:272:GLU:HB2 | 1.85 | 0.57 |
| 1:C:1600:LEU:HD13 | 1:C:1657:HIS:HA | 1.87 | 0.57 |
| 2:H:736:ARG:NH1 | 2:H:769:SER:O | 2.36 | 0.57 |
| 2:G:1010:PRO:O | 2:G:1011:MET:HB2 | 2.05 | 0.57 |
| 1:C:771:PHE:CD1 | 1:C:825:PRO:HG3 | 2.40 | 0.57 |
| 2:H:89:THR:O | 2:H:93:ASN:HB2 | 2.04 | 0.57 |
| 2:I:1130:THR:H | 2:I:1133:THR:HG23 | 1.69 | 0.57 |
| 1:C:1189:ILE:HD12 | 1:C:1380:GLN:HG3 | 1.86 | 0.57 |
| 1:C:251:GLN:HA | 1:C:256:LEU:H | 1.69 | 0.57 |
| 2:I:2038:ILE:O | 2:I:2042:ILE:HG12 | 2.04 | 0.57 |
| 2:G:1314:ARG:CG | 2:G:1314:ARG:NH1 | 2.61 | 0.57 |
| 1:C:1473:GLU:O | 1:C:1478:PRO:HD3 | 2.05 | 0.57 |
| 2:H:732:TRP:CG | 2:H:750:MET:HE1 | 2.40 | 0.57 |
| 2:G:1954:LYS:HD3 | 2:G:1958:LEU:HD13 | 1.86 | 0.57 |
| 1:A:828:PRO:HG3 | 1:A:868:ILE:HG22 | 1.86 | 0.57 |
| 2:I:813:THR:HB | 2:I:818:LYS:HE3 | 1.85 | 0.57 |
| 2:H:1782:THR:HG22 | 2:H:1827:LEU:HD21 | 1.86 | 0.57 |
| 1:C:1184:LEU:HB2 | 1:C:1352:THR:HG21 | 1.85 | 0.57 |
| 1:B:980:VAL:HG21 | 2:H:952:ARG:HH21 | 1.70 | 0.57 |
| 1:A:604:ALA:HB3 | 1:A:612:GLU:HG2 | 1.86 | 0.57 |
| 2:G:517:HIS:C | 2:G:517:HIS:CD2 | 2.78 | 0.57 |
| 2:G:741:HIS:HE1 | 2:G:845:THR:HG22 | 1.58 | 0.57 |
| 2:G:1778:GLN:HB3 | 2:G:1831:VAL:HG13 | 1.85 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:988:ILE:HA | 1:A:1048:GLU:HG2 | 1.84 | 0.57 |
| 1:A:655:LEU:CD2 | 1:A:916:LEU:HD11 | 2.35 | 0.57 |
| 2:H:561:TRP:CD1 | 2:H:754:TYR:HE2 | 2.22 | 0.57 |
| 2:H:61:VAL:HG21 | 2:H:95:TYR:HE1 | 1.69 | 0.57 |
| 2:G:1775:GLN:HG2 | 2:G:1836:MET:SD | 2.44 | 0.57 |
| 2:I:665:LEU:O | 2:I:669:LEU:HB2 | 2.05 | 0.57 |
| 2:G:1890:ASN:HB2 | 2:G:1899:VAL:HB | 1.86 | 0.57 |
| 2:H:166:THR:HG22 | 2:H:168:ASP:N | 2.19 | 0.57 |
| 2:I:273:HIS:HB3 | 2:I:512:LEU:HD22 | 1.87 | 0.57 |
| 1:A:1474:ALA:O | 1:A:1478:PRO:HD2 | 2.04 | 0.57 |
| 2:G:703:LEU:HD21 | 2:G:705:LEU:HD21 | 1.86 | 0.57 |
| 2:H:2029:VAL:O | 2:H:2033:THR:HG22 | 2.05 | 0.57 |
| 2:H:1100:VAL:HG21 | 2:H:1147:ILE:CD1 | 2.34 | 0.57 |
| 2:H:732:TRP:CD2 | 2:H:750:MET:CE | 2.87 | 0.57 |
| 2:G:1266:TYR:CG | 2:G:1347:LEU:HD23 | 2.40 | 0.57 |
| 2:I:353:VAL:HG23 | 2:I:357:ASN:HD22 | 1.69 | 0.57 |
| 1:B:440:MET:HE3 | 1:B:483:VAL:HG21 | 1.87 | 0.57 |
| 1:A:1285:ALA:O | 1:A:1289:MET:HG3 | 2.04 | 0.57 |
| 2:I:1292:ILE:O | 2:I:1368:VAL:O | 2.23 | 0.57 |
| 1:A:680:ILE:HG13 | 1:A:769:ILE:HB | 1.87 | 0.57 |
| 2:H:1123:ASP:OD1 | 2:H:1123:ASP:N | 2.36 | 0.57 |
| 2:H:1575:LEU:HD13 | 2:H:1579:ILE:HD12 | 1.85 | 0.57 |
| 1:B:140:ILE:HD13 | 1:B:255:GLY:O | 2.05 | 0.57 |
| 2:H:127:ILE:O | 2:H:131:ILE:HG13 | 2.04 | 0.57 |
| 2:I:1199:GLU:OE2 | 2:I:1567:ARG:NH1 | 2.37 | 0.57 |
| 2:H:1589:VAL:HG11 | 2:H:1640:PHE:CE1 | 2.39 | 0.57 |
| 2:G:667:LYS:HB2 | 2:G:698:LEU:HD23 | 1.85 | 0.57 |
| 1:C:1474:ALA:O | 1:C:1478:PRO:HD2 | 2.04 | 0.57 |
| 2:H:777:THR:CG2 | 2:H:1081:HIS:CE1 | 2.88 | 0.57 |
| 2:I:777:THR:CG2 | 2:I:1081:HIS:CE1 | 2.88 | 0.57 |
| 2:G:455:ILE:HG13 | 2:G:469:ARG:HD3 | 1.86 | 0.57 |
| 2:G:1168:ASN:ND2 | 2:G:1171:ARG:HB2 | 2.20 | 0.57 |
| 2:G:584:SER:HA | 2:G:587:ILE:HG23 | 1.87 | 0.57 |
| 1:A:415:SER:O | 1:A:419:GLU:HB2 | 2.05 | 0.57 |
| 2:I:807:ILE:CG2 | 2:I:1066:ILE:HA | 2.35 | 0.57 |
| 2:G:89:THR:O | 2:G:93:ASN:HB2 | 2.05 | 0.57 |
| 2:G:1547:PRO:HD3 | 2:G:1584:PHE:CE2 | 2.40 | 0.57 |
| 1:A:80:CYS:SG | 1:A:82:SER:HB3 | 2.45 | 0.57 |
| 2:G:463:PHE:HD1 | 2:G:486:LEU:HD13 | 1.70 | 0.57 |
| 2:I:463:PHE:HD1 | 2:I:486:LEU:HD13 | 1.70 | 0.57 |
| 2:I:2029:VAL:O | 2:I:2033:THR:HG22 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1871:LEU:HD22 | 2:H:1888:ILE:HD11 | 1.85 | 0.57 |
| 2:I:607:VAL:HA | 2:I:617:ILE:HD13 | 1.86 | 0.57 |
| 1:B:529:MET:HE3 | 1:B:529:MET:CA | 2.31 | 0.57 |
| 2:H:565:TYR:OH | 2:H:758:ARG:HD2 | 2.04 | 0.57 |
| 2:G:1675:GLY:O | 2:G:1678:MET:HB2 | 2.05 | 0.57 |
| 1:B:742:LYS:HD3 | 1:B:746:GLU:OE2 | 2.05 | 0.57 |
| 2:H:1266:TYR:CG | 2:H:1347:LEU:HD23 | 2.40 | 0.57 |
| 1:B:1431:GLU:HB3 | 1:B:1520:ALA:HB2 | 1.86 | 0.57 |
| 1:C:341:GLN:O | 1:C:345:VAL:HG12 | 2.05 | 0.57 |
| 2:I:1210:ILE:HB | 2:I:1222:GLU:HB3 | 1.85 | 0.57 |
| 2:H:1976:PHE:HA | 2:H:1981:LEU:HD22 | 1.86 | 0.57 |
| 2:I:1231:GLY:O | 2:I:1233:PRO:HD3 | 2.05 | 0.57 |
| 2:H:740:HIS:CE1 | 2:H:852:GLU:OE1 | 2.58 | 0.56 |
| 2:H:56:THR:HG23 | 2:H:59:GLU:CG | 2.32 | 0.56 |
| 1:B:152:HIS:HD2 | 1:B:163:LEU:HB2 | 1.66 | 0.56 |
| 1:B:251:GLN:HA | 1:B:256:LEU:H | 1.70 | 0.56 |
| 1:C:893:VAL:HG11 | 1:C:930:LEU:HD23 | 1.87 | 0.56 |
| 1:B:964:GLU:HG2 | 2:H:1515:PRO:HB3 | 1.86 | 0.56 |
| 1:A:742:LYS:HD3 | 1:A:746:GLU:OE2 | 2.05 | 0.56 |
| 2:I:120:LYS:O | 2:I:124:LYS:HG3 | 2.05 | 0.56 |
| 2:H:517:HIS:CD2 | 2:H:517:HIS:C | 2.78 | 0.56 |
| 2:G:653:TYR:CD1 | 2:G:659:LEU:HD21 | 2.39 | 0.56 |
| 2:H:653:TYR:CD1 | 2:H:659:LEU:HD21 | 2.40 | 0.56 |
| 1:A:263:GLY:O | 1:A:267:VAL:HG23 | 2.05 | 0.56 |
| 2:G:1868:GLN:HG3 | 2:G:1898:TYR:OH | 2.04 | 0.56 |
| 1:B:1524:GLY:O | 1:B:1528:THR:HG23 | 2.05 | 0.56 |
| 2:I:2030:TYR:CE1 | 2:I:2034:GLY:HA2 | 2.39 | 0.56 |
| 2:G:28:PHE:HZ | 2:H:7:ARG:NE | 2.02 | 0.56 |
| 1:C:20:TYR:HE1 | 2:I:2035:SER:HB2 | 1.69 | 0.56 |
| 2:I:741:HIS:HB3 | 2:I:853:PRO:HB2 | 1.86 | 0.56 |
| 2:H:638:VAL:HA | 2:H:641:ILE:HG22 | 1.86 | 0.56 |
| 2:G:1567:ARG:HG3 | 2:G:1568:HIS:N | 2.20 | 0.56 |
| 2:H:839:PRO:HA | 2:H:844:VAL:HG13 | 1.86 | 0.56 |
| 2:H:1352:HIS:HE1 | 2:H:1583:MET:HE1 | 1.69 | 0.56 |
| 1:A:419:GLU:HG2 | 1:A:424:VAL:HB | 1.86 | 0.56 |
| 1:C:1524:GLY:O | 1:C:1528:THR:HG23 | 2.05 | 0.56 |
| 1:C:626:VAL:HG23 | 1:C:664:GLU:OE2 | 2.05 | 0.56 |
| 1:C:1538:VAL:HB | 1:C:1639:VAL:HG22 | 1.86 | 0.56 |
| 2:H:926:LEU:HD13 | 2:H:947:THR:HG22 | 1.86 | 0.56 |
| 2:I:281:VAL:HG23 | 2:I:459:VAL:HG11 | 1.87 | 0.56 |
| 2:I:197:GLU:OE1 | 2:I:197:GLU:HA | 2.05 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:89:THR:O | 2:I:93:ASN:HB2 | 2.05 | 0.56 |
| 2:I:1223:MET:HE3 | 2:I:1238:LEU:HD12 | 1.87 | 0.56 |
| 2:G:1804:PHE:CZ | 2:G:2010:TYR:HB2 | 2.40 | 0.56 |
| 1:C:1326:ILE:HG12 | 1:C:1388:MET:HG3 | 1.86 | 0.56 |
| 2:G:654:VAL:HG23 | 2:G:683:ALA:HB1 | 1.87 | 0.56 |
| 2:I:490:TRP:CH2 | 2:I:512:LEU:HD21 | 2.40 | 0.56 |
| 2:H:702:TYR:CB | 2:H:727:PRO:HB2 | 2.36 | 0.56 |
| 1:A:1014:ASP:N | 1:A:1510:ASN:HD21 | 1.92 | 0.56 |
| 2:G:1989:LYS:O | 2:G:1993:LYS:HG3 | 2.05 | 0.56 |
| 1:B:152:HIS:CE1 | 1:B:168:MET:HG3 | 2.40 | 0.56 |
| 2:I:443:LEU:HD22 | 2:I:448:VAL:HG11 | 1.87 | 0.56 |
| 2:I:1149:TRP:CD1 | 2:I:1213:LEU:CD1 | 2.88 | 0.56 |
| 2:I:543:PHE:CB | 2:I:545:GLN:HE22 | 2.17 | 0.56 |
| 2:H:522:GLY:HA3 | 2:H:561:TRP:CZ3 | 2.40 | 0.56 |
| 2:H:561:TRP:O | 2:H:562:LEU:C | 2.42 | 0.56 |
| 2:G:1194:VAL:HG12 | 2:G:1194:VAL:O | 2.05 | 0.56 |
| 2:G:663:ILE:HG13 | 2:G:694:TYR:HE1 | 1.70 | 0.56 |
| 2:G:1086:LEU:HD12 | 2:G:1090:TYR:CB | 2.35 | 0.56 |
| 2:I:481:ASP:OD2 | 2:I:485:ARG:NH1 | 2.38 | 0.56 |
| 2:H:1834:ARG:NH1 | 2:H:1834:ARG:CG | 2.60 | 0.56 |
| 2:H:835:THR:HG22 | 2:H:844:VAL:C | 2.26 | 0.56 |
| 2:H:1223:MET:CE | 2:H:1238:LEU:HD12 | 2.35 | 0.56 |
| 2:G:813:THR:HB | 2:G:818:LYS:HE3 | 1.87 | 0.56 |
| 1:B:488:PRO:HG3 | 1:B:728:LYS:HG3 | 1.87 | 0.56 |
| 2:I:1804:PHE:CZ | 2:I:2010:TYR:HB2 | 2.40 | 0.56 |
| 2:H:376:ASN:HD22 | 2:H:377:LEU:N | 2.03 | 0.56 |
| 2:I:1722:GLY:N | 2:I:1726:GLY:HA3 | 2.21 | 0.56 |
| 1:C:635:ILE:HG22 | 1:C:651:TYR:CD1 | 2.41 | 0.56 |
| 2:G:1834:ARG:HH11 | 2:G:1834:ARG:CG | 2.03 | 0.56 |
| 2:G:758:ARG:NH2 | 2:G:797:ASP:OD1 | 2.33 | 0.56 |
| 1:C:152:HIS:HD2 | 1:C:163:LEU:HB2 | 1.63 | 0.56 |
| 2:G:543:PHE:CB | 2:G:545:GLN:HE22 | 2.17 | 0.56 |
| 1:A:21:GLN:O | 2:G:1977:HIS:CD2 | 2.59 | 0.56 |
| 1:B:411:GLN:HE22 | 1:B:1628:SER:H | 1.52 | 0.56 |
| 2:H:120:LYS:O | 2:H:124:LYS:HG3 | 2.06 | 0.56 |
| 1:A:1009:LEU:HA | 1:A:1445:MET:HE2 | 1.87 | 0.56 |
| 2:H:606:PHE:HZ | 2:H:805:VAL:HG11 | 1.68 | 0.56 |
| 2:H:1920:GLN:HG2 | 2:H:1922:ILE:HD11 | 1.87 | 0.56 |
| 1:A:1057:MET:SD | 1:A:1097:ILE:HG23 | 2.45 | 0.56 |
| 1:B:1419:PRO:HB3 | 1:B:1646:PHE:CZ | 2.40 | 0.56 |
| 1:C:741:SER:HB3 | 1:C:744:ASP:HB2 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:221:LEU:O | 1:A:225:SER:HB3 | 2.05 | 0.56 |
| 1:C:1022:THR:HG22 | 1:C:1226:SER:HB2 | 1.87 | 0.56 |
| 2:I:835:THR:HG23 | 2:I:843:ILE:O | 2.05 | 0.56 |
| 2:I:1567:ARG:HH12 | 2:I:1568:HIS:HB3 | 1.71 | 0.56 |
| 2:H:443:LEU:HD22 | 2:H:448:VAL:HG11 | 1.86 | 0.56 |
| 2:G:634:ILE:HD11 | 2:G:649:ILE:CD1 | 2.34 | 0.56 |
| 1:C:695:GLY:HA3 | 1:C:906:LEU:HD11 | 1.88 | 0.56 |
| 1:B:1009:LEU:HG | 1:B:1664:ALA:HB2 | 1.87 | 0.56 |
| 2:H:463:PHE:HD1 | 2:H:486:LEU:HD13 | 1.71 | 0.56 |
| 2:H:1890:ASN:HB2 | 2:H:1899:VAL:HB | 1.88 | 0.56 |
| 2:G:1722:GLY:N | 2:G:1726:GLY:HA3 | 2.21 | 0.56 |
| 2:I:601:THR:HG22 | 2:I:620:ALA:H | 1.71 | 0.56 |
| 2:G:599:PRO:HD2 | 4:G:3051:FMN:H6 | 1.88 | 0.56 |
| 2:I:702:TYR:CB | 2:I:727:PRO:HB2 | 2.36 | 0.56 |
| 2:H:607:VAL:HA | 2:H:617:ILE:HD13 | 1.88 | 0.56 |
| 1:A:152:HIS:CE1 | 1:A:168:MET:HG3 | 2.41 | 0.56 |
| 2:I:774:ALA:HB1 | 2:I:1081:HIS:CD2 | 2.33 | 0.56 |
| 2:G:589:ARG:HB3 | 2:G:590:PRO:HD2 | 1.87 | 0.56 |
| 2:I:732:TRP:CG | 2:I:750:MET:HE3 | 2.39 | 0.56 |
| 1:A:251:GLN:HA | 1:A:256:LEU:H | 1.68 | 0.56 |
| 1:B:644:THR:HG22 | 1:B:648:ASP:O | 2.06 | 0.56 |
| 1:B:1492:GLU:O | 1:B:1496:GLU:HG3 | 2.06 | 0.56 |
| 1:A:1036:ARG:NH1 | 1:A:1040:GLU:OE1 | 2.39 | 0.56 |
| 2:H:1868:GLN:HG3 | 2:H:1898:TYR:OH | 2.05 | 0.56 |
| 1:B:1138:LYS:HG3 | 1:B:1163:TYR:CE1 | 2.41 | 0.56 |
| 2:I:871:THR:HB | 2:I:872:ILE:HD12 | 1.88 | 0.56 |
| 2:G:577:ILE:HD13 | 2:G:1097:ILE:CD1 | 2.35 | 0.56 |
| 2:H:1989:LYS:O | 2:H:1993:LYS:HG3 | 2.06 | 0.56 |
| 2:G:1567:ARG:HH12 | 2:G:1568:HIS:HB3 | 1.71 | 0.56 |
| 2:G:702:TYR:CB | 2:G:727:PRO:HB2 | 2.35 | 0.56 |
| 1:B:529:MET:HG2 | 1:B:638:LEU:CD1 | 2.35 | 0.56 |
| 2:I:1931:LEU:HD22 | 2:I:1935:GLU:HG2 | 1.86 | 0.56 |
| 1:C:329:GLU:O | 1:C:333:LYS:HG3 | 2.06 | 0.56 |
| 2:H:1194:VAL:O | 2:H:1194:VAL:HG12 | 2.05 | 0.56 |
| 1:C:881:ASN:HA | 1:C:944:ARG:HH21 | 1.70 | 0.56 |
| 2:H:1100:VAL:HG21 | 2:H:1147:ILE:HD13 | 1.88 | 0.56 |
| 1:C:1259:GLY:HA2 | 1:C:1263:ASP:HB2 | 1.87 | 0.56 |
| 1:C:531:LEU:HD21 | 1:C:629:THR:HG22 | 1.88 | 0.56 |
| 2:H:553:ASN:O | 2:H:556:LYS:HE3 | 2.06 | 0.56 |
| 2:G:1130:THR:H | 2:G:1133:THR:HG23 | 1.70 | 0.56 |
| 2:H:1778:GLN:HB3 | 2:H:1831:VAL:HG13 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1749:THR:CA | 1:C:1874:ASP:HB3 | 2.32 | 0.56 |
| 2:G:1874:VAL:O | 2:G:1878:VAL:HG12 | 2.05 | 0.56 |
| 2:I:1589:VAL:HG11 | 2:I:1640:PHE:CE1 | 2.41 | 0.56 |
| 1:A:1665:ILE:CG1 | 1:A:1669:ARG:HD3 | 2.36 | 0.56 |
| 1:A:1498:GLU:CB | 1:A:1876:LEU:HD13 | 1.83 | 0.56 |
| 2:G:120:LYS:O | 2:G:124:LYS:HG3 | 2.05 | 0.56 |
| 2:I:732:TRP:CD1 | 2:I:750:MET:HE3 | 2.40 | 0.56 |
| 2:I:826:GLY:HA2 | 2:I:1060:ALA:HB3 | 1.88 | 0.56 |
| 1:A:1052:GLU:O | 1:A:1056:ILE:HG23 | 2.06 | 0.56 |
| 2:H:1328:VAL:HG23 | 2:H:1557:SER:HA | 1.88 | 0.56 |
| 1:C:1419:PRO:HB3 | 1:C:1646:PHE:CZ | 2.41 | 0.56 |
| 2:I:577:ILE:HD13 | 2:I:1097:ILE:CD1 | 2.36 | 0.56 |
| 2:G:1308:CYS:HB3 | 2:G:1311:PHE:CD2 | 2.41 | 0.56 |
| 2:H:1308:CYS:HB3 | 2:H:1311:PHE:CD2 | 2.41 | 0.56 |
| 1:A:295:ALA:HB2 | 1:A:302:LEU:HD11 | 1.87 | 0.55 |
| 2:I:7:ARG:NH1 | 2:I:24:THR:HA | 2.20 | 0.55 |
| 1:B:11:HIS:O | 1:B:15:THR:HG22 | 2.06 | 0.55 |
| 2:H:239:PRO:HG3 | 2:H:304:PHE:HA | 1.88 | 0.55 |
| 2:G:732:TRP:CD2 | 2:G:750:MET:HE1 | 2.41 | 0.55 |
| 2:I:653:TYR:CD1 | 2:I:659:LEU:HD21 | 2.40 | 0.55 |
| 2:G:1475:LYS:HG3 | 2:G:1481:SER:HB2 | 1.88 | 0.55 |
| 1:C:1496:GLU:O | 1:C:1500:GLN:HG3 | 2.06 | 0.55 |
| 1:A:1524:GLY:HA2 | 1:A:1527:ALA:HB3 | 1.89 | 0.55 |
| 2:G:1561:ASN:OD1 | 2:G:1563:ILE:HB | 2.05 | 0.55 |
| 1:C:29:ILE:HG13 | 2:I:1891:TYR:O | 2.06 | 0.55 |
| 2:H:1493:LEU:HD11 | 2:H:1499:VAL:CG2 | 2.36 | 0.55 |
| 2:I:1308:CYS:HB3 | 2:I:1311:PHE:CD2 | 2.40 | 0.55 |
| 1:B:1233:GLU:OE2 | 1:B:1680:ARG:NH2 | 2.40 | 0.55 |
| 2:H:16:LEU:HG | 2:H:48:PHE:CZ | 2.40 | 0.55 |
| 2:H:7:ARG:NH1 | 2:H:24:THR:HA | 2.21 | 0.55 |
| 2:G:652:ILE:HB | 2:G:658:MET:CE | 2.36 | 0.55 |
| 2:I:1931:LEU:HB3 | 2:I:1935:GLU:CG | 2.35 | 0.55 |
| 1:C:335:HIS:HD2 | 1:C:335:HIS:O | 1.89 | 0.55 |
| 2:I:232:LEU:HD23 | 2:I:232:LEU:O | 2.06 | 0.55 |
| 1:A:864:VAL:CG2 | 1:A:921:PRO:HB3 | 2.36 | 0.55 |
| 1:B:733:ILE:HD12 | 1:B:761:LEU:HD21 | 1.88 | 0.55 |
| 1:B:1538:VAL:HB | 1:B:1639:VAL:HG22 | 1.87 | 0.55 |
| 1:A:1114:TYR:CD1 | 1:A:1337:GLU:HG3 | 2.41 | 0.55 |
| 1:A:1555:ALA:HA | 1:A:1621:PHE:CE1 | 2.41 | 0.55 |
| 1:B:988:ILE:HD13 | 1:B:1048:GLU:HB3 | 1.89 | 0.55 |
| 2:H:490:TRP:HA | 2:H:493:THR:CG2 | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:12:ILE:HA | 1:C:15:THR:HG23 | 1.88 | 0.55 |
| 2:G:2036:GLU:O | 2:G:2039:LYS:HG2 | 2.06 | 0.55 |
| 2:G:1931:LEU:HB3 | 2:G:1935:GLU:CG | 2.33 | 0.55 |
| 2:I:634:ILE:HD11 | 2:I:649:ILE:CD1 | 2.35 | 0.55 |
| 1:A:1665:ILE:HD11 | 1:A:1669:ARG:HG2 | 1.88 | 0.55 |
| 1:B:1665:ILE:HD11 | 1:B:1669:ARG:HG2 | 1.88 | 0.55 |
| 2:I:124:LYS:HG2 | 2:I:179:THR:HA | 1.87 | 0.55 |
| 2:G:722:ALA:HB1 | 2:G:723:HIS:CE1 | 2.42 | 0.55 |
| 1:C:417:TYR:OH | 1:C:458:THR:HG22 | 2.06 | 0.55 |
| 2:H:1822:MET:HE2 | 2:H:1996:ILE:HG12 | 1.89 | 0.55 |
| 1:B:433:VAL:O | 1:B:437:ILE:HG13 | 2.07 | 0.55 |
| 2:G:1678:MET:CE | 2:G:1707:LEU:HD22 | 2.35 | 0.55 |
| 1:C:1:MET:HE3 | 1:C:9:LEU:HD12 | 1.89 | 0.55 |
| 1:B:1036:ARG:NH1 | 1:B:1040:GLU:OE1 | 2.40 | 0.55 |
| 2:G:665:LEU:O | 2:G:669:LEU:HB2 | 2.06 | 0.55 |
| 1:A:825:PRO:HB2 | 1:A:843:LYS:NZ | 2.21 | 0.55 |
| 1:C:1347:LYS:O | 1:C:1347:LYS:HD3 | 2.05 | 0.55 |
| 2:H:1431:TYR:CE1 | 2:H:1526:THR:HG23 | 2.41 | 0.55 |
| 1:C:1498:GLU:CG | 1:C:1876:LEU:CB | 2.64 | 0.55 |
| 1:C:807:LYS:HG3 | 1:C:858:TRP:HB3 | 1.87 | 0.55 |
| 1:C:254:TRP:CZ3 | 1:C:302:LEU:HD13 | 2.41 | 0.55 |
| 2:I:638:VAL:HA | 2:I:641:ILE:HG22 | 1.88 | 0.55 |
| 2:H:2038:ILE:HG22 | 2:H:2042:ILE:CD1 | 2.36 | 0.55 |
| 1:C:27:ARG:HD2 | 1:C:30:GLU:OE2 | 2.06 | 0.55 |
| 2:I:926:LEU:HB3 | 2:I:947:THR:HG22 | 1.88 | 0.55 |
| 2:G:1475:LYS:HB2 | 2:G:1481:SER:HB2 | 1.89 | 0.55 |
| 2:I:61:VAL:HG21 | 2:I:95:TYR:HE1 | 1.72 | 0.55 |
| 2:I:166:THR:HG22 | 2:I:168:ASP:N | 2.21 | 0.55 |
| 2:H:1166:VAL:HG12 | 2:H:1167:SER:N | 2.21 | 0.55 |
| 1:C:11:HIS:O | 1:C:15:THR:HG22 | 2.06 | 0.55 |
| 1:C:152:HIS:CE1 | 1:C:168:MET:HG3 | 2.41 | 0.55 |
| 2:G:1496:LYS:HE2 | 2:G:1693:ARG:NH2 | 2.20 | 0.55 |
| 2:I:2015:THR:HG22 | 2:I:2017:LYS:N | 2.21 | 0.55 |
| 1:A:1498:GLU:CB | 1:A:1876:LEU:CD1 | 2.63 | 0.55 |
| 1:A:1238:VAL:HG12 | 1:A:1239:HIS:N | 2.21 | 0.55 |
| 2:H:807:ILE:CG2 | 2:H:1066:ILE:HA | 2.36 | 0.55 |
| 2:H:1359:MET:HE3 | 2:H:1359:MET:HA | 1.88 | 0.55 |
| 1:C:1125:VAL:HG21 | 1:C:1175:ILE:HD12 | 1.88 | 0.55 |
| 2:G:197:GLU:OE1 | 2:G:197:GLU:HA | 2.06 | 0.55 |
| 1:C:383:GLY:O | 1:C:387:VAL:HG23 | 2.07 | 0.55 |
| 1:A:12:ILE:HD11 | 2:G:2041:ILE:HD11 | 1.83 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:603:SER:O | 2:I:607:VAL:HG12 | 2.06 | 0.55 |
| 2:H:707:PRO:HG2 | 2:H:730:LEU:HD13 | 1.89 | 0.55 |
| 1:A:529:MET:HG2 | 1:A:638:LEU:CD1 | 2.36 | 0.55 |
| 1:A:1473:GLU:O | 1:A:1478:PRO:HD3 | 2.06 | 0.55 |
| 1:B:328:LEU:C | 1:B:328:LEU:HD22 | 2.28 | 0.55 |
| 1:A:332:THR:HG22 | 1:B:331:ILE:CD1 | 2.36 | 0.55 |
| 2:H:584:SER:HA | 2:H:587:ILE:HG23 | 1.89 | 0.55 |
| 2:G:239:PRO:HG3 | 2:G:304:PHE:HA | 1.88 | 0.55 |
| 1:A:1056:ILE:HD13 | 1:A:1193:TRP:CD1 | 2.42 | 0.55 |
| 1:A:771:PHE:CD1 | 1:A:825:PRO:HG3 | 2.42 | 0.55 |
| 2:I:1432:GLN:HB2 | 2:I:1527:LEU:HD12 | 1.88 | 0.55 |
| 1:B:1285:ALA:O | 1:B:1289:MET:HG3 | 2.07 | 0.55 |
| 1:A:1233:GLU:OE2 | 1:A:1680:ARG:NH2 | 2.40 | 0.55 |
| 2:I:1873:TYR:HE1 | 2:I:1877:ARG:HH21 | 1.54 | 0.55 |
| 1:C:883:ILE:HD12 | 1:C:947:LEU:HD12 | 1.88 | 0.55 |
| 1:B:1432:HIS:CE1 | 1:B:1434:SER:OG | 2.60 | 0.55 |
| 2:H:740:HIS:HA | 2:H:854:ILE:HD13 | 1.89 | 0.55 |
| 2:I:741:HIS:CE1 | 2:I:855:HIS:CD2 | 2.95 | 0.55 |
| 2:G:777:THR:CG2 | 2:G:1081:HIS:CE1 | 2.89 | 0.55 |
| 2:H:1173:VAL:CG2 | 2:H:1221:MET:HE1 | 2.35 | 0.55 |
| 2:G:1822:MET:CE | 2:G:1996:ILE:HG12 | 2.37 | 0.55 |
| 1:C:635:ILE:HG22 | 1:C:651:TYR:CG | 2.42 | 0.55 |
| 2:H:1822:MET:CE | 2:H:1996:ILE:HG12 | 2.37 | 0.55 |
| 2:H:264:ARG:NH1 | 2:H:456:GLN:HG3 | 2.22 | 0.55 |
| 2:I:1427:VAL:O | 2:I:1427:VAL:HG12 | 2.07 | 0.55 |
| 2:G:127:ILE:O | 2:G:131:ILE:HG13 | 2.07 | 0.55 |
| 2:H:1567:ARG:NH1 | 2:H:1567:ARG:CG | 2.50 | 0.55 |
| 2:G:1624:THR:HB | 2:G:1642:THR:HG23 | 1.86 | 0.55 |
| 2:G:835:THR:HG23 | 2:G:843:ILE:O | 2.06 | 0.55 |
| 2:H:1844:ARG:CG | 2:H:1844:ARG:NH1 | 2.58 | 0.55 |
| 2:I:1168:ASN:ND2 | 2:I:1171:ARG:HB2 | 2.22 | 0.55 |
| 1:A:982:ILE:HG13 | 2:G:965:SER:N | 2.22 | 0.55 |
| 2:G:747:HIS:O | 2:G:751:LEU:HB2 | 2.07 | 0.55 |
| 2:H:1350:LEU:HD11 | 2:H:1410:PHE:HB3 | 1.89 | 0.55 |
| 2:H:1697:HIS:CE1 | 2:H:1829:GLU:HG2 | 2.42 | 0.55 |
| 1:C:176:VAL:HG12 | 1:C:178:GLY:H | 1.72 | 0.55 |
| 1:C:50:SER:HB2 | 1:C:51:PRO:HD3 | 1.88 | 0.55 |
| 2:I:1010:PRO:O | 2:I:1011:MET:HB2 | 2.05 | 0.55 |
| 2:H:402:LEU:O | 2:H:402:LEU:HD13 | 2.07 | 0.55 |
| 1:A:56:MET:HG3 | 2:G:1893:VAL:CG2 | 2.37 | 0.55 |
| 2:I:1624:THR:HB | 2:I:1642:THR:OG1 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:2036:GLU:O | 2:H:2039:LYS:HG2 | 2.07 | 0.55 |
| 2:I:260:PRO:HD3 | 2:I:289:TRP:CE2 | 2.42 | 0.55 |
| 2:I:1293:THR:HG22 | 2:I:1296:GLU:CD | 2.28 | 0.55 |
| 1:C:1455:ARG:NH2 | 1:C:1459:ILE:HG12 | 2.22 | 0.55 |
| 2:H:1475:LYS:HB2 | 2:H:1481:SER:HB2 | 1.88 | 0.55 |
| 1:B:49:PRO:O | 1:B:82:SER:HB2 | 2.07 | 0.55 |
| 1:C:1009:LEU:HD13 | 1:C:1445:MET:HE1 | 1.89 | 0.55 |
| 1:A:1392:LEU:HD22 | 1:A:1396:MET:HG3 | 1.89 | 0.55 |
| 1:B:1566:ARG:HB3 | 1:B:1623:TYR:CE1 | 2.42 | 0.55 |
| 1:B:1123:GLN:HG3 | 1:B:1124:GLU:N | 2.22 | 0.55 |
| 2:G:264:ARG:NH1 | 2:G:456:GLN:HG3 | 2.22 | 0.55 |
| 1:C:1501:LEU:O | 1:C:1505:GLN:HG3 | 2.07 | 0.54 |
| 2:G:598:THR:HG23 | 4:G:3051:FMN:O4 | 2.06 | 0.54 |
| 2:G:1227:ARG:CG | 2:G:1227:ARG:NH1 | 2.56 | 0.54 |
| 2:G:1313:SER:O | 2:G:1314:ARG:HD3 | 2.07 | 0.54 |
| 2:H:1159:ILE:HG12 | 2:H:1169:PRO:CD | 2.36 | 0.54 |
| 1:B:1373:ARG:HB2 | 1:B:1545:SER:O | 2.07 | 0.54 |
| 1:C:1:MET:HE3 | 1:C:5:VAL:HG12 | 1.88 | 0.54 |
| 1:A:1194:ASN:HB3 | 1:A:1197:THR:HG22 | 1.88 | 0.54 |
| 2:I:1493:LEU:HD11 | 2:I:1499:VAL:CG2 | 2.37 | 0.54 |
| 2:G:1859:PRO:CG | 2:G:1871:LEU:HD12 | 2.20 | 0.54 |
| 2:I:145:LEU:HD21 | 2:I:156:LEU:HD21 | 1.89 | 0.54 |
| 2:I:131:ILE:HD12 | 2:I:182:VAL:CB | 2.33 | 0.54 |
| 2:H:1293:THR:HG22 | 2:H:1296:GLU:CD | 2.28 | 0.54 |
| 1:A:733:ILE:CD1 | 1:A:761:LEU:HD11 | 2.37 | 0.54 |
| 2:I:1331:TRP:CE2 | 2:I:1335:ILE:HG13 | 2.42 | 0.54 |
| 1:C:1373:ARG:HB2 | 1:C:1545:SER:O | 2.07 | 0.54 |
| 1:A:1455:ARG:NH2 | 1:A:1459:ILE:HG12 | 2.22 | 0.54 |
| 1:A:236:LYS:HE2 | 1:A:273:PRO:O | 2.07 | 0.54 |
| 2:G:464:ASP:HB3 | 2:G:466:SER:HB3 | 1.88 | 0.54 |
| 1:B:263:GLY:O | 1:B:267:VAL:HG23 | 2.07 | 0.54 |
| 2:H:1976:PHE:HB3 | 2:H:1981:LEU:HD21 | 1.89 | 0.54 |
| 1:A:741:SER:HB3 | 1:A:744:ASP:HB2 | 1.89 | 0.54 |
| 1:B:771:PHE:CD1 | 1:B:825:PRO:HG3 | 2.42 | 0.54 |
| 1:C:286:PHE:O | 1:C:290:MET:HG2 | 2.07 | 0.54 |
| 2:I:606:PHE:HZ | 2:I:805:VAL:HG11 | 1.71 | 0.54 |
| 2:I:1567:ARG:CG | 2:I:1567:ARG:NH1 | 2.50 | 0.54 |
| 2:H:2015:THR:HG22 | 2:H:2017:LYS:N | 2.21 | 0.54 |
| 2:H:732:TRP:CD2 | 2:H:750:MET:HE3 | 2.43 | 0.54 |
| 2:G:462:THR:HB | 2:G:482:CYS:SG | 2.48 | 0.54 |
| 2:G:332:GLU:OE2 | 2:G:394:ARG:HD3 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1497:GLU:OE1 | 2:H:2002:LYS:HE3 | 2.07 | 0.54 |
| 1:A:430:ARG:NH2 | 1:A:605:LEU:HD13 | 2.23 | 0.54 |
| 2:G:1292:ILE:O | 2:G:1368:VAL:O | 2.25 | 0.54 |
| 2:I:517:HIS:CD2 | 2:I:517:HIS:C | 2.80 | 0.54 |
| 2:H:490:TRP:HE1 | 2:H:516:THR:CG2 | 2.01 | 0.54 |
| 2:I:490:TRP:HA | 2:I:493:THR:CG2 | 2.38 | 0.54 |
| 2:H:611:THR:CG2 | 2:H:641:ILE:HG13 | 2.38 | 0.54 |
| 1:A:20:TYR:CD1 | 2:G:2033:THR:HG21 | 2.42 | 0.54 |
| 2:H:1102:TYR:HB3 | 2:H:1244:PRO:HA | 1.90 | 0.54 |
| 1:A:733:ILE:HD12 | 1:A:761:LEU:HD21 | 1.89 | 0.54 |
| 1:A:1475:GLU:HG2 | 1:A:1761:LYS:O | 2.06 | 0.54 |
| 2:I:1166:VAL:HG12 | 2:I:1167:SER:N | 2.23 | 0.54 |
| 1:A:1748:ASN:C | 1:A:1750:ILE:H | 2.11 | 0.54 |
| 2:I:1093:ASP:HB3 | 2:I:1096:LYS:HG3 | 1.89 | 0.54 |
| 1:B:1749:THR:CB | 1:B:1874:ASP:HA | 2.33 | 0.54 |
| 1:A:1501:LEU:CD1 | 1:A:1775:LEU:CG | 2.86 | 0.54 |
| 1:B:1501:LEU:O | 1:B:1505:GLN:HG3 | 2.08 | 0.54 |
| 2:H:85:ASN:HD22 | 2:H:135:ARG:NH1 | 2.02 | 0.54 |
| 2:I:584:SER:HA | 2:I:587:ILE:HG23 | 1.89 | 0.54 |
| 1:A:183:GLN:O | 1:A:187:LEU:HG | 2.08 | 0.54 |
| 2:I:1475:LYS:HB2 | 2:I:1481:SER:HB2 | 1.89 | 0.54 |
| 1:C:479:ASN:O | 1:C:483:VAL:HG23 | 2.07 | 0.54 |
| 1:B:1401:TYR:C | 1:B:1658:PRO:HG3 | 2.27 | 0.54 |
| 1:A:1657:HIS:ND1 | 1:A:1658:PRO:HD2 | 2.21 | 0.54 |
| 2:I:2046:GLU:C | 2:I:2048:TYR:H | 2.11 | 0.54 |
| 2:I:1547:PRO:HD3 | 2:I:1584:PHE:CE2 | 2.43 | 0.54 |
| 2:G:1575:LEU:HD13 | 2:G:1579:ILE:HD12 | 1.89 | 0.54 |
| 2:G:344:LEU:HB3 | 2:G:349:VAL:HG23 | 1.90 | 0.54 |
| 2:I:611:THR:CG2 | 2:I:641:ILE:HG13 | 2.37 | 0.54 |
| 2:I:652:ILE:HB | 2:I:658:MET:CE | 2.37 | 0.54 |
| 1:A:328:LEU:C | 1:A:328:LEU:HD22 | 2.28 | 0.54 |
| 2:I:123:ILE:HD11 | 2:I:533:LEU:CD2 | 2.37 | 0.54 |
| 2:I:1778:GLN:HB3 | 2:I:1831:VAL:HG13 | 1.88 | 0.54 |
| 1:A:1234:MET:CE | 1:A:1326:ILE:HG21 | 2.38 | 0.54 |
| 1:B:824:LEU:HD11 | 1:B:849:LEU:HD12 | 1.89 | 0.54 |
| 2:H:464:ASP:HB3 | 2:H:466:SER:HB3 | 1.90 | 0.54 |
| 2:G:807:ILE:HG21 | 2:G:1066:ILE:HA | 1.88 | 0.54 |
| 2:G:2030:TYR:CE1 | 2:G:2034:GLY:HA2 | 2.43 | 0.54 |
| 2:H:1547:PRO:HD3 | 2:H:1584:PHE:CE2 | 2.42 | 0.54 |
| 2:G:1697:HIS:CE1 | 2:G:1829:GLU:HG2 | 2.43 | 0.54 |
| 1:B:385:PHE:HD2 | 1:B:787:LYS:HA | 1.73 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1123:GLN:HG3 | 1:C:1124:GLU:N | 2.23 | 0.54 |
| 2:I:1417:THR:O | 2:I:1419:PHE:N | 2.30 | 0.54 |
| 1:B:23:ALA:O | 2:H:1977:HIS:HA | 2.07 | 0.54 |
| 2:G:1749:GLU:OE2 | 2:G:1840:VAL:CG1 | 2.56 | 0.54 |
| 1:A:1184:LEU:HB2 | 1:A:1352:THR:HG21 | 1.89 | 0.54 |
| 2:G:1428:GLU:HB2 | 2:G:1468:THR:HG22 | 1.88 | 0.54 |
| 2:G:601:THR:CG2 | 2:G:618:GLU:O | 2.41 | 0.54 |
| 2:I:722:ALA:HB1 | 2:I:723:HIS:CE1 | 2.42 | 0.54 |
| 2:I:545:GLN:NE2 | 2:I:545:GLN:H | 2.06 | 0.54 |
| 1:B:655:LEU:CD2 | 1:B:916:LEU:HD11 | 2.38 | 0.54 |
| 2:H:964:LEU:N | 2:H:964:LEU:CD2 | 2.70 | 0.54 |
| 2:H:1378:ILE:HD11 | 2:H:1381:VAL:HG21 | 1.90 | 0.54 |
| 2:I:99:ASN:HA | 2:I:550:VAL:HG21 | 1.90 | 0.54 |
| 1:B:236:LYS:HE2 | 1:B:273:PRO:O | 2.07 | 0.54 |
| 1:B:280:GLU:O | 1:B:280:GLU:HG2 | 2.08 | 0.54 |
| 1:C:1748:ASN:C | 1:C:1750:ILE:H | 2.12 | 0.54 |
| 2:I:1452:LEU:HA | 2:I:1502:GLY:HA3 | 1.88 | 0.54 |
| 1:C:1477:ILE:H | 1:C:1478:PRO:CD | 2.20 | 0.54 |
| 2:I:826:GLY:O | 2:I:827:VAL:HG23 | 2.07 | 0.54 |
| 1:B:695:GLY:HA3 | 1:B:906:LEU:HD11 | 1.90 | 0.54 |
| 1:C:37:LYS:HB2 | 1:C:65:TYR:HE1 | 1.72 | 0.54 |
| 1:A:1496:GLU:O | 1:A:1500:GLN:HG3 | 2.07 | 0.54 |
| 1:A:340:ARG:HH12 | 1:A:344:GLN:NE2 | 2.06 | 0.54 |
| 2:I:1054:LEU:CB | 4:I:3051:FMN:C7M | 2.85 | 0.54 |
| 1:C:516:ARG:NH2 | 1:C:889:GLU:OE1 | 2.41 | 0.54 |
| 1:A:644:THR:HG22 | 1:A:648:ASP:O | 2.08 | 0.54 |
| 1:B:1600:LEU:HD13 | 1:B:1657:HIS:HA | 1.90 | 0.54 |
| 1:B:635:ILE:HG22 | 1:B:651:TYR:CG | 2.43 | 0.54 |
| 1:A:625:THR:HG23 | 1:A:661:ASP:OD1 | 2.08 | 0.54 |
| 2:I:1172:LYS:HE3 | 2:I:1574:ASN:OD1 | 2.08 | 0.54 |
| 1:A:1138:LYS:HG3 | 1:A:1163:TYR:CE1 | 2.43 | 0.54 |
| 2:I:332:GLU:OE2 | 2:I:394:ARG:HD3 | 2.08 | 0.54 |
| 2:G:1231:GLY:O | 2:G:1233:PRO:HD3 | 2.08 | 0.54 |
| 2:I:868:PHE:HB3 | 2:I:873:PHE:CE2 | 2.43 | 0.54 |
| 1:C:1682:LYS:HB3 | 2:I:994:PHE:CE2 | 2.43 | 0.54 |
| 2:H:146:PHE:HA | 2:H:149:VAL:HG12 | 1.89 | 0.53 |
| 2:H:1313:SER:O | 2:H:1314:ARG:HD3 | 2.09 | 0.53 |
| 1:C:529:MET:HG2 | 1:C:638:LEU:CD1 | 2.39 | 0.53 |
| 2:I:754:TYR:CD2 | 2:I:794:MET:HG3 | 2.42 | 0.53 |
| 2:H:1325:PHE:CE1 | 2:H:1328:VAL:HG11 | 2.43 | 0.53 |
| 1:C:1194:ASN:HB3 | 1:C:1197:THR:HG22 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1010:GLU:HA | 1:B:1664:ALA:HA | 1.89 | 0.53 |
| 1:A:1125:VAL:HG21 | 1:A:1175:ILE:HD12 | 1.88 | 0.53 |
| 1:B:807:LYS:HG3 | 1:B:858:TRP:HB3 | 1.90 | 0.53 |
| 2:H:1177:SER:O | 2:H:1180:MET:HG2 | 2.08 | 0.53 |
| 2:I:615:TYR:CZ | 2:I:1074:MET:HB3 | 2.42 | 0.53 |
| 1:A:1120:GLU:O | 1:A:1121:MET:CG | 2.56 | 0.53 |
| 2:I:1844:ARG:NH1 | 2:I:1844:ARG:CG | 2.61 | 0.53 |
| 2:G:1331:TRP:CE2 | 2:G:1335:ILE:HG13 | 2.43 | 0.53 |
| 2:I:1954:LYS:HD3 | 2:I:1958:LEU:HD13 | 1.89 | 0.53 |
| 1:C:825:PRO:HB2 | 1:C:843:LYS:NZ | 2.24 | 0.53 |
| 2:H:606:PHE:CE1 | 2:H:811:VAL:HG13 | 2.43 | 0.53 |
| 1:A:1566:ARG:HB3 | 1:A:1623:TYR:CE1 | 2.42 | 0.53 |
| 2:I:491:GLU:HA | 2:I:494:THR:HG22 | 1.89 | 0.53 |
| 2:H:674:TYR:HB3 | 2:H:676:ILE:HG22 | 1.88 | 0.53 |
| 2:I:234:ILE:CG1 | 2:I:235:PRO:HD3 | 2.38 | 0.53 |
| 2:H:826:GLY:O | 2:H:827:VAL:HG23 | 2.07 | 0.53 |
| 1:B:1194:ASN:O | 1:B:1197:THR:HG23 | 2.08 | 0.53 |
| 1:A:1392:LEU:CD2 | 1:A:1396:MET:HG3 | 2.38 | 0.53 |
| 2:I:873:PHE:CD1 | 2:I:1026:GLU:HB2 | 2.43 | 0.53 |
| 1:A:1153:ASP:OD2 | 1:B:359:ARG:NH2 | 2.41 | 0.53 |
| 2:G:1269:LEU:O | 2:G:1560:LEU:HD23 | 2.08 | 0.53 |
| 2:H:281:VAL:HG23 | 2:H:459:VAL:HG11 | 1.90 | 0.53 |
| 2:I:582:LYS:HE2 | 2:I:1108:PRO:HB3 | 1.91 | 0.53 |
| 1:A:1123:GLN:HB2 | 1:A:1177:LYS:HE2 | 1.90 | 0.53 |
| 1:C:236:LYS:HE2 | 1:C:273:PRO:O | 2.08 | 0.53 |
| 2:G:892:ILE:HG12 | 2:G:903:TRP:CG | 2.43 | 0.53 |
| 1:A:807:LYS:HG3 | 1:A:858:TRP:HB3 | 1.91 | 0.53 |
| 2:H:55:THR:CG2 | 2:H:56:THR:HG22 | 2.30 | 0.53 |
| 2:G:741:HIS:CB | 2:G:853:PRO:HB2 | 2.38 | 0.53 |
| 2:G:964:LEU:CD2 | 2:G:964:LEU:N | 2.68 | 0.53 |
| 1:A:1373:ARG:HB2 | 1:A:1545:SER:O | 2.08 | 0.53 |
| 1:C:824:LEU:HD11 | 1:C:849:LEU:HD12 | 1.90 | 0.53 |
| 2:I:271:THR:OG1 | 2:I:460:TYR:HB2 | 2.08 | 0.53 |
| 1:B:1392:LEU:CD2 | 1:B:1396:MET:HG3 | 2.38 | 0.53 |
| 1:C:263:GLY:O | 1:C:267:VAL:HG23 | 2.08 | 0.53 |
| 2:I:1745:LYS:HE2 | 2:I:1747:LYS:HG2 | 1.91 | 0.53 |
| 1:B:1020:VAL:HG13 | 1:B:1400:ILE:HG23 | 1.91 | 0.53 |
| 2:I:1177:SER:O | 2:I:1180:MET:HG2 | 2.09 | 0.53 |
| 2:I:1567:ARG:HG3 | 2:I:1568:HIS:N | 2.22 | 0.53 |
| 2:I:1314:ARG:CG | 2:I:1314:ARG:NH1 | 2.63 | 0.53 |
| 2:G:707:PRO:HG2 | 2:G:730:LEU:HD13 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1102:TYR:HB3 | 2:I:1244:PRO:HA | 1.91 | 0.53 |
| 1:B:1665:ILE:CG1 | 1:B:1669:ARG:HD3 | 2.36 | 0.53 |
| 1:C:985:ARG:HH12 | 2:I:953:ARG:CZ | 2.21 | 0.53 |
| 1:B:751:PHE:CZ | 1:B:761:LEU:HD13 | 2.42 | 0.53 |
| 1:A:421:ILE:HG13 | 1:A:469:VAL:HG21 | 1.89 | 0.53 |
| 1:C:1401:TYR:C | 1:C:1658:PRO:HG3 | 2.29 | 0.53 |
| 2:H:173:LEU:HD13 | 2:H:219:LEU:HD21 | 1.90 | 0.53 |
| 1:C:158:LYS:HD3 | 1:C:185:GLU:HB3 | 1.91 | 0.53 |
| 2:I:1431:TYR:CE1 | 2:I:1526:THR:HG22 | 2.44 | 0.53 |
| 2:I:526:ARG:HH11 | 2:I:558:ASN:HD21 | 1.55 | 0.53 |
| 2:H:816:ASP:HB3 | 2:H:1048:VAL:HG21 | 1.91 | 0.53 |
| 1:B:607:LYS:HG2 | 1:B:608:ASP:N | 2.23 | 0.53 |
| 2:H:1804:PHE:CZ | 2:H:2010:TYR:HB2 | 2.44 | 0.53 |
| 2:I:2036:GLU:HG2 | 2:I:2039:LYS:NZ | 2.23 | 0.53 |
| 2:H:1567:ARG:HG3 | 2:H:1568:HIS:N | 2.23 | 0.53 |
| 2:H:652:ILE:HB | 2:H:658:MET:CE | 2.39 | 0.53 |
| 1:A:529:MET:CE | 1:A:894:ARG:HD2 | 2.38 | 0.53 |
| 2:I:1173:VAL:CG2 | 2:I:1221:MET:HE1 | 2.39 | 0.53 |
| 2:I:1293:THR:HG22 | 2:I:1296:GLU:CG | 2.39 | 0.53 |
| 1:A:1665:ILE:HG12 | 1:A:1666:THR:N | 2.23 | 0.53 |
| 2:G:2015:THR:HG22 | 2:G:2017:LYS:N | 2.22 | 0.53 |
| 1:A:50:SER:HB2 | 1:A:51:PRO:CD | 2.39 | 0.53 |
| 1:C:825:PRO:HB2 | 1:C:843:LYS:HZ2 | 1.73 | 0.53 |
| 1:A:635:ILE:HG22 | 1:A:651:TYR:CG | 2.43 | 0.53 |
| 1:A:1020:VAL:HG13 | 1:A:1400:ILE:HG23 | 1.90 | 0.53 |
| 2:G:913:ASP:H | 2:G:916:THR:CG2 | 2.22 | 0.53 |
| 2:H:774:ALA:HB1 | 2:H:1081:HIS:CD2 | 2.32 | 0.53 |
| 2:I:1327:ILE:HG12 | 2:I:1583:MET:HE3 | 1.91 | 0.53 |
| 2:H:1913:VAL:O | 2:H:1917:ILE:HG13 | 2.08 | 0.53 |
| 1:C:1037:TRP:HB2 | 1:C:1598:GLN:OE1 | 2.09 | 0.53 |
| 1:B:1577:GLN:HE22 | 1:B:1591:TRP:C | 2.12 | 0.53 |
| 1:C:1012:LEU:HD23 | 1:C:1445:MET:CE | 2.39 | 0.53 |
| 2:G:346:GLN:HA | 2:G:377:LEU:HD21 | 1.89 | 0.53 |
| 2:H:402:LEU:HD12 | 2:H:404:GLN:HG2 | 1.90 | 0.53 |
| 1:B:1123:GLN:HB2 | 1:B:1177:LYS:HE2 | 1.91 | 0.53 |
| 1:A:1492:GLU:O | 1:A:1496:GLU:HG3 | 2.09 | 0.53 |
| 2:G:606:PHE:HZ | 2:G:805:VAL:HG11 | 1.74 | 0.53 |
| 2:G:1166:VAL:HG12 | 2:G:1167:SER:N | 2.23 | 0.53 |
| 2:G:490:TRP:CH2 | 2:G:512:LEU:HD21 | 2.43 | 0.53 |
| 2:I:2038:ILE:HG22 | 2:I:2042:ILE:CD1 | 2.37 | 0.53 |
| 2:I:892:ILE:HG12 | 2:I:903:TRP:CG | 2.44 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1014:ASP:H | 1:A:1510:ASN:ND2 | 1.93 | 0.53 |
| 2:I:1441:ILE:HD11 | 2:I:1445:ARG:NH2 | 2.23 | 0.53 |
| 1:B:12:ILE:HA | 1:B:15:THR:HG23 | 1.90 | 0.53 |
| 1:A:483:VAL:O | 1:A:486:VAL:N | 2.42 | 0.53 |
| 2:G:85:ASN:HD22 | 2:G:135:ARG:NH1 | 2.03 | 0.53 |
| 2:G:750:MET:CG | 2:G:796:PHE:HZ | 2.21 | 0.53 |
| 2:H:1954:LYS:HD3 | 2:H:1958:LEU:HD13 | 1.90 | 0.53 |
| 1:C:1524:GLY:HA2 | 1:C:1527:ALA:HB3 | 1.91 | 0.53 |
| 2:H:346:GLN:HA | 2:H:377:LEU:HD21 | 1.91 | 0.53 |
| 2:H:1040:LEU:HD21 | 2:H:1048:VAL:HA | 1.89 | 0.53 |
| 2:H:1452:LEU:HA | 2:H:1502:GLY:HA3 | 1.90 | 0.53 |
| 1:A:385:PHE:HD2 | 1:A:787:LYS:HA | 1.74 | 0.53 |
| 2:I:1040:LEU:HD21 | 2:I:1048:VAL:HA | 1.90 | 0.53 |
| 2:I:1861:ARG:HD2 | 2:I:1964:PHE:O | 2.08 | 0.53 |
| 2:I:2035:SER:HB3 | 2:I:2038:ILE:CG1 | 2.37 | 0.53 |
| 1:A:12:ILE:HA | 1:A:15:THR:HG23 | 1.88 | 0.53 |
| 2:G:2038:ILE:HG22 | 2:G:2042:ILE:CD1 | 2.37 | 0.53 |
| 1:C:1036:ARG:NH1 | 1:C:1040:GLU:OE1 | 2.41 | 0.53 |
| 2:I:1266:TYR:CG | 2:I:1347:LEU:HD23 | 2.43 | 0.53 |
| 1:A:1455:ARG:O | 1:A:1459:ILE:HG13 | 2.08 | 0.53 |
| 2:G:1040:LEU:HD21 | 2:G:1048:VAL:HA | 1.90 | 0.53 |
| 2:I:871:THR:HG21 | 2:I:887:LYS:NZ | 2.24 | 0.53 |
| 2:G:281:VAL:HG23 | 2:G:459:VAL:HG11 | 1.91 | 0.53 |
| 2:H:1745:LYS:HE2 | 2:H:1747:LYS:HG2 | 1.91 | 0.53 |
| 2:I:240:LEU:O | 2:I:244:ILE:HG13 | 2.08 | 0.53 |
| 2:H:455:ILE:HG12 | 2:H:469:ARG:HG2 | 1.91 | 0.53 |
| 2:G:1173:VAL:CG2 | 2:G:1221:MET:HE1 | 2.38 | 0.53 |
| 2:H:234:ILE:CG1 | 2:H:235:PRO:HD3 | 2.39 | 0.53 |
| 2:H:1101:GLU:HB2 | 2:H:1147:ILE:O | 2.09 | 0.53 |
| 2:G:102:HIS:HE1 | 2:G:180:TYR:OH | 1.92 | 0.53 |
| 1:B:1326:ILE:HG12 | 1:B:1388:MET:HG3 | 1.91 | 0.53 |
| 2:H:1697:HIS:HE1 | 2:H:1829:GLU:HG2 | 1.74 | 0.53 |
| 1:C:625:THR:HG23 | 1:C:661:ASP:OD1 | 2.09 | 0.53 |
| 2:I:264:ARG:NH1 | 2:I:456:GLN:HG3 | 2.24 | 0.53 |
| 2:G:1861:ARG:HD2 | 2:G:1964:PHE:O | 2.09 | 0.53 |
| 1:C:1285:ALA:O | 1:C:1289:MET:HG3 | 2.09 | 0.53 |
| 2:G:55:THR:CG2 | 2:G:56:THR:HG22 | 2.33 | 0.52 |
| 1:A:529:MET:HG2 | 1:A:638:LEU:HG | 1.89 | 0.52 |
| 1:B:340:ARG:HH12 | 1:B:344:GLN:NE2 | 2.08 | 0.52 |
| 2:G:1418:ASP:C | 2:G:1420:GLU:N | 2.63 | 0.52 |
| 1:C:864:VAL:CG2 | 1:C:921:PRO:HB3 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1418:ASP:O | 2:H:1419:PHE:C | 2.46 | 0.52 |
| 2:I:606:PHE:CE1 | 2:I:811:VAL:HG13 | 2.44 | 0.52 |
| 2:I:1040:LEU:O | 2:I:1046:GLN:HG3 | 2.09 | 0.52 |
| 1:C:929:GLY:C | 1:C:931:GLN:H | 2.13 | 0.52 |
| 1:C:1749:THR:C | 1:C:1874:ASP:HB3 | 2.29 | 0.52 |
| 2:H:145:LEU:O | 2:H:149:VAL:HG12 | 2.10 | 0.52 |
| 2:I:465:GLY:HA2 | 2:I:493:THR:HA | 1.91 | 0.52 |
| 2:I:2036:GLU:O | 2:I:2039:LYS:HG2 | 2.09 | 0.52 |
| 2:H:2026:PHE:CD2 | 2:H:2045:TRP:HZ3 | 2.27 | 0.52 |
| 1:B:12:ILE:HD11 | 2:H:2041:ILE:HD11 | 1.89 | 0.52 |
| 2:I:598:THR:O | 2:I:602:VAL:HB | 2.09 | 0.52 |
| 2:H:1159:ILE:CG1 | 2:H:1169:PRO:CD | 2.87 | 0.52 |
| 1:B:1234:MET:CE | 1:B:1326:ILE:HG21 | 2.40 | 0.52 |
| 1:A:986:ALA:CA | 1:A:1047:LEU:HD13 | 2.39 | 0.52 |
| 2:H:1697:HIS:HE1 | 2:H:1829:GLU:CG | 2.22 | 0.52 |
| 2:H:1427:VAL:O | 2:H:1427:VAL:HG12 | 2.08 | 0.52 |
| 1:A:341:GLN:O | 1:A:345:VAL:HG12 | 2.09 | 0.52 |
| 1:A:156:ALA:HA | 1:A:166:ILE:CD1 | 2.39 | 0.52 |
| 2:G:615:TYR:CZ | 2:G:1074:MET:HB3 | 2.44 | 0.52 |
| 2:H:194:THR:CG2 | 2:H:300:ILE:HD11 | 2.39 | 0.52 |
| 1:C:1056:ILE:HD13 | 1:C:1193:TRP:CD1 | 2.41 | 0.52 |
| 2:H:768:GLY:HA3 | 2:H:800:LEU:CD2 | 2.39 | 0.52 |
| 1:C:1305:CYS:SG | 1:C:1583:HIS:NE2 | 2.82 | 0.52 |
| 1:B:980:VAL:HG21 | 2:H:952:ARG:NH2 | 2.24 | 0.52 |
| 2:I:418:ASN:HD22 | 2:I:418:ASN:N | 2.07 | 0.52 |
| 1:B:784:ILE:HG23 | 1:B:788:SER:HB2 | 1.92 | 0.52 |
| 2:G:490:TRP:HA | 2:G:493:THR:CG2 | 2.40 | 0.52 |
| 1:C:260:ARG:HH12 | 1:C:300:VAL:CG2 | 2.22 | 0.52 |
| 2:G:1438:SER:O | 2:G:1441:ILE:HG23 | 2.09 | 0.52 |
| 1:C:530:ALA:HA | 1:C:636:PRO:HB3 | 1.91 | 0.52 |
| 1:A:335:HIS:HD2 | 1:A:335:HIS:O | 1.92 | 0.52 |
| 1:B:329:GLU:O | 1:B:333:LYS:HG3 | 2.08 | 0.52 |
| 2:G:1159:ILE:HG12 | 2:G:1169:PRO:CD | 2.39 | 0.52 |
| 2:G:1359:MET:CE | 2:G:1404:MET:HB3 | 2.39 | 0.52 |
| 1:A:824:LEU:HD11 | 1:A:849:LEU:HD12 | 1.89 | 0.52 |
| 2:I:1486:PHE:HA | 2:I:1504:VAL:O | 2.10 | 0.52 |
| 2:H:955:GLU:HG2 | 2:H:987:TYR:CE2 | 2.45 | 0.52 |
| 1:C:1411:THR:HG22 | 1:C:1412:ASP:N | 2.24 | 0.52 |
| 2:G:145:LEU:HD21 | 2:G:156:LEU:HD21 | 1.91 | 0.52 |
| 2:I:741:HIS:HE1 | 2:I:855:HIS:NE2 | 2.06 | 0.52 |
| 2:I:1438:SER:O | 2:I:1441:ILE:HG23 | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1774:THR:HA | 2:I:1777:THR:HB | 1.92 | 0.52 |
| 1:A:988:ILE:HD13 | 1:A:1048:GLU:CA | 2.39 | 0.52 |
| 2:I:1350:LEU:HD11 | 2:I:1410:PHE:HB3 | 1.91 | 0.52 |
| 2:H:754:TYR:CD2 | 2:H:794:MET:HG3 | 2.44 | 0.52 |
| 2:I:1475:LYS:HG3 | 2:I:1481:SER:HB2 | 1.92 | 0.52 |
| 2:G:871:THR:HG21 | 2:G:887:LYS:NZ | 2.25 | 0.52 |
| 2:I:1300:PHE:CA | 2:I:1556:VAL:HG11 | 2.40 | 0.52 |
| 1:C:465:ASN:O | 1:C:469:VAL:HG23 | 2.10 | 0.52 |
| 2:H:1722:GLY:N | 2:H:1726:GLY:HA3 | 2.24 | 0.52 |
| 2:G:1389:ILE:HG13 | 2:G:1411:PHE:HD1 | 1.75 | 0.52 |
| 1:C:406:TRP:CE3 | 1:C:1619:GLU:HG3 | 2.44 | 0.52 |
| 2:I:702:TYR:HB2 | 2:I:727:PRO:HB2 | 1.92 | 0.52 |
| 2:G:1567:ARG:HG2 | 2:G:1567:ARG:HH11 | 1.72 | 0.52 |
| 1:A:1477:ILE:H | 1:A:1478:PRO:CD | 2.21 | 0.52 |
| 2:I:964:LEU:CD2 | 2:I:964:LEU:N | 2.72 | 0.52 |
| 2:G:1475:LYS:CB | 2:G:1481:SER:HB2 | 2.39 | 0.52 |
| 2:H:1359:MET:HE3 | 2:H:1404:MET:HB3 | 1.92 | 0.52 |
| 2:G:1932:SER:O | 2:G:1936:VAL:HG22 | 2.10 | 0.52 |
| 1:A:501:THR:N | 1:A:886:GLU:OE1 | 2.30 | 0.52 |
| 1:A:998:TYR:CE2 | 1:A:1667:GLU:HB2 | 2.44 | 0.52 |
| 1:B:341:GLN:O | 1:B:345:VAL:HG12 | 2.10 | 0.52 |
| 2:G:1593:ILE:HD13 | 2:G:1626:ILE:HD13 | 1.92 | 0.52 |
| 2:H:615:TYR:CZ | 2:H:1074:MET:HB3 | 2.43 | 0.52 |
| 2:G:2026:PHE:CD2 | 2:G:2045:TRP:HZ3 | 2.27 | 0.52 |
| 2:I:1159:ILE:HG12 | 2:I:1169:PRO:CD | 2.39 | 0.52 |
| 1:A:2:LYS:CD | 2:G:2050:GLN:HB3 | 2.38 | 0.52 |
| 2:H:1776:PHE:O | 2:H:1779:PRO:HD2 | 2.09 | 0.52 |
| 2:H:747:HIS:O | 2:H:751:LEU:HB2 | 2.10 | 0.52 |
| 1:A:1305:CYS:SG | 1:A:1583:HIS:NE2 | 2.83 | 0.52 |
| 1:A:430:ARG:NH1 | 1:A:493:VAL:O | 2.40 | 0.52 |
| 1:A:59:ARG:HH11 | 2:G:1896:GLN:NE2 | 2.07 | 0.52 |
| 2:I:1004:LEU:HD21 | 2:I:1020:VAL:HG23 | 1.91 | 0.52 |
| 2:H:1292:ILE:O | 2:H:1368:VAL:O | 2.27 | 0.52 |
| 2:I:913:ASP:H | 2:I:916:THR:CG2 | 2.23 | 0.52 |
| 2:G:955:GLU:HG2 | 2:G:987:TYR:CE2 | 2.45 | 0.52 |
| 2:H:599:PRO:HD2 | 4:H:3051:FMN:H6 | 1.92 | 0.52 |
| 2:G:1177:SER:O | 2:G:1180:MET:HG2 | 2.09 | 0.52 |
| 1:B:529:MET:HG2 | 1:B:638:LEU:HG | 1.92 | 0.52 |
| 1:C:1431:GLU:CD | 1:C:1433:HIS:CE1 | 2.83 | 0.52 |
| 1:B:893:VAL:HG11 | 1:B:930:LEU:CD2 | 2.36 | 0.52 |
| 2:I:1282:ARG:HH21 | 2:I:1423:PHE:HB3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:27:ARG:HB2 | 2:I:2016:ALA:HB2 | 1.91 | 0.52 |
| 2:I:751:LEU:HD23 | 2:I:791:TYR:CZ | 2.44 | 0.52 |
| 2:I:1597:ALA:HB1 | 2:I:1638:ILE:CD1 | 2.39 | 0.52 |
| 2:G:926:LEU:HB3 | 2:G:947:THR:HG22 | 1.92 | 0.52 |
| 2:I:1918:LYS:HG2 | 2:I:1919:LEU:HD23 | 1.92 | 0.52 |
| 2:H:418:ASN:HD22 | 2:H:418:ASN:N | 2.08 | 0.52 |
| 1:C:607:LYS:HG2 | 1:C:608:ASP:N | 2.24 | 0.52 |
| 2:I:273:HIS:CB | 2:I:512:LEU:HD22 | 2.40 | 0.52 |
| 1:C:340:ARG:HH12 | 1:C:344:GLN:NE2 | 2.08 | 0.52 |
| 2:G:121:GLU:HA | 2:G:124:LYS:HD2 | 1.91 | 0.52 |
| 2:I:747:HIS:O | 2:I:751:LEU:HB2 | 2.10 | 0.52 |
| 2:G:768:GLY:HA3 | 2:G:800:LEU:CD2 | 2.38 | 0.52 |
| 2:G:176:LEU:HD22 | 2:G:247:ALA:HB1 | 1.90 | 0.52 |
| 1:A:705:VAL:CG2 | 1:A:732:LEU:HD21 | 2.39 | 0.52 |
| 1:A:1475:GLU:HG3 | 1:A:1761:LYS:O | 2.10 | 0.52 |
| 1:C:705:VAL:CG2 | 1:C:732:LEU:HD21 | 2.40 | 0.52 |
| 1:C:1577:GLN:HE22 | 1:C:1591:TRP:C | 2.13 | 0.52 |
| 2:I:1223:MET:CE | 2:I:1238:LEU:HD12 | 2.40 | 0.52 |
| 2:H:553:ASN:O | 2:H:556:LYS:CE | 2.58 | 0.52 |
| 1:A:521:LYS:HE2 | 1:A:605:LEU:HD11 | 1.92 | 0.52 |
| 2:G:1745:LYS:HD3 | 2:G:1747:LYS:HE2 | 1.91 | 0.52 |
| 2:G:1873:TYR:CE1 | 2:G:1877:ARG:NE | 2.75 | 0.52 |
| 2:H:278:VAL:HG11 | 2:H:303:LEU:HD13 | 1.92 | 0.52 |
| 2:G:1093:ASP:HB3 | 2:G:1096:LYS:HG3 | 1.90 | 0.52 |
| 2:I:2026:PHE:CD2 | 2:I:2045:TRP:HZ3 | 2.27 | 0.52 |
| 2:I:1871:LEU:HD22 | 2:I:1888:ILE:HD11 | 1.92 | 0.52 |
| 2:H:892:ILE:HG12 | 2:H:903:TRP:CG | 2.45 | 0.52 |
| 1:A:1577:GLN:HE22 | 1:A:1591:TRP:C | 2.13 | 0.52 |
| 2:H:281:VAL:HG12 | 2:H:282:ALA:N | 2.24 | 0.52 |
| 1:C:156:ALA:HA | 1:C:166:ILE:CD1 | 2.40 | 0.52 |
| 1:A:280:GLU:O | 1:A:280:GLU:HG2 | 2.10 | 0.52 |
| 2:H:577:ILE:HD13 | 2:H:1097:ILE:CD1 | 2.40 | 0.52 |
| 1:A:674:LYS:O | 1:A:675:ASP:HB2 | 2.09 | 0.52 |
| 2:G:278:VAL:HG11 | 2:G:303:LEU:HD13 | 1.92 | 0.52 |
| 1:A:607:LYS:HG2 | 1:A:608:ASP:N | 2.25 | 0.52 |
| 1:A:1183:ARG:NH1 | 1:A:1344:GLY:HA2 | 2.24 | 0.52 |
| 2:H:1673:GLU:N | 2:H:1676:MET:HE3 | 2.25 | 0.51 |
| 2:G:1774:THR:HA | 2:G:1777:THR:HB | 1.90 | 0.51 |
| 1:C:1665:ILE:CG1 | 1:C:1669:ARG:HD3 | 2.36 | 0.51 |
| 1:B:1238:VAL:HG12 | 1:B:1239:HIS:N | 2.25 | 0.51 |
| 2:G:234:ILE:CG1 | 2:G:235:PRO:HD3 | 2.40 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1056:ILE:CD1 | 1:B:1193:TRP:HD1 | 2.22 | 0.51 |
| 2:I:1745:LYS:HD3 | 2:I:1747:LYS:HE2 | 1.93 | 0.51 |
| 2:H:654:VAL:HG23 | 2:H:683:ALA:HB1 | 1.92 | 0.51 |
| 1:B:1748:ASN:C | 1:B:1750:ILE:H | 2.13 | 0.51 |
| 1:A:881:ASN:HA | 1:A:944:ARG:NH2 | 2.25 | 0.51 |
| 1:B:985:ARG:HH12 | 2:H:953:ARG:NH2 | 2.07 | 0.51 |
| 2:H:131:ILE:CD1 | 2:H:182:VAL:CG1 | 2.88 | 0.51 |
| 2:I:715:GLN:O | 2:I:719:ILE:HG12 | 2.10 | 0.51 |
| 1:C:1303:GLY:N | 1:C:1307:THR:HG22 | 2.26 | 0.51 |
| 1:C:1238:VAL:HG12 | 1:C:1239:HIS:N | 2.25 | 0.51 |
| 1:B:1665:ILE:HG12 | 1:B:1666:THR:N | 2.25 | 0.51 |
| 2:I:1868:GLN:HG3 | 2:I:1898:TYR:CZ | 2.45 | 0.51 |
| 2:G:376:ASN:C | 2:G:376:ASN:HD22 | 2.13 | 0.51 |
| 1:A:1123:GLN:HG3 | 1:A:1124:GLU:N | 2.24 | 0.51 |
| 1:C:156:ALA:HA | 1:C:166:ILE:HD12 | 1.92 | 0.51 |
| 1:B:1104:ARG:O | 1:B:1185:VAL:HG13 | 2.11 | 0.51 |
| 1:C:1840:VAL:HG23 | 1:C:1848:ALA:HB3 | 1.92 | 0.51 |
| 1:A:1411:THR:HG22 | 1:A:1412:ASP:N | 2.25 | 0.51 |
| 2:I:1697:HIS:CE1 | 2:I:1829:GLU:HG2 | 2.45 | 0.51 |
| 2:G:489:LYS:O | 2:G:493:THR:HG22 | 2.10 | 0.51 |
| 2:G:702:TYR:HB2 | 2:G:727:PRO:HB2 | 1.93 | 0.51 |
| 2:H:758:ARG:NH2 | 2:H:797:ASP:OD1 | 2.35 | 0.51 |
| 1:A:1474:ALA:HA | 1:A:1478:PRO:CD | 2.41 | 0.51 |
| 2:G:1293:THR:HG22 | 2:G:1296:GLU:CG | 2.40 | 0.51 |
| 2:H:545:GLN:NE2 | 2:H:545:GLN:H | 2.07 | 0.51 |
| 2:H:1293:THR:HG22 | 2:H:1296:GLU:CG | 2.41 | 0.51 |
| 1:A:1303:GLY:N | 1:A:1307:THR:HG22 | 2.25 | 0.51 |
| 2:G:124:LYS:HG2 | 2:G:179:THR:HA | 1.90 | 0.51 |
| 2:H:1475:LYS:CB | 2:H:1481:SER:HB2 | 2.40 | 0.51 |
| 2:G:1328:VAL:HG23 | 2:G:1557:SER:HA | 1.92 | 0.51 |
| 1:B:985:ARG:NH1 | 2:H:953:ARG:CZ | 2.73 | 0.51 |
| 1:A:1411:THR:HG22 | 1:A:1412:ASP:H | 1.76 | 0.51 |
| 1:C:46:GLU:OE1 | 1:C:53:LEU:HB2 | 2.11 | 0.51 |
| 2:G:1493:LEU:HD11 | 2:G:1499:VAL:CG2 | 2.40 | 0.51 |
| 1:C:674:LYS:O | 1:C:675:ASP:HB2 | 2.11 | 0.51 |
| 2:G:213:LEU:HG | 2:G:213:LEU:O | 2.10 | 0.51 |
| 1:A:12:ILE:CD1 | 2:G:2041:ILE:CD1 | 2.83 | 0.51 |
| 2:I:652:ILE:HD12 | 2:I:652:ILE:N | 2.25 | 0.51 |
| 2:H:1081:HIS:O | 2:H:1085:LEU:HB2 | 2.10 | 0.51 |
| 2:G:1081:HIS:O | 2:G:1085:LEU:HB2 | 2.10 | 0.51 |
| 1:B:335:HIS:HD2 | 1:B:335:HIS:O | 1.93 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:732:TRP:CD2 | 2:I:750:MET:HE1 | 2.43 | 0.51 |
| 2:I:732:TRP:CD2 | 2:I:750:MET:HE3 | 2.45 | 0.51 |
| 2:I:1475:LYS:CB | 2:I:1481:SER:HB2 | 2.41 | 0.51 |
| 2:H:1491:VAL:HB | 2:H:1501:ILE:HD12 | 1.92 | 0.51 |
| 2:H:1475:LYS:HG3 | 2:H:1481:SER:HB2 | 1.93 | 0.51 |
| 2:G:654:VAL:HG12 | 2:G:654:VAL:O | 2.09 | 0.51 |
| 2:H:582:LYS:HE2 | 2:H:1108:PRO:HB3 | 1.92 | 0.51 |
| 1:B:1411:THR:HG22 | 1:B:1412:ASP:N | 2.26 | 0.51 |
| 1:C:983:GLN:NE2 | 2:I:962:LYS:HD2 | 2.25 | 0.51 |
| 2:I:460:TYR:HA | 2:I:466:SER:O | 2.11 | 0.51 |
| 2:G:816:ASP:HB3 | 2:G:1048:VAL:CG2 | 2.41 | 0.51 |
| 2:H:1561:ASN:OD1 | 2:H:1563:ILE:HB | 2.10 | 0.51 |
| 2:G:145:LEU:O | 2:G:149:VAL:HG12 | 2.10 | 0.51 |
| 2:H:55:THR:HB | 2:H:59:GLU:OE2 | 2.10 | 0.51 |
| 1:B:1477:ILE:H | 1:B:1478:PRO:CD | 2.24 | 0.51 |
| 1:B:338:LEU:O | 1:B:342:GLN:HG3 | 2.10 | 0.51 |
| 1:C:328:LEU:HD22 | 1:C:328:LEU:C | 2.30 | 0.51 |
| 2:I:1015:VAL:HG11 | 2:I:1017:PHE:CE1 | 2.45 | 0.51 |
| 2:G:1417:THR:CG2 | 2:G:1419:PHE:CE2 | 2.93 | 0.51 |
| 1:B:1194:ASN:HB3 | 1:B:1197:THR:HG22 | 1.91 | 0.51 |
| 1:A:157:HIS:HE1 | 1:A:228:LEU:HD22 | 1.76 | 0.51 |
| 1:C:644:THR:HG22 | 1:C:648:ASP:O | 2.10 | 0.51 |
| 1:B:415:SER:O | 1:B:419:GLU:HB2 | 2.10 | 0.51 |
| 2:H:1493:LEU:HD11 | 2:H:1499:VAL:HG21 | 1.93 | 0.51 |
| 1:A:1840:VAL:HG23 | 1:A:1848:ALA:HB3 | 1.91 | 0.51 |
| 1:B:1840:VAL:HG23 | 1:B:1848:ALA:HB3 | 1.92 | 0.51 |
| 2:G:1427:VAL:HG12 | 2:G:1427:VAL:O | 2.09 | 0.51 |
| 2:H:432:LEU:HB3 | 2:H:484:ILE:HG23 | 1.92 | 0.51 |
| 2:H:1054:LEU:HB3 | 4:H:3051:FMN:HM82 | 1.93 | 0.51 |
| 2:I:1566:SER:HB3 | 2:I:1568:HIS:CE1 | 2.45 | 0.51 |
| 2:G:1589:VAL:HG11 | 2:G:1640:PHE:CE1 | 2.45 | 0.51 |
| 2:G:1764:PHE:HB2 | 2:G:1770:LEU:HD21 | 1.93 | 0.51 |
| 2:H:260:PRO:HD3 | 2:H:289:TRP:CZ2 | 2.46 | 0.51 |
| 2:H:1716:ASN:OD1 | 2:H:1765:ARG:HA | 2.11 | 0.51 |
| 1:A:1310:GLU:OE1 | 1:A:1649:LYS:CE | 2.56 | 0.51 |
| 2:H:732:TRP:CD1 | 2:H:750:MET:HE3 | 2.46 | 0.51 |
| 2:H:1419:PHE:O | 2:H:1420:GLU:C | 2.49 | 0.51 |
| 2:G:1579:ILE:HD11 | 2:G:1615:MET:SD | 2.51 | 0.51 |
| 2:I:306:ILE:HA | 2:I:439:ILE:CD1 | 2.40 | 0.51 |
| 2:I:1428:GLU:HB2 | 2:I:1468:THR:HG22 | 1.93 | 0.51 |
| 2:G:1431:TYR:CE1 | 2:G:1526:THR:HG23 | 2.45 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:254:TRP:HZ3 | 1:A:292:GLN:HG3 | 1.75 | 0.51 |
| 2:G:1986:LYS:HA | 2:G:1989:LYS:HB3 | 1.92 | 0.51 |
| 2:H:667:LYS:HD2 | 2:H:697:THR:CG2 | 2.35 | 0.51 |
| 2:H:533:LEU:HD13 | 2:H:545:GLN:HG3 | 1.92 | 0.51 |
| 1:A:1498:GLU:HB2 | 1:A:1876:LEU:CD1 | 2.37 | 0.51 |
| 2:I:950:PHE:O | 2:I:954:VAL:HG23 | 2.11 | 0.51 |
| 1:C:513:GLU:OE2 | 1:C:873:ARG:NH1 | 2.44 | 0.51 |
| 1:B:864:VAL:CG2 | 1:B:921:PRO:HB3 | 2.40 | 0.51 |
| 1:A:465:ASN:O | 1:A:469:VAL:HG23 | 2.11 | 0.51 |
| 2:H:1236:LEU:HD11 | 2:H:1262:ILE:HG12 | 1.92 | 0.51 |
| 1:C:1009:LEU:HG | 1:C:1664:ALA:HB2 | 1.93 | 0.51 |
| 2:I:346:GLN:HA | 2:I:377:LEU:HD21 | 1.92 | 0.51 |
| 1:C:1123:GLN:HB2 | 1:C:1177:LYS:HE2 | 1.93 | 0.51 |
| 1:C:1411:THR:HG22 | 1:C:1412:ASP:H | 1.75 | 0.51 |
| 2:I:157:VAL:HG11 | 2:I:496:PHE:CZ | 2.46 | 0.51 |
| 2:I:1313:SER:O | 2:I:1314:ARG:HD3 | 2.11 | 0.51 |
| 2:G:1422:THR:O | 2:G:1422:THR:CG2 | 2.59 | 0.51 |
| 2:G:443:LEU:HD22 | 2:G:448:VAL:CG1 | 2.41 | 0.51 |
| 2:G:566:HIS:O | 2:G:568:LYS:HG3 | 2.10 | 0.51 |
| 2:G:786:SER:CB | 2:G:794:MET:HE2 | 2.41 | 0.51 |
| 1:C:733:ILE:CD1 | 1:C:761:LEU:HD11 | 2.40 | 0.51 |
| 2:H:807:ILE:HG21 | 2:H:1066:ILE:HA | 1.92 | 0.51 |
| 2:H:461:ASP:HB3 | 2:H:464:ASP:HB2 | 1.93 | 0.51 |
| 2:I:807:ILE:HG21 | 2:I:1066:ILE:HA | 1.93 | 0.51 |
| 2:G:16:LEU:HG | 2:G:48:PHE:CZ | 2.45 | 0.51 |
| 2:H:2046:GLU:C | 2:H:2048:TYR:H | 2.14 | 0.51 |
| 2:I:1359:MET:HA | 2:I:1359:MET:HE3 | 1.92 | 0.51 |
| 2:H:332:GLU:OE2 | 2:H:394:ARG:HD3 | 2.10 | 0.51 |
| 1:B:1705:PRO:HB2 | 1:B:1733:PHE:CE1 | 2.46 | 0.51 |
| 1:A:400:ARG:HH11 | 1:A:400:ARG:HG3 | 1.67 | 0.51 |
| 2:G:1135:GLU:OE2 | 2:G:1175:LYS:HE3 | 2.11 | 0.51 |
| 2:H:741:HIS:HB2 | 2:H:853:PRO:O | 2.11 | 0.51 |
| 2:H:2026:PHE:HD2 | 2:H:2045:TRP:HZ3 | 1.59 | 0.51 |
| 2:H:1678:MET:CE | 2:H:1707:LEU:HD22 | 2.40 | 0.51 |
| 2:G:751:LEU:HD23 | 2:G:791:TYR:CZ | 2.46 | 0.51 |
| 1:A:889:GLU:HG3 | 1:A:893:VAL:O | 2.11 | 0.51 |
| 1:B:1455:ARG:NH2 | 1:B:1459:ILE:HG12 | 2.26 | 0.51 |
| 1:B:822:VAL:HG12 | 1:B:824:LEU:HD22 | 1.93 | 0.51 |
| 2:H:460:TYR:HA | 2:H:466:SER:O | 2.11 | 0.51 |
| 1:C:411:GLN:HE22 | 1:C:1628:SER:H | 1.58 | 0.51 |
| 2:G:418:ASN:N | 2:G:418:ASN:HD22 | 2.09 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:868:PHE:HB3 | 2:G:873:PHE:CE2 | 2.46 | 0.51 |
| 2:G:1452:LEU:HA | 2:G:1502:GLY:HA3 | 1.92 | 0.51 |
| 2:H:233:SER:HA | 2:H:424:ALA:CB | 2.41 | 0.51 |
| 1:C:157:HIS:HE1 | 1:C:228:LEU:HD22 | 1.75 | 0.51 |
| 2:G:601:THR:HG22 | 2:G:620:ALA:H | 1.75 | 0.50 |
| 2:I:1776:PHE:O | 2:I:1779:PRO:HD2 | 2.10 | 0.50 |
| 2:G:194:THR:CG2 | 2:G:300:ILE:HD11 | 2.41 | 0.50 |
| 2:G:1223:MET:CE | 2:G:1238:LEU:HD12 | 2.40 | 0.50 |
| 1:B:50:SER:HB2 | 1:B:51:PRO:CD | 2.40 | 0.50 |
| 1:B:1524:GLY:HA2 | 1:B:1527:ALA:HB3 | 1.93 | 0.50 |
| 2:I:1493:LEU:HD11 | 2:I:1499:VAL:HG21 | 1.93 | 0.50 |
| 2:G:1697:HIS:HE1 | 2:G:1829:GLU:HG2 | 1.74 | 0.50 |
| 1:A:635:ILE:HG22 | 1:A:651:TYR:CD1 | 2.46 | 0.50 |
| 1:A:1105:LEU:HD23 | 1:A:1185:VAL:HG22 | 1.93 | 0.50 |
| 2:H:1265:MET:HE1 | 2:H:1562:PRO:HG2 | 1.92 | 0.50 |
| 1:B:386:PHE:O | 1:B:390:VAL:HB | 2.11 | 0.50 |
| 2:H:408:PRO:HG3 | 2:H:836:TYR:CD2 | 2.46 | 0.50 |
| 1:A:985:ARG:NH1 | 2:G:953:ARG:CZ | 2.74 | 0.50 |
| 2:G:7:ARG:CZ | 2:G:24:THR:HA | 2.41 | 0.50 |
| 2:I:611:THR:HA | 2:I:615:TYR:O | 2.11 | 0.50 |
| 1:A:1533:ILE:HD11 | 1:A:1564:LEU:HD13 | 1.93 | 0.50 |
| 2:H:1597:ALA:HB1 | 2:H:1638:ILE:CD1 | 2.41 | 0.50 |
| 2:I:85:ASN:HD22 | 2:I:135:ARG:NH1 | 2.04 | 0.50 |
| 2:I:750:MET:CG | 2:I:796:PHE:HZ | 2.24 | 0.50 |
| 1:C:655:LEU:CD2 | 1:C:916:LEU:HD11 | 2.41 | 0.50 |
| 2:I:281:VAL:HG12 | 2:I:282:ALA:N | 2.25 | 0.50 |
| 1:B:635:ILE:HG22 | 1:B:651:TYR:CD1 | 2.46 | 0.50 |
| 2:G:281:VAL:HG12 | 2:G:282:ALA:N | 2.26 | 0.50 |
| 1:B:1411:THR:HG22 | 1:B:1412:ASP:H | 1.75 | 0.50 |
| 1:B:1196:LYS:HE3 | 1:B:1202:ASP:CG | 2.31 | 0.50 |
| 1:C:34:VAL:O | 1:C:38:ASP:HB2 | 2.11 | 0.50 |
| 2:H:1861:ARG:HD2 | 2:H:1964:PHE:O | 2.12 | 0.50 |
| 2:G:526:ARG:HH11 | 2:G:558:ASN:HD21 | 1.59 | 0.50 |
| 1:C:828:PRO:HG3 | 1:C:868:ILE:HG22 | 1.94 | 0.50 |
| 1:A:433:VAL:O | 1:A:437:ILE:HG13 | 2.12 | 0.50 |
| 1:B:1158:PRO:HD2 | 1:B:1159:GLU:OE2 | 2.10 | 0.50 |
| 2:H:491:GLU:HA | 2:H:494:THR:HG22 | 1.93 | 0.50 |
| 1:A:20:TYR:CE1 | 2:G:2033:THR:HG21 | 2.47 | 0.50 |
| 2:G:652:ILE:CD1 | 2:G:658:MET:HE3 | 2.42 | 0.50 |
| 2:H:1774:THR:HA | 2:H:1777:THR:HB | 1.93 | 0.50 |
| 1:A:24:SER:O | 2:G:1977:HIS:CD2 | 2.65 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:376:ASN:C | 2:I:376:ASN:HD22 | 2.14 | 0.50 |
| 1:A:59:ARG:HH11 | 2:G:1896:GLN:HE22 | 1.58 | 0.50 |
| 2:I:1027:ILE:O | 2:I:1031:LYS:HB2 | 2.11 | 0.50 |
| 2:H:1775:GLN:HG2 | 2:H:1836:MET:SD | 2.51 | 0.50 |
| 2:I:1945:ASP:O | 2:I:1949:LYS:HG3 | 2.10 | 0.50 |
| 2:I:173:LEU:HD13 | 2:I:219:LEU:HD21 | 1.94 | 0.50 |
| 2:H:344:LEU:HB3 | 2:H:349:VAL:HG23 | 1.94 | 0.50 |
| 2:G:1272:ASP:O | 2:G:1273:GLU:HG3 | 2.11 | 0.50 |
| 1:A:34:VAL:O | 1:A:38:ASP:HB2 | 2.10 | 0.50 |
| 2:G:1918:LYS:HG2 | 2:G:1919:LEU:HD23 | 1.93 | 0.50 |
| 2:G:545:GLN:NE2 | 2:G:545:GLN:H | 2.09 | 0.50 |
| 2:H:1102:TYR:CE2 | 2:H:1152:ALA:HB2 | 2.47 | 0.50 |
| 1:B:1303:GLY:N | 1:B:1307:THR:HG22 | 2.25 | 0.50 |
| 2:I:1491:VAL:HB | 2:I:1501:ILE:HD12 | 1.93 | 0.50 |
| 1:B:421:ILE:HG12 | 1:B:469:VAL:HG21 | 1.93 | 0.50 |
| 1:C:415:SER:O | 1:C:419:GLU:HB2 | 2.12 | 0.50 |
| 1:C:1116:PRO:HB2 | 1:C:1184:LEU:HD12 | 1.93 | 0.50 |
| 1:A:286:PHE:O | 1:A:290:MET:HG2 | 2.10 | 0.50 |
| 2:H:463:PHE:CE1 | 2:H:486:LEU:HD22 | 2.47 | 0.50 |
| 1:C:702:LYS:HE2 | 1:C:729:GLY:O | 2.11 | 0.50 |
| 2:H:1389:ILE:HG13 | 2:H:1411:PHE:HD1 | 1.76 | 0.50 |
| 1:C:280:GLU:O | 1:C:280:GLU:HG2 | 2.11 | 0.50 |
| 2:H:1435:ILE:HG22 | 2:H:1435:ILE:O | 2.10 | 0.50 |
| 2:H:1148:ASN:ND2 | 2:H:1151:HIS:H | 2.08 | 0.50 |
| 2:G:1871:LEU:HD22 | 2:G:1888:ILE:HD11 | 1.93 | 0.50 |
| 2:I:2035:SER:HB3 | 2:I:2038:ILE:CD1 | 2.40 | 0.50 |
| 2:I:1135:GLU:OE2 | 2:I:1175:LYS:HE3 | 2.12 | 0.50 |
| 1:C:1431:GLU:HB3 | 1:C:1520:ALA:HB2 | 1.92 | 0.50 |
| 2:G:611:THR:HA | 2:G:615:TYR:O | 2.11 | 0.50 |
| 2:G:732:TRP:CG | 2:G:750:MET:HE3 | 2.46 | 0.50 |
| 2:G:663:ILE:HB | 2:G:664:PRO:CD | 2.40 | 0.50 |
| 2:G:676:ILE:HG12 | 2:G:676:ILE:O | 2.11 | 0.50 |
| 1:A:1004:ILE:HG22 | 1:A:1660:TYR:CE2 | 2.46 | 0.50 |
| 2:I:1716:ASN:OD1 | 2:I:1765:ARG:HA | 2.11 | 0.50 |
| 2:G:784:GLU:O | 2:G:787:THR:HB | 2.11 | 0.50 |
| 2:I:955:GLU:HG2 | 2:I:987:TYR:CE2 | 2.46 | 0.50 |
| 2:H:1428:GLU:HB2 | 2:H:1468:THR:HG22 | 1.94 | 0.50 |
| 1:B:156:ALA:HA | 1:B:166:ILE:CD1 | 2.41 | 0.50 |
| 1:B:156:ALA:HA | 1:B:166:ILE:HD12 | 1.93 | 0.50 |
| 1:A:1523:ARG:NH2 | 1:A:1564:LEU:O | 2.45 | 0.50 |
| 2:I:712:ALA:O | 2:I:715:GLN:HB3 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1474:ALA:HA | 1:C:1478:PRO:CD | 2.42 | 0.50 |
| 2:H:2036:GLU:HG2 | 2:H:2039:LYS:NZ | 2.27 | 0.50 |
| 2:G:774:ALA:HB1 | 2:G:1081:HIS:CD2 | 2.37 | 0.50 |
| 1:C:985:ARG:HH12 | 2:I:953:ARG:NH2 | 2.09 | 0.50 |
| 2:H:826:GLY:HA2 | 2:H:1060:ALA:HB3 | 1.94 | 0.50 |
| 2:G:1350:LEU:HD11 | 2:G:1410:PHE:HB3 | 1.94 | 0.50 |
| 2:G:1840:VAL:O | 2:G:1840:VAL:HG12 | 2.11 | 0.50 |
| 2:I:866:LYS:O | 2:I:870:GLU:HG3 | 2.12 | 0.50 |
| 1:B:1009:LEU:HA | 1:B:1445:MET:HE2 | 1.93 | 0.50 |
| 2:I:1953:VAL:HG12 | 2:I:1953:VAL:O | 2.11 | 0.50 |
| 1:A:487:ASP:O | 1:A:488:PRO:O | 2.30 | 0.50 |
| 1:C:1019:ILE:HG21 | 1:C:1316:VAL:HG22 | 1.94 | 0.50 |
| 1:C:13:LEU:HB2 | 2:I:2026:PHE:CE1 | 2.45 | 0.50 |
| 2:I:1986:LYS:HA | 2:I:1989:LYS:HB3 | 1.93 | 0.50 |
| 2:H:638:VAL:HG22 | 2:H:675:PRO:HG2 | 1.93 | 0.50 |
| 1:A:12:ILE:CD1 | 2:G:2041:ILE:HD11 | 2.41 | 0.50 |
| 1:B:20:TYR:OH | 2:H:2035:SER:HB2 | 2.12 | 0.50 |
| 2:G:949:ASP:CB | 2:G:1006:MET:HE2 | 2.38 | 0.50 |
| 2:H:161:GLY:HA3 | 2:H:506:PRO:HD2 | 1.93 | 0.50 |
| 2:G:894:ARG:NH1 | 2:G:898:ASP:OD2 | 2.43 | 0.50 |
| 2:H:121:GLU:HA | 2:H:124:LYS:HD2 | 1.93 | 0.50 |
| 1:B:825:PRO:HB2 | 1:B:843:LYS:NZ | 2.27 | 0.50 |
| 1:A:1104:ARG:O | 1:A:1185:VAL:HG13 | 2.12 | 0.50 |
| 1:A:359:ARG:NH2 | 1:C:1153:ASP:OD2 | 2.43 | 0.50 |
| 1:B:1347:LYS:O | 1:B:1347:LYS:HD3 | 2.11 | 0.50 |
| 2:G:440:ASN:ND2 | 2:G:477:GLU:HG2 | 2.26 | 0.50 |
| 2:G:24:THR:O | 2:G:26:SER:N | 2.44 | 0.50 |
| 2:G:2035:SER:HB3 | 2:G:2038:ILE:CD1 | 2.42 | 0.50 |
| 2:H:2035:SER:HB3 | 2:H:2038:ILE:CD1 | 2.42 | 0.50 |
| 1:C:328:LEU:HD13 | 1:C:329:GLU:N | 2.27 | 0.50 |
| 2:G:1776:PHE:O | 2:G:1779:PRO:HD2 | 2.12 | 0.50 |
| 2:H:747:HIS:HE1 | 2:H:780:TYR:OH | 1.95 | 0.50 |
| 1:A:930:LEU:HD22 | 1:A:933:VAL:HG11 | 1.93 | 0.50 |
| 2:G:60:LEU:O | 2:G:63:LYS:HB2 | 2.12 | 0.50 |
| 1:B:408:TRP:CZ3 | 1:B:1628:SER:HB3 | 2.47 | 0.50 |
| 2:G:682:GLY:O | 2:G:683:ALA:HB3 | 2.12 | 0.50 |
| 2:I:1417:THR:C | 2:I:1419:PHE:H | 2.14 | 0.50 |
| 2:G:606:PHE:CE1 | 2:G:811:VAL:HG13 | 2.46 | 0.50 |
| 1:C:157:HIS:CE1 | 1:C:228:LEU:HD22 | 2.47 | 0.50 |
| 1:C:702:LYS:HD3 | 1:C:731:THR:CG2 | 2.41 | 0.50 |
| 2:I:344:LEU:HB3 | 2:I:349:VAL:HG23 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:306:ILE:HA | 2:G:439:ILE:CD1 | 2.42 | 0.50 |
| 2:H:7:ARG:CZ | 2:H:24:THR:HA | 2.42 | 0.50 |
| 1:C:1460:LYS:CE | 1:C:1774:GLU:OE1 | 2.59 | 0.50 |
| 2:I:777:THR:HG23 | 2:I:1081:HIS:CE1 | 2.47 | 0.50 |
| 2:I:1673:GLU:N | 2:I:1676:MET:HE3 | 2.25 | 0.50 |
| 2:I:455:ILE:HG12 | 2:I:469:ARG:HG2 | 1.93 | 0.50 |
| 2:H:1004:LEU:HD21 | 2:H:1020:VAL:CG2 | 2.41 | 0.50 |
| 2:G:1552:PRO:O | 2:G:1556:VAL:HG23 | 2.12 | 0.50 |
| 1:A:1459:ILE:O | 1:A:1463:VAL:HG23 | 2.12 | 0.50 |
| 2:G:428:HIS:CD2 | 2:G:488:VAL:HG23 | 2.47 | 0.50 |
| 2:G:1697:HIS:HE1 | 2:G:1829:GLU:CG | 2.25 | 0.50 |
| 1:A:1116:PRO:HB2 | 1:A:1184:LEU:HD12 | 1.94 | 0.50 |
| 1:A:1125:VAL:HG21 | 1:A:1175:ILE:CD1 | 2.42 | 0.50 |
| 1:A:156:ALA:HA | 1:A:166:ILE:HD12 | 1.93 | 0.50 |
| 1:C:1566:ARG:HB3 | 1:C:1623:TYR:CE1 | 2.46 | 0.50 |
| 2:H:2030:TYR:CE1 | 2:H:2034:GLY:HA2 | 2.46 | 0.50 |
| 1:B:46:GLU:OE1 | 1:B:53:LEU:HB2 | 2.12 | 0.50 |
| 1:A:1347:LYS:HD3 | 1:A:1347:LYS:O | 2.11 | 0.50 |
| 2:G:1716:ASN:OD1 | 2:G:1765:ARG:HA | 2.12 | 0.50 |
| 1:C:385:PHE:HD2 | 1:C:787:LYS:HA | 1.77 | 0.50 |
| 1:C:1705:PRO:HB2 | 1:C:1733:PHE:CE1 | 2.46 | 0.50 |
| 2:H:441:LYS:O | 2:H:444:VAL:HG12 | 2.12 | 0.50 |
| 2:G:131:ILE:CB | 2:G:182:VAL:CG1 | 2.85 | 0.49 |
| 2:I:7:ARG:HE | 2:I:27:PHE:CB | 2.24 | 0.49 |
| 2:H:1227:ARG:HG3 | 2:H:1227:ARG:NH1 | 2.01 | 0.49 |
| 2:G:2029:VAL:O | 2:G:2033:THR:HG22 | 2.12 | 0.49 |
| 1:B:1533:ILE:HG13 | 1:B:1564:LEU:HB3 | 1.94 | 0.49 |
| 2:G:1441:ILE:HD11 | 2:G:1445:ARG:NH2 | 2.25 | 0.49 |
| 2:H:777:THR:HG23 | 2:H:1081:HIS:CE1 | 2.47 | 0.49 |
| 1:C:1665:ILE:HG12 | 1:C:1666:THR:N | 2.27 | 0.49 |
| 1:A:142:ASP:CG | 1:A:257:PRO:HB2 | 2.32 | 0.49 |
| 1:B:413:LEU:HB2 | 1:B:439:ILE:HD13 | 1.94 | 0.49 |
| 2:G:1868:GLN:HG3 | 2:G:1898:TYR:CZ | 2.48 | 0.49 |
| 1:C:267:VAL:O | 1:C:290:MET:HE1 | 2.12 | 0.49 |
| 1:B:1451:GLN:OE1 | 1:B:1451:GLN:HA | 2.12 | 0.49 |
| 2:I:1632:ILE:HG23 | 2:I:1632:ILE:O | 2.12 | 0.49 |
| 2:I:72:VAL:HG12 | 2:I:73:GLU:N | 2.27 | 0.49 |
| 1:A:1460:LYS:HE3 | 1:A:1774:GLU:HA | 1.94 | 0.49 |
| 2:H:7:ARG:HE | 2:H:27:PHE:CB | 2.26 | 0.49 |
| 2:I:24:THR:O | 2:I:26:SER:N | 2.45 | 0.49 |
| 2:H:28:PHE:CE1 | 2:I:27:PHE:CE2 | 3.00 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1474:ALA:HA | 1:B:1478:PRO:CD | 2.41 | 0.49 |
| 1:A:335:HIS:O | 1:A:338:LEU:HB3 | 2.12 | 0.49 |
| 2:I:259:THR:HG22 | 2:I:262:GLU:CB | 2.41 | 0.49 |
| 2:I:60:LEU:O | 2:I:63:LYS:HB2 | 2.11 | 0.49 |
| 2:H:871:THR:HG21 | 2:H:887:LYS:NZ | 2.26 | 0.49 |
| 2:G:871:THR:HG21 | 2:G:887:LYS:HZ2 | 1.77 | 0.49 |
| 1:B:1125:VAL:HG21 | 1:B:1175:ILE:CD1 | 2.42 | 0.49 |
| 2:I:274:SER:OG | 2:I:428:HIS:HE1 | 1.95 | 0.49 |
| 2:H:1745:LYS:HD3 | 2:H:1747:LYS:HE2 | 1.94 | 0.49 |
| 2:H:1148:ASN:HD22 | 2:H:1151:HIS:H | 1.60 | 0.49 |
| 1:B:674:LYS:O | 1:B:675:ASP:HB2 | 2.11 | 0.49 |
| 2:H:1162:ASP:O | 2:H:1163:LYS:HB2 | 2.11 | 0.49 |
| 1:A:1501:LEU:CD1 | 1:A:1775:LEU:HG | 2.43 | 0.49 |
| 1:C:1455:ARG:O | 1:C:1459:ILE:HG13 | 2.12 | 0.49 |
| 1:C:889:GLU:HG3 | 1:C:893:VAL:O | 2.13 | 0.49 |
| 2:I:1352:HIS:HE1 | 2:I:1583:MET:CE | 2.25 | 0.49 |
| 2:I:751:LEU:HA | 2:I:794:MET:HE3 | 1.94 | 0.49 |
| 2:I:324:LEU:HD12 | 2:I:324:LEU:O | 2.12 | 0.49 |
| 2:H:894:ARG:NH1 | 2:H:898:ASP:OD2 | 2.41 | 0.49 |
| 2:G:463:PHE:CE1 | 2:G:486:LEU:HD22 | 2.47 | 0.49 |
| 2:G:463:PHE:O | 2:G:463:PHE:HD2 | 1.95 | 0.49 |
| 1:C:1264:ARG:NH1 | 1:C:1270:VAL:HB | 2.27 | 0.49 |
| 2:G:1493:LEU:HD11 | 2:G:1499:VAL:HG21 | 1.93 | 0.49 |
| 2:G:1486:PHE:HA | 2:G:1504:VAL:O | 2.12 | 0.49 |
| 1:A:1276:GLN:O | 1:A:1282:THR:HG21 | 2.13 | 0.49 |
| 1:A:1460:LYS:CG | 1:A:1773:VAL:O | 2.60 | 0.49 |
| 2:H:273:HIS:CB | 2:H:512:LEU:HD22 | 2.41 | 0.49 |
| 2:G:677:GLN:O | 2:G:678:PHE:HB3 | 2.13 | 0.49 |
| 2:H:942:THR:HG21 | 2:H:1012:GLN:HA | 1.95 | 0.49 |
| 2:H:1889:VAL:HG13 | 2:H:1977:HIS:HB3 | 1.93 | 0.49 |
| 2:I:1293:THR:CG2 | 2:I:1296:GLU:H | 2.20 | 0.49 |
| 2:I:238:CYS:CB | 2:I:239:PRO:HD3 | 2.40 | 0.49 |
| 2:I:1678:MET:CE | 2:I:1707:LEU:HD22 | 2.41 | 0.49 |
| 1:C:1392:LEU:HD22 | 1:C:1396:MET:HG3 | 1.93 | 0.49 |
| 1:A:1189:ILE:HG23 | 1:A:1190:PRO:HD2 | 1.95 | 0.49 |
| 1:A:1009:LEU:HD13 | 1:A:1445:MET:HE1 | 1.94 | 0.49 |
| 2:H:682:GLY:O | 2:H:683:ALA:HB3 | 2.13 | 0.49 |
| 2:G:1427:VAL:HG22 | 2:G:1469:GLU:HG2 | 1.94 | 0.49 |
| 2:G:950:PHE:O | 2:G:954:VAL:HG23 | 2.13 | 0.49 |
| 2:G:706:LYS:HE2 | 2:G:731:GLN:OE1 | 2.13 | 0.49 |
| 1:C:790:PHE:CE2 | 1:C:794:ILE:HD11 | 2.48 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:598:THR:O | 2:H:602:VAL:HB | 2.11 | 0.49 |
| 1:B:1460:LYS:HE3 | 1:B:1774:GLU:CD | 2.33 | 0.49 |
| 1:A:20:TYR:CD1 | 2:G:2033:THR:OG1 | 2.59 | 0.49 |
| 2:H:1303:ALA:HB2 | 2:H:1556:VAL:HG21 | 1.93 | 0.49 |
| 2:G:1738:PHE:HE1 | 2:G:1837:THR:HG23 | 1.76 | 0.49 |
| 1:B:1305:CYS:SG | 1:B:1583:HIS:NE2 | 2.85 | 0.49 |
| 1:A:1234:MET:HG2 | 1:A:1326:ILE:HD12 | 1.94 | 0.49 |
| 2:H:1417:THR:O | 2:H:1419:PHE:N | 2.45 | 0.49 |
| 1:B:435:GLU:O | 1:B:439:ILE:HG13 | 2.12 | 0.49 |
| 1:C:50:SER:HB2 | 1:C:51:PRO:CD | 2.43 | 0.49 |
| 1:C:1050:CYS:HB3 | 1:C:1089:VAL:HG12 | 1.94 | 0.49 |
| 1:A:46:GLU:OE1 | 1:A:53:LEU:HB2 | 2.12 | 0.49 |
| 2:H:7:ARG:HH11 | 2:H:24:THR:HG23 | 1.75 | 0.49 |
| 2:H:22:VAL:HG11 | 2:H:27:PHE:HA | 1.94 | 0.49 |
| 2:G:465:GLY:HA2 | 2:G:493:THR:HA | 1.95 | 0.49 |
| 2:I:7:ARG:CZ | 2:I:24:THR:HA | 2.42 | 0.49 |
| 2:H:1566:SER:HB3 | 2:H:1568:HIS:CE1 | 2.47 | 0.49 |
| 2:I:55:THR:CG2 | 2:I:56:THR:HG22 | 2.33 | 0.49 |
| 2:H:715:GLN:O | 2:H:719:ILE:HG12 | 2.13 | 0.49 |
| 2:H:369:SER:O | 2:H:370:LEU:HD23 | 2.13 | 0.49 |
| 2:I:1015:VAL:HG13 | 2:I:1017:PHE:CE2 | 2.47 | 0.49 |
| 2:I:161:GLY:HA3 | 2:I:506:PRO:HD2 | 1.93 | 0.49 |
| 2:H:949:ASP:CB | 2:H:1006:MET:HE2 | 2.42 | 0.49 |
| 2:I:1265:MET:CE | 2:I:1562:PRO:HG2 | 2.41 | 0.49 |
| 1:A:157:HIS:CE1 | 1:A:228:LEU:HD22 | 2.48 | 0.49 |
| 1:B:1600:LEU:HD11 | 1:B:1655:VAL:HG12 | 1.94 | 0.49 |
| 1:B:170:LYS:HD3 | 1:B:175:LEU:HD23 | 1.93 | 0.49 |
| 1:B:1362:PRO:HA | 1:B:1365:MET:HG3 | 1.94 | 0.49 |
| 1:A:489:VAL:HG22 | 1:A:671:VAL:N | 2.28 | 0.49 |
| 1:A:1451:GLN:HA | 1:A:1451:GLN:OE1 | 2.12 | 0.49 |
| 2:I:1435:ILE:O | 2:I:1435:ILE:HG22 | 2.12 | 0.49 |
| 1:B:764:ASP:OD2 | 1:B:818:ARG:HD3 | 2.11 | 0.49 |
| 2:H:138:ASP:O | 2:H:139:LYS:HG3 | 2.12 | 0.49 |
| 2:I:16:LEU:HG | 2:I:48:PHE:CZ | 2.48 | 0.49 |
| 2:G:618:GLU:HG2 | 2:G:678:PHE:CZ | 2.48 | 0.49 |
| 1:C:636:PRO:HB2 | 1:C:638:LEU:O | 2.13 | 0.49 |
| 1:A:328:LEU:HD13 | 1:A:329:GLU:N | 2.27 | 0.49 |
| 2:I:1169:PRO:O | 2:I:1173:VAL:HG23 | 2.13 | 0.49 |
| 2:H:455:ILE:HD11 | 2:H:469:ARG:NE | 2.27 | 0.49 |
| 1:A:256:LEU:HD22 | 1:A:260:ARG:HB3 | 1.94 | 0.49 |
| 2:H:161:GLY:N | 2:H:505:GLY:HA3 | 2.25 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1266:TYR:HB2 | 2:G:1347:LEU:HD23 | 1.95 | 0.49 |
| 1:A:1264:ARG:NH1 | 1:A:1270:VAL:HB | 2.28 | 0.49 |
| 2:H:463:PHE:O | 2:H:463:PHE:HD2 | 1.96 | 0.49 |
| 2:I:1873:TYR:CE2 | 2:I:1940:LEU:HD21 | 2.47 | 0.49 |
| 1:B:1105:LEU:HD23 | 1:B:1185:VAL:HG22 | 1.94 | 0.49 |
| 1:C:980:VAL:HG23 | 2:I:968:GLN:OE1 | 2.13 | 0.49 |
| 2:I:740:HIS:CE1 | 2:I:852:GLU:OE1 | 2.65 | 0.49 |
| 2:H:1873:TYR:HE1 | 2:H:1877:ARG:HH21 | 1.59 | 0.49 |
| 1:A:1705:PRO:HB2 | 1:A:1733:PHE:CE1 | 2.47 | 0.49 |
| 1:A:18:LEU:HD21 | 2:G:1815:LEU:HD12 | 1.95 | 0.49 |
| 2:I:597:MET:H | 2:I:601:THR:HB | 1.78 | 0.49 |
| 2:G:491:GLU:HA | 2:G:494:THR:HG22 | 1.95 | 0.49 |
| 2:H:702:TYR:HB2 | 2:H:727:PRO:HB2 | 1.94 | 0.49 |
| 2:H:932:ILE:HD12 | 2:H:939:PHE:HD1 | 1.78 | 0.49 |
| 2:H:1593:ILE:O | 2:H:1597:ALA:HB3 | 2.12 | 0.49 |
| 1:A:21:GLN:HG3 | 2:G:2013:ASN:HB2 | 1.93 | 0.49 |
| 2:G:732:TRP:CD1 | 2:G:750:MET:HE3 | 2.47 | 0.49 |
| 2:H:569:LEU:HD12 | 2:H:1090:TYR:CD1 | 2.48 | 0.49 |
| 2:I:949:ASP:CB | 2:I:1006:MET:HE2 | 2.43 | 0.49 |
| 2:H:173:LEU:O | 2:H:173:LEU:HD22 | 2.13 | 0.49 |
| 1:C:982:ILE:HD11 | 2:I:965:SER:HB2 | 1.95 | 0.49 |
| 2:H:1666:PHE:CD1 | 2:H:1814:ALA:HA | 2.48 | 0.49 |
| 2:I:11:LEU:HD11 | 2:I:64:PHE:CD2 | 2.48 | 0.49 |
| 2:H:1634:GLY:HA3 | 2:H:1799:PRO:HA | 1.94 | 0.49 |
| 1:B:1642:THR:HG22 | 1:B:1652:GLN:HG3 | 1.93 | 0.49 |
| 2:G:157:VAL:HG11 | 2:G:496:PHE:CZ | 2.47 | 0.49 |
| 2:I:573:LYS:HE3 | 2:I:1101:GLU:OE1 | 2.12 | 0.49 |
| 1:C:1114:TYR:CD1 | 1:C:1337:GLU:HG3 | 2.48 | 0.49 |
| 2:G:273:HIS:CB | 2:G:512:LEU:HD22 | 2.42 | 0.49 |
| 1:C:20:TYR:CD2 | 2:I:2033:THR:OG1 | 2.66 | 0.49 |
| 2:I:1567:ARG:HH11 | 2:I:1567:ARG:HG2 | 1.70 | 0.49 |
| 1:A:1219:VAL:CA | 1:A:1384:ILE:HD11 | 2.31 | 0.49 |
| 2:G:161:GLY:N | 2:G:505:GLY:HA3 | 2.24 | 0.49 |
| 1:C:1020:VAL:CG1 | 1:C:1400:ILE:HG23 | 2.42 | 0.49 |
| 2:H:428:HIS:HD2 | 2:H:486:LEU:O | 1.96 | 0.49 |
| 2:G:1130:THR:H | 2:G:1133:THR:CG2 | 2.26 | 0.49 |
| 1:C:267:VAL:HG12 | 1:C:290:MET:CE | 2.42 | 0.49 |
| 2:I:306:ILE:HA | 2:I:439:ILE:HD13 | 1.94 | 0.49 |
| 2:I:173:LEU:O | 2:I:173:LEU:HD22 | 2.13 | 0.49 |
| 1:B:186:ILE:O | 1:B:190:LEU:HG | 2.13 | 0.49 |
| 2:H:1749:GLU:OE2 | 2:H:1840:VAL:HG13 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:18:LEU:HD21 | 2:I:1815:LEU:HD12 | 1.94 | 0.49 |
| 1:A:1362:PRO:HA | 1:A:1365:MET:HG3 | 1.95 | 0.49 |
| 1:A:1749:THR:CB | 1:A:1874:ASP:N | 2.75 | 0.49 |
| 2:G:2036:GLU:HG2 | 2:G:2039:LYS:NZ | 2.28 | 0.49 |
| 2:I:1567:ARG:NH1 | 2:I:1568:HIS:HB3 | 2.28 | 0.49 |
| 1:C:335:HIS:O | 1:C:335:HIS:CD2 | 2.65 | 0.49 |
| 2:G:259:THR:HG22 | 2:G:262:GLU:CB | 2.43 | 0.49 |
| 2:G:560:ASN:OD1 | 2:G:560:ASN:O | 2.30 | 0.49 |
| 2:G:1913:VAL:O | 2:G:1917:ILE:HG13 | 2.12 | 0.49 |
| 1:B:1312:VAL:CG2 | 1:B:1329:VAL:HG11 | 2.39 | 0.49 |
| 1:C:32:GLN:NE2 | 1:C:57:ALA:HA | 2.28 | 0.49 |
| 2:H:1002:HIS:NE2 | 2:H:1006:MET:HE3 | 2.27 | 0.49 |
| 1:A:1022:THR:HG22 | 1:A:1226:SER:CB | 2.43 | 0.49 |
| 2:G:715:GLN:O | 2:G:719:ILE:HG12 | 2.13 | 0.49 |
| 2:H:860:ARG:HB2 | 2:H:1049:GLN:HG3 | 1.94 | 0.49 |
| 2:G:807:ILE:HD12 | 2:G:1063:THR:HG23 | 1.95 | 0.49 |
| 2:I:428:HIS:HD2 | 2:I:486:LEU:O | 1.95 | 0.49 |
| 2:G:653:TYR:HD1 | 2:G:659:LEU:HD21 | 1.78 | 0.49 |
| 1:A:1009:LEU:HG | 1:A:1664:ALA:HB2 | 1.95 | 0.49 |
| 2:G:1666:PHE:CD1 | 2:G:1814:ALA:HA | 2.48 | 0.49 |
| 2:G:173:LEU:HD22 | 2:G:173:LEU:O | 2.13 | 0.49 |
| 2:I:881:VAL:N | 2:I:882:PRO:CD | 2.76 | 0.49 |
| 2:H:465:GLY:HA2 | 2:H:493:THR:HA | 1.95 | 0.48 |
| 2:H:739:GLY:HA2 | 2:H:1054:LEU:HG | 1.95 | 0.48 |
| 2:G:598:THR:O | 2:G:602:VAL:HB | 2.13 | 0.48 |
| 2:I:835:THR:HG22 | 2:I:844:VAL:HA | 1.95 | 0.48 |
| 2:H:1931:LEU:HB3 | 2:H:1935:GLU:CG | 2.36 | 0.48 |
| 1:C:1693:ILE:CD1 | 2:I:998:GLN:HB2 | 2.40 | 0.48 |
| 1:B:916:LEU:HD22 | 1:B:922:VAL:HG22 | 1.94 | 0.48 |
| 1:A:1312:VAL:CG2 | 1:A:1329:VAL:HG11 | 2.41 | 0.48 |
| 2:I:663:ILE:HB | 2:I:664:PRO:CD | 2.42 | 0.48 |
| 2:I:161:GLY:N | 2:I:505:GLY:HA3 | 2.24 | 0.48 |
| 1:A:1021:VAL:HG22 | 1:A:1387:ILE:HG22 | 1.95 | 0.48 |
| 2:G:402:LEU:HD12 | 2:G:404:GLN:HG2 | 1.95 | 0.48 |
| 2:I:1697:HIS:HE1 | 2:I:1829:GLU:CG | 2.26 | 0.48 |
| 1:B:182:VAL:O | 1:B:186:ILE:HG13 | 2.12 | 0.48 |
| 1:C:1105:LEU:HD23 | 1:C:1185:VAL:HG22 | 1.94 | 0.48 |
| 1:B:1753:ALA:HB2 | 1:B:1872:SER:OG | 2.13 | 0.48 |
| 2:G:597:MET:H | 2:G:601:THR:HB | 1.77 | 0.48 |
| 2:H:259:THR:HG22 | 2:H:262:GLU:CB | 2.42 | 0.48 |
| 2:H:786:SER:CB | 2:H:794:MET:HE2 | 2.43 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:187:LEU:HD22 | 1:B:201:PRO:HB2 | 1.94 | 0.48 |
| 1:B:465:ASN:O | 1:B:469:VAL:HG23 | 2.12 | 0.48 |
| 2:G:376:ASN:C | 2:G:376:ASN:ND2 | 2.67 | 0.48 |
| 2:I:682:GLY:O | 2:I:683:ALA:HB3 | 2.13 | 0.48 |
| 2:H:1868:GLN:HG3 | 2:H:1898:TYR:CZ | 2.48 | 0.48 |
| 2:G:1745:LYS:HE2 | 2:G:1747:LYS:HG2 | 1.95 | 0.48 |
| 2:H:306:ILE:HA | 2:H:439:ILE:CD1 | 2.42 | 0.48 |
| 2:H:1272:ASP:O | 2:H:1273:GLU:HG3 | 2.13 | 0.48 |
| 2:G:2046:GLU:C | 2:G:2048:TYR:H | 2.15 | 0.48 |
| 2:I:629:GLY:O | 2:I:632:ALA:HB3 | 2.13 | 0.48 |
| 2:H:901:LYS:NZ | 2:H:1031:LYS:O | 2.46 | 0.48 |
| 2:I:1674:GLN:OE1 | 2:I:1712:ASN:HA | 2.13 | 0.48 |
| 2:G:11:LEU:HD11 | 2:G:64:PHE:CD2 | 2.48 | 0.48 |
| 2:I:970:TYR:O | 2:I:973:LEU:HB2 | 2.14 | 0.48 |
| 1:C:256:LEU:HD22 | 1:C:260:ARG:HB3 | 1.95 | 0.48 |
| 2:G:7:ARG:HE | 2:G:27:PHE:CB | 2.25 | 0.48 |
| 1:C:1523:ARG:NH2 | 1:C:1564:LEU:O | 2.46 | 0.48 |
| 1:A:1477:ILE:H | 1:A:1478:PRO:HD3 | 1.78 | 0.48 |
| 2:G:533:LEU:HD13 | 2:G:545:GLN:HG3 | 1.94 | 0.48 |
| 2:G:754:TYR:CE2 | 2:G:794:MET:HG3 | 2.48 | 0.48 |
| 1:B:2:LYS:HE2 | 1:B:4:GLU:CD | 2.34 | 0.48 |
| 2:I:786:SER:CB | 2:I:794:MET:HE2 | 2.42 | 0.48 |
| 2:H:33:LEU:HD21 | 2:H:80:PHE:CE2 | 2.49 | 0.48 |
| 1:C:1305:CYS:SG | 3:C:2748:CER:C5 | 3.01 | 0.48 |
| 2:G:1330:GLY:HA2 | 2:G:1374:THR:HG21 | 1.94 | 0.48 |
| 1:B:157:HIS:HE1 | 1:B:228:LEU:HD22 | 1.77 | 0.48 |
| 1:B:413:LEU:C | 1:B:415:SER:H | 2.17 | 0.48 |
| 2:I:1130:THR:H | 2:I:1133:THR:CG2 | 2.25 | 0.48 |
| 2:H:463:PHE:CD1 | 2:H:486:LEU:HD22 | 2.48 | 0.48 |
| 2:I:1873:TYR:CE1 | 2:I:1877:ARG:NE | 2.77 | 0.48 |
| 2:G:1428:GLU:HG2 | 2:G:1470:THR:HG22 | 1.94 | 0.48 |
| 2:H:955:GLU:HG2 | 2:H:987:TYR:HE2 | 1.78 | 0.48 |
| 2:H:40:ILE:O | 2:H:42:PRO:HD3 | 2.13 | 0.48 |
| 2:I:278:VAL:HG11 | 2:I:303:LEU:HD13 | 1.95 | 0.48 |
| 2:I:146:PHE:HA | 2:I:149:VAL:HG12 | 1.92 | 0.48 |
| 2:H:1624:THR:HB | 2:H:1642:THR:OG1 | 2.14 | 0.48 |
| 1:A:340:ARG:HH12 | 1:A:344:GLN:HE21 | 1.60 | 0.48 |
| 2:H:1422:THR:HG23 | 2:H:1474:PHE:CD1 | 2.48 | 0.48 |
| 2:I:995:LEU:HB3 | 2:I:1000:ILE:HD11 | 1.95 | 0.48 |
| 2:H:995:LEU:HB3 | 2:H:1000:ILE:HD11 | 1.94 | 0.48 |
| 1:B:335:HIS:O | 1:B:338:LEU:HB3 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:328:LEU:HD13 | 1:B:329:GLU:N | 2.29 | 0.48 |
| 1:B:332:THR:HG22 | 1:C:331:ILE:CD1 | 2.44 | 0.48 |
| 1:C:331:ILE:HG23 | 1:C:332:THR:N | 2.28 | 0.48 |
| 2:I:455:ILE:O | 2:I:455:ILE:HG13 | 2.13 | 0.48 |
| 2:G:455:ILE:HG12 | 2:G:469:ARG:HG2 | 1.94 | 0.48 |
| 2:I:593:LEU:HD21 | 2:I:800:LEU:HB3 | 1.95 | 0.48 |
| 2:G:1980:TYR:HD1 | 2:G:1981:LEU:HD12 | 1.79 | 0.48 |
| 2:I:402:LEU:HD12 | 2:I:404:GLN:HG2 | 1.94 | 0.48 |
| 2:H:428:HIS:CD2 | 2:H:488:VAL:HG23 | 2.49 | 0.48 |
| 1:B:702:LYS:HD3 | 1:B:731:THR:CG2 | 2.44 | 0.48 |
| 2:G:720:ALA:HA | 2:G:728:ILE:CD1 | 2.43 | 0.48 |
| 2:I:551:THR:HG22 | 2:I:552:SER:N | 2.29 | 0.48 |
| 2:I:249:TYR:CD2 | 2:I:283:ILE:HD11 | 2.48 | 0.48 |
| 2:I:1850:SER:HB2 | 2:I:1973:SER:HB2 | 1.95 | 0.48 |
| 2:H:145:LEU:HD21 | 2:H:156:LEU:HD21 | 1.95 | 0.48 |
| 2:H:1986:LYS:HA | 2:H:1989:LYS:HB3 | 1.95 | 0.48 |
| 2:G:1567:ARG:CG | 2:G:1567:ARG:NH1 | 2.51 | 0.48 |
| 1:C:1477:ILE:H | 1:C:1478:PRO:HD3 | 1.78 | 0.48 |
| 2:I:1382:VAL:HA | 2:I:1422:THR:OG1 | 2.12 | 0.48 |
| 2:I:1081:HIS:O | 2:I:1085:LEU:HB2 | 2.14 | 0.48 |
| 2:G:995:LEU:HB3 | 2:G:1000:ILE:HD11 | 1.96 | 0.48 |
| 1:A:1714:VAL:HG22 | 1:A:1738:ILE:HD11 | 1.96 | 0.48 |
| 2:I:569:LEU:HD12 | 2:I:1090:TYR:CD1 | 2.48 | 0.48 |
| 2:H:1100:VAL:CG2 | 2:H:1147:ILE:HG21 | 2.43 | 0.48 |
| 1:B:21:GLN:HG3 | 2:H:2013:ASN:HB2 | 1.95 | 0.48 |
| 2:I:1266:TYR:HB2 | 2:I:1347:LEU:HD23 | 1.95 | 0.48 |
| 1:B:408:TRP:CH2 | 1:B:1628:SER:HB3 | 2.47 | 0.48 |
| 1:C:988:ILE:HD13 | 1:C:1048:GLU:CB | 2.43 | 0.48 |
| 2:H:1918:LYS:HG2 | 2:H:1919:LEU:HD23 | 1.96 | 0.48 |
| 2:H:1953:VAL:O | 2:H:1953:VAL:HG12 | 2.14 | 0.48 |
| 1:C:1642:THR:HG22 | 1:C:1652:GLN:HG3 | 1.96 | 0.48 |
| 1:B:998:TYR:CE2 | 1:B:1667:GLU:HB2 | 2.49 | 0.48 |
| 2:I:7:ARG:HH11 | 2:I:24:THR:HG23 | 1.77 | 0.48 |
| 1:A:20:TYR:CE1 | 2:G:2033:THR:CG2 | 2.97 | 0.48 |
| 1:A:444:ASN:HB2 | 1:A:447:LEU:N | 2.14 | 0.48 |
| 2:I:1159:ILE:CG1 | 2:I:1169:PRO:CD | 2.90 | 0.48 |
| 2:I:533:LEU:HG | 2:I:533:LEU:O | 2.13 | 0.48 |
| 2:G:1213:LEU:O | 2:G:1214:LEU:HD23 | 2.12 | 0.48 |
| 2:G:593:LEU:HD21 | 2:G:800:LEU:HB3 | 1.96 | 0.48 |
| 2:G:569:LEU:HD12 | 2:G:1090:TYR:CD1 | 2.48 | 0.48 |
| 2:I:121:GLU:HA | 2:I:124:LYS:HD2 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1401:TYR:C | 1:A:1658:PRO:HG3 | 2.33 | 0.48 |
| 2:I:1738:PHE:CE1 | 2:I:1837:THR:HG23 | 2.48 | 0.48 |
| 2:H:99:ASN:HA | 2:H:550:VAL:HG21 | 1.95 | 0.48 |
| 2:G:72:VAL:HG12 | 2:G:73:GLU:N | 2.28 | 0.48 |
| 1:B:503:ILE:HD12 | 1:B:950:THR:HG21 | 1.96 | 0.48 |
| 2:I:586:LEU:HD12 | 2:I:764:MET:SD | 2.54 | 0.48 |
| 1:C:764:ASP:OD2 | 1:C:818:ARG:HD3 | 2.12 | 0.48 |
| 2:H:784:GLU:O | 2:H:787:THR:HB | 2.13 | 0.48 |
| 2:G:1148:ASN:HD22 | 2:G:1148:ASN:C | 2.17 | 0.48 |
| 1:A:19:ALA:O | 1:A:22:PHE:HB2 | 2.14 | 0.48 |
| 2:H:1632:ILE:O | 2:H:1632:ILE:HG23 | 2.13 | 0.48 |
| 2:H:397:LYS:HB3 | 2:H:416:PHE:CE2 | 2.48 | 0.48 |
| 1:C:430:ARG:NH1 | 1:C:493:VAL:O | 2.44 | 0.48 |
| 1:C:852:ARG:CG | 1:C:852:ARG:NH1 | 2.66 | 0.48 |
| 2:I:762:ASN:HD22 | 2:I:762:ASN:N | 1.88 | 0.48 |
| 2:G:2026:PHE:HD2 | 2:G:2045:TRP:HZ3 | 1.59 | 0.48 |
| 2:I:667:LYS:HD2 | 2:I:697:THR:CG2 | 2.35 | 0.48 |
| 1:A:988:ILE:HA | 1:A:1048:GLU:CG | 2.44 | 0.48 |
| 1:C:1617:ILE:O | 1:C:1620:GLN:HG2 | 2.13 | 0.48 |
| 2:H:561:TRP:CZ3 | 2:H:792:PRO:HB2 | 2.49 | 0.48 |
| 2:H:751:LEU:HD23 | 2:H:791:TYR:CZ | 2.49 | 0.48 |
| 1:C:1312:VAL:CG2 | 1:C:1329:VAL:HG11 | 2.44 | 0.48 |
| 1:A:420:ILE:HG22 | 1:A:469:VAL:HG22 | 1.96 | 0.48 |
| 1:C:1396:MET:O | 1:C:1680:ARG:NH1 | 2.46 | 0.48 |
| 2:I:1697:HIS:HE1 | 2:I:1829:GLU:HG2 | 1.77 | 0.48 |
| 1:C:1276:GLN:O | 1:C:1282:THR:HG21 | 2.13 | 0.48 |
| 1:C:1451:GLN:OE1 | 1:C:1451:GLN:HA | 2.13 | 0.48 |
| 2:G:240:LEU:O | 2:G:244:ILE:HG13 | 2.13 | 0.48 |
| 1:C:1300:THR:HA | 1:C:1301:PRO:HD3 | 1.67 | 0.48 |
| 2:G:1590:ARG:HG3 | 2:G:1608:TYR:CD2 | 2.48 | 0.48 |
| 2:H:1674:GLN:OE1 | 2:H:1712:ASN:HA | 2.12 | 0.48 |
| 1:A:182:VAL:O | 1:A:186:ILE:HG13 | 2.14 | 0.48 |
| 2:H:490:TRP:HA | 2:H:493:THR:HG22 | 1.96 | 0.48 |
| 2:H:597:MET:H | 2:H:601:THR:HB | 1.78 | 0.48 |
| 2:I:845:THR:HG22 | 2:I:855:HIS:CD2 | 2.49 | 0.48 |
| 2:G:1180:MET:HB2 | 2:G:1197:LEU:HD21 | 1.95 | 0.48 |
| 2:H:317:THR:HG21 | 2:I:1309:GLU:CG | 2.42 | 0.48 |
| 1:C:888:ILE:HD12 | 1:C:939:PHE:CE2 | 2.47 | 0.48 |
| 1:A:1037:TRP:HB2 | 1:A:1598:GLN:OE1 | 2.13 | 0.48 |
| 1:B:1056:ILE:HD13 | 1:B:1193:TRP:CD1 | 2.45 | 0.48 |
| 2:I:1325:PHE:CE1 | 2:I:1328:VAL:HG11 | 2.49 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1040:LEU:O | 2:H:1046:GLN:HG3 | 2.13 | 0.48 |
| 1:B:625:THR:HG23 | 1:B:661:ASP:OD1 | 2.13 | 0.48 |
| 1:B:1183:ARG:NH1 | 1:B:1344:GLY:HA2 | 2.29 | 0.48 |
| 1:C:1738:ILE:O | 1:C:1739:GLN:HB2 | 2.14 | 0.48 |
| 2:H:214:ASN:ND2 | 2:H:217:GLU:HB2 | 2.27 | 0.48 |
| 2:I:1586:SER:O | 2:I:1590:ARG:HB2 | 2.14 | 0.48 |
| 1:B:790:PHE:CE2 | 1:B:794:ILE:HD11 | 2.47 | 0.48 |
| 1:A:539:SER:O | 1:A:540:GLN:C | 2.52 | 0.48 |
| 2:H:169:TYR:CG | 2:H:170:PHE:N | 2.81 | 0.48 |
| 2:H:489:LYS:O | 2:H:493:THR:HG22 | 2.13 | 0.48 |
| 2:I:1159:ILE:HG22 | 2:I:1160:THR:N | 2.28 | 0.48 |
| 1:A:427:ASN:HB2 | 1:A:468:LEU:HD21 | 1.95 | 0.48 |
| 2:G:306:ILE:HA | 2:G:439:ILE:HD13 | 1.96 | 0.48 |
| 2:G:432:LEU:HB3 | 2:G:484:ILE:HG23 | 1.96 | 0.48 |
| 2:I:772:GLY:O | 2:I:804:ARG:HD3 | 2.14 | 0.48 |
| 2:G:481:ASP:OD2 | 2:G:485:ARG:NH1 | 2.47 | 0.48 |
| 2:H:868:PHE:HB3 | 2:H:873:PHE:CE2 | 2.48 | 0.48 |
| 1:B:243:ILE:O | 1:B:247:ARG:HG3 | 2.13 | 0.48 |
| 1:A:695:GLY:HA3 | 1:A:906:LEU:HD11 | 1.94 | 0.48 |
| 2:I:489:LYS:O | 2:I:493:THR:HG22 | 2.13 | 0.48 |
| 2:I:2026:PHE:HD2 | 2:I:2045:TRP:HZ3 | 1.60 | 0.48 |
| 1:B:930:LEU:HD23 | 1:B:930:LEU:HA | 1.67 | 0.48 |
| 1:A:328:LEU:N | 1:A:330:GLU:H | 2.12 | 0.48 |
| 1:B:328:LEU:N | 1:B:330:GLU:H | 2.11 | 0.48 |
| 2:I:753:MET:O | 2:I:757:ILE:HG13 | 2.14 | 0.48 |
| 1:C:751:PHE:CZ | 1:C:761:LEU:HD13 | 2.49 | 0.48 |
| 2:H:232:LEU:HD21 | 2:H:423:VAL:HA | 1.95 | 0.48 |
| 2:G:1325:PHE:CE1 | 2:G:1328:VAL:HG11 | 2.48 | 0.48 |
| 2:G:461:ASP:HB3 | 2:G:464:ASP:HB2 | 1.95 | 0.48 |
| 1:A:1639:VAL:HG12 | 1:A:1640:SER:N | 2.28 | 0.48 |
| 2:G:173:LEU:HD13 | 2:G:219:LEU:HD21 | 1.94 | 0.48 |
| 2:G:1148:ASN:ND2 | 2:G:1151:HIS:H | 2.12 | 0.48 |
| 1:A:927:ASN:O | 1:A:929:GLY:N | 2.41 | 0.48 |
| 2:H:706:LYS:HE2 | 2:H:731:GLN:OE1 | 2.14 | 0.48 |
| 1:C:386:PHE:O | 1:C:390:VAL:HB | 2.14 | 0.48 |
| 1:B:683:ALA:HA | 1:B:689:GLY:HA3 | 1.95 | 0.48 |
| 2:I:214:ASN:ND2 | 2:I:217:GLU:HB2 | 2.28 | 0.48 |
| 1:B:1319:ILE:HA | 1:B:1324:ALA:O | 2.13 | 0.48 |
| 2:H:157:VAL:HG11 | 2:H:496:PHE:CZ | 2.49 | 0.48 |
| 2:I:1834:ARG:NH1 | 2:I:1834:ARG:CG | 2.66 | 0.47 |
| 2:G:22:VAL:HG11 | 2:G:27:PHE:HA | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:594:VAL:CG2 | 2:I:610:THR:HG21 | 2.44 | 0.47 |
| 2:G:1566:SER:HB3 | 2:G:1568:HIS:CE1 | 2.49 | 0.47 |
| 1:C:529:MET:HG2 | 1:C:638:LEU:HG | 1.95 | 0.47 |
| 2:H:943:TRP:CZ2 | 2:H:1016:PRO:HG3 | 2.49 | 0.47 |
| 2:I:1015:VAL:HA | 2:I:1016:PRO:HD3 | 1.74 | 0.47 |
| 2:G:567:PRO:HG3 | 2:G:781:LEU:CD1 | 2.44 | 0.47 |
| 1:B:1:MET:HE3 | 1:B:9:LEU:HD12 | 1.96 | 0.47 |
| 2:I:1002:HIS:NE2 | 2:I:1006:MET:HE3 | 2.29 | 0.47 |
| 1:A:187:LEU:HD22 | 1:A:201:PRO:HB2 | 1.96 | 0.47 |
| 2:I:176:LEU:HD22 | 2:I:247:ALA:HB1 | 1.96 | 0.47 |
| 1:C:440:MET:HE3 | 1:C:483:VAL:HG21 | 1.95 | 0.47 |
| 1:B:1646:PHE:CE1 | 3:B:2748:CER:H31 | 2.49 | 0.47 |
| 1:C:1392:LEU:CD2 | 1:C:1396:MET:HG3 | 2.44 | 0.47 |
| 2:H:873:PHE:CD1 | 2:H:1026:GLU:HB2 | 2.49 | 0.47 |
| 2:H:1590:ARG:NH2 | 2:H:1594:GLU:OE2 | 2.47 | 0.47 |
| 2:G:1027:ILE:O | 2:G:1031:LYS:HB2 | 2.14 | 0.47 |
| 2:I:900:GLN:NE2 | 2:I:1051:THR:HA | 2.28 | 0.47 |
| 2:H:159:ILE:CG2 | 2:H:501:ILE:HG22 | 2.44 | 0.47 |
| 1:B:1367:ARG:HH12 | 1:B:1372:THR:CB | 2.20 | 0.47 |
| 1:A:1501:LEU:O | 1:A:1505:GLN:HG3 | 2.14 | 0.47 |
| 1:B:256:LEU:HD22 | 1:B:260:ARG:HB3 | 1.95 | 0.47 |
| 2:G:777:THR:HG23 | 2:G:1081:HIS:CE1 | 2.49 | 0.47 |
| 1:C:427:ASN:HB2 | 1:C:468:LEU:HD21 | 1.95 | 0.47 |
| 1:C:1021:VAL:HG11 | 1:C:1597:LEU:CD1 | 2.44 | 0.47 |
| 2:H:732:TRP:CD2 | 2:H:750:MET:HE1 | 2.49 | 0.47 |
| 1:C:1125:VAL:HG21 | 1:C:1175:ILE:CD1 | 2.43 | 0.47 |
| 2:H:950:PHE:O | 2:H:954:VAL:HG23 | 2.13 | 0.47 |
| 2:H:1749:GLU:OE2 | 2:H:1840:VAL:CG1 | 2.62 | 0.47 |
| 2:G:40:ILE:O | 2:G:42:PRO:HD3 | 2.14 | 0.47 |
| 2:H:213:LEU:HG | 2:H:213:LEU:O | 2.14 | 0.47 |
| 1:A:176:VAL:HG12 | 1:A:178:GLY:H | 1.79 | 0.47 |
| 1:A:852:ARG:HB3 | 1:A:858:TRP:HZ2 | 1.80 | 0.47 |
| 2:G:1624:THR:HB | 2:G:1642:THR:OG1 | 2.15 | 0.47 |
| 2:H:1438:SER:O | 2:H:1441:ILE:HG23 | 2.13 | 0.47 |
| 2:H:589:ARG:HB3 | 2:H:590:PRO:CD | 2.43 | 0.47 |
| 1:A:1303:GLY:C | 1:A:1307:THR:HG22 | 2.35 | 0.47 |
| 1:A:1238:VAL:CG1 | 1:A:1242:GLU:HB2 | 2.44 | 0.47 |
| 2:I:926:LEU:HB3 | 2:I:947:THR:CG2 | 2.43 | 0.47 |
| 1:B:1116:PRO:HB2 | 1:B:1184:LEU:HD12 | 1.95 | 0.47 |
| 2:I:1579:ILE:HD11 | 2:I:1615:MET:SD | 2.53 | 0.47 |
| 1:C:1010:GLU:HA | 1:C:1664:ALA:HA | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:428:HIS:HD2 | 2:G:486:LEU:O | 1.97 | 0.47 |
| 2:G:1666:PHE:CD1 | 2:G:1814:ALA:HB2 | 2.49 | 0.47 |
| 1:B:530:ALA:HA | 1:B:636:PRO:HB3 | 1.97 | 0.47 |
| 1:A:683:ALA:HA | 1:A:689:GLY:HA3 | 1.95 | 0.47 |
| 2:I:1752:PHE:HZ | 2:I:1836:MET:HE3 | 1.80 | 0.47 |
| 2:G:804:ARG:NH2 | 2:G:1068:GLU:OE1 | 2.48 | 0.47 |
| 1:B:1209:ASP:OD2 | 1:B:1253:GLY:HA2 | 2.14 | 0.47 |
| 1:C:1516:ASP:HA | 1:C:1517:PRO:HD3 | 1.66 | 0.47 |
| 2:H:597:MET:HA | 4:H:3051:FMN:N5 | 2.30 | 0.47 |
| 2:H:677:GLN:O | 2:H:678:PHE:HB3 | 2.15 | 0.47 |
| 2:G:512:LEU:O | 2:G:516:THR:HG23 | 2.15 | 0.47 |
| 2:H:634:ILE:HD11 | 2:H:649:ILE:CD1 | 2.40 | 0.47 |
| 1:C:987:ASN:HD22 | 2:I:957:ARG:CD | 2.26 | 0.47 |
| 2:G:33:LEU:HD21 | 2:G:80:PHE:CE2 | 2.50 | 0.47 |
| 2:H:1472:VAL:CG2 | 2:H:1483:VAL:HG22 | 2.44 | 0.47 |
| 1:C:526:VAL:HG12 | 1:C:626:VAL:HG11 | 1.96 | 0.47 |
| 2:I:1804:PHE:CD2 | 2:I:1818:LEU:HD22 | 2.49 | 0.47 |
| 1:C:1133:PRO:HG3 | 1:C:1166:LYS:HG3 | 1.96 | 0.47 |
| 1:C:998:TYR:CE2 | 1:C:1667:GLU:HB2 | 2.49 | 0.47 |
| 2:I:562:LEU:HG | 2:I:793:PRO:CB | 2.44 | 0.47 |
| 2:H:1425:LYS:HG2 | 2:H:1471:GLU:HG3 | 1.95 | 0.47 |
| 2:H:1486:PHE:HA | 2:H:1504:VAL:O | 2.14 | 0.47 |
| 2:G:169:TYR:CG | 2:G:170:PHE:N | 2.83 | 0.47 |
| 1:C:1138:LYS:HG3 | 1:C:1163:TYR:CE1 | 2.48 | 0.47 |
| 1:C:370:GLU:O | 1:C:373:ALA:HB3 | 2.14 | 0.47 |
| 2:I:233:SER:HA | 2:I:424:ALA:CB | 2.44 | 0.47 |
| 1:C:142:ASP:CG | 1:C:257:PRO:HB2 | 2.34 | 0.47 |
| 2:I:2037:PRO:O | 2:I:2041:ILE:HG13 | 2.14 | 0.47 |
| 2:G:1651:LEU:O | 2:G:1652:THR:HG23 | 2.14 | 0.47 |
| 2:I:55:THR:HB | 2:I:59:GLU:OE2 | 2.13 | 0.47 |
| 1:B:1477:ILE:H | 1:B:1478:PRO:HD3 | 1.79 | 0.47 |
| 1:B:20:TYR:CG | 2:H:2033:THR:OG1 | 2.67 | 0.47 |
| 1:C:1303:GLY:CA | 1:C:1649:LYS:HE2 | 2.36 | 0.47 |
| 2:H:2037:PRO:O | 2:H:2041:ILE:HG13 | 2.15 | 0.47 |
| 1:B:331:ILE:HG23 | 1:B:332:THR:N | 2.29 | 0.47 |
| 1:C:328:LEU:N | 1:C:330:GLU:H | 2.12 | 0.47 |
| 2:G:123:ILE:CD1 | 2:G:533:LEU:CD2 | 2.93 | 0.47 |
| 2:H:455:ILE:HG13 | 2:H:455:ILE:O | 2.13 | 0.47 |
| 1:A:1208:VAL:HG11 | 1:A:1212:THR:HB | 1.96 | 0.47 |
| 2:G:732:TRP:CD2 | 2:G:750:MET:HE3 | 2.48 | 0.47 |
| 2:I:1378:ILE:O | 2:I:1378:ILE:HG12 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:750:MET:CG | 2:H:796:PHE:HZ | 2.25 | 0.47 |
| 2:H:860:ARG:H | 2:H:1049:GLN:HG3 | 1.79 | 0.47 |
| 2:I:350:GLN:HA | 2:I:353:VAL:HG13 | 1.96 | 0.47 |
| 2:G:463:PHE:CD1 | 2:G:486:LEU:HD22 | 2.48 | 0.47 |
| 2:H:376:ASN:C | 2:H:376:ASN:HD22 | 2.18 | 0.47 |
| 1:A:1012:LEU:HD23 | 1:A:1445:MET:CE | 2.43 | 0.47 |
| 2:I:873:PHE:CE1 | 2:I:1026:GLU:HB2 | 2.49 | 0.47 |
| 1:B:531:LEU:HD21 | 1:B:629:THR:HG22 | 1.97 | 0.47 |
| 2:G:1949:LYS:O | 2:G:1953:VAL:HG23 | 2.15 | 0.47 |
| 1:A:1319:ILE:HA | 1:A:1324:ALA:O | 2.14 | 0.47 |
| 2:H:652:ILE:N | 2:H:652:ILE:HD12 | 2.30 | 0.47 |
| 2:G:1422:THR:O | 2:G:1422:THR:HG23 | 2.14 | 0.47 |
| 1:C:335:HIS:O | 1:C:338:LEU:HB3 | 2.14 | 0.47 |
| 2:I:455:ILE:HD11 | 2:I:469:ARG:NE | 2.29 | 0.47 |
| 2:H:355:LYS:HB3 | 2:H:355:LYS:HE2 | 1.65 | 0.47 |
| 2:H:579:VAL:CG2 | 2:H:1078:HIS:CD2 | 2.95 | 0.47 |
| 1:A:983:GLN:HE22 | 2:G:962:LYS:HD2 | 1.77 | 0.47 |
| 2:I:748:THR:CB | 2:I:749:PRO:HD3 | 2.44 | 0.47 |
| 2:H:751:LEU:HD23 | 2:H:791:TYR:CD2 | 2.49 | 0.47 |
| 1:B:1305:CYS:SG | 3:B:2748:CER:C5 | 3.03 | 0.47 |
| 1:B:157:HIS:CE1 | 1:B:228:LEU:HD22 | 2.49 | 0.47 |
| 2:I:553:ASN:O | 2:I:556:LYS:HE3 | 2.15 | 0.47 |
| 2:I:1590:ARG:NH2 | 2:I:1594:GLU:OE2 | 2.48 | 0.47 |
| 2:H:1854:MET:CG | 2:H:1901:ALA:HB2 | 2.45 | 0.47 |
| 2:I:706:LYS:HE2 | 2:I:731:GLN:OE1 | 2.15 | 0.47 |
| 2:I:1103:PHE:O | 2:I:1247:GLY:HA3 | 2.14 | 0.47 |
| 2:I:1389:ILE:HG13 | 2:I:1411:PHE:HD1 | 1.80 | 0.47 |
| 2:I:22:VAL:HG11 | 2:I:27:PHE:HA | 1.97 | 0.47 |
| 1:C:254:TRP:HZ3 | 1:C:292:GLN:HG3 | 1.77 | 0.47 |
| 2:G:1567:ARG:NH1 | 2:G:1568:HIS:HB3 | 2.28 | 0.47 |
| 2:H:741:HIS:HE1 | 2:H:845:THR:HG21 | 1.61 | 0.47 |
| 2:I:443:LEU:HD22 | 2:I:448:VAL:CG1 | 2.45 | 0.47 |
| 1:B:889:GLU:HG3 | 1:B:893:VAL:O | 2.15 | 0.47 |
| 2:G:369:SER:O | 2:G:370:LEU:HD23 | 2.14 | 0.47 |
| 1:C:338:LEU:O | 1:C:342:GLN:HG3 | 2.15 | 0.47 |
| 2:G:1102:TYR:HB3 | 2:G:1244:PRO:CA | 2.44 | 0.47 |
| 2:H:1819:ALA:CA | 2:H:2005:ARG:HH11 | 2.26 | 0.47 |
| 2:I:732:TRP:CE2 | 2:I:750:MET:HE3 | 2.50 | 0.47 |
| 2:I:747:HIS:HE1 | 2:I:780:TYR:OH | 1.97 | 0.47 |
| 2:H:560:ASN:OD1 | 2:H:560:ASN:O | 2.33 | 0.47 |
| 2:G:732:TRP:CE2 | 2:G:750:MET:HE3 | 2.50 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:968:VAL:O | 2:H:1512:HIS:HB2 | 2.14 | 0.47 |
| 2:H:1378:ILE:HG12 | 2:H:1378:ILE:O | 2.13 | 0.47 |
| 2:I:768:GLY:HA3 | 2:I:800:LEU:CD2 | 2.41 | 0.47 |
| 1:A:930:LEU:CD2 | 1:A:933:VAL:HG11 | 2.44 | 0.47 |
| 2:H:176:LEU:HD22 | 2:H:247:ALA:HB1 | 1.95 | 0.47 |
| 2:G:232:LEU:HD21 | 2:G:423:VAL:HA | 1.97 | 0.47 |
| 1:A:413:LEU:HD13 | 1:A:451:MET:HG2 | 1.97 | 0.47 |
| 2:I:461:ASP:HB3 | 2:I:464:ASP:HB2 | 1.95 | 0.47 |
| 1:C:1305:CYS:SG | 1:C:1585:LYS:HA | 2.55 | 0.47 |
| 2:H:1130:THR:H | 2:H:1133:THR:CG2 | 2.27 | 0.47 |
| 1:B:705:VAL:CG2 | 1:B:732:LEU:HD21 | 2.43 | 0.47 |
| 2:H:1980:TYR:HD1 | 2:H:1981:LEU:HD12 | 1.79 | 0.47 |
| 1:A:1010:GLU:HA | 1:A:1664:ALA:HA | 1.97 | 0.47 |
| 2:H:606:PHE:HZ | 2:H:805:VAL:CG1 | 2.28 | 0.47 |
| 2:I:1004:LEU:CD2 | 2:I:1019:PRO:HB2 | 2.44 | 0.47 |
| 2:I:955:GLU:HG2 | 2:I:987:TYR:HE2 | 1.79 | 0.47 |
| 1:C:1183:ARG:NH1 | 1:C:1344:GLY:HA2 | 2.30 | 0.47 |
| 1:B:34:VAL:O | 1:B:38:ASP:HB2 | 2.14 | 0.47 |
| 1:B:827:SER:HA | 1:B:828:PRO:HD3 | 1.73 | 0.47 |
| 1:A:243:ILE:O | 1:A:247:ARG:HG3 | 2.14 | 0.47 |
| 1:A:1061:SER:HB2 | 1:A:1078:SER:HB3 | 1.96 | 0.47 |
| 1:B:776:GLU:OE1 | 1:B:795:MET:HE1 | 2.13 | 0.47 |
| 2:H:11:LEU:HD11 | 2:H:64:PHE:CD2 | 2.50 | 0.47 |
| 2:I:1148:ASN:ND2 | 2:I:1151:HIS:H | 2.13 | 0.47 |
| 1:B:1276:GLN:O | 1:B:1282:THR:HG21 | 2.14 | 0.47 |
| 1:A:406:TRP:CE3 | 1:A:1619:GLU:HG3 | 2.49 | 0.47 |
| 2:H:967:ILE:HD12 | 2:H:972:LEU:HD22 | 1.96 | 0.47 |
| 1:A:1158:PRO:HD2 | 1:A:1159:GLU:OE2 | 2.14 | 0.47 |
| 2:G:629:GLY:O | 2:G:632:ALA:HB3 | 2.15 | 0.47 |
| 1:B:253:ARG:O | 1:B:254:TRP:CD1 | 2.68 | 0.47 |
| 2:G:55:THR:HB | 2:G:59:GLU:OE2 | 2.14 | 0.47 |
| 1:B:1523:ARG:NH2 | 1:B:1564:LEU:O | 2.48 | 0.47 |
| 1:A:529:MET:HE3 | 1:A:529:MET:CA | 2.36 | 0.47 |
| 1:B:142:ASP:CG | 1:B:257:PRO:HB2 | 2.35 | 0.47 |
| 1:A:988:ILE:HD13 | 1:A:1048:GLU:HA | 1.97 | 0.47 |
| 2:G:1159:ILE:CG1 | 2:G:1169:PRO:CD | 2.93 | 0.47 |
| 2:H:1004:LEU:CD2 | 2:H:1019:PRO:HB2 | 2.44 | 0.47 |
| 2:I:194:THR:CG2 | 2:I:300:ILE:HD11 | 2.40 | 0.47 |
| 1:C:1544:THR:O | 1:C:1545:SER:HB3 | 2.15 | 0.47 |
| 2:H:826:GLY:HA3 | 2:H:1061:GLN:CB | 2.44 | 0.47 |
| 2:I:376:ASN:C | 2:I:376:ASN:ND2 | 2.68 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1873:TYR:CE2 | 2:G:1940:LEU:HD21 | 2.49 | 0.47 |
| 2:G:1666:PHE:CE1 | 2:G:1814:ALA:HA | 2.50 | 0.47 |
| 2:H:586:LEU:HD12 | 2:H:764:MET:SD | 2.55 | 0.47 |
| 2:I:42:PRO:HG2 | 2:I:52:ASP:CG | 2.35 | 0.47 |
| 2:I:1418:ASP:C | 2:I:1420:GLU:H | 2.18 | 0.47 |
| 2:H:127:ILE:HD12 | 2:H:180:TYR:HD2 | 1.80 | 0.47 |
| 2:H:131:ILE:CD1 | 2:H:182:VAL:CB | 2.71 | 0.47 |
| 2:G:730:LEU:C | 2:G:730:LEU:HD12 | 2.35 | 0.47 |
| 2:I:1553:TYR:OH | 2:I:1583:MET:HB3 | 2.15 | 0.47 |
| 2:G:826:GLY:HA2 | 2:G:1060:ALA:HB3 | 1.97 | 0.47 |
| 1:B:1305:CYS:SG | 3:B:2748:CER:H51 | 2.54 | 0.47 |
| 1:C:237:MET:HG3 | 1:C:241:PHE:HB3 | 1.95 | 0.47 |
| 1:C:1012:LEU:HD23 | 1:C:1445:MET:HE3 | 1.97 | 0.47 |
| 2:I:606:PHE:HZ | 2:I:805:VAL:CG1 | 2.28 | 0.47 |
| 1:C:18:LEU:HD21 | 2:I:1815:LEU:CD1 | 2.45 | 0.47 |
| 2:G:772:GLY:O | 2:G:804:ARG:HD3 | 2.15 | 0.47 |
| 2:G:1850:SER:HB2 | 2:G:1973:SER:HB2 | 1.96 | 0.47 |
| 2:I:490:TRP:HA | 2:I:493:THR:HG22 | 1.96 | 0.47 |
| 2:H:1054:LEU:HB2 | 4:H:3051:FMN:HM71 | 1.96 | 0.47 |
| 2:G:739:GLY:HA2 | 2:G:1054:LEU:HG | 1.97 | 0.47 |
| 1:B:254:TRP:HZ3 | 1:B:292:GLN:HG3 | 1.76 | 0.47 |
| 2:G:1844:ARG:NH1 | 2:G:1844:ARG:HG2 | 2.09 | 0.47 |
| 1:A:36:LEU:CD2 | 1:A:61:LEU:HD21 | 2.37 | 0.47 |
| 2:H:1764:PHE:HB2 | 2:H:1770:LEU:HD21 | 1.97 | 0.47 |
| 2:H:238:CYS:CB | 2:H:239:PRO:HD3 | 2.43 | 0.47 |
| 2:H:1015:VAL:HG11 | 2:H:1017:PHE:CE1 | 2.50 | 0.47 |
| 2:G:745:ASP:HA | 2:G:832:TRP:CH2 | 2.48 | 0.47 |
| 2:H:1473:THR:O | 2:H:1481:SER:HB3 | 2.15 | 0.47 |
| 1:B:32:GLN:NE2 | 1:B:57:ALA:HA | 2.29 | 0.47 |
| 1:C:1189:ILE:HG23 | 1:C:1190:PRO:HD2 | 1.97 | 0.47 |
| 1:B:1009:LEU:HD13 | 1:B:1445:MET:HE1 | 1.97 | 0.47 |
| 2:G:1493:LEU:HB3 | 2:G:1494:PRO:HD2 | 1.96 | 0.47 |
| 2:G:1273:GLU:HB3 | 2:G:1274:PRO:CD | 2.45 | 0.47 |
| 2:H:1428:GLU:HG2 | 2:H:1470:THR:HG22 | 1.97 | 0.47 |
| 2:H:1273:GLU:HB3 | 2:H:1274:PRO:CD | 2.45 | 0.47 |
| 2:I:1148:ASN:C | 2:I:1148:ASN:HD22 | 2.19 | 0.47 |
| 2:H:720:ALA:HA | 2:H:728:ILE:CD1 | 2.45 | 0.47 |
| 1:A:1830:GLY:HA2 | 1:A:1831:GLY:HA2 | 1.57 | 0.47 |
| 1:A:1430:ARG:HG2 | 1:A:1430:ARG:O | 2.15 | 0.47 |
| 1:B:883:ILE:HD12 | 1:B:947:LEU:HD12 | 1.97 | 0.47 |
| 2:G:881:VAL:N | 2:G:882:PRO:CD | 2.78 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:29:ILE:HG13 | 2:G:1891:TYR:O | 2.15 | 0.47 |
| 2:H:7:ARG:NH2 | 2:H:24:THR:O | 2.48 | 0.46 |
| 2:G:2035:SER:HB3 | 2:G:2038:ILE:CG1 | 2.41 | 0.46 |
| 2:I:533:LEU:HD13 | 2:I:545:GLN:HG3 | 1.97 | 0.46 |
| 1:C:930:LEU:CD2 | 1:C:933:VAL:HG11 | 2.45 | 0.46 |
| 1:B:1544:THR:O | 1:B:1545:SER:HB3 | 2.15 | 0.46 |
| 2:I:1913:VAL:O | 2:I:1917:ILE:HG13 | 2.15 | 0.46 |
| 2:G:1015:VAL:HG11 | 2:G:1017:PHE:CE1 | 2.50 | 0.46 |
| 2:I:99:ASN:HA | 2:I:550:VAL:HG23 | 1.97 | 0.46 |
| 2:I:573:LYS:C | 2:I:575:GLY:H | 2.19 | 0.46 |
| 1:A:186:ILE:O | 1:A:190:LEU:HG | 2.14 | 0.46 |
| 2:G:249:TYR:CD2 | 2:G:283:ILE:HD11 | 2.50 | 0.46 |
| 1:C:709:ARG:O | 1:C:714:VAL:HG21 | 2.16 | 0.46 |
| 2:H:440:ASN:ND2 | 2:H:477:GLU:HG2 | 2.30 | 0.46 |
| 1:A:702:LYS:HD3 | 1:A:731:THR:CG2 | 2.44 | 0.46 |
| 2:G:598:THR:CB | 2:G:599:PRO:HD3 | 2.46 | 0.46 |
| 2:G:652:ILE:HD12 | 2:G:652:ILE:N | 2.29 | 0.46 |
| 1:C:1303:GLY:C | 1:C:1307:THR:HG22 | 2.35 | 0.46 |
| 2:G:1293:THR:HG22 | 2:G:1296:GLU:CD | 2.35 | 0.46 |
| 2:I:345:THR:HG22 | 2:I:347:GLU:N | 2.23 | 0.46 |
| 1:A:1238:VAL:CG1 | 1:A:1239:HIS:N | 2.78 | 0.46 |
| 1:C:499:PRO:HD3 | 1:C:516:ARG:HH21 | 1.80 | 0.46 |
| 2:G:751:LEU:HA | 2:G:794:MET:HE3 | 1.96 | 0.46 |
| 1:A:1056:ILE:HG13 | 1:A:1057:MET:N | 2.30 | 0.46 |
| 1:A:183:GLN:NE2 | 1:A:202:GLU:HG2 | 2.29 | 0.46 |
| 2:H:218:TRP:HB3 | 2:H:225:THR:OG1 | 2.15 | 0.46 |
| 2:I:758:ARG:NH2 | 2:I:797:ASP:OD1 | 2.38 | 0.46 |
| 1:C:1646:PHE:CE1 | 3:C:2748:CER:H31 | 2.50 | 0.46 |
| 2:H:1258:ARG:O | 2:H:1262:ILE:HG13 | 2.15 | 0.46 |
| 2:H:736:ARG:H | 2:H:736:ARG:HG3 | 1.55 | 0.46 |
| 2:H:926:LEU:HB3 | 2:H:947:THR:HG22 | 1.97 | 0.46 |
| 2:H:1804:PHE:CD2 | 2:H:1818:LEU:HD22 | 2.50 | 0.46 |
| 2:I:1148:ASN:HD22 | 2:I:1151:HIS:H | 1.63 | 0.46 |
| 2:G:279:THR:O | 2:G:283:ILE:HB | 2.15 | 0.46 |
| 1:A:908:LEU:HA | 1:A:913:VAL:HG21 | 1.96 | 0.46 |
| 2:I:1080:GLY:O | 2:I:1084:LYS:HG3 | 2.15 | 0.46 |
| 2:H:1269:LEU:O | 2:H:1560:LEU:HD23 | 2.15 | 0.46 |
| 2:H:101:ILE:H | 2:H:101:ILE:HG13 | 1.30 | 0.46 |
| 1:C:293:LYS:O | 1:C:297:ILE:HG13 | 2.15 | 0.46 |
| 2:I:213:LEU:HG | 2:I:213:LEU:O | 2.16 | 0.46 |
| 1:B:1133:PRO:HG3 | 1:B:1166:LYS:HG3 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:598:THR:CB | 2:H:599:PRO:HD3 | 2.44 | 0.46 |
| 2:G:7:ARG:NH2 | 2:G:24:THR:O | 2.48 | 0.46 |
| 2:G:9:LEU:HB2 | 2:G:27:PHE:HE1 | 1.81 | 0.46 |
| 2:G:1422:THR:HG23 | 2:G:1474:PHE:CD1 | 2.51 | 0.46 |
| 1:B:1303:GLY:C | 1:B:1307:THR:HG22 | 2.35 | 0.46 |
| 1:B:1239:HIS:CD2 | 1:B:1241:SER:H | 2.33 | 0.46 |
| 1:B:14:LEU:HD11 | 2:H:1821:VAL:HG11 | 1.97 | 0.46 |
| 2:H:1552:PRO:O | 2:H:1556:VAL:HG23 | 2.15 | 0.46 |
| 2:I:826:GLY:HA3 | 2:I:1061:GLN:CB | 2.46 | 0.46 |
| 2:G:826:GLY:HA3 | 2:G:1061:GLN:CB | 2.44 | 0.46 |
| 2:I:1593:ILE:HD13 | 2:I:1626:ILE:HD13 | 1.97 | 0.46 |
| 2:H:350:GLN:HA | 2:H:353:VAL:HG13 | 1.97 | 0.46 |
| 1:B:237:MET:HG3 | 1:B:241:PHE:HB3 | 1.97 | 0.46 |
| 1:A:232:LEU:HD13 | 1:A:272:GLU:CB | 2.44 | 0.46 |
| 1:C:420:ILE:HG22 | 1:C:469:VAL:HG22 | 1.96 | 0.46 |
| 1:B:1639:VAL:CG1 | 1:B:1640:SER:N | 2.79 | 0.46 |
| 2:H:1359:MET:CE | 2:H:1404:MET:HB3 | 2.44 | 0.46 |
| 2:G:1579:ILE:HG22 | 2:G:1580:THR:O | 2.15 | 0.46 |
| 2:H:1945:ASP:O | 2:H:1949:LYS:HG3 | 2.15 | 0.46 |
| 1:A:702:LYS:HE2 | 1:A:729:GLY:O | 2.15 | 0.46 |
| 2:H:1079:ASP:O | 2:H:1082:ILE:HG22 | 2.16 | 0.46 |
| 1:C:908:LEU:HA | 1:C:913:VAL:HG21 | 1.96 | 0.46 |
| 1:C:186:ILE:O | 1:C:190:LEU:HG | 2.15 | 0.46 |
| 1:C:1004:ILE:HG22 | 1:C:1660:TYR:CE2 | 2.49 | 0.46 |
| 2:H:879:LYS:HA | 2:H:879:LYS:HD3 | 1.71 | 0.46 |
| 2:H:72:VAL:HG12 | 2:H:73:GLU:N | 2.30 | 0.46 |
| 1:B:1114:TYR:CD1 | 1:B:1337:GLU:HG3 | 2.50 | 0.46 |
| 2:I:1624:THR:HB | 2:I:1642:THR:CG2 | 2.43 | 0.46 |
| 2:I:131:ILE:HG21 | 2:I:182:VAL:HG12 | 1.97 | 0.46 |
| 1:A:338:LEU:O | 1:A:342:GLN:HG3 | 2.16 | 0.46 |
| 2:I:1764:PHE:HB2 | 2:I:1770:LEU:HD21 | 1.97 | 0.46 |
| 2:G:355:LYS:HE2 | 2:G:355:LYS:HB3 | 1.64 | 0.46 |
| 1:C:1238:VAL:CG1 | 1:C:1242:GLU:HB2 | 2.45 | 0.46 |
| 1:A:1544:THR:O | 1:A:1545:SER:HB3 | 2.15 | 0.46 |
| 2:H:573:LYS:HE3 | 2:H:1101:GLU:OE1 | 2.15 | 0.46 |
| 2:G:1749:GLU:OE2 | 2:G:1840:VAL:HG13 | 2.16 | 0.46 |
| 2:H:1266:TYR:HB2 | 2:H:1347:LEU:HD23 | 1.97 | 0.46 |
| 1:B:1305:CYS:SG | 1:B:1585:LYS:HA | 2.56 | 0.46 |
| 2:H:807:ILE:HD12 | 2:H:1063:THR:HG23 | 1.96 | 0.46 |
| 1:A:1646:PHE:CE1 | 3:A:2748:CER:H31 | 2.50 | 0.46 |
| 1:A:986:ALA:CB | 1:A:1047:LEU:HD13 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:451:MET:HE2 | 1:C:451:MET:HB3 | 1.71 | 0.46 |
| 1:A:1639:VAL:CG1 | 1:A:1640:SER:N | 2.78 | 0.46 |
| 2:H:1908:ASP:HA | 2:H:1911:THR:HG22 | 1.98 | 0.46 |
| 2:H:1666:PHE:CD1 | 2:H:1814:ALA:HB2 | 2.49 | 0.46 |
| 2:H:42:PRO:HG2 | 2:H:52:ASP:CG | 2.36 | 0.46 |
| 2:I:1272:ASP:O | 2:I:1273:GLU:HG3 | 2.15 | 0.46 |
| 1:B:741:SER:HB3 | 1:B:744:ASP:HB2 | 1.97 | 0.46 |
| 2:H:881:VAL:N | 2:H:882:PRO:CD | 2.79 | 0.46 |
| 1:C:784:ILE:HG23 | 1:C:788:SER:HB2 | 1.98 | 0.46 |
| 2:G:1834:ARG:NH1 | 2:G:1834:ARG:CG | 2.68 | 0.46 |
| 1:C:256:LEU:HA | 1:C:257:PRO:HD3 | 1.72 | 0.46 |
| 2:H:1567:ARG:NH1 | 2:H:1568:HIS:HB3 | 2.29 | 0.46 |
| 1:C:2:LYS:HE2 | 1:C:4:GLU:CD | 2.35 | 0.46 |
| 2:G:702:TYR:HB3 | 2:G:727:PRO:HB2 | 1.97 | 0.46 |
| 2:H:1441:ILE:HD11 | 2:H:1445:ARG:NH2 | 2.27 | 0.46 |
| 2:H:1169:PRO:O | 2:H:1173:VAL:HG23 | 2.15 | 0.46 |
| 2:I:584:SER:CB | 2:I:591:PRO:HG3 | 2.41 | 0.46 |
| 2:H:1638:ILE:HD12 | 2:H:1657:ILE:CG1 | 2.43 | 0.46 |
| 2:G:455:ILE:O | 2:G:455:ILE:HG13 | 2.14 | 0.46 |
| 2:G:109:LEU:HD11 | 2:G:116:LEU:CD2 | 2.41 | 0.46 |
| 2:H:1195:VAL:HG13 | 2:H:1211:LEU:CB | 2.44 | 0.46 |
| 1:B:183:GLN:NE2 | 1:B:202:GLU:HG2 | 2.29 | 0.46 |
| 1:B:1618:LEU:HD23 | 1:B:1621:PHE:CE2 | 2.51 | 0.46 |
| 1:B:451:MET:HE2 | 1:B:451:MET:HB3 | 1.73 | 0.46 |
| 1:A:26:VAL:CG2 | 2:G:1890:ASN:ND2 | 2.78 | 0.46 |
| 2:G:873:PHE:CD1 | 2:G:1026:GLU:HB2 | 2.50 | 0.46 |
| 2:I:1666:PHE:CD1 | 2:I:1814:ALA:HA | 2.50 | 0.46 |
| 1:A:1050:CYS:HB3 | 1:A:1089:VAL:HG12 | 1.98 | 0.46 |
| 1:C:1367:ARG:HH12 | 1:C:1372:THR:CB | 2.20 | 0.46 |
| 2:I:2026:PHE:HB3 | 2:I:2042:ILE:HD13 | 1.98 | 0.46 |
| 2:I:843:ILE:HD11 | 2:I:1055:HIS:HB3 | 1.98 | 0.46 |
| 2:G:1886:VAL:HG22 | 2:G:1906:ALA:HB1 | 1.97 | 0.46 |
| 1:C:1533:ILE:HD11 | 1:C:1564:LEU:HD13 | 1.98 | 0.46 |
| 2:G:844:VAL:HG22 | 2:G:858:ALA:HB2 | 1.98 | 0.46 |
| 1:B:1303:GLY:CA | 1:B:1649:LYS:HE2 | 2.40 | 0.46 |
| 1:A:2:LYS:HE2 | 1:A:4:GLU:CD | 2.36 | 0.46 |
| 2:G:719:ILE:H | 2:G:719:ILE:HG12 | 1.57 | 0.46 |
| 2:G:669:LEU:HD12 | 2:G:669:LEU:HA | 1.62 | 0.46 |
| 2:G:209:PHE:CE2 | 2:G:213:LEU:HD22 | 2.51 | 0.46 |
| 2:H:582:LYS:HE2 | 2:H:761:PRO:O | 2.16 | 0.46 |
| 1:B:702:LYS:HE2 | 1:B:729:GLY:O | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:243:ILE:O | 1:C:247:ARG:HG3 | 2.16 | 0.46 |
| 2:I:1071:LYS:HE3 | 2:I:1075:ASP:OD2 | 2.14 | 0.46 |
| 1:C:1362:PRO:HA | 1:C:1365:MET:HG3 | 1.97 | 0.46 |
| 2:G:309:ARG:HA | 2:G:309:ARG:HD3 | 1.64 | 0.46 |
| 2:I:1932:SER:O | 2:I:1936:VAL:HG22 | 2.16 | 0.46 |
| 2:H:321:PRO:HD2 | 2:I:1599:ASP:OD1 | 2.16 | 0.46 |
| 2:G:214:ASN:ND2 | 2:G:217:GLU:HB2 | 2.30 | 0.46 |
| 2:G:441:LYS:O | 2:G:444:VAL:HG12 | 2.15 | 0.46 |
| 1:A:170:LYS:HD3 | 1:A:175:LEU:HD23 | 1.97 | 0.46 |
| 1:C:1319:ILE:HA | 1:C:1324:ALA:O | 2.14 | 0.46 |
| 2:H:1180:MET:HB2 | 2:H:1197:LEU:HD21 | 1.98 | 0.46 |
| 2:H:845:THR:HG22 | 2:H:855:HIS:CD2 | 2.51 | 0.46 |
| 2:H:1624:THR:HB | 2:H:1642:THR:CG2 | 2.45 | 0.46 |
| 1:B:11:HIS:C | 1:B:11:HIS:CD2 | 2.89 | 0.46 |
| 1:A:1617:ILE:O | 1:A:1620:GLN:HG2 | 2.16 | 0.46 |
| 2:I:109:LEU:HD11 | 2:I:116:LEU:CD2 | 2.43 | 0.46 |
| 2:I:109:LEU:HD22 | 2:I:114:THR:HG23 | 1.96 | 0.46 |
| 2:I:653:TYR:HD1 | 2:I:659:LEU:HD21 | 1.79 | 0.46 |
| 2:G:1378:ILE:O | 2:G:1378:ILE:HG12 | 2.13 | 0.46 |
| 1:A:1270:VAL:HG11 | 1:A:1274:ILE:HD13 | 1.97 | 0.46 |
| 2:I:860:ARG:HB2 | 2:I:1049:GLN:HG3 | 1.97 | 0.46 |
| 2:I:589:ARG:HB3 | 2:I:590:PRO:CD | 2.43 | 0.46 |
| 1:C:1577:GLN:NE2 | 1:C:1591:TRP:HB3 | 2.30 | 0.46 |
| 1:C:1233:GLU:CD | 1:C:1680:ARG:HH21 | 2.19 | 0.46 |
| 2:H:653:TYR:HD1 | 2:H:659:LEU:HD21 | 1.80 | 0.46 |
| 1:C:1263:ASP:HB2 | 1:C:1270:VAL:HG21 | 1.98 | 0.46 |
| 2:H:306:ILE:HA | 2:H:439:ILE:HD13 | 1.96 | 0.46 |
| 2:I:1418:ASP:C | 2:I:1420:GLU:N | 2.68 | 0.46 |
| 2:G:553:ASN:O | 2:G:556:LYS:HE3 | 2.16 | 0.46 |
| 2:H:1738:PHE:CE1 | 2:H:1837:THR:HG23 | 2.50 | 0.46 |
| 1:A:1487:LEU:C | 1:A:1487:LEU:HD23 | 2.35 | 0.46 |
| 2:H:1850:SER:HB2 | 2:H:1973:SER:HB2 | 1.97 | 0.46 |
| 1:C:774:ILE:HA | 1:C:775:PRO:HD3 | 1.74 | 0.46 |
| 2:H:481:ASP:OD2 | 2:H:485:ARG:NH1 | 2.48 | 0.46 |
| 1:B:792:HIS:CE1 | 1:B:796:LEU:HD23 | 2.51 | 0.46 |
| 2:H:1858:ASN:HA | 2:H:1896:GLN:O | 2.16 | 0.46 |
| 1:A:709:ARG:O | 1:A:714:VAL:HG21 | 2.16 | 0.46 |
| 2:G:1854:MET:CG | 2:G:1901:ALA:HB2 | 2.46 | 0.46 |
| 2:I:490:TRP:CZ2 | 2:I:512:LEU:HD21 | 2.51 | 0.46 |
| 2:G:131:ILE:CG2 | 2:G:182:VAL:HG11 | 2.43 | 0.46 |
| 2:G:2037:PRO:O | 2:G:2041:ILE:HG13 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1180:MET:HB3 | 2:I:1199:GLU:HG2 | 1.98 | 0.46 |
| 2:H:1651:LEU:O | 2:H:1652:THR:HG23 | 2.16 | 0.46 |
| 2:G:845:THR:HG22 | 2:G:855:HIS:CD2 | 2.50 | 0.46 |
| 2:G:1168:ASN:HA | 2:G:1169:PRO:HD3 | 1.81 | 0.46 |
| 1:A:427:ASN:ND2 | 1:A:610:THR:H | 2.08 | 0.46 |
| 2:G:785:TRP:CG | 2:G:786:SER:N | 2.83 | 0.46 |
| 2:H:60:LEU:O | 2:H:63:LYS:HB2 | 2.16 | 0.46 |
| 2:G:1303:ALA:HB2 | 2:G:1556:VAL:HG21 | 1.98 | 0.46 |
| 2:H:1491:VAL:HB | 2:H:1501:ILE:CD1 | 2.45 | 0.46 |
| 1:B:1021:VAL:HG22 | 1:B:1387:ILE:HG22 | 1.98 | 0.46 |
| 1:A:37:LYS:HB2 | 1:A:65:TYR:CE1 | 2.48 | 0.46 |
| 1:A:49:PRO:O | 1:A:82:SER:HB2 | 2.16 | 0.46 |
| 2:H:551:THR:HG22 | 2:H:552:SER:N | 2.30 | 0.46 |
| 2:H:1427:VAL:HG22 | 2:H:1469:GLU:HG2 | 1.96 | 0.46 |
| 2:G:955:GLU:HG2 | 2:G:987:TYR:HE2 | 1.80 | 0.46 |
| 2:H:1873:TYR:CE1 | 2:H:1877:ARG:NE | 2.77 | 0.46 |
| 1:C:182:VAL:O | 1:C:186:ILE:HG13 | 2.16 | 0.46 |
| 2:H:1846:GLU:C | 2:H:1848:GLY:H | 2.19 | 0.46 |
| 2:I:1543:ASP:OD1 | 2:I:1623:LYS:HG2 | 2.15 | 0.46 |
| 1:B:1595:GLY:O | 1:B:1599:ILE:HG13 | 2.15 | 0.46 |
| 2:H:1344:ASP:O | 2:H:1416:TYR:HE2 | 1.99 | 0.46 |
| 2:H:490:TRP:CZ2 | 2:H:512:LEU:HD21 | 2.51 | 0.46 |
| 1:C:11:HIS:C | 1:C:11:HIS:CD2 | 2.89 | 0.46 |
| 2:H:1227:ARG:NE | 2:H:1565:VAL:HG12 | 2.30 | 0.46 |
| 2:H:702:TYR:HB3 | 2:H:727:PRO:HB2 | 1.97 | 0.46 |
| 1:A:35:PHE:HA | 1:A:39:PHE:HD2 | 1.81 | 0.46 |
| 1:A:331:ILE:HG23 | 1:A:332:THR:N | 2.31 | 0.46 |
| 2:I:1054:LEU:HB3 | 4:I:3051:FMN:HM82 | 1.98 | 0.46 |
| 2:G:123:ILE:HD11 | 2:G:533:LEU:HD22 | 1.98 | 0.46 |
| 1:C:1209:ASP:OD2 | 1:C:1253:GLY:HA2 | 2.16 | 0.46 |
| 2:G:1418:ASP:O | 2:G:1421:ASN:N | 2.43 | 0.46 |
| 2:H:1374:THR:HG23 | 2:H:1396:LEU:CD1 | 2.46 | 0.46 |
| 2:I:860:ARG:H | 2:I:1049:GLN:HG3 | 1.80 | 0.46 |
| 2:H:1236:LEU:HA | 2:H:1237:PRO:HD3 | 1.78 | 0.46 |
| 2:I:1031:LYS:O | 2:I:1032:ASP:C | 2.54 | 0.46 |
| 1:A:489:VAL:CG2 | 1:A:670:GLY:C | 2.84 | 0.46 |
| 2:I:740:HIS:HE1 | 2:I:852:GLU:OE1 | 1.99 | 0.46 |
| 2:I:1418:ASP:O | 2:I:1420:GLU:N | 2.49 | 0.46 |
| 2:G:970:TYR:O | 2:G:973:LEU:HB2 | 2.16 | 0.46 |
| 1:A:507:GLY:N | 1:A:954:ARG:HG2 | 2.31 | 0.46 |
| 2:I:1228:THR:HG21 | 2:I:1234:VAL:HG23 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1196:LYS:HE3 | 1:C:1202:ASP:CG | 2.37 | 0.46 |
| 2:I:844:VAL:HG22 | 2:I:858:ALA:HB2 | 1.97 | 0.46 |
| 2:I:670:ARG:HD2 | 2:I:676:ILE:O | 2.16 | 0.46 |
| 1:B:143:GLU:H | 1:B:260:ARG:HG2 | 1.81 | 0.46 |
| 2:H:913:ASP:H | 2:H:916:THR:CG2 | 2.29 | 0.46 |
| 1:C:1459:ILE:O | 1:C:1463:VAL:HG23 | 2.16 | 0.46 |
| 2:I:1282:ARG:NH2 | 2:I:1423:PHE:HB3 | 2.31 | 0.46 |
| 2:G:1002:HIS:NE2 | 2:G:1006:MET:CE | 2.79 | 0.46 |
| 2:I:751:LEU:HD11 | 2:I:789:PHE:CD1 | 2.51 | 0.46 |
| 2:I:785:TRP:CG | 2:I:786:SER:N | 2.84 | 0.46 |
| 2:I:232:LEU:HD21 | 2:I:423:VAL:HA | 1.98 | 0.46 |
| 2:I:1561:ASN:OD1 | 2:I:1563:ILE:HB | 2.15 | 0.46 |
| 2:I:1222:GLU:HG3 | 2:I:1235:SER:OG | 2.16 | 0.46 |
| 2:G:1311:PHE:HD1 | 2:G:1320:LEU:O | 1.99 | 0.46 |
| 2:I:391:LEU:CD2 | 2:I:394:ARG:NH2 | 2.78 | 0.46 |
| 1:A:386:PHE:O | 1:A:390:VAL:HB | 2.16 | 0.46 |
| 1:C:539:SER:O | 1:C:540:GLN:C | 2.52 | 0.46 |
| 2:H:1021:LEU:HA | 2:H:1021:LEU:HD22 | 1.58 | 0.46 |
| 2:G:1435:ILE:O | 2:G:1435:ILE:HG22 | 2.15 | 0.46 |
| 1:A:1709:GLU:HG3 | 1:A:1709:GLU:H | 1.46 | 0.46 |
| 2:G:233:SER:HA | 2:G:424:ALA:CB | 2.46 | 0.46 |
| 1:B:601:VAL:O | 1:B:602:GLU:C | 2.54 | 0.46 |
| 2:G:159:ILE:CG2 | 2:G:501:ILE:HG22 | 2.46 | 0.45 |
| 2:H:1135:GLU:OE2 | 2:H:1175:LYS:HE3 | 2.15 | 0.45 |
| 1:C:400:ARG:HH11 | 1:C:400:ARG:HG3 | 1.72 | 0.45 |
| 1:A:1533:ILE:HG13 | 1:A:1564:LEU:HB3 | 1.98 | 0.45 |
| 2:H:730:LEU:HD12 | 2:H:730:LEU:C | 2.36 | 0.45 |
| 1:B:516:ARG:NH2 | 1:B:889:GLU:OE1 | 2.49 | 0.45 |
| 2:H:2026:PHE:HB3 | 2:H:2042:ILE:HD13 | 1.98 | 0.45 |
| 2:I:738:GLY:HA3 | 4:I:3051:FMN:HM81 | 1.98 | 0.45 |
| 1:B:881:ASN:HA | 1:B:944:ARG:HH22 | 1.78 | 0.45 |
| 2:H:1593:ILE:HD13 | 2:H:1626:ILE:HD13 | 1.97 | 0.45 |
| 1:C:1040:GLU:HB2 | 1:C:1580:LEU:HD12 | 1.98 | 0.45 |
| 1:C:1376:PHE:CB | 1:C:1544:THR:HG22 | 2.45 | 0.45 |
| 2:G:1738:PHE:CD1 | 2:G:1837:THR:HG23 | 2.51 | 0.45 |
| 1:A:411:GLN:NE2 | 1:A:1628:SER:H | 2.13 | 0.45 |
| 2:H:1388:LYS:HE3 | 2:H:1418:ASP:OD2 | 2.16 | 0.45 |
| 2:H:1417:THR:C | 2:H:1419:PHE:H | 2.19 | 0.45 |
| 1:B:1234:MET:HG2 | 1:B:1326:ILE:CD1 | 2.46 | 0.45 |
| 2:I:807:ILE:HD12 | 2:I:1063:THR:HG23 | 1.98 | 0.45 |
| 2:H:391:LEU:CD2 | 2:H:394:ARG:NH2 | 2.80 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1873:TYR:CE1 | 2:H:1877:ARG:NH2 | 2.83 | 0.45 |
| 2:H:1666:PHE:CE1 | 2:H:1814:ALA:HA | 2.50 | 0.45 |
| 2:H:1031:LYS:O | 2:H:1032:ASP:C | 2.54 | 0.45 |
| 2:G:1586:SER:O | 2:G:1590:ARG:HB2 | 2.16 | 0.45 |
| 1:A:1557:ILE:HD11 | 1:A:1642:THR:HG21 | 1.97 | 0.45 |
| 1:C:1573:ILE:HG23 | 1:C:1627:PRO:HG3 | 1.98 | 0.45 |
| 1:A:792:HIS:CE1 | 1:A:796:LEU:HD23 | 2.51 | 0.45 |
| 2:I:601:THR:HB | 2:I:620:ALA:HB2 | 1.98 | 0.45 |
| 2:H:612:ASN:HD21 | 2:H:641:ILE:HA | 1.81 | 0.45 |
| 2:I:369:SER:O | 2:I:370:LEU:HD23 | 2.16 | 0.45 |
| 1:C:529:MET:CE | 1:C:894:ARG:HD2 | 2.46 | 0.45 |
| 2:G:1673:GLU:N | 2:G:1676:MET:HE3 | 2.25 | 0.45 |
| 2:G:1219:ILE:HD11 | 2:G:1242:PHE:HB2 | 1.98 | 0.45 |
| 2:G:191:SER:HA | 2:G:194:THR:CG2 | 2.46 | 0.45 |
| 2:G:161:GLY:HA3 | 2:G:506:PRO:HD2 | 1.98 | 0.45 |
| 1:B:2:LYS:HE2 | 1:B:4:GLU:OE1 | 2.15 | 0.45 |
| 2:G:1976:PHE:HA | 2:G:1981:LEU:CD2 | 2.46 | 0.45 |
| 1:B:26:VAL:HG13 | 2:H:2013:ASN:ND2 | 2.31 | 0.45 |
| 1:A:408:TRP:CZ3 | 1:A:1628:SER:HB3 | 2.51 | 0.45 |
| 1:B:1431:GLU:OE2 | 1:B:1433:HIS:HE1 | 2.00 | 0.45 |
| 2:G:1472:VAL:CG2 | 2:G:1483:VAL:HG22 | 2.46 | 0.45 |
| 2:H:324:LEU:O | 2:H:324:LEU:HD12 | 2.16 | 0.45 |
| 2:G:1222:GLU:HG3 | 2:G:1235:SER:OG | 2.16 | 0.45 |
| 2:I:669:LEU:HA | 2:I:669:LEU:HD12 | 1.65 | 0.45 |
| 2:H:1579:ILE:HG22 | 2:H:1580:THR:O | 2.16 | 0.45 |
| 1:A:1114:TYR:CE1 | 1:A:1337:GLU:HG3 | 2.50 | 0.45 |
| 2:I:1359:MET:HE3 | 2:I:1404:MET:HB3 | 1.98 | 0.45 |
| 1:C:430:ARG:NH2 | 1:C:605:LEU:HD13 | 2.31 | 0.45 |
| 1:B:719:GLN:HG3 | 1:B:720:SER:N | 2.31 | 0.45 |
| 1:C:170:LYS:HD3 | 1:C:175:LEU:HD23 | 1.97 | 0.45 |
| 2:H:246:LEU:HD12 | 2:H:246:LEU:HA | 1.85 | 0.45 |
| 2:H:1768:LYS:HE2 | 2:H:1772:SER:HB3 | 1.98 | 0.45 |
| 1:A:764:ASP:OD2 | 1:A:818:ARG:HD3 | 2.17 | 0.45 |
| 1:B:19:ALA:O | 1:B:22:PHE:HB2 | 2.15 | 0.45 |
| 2:I:618:GLU:HG2 | 2:I:678:PHE:CZ | 2.51 | 0.45 |
| 1:A:1367:ARG:HH12 | 1:A:1372:THR:CB | 2.18 | 0.45 |
| 2:I:1180:MET:HB2 | 2:I:1197:LEU:HD21 | 1.97 | 0.45 |
| 1:B:444:ASN:HB2 | 1:B:447:LEU:N | 2.15 | 0.45 |
| 1:A:1431:GLU:OE2 | 1:A:1523:ARG:NH1 | 2.48 | 0.45 |
| 2:I:739:GLY:HA2 | 2:I:1054:LEU:HG | 1.97 | 0.45 |
| 2:I:1854:MET:CG | 2:I:1901:ALA:HB2 | 2.47 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1776:PHE:C | 2:H:1779:PRO:HD2 | 2.37 | 0.45 |
| 2:G:562:LEU:HG | 2:G:793:PRO:CG | 2.43 | 0.45 |
| 1:A:751:PHE:CZ | 1:A:761:LEU:HD13 | 2.51 | 0.45 |
| 2:H:562:LEU:HG | 2:H:793:PRO:CB | 2.47 | 0.45 |
| 2:G:247:ALA:O | 2:G:251:VAL:HG13 | 2.15 | 0.45 |
| 2:G:460:TYR:HA | 2:G:466:SER:O | 2.17 | 0.45 |
| 1:B:37:LYS:HB2 | 1:B:65:TYR:CE1 | 2.51 | 0.45 |
| 2:G:860:ARG:HB2 | 2:G:1049:GLN:HG3 | 1.97 | 0.45 |
| 1:B:1639:VAL:HG12 | 1:B:1640:SER:N | 2.31 | 0.45 |
| 2:H:439:ILE:HD12 | 2:H:484:ILE:CD1 | 2.46 | 0.45 |
| 1:C:827:SER:HA | 1:C:828:PRO:HD3 | 1.70 | 0.45 |
| 1:A:18:LEU:HD21 | 2:G:1815:LEU:CD1 | 2.46 | 0.45 |
| 1:C:982:ILE:HD11 | 2:I:965:SER:CB | 2.46 | 0.45 |
| 2:H:1590:ARG:HG3 | 2:H:1608:TYR:CD2 | 2.51 | 0.45 |
| 2:I:1775:GLN:HG2 | 2:I:1836:MET:SD | 2.57 | 0.45 |
| 2:G:1953:VAL:O | 2:G:1953:VAL:HG12 | 2.16 | 0.45 |
| 2:H:249:TYR:CD2 | 2:H:283:ILE:HD11 | 2.52 | 0.45 |
| 1:B:235:SER:HA | 1:B:276:ARG:NH2 | 2.32 | 0.45 |
| 2:H:601:THR:O | 2:H:601:THR:CG2 | 2.65 | 0.45 |
| 2:G:1844:ARG:HA | 2:G:1849:ARG:O | 2.16 | 0.45 |
| 2:I:1199:GLU:OE2 | 2:I:1567:ARG:CZ | 2.65 | 0.45 |
| 2:H:835:THR:CB | 2:H:845:THR:HG23 | 2.43 | 0.45 |
| 1:C:1533:ILE:HG13 | 1:C:1564:LEU:HB3 | 1.98 | 0.45 |
| 1:A:168:MET:HA | 1:A:206:LEU:HB2 | 1.98 | 0.45 |
| 2:G:1314:ARG:HA | 2:G:1314:ARG:HD3 | 1.62 | 0.45 |
| 1:B:1310:GLU:OE1 | 1:B:1649:LYS:CE | 2.62 | 0.45 |
| 2:I:1327:ILE:HA | 2:I:1327:ILE:HD12 | 1.80 | 0.45 |
| 2:G:1015:VAL:HG13 | 2:G:1017:PHE:CE2 | 2.52 | 0.45 |
| 1:A:413:LEU:C | 1:A:415:SER:H | 2.18 | 0.45 |
| 1:B:32:GLN:NE2 | 1:B:57:ALA:CA | 2.80 | 0.45 |
| 2:G:807:ILE:HA | 2:G:818:LYS:HG2 | 1.97 | 0.45 |
| 2:I:463:PHE:CE1 | 2:I:486:LEU:HD22 | 2.51 | 0.45 |
| 2:H:463:PHE:CD2 | 2:H:463:PHE:C | 2.90 | 0.45 |
| 1:B:988:ILE:HD13 | 1:B:1048:GLU:CB | 2.47 | 0.45 |
| 1:A:625:THR:HG23 | 1:A:627:SER:H | 1.82 | 0.45 |
| 2:G:582:LYS:HE2 | 2:G:1108:PRO:HB3 | 1.97 | 0.45 |
| 2:G:1148:ASN:HD22 | 2:G:1151:HIS:H | 1.63 | 0.45 |
| 1:A:630:ILE:O | 1:A:653:ARG:NH2 | 2.48 | 0.45 |
| 2:H:1735:ALA:O | 2:H:1737:ILE:HG13 | 2.16 | 0.45 |
| 2:I:1609:THR:O | 2:I:1653:GLY:HA3 | 2.16 | 0.45 |
| 1:A:798:ASN:HA | 1:A:801:ARG:HB2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:24:THR:O | 2:H:26:SER:N | 2.49 | 0.45 |
| 1:B:1464:GLU:HG3 | 1:B:1773:VAL:HG11 | 1.91 | 0.45 |
| 2:I:2036:GLU:HG2 | 2:I:2039:LYS:HZ3 | 1.82 | 0.45 |
| 2:H:611:THR:HA | 2:H:615:TYR:O | 2.16 | 0.45 |
| 2:I:1776:PHE:C | 2:I:1779:PRO:HD2 | 2.37 | 0.45 |
| 2:H:754:TYR:CE2 | 2:H:794:MET:HG3 | 2.52 | 0.45 |
| 1:B:1376:PHE:CB | 1:B:1544:THR:HG22 | 2.45 | 0.45 |
| 1:A:143:GLU:H | 1:A:260:ARG:HG2 | 1.81 | 0.45 |
| 2:G:357:ASN:OD1 | 2:G:365:GLN:HB3 | 2.16 | 0.45 |
| 2:I:1976:PHE:CB | 2:I:1981:LEU:CD2 | 2.94 | 0.45 |
| 1:A:1196:LYS:HE3 | 1:A:1202:ASP:CG | 2.36 | 0.45 |
| 2:I:894:ARG:NH1 | 2:I:898:ASP:OD2 | 2.42 | 0.45 |
| 2:H:1383:ASN:HD21 | 2:H:1418:ASP:CB | 2.30 | 0.45 |
| 2:H:659:LEU:HA | 2:H:659:LEU:HD12 | 1.82 | 0.45 |
| 1:C:1682:LYS:HB3 | 2:I:994:PHE:CD2 | 2.51 | 0.45 |
| 1:B:1020:VAL:CG1 | 1:B:1400:ILE:HG23 | 2.46 | 0.45 |
| 1:C:1104:ARG:O | 1:C:1185:VAL:HG13 | 2.17 | 0.45 |
| 2:H:1027:ILE:O | 2:H:1031:LYS:HB2 | 2.16 | 0.45 |
| 1:A:293:LYS:O | 1:A:297:ILE:HG13 | 2.16 | 0.45 |
| 2:H:319:LEU:HD22 | 2:H:319:LEU:HA | 1.68 | 0.45 |
| 2:I:938:TRP:CD1 | 2:I:944:ARG:HG3 | 2.52 | 0.45 |
| 1:B:1019:ILE:HG21 | 1:B:1316:VAL:HG22 | 1.98 | 0.45 |
| 1:B:1061:SER:HB2 | 1:B:1078:SER:HB3 | 1.99 | 0.45 |
| 1:C:776:GLU:OE1 | 1:C:795:MET:HE1 | 2.17 | 0.45 |
| 2:H:618:GLU:HG2 | 2:H:678:PHE:CZ | 2.52 | 0.45 |
| 1:C:143:GLU:H | 1:C:260:ARG:HG2 | 1.81 | 0.45 |
| 1:C:197:THR:HG22 | 1:C:198:PRO:O | 2.15 | 0.45 |
| 2:G:315:PRO:O | 2:H:1314:ARG:NH2 | 2.50 | 0.45 |
| 1:B:1533:ILE:HD11 | 1:B:1564:LEU:HD13 | 1.98 | 0.45 |
| 1:A:1120:GLU:O | 1:A:1121:MET:HG3 | 2.16 | 0.45 |
| 2:H:1085:LEU:HD12 | 2:H:1085:LEU:HA | 1.85 | 0.45 |
| 1:B:332:THR:HG22 | 1:C:331:ILE:HD11 | 1.98 | 0.45 |
| 2:H:1159:ILE:HG22 | 2:H:1160:THR:N | 2.32 | 0.45 |
| 1:A:658:LEU:HD13 | 1:A:916:LEU:HD12 | 1.99 | 0.45 |
| 2:H:785:TRP:CG | 2:H:786:SER:N | 2.84 | 0.45 |
| 2:I:1195:VAL:HG13 | 2:I:1211:LEU:CB | 2.46 | 0.45 |
| 2:G:1976:PHE:CB | 2:G:1981:LEU:CD2 | 2.95 | 0.45 |
| 2:H:1325:PHE:O | 2:H:1328:VAL:HG12 | 2.16 | 0.45 |
| 2:G:712:ALA:O | 2:G:715:GLN:HB3 | 2.16 | 0.45 |
| 1:C:225:SER:OG | 1:C:266:LEU:HD21 | 2.16 | 0.45 |
| 2:G:142:ASN:HB2 | 2:G:550:VAL:HG13 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:776:GLU:OE1 | 1:A:795:MET:HE1 | 2.16 | 0.45 |
| 2:I:23:PRO:HG2 | 2:I:86:LEU:HD11 | 1.98 | 0.45 |
| 2:G:1466:PHE:HE2 | 2:G:1489:ILE:HD13 | 1.81 | 0.45 |
| 1:C:1491:ARG:NH1 | 1:C:1744:TYR:O | 2.50 | 0.45 |
| 2:I:1637:LEU:HD23 | 2:I:1637:LEU:HA | 1.79 | 0.45 |
| 2:I:440:ASN:ND2 | 2:I:477:GLU:HG2 | 2.31 | 0.45 |
| 2:G:1241:ASN:N | 2:G:1252:SER:O | 2.49 | 0.45 |
| 2:G:1080:GLY:O | 2:G:1084:LYS:HG3 | 2.16 | 0.45 |
| 2:H:594:VAL:CG2 | 2:H:610:THR:HG21 | 2.45 | 0.45 |
| 2:H:2035:SER:HB3 | 2:H:2038:ILE:CG1 | 2.44 | 0.45 |
| 2:H:1678:MET:HE3 | 2:H:1707:LEU:CD2 | 2.41 | 0.45 |
| 2:G:754:TYR:CG | 2:G:794:MET:HG2 | 2.51 | 0.45 |
| 1:C:21:GLN:HG3 | 2:I:2013:ASN:HB2 | 1.98 | 0.45 |
| 1:C:1305:CYS:SG | 3:C:2748:CER:H51 | 2.57 | 0.45 |
| 2:G:665:LEU:O | 2:G:665:LEU:HD22 | 2.17 | 0.45 |
| 2:G:1858:ASN:ND2 | 2:G:1861:ARG:HG3 | 2.32 | 0.45 |
| 2:G:1873:TYR:HE1 | 2:G:1877:ARG:HH21 | 1.59 | 0.45 |
| 2:I:1949:LYS:O | 2:I:1953:VAL:HG23 | 2.17 | 0.45 |
| 1:C:521:LYS:HB3 | 1:C:523:SER:HB3 | 1.98 | 0.45 |
| 2:I:1162:ASP:O | 2:I:1163:LYS:HB2 | 2.16 | 0.45 |
| 1:B:66:GLU:HA | 1:B:66:GLU:OE1 | 2.15 | 0.45 |
| 2:I:478:ARG:O | 2:I:482:CYS:HB2 | 2.17 | 0.45 |
| 1:C:1670:TYR:O | 1:C:1674:VAL:HG23 | 2.17 | 0.45 |
| 2:I:784:GLU:O | 2:I:787:THR:HB | 2.17 | 0.45 |
| 1:A:1300:THR:HA | 1:A:1301:PRO:HD3 | 1.70 | 0.45 |
| 2:I:677:GLN:O | 2:I:678:PHE:HB3 | 2.17 | 0.45 |
| 2:H:1845:ASP:HB2 | 2:H:1849:ARG:N | 2.15 | 0.45 |
| 2:G:455:ILE:HD11 | 2:G:469:ARG:NE | 2.32 | 0.45 |
| 1:B:1239:HIS:HE1 | 1:B:1714:VAL:O | 2.00 | 0.45 |
| 2:I:355:LYS:HE2 | 2:I:355:LYS:HB3 | 1.70 | 0.45 |
| 2:I:943:TRP:CZ2 | 2:I:1016:PRO:HG3 | 2.52 | 0.45 |
| 1:A:1239:HIS:CD2 | 1:A:1241:SER:H | 2.35 | 0.45 |
| 2:H:751:LEU:HA | 2:H:794:MET:HE3 | 1.98 | 0.45 |
| 2:H:1100:VAL:HG23 | 2:H:1147:ILE:HB | 1.99 | 0.45 |
| 2:I:161:GLY:H | 2:I:505:GLY:CA | 2.28 | 0.45 |
| 2:I:1002:HIS:NE2 | 2:I:1006:MET:CE | 2.80 | 0.45 |
| 2:G:350:GLN:HA | 2:G:353:VAL:HG13 | 1.97 | 0.45 |
| 1:B:1584:PRO:CG | 1:B:1591:TRP:CZ3 | 3.00 | 0.45 |
| 1:B:1459:ILE:O | 1:B:1463:VAL:HG23 | 2.17 | 0.45 |
| 2:G:218:TRP:HB3 | 2:G:225:THR:OG1 | 2.16 | 0.45 |
| 2:I:654:VAL:HG12 | 2:I:654:VAL:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1308:CYS:HB3 | 2:I:1311:PHE:CE2 | 2.51 | 0.45 |
| 2:G:1265:MET:HE1 | 2:G:1562:PRO:HG2 | 1.98 | 0.45 |
| 2:I:1258:ARG:O | 2:I:1262:ILE:HG13 | 2.17 | 0.45 |
| 1:B:1004:ILE:HG22 | 1:B:1660:TYR:CE2 | 2.52 | 0.45 |
| 2:G:879:LYS:HA | 2:G:879:LYS:HD3 | 1.68 | 0.45 |
| 1:A:1443:LEU:HA | 1:A:1443:LEU:HD23 | 1.75 | 0.45 |
| 2:G:101:ILE:HG13 | 2:G:101:ILE:H | 1.31 | 0.45 |
| 2:H:512:LEU:O | 2:H:516:THR:HG23 | 2.17 | 0.45 |
| 2:G:1227:ARG:CZ | 2:G:1565:VAL:HG12 | 2.47 | 0.45 |
| 1:B:340:ARG:HH12 | 1:B:344:GLN:HE21 | 1.64 | 0.45 |
| 1:A:483:VAL:O | 1:A:484:LEU:C | 2.56 | 0.45 |
| 1:B:1617:ILE:O | 1:B:1620:GLN:HG2 | 2.17 | 0.45 |
| 2:I:653:TYR:OH | 2:I:690:VAL:HG11 | 2.17 | 0.45 |
| 2:G:1491:VAL:HB | 2:G:1501:ILE:HD12 | 1.99 | 0.45 |
| 2:H:1327:ILE:HG12 | 2:H:1583:MET:HE3 | 1.99 | 0.45 |
| 2:I:1491:VAL:HB | 2:I:1501:ILE:CD1 | 2.47 | 0.45 |
| 1:B:420:ILE:HG22 | 1:B:469:VAL:HG22 | 1.99 | 0.45 |
| 1:C:927:ASN:O | 1:C:929:GLY:N | 2.41 | 0.45 |
| 1:A:929:GLY:C | 1:A:931:GLN:H | 2.19 | 0.45 |
| 1:C:378:LEU:HA | 1:C:378:LEU:HD12 | 1.84 | 0.45 |
| 2:G:1543:ASP:OD1 | 2:G:1623:LYS:HG2 | 2.16 | 0.45 |
| 2:G:624:TYR:HB2 | 2:G:630:MET:HE3 | 1.99 | 0.45 |
| 2:H:641:ILE:HG12 | 2:H:645:SER:CB | 2.46 | 0.45 |
| 2:I:298:LYS:HG2 | 2:I:448:VAL:CG2 | 2.38 | 0.45 |
| 1:A:335:HIS:CD2 | 1:A:335:HIS:O | 2.69 | 0.45 |
| 1:B:44:VAL:HG13 | 1:B:78:ILE:HG12 | 1.98 | 0.45 |
| 2:G:1002:HIS:NE2 | 2:G:1006:MET:HE3 | 2.32 | 0.45 |
| 2:G:109:LEU:HA | 2:G:109:LEU:HD23 | 1.79 | 0.45 |
| 1:C:916:LEU:HD22 | 1:C:922:VAL:HG22 | 1.99 | 0.45 |
| 2:G:1417:THR:C | 2:G:1419:PHE:N | 2.69 | 0.45 |
| 2:G:1418:ASP:C | 2:G:1420:GLU:H | 2.19 | 0.45 |
| 2:G:1325:PHE:O | 2:G:1328:VAL:HG12 | 2.17 | 0.45 |
| 1:B:32:GLN:HE21 | 1:B:57:ALA:HB2 | 1.82 | 0.45 |
| 2:G:1389:ILE:HG13 | 2:G:1411:PHE:CD1 | 2.52 | 0.45 |
| 1:B:43:ARG:O | 2:H:1662:THR:HA | 2.16 | 0.45 |
| 2:G:42:PRO:HG2 | 2:G:52:ASP:CG | 2.38 | 0.45 |
| 1:C:1061:SER:HB2 | 1:C:1078:SER:HB3 | 1.99 | 0.45 |
| 2:I:1256:GLU:O | 2:I:1257:ASP:HB2 | 2.17 | 0.45 |
| 1:B:1592:MET:HE2 | 1:B:1641:ILE:HG23 | 1.98 | 0.45 |
| 1:B:67:SER:OG | 2:G:359:HIS:HE1 | 1.99 | 0.45 |
| 1:A:204:THR:HA | 1:A:205:PRO:HD3 | 1.85 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:478:GLU:OE1 | 1:C:478:GLU:HA | 2.17 | 0.45 |
| 1:B:1119:LYS:HE2 | 1:B:1341:PHE:CG | 2.52 | 0.45 |
| 1:B:1300:THR:HA | 1:B:1301:PRO:HD3 | 1.69 | 0.45 |
| 1:B:196:THR:O | 1:B:213:PHE:HE2 | 2.00 | 0.45 |
| 1:A:1516:ASP:HA | 1:A:1517:PRO:HD3 | 1.61 | 0.45 |
| 2:I:231:LEU:HA | 2:I:236:ILE:HD12 | 1.99 | 0.45 |
| 1:C:253:ARG:O | 1:C:254:TRP:CD1 | 2.70 | 0.44 |
| 2:G:741:HIS:HB3 | 2:G:853:PRO:HB2 | 1.98 | 0.44 |
| 2:G:741:HIS:HE1 | 2:G:855:HIS:NE2 | 2.13 | 0.44 |
| 2:G:607:VAL:O | 2:G:611:THR:HB | 2.17 | 0.44 |
| 2:I:1589:VAL:HG21 | 2:I:1651:LEU:HD12 | 1.99 | 0.44 |
| 1:A:636:PRO:HB2 | 1:A:638:LEU:O | 2.16 | 0.44 |
| 1:B:13:LEU:HB2 | 2:H:2026:PHE:CE1 | 2.52 | 0.44 |
| 2:I:1159:ILE:CG2 | 2:I:1160:THR:N | 2.81 | 0.44 |
| 2:H:443:LEU:HD22 | 2:H:448:VAL:CG1 | 2.46 | 0.44 |
| 1:C:1494:HIS:CE1 | 1:C:1877:GLN:CG | 2.99 | 0.44 |
| 2:H:109:LEU:HD22 | 2:H:114:THR:HG23 | 1.99 | 0.44 |
| 1:B:427:ASN:HB2 | 1:B:468:LEU:HD21 | 1.99 | 0.44 |
| 1:B:733:ILE:CD1 | 1:B:761:LEU:HD11 | 2.46 | 0.44 |
| 1:B:1455:ARG:HD2 | 1:B:1455:ARG:HA | 1.86 | 0.44 |
| 2:G:926:LEU:HB3 | 2:G:947:THR:CG2 | 2.46 | 0.44 |
| 1:B:612:GLU:O | 1:B:615:SER:HB3 | 2.17 | 0.44 |
| 1:B:411:GLN:NE2 | 1:B:1628:SER:H | 2.15 | 0.44 |
| 2:H:1308:CYS:HB3 | 2:H:1311:PHE:CE2 | 2.52 | 0.44 |
| 2:G:1294:ALA:HA | 2:G:1368:VAL:CG2 | 2.47 | 0.44 |
| 2:G:717:ILE:O | 2:G:720:ALA:HB3 | 2.18 | 0.44 |
| 2:H:1529:GLN:O | 2:H:1632:ILE:HG13 | 2.16 | 0.44 |
| 1:A:242:THR:HG22 | 1:A:243:ILE:H | 1.81 | 0.44 |
| 1:B:626:VAL:HG23 | 1:B:664:GLU:OE2 | 2.17 | 0.44 |
| 1:A:1283:MET:O | 1:A:1287:VAL:HG23 | 2.18 | 0.44 |
| 1:B:1029:PRO:HA | 1:B:1188:GLN:O | 2.17 | 0.44 |
| 2:I:272:GLY:HA3 | 2:I:276:GLY:C | 2.37 | 0.44 |
| 2:G:1855:ILE:HB | 2:G:1907:LEU:HD12 | 2.00 | 0.44 |
| 1:C:1257:LEU:HA | 1:C:1257:LEU:HD23 | 1.83 | 0.44 |
| 2:H:1321:ALA:HA | 2:H:1322:PRO:HD3 | 1.84 | 0.44 |
| 1:C:641:ARG:HD3 | 1:C:649:TRP:O | 2.17 | 0.44 |
| 2:G:1071:LYS:HE3 | 2:G:1075:ASP:OD2 | 2.16 | 0.44 |
| 2:H:854:ILE:HG22 | 2:H:856:LYS:HG3 | 1.99 | 0.44 |
| 2:G:7:ARG:HH11 | 2:G:24:THR:HG23 | 1.76 | 0.44 |
| 2:I:1314:ARG:HD3 | 2:I:1314:ARG:HA | 1.64 | 0.44 |
| 1:B:168:MET:HA | 1:B:206:LEU:HB2 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:256:LEU:HA | 1:B:257:PRO:HD3 | 1.73 | 0.44 |
| 1:B:330:GLU:O | 1:B:330:GLU:HG2 | 2.16 | 0.44 |
| 1:A:1666:THR:HG23 | 1:A:1669:ARG:CB | 2.47 | 0.44 |
| 1:C:1238:VAL:CG1 | 1:C:1239:HIS:N | 2.80 | 0.44 |
| 2:I:191:SER:HA | 2:I:194:THR:CG2 | 2.43 | 0.44 |
| 2:H:560:ASN:H | 2:H:564:GLU:HG2 | 1.82 | 0.44 |
| 2:H:786:SER:HB2 | 2:H:794:MET:HE2 | 1.99 | 0.44 |
| 2:I:659:LEU:HA | 2:I:659:LEU:HD12 | 1.84 | 0.44 |
| 1:A:1373:ARG:NE | 1:A:1550:ASP:HB2 | 2.32 | 0.44 |
| 2:G:595:PRO:HD3 | 2:G:800:LEU:HB2 | 1.99 | 0.44 |
| 2:H:1330:GLY:HA2 | 2:H:1374:THR:HG21 | 1.98 | 0.44 |
| 2:I:1303:ALA:HB2 | 2:I:1556:VAL:HG21 | 1.98 | 0.44 |
| 2:H:120:LYS:HB3 | 2:H:124:LYS:HE3 | 1.99 | 0.44 |
| 2:G:463:PHE:C | 2:G:463:PHE:CD2 | 2.90 | 0.44 |
| 1:C:1234:MET:HG2 | 1:C:1326:ILE:HD12 | 1.98 | 0.44 |
| 1:A:1012:LEU:HD23 | 1:A:1445:MET:HE2 | 1.99 | 0.44 |
| 1:A:225:SER:OG | 1:A:266:LEU:HD21 | 2.16 | 0.44 |
| 2:G:1609:THR:O | 2:G:1653:GLY:HA3 | 2.16 | 0.44 |
| 2:I:441:LYS:O | 2:I:444:VAL:HG12 | 2.17 | 0.44 |
| 2:H:1543:ASP:OD1 | 2:H:1623:LYS:HG2 | 2.17 | 0.44 |
| 2:H:607:VAL:O | 2:H:611:THR:HB | 2.17 | 0.44 |
| 1:A:1431:GLU:HB3 | 1:A:1520:ALA:HB2 | 1.99 | 0.44 |
| 2:I:703:LEU:HD21 | 2:I:705:LEU:CD2 | 2.45 | 0.44 |
| 1:A:27:ARG:HH21 | 2:G:2015:THR:HA | 1.82 | 0.44 |
| 1:B:833:PHE:O | 1:B:834:GLY:O | 2.35 | 0.44 |
| 2:G:120:LYS:HB3 | 2:G:124:LYS:HE3 | 1.99 | 0.44 |
| 2:G:566:HIS:O | 2:G:567:PRO:O | 2.34 | 0.44 |
| 1:B:655:LEU:HD23 | 1:B:655:LEU:HA | 1.82 | 0.44 |
| 2:I:780:TYR:HB2 | 2:I:799:PHE:CE2 | 2.53 | 0.44 |
| 2:H:161:GLY:H | 2:H:505:GLY:CA | 2.29 | 0.44 |
| 1:B:183:GLN:O | 1:B:187:LEU:HG | 2.17 | 0.44 |
| 2:G:1015:VAL:HA | 2:G:1016:PRO:HD3 | 1.79 | 0.44 |
| 1:B:225:SER:OG | 1:B:266:LEU:HD21 | 2.18 | 0.44 |
| 1:B:479:ASN:O | 1:B:483:VAL:HG23 | 2.17 | 0.44 |
| 1:C:180:SER:O | 1:C:183:GLN:N | 2.50 | 0.44 |
| 1:A:267:VAL:HG12 | 1:A:290:MET:CE | 2.48 | 0.44 |
| 2:H:427:PHE:HB3 | 2:H:428:HIS:ND1 | 2.32 | 0.44 |
| 2:I:901:LYS:NZ | 2:I:1031:LYS:O | 2.51 | 0.44 |
| 2:G:231:LEU:HA | 2:G:236:ILE:HD12 | 2.00 | 0.44 |
| 1:B:539:SER:O | 1:B:540:GLN:C | 2.54 | 0.44 |
| 2:I:1735:ALA:O | 2:I:1737:ILE:HG13 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:1757:GLU:H | 2:I:1757:GLU:HG3 | 1.50 | 0.44 |
| 1:C:1487:LEU:C | 1:C:1487:LEU:HD23 | 2.38 | 0.44 |
| 2:G:932:ILE:HD12 | 2:G:939:PHE:HD1 | 1.83 | 0.44 |
| 2:I:1651:LEU:HA | 2:I:1651:LEU:HD23 | 1.73 | 0.44 |
| 2:I:1054:LEU:CB | 4:I:3051:FMN:HM71 | 2.46 | 0.44 |
| 1:C:930:LEU:HD23 | 1:C:930:LEU:HA | 1.76 | 0.44 |
| 2:H:663:ILE:HB | 2:H:664:PRO:CD | 2.44 | 0.44 |
| 1:A:1056:ILE:CD1 | 1:A:1193:TRP:CD1 | 3.00 | 0.44 |
| 1:B:1040:GLU:OE2 | 1:B:1577:GLN:HB2 | 2.18 | 0.44 |
| 2:G:1908:ASP:HA | 2:G:1911:THR:HG22 | 2.00 | 0.44 |
| 1:B:32:GLN:HE22 | 1:B:57:ALA:N | 2.16 | 0.44 |
| 1:C:1657:HIS:CG | 1:C:1658:PRO:HD2 | 2.53 | 0.44 |
| 2:I:1330:GLY:HA2 | 2:I:1374:THR:HG21 | 1.99 | 0.44 |
| 1:B:232:LEU:HD13 | 1:B:272:GLU:CB | 2.47 | 0.44 |
| 2:G:1752:PHE:HZ | 2:G:1836:MET:HE3 | 1.82 | 0.44 |
| 2:I:665:LEU:HD22 | 2:I:665:LEU:O | 2.18 | 0.44 |
| 1:C:1022:THR:HG22 | 1:C:1226:SER:CB | 2.47 | 0.44 |
| 2:H:1311:PHE:HD1 | 2:H:1320:LEU:O | 2.00 | 0.44 |
| 2:H:1697:HIS:CE1 | 2:H:1829:GLU:CG | 3.00 | 0.44 |
| 1:A:1020:VAL:CG1 | 1:A:1400:ILE:HG23 | 2.47 | 0.44 |
| 1:C:625:THR:HG23 | 1:C:627:SER:H | 1.83 | 0.44 |
| 2:G:1873:TYR:CE1 | 2:G:1877:ARG:NH2 | 2.84 | 0.44 |
| 2:G:1590:ARG:NH2 | 2:G:1594:GLU:OE2 | 2.50 | 0.44 |
| 2:H:209:PHE:CE2 | 2:H:213:LEU:HD22 | 2.52 | 0.44 |
| 2:G:1945:ASP:O | 2:G:1949:LYS:HG3 | 2.17 | 0.44 |
| 2:I:1418:ASP:OD1 | 2:I:1420:GLU:HG3 | 2.17 | 0.44 |
| 1:A:66:GLU:HA | 1:A:66:GLU:OE1 | 2.17 | 0.44 |
| 2:H:778:TYR:N | 2:H:779:PRO:CD | 2.80 | 0.44 |
| 2:G:490:TRP:HA | 2:G:493:THR:HG22 | 1.98 | 0.44 |
| 2:G:297:ARG:O | 2:G:301:THR:HG22 | 2.17 | 0.44 |
| 2:I:9:LEU:HB2 | 2:I:27:PHE:HE1 | 1.82 | 0.44 |
| 2:I:835:THR:HG22 | 2:I:844:VAL:CA | 2.48 | 0.44 |
| 2:H:641:ILE:CG1 | 2:H:645:SER:HB2 | 2.45 | 0.44 |
| 2:H:109:LEU:HD11 | 2:H:116:LEU:CD2 | 2.43 | 0.44 |
| 2:G:589:ARG:HB3 | 2:G:590:PRO:CD | 2.48 | 0.44 |
| 2:G:109:LEU:HD22 | 2:G:114:THR:HG23 | 2.00 | 0.44 |
| 2:I:245:GLN:HG2 | 2:I:505:GLY:HA2 | 2.00 | 0.44 |
| 1:C:44:VAL:HG13 | 1:C:78:ILE:HG12 | 1.99 | 0.44 |
| 1:C:503:ILE:HD12 | 1:C:950:THR:HG21 | 1.98 | 0.44 |
| 2:I:1590:ARG:HG3 | 2:I:1608:TYR:CD2 | 2.53 | 0.44 |
| 2:G:1632:ILE:O | 2:G:1632:ILE:HG23 | 2.16 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:468:LEU:O | 2:I:471:LEU:HB2 | 2.18 | 0.44 |
| 1:B:496:PRO:HB2 | 1:B:519:VAL:HG12 | 1.99 | 0.44 |
| 2:I:1846:GLU:C | 2:I:1848:GLY:H | 2.20 | 0.44 |
| 2:I:159:ILE:CG2 | 2:I:501:ILE:HG22 | 2.47 | 0.44 |
| 2:I:1896:GLN:HE21 | 2:I:1896:GLN:HB3 | 1.58 | 0.44 |
| 1:B:1238:VAL:CG1 | 1:B:1239:HIS:N | 2.81 | 0.44 |
| 2:G:751:LEU:HD23 | 2:G:791:TYR:CD2 | 2.53 | 0.44 |
| 2:G:751:LEU:HD11 | 2:G:789:PHE:CD1 | 2.53 | 0.44 |
| 2:H:305:PHE:CD1 | 2:H:442:ASP:HB3 | 2.53 | 0.44 |
| 2:G:1784:MET:HE2 | 2:G:1784:MET:O | 2.17 | 0.44 |
| 2:I:305:PHE:CD1 | 2:I:442:ASP:HB3 | 2.52 | 0.44 |
| 1:A:1022:THR:CG2 | 1:A:1226:SER:OG | 2.66 | 0.44 |
| 2:H:807:ILE:HA | 2:H:818:LYS:HG2 | 1.99 | 0.44 |
| 1:A:1305:CYS:SG | 1:A:1585:LYS:HA | 2.57 | 0.44 |
| 1:B:267:VAL:HG12 | 1:B:290:MET:CE | 2.48 | 0.44 |
| 1:C:503:ILE:HD11 | 1:C:947:LEU:HD22 | 1.98 | 0.44 |
| 2:H:1389:ILE:HG13 | 2:H:1411:PHE:CD1 | 2.52 | 0.44 |
| 1:C:1557:ILE:HD11 | 1:C:1642:THR:HG21 | 2.00 | 0.44 |
| 1:A:1135:GLU:CD | 1:B:242:THR:HG21 | 2.38 | 0.44 |
| 2:I:40:ILE:O | 2:I:42:PRO:HD3 | 2.17 | 0.44 |
| 2:G:551:THR:C | 2:G:553:ASN:H | 2.20 | 0.44 |
| 2:G:551:THR:HG22 | 2:G:552:SER:N | 2.31 | 0.44 |
| 2:I:1257:ASP:O | 2:I:1261:ARG:HG3 | 2.17 | 0.44 |
| 2:I:720:ALA:HA | 2:I:728:ILE:CD1 | 2.47 | 0.44 |
| 1:B:1516:ASP:HA | 1:B:1517:PRO:HD3 | 1.65 | 0.44 |
| 1:A:1464:GLU:HG3 | 1:A:1773:VAL:HG11 | 1.77 | 0.44 |
| 2:I:297:ARG:O | 2:I:301:THR:HG22 | 2.18 | 0.44 |
| 2:I:1739:GLU:HB2 | 2:I:1987:PRO:CB | 2.29 | 0.44 |
| 2:H:455:ILE:C | 2:H:455:ILE:HD12 | 2.38 | 0.44 |
| 1:B:29:ILE:HG12 | 2:H:1892:ASN:C | 2.37 | 0.44 |
| 2:I:184:VAL:HG12 | 2:I:188:ILE:HG12 | 1.99 | 0.44 |
| 2:I:1976:PHE:HB3 | 2:I:1981:LEU:CD2 | 2.48 | 0.44 |
| 1:A:1194:ASN:OD1 | 1:A:1196:LYS:HB2 | 2.18 | 0.44 |
| 1:A:458:THR:OG1 | 1:A:470:LYS:HD2 | 2.18 | 0.44 |
| 2:H:1579:ILE:HD11 | 2:H:1615:MET:SD | 2.58 | 0.44 |
| 2:H:376:ASN:C | 2:H:376:ASN:ND2 | 2.70 | 0.44 |
| 1:B:1012:LEU:HD23 | 1:B:1445:MET:CE | 2.48 | 0.44 |
| 2:I:517:HIS:CE1 | 2:I:540:ASP:O | 2.71 | 0.44 |
| 2:H:1148:ASN:HD22 | 2:H:1148:ASN:C | 2.21 | 0.44 |
| 2:H:272:GLY:HA3 | 2:H:276:GLY:C | 2.38 | 0.44 |
| 1:B:1195:ALA:HB1 | 1:B:1200:ILE:HD12 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1220:VAL:O | 1:A:1224:ILE:HG12 | 2.18 | 0.44 |
| 1:C:1673:TYR:CZ | 1:C:1677:VAL:HG21 | 2.51 | 0.44 |
| 1:C:852:ARG:HB3 | 1:C:858:TRP:HZ2 | 1.83 | 0.44 |
| 1:A:11:HIS:CD2 | 1:A:11:HIS:C | 2.92 | 0.44 |
| 2:G:1589:VAL:HG21 | 2:G:1651:LEU:HD12 | 1.99 | 0.44 |
| 2:I:1886:VAL:HG22 | 2:I:1906:ALA:HB1 | 1.98 | 0.44 |
| 2:G:615:TYR:CE2 | 2:G:1074:MET:HB3 | 2.52 | 0.44 |
| 1:A:530:ALA:HA | 1:A:636:PRO:HB3 | 1.99 | 0.44 |
| 1:B:20:TYR:CD2 | 2:H:2033:THR:OG1 | 2.71 | 0.44 |
| 2:G:1776:PHE:C | 2:G:1779:PRO:HD2 | 2.38 | 0.44 |
| 2:H:780:TYR:HB2 | 2:H:799:PHE:CE2 | 2.53 | 0.44 |
| 1:A:499:PRO:HD3 | 1:A:516:ARG:HH21 | 1.83 | 0.44 |
| 2:H:184:VAL:HG12 | 2:H:188:ILE:HG12 | 2.00 | 0.44 |
| 2:G:1551:GLU:HB2 | 2:G:1552:PRO:HD3 | 2.00 | 0.44 |
| 2:H:732:TRP:CE2 | 2:H:750:MET:HE3 | 2.52 | 0.44 |
| 1:B:1455:ARG:O | 1:B:1459:ILE:HG13 | 2.18 | 0.44 |
| 1:B:1037:TRP:HB2 | 1:B:1598:GLN:OE1 | 2.18 | 0.44 |
| 2:I:1579:ILE:HG22 | 2:I:1580:THR:O | 2.18 | 0.44 |
| 1:B:1842:VAL:O | 1:B:1843:ASN:C | 2.57 | 0.44 |
| 2:I:142:ASN:HB2 | 2:I:550:VAL:HG13 | 1.99 | 0.44 |
| 1:C:187:LEU:HD22 | 1:C:201:PRO:HB2 | 1.99 | 0.44 |
| 1:C:1234:MET:CE | 1:C:1326:ILE:HG21 | 2.48 | 0.44 |
| 1:C:1270:VAL:HG11 | 1:C:1274:ILE:HD13 | 1.99 | 0.44 |
| 2:I:1666:PHE:CE1 | 2:I:1814:ALA:HA | 2.53 | 0.44 |
| 2:G:1662:THR:HB | 2:G:1799:PRO:HG2 | 1.99 | 0.44 |
| 1:B:42:GLU:O | 1:B:77:GLU:N | 2.47 | 0.44 |
| 2:H:938:TRP:CE2 | 2:H:944:ARG:HG3 | 2.52 | 0.44 |
| 1:A:1133:PRO:HG3 | 1:A:1166:LYS:HG3 | 1.99 | 0.44 |
| 1:C:706:THR:HB | 1:C:737:PHE:HB3 | 2.00 | 0.44 |
| 2:H:1228:THR:HG21 | 2:H:1234:VAL:HG23 | 2.00 | 0.44 |
| 2:G:1257:ASP:O | 2:G:1261:ARG:HG3 | 2.18 | 0.44 |
| 1:C:601:VAL:O | 1:C:602:GLU:C | 2.56 | 0.44 |
| 2:H:102:HIS:HE1 | 2:H:180:TYR:OH | 2.00 | 0.44 |
| 2:G:159:ILE:HD11 | 2:G:512:LEU:CG | 2.48 | 0.44 |
| 1:C:295:ALA:HB1 | 1:C:300:VAL:O | 2.18 | 0.44 |
| 2:H:1739:GLU:HB2 | 2:H:1987:PRO:CB | 2.30 | 0.44 |
| 1:A:1501:LEU:HD11 | 1:A:1775:LEU:CG | 2.47 | 0.44 |
| 2:H:1496:LYS:HE2 | 2:H:1693:ARG:HH21 | 1.82 | 0.44 |
| 2:G:566:HIS:O | 2:G:567:PRO:C | 2.57 | 0.44 |
| 2:G:1004:LEU:CD2 | 2:G:1019:PRO:HB2 | 2.48 | 0.44 |
| 2:G:1352:HIS:HE1 | 2:G:1583:MET:CE | 2.27 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:833:PHE:O | 1:C:834:GLY:O | 2.36 | 0.44 |
| 1:A:1842:VAL:O | 1:A:1843:ASN:C | 2.57 | 0.44 |
| 2:I:218:TRP:HB3 | 2:I:225:THR:OG1 | 2.18 | 0.44 |
| 1:B:267:VAL:O | 1:B:290:MET:HE1 | 2.17 | 0.44 |
| 2:I:1493:LEU:HB3 | 2:I:1494:PRO:CD | 2.48 | 0.44 |
| 2:G:459:VAL:HG12 | 2:G:468:LEU:HD12 | 2.00 | 0.44 |
| 2:G:901:LYS:NZ | 2:G:1031:LYS:O | 2.50 | 0.44 |
| 1:C:1181:PHE:CZ | 1:C:1341:PHE:HA | 2.53 | 0.44 |
| 2:I:914:LEU:HD21 | 2:I:1003:PHE:CD2 | 2.53 | 0.44 |
| 1:B:1430:ARG:HG2 | 1:B:1430:ARG:O | 2.18 | 0.44 |
| 1:C:1291:LEU:HD21 | 1:C:1698:PHE:CE1 | 2.53 | 0.44 |
| 2:I:1684:SER:O | 2:I:1688:GLN:HG3 | 2.18 | 0.44 |
| 2:I:246:LEU:O | 2:I:250:VAL:HG23 | 2.18 | 0.44 |
| 2:H:9:LEU:HB2 | 2:H:27:PHE:HE1 | 1.83 | 0.43 |
| 1:B:1460:LYS:CE | 1:B:1774:GLU:CD | 2.86 | 0.43 |
| 2:H:670:ARG:HD2 | 2:H:676:ILE:O | 2.18 | 0.43 |
| 2:G:726:PHE:HA | 2:G:727:PRO:HD3 | 1.89 | 0.43 |
| 2:I:932:ILE:HD12 | 2:I:939:PHE:HD1 | 1.83 | 0.43 |
| 2:H:123:ILE:HD11 | 2:H:533:LEU:CD2 | 2.48 | 0.43 |
| 2:G:543:PHE:CB | 2:G:545:GLN:NE2 | 2.81 | 0.43 |
| 2:H:1638:ILE:CD1 | 2:H:1657:ILE:HG13 | 2.41 | 0.43 |
| 2:G:753:MET:O | 2:G:757:ILE:HG13 | 2.18 | 0.43 |
| 2:G:566:HIS:ND1 | 2:G:567:PRO:HD2 | 2.33 | 0.43 |
| 2:G:245:GLN:HG2 | 2:G:505:GLY:HA2 | 1.99 | 0.43 |
| 1:B:888:ILE:HD12 | 1:B:939:PHE:CE2 | 2.43 | 0.43 |
| 2:H:567:PRO:CG | 2:H:781:LEU:CD1 | 2.94 | 0.43 |
| 1:C:1373:ARG:NE | 1:C:1550:ASP:HB2 | 2.33 | 0.43 |
| 1:A:933:VAL:HG22 | 1:A:933:VAL:O | 2.18 | 0.43 |
| 2:I:1782:THR:CG2 | 2:I:1827:LEU:HD21 | 2.45 | 0.43 |
| 1:A:181:THR:O | 1:A:185:GLU:HG3 | 2.18 | 0.43 |
| 2:I:1551:GLU:HB2 | 2:I:1552:PRO:HD3 | 2.00 | 0.43 |
| 1:B:35:PHE:HA | 1:B:39:PHE:HD2 | 1.83 | 0.43 |
| 1:C:413:LEU:C | 1:C:415:SER:H | 2.21 | 0.43 |
| 1:C:1332:TYR:HB3 | 1:C:1382:ALA:CB | 2.48 | 0.43 |
| 2:H:1222:GLU:HG3 | 2:H:1235:SER:OG | 2.17 | 0.43 |
| 2:I:427:PHE:HB3 | 2:I:428:HIS:ND1 | 2.33 | 0.43 |
| 2:I:1427:VAL:HG22 | 2:I:1469:GLU:HG2 | 1.99 | 0.43 |
| 2:I:432:LEU:HB3 | 2:I:484:ILE:HG23 | 2.00 | 0.43 |
| 2:H:1586:SER:O | 2:H:1590:ARG:HB2 | 2.17 | 0.43 |
| 1:A:406:TRP:CE3 | 1:A:407:ASN:HB2 | 2.53 | 0.43 |
| 1:B:1129:GLU:OE1 | 1:C:348:ARG:HD3 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:866:LYS:O | 2:G:870:GLU:HG3 | 2.18 | 0.43 |
| 2:G:1236:LEU:HD11 | 2:G:1262:ILE:HG12 | 1.99 | 0.43 |
| 1:C:1720:ALA:O | 1:C:1721:ARG:HG2 | 2.17 | 0.43 |
| 2:G:1227:ARG:CD | 2:G:1565:VAL:HG11 | 2.44 | 0.43 |
| 1:C:168:MET:HA | 1:C:206:LEU:HB2 | 2.00 | 0.43 |
| 2:H:666:ILE:HG22 | 2:H:698:LEU:HD22 | 2.00 | 0.43 |
| 2:I:1778:GLN:HB2 | 2:I:1779:PRO:HD3 | 2.00 | 0.43 |
| 2:G:754:TYR:CD2 | 2:G:794:MET:CG | 3.01 | 0.43 |
| 2:I:751:LEU:HD23 | 2:I:791:TYR:CD2 | 2.53 | 0.43 |
| 1:A:930:LEU:HD23 | 1:A:930:LEU:HA | 1.75 | 0.43 |
| 2:G:1195:VAL:HG13 | 2:G:1211:LEU:CB | 2.48 | 0.43 |
| 2:I:1976:PHE:HA | 2:I:1981:LEU:CD2 | 2.48 | 0.43 |
| 1:A:1584:PRO:CG | 1:A:1591:TRP:CZ3 | 3.02 | 0.43 |
| 2:I:428:HIS:CD2 | 2:I:488:VAL:HG23 | 2.53 | 0.43 |
| 1:C:1279:PHE:HB2 | 1:C:1282:THR:HG23 | 2.00 | 0.43 |
| 1:B:1279:PHE:HB2 | 1:B:1282:THR:HG23 | 2.00 | 0.43 |
| 2:I:938:TRP:CE2 | 2:I:944:ARG:HG3 | 2.53 | 0.43 |
| 2:G:195:LEU:O | 2:G:199:ILE:HG13 | 2.18 | 0.43 |
| 2:G:581:THR:O | 2:G:585:LYS:HB2 | 2.18 | 0.43 |
| 1:C:196:THR:O | 1:C:213:PHE:HE2 | 2.01 | 0.43 |
| 1:A:626:VAL:HG23 | 1:A:664:GLU:OE2 | 2.18 | 0.43 |
| 2:G:900:GLN:NE2 | 2:G:1051:THR:HA | 2.32 | 0.43 |
| 2:I:159:ILE:HG12 | 2:I:512:LEU:HD23 | 2.01 | 0.43 |
| 2:H:856:LYS:CE | 2:H:1052:CYS:SG | 3.06 | 0.43 |
| 1:B:807:LYS:HD3 | 1:B:807:LYS:C | 2.39 | 0.43 |
| 2:I:843:ILE:HD13 | 2:I:1055:HIS:O | 2.18 | 0.43 |
| 2:I:1624:THR:CB | 2:I:1642:THR:HG23 | 2.47 | 0.43 |
| 1:C:340:ARG:HH12 | 1:C:344:GLN:HE21 | 1.65 | 0.43 |
| 2:H:369:SER:C | 2:H:370:LEU:HD23 | 2.38 | 0.43 |
| 1:B:1014:ASP:N | 1:B:1510:ASN:HD21 | 2.06 | 0.43 |
| 2:I:572:ASN:CB | 2:I:576:LYS:H | 2.27 | 0.43 |
| 2:I:754:TYR:CG | 2:I:794:MET:HG2 | 2.53 | 0.43 |
| 2:G:1473:THR:O | 2:G:1481:SER:HB3 | 2.18 | 0.43 |
| 1:C:1056:ILE:CD1 | 1:C:1193:TRP:CD1 | 2.99 | 0.43 |
| 2:G:1327:ILE:HD12 | 2:G:1327:ILE:HA | 1.79 | 0.43 |
| 2:H:732:TRP:CH2 | 2:H:749:PRO:HG2 | 2.53 | 0.43 |
| 1:A:237:MET:HG3 | 1:A:241:PHE:HB3 | 2.00 | 0.43 |
| 1:A:411:GLN:O | 1:A:415:SER:HB2 | 2.18 | 0.43 |
| 1:C:421:ILE:HG12 | 1:C:469:VAL:HG21 | 1.98 | 0.43 |
| 1:C:627:SER:HB3 | 1:C:661:ASP:OD1 | 2.18 | 0.43 |
| 2:H:439:ILE:HD12 | 2:H:484:ILE:HD11 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:28:TRP:HB3 | 2:G:1892:ASN:HA | 2.00 | 0.43 |
| 2:I:551:THR:C | 2:I:553:ASN:H | 2.22 | 0.43 |
| 1:C:988:ILE:HD13 | 1:C:1048:GLU:HB3 | 2.01 | 0.43 |
| 1:B:1248:GLY:HA3 | 1:B:1301:PRO:HD2 | 1.99 | 0.43 |
| 2:I:1241:ASN:N | 2:I:1252:SER:O | 2.50 | 0.43 |
| 1:C:639:HIS:HB2 | 1:C:656:SER:OG | 2.18 | 0.43 |
| 2:G:1768:LYS:HE2 | 2:G:1772:SER:HB3 | 2.00 | 0.43 |
| 1:A:1209:ASP:OD2 | 1:A:1253:GLY:HA2 | 2.19 | 0.43 |
| 1:A:235:SER:HA | 1:A:276:ARG:NH2 | 2.32 | 0.43 |
| 2:H:970:TYR:O | 2:H:973:LEU:HB2 | 2.18 | 0.43 |
| 2:H:772:GLY:O | 2:H:804:ARG:HD3 | 2.18 | 0.43 |
| 2:I:835:THR:HG21 | 2:I:855:HIS:NE2 | 2.33 | 0.43 |
| 2:G:1846:GLU:C | 2:G:1848:GLY:H | 2.20 | 0.43 |
| 2:G:455:ILE:C | 2:G:455:ILE:HD12 | 2.39 | 0.43 |
| 2:G:1678:MET:HE3 | 2:G:1707:LEU:CD2 | 2.43 | 0.43 |
| 2:G:1016:PRO:HD2 | 2:G:1017:PHE:CE2 | 2.53 | 0.43 |
| 2:I:1325:PHE:O | 2:I:1328:VAL:HG12 | 2.18 | 0.43 |
| 2:G:1040:LEU:O | 2:G:1046:GLN:HG3 | 2.19 | 0.43 |
| 2:G:1223:MET:HE3 | 2:G:1238:LEU:CD1 | 2.49 | 0.43 |
| 2:I:1210:ILE:O | 2:I:1210:ILE:HG22 | 2.18 | 0.43 |
| 2:G:1804:PHE:CD2 | 2:G:1818:LEU:HD22 | 2.53 | 0.43 |
| 2:G:1308:CYS:HB3 | 2:G:1311:PHE:CE2 | 2.53 | 0.43 |
| 2:I:439:ILE:HD12 | 2:I:484:ILE:CD1 | 2.48 | 0.43 |
| 2:I:1428:GLU:HG2 | 2:I:1470:THR:HG22 | 1.99 | 0.43 |
| 1:C:980:VAL:HG21 | 2:I:952:ARG:HH21 | 1.83 | 0.43 |
| 1:B:176:VAL:HG12 | 1:B:178:GLY:H | 1.83 | 0.43 |
| 2:I:430:HIS:CE1 | 2:I:431:LEU:HD13 | 2.53 | 0.43 |
| 2:H:309:ARG:HD3 | 2:H:309:ARG:HA | 1.63 | 0.43 |
| 2:G:967:ILE:HD12 | 2:G:972:LEU:HD22 | 2.00 | 0.43 |
| 1:B:1244:GLY:C | 1:B:1327:CYS:HB2 | 2.38 | 0.43 |
| 2:G:1162:ASP:O | 2:G:1163:LYS:HB2 | 2.19 | 0.43 |
| 2:G:1674:GLN:OE1 | 2:G:1712:ASN:HA | 2.18 | 0.43 |
| 1:A:254:TRP:CZ3 | 1:A:302:LEU:HD13 | 2.53 | 0.43 |
| 2:G:156:LEU:HD23 | 2:G:500:HIS:HB2 | 1.99 | 0.43 |
| 2:H:726:PHE:HA | 2:H:727:PRO:HD3 | 1.88 | 0.43 |
| 2:I:1651:LEU:O | 2:I:1652:THR:HG23 | 2.17 | 0.43 |
| 2:H:1422:THR:CG2 | 2:H:1422:THR:O | 2.66 | 0.43 |
| 2:I:1496:LYS:CE | 2:I:1693:ARG:HH21 | 2.31 | 0.43 |
| 1:A:1553:GLU:HA | 1:A:1556:THR:HG23 | 2.01 | 0.43 |
| 1:A:1556:THR:O | 1:A:1560:MET:HG2 | 2.18 | 0.43 |
| 1:C:1021:VAL:HG22 | 1:C:1387:ILE:HG22 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:893:VAL:HG11 | 1:A:930:LEU:CD2 | 2.46 | 0.43 |
| 2:H:1015:VAL:HG13 | 2:H:1017:PHE:CE2 | 2.53 | 0.43 |
| 1:A:413:LEU:HG | 1:A:413:LEU:O | 2.17 | 0.43 |
| 2:H:745:ASP:HA | 2:H:832:TRP:CH2 | 2.51 | 0.43 |
| 1:C:221:LEU:HA | 1:C:221:LEU:HD23 | 1.89 | 0.43 |
| 2:G:653:TYR:OH | 2:G:690:VAL:HG11 | 2.18 | 0.43 |
| 2:G:1493:LEU:HB3 | 2:G:1494:PRO:CD | 2.48 | 0.43 |
| 2:I:439:ILE:HD12 | 2:I:484:ILE:HD11 | 1.99 | 0.43 |
| 2:I:852:GLU:HG3 | 2:I:852:GLU:H | 1.39 | 0.43 |
| 1:B:242:THR:HB | 1:B:244:THR:HB | 2.01 | 0.43 |
| 2:I:562:LEU:HD23 | 2:I:562:LEU:HA | 1.79 | 0.43 |
| 1:C:1625:LEU:O | 1:C:1627:PRO:HD3 | 2.18 | 0.43 |
| 1:A:1375:GLY:HA2 | 1:A:1546:THR:HG22 | 2.01 | 0.43 |
| 1:A:1291:LEU:HD21 | 1:A:1698:PHE:CE1 | 2.53 | 0.43 |
| 2:G:397:LYS:HB3 | 2:G:416:PHE:CE2 | 2.53 | 0.43 |
| 1:A:1673:TYR:CZ | 1:A:1677:VAL:HG21 | 2.53 | 0.43 |
| 1:A:496:PRO:HB2 | 1:A:519:VAL:HG12 | 2.01 | 0.43 |
| 2:I:397:LYS:HB3 | 2:I:416:PHE:CE2 | 2.53 | 0.43 |
| 2:I:972:LEU:HD23 | 2:I:979:ALA:HB2 | 2.00 | 0.43 |
| 1:C:235:SER:HA | 1:C:276:ARG:NH2 | 2.33 | 0.43 |
| 2:G:1458:ASP:O | 2:G:1462:LYS:HE3 | 2.19 | 0.43 |
| 2:G:272:GLY:HA3 | 2:G:276:GLY:C | 2.38 | 0.43 |
| 2:G:1889:VAL:HG13 | 2:G:1977:HIS:HB3 | 1.97 | 0.43 |
| 1:B:1208:VAL:HG11 | 1:B:1212:THR:HB | 1.97 | 0.43 |
| 2:H:1419:PHE:C | 2:H:1421:ASN:N | 2.71 | 0.43 |
| 1:B:1270:VAL:HG11 | 1:B:1274:ILE:HD13 | 2.00 | 0.43 |
| 1:C:232:LEU:HD13 | 1:C:272:GLU:CB | 2.48 | 0.43 |
| 2:I:1236:LEU:HD22 | 2:I:1238:LEU:HG | 1.99 | 0.43 |
| 1:C:1234:MET:HE3 | 1:C:1326:ILE:HG21 | 2.01 | 0.43 |
| 2:I:871:THR:HG21 | 2:I:887:LYS:HZ1 | 1.83 | 0.43 |
| 1:A:627:SER:HB2 | 1:A:657:SER:CB | 2.48 | 0.43 |
| 2:I:279:THR:O | 2:I:283:ILE:HB | 2.19 | 0.43 |
| 1:A:242:THR:HB | 1:A:244:THR:HB | 2.00 | 0.43 |
| 2:H:73:GLU:OE2 | 2:H:76:LYS:HD2 | 2.18 | 0.43 |
| 2:G:99:ASN:HA | 2:G:550:VAL:CG2 | 2.49 | 0.43 |
| 1:A:641:ARG:HD3 | 1:A:649:TRP:O | 2.18 | 0.43 |
| 2:I:1079:ASP:O | 2:I:1082:ILE:HG22 | 2.19 | 0.43 |
| 2:H:360:LEU:HA | 2:H:361:PRO:HD3 | 1.90 | 0.43 |
| 1:C:1446:LYS:O | 1:C:1450:ARG:HG3 | 2.18 | 0.43 |
| 2:I:1959:LYS:HG2 | 2:I:1959:LYS:O | 2.19 | 0.43 |
| 1:A:790:PHE:CE2 | 1:A:794:ILE:HD11 | 2.53 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:419:ARG:HG3 | 2:G:420:PHE:N | 2.33 | 0.43 |
| 2:H:160:PHE:CE2 | 2:H:504:PHE:HB2 | 2.54 | 0.43 |
| 2:H:1241:ASN:N | 2:H:1252:SER:O | 2.51 | 0.43 |
| 2:G:854:ILE:HG22 | 2:G:856:LYS:HG3 | 2.01 | 0.43 |
| 2:I:7:ARG:NH2 | 2:I:24:THR:O | 2.52 | 0.43 |
| 1:B:1219:VAL:CA | 1:B:1384:ILE:HD11 | 2.32 | 0.43 |
| 2:I:607:VAL:O | 2:I:611:THR:HB | 2.18 | 0.43 |
| 1:A:1431:GLU:OE2 | 1:A:1433:HIS:HE1 | 2.02 | 0.43 |
| 2:G:652:ILE:HD13 | 2:G:658:MET:HE3 | 1.99 | 0.43 |
| 1:A:988:ILE:CD1 | 1:A:1048:GLU:HA | 2.48 | 0.43 |
| 1:C:1553:GLU:HA | 1:C:1556:THR:HG23 | 2.01 | 0.43 |
| 2:G:566:HIS:C | 2:G:566:HIS:ND1 | 2.72 | 0.43 |
| 2:H:573:LYS:C | 2:H:575:GLY:H | 2.21 | 0.43 |
| 2:G:184:VAL:O | 2:G:184:VAL:HG12 | 2.19 | 0.43 |
| 2:G:184:VAL:HG12 | 2:G:188:ILE:HG12 | 2.00 | 0.43 |
| 2:G:324:LEU:O | 2:G:324:LEU:HD12 | 2.18 | 0.43 |
| 2:H:1223:MET:HE3 | 2:H:1238:LEU:CD1 | 2.46 | 0.43 |
| 1:C:49:PRO:O | 1:C:82:SER:HB2 | 2.19 | 0.43 |
| 2:H:653:TYR:OH | 2:H:690:VAL:HG11 | 2.18 | 0.43 |
| 1:A:267:VAL:O | 1:A:290:MET:HE1 | 2.19 | 0.43 |
| 1:B:1233:GLU:CD | 1:B:1680:ARG:HH21 | 2.22 | 0.43 |
| 2:H:643:LYS:HA | 2:H:1163:LYS:HG2 | 1.99 | 0.43 |
| 1:C:1248:GLY:HA3 | 1:C:1301:PRO:HD2 | 2.01 | 0.43 |
| 2:H:629:GLY:O | 2:H:632:ALA:HB3 | 2.18 | 0.43 |
| 1:C:1539:ALA:O | 1:C:1574:GLY:HA2 | 2.18 | 0.43 |
| 2:G:573:LYS:C | 2:G:575:GLY:H | 2.21 | 0.43 |
| 1:B:370:GLU:O | 1:B:373:ALA:HB3 | 2.19 | 0.43 |
| 1:C:1375:GLY:HA2 | 1:C:1546:THR:HG22 | 1.99 | 0.43 |
| 1:C:1599:ILE:HD11 | 1:C:1606:PRO:HD2 | 2.01 | 0.43 |
| 2:G:601:THR:O | 2:G:601:THR:CG2 | 2.67 | 0.43 |
| 2:H:1567:ARG:HH11 | 2:H:1567:ARG:HG2 | 1.72 | 0.43 |
| 2:G:1175:LYS:HG3 | 2:G:1176:PRO:HD2 | 2.00 | 0.43 |
| 1:A:335:HIS:ND1 | 1:C:335:HIS:HE1 | 2.17 | 0.43 |
| 2:I:1168:ASN:HA | 2:I:1169:PRO:HD3 | 1.84 | 0.43 |
| 2:G:786:SER:HB3 | 2:G:794:MET:HE2 | 2.01 | 0.43 |
| 2:G:1004:LEU:HD21 | 2:G:1020:VAL:CG2 | 2.48 | 0.43 |
| 2:I:846:VAL:CG1 | 2:I:865:TRP:NE1 | 2.82 | 0.43 |
| 2:G:324:LEU:O | 2:G:328:LEU:HG | 2.18 | 0.43 |
| 1:A:644:THR:HG23 | 1:A:648:ASP:N | 2.34 | 0.43 |
| 2:I:1552:PRO:O | 2:I:1556:VAL:HG23 | 2.19 | 0.43 |
| 2:G:860:ARG:H | 2:G:1049:GLN:HG3 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:827:SER:HA | 1:A:828:PRO:HD3 | 1.70 | 0.43 |
| 2:I:2030:TYR:CD1 | 2:I:2034:GLY:HA2 | 2.54 | 0.43 |
| 1:A:1009:LEU:CD1 | 1:A:1445:MET:HE1 | 2.48 | 0.43 |
| 2:H:654:VAL:HG12 | 2:H:654:VAL:O | 2.18 | 0.43 |
| 1:C:1158:PRO:HD2 | 1:C:1159:GLU:OE2 | 2.18 | 0.43 |
| 1:B:1446:LYS:O | 1:B:1450:ARG:HG3 | 2.19 | 0.43 |
| 2:I:169:TYR:CG | 2:I:170:PHE:N | 2.87 | 0.43 |
| 2:H:1940:LEU:HD12 | 2:H:1941:PHE:N | 2.34 | 0.43 |
| 1:B:1375:GLY:HA2 | 1:B:1546:THR:HG22 | 2.01 | 0.43 |
| 1:C:384:GLU:O | 1:C:388:ASN:HB2 | 2.19 | 0.43 |
| 1:B:1498:GLU:HG2 | 1:B:1876:LEU:HB3 | 1.89 | 0.43 |
| 1:B:681:THR:HA | 1:B:706:THR:OG1 | 2.19 | 0.43 |
| 2:I:425:SER:HA | 2:I:426:PRO:HD3 | 1.78 | 0.43 |
| 2:G:28:PHE:CE2 | 2:H:7:ARG:CD | 2.73 | 0.43 |
| 2:H:1862:VAL:HG22 | 2:H:1863:ALA:N | 2.33 | 0.43 |
| 2:I:702:TYR:HB3 | 2:I:727:PRO:HB2 | 2.00 | 0.43 |
| 2:G:2042:ILE:HG12 | 2:G:2042:ILE:H | 1.39 | 0.43 |
| 2:I:615:TYR:CE2 | 2:I:1074:MET:HB3 | 2.53 | 0.43 |
| 2:G:1875:VAL:HG22 | 2:G:1910:VAL:HG11 | 2.01 | 0.43 |
| 1:A:1431:GLU:CG | 1:A:1433:HIS:CE1 | 3.00 | 0.43 |
| 2:G:835:THR:HG22 | 2:G:844:VAL:HA | 2.00 | 0.43 |
| 2:H:543:PHE:CB | 2:H:545:GLN:NE2 | 2.81 | 0.43 |
| 2:G:1219:ILE:HB | 2:G:1240:TYR:HB2 | 2.01 | 0.43 |
| 1:B:460:GLU:CG | 1:B:470:LYS:HD3 | 2.48 | 0.43 |
| 2:I:1561:ASN:HA | 2:I:1562:PRO:HD3 | 1.80 | 0.43 |
| 1:B:1431:GLU:CG | 1:B:1433:HIS:CE1 | 3.02 | 0.43 |
| 1:B:1657:HIS:HA | 1:B:1658:PRO:HD3 | 1.89 | 0.43 |
| 1:C:1600:LEU:HD11 | 1:C:1655:VAL:HG12 | 2.00 | 0.43 |
| 2:G:486:LEU:HA | 2:G:487:PRO:HD3 | 1.90 | 0.43 |
| 2:I:1873:TYR:CE1 | 2:I:1877:ARG:NH2 | 2.81 | 0.43 |
| 2:G:15:SER:H | 2:G:48:PHE:HE2 | 1.67 | 0.43 |
| 2:I:573:LYS:C | 2:I:575:GLY:N | 2.72 | 0.43 |
| 2:I:209:PHE:CE2 | 2:I:213:LEU:HD22 | 2.53 | 0.43 |
| 2:I:967:ILE:HD12 | 2:I:972:LEU:HD22 | 2.00 | 0.43 |
| 1:A:833:PHE:HA | 1:A:937:LYS:HD2 | 2.00 | 0.43 |
| 1:A:1670:TYR:O | 1:A:1674:VAL:HG23 | 2.18 | 0.43 |
| 2:H:717:ILE:HG23 | 2:H:760:HIS:CE1 | 2.54 | 0.43 |
| 2:G:884:LEU:HD22 | 2:G:1021:LEU:CD1 | 2.49 | 0.43 |
| 2:I:1662:THR:HB | 2:I:1799:PRO:HG2 | 2.00 | 0.43 |
| 1:C:852:ARG:NH1 | 1:C:856:GLU:OE1 | 2.52 | 0.43 |
| 2:I:652:ILE:CD1 | 2:I:658:MET:HE3 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:260:ARG:HH12 | 1:B:300:VAL:CG2 | 2.20 | 0.43 |
| 1:A:32:GLN:HE22 | 1:A:57:ALA:N | 2.16 | 0.43 |
| 1:B:335:HIS:C | 1:B:335:HIS:CD2 | 2.92 | 0.43 |
| 2:G:634:ILE:CD1 | 2:G:649:ILE:HD11 | 2.43 | 0.43 |
| 2:H:1293:THR:CG2 | 2:H:1296:GLU:H | 2.24 | 0.43 |
| 1:A:1498:GLU:HG2 | 1:A:1876:LEU:HB3 | 1.68 | 0.43 |
| 1:B:1553:GLU:HA | 1:B:1556:THR:HG23 | 2.00 | 0.43 |
| 1:A:44:VAL:HG11 | 1:A:78:ILE:HG12 | 1.96 | 0.43 |
| 1:C:1208:VAL:HG11 | 1:C:1212:THR:HB | 1.98 | 0.43 |
| 2:I:950:PHE:O | 2:I:953:ARG:HB3 | 2.19 | 0.43 |
| 2:H:595:PRO:HD3 | 2:H:800:LEU:HB2 | 2.01 | 0.43 |
| 2:G:1327:ILE:HG12 | 2:G:1583:MET:HE3 | 2.01 | 0.43 |
| 1:A:460:GLU:CG | 1:A:470:LYS:HD3 | 2.49 | 0.43 |
| 2:G:1339:PHE:N | 2:G:1340:PRO:CD | 2.82 | 0.43 |
| 1:B:411:GLN:O | 1:B:415:SER:HB2 | 2.18 | 0.43 |
| 2:G:1858:ASN:HA | 2:G:1896:GLN:O | 2.18 | 0.43 |
| 2:G:441:LYS:O | 2:G:445:LYS:HG3 | 2.18 | 0.43 |
| 2:G:339:LEU:HD23 | 2:G:419:ARG:O | 2.19 | 0.43 |
| 1:A:196:THR:O | 1:A:213:PHE:HE2 | 2.01 | 0.43 |
| 1:A:1107:GLU:HA | 1:A:1108:PRO:HD3 | 1.90 | 0.43 |
| 1:B:1283:MET:O | 1:B:1287:VAL:HG23 | 2.18 | 0.43 |
| 2:G:1348:LEU:HD12 | 2:G:1348:LEU:HA | 1.81 | 0.43 |
| 1:C:1107:GLU:HA | 1:C:1108:PRO:HD3 | 1.89 | 0.43 |
| 1:C:1047:LEU:O | 1:C:1051:VAL:HG23 | 2.19 | 0.43 |
| 2:I:516:THR:O | 2:I:519:ASN:HB2 | 2.19 | 0.42 |
| 2:I:7:ARG:CG | 2:I:22:VAL:O | 2.67 | 0.42 |
| 2:I:835:THR:HB | 2:I:845:THR:HG23 | 2.01 | 0.42 |
| 2:I:1878:VAL:CG1 | 2:I:1910:VAL:HG22 | 2.36 | 0.42 |
| 2:H:1847:LEU:H | 2:H:1847:LEU:CD1 | 2.12 | 0.42 |
| 1:B:335:HIS:CD2 | 1:B:335:HIS:O | 2.70 | 0.42 |
| 1:A:2:LYS:HE2 | 1:A:4:GLU:OE1 | 2.19 | 0.42 |
| 2:G:561:TRP:O | 2:G:563:GLU:N | 2.51 | 0.42 |
| 2:H:1257:ASP:O | 2:H:1261:ARG:HG3 | 2.19 | 0.42 |
| 2:I:1868:GLN:HG3 | 2:I:1898:TYR:HH | 1.83 | 0.42 |
| 1:A:705:VAL:HG23 | 1:A:732:LEU:CD2 | 2.48 | 0.42 |
| 1:B:1263:ASP:HB2 | 1:B:1270:VAL:HG21 | 2.00 | 0.42 |
| 2:I:736:ARG:HG3 | 2:I:736:ARG:H | 1.57 | 0.42 |
| 2:H:551:THR:C | 2:H:553:ASN:H | 2.21 | 0.42 |
| 2:I:1311:PHE:HD1 | 2:I:1320:LEU:O | 2.02 | 0.42 |
| 1:C:1175:ILE:HA | 1:C:1176:PRO:HD3 | 1.89 | 0.42 |
| 1:A:1396:MET:O | 1:A:1680:ARG:NH1 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:155:VAL:O | 1:A:159:LEU:HG | 2.19 | 0.42 |
| 1:B:350:LEU:HB2 | 1:B:352:MET:HG2 | 2.01 | 0.42 |
| 2:H:1458:ASP:O | 2:H:1462:LYS:HE3 | 2.19 | 0.42 |
| 2:G:23:PRO:HG2 | 2:G:86:LEU:HD11 | 2.00 | 0.42 |
| 1:B:1050:CYS:HB3 | 1:B:1089:VAL:HG12 | 2.00 | 0.42 |
| 1:B:1406:MET:HE1 | 1:B:1428:THR:HB | 2.01 | 0.42 |
| 1:A:1539:ALA:O | 1:A:1574:GLY:HA2 | 2.18 | 0.42 |
| 1:B:430:ARG:NH2 | 1:B:605:LEU:HD13 | 2.33 | 0.42 |
| 1:C:1243:VAL:O | 1:C:1296:GLY:HA3 | 2.18 | 0.42 |
| 2:H:127:ILE:HD12 | 2:H:180:TYR:CD2 | 2.54 | 0.42 |
| 2:H:1070:ILE:CD1 | 2:H:1074:MET:HG2 | 2.49 | 0.42 |
| 2:G:612:ASN:HD21 | 2:G:641:ILE:HA | 1.85 | 0.42 |
| 1:B:12:ILE:CD1 | 2:H:2041:ILE:HD11 | 2.49 | 0.42 |
| 1:A:32:GLN:NE2 | 1:A:57:ALA:HA | 2.34 | 0.42 |
| 2:I:856:LYS:CE | 2:I:1052:CYS:SG | 3.07 | 0.42 |
| 2:H:1149:TRP:HA | 2:H:1242:PHE:CD1 | 2.54 | 0.42 |
| 1:C:1239:HIS:HE1 | 1:C:1714:VAL:O | 2.02 | 0.42 |
| 2:H:1335:ILE:O | 2:H:1338:ILE:HG12 | 2.19 | 0.42 |
| 2:G:238:CYS:CB | 2:G:239:PRO:HD3 | 2.45 | 0.42 |
| 2:H:245:GLN:HG2 | 2:H:505:GLY:HA2 | 2.00 | 0.42 |
| 1:B:417:TYR:HH | 1:B:458:THR:HG22 | 1.84 | 0.42 |
| 1:C:1618:LEU:HD23 | 1:C:1621:PHE:CE2 | 2.55 | 0.42 |
| 1:C:1657:HIS:CE1 | 1:C:1658:PRO:HD2 | 2.54 | 0.42 |
| 2:H:665:LEU:HD22 | 2:H:665:LEU:O | 2.19 | 0.42 |
| 2:H:274:SER:OG | 2:H:428:HIS:HE1 | 2.02 | 0.42 |
| 2:G:1320:LEU:HD12 | 2:G:1320:LEU:HA | 1.88 | 0.42 |
| 2:I:538:ASP:HB2 | 2:I:540:ASP:HB2 | 2.01 | 0.42 |
| 2:I:1666:PHE:CD1 | 2:I:1814:ALA:HB2 | 2.54 | 0.42 |
| 2:H:279:THR:O | 2:H:283:ILE:HB | 2.20 | 0.42 |
| 1:B:1119:LYS:HE2 | 1:B:1341:PHE:CD1 | 2.54 | 0.42 |
| 2:H:938:TRP:CD1 | 2:H:944:ARG:HG3 | 2.53 | 0.42 |
| 2:I:810:GLU:OE2 | 2:I:1070:ILE:N | 2.43 | 0.42 |
| 1:A:1195:ALA:HB1 | 1:A:1200:ILE:HD12 | 2.02 | 0.42 |
| 1:A:1495:ASN:HD22 | 1:A:1495:ASN:HA | 1.67 | 0.42 |
| 2:H:866:LYS:O | 2:H:870:GLU:HG3 | 2.19 | 0.42 |
| 1:C:1308:SER:HB3 | 1:C:1589:GLY:HA3 | 2.01 | 0.42 |
| 1:C:949:GLU:O | 1:C:953:VAL:CG1 | 2.67 | 0.42 |
| 2:I:503:ASP:O | 2:I:530:ALA:HB3 | 2.19 | 0.42 |
| 2:I:1321:ALA:HA | 2:I:1322:PRO:HD3 | 1.83 | 0.42 |
| 2:I:896:ASN:O | 2:I:1050:ARG:NH2 | 2.52 | 0.42 |
| 2:I:726:PHE:HA | 2:I:727:PRO:HD3 | 1.86 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1986:LYS:N | 2:G:1987:PRO:CD | 2.82 | 0.42 |
| 2:G:2026:PHE:HB3 | 2:G:2042:ILE:HD13 | 2.00 | 0.42 |
| 2:I:1085:LEU:HD12 | 2:I:1085:LEU:HA | 1.82 | 0.42 |
| 1:C:330:GLU:O | 1:C:330:GLU:HG2 | 2.18 | 0.42 |
| 2:H:1159:ILE:CG2 | 2:H:1160:THR:N | 2.82 | 0.42 |
| 2:G:543:PHE:HB2 | 2:G:545:GLN:NE2 | 2.25 | 0.42 |
| 2:H:1551:GLU:HB2 | 2:H:1552:PRO:HD3 | 2.00 | 0.42 |
| 2:I:190:PHE:O | 2:I:194:THR:HG22 | 2.19 | 0.42 |
| 2:I:234:ILE:HG13 | 2:I:235:PRO:CD | 2.46 | 0.42 |
| 2:H:1383:ASN:HD21 | 2:H:1418:ASP:HB3 | 1.84 | 0.42 |
| 1:C:408:TRP:CH2 | 1:C:1628:SER:HB3 | 2.55 | 0.42 |
| 1:A:290:MET:HB3 | 1:A:290:MET:HE2 | 1.93 | 0.42 |
| 2:H:1497:GLU:OE1 | 2:H:2002:LYS:CE | 2.66 | 0.42 |
| 1:B:280:GLU:O | 1:B:284:LYS:HG3 | 2.20 | 0.42 |
| 1:C:1114:TYR:CE1 | 1:C:1337:GLU:HG3 | 2.55 | 0.42 |
| 1:B:155:VAL:HG22 | 1:B:186:ILE:CG2 | 2.50 | 0.42 |
| 2:G:1031:LYS:O | 2:G:1032:ASP:C | 2.57 | 0.42 |
| 1:B:828:PRO:HG3 | 1:B:868:ILE:HG22 | 2.00 | 0.42 |
| 2:H:967:ILE:CD1 | 2:H:972:LEU:HD22 | 2.50 | 0.42 |
| 1:A:1132:GLU:HA | 1:A:1133:PRO:HD3 | 1.94 | 0.42 |
| 2:H:1080:GLY:O | 2:H:1084:LYS:HG3 | 2.19 | 0.42 |
| 2:H:38:ASN:HA | 2:H:41:LEU:HD12 | 2.01 | 0.42 |
| 1:B:908:LEU:HA | 1:B:913:VAL:HG21 | 2.00 | 0.42 |
| 2:G:586:LEU:HD12 | 2:G:764:MET:SD | 2.59 | 0.42 |
| 1:A:1131:LEU:HD12 | 1:A:1131:LEU:HA | 1.76 | 0.42 |
| 2:I:309:ARG:HD3 | 2:I:309:ARG:HA | 1.61 | 0.42 |
| 2:H:258:PHE:CD1 | 2:H:258:PHE:N | 2.87 | 0.42 |
| 2:G:421:LEU:HA | 2:G:422:PRO:HD3 | 1.81 | 0.42 |
| 2:I:778:TYR:N | 2:I:779:PRO:CD | 2.82 | 0.42 |
| 1:B:1145:LYS:HD3 | 1:B:1154:ILE:HG12 | 2.01 | 0.42 |
| 2:H:240:LEU:HA | 2:H:240:LEU:HD12 | 1.78 | 0.42 |
| 1:B:1420:ALA:HA | 1:B:1421:PRO:HD3 | 1.74 | 0.42 |
| 2:I:2042:ILE:HG12 | 2:I:2042:ILE:H | 1.36 | 0.42 |
| 2:H:1986:LYS:N | 2:H:1987:PRO:CD | 2.81 | 0.42 |
| 1:C:1219:VAL:CA | 1:C:1384:ILE:CD1 | 2.94 | 0.42 |
| 2:I:674:TYR:HA | 2:I:675:PRO:HD3 | 1.69 | 0.42 |
| 2:I:1175:LYS:HG3 | 2:I:1176:PRO:HD2 | 2.00 | 0.42 |
| 2:G:1878:VAL:CG1 | 2:G:1910:VAL:HG22 | 2.34 | 0.42 |
| 2:H:741:HIS:CE1 | 2:H:855:HIS:NE2 | 2.88 | 0.42 |
| 2:H:1159:ILE:HG13 | 2:H:1169:PRO:CD | 2.50 | 0.42 |
| 2:I:1102:TYR:HB3 | 2:I:1244:PRO:CA | 2.49 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:176:LEU:CD2 | 2:H:184:VAL:HG21 | 2.50 | 0.42 |
| 1:C:21:GLN:HB3 | 1:C:21:GLN:HE21 | 1.69 | 0.42 |
| 1:A:460:GLU:H | 1:A:460:GLU:HG3 | 1.34 | 0.42 |
| 2:I:120:LYS:HB3 | 2:I:124:LYS:HE3 | 2.01 | 0.42 |
| 1:A:1002:LYS:HZ1 | 1:A:1782:GLU:HG2 | 1.83 | 0.42 |
| 2:H:536:ASN:HD21 | 2:H:540:ASP:HB3 | 1.84 | 0.42 |
| 2:H:1427:VAL:HG22 | 2:H:1469:GLU:CG | 2.50 | 0.42 |
| 1:C:406:TRP:CE3 | 1:C:407:ASN:HB2 | 2.53 | 0.42 |
| 2:I:1590:ARG:HG3 | 2:I:1608:TYR:CG | 2.54 | 0.42 |
| 2:I:441:LYS:O | 2:I:445:LYS:HG3 | 2.19 | 0.42 |
| 2:G:503:ASP:OD2 | 2:G:513:GLY:N | 2.50 | 0.42 |
| 1:B:874:GLY:O | 1:B:875:THR:C | 2.58 | 0.42 |
| 2:H:520:LYS:O | 2:H:521:ASP:C | 2.58 | 0.42 |
| 1:C:798:ASN:HA | 1:C:801:ARG:HB2 | 2.02 | 0.42 |
| 2:I:835:THR:HG22 | 2:I:844:VAL:C | 2.40 | 0.42 |
| 2:H:676:ILE:O | 2:H:676:ILE:HG12 | 2.17 | 0.42 |
| 2:G:1135:GLU:HG2 | 2:G:1176:PRO:HG2 | 2.02 | 0.42 |
| 2:I:730:LEU:C | 2:I:730:LEU:HD12 | 2.40 | 0.42 |
| 2:G:638:VAL:HG22 | 2:G:675:PRO:HG2 | 2.01 | 0.42 |
| 1:B:20:TYR:HE1 | 2:H:2035:SER:HB2 | 1.82 | 0.42 |
| 2:H:1149:TRP:NE1 | 2:H:1213:LEU:HD12 | 2.34 | 0.42 |
| 1:C:1455:ARG:HD2 | 1:C:1455:ARG:HA | 1.82 | 0.42 |
| 2:I:786:SER:HB3 | 2:I:794:MET:HE2 | 2.01 | 0.42 |
| 2:I:754:TYR:CE2 | 2:I:794:MET:HG3 | 2.53 | 0.42 |
| 2:H:751:LEU:HD11 | 2:H:789:PHE:CD1 | 2.55 | 0.42 |
| 1:C:32:GLN:NE2 | 1:C:57:ALA:CA | 2.82 | 0.42 |
| 1:B:1234:MET:HE3 | 1:B:1326:ILE:HG21 | 2.01 | 0.42 |
| 1:C:408:TRP:CZ3 | 1:C:1628:SER:HB3 | 2.54 | 0.42 |
| 1:C:413:LEU:O | 1:C:413:LEU:HG | 2.19 | 0.42 |
| 1:B:157:HIS:CE1 | 1:B:269:LEU:HD11 | 2.55 | 0.42 |
| 1:B:272:GLU:HA | 1:B:273:PRO:HD3 | 1.92 | 0.42 |
| 1:B:1022:THR:HG22 | 1:B:1226:SER:CB | 2.49 | 0.42 |
| 2:G:517:HIS:CE1 | 2:G:540:ASP:O | 2.73 | 0.42 |
| 2:I:463:PHE:CD1 | 2:I:486:LEU:HD22 | 2.54 | 0.42 |
| 1:B:1534:ASP:OD1 | 1:B:1566:ARG:HD3 | 2.19 | 0.42 |
| 2:H:1294:ALA:HA | 2:H:1368:VAL:CG2 | 2.49 | 0.42 |
| 1:A:1195:ALA:CB | 1:A:1213:LEU:HD13 | 2.49 | 0.42 |
| 1:C:1592:MET:HE2 | 1:C:1641:ILE:HG23 | 2.00 | 0.42 |
| 1:A:382:LEU:HA | 1:A:382:LEU:HD23 | 1.79 | 0.42 |
| 1:B:1385:GLN:HE21 | 1:B:1385:GLN:HB3 | 1.66 | 0.42 |
| 2:G:1180:MET:HB3 | 2:G:1199:GLU:HG2 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:529:MET:HG2 | 1:A:638:LEU:CG | 2.50 | 0.42 |
| 2:I:298:LYS:HA | 2:I:448:VAL:CG2 | 2.49 | 0.42 |
| 2:H:345:THR:HG22 | 2:H:347:GLU:N | 2.25 | 0.42 |
| 1:B:1239:HIS:CD2 | 1:B:1241:SER:OG | 2.59 | 0.42 |
| 2:G:786:SER:HB2 | 2:G:794:MET:HE2 | 2.00 | 0.42 |
| 2:H:562:LEU:HG | 2:H:793:PRO:HG2 | 2.02 | 0.42 |
| 2:H:60:LEU:O | 2:H:60:LEU:HD23 | 2.20 | 0.42 |
| 2:G:1418:ASP:O | 2:G:1419:PHE:C | 2.58 | 0.42 |
| 2:I:33:LEU:HD21 | 2:I:80:PHE:CE2 | 2.54 | 0.42 |
| 1:C:1639:VAL:CG1 | 1:C:1640:SER:N | 2.82 | 0.42 |
| 1:C:406:TRP:CD2 | 1:C:1619:GLU:HG3 | 2.55 | 0.42 |
| 2:I:1359:MET:CE | 2:I:1404:MET:HB3 | 2.50 | 0.42 |
| 1:B:706:THR:HB | 1:B:737:PHE:HB3 | 2.01 | 0.42 |
| 2:I:1344:ASP:O | 2:I:1416:TYR:HE2 | 2.02 | 0.42 |
| 1:C:475:GLN:CD | 1:C:614:ALA:HB2 | 2.40 | 0.42 |
| 2:I:1217:ASN:HD22 | 2:I:1217:ASN:HA | 1.60 | 0.42 |
| 1:B:982:ILE:HG23 | 2:H:956:GLU:HG2 | 2.01 | 0.42 |
| 1:A:1420:ALA:HA | 1:A:1421:PRO:HD3 | 1.75 | 0.42 |
| 1:B:1784:ASP:O | 1:B:1788:GLU:HB2 | 2.20 | 0.42 |
| 2:H:900:GLN:NE2 | 2:H:1051:THR:HA | 2.34 | 0.42 |
| 1:C:1220:VAL:O | 1:C:1224:ILE:HG12 | 2.19 | 0.42 |
| 2:G:856:LYS:CE | 2:G:1052:CYS:SG | 3.08 | 0.42 |
| 2:I:1989:LYS:NZ | 2:I:2037:PRO:HG2 | 2.35 | 0.42 |
| 2:H:1175:LYS:HG3 | 2:H:1176:PRO:HD2 | 2.02 | 0.42 |
| 2:I:703:LEU:CD2 | 2:I:705:LEU:HG | 2.50 | 0.42 |
| 2:H:712:ALA:O | 2:H:716:VAL:HG23 | 2.20 | 0.42 |
| 1:B:1238:VAL:CG1 | 1:B:1242:GLU:HB2 | 2.49 | 0.42 |
| 2:G:1149:TRP:NE1 | 2:G:1213:LEU:HD12 | 2.35 | 0.42 |
| 2:I:1129:ALA:HB2 | 2:I:1138:TRP:CH2 | 2.55 | 0.42 |
| 2:H:567:PRO:HG3 | 2:H:781:LEU:HD11 | 1.99 | 0.42 |
| 2:H:754:TYR:CG | 2:H:794:MET:HG2 | 2.55 | 0.42 |
| 1:A:1:MET:HE3 | 1:A:9:LEU:HD12 | 2.01 | 0.42 |
| 2:I:44:PRO:HA | 2:I:53:GLU:OE2 | 2.19 | 0.42 |
| 2:H:1002:HIS:NE2 | 2:H:1006:MET:CE | 2.82 | 0.42 |
| 2:H:949:ASP:HB3 | 2:H:1006:MET:CE | 2.47 | 0.42 |
| 1:A:181:THR:HG22 | 1:A:185:GLU:OE2 | 2.19 | 0.42 |
| 1:A:1263:ASP:HB2 | 1:A:1270:VAL:HG21 | 2.01 | 0.42 |
| 2:I:745:ASP:HA | 2:I:832:TRP:CH2 | 2.49 | 0.42 |
| 2:H:1339:PHE:N | 2:H:1340:PRO:CD | 2.83 | 0.42 |
| 1:B:1264:ARG:NH1 | 1:B:1270:VAL:HB | 2.35 | 0.42 |
| 2:I:2046:GLU:C | 2:I:2048:TYR:N | 2.73 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:I:73:GLU:OE2 | 2:I:76:LYS:HD2 | 2.18 | 0.42 |
| 1:A:489:VAL:CG2 | 1:A:671:VAL:N | 2.83 | 0.42 |
| 2:I:740:HIS:HA | 2:I:854:ILE:HD13 | 2.01 | 0.42 |
| 1:B:625:THR:HG23 | 1:B:627:SER:H | 1.84 | 0.42 |
| 1:B:242:THR:HG22 | 1:B:243:ILE:H | 1.83 | 0.42 |
| 2:I:1273:GLU:HB3 | 2:I:1274:PRO:CD | 2.50 | 0.42 |
| 2:H:804:ARG:NH1 | 2:H:1062:PHE:O | 2.52 | 0.42 |
| 1:B:1244:GLY:O | 1:B:1327:CYS:HB2 | 2.20 | 0.42 |
| 1:C:1067:LEU:HA | 1:C:1067:LEU:HD23 | 1.76 | 0.42 |
| 1:C:438:ASN:HD21 | 1:C:698:GLN:HE21 | 1.66 | 0.42 |
| 2:G:938:TRP:CE2 | 2:G:944:ARG:HG3 | 2.54 | 0.42 |
| 2:I:1343:VAL:HG22 | 2:I:1343:VAL:O | 2.20 | 0.42 |
| 2:H:581:THR:O | 2:H:585:LYS:HB2 | 2.20 | 0.42 |
| 2:G:1044:VAL:HG21 | 2:G:1050:ARG:NE | 2.34 | 0.42 |
| 1:A:1019:ILE:HG13 | 1:A:1316:VAL:HG13 | 2.01 | 0.42 |
| 2:G:507:GLY:O | 2:G:508:GLY:C | 2.58 | 0.42 |
| 1:B:1682:LYS:HB3 | 2:H:994:PHE:CE2 | 2.54 | 0.42 |
| 2:G:810:GLU:OE2 | 2:G:1070:ILE:N | 2.44 | 0.42 |
| 2:G:7:ARG:NH1 | 2:G:24:THR:CG2 | 2.79 | 0.42 |
| 2:H:844:VAL:HG22 | 2:H:858:ALA:HB2 | 2.01 | 0.42 |
| 1:C:2:LYS:HE2 | 1:C:4:GLU:OE1 | 2.19 | 0.42 |
| 2:H:1642:THR:HB | 2:H:1651:LEU:HB2 | 2.01 | 0.42 |
| 1:C:1310:GLU:OE1 | 1:C:1649:LYS:CE | 2.65 | 0.42 |
| 1:A:655:LEU:HA | 1:A:655:LEU:HD23 | 1.81 | 0.42 |
| 2:G:237:SER:O | 2:G:241:ILE:HG13 | 2.20 | 0.42 |
| 2:I:732:TRP:CH2 | 2:I:749:PRO:HG2 | 2.55 | 0.42 |
| 2:G:732:TRP:CH2 | 2:G:749:PRO:HG2 | 2.55 | 0.42 |
| 2:G:827:VAL:HG21 | 2:G:840:THR:CG2 | 2.49 | 0.42 |
| 1:B:458:THR:OG1 | 1:B:470:LYS:HD2 | 2.20 | 0.42 |
| 2:H:33:LEU:HD13 | 2:H:68:VAL:HG22 | 2.02 | 0.42 |
| 1:A:408:TRP:CH2 | 1:A:1628:SER:HB3 | 2.55 | 0.42 |
| 1:A:1260:MET:HB2 | 1:A:1274:ILE:HD12 | 2.02 | 0.42 |
| 1:C:1842:VAL:O | 1:C:1843:ASN:C | 2.57 | 0.42 |
| 1:A:987:ASN:HD22 | 2:G:957:ARG:CD | 2.30 | 0.42 |
| 1:B:1012:LEU:HD23 | 1:B:1445:MET:HE3 | 2.00 | 0.42 |
| 1:C:37:LYS:HB2 | 1:C:65:TYR:CE1 | 2.52 | 0.42 |
| 2:G:1014:PRO:HG2 | 2:G:1032:ASP:HB2 | 2.01 | 0.42 |
| 1:C:155:VAL:O | 1:C:159:LEU:HG | 2.19 | 0.42 |
| 2:H:624:TYR:HB2 | 2:H:630:MET:HE3 | 2.02 | 0.42 |
| 2:G:1383:ASN:OD1 | 2:G:1388:LYS:HG3 | 2.20 | 0.42 |
| 1:B:1830:GLY:HA2 | 1:B:1831:GLY:HA2 | 1.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1217:ASN:HA | 2:G:1217:ASN:HD22 | 1.62 | 0.42 |
| 2:G:258:PHE:HD1 | 2:G:258:PHE:N | 2.18 | 0.42 |
| 1:A:800:LEU:HA | 1:A:800:LEU:HD23 | 1.84 | 0.42 |
| 2:G:1079:ASP:O | 2:G:1082:ILE:HG22 | 2.19 | 0.42 |
| 1:B:798:ASN:HA | 1:B:801:ARG:HB2 | 2.02 | 0.42 |
| 2:G:892:ILE:HD11 | 2:G:903:TRP:CD2 | 2.51 | 0.42 |
| 2:H:641:ILE:CD1 | 2:H:645:SER:HB2 | 2.50 | 0.42 |
| 2:G:2036:GLU:HB2 | 2:G:2037:PRO:CD | 2.48 | 0.42 |
| 2:I:1135:GLU:HG2 | 2:I:1176:PRO:HG2 | 2.02 | 0.42 |
| 1:A:444:ASN:CB | 1:A:446:ALA:H | 2.32 | 0.42 |
| 1:B:31:THR:CG2 | 2:H:2011:ILE:HG21 | 2.40 | 0.42 |
| 1:B:20:TYR:CZ | 2:H:2035:SER:HB2 | 2.53 | 0.42 |
| 2:H:995:LEU:HB3 | 2:H:1000:ILE:CD1 | 2.50 | 0.42 |
| 1:A:335:HIS:CD2 | 1:A:335:HIS:C | 2.92 | 0.42 |
| 2:H:1889:VAL:HG22 | 2:H:1977:HIS:O | 2.19 | 0.42 |
| 1:B:44:VAL:HG11 | 1:B:78:ILE:HG12 | 2.00 | 0.42 |
| 1:B:1:MET:HE3 | 1:B:6:GLU:HA | 2.01 | 0.42 |
| 2:I:1593:ILE:O | 2:I:1597:ALA:HB3 | 2.20 | 0.42 |
| 2:G:1840:VAL:O | 2:G:1840:VAL:HG13 | 2.18 | 0.42 |
| 1:B:1189:ILE:HG23 | 1:B:1190:PRO:HD2 | 2.01 | 0.42 |
| 1:C:1012:LEU:HD23 | 1:C:1445:MET:HE2 | 2.02 | 0.42 |
| 1:A:1332:TYR:HB3 | 1:A:1382:ALA:CB | 2.50 | 0.42 |
| 2:I:1223:MET:HE3 | 2:I:1238:LEU:CD1 | 2.49 | 0.42 |
| 1:A:1618:LEU:HD23 | 1:A:1621:PHE:CE2 | 2.54 | 0.42 |
| 1:B:1705:PRO:HB2 | 1:B:1733:PHE:CD1 | 2.55 | 0.42 |
| 2:G:1666:PHE:CD1 | 2:G:1814:ALA:CB | 3.02 | 0.42 |
| 1:A:155:VAL:HG22 | 1:A:186:ILE:CG2 | 2.50 | 0.42 |
| 1:C:1244:GLY:HA3 | 1:C:1297:PRO:HD2 | 2.02 | 0.42 |
| 2:I:360:LEU:HA | 2:I:361:PRO:HD3 | 1.89 | 0.42 |
| 2:I:879:LYS:HA | 2:I:879:LYS:HD3 | 1.73 | 0.42 |
| 1:C:1154:ILE:O | 1:C:1154:ILE:HG13 | 2.20 | 0.42 |
| 1:B:780:GLU:O | 1:B:781:LEU:C | 2.58 | 0.42 |
| 2:H:433:VAL:N | 2:H:434:PRO:CD | 2.83 | 0.42 |
| 1:B:1539:ALA:O | 1:B:1574:GLY:HA2 | 2.20 | 0.42 |
| 1:A:453:TYR:O | 1:A:457:ASN:HB2 | 2.20 | 0.42 |
| 2:H:1180:MET:HB3 | 2:H:1199:GLU:HG2 | 2.02 | 0.42 |
| 2:H:2036:GLU:HB2 | 2:H:2037:PRO:CD | 2.47 | 0.42 |
| 2:G:298:LYS:HA | 2:G:448:VAL:CG2 | 2.50 | 0.42 |
| 1:A:32:GLN:HE21 | 1:A:57:ALA:HB2 | 1.85 | 0.42 |
| 2:I:1214:LEU:HD11 | 2:I:1220:GLN:NE2 | 2.35 | 0.42 |
| 2:I:1335:ILE:O | 2:I:1338:ILE:HG12 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:234:ILE:HG13 | 2:H:235:PRO:CD | 2.47 | 0.42 |
| 2:G:670:ARG:HD2 | 2:G:676:ILE:O | 2.20 | 0.42 |
| 2:G:736:ARG:H | 2:G:736:ARG:HG3 | 1.59 | 0.42 |
| 1:B:438:ASN:ND2 | 1:B:698:GLN:HE21 | 2.14 | 0.42 |
| 2:G:1360:ILE:HA | 2:G:1361:PRO:HD3 | 1.91 | 0.42 |
| 2:G:1782:THR:CG2 | 2:G:1827:LEU:HD21 | 2.48 | 0.42 |
| 1:A:1234:MET:HE3 | 1:A:1326:ILE:HG21 | 2.02 | 0.42 |
| 1:B:1175:ILE:HA | 1:B:1176:PRO:HD3 | 1.89 | 0.42 |
| 1:B:140:ILE:CG2 | 1:B:141:ALA:N | 2.83 | 0.42 |
| 2:G:427:PHE:HB3 | 2:G:428:HIS:ND1 | 2.34 | 0.42 |
| 1:A:521:LYS:HB3 | 1:A:523:SER:HB3 | 2.01 | 0.42 |
| 2:G:468:LEU:O | 2:G:471:LEU:HB2 | 2.20 | 0.42 |
| 1:A:998:TYR:CD2 | 1:A:1667:GLU:HG3 | 2.55 | 0.42 |
| 2:H:1666:PHE:CD1 | 2:H:1814:ALA:CB | 3.03 | 0.42 |
| 2:I:1738:PHE:HE1 | 2:I:1837:THR:HG23 | 1.85 | 0.42 |
| 2:I:804:ARG:NH2 | 2:I:1068:GLU:OE1 | 2.53 | 0.42 |
| 2:G:1236:LEU:HA | 2:G:1237:PRO:HD3 | 1.76 | 0.42 |
| 1:C:19:ALA:O | 1:C:22:PHE:HB2 | 2.19 | 0.42 |
| 1:C:1029:PRO:HA | 1:C:1188:GLN:O | 2.20 | 0.42 |
| 2:H:1855:ILE:HB | 2:H:1907:LEU:HD12 | 2.01 | 0.42 |
| 2:H:1343:VAL:HG22 | 2:H:1343:VAL:O | 2.20 | 0.42 |
| 2:I:258:PHE:N | 2:I:258:PHE:CD1 | 2.87 | 0.42 |
| 1:A:780:GLU:O | 1:A:781:LEU:C | 2.59 | 0.42 |
| 2:H:23:PRO:HG2 | 2:H:86:LEU:HD11 | 2.01 | 0.42 |
| 1:C:1370:THR:HG22 | 1:C:1371:THR:N | 2.35 | 0.42 |
| 2:H:421:LEU:HA | 2:H:422:PRO:HD3 | 1.78 | 0.42 |
| 1:A:350:LEU:HD23 | 1:A:350:LEU:HA | 1.89 | 0.42 |
| 2:I:512:LEU:O | 2:I:516:THR:HG23 | 2.20 | 0.41 |
| 1:C:12:ILE:HD11 | 2:I:2041:ILE:HD11 | 2.01 | 0.41 |
| 1:C:1215:VAL:O | 1:C:1219:VAL:HG23 | 2.20 | 0.41 |
| 2:G:638:VAL:HA | 2:G:641:ILE:CG2 | 2.50 | 0.41 |
| 1:A:32:GLN:NE2 | 1:A:57:ALA:CA | 2.83 | 0.41 |
| 2:G:1496:LYS:CE | 2:G:1693:ARG:HH21 | 2.28 | 0.41 |
| 2:I:659:LEU:O | 2:I:663:ILE:HG12 | 2.20 | 0.41 |
| 2:I:1980:TYR:HD1 | 2:I:1981:LEU:HD12 | 1.85 | 0.41 |
| 1:A:1657:HIS:CG | 1:A:1658:PRO:HD2 | 2.55 | 0.41 |
| 1:C:635:ILE:CG2 | 1:C:651:TYR:CG | 3.03 | 0.41 |
| 2:G:1579:ILE:CD1 | 2:G:1615:MET:SD | 3.08 | 0.41 |
| 2:H:2010:TYR:O | 2:H:2012:PRO:HD3 | 2.20 | 0.41 |
| 2:I:1697:HIS:CE1 | 2:I:1829:GLU:CG | 3.03 | 0.41 |
| 2:G:439:ILE:HD12 | 2:G:484:ILE:HD11 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1279:PHE:HB2 | 1:A:1282:THR:HG23 | 2.01 | 0.41 |
| 2:I:1815:LEU:O | 2:I:1821:VAL:HG23 | 2.20 | 0.41 |
| 1:B:1019:ILE:HG13 | 1:B:1316:VAL:HG13 | 2.02 | 0.41 |
| 2:I:441:LYS:HG2 | 2:I:445:LYS:HE3 | 2.02 | 0.41 |
| 2:H:258:PHE:N | 2:H:258:PHE:HD1 | 2.18 | 0.41 |
| 2:H:240:LEU:O | 2:H:244:ILE:HG13 | 2.19 | 0.41 |
| 1:A:1019:ILE:HG21 | 1:A:1316:VAL:HG22 | 2.01 | 0.41 |
| 1:C:616:LEU:HB2 | 1:C:617:PRO:HD3 | 2.01 | 0.41 |
| 1:B:1673:TYR:CZ | 1:B:1677:VAL:HG21 | 2.55 | 0.41 |
| 2:H:896:ASN:O | 2:H:1050:ARG:NH2 | 2.53 | 0.41 |
| 1:A:1308:SER:HB3 | 1:A:1589:GLY:HA3 | 2.01 | 0.41 |
| 2:G:1128:LYS:HG2 | 2:G:1181:VAL:HG22 | 2.02 | 0.41 |
| 1:C:12:ILE:O | 1:C:15:THR:HG23 | 2.20 | 0.41 |
| 2:G:2035:SER:OG | 2:G:2037:PRO:HD2 | 2.21 | 0.41 |
| 1:A:340:ARG:NH1 | 1:A:344:GLN:CG | 2.70 | 0.41 |
| 2:I:1495:THR:O | 2:I:1496:LYS:HB2 | 2.20 | 0.41 |
| 2:I:1149:TRP:HA | 2:I:1242:PHE:CD1 | 2.54 | 0.41 |
| 2:H:584:SER:CB | 2:H:591:PRO:HG3 | 2.46 | 0.41 |
| 1:C:889:GLU:C | 1:C:891:MET:H | 2.24 | 0.41 |
| 2:I:84:LEU:HA | 2:I:84:LEU:HD23 | 1.89 | 0.41 |
| 1:A:983:GLN:HE21 | 2:G:962:LYS:HD2 | 1.80 | 0.41 |
| 2:G:1553:TYR:OH | 2:G:1583:MET:HB3 | 2.20 | 0.41 |
| 1:C:1584:PRO:CG | 1:C:1591:TRP:CZ3 | 3.03 | 0.41 |
| 1:A:50:SER:CB | 1:A:51:PRO:CD | 2.98 | 0.41 |
| 1:B:290:MET:HE2 | 1:B:290:MET:HB3 | 1.96 | 0.41 |
| 2:H:15:SER:H | 2:H:48:PHE:HE2 | 1.66 | 0.41 |
| 1:A:1233:GLU:CD | 1:A:1680:ARG:HH21 | 2.24 | 0.41 |
| 2:I:524:GLY:HA2 | 2:I:558:ASN:O | 2.20 | 0.41 |
| 1:A:280:GLU:O | 1:A:284:LYS:HG3 | 2.21 | 0.41 |
| 1:A:28:TRP:CE2 | 1:A:53:LEU:HD22 | 2.55 | 0.41 |
| 2:G:717:ILE:HG23 | 2:G:760:HIS:CE1 | 2.55 | 0.41 |
| 2:H:142:ASN:HB2 | 2:H:550:VAL:HG13 | 2.01 | 0.41 |
| 1:A:29:ILE:HD13 | 2:G:1894:GLU:HA | 2.01 | 0.41 |
| 2:G:1755:ILE:HD11 | 2:G:1762:TYR:HB2 | 2.03 | 0.41 |
| 2:G:992:GLU:HA | 2:G:992:GLU:OE1 | 2.20 | 0.41 |
| 2:I:592:LEU:O | 2:I:616:THR:HG23 | 2.19 | 0.41 |
| 2:H:1713:ASN:HA | 2:H:1714:PRO:HD3 | 1.89 | 0.41 |
| 2:G:888:ARG:O | 2:G:892:ILE:HB | 2.21 | 0.41 |
| 1:B:852:ARG:HB3 | 1:B:858:TRP:HZ2 | 1.83 | 0.41 |
| 2:G:1624:THR:HB | 2:G:1642:THR:CG2 | 2.50 | 0.41 |
| 2:H:1314:ARG:HD3 | 2:H:1314:ARG:HA | 1.63 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:667:LYS:HD2 | 2:G:697:THR:CG2 | 2.38 | 0.41 |
| 1:C:335:HIS:C | 1:C:335:HIS:CD2 | 2.91 | 0.41 |
| 1:A:1666:THR:HG23 | 1:A:1669:ARG:HB2 | 2.01 | 0.41 |
| 1:C:1208:VAL:HG13 | 1:C:1209:ASP:O | 2.20 | 0.41 |
| 2:G:1359:MET:HB3 | 2:G:1606:ARG:NH2 | 2.35 | 0.41 |
| 2:I:807:ILE:HA | 2:I:818:LYS:HG2 | 2.02 | 0.41 |
| 2:I:1493:LEU:HB3 | 2:I:1494:PRO:HD2 | 2.02 | 0.41 |
| 2:G:1258:ARG:O | 2:G:1262:ILE:HG13 | 2.20 | 0.41 |
| 1:C:1047:LEU:HD23 | 1:C:1047:LEU:HA | 1.89 | 0.41 |
| 2:G:1380:SER:HB3 | 2:G:1424:GLN:HB2 | 2.02 | 0.41 |
| 1:B:455:ILE:HD13 | 1:B:455:ILE:HA | 1.84 | 0.41 |
| 1:A:1784:ASP:O | 1:A:1788:GLU:HB2 | 2.20 | 0.41 |
| 2:I:581:THR:O | 2:I:585:LYS:HB2 | 2.20 | 0.41 |
| 2:I:195:LEU:O | 2:I:199:ILE:HG13 | 2.20 | 0.41 |
| 1:B:1047:LEU:O | 1:B:1051:VAL:HG23 | 2.20 | 0.41 |
| 2:G:520:LYS:O | 2:G:521:ASP:C | 2.58 | 0.41 |
| 2:I:507:GLY:O | 2:I:508:GLY:C | 2.59 | 0.41 |
| 2:I:339:LEU:HD23 | 2:I:419:ARG:O | 2.20 | 0.41 |
| 1:C:792:HIS:CE1 | 1:C:796:LEU:HD23 | 2.55 | 0.41 |
| 2:H:601:THR:HB | 2:H:620:ALA:HB2 | 2.01 | 0.41 |
| 1:A:1720:ALA:O | 1:A:1721:ARG:HG2 | 2.21 | 0.41 |
| 2:I:156:LEU:HD23 | 2:I:500:HIS:HB2 | 2.02 | 0.41 |
| 1:A:807:LYS:C | 1:A:807:LYS:HD3 | 2.40 | 0.41 |
| 1:A:12:ILE:O | 1:A:15:THR:HG23 | 2.20 | 0.41 |
| 2:H:1886:VAL:HG22 | 2:H:1906:ALA:HB1 | 2.02 | 0.41 |
| 1:A:330:GLU:O | 1:A:330:GLU:HG2 | 2.20 | 0.41 |
| 2:H:455:ILE:HG12 | 2:H:469:ARG:CG | 2.49 | 0.41 |
| 2:H:561:TRP:CG | 2:H:754:TYR:HE2 | 2.39 | 0.41 |
| 2:I:949:ASP:HB3 | 2:I:1006:MET:CE | 2.48 | 0.41 |
| 2:I:1457:PHE:CD2 | 2:I:1459:LEU:HD23 | 2.55 | 0.41 |
| 1:B:992:PHE:CD2 | 1:B:1399:PRO:HG3 | 2.55 | 0.41 |
| 2:G:846:VAL:HG13 | 2:G:865:TRP:CD1 | 2.55 | 0.41 |
| 1:A:1305:CYS:SG | 3:A:2748:CER:C5 | 3.08 | 0.41 |
| 2:I:654:VAL:CG2 | 2:I:683:ALA:HB1 | 2.50 | 0.41 |
| 2:G:950:PHE:O | 2:G:953:ARG:HB3 | 2.20 | 0.41 |
| 2:H:1752:PHE:HZ | 2:H:1836:MET:HE3 | 1.84 | 0.41 |
| 2:G:439:ILE:HD12 | 2:G:484:ILE:CD1 | 2.50 | 0.41 |
| 1:A:28:TRP:CZ2 | 1:A:53:LEU:HD22 | 2.56 | 0.41 |
| 2:G:760:HIS:HA | 2:G:761:PRO:HD3 | 1.85 | 0.41 |
| 1:C:521:LYS:HE2 | 1:C:605:LEU:HD11 | 2.02 | 0.41 |
| 2:I:258:PHE:HD1 | 2:I:258:PHE:N | 2.18 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1448:ARG:HD2 | 1:B:1508:TRP:O | 2.21 | 0.41 |
| 1:C:719:GLN:HG3 | 1:C:720:SER:N | 2.35 | 0.41 |
| 1:B:1216:LEU:HD23 | 1:B:1216:LEU:HA | 1.93 | 0.41 |
| 2:I:1021:LEU:HD22 | 2:I:1021:LEU:HA | 1.61 | 0.41 |
| 1:A:1154:ILE:O | 1:A:1154:ILE:HG13 | 2.19 | 0.41 |
| 1:B:378:LEU:HA | 1:B:378:LEU:HD12 | 1.75 | 0.41 |
| 2:I:1458:ASP:O | 2:I:1462:LYS:HE3 | 2.21 | 0.41 |
| 2:H:1071:LYS:HE3 | 2:H:1075:ASP:OD2 | 2.20 | 0.41 |
| 1:C:495:LYS:HA | 1:C:496:PRO:HD3 | 1.86 | 0.41 |
| 1:C:496:PRO:HB2 | 1:C:519:VAL:HG12 | 2.02 | 0.41 |
| 2:G:1862:VAL:HG22 | 2:G:1863:ALA:N | 2.36 | 0.41 |
| 1:A:12:ILE:O | 1:A:16:GLU:HG2 | 2.20 | 0.41 |
| 2:I:712:ALA:O | 2:I:716:VAL:HG23 | 2.21 | 0.41 |
| 1:A:1477:ILE:N | 1:A:1478:PRO:CD | 2.83 | 0.41 |
| 2:G:1676:MET:HE1 | 2:G:1781:LEU:CD2 | 2.47 | 0.41 |
| 1:B:1303:GLY:H | 1:B:1307:THR:CG2 | 2.31 | 0.41 |
| 2:I:572:ASN:HA | 2:I:572:ASN:HD22 | 1.70 | 0.41 |
| 2:I:177:TYR:CD1 | 2:I:188:ILE:HG21 | 2.55 | 0.41 |
| 1:B:1232:TYR:CE2 | 1:B:1701:LYS:HD2 | 2.55 | 0.41 |
| 1:B:2:LYS:CD | 2:H:2050:GLN:HB3 | 2.44 | 0.41 |
| 2:I:780:TYR:HB2 | 2:I:799:PHE:HE2 | 1.85 | 0.41 |
| 2:I:786:SER:HB2 | 2:I:794:MET:HE2 | 2.02 | 0.41 |
| 1:A:9:LEU:HD21 | 2:G:2047:LYS:HD2 | 2.02 | 0.41 |
| 2:I:800:LEU:H | 2:I:800:LEU:HD23 | 1.85 | 0.41 |
| 1:B:504:ASP:CB | 1:B:508:ASN:HB2 | 2.49 | 0.41 |
| 1:A:82:SER:OG | 1:A:83:LYS:HG3 | 2.20 | 0.41 |
| 2:I:1940:LEU:HD12 | 2:I:1941:PHE:N | 2.35 | 0.41 |
| 1:B:1244:GLY:HA3 | 1:B:1297:PRO:HD2 | 2.03 | 0.41 |
| 1:C:242:THR:HB | 1:C:244:THR:HB | 2.02 | 0.41 |
| 1:B:453:TYR:O | 1:B:457:ASN:HB2 | 2.21 | 0.41 |
| 2:H:478:ARG:O | 2:H:482:CYS:HB2 | 2.20 | 0.41 |
| 1:C:1830:GLY:HA2 | 1:C:1831:GLY:HA2 | 1.57 | 0.41 |
| 2:I:566:HIS:ND1 | 2:I:567:PRO:HD2 | 2.35 | 0.41 |
| 2:G:1706:ILE:HD12 | 2:G:1706:ILE:HA | 1.89 | 0.41 |
| 1:B:1257:LEU:HD23 | 1:B:1257:LEU:HA | 1.76 | 0.41 |
| 1:C:1443:LEU:HA | 1:C:1443:LEU:HD23 | 1.77 | 0.41 |
| 1:B:1308:SER:HB3 | 1:B:1589:GLY:HA3 | 2.03 | 0.41 |
| 1:B:949:GLU:O | 1:B:953:VAL:HG12 | 2.21 | 0.41 |
| 1:A:601:VAL:O | 1:A:602:GLU:C | 2.59 | 0.41 |
| 2:H:339:LEU:HD23 | 2:H:419:ARG:O | 2.20 | 0.41 |
| 2:H:231:LEU:HA | 2:H:236:ILE:HD12 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1408:ALA:O | 1:C:1651:GLY:HA2 | 2.21 | 0.41 |
| 2:G:597:MET:HA | 4:G:3051:FMN:C5A | 2.51 | 0.41 |
| 2:G:490:TRP:CZ2 | 2:G:512:LEU:HD21 | 2.55 | 0.41 |
| 2:I:638:VAL:HG22 | 2:I:675:PRO:HG2 | 2.03 | 0.41 |
| 2:G:1642:THR:HB | 2:G:1651:LEU:HB2 | 2.01 | 0.41 |
| 2:H:712:ALA:O | 2:H:715:GLN:HB3 | 2.20 | 0.41 |
| 2:H:722:ALA:CB | 2:H:723:HIS:CE1 | 3.04 | 0.41 |
| 1:A:529:MET:HE1 | 1:A:894:ARG:HD2 | 2.00 | 0.41 |
| 2:I:1054:LEU:HD22 | 4:I:3051:FMN:HM72 | 2.03 | 0.41 |
| 2:G:1495:THR:O | 2:G:1496:LYS:HB2 | 2.20 | 0.41 |
| 2:I:1423:PHE:N | 2:I:1423:PHE:CD1 | 2.71 | 0.41 |
| 2:G:1169:PRO:O | 2:G:1173:VAL:HG23 | 2.20 | 0.41 |
| 2:H:1680:LEU:HD13 | 2:H:1687:ALA:CB | 2.45 | 0.41 |
| 2:G:754:TYR:CG | 2:G:794:MET:CG | 3.04 | 0.41 |
| 2:I:663:ILE:HG13 | 2:I:694:TYR:CE1 | 2.51 | 0.41 |
| 2:G:1352:HIS:HD2 | 2:G:1410:PHE:CD2 | 2.38 | 0.41 |
| 1:A:932:PHE:O | 1:A:934:PRO:HD3 | 2.20 | 0.41 |
| 1:A:1842:VAL:O | 1:A:1843:ASN:O | 2.39 | 0.41 |
| 2:H:1236:LEU:HD22 | 2:H:1238:LEU:HG | 2.03 | 0.41 |
| 1:A:825:PRO:HB2 | 1:A:843:LYS:HZ2 | 1.86 | 0.41 |
| 2:I:1417:THR:C | 2:I:1419:PHE:N | 2.74 | 0.41 |
| 2:H:950:PHE:O | 2:H:953:ARG:HB3 | 2.20 | 0.41 |
| 2:G:1815:LEU:O | 2:G:1821:VAL:HG23 | 2.20 | 0.41 |
| 1:B:495:LYS:HA | 1:B:496:PRO:HD3 | 1.89 | 0.41 |
| 2:H:717:ILE:CG2 | 2:H:760:HIS:CE1 | 3.04 | 0.41 |
| 2:H:624:TYR:CD1 | 2:H:630:MET:HE2 | 2.56 | 0.41 |
| 1:A:370:GLU:O | 1:A:373:ALA:HB3 | 2.20 | 0.41 |
| 1:B:238:PRO:CG | 1:B:283:ALA:HB2 | 2.50 | 0.41 |
| 1:C:1709:GLU:H | 1:C:1709:GLU:HG3 | 1.42 | 0.41 |
| 2:G:1979:THR:O | 2:G:1982:MET:HB2 | 2.21 | 0.41 |
| 1:C:1784:ASP:O | 1:C:1788:GLU:HB2 | 2.20 | 0.41 |
| 1:B:1066:ASN:HD22 | 1:B:1071:PRO:HA | 1.86 | 0.41 |
| 1:B:406:TRP:CD2 | 1:B:1619:GLU:HG3 | 2.55 | 0.41 |
| 2:I:159:ILE:HD11 | 2:I:512:LEU:CG | 2.49 | 0.41 |
| 2:G:843:ILE:CD1 | 2:G:1055:HIS:HB3 | 2.50 | 0.41 |
| 2:G:835:THR:HG21 | 2:G:855:HIS:NE2 | 2.35 | 0.41 |
| 2:I:1642:THR:HB | 2:I:1651:LEU:HB2 | 2.03 | 0.41 |
| 1:A:32:GLN:O | 1:A:36:LEU:HB2 | 2.21 | 0.41 |
| 2:I:634:ILE:CD1 | 2:I:649:ILE:HD11 | 2.44 | 0.41 |
| 1:A:988:ILE:HD13 | 1:A:1048:GLU:CG | 2.50 | 0.41 |
| 1:B:1666:THR:HG23 | 1:B:1669:ARG:CB | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:587:ILE:HD11 | 2:G:589:ARG:HB2 | 2.03 | 0.41 |
| 2:I:595:PRO:HD3 | 2:I:800:LEU:HB2 | 2.01 | 0.41 |
| 2:H:827:VAL:HG12 | 2:H:828:PRO:O | 2.19 | 0.41 |
| 1:C:35:PHE:HA | 1:C:39:PHE:HD2 | 1.86 | 0.41 |
| 2:I:1981:LEU:HD12 | 2:I:1981:LEU:N | 2.36 | 0.41 |
| 1:C:1418:VAL:N | 1:C:1419:PRO:CD | 2.83 | 0.41 |
| 2:H:821:ILE:HA | 2:H:857:ILE:HD11 | 2.02 | 0.41 |
| 2:I:463:PHE:O | 2:I:463:PHE:HD2 | 2.04 | 0.41 |
| 1:B:1105:LEU:HA | 1:B:1105:LEU:HD23 | 1.89 | 0.41 |
| 2:G:1427:VAL:HG22 | 2:G:1469:GLU:CG | 2.51 | 0.41 |
| 2:H:1503:ILE:HG22 | 2:H:1504:VAL:C | 2.41 | 0.41 |
| 2:H:11:LEU:HD23 | 2:H:11:LEU:HA | 1.93 | 0.41 |
| 1:C:1119:LYS:HE2 | 1:C:1341:PHE:CG | 2.55 | 0.41 |
| 2:H:236:ILE:HD13 | 2:H:236:ILE:C | 2.40 | 0.41 |
| 1:A:774:ILE:HA | 1:A:775:PRO:HD3 | 1.76 | 0.41 |
| 2:I:1357:TYR:HD1 | 2:I:1406:VAL:HG22 | 1.85 | 0.41 |
| 2:G:571:LYS:HB2 | 2:G:1099:ALA:HB2 | 2.02 | 0.41 |
| 2:G:246:LEU:HD12 | 2:G:246:LEU:HA | 1.82 | 0.41 |
| 1:C:1131:LEU:HA | 1:C:1131:LEU:HD12 | 1.69 | 0.41 |
| 2:H:1128:LYS:HG2 | 2:H:1181:VAL:HG22 | 2.01 | 0.41 |
| 1:B:1126:ILE:CD1 | 1:B:1172:THR:HG22 | 2.51 | 0.41 |
| 2:G:425:SER:HA | 2:G:426:PRO:HD3 | 1.79 | 0.41 |
| 2:G:1344:ASP:O | 2:G:1416:TYR:HE2 | 2.03 | 0.41 |
| 2:H:159:ILE:HG12 | 2:H:512:LEU:HD23 | 2.02 | 0.41 |
| 2:G:131:ILE:HD12 | 2:G:182:VAL:CG1 | 2.49 | 0.41 |
| 2:I:2035:SER:OG | 2:I:2037:PRO:HD2 | 2.21 | 0.41 |
| 2:H:674:TYR:HA | 2:H:675:PRO:HD3 | 1.73 | 0.41 |
| 1:A:16:GLU:HA | 1:A:16:GLU:OE2 | 2.21 | 0.41 |
| 2:I:705:LEU:HD23 | 2:I:705:LEU:HA | 1.80 | 0.41 |
| 2:H:719:ILE:H | 2:H:719:ILE:HG12 | 1.63 | 0.41 |
| 2:G:123:ILE:CD1 | 2:G:533:LEU:HD23 | 2.50 | 0.41 |
| 1:A:1239:HIS:HE1 | 1:A:1714:VAL:O | 2.03 | 0.41 |
| 1:C:658:LEU:HD13 | 1:C:916:LEU:HD12 | 2.02 | 0.41 |
| 2:I:1374:THR:HG23 | 2:I:1396:LEU:CD1 | 2.49 | 0.41 |
| 2:H:805:VAL:HG12 | 2:H:805:VAL:O | 2.21 | 0.41 |
| 2:G:1428:GLU:CG | 2:G:1468:THR:HG22 | 2.51 | 0.41 |
| 2:G:270:ALA:O | 2:G:459:VAL:HA | 2.20 | 0.41 |
| 1:A:441:ASN:OD1 | 1:A:488:PRO:HA | 2.21 | 0.41 |
| 2:H:1662:THR:HB | 2:H:1799:PRO:HG2 | 2.02 | 0.41 |
| 2:G:236:ILE:HG12 | 2:G:240:LEU:HD22 | 2.02 | 0.41 |
| 2:H:320:PRO:HA | 2:H:321:PRO:HD3 | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1070:ILE:O | 2:G:1070:ILE:HD13 | 2.21 | 0.41 |
| 1:B:949:GLU:O | 1:B:953:VAL:CG1 | 2.68 | 0.41 |
| 2:H:1959:LYS:HG2 | 2:H:1959:LYS:O | 2.20 | 0.41 |
| 1:A:91:THR:HA | 1:A:92:PRO:HD3 | 1.81 | 0.41 |
| 1:B:521:LYS:HB3 | 1:B:523:SER:HB3 | 2.03 | 0.41 |
| 1:C:1420:ALA:HA | 1:C:1421:PRO:HD3 | 1.78 | 0.41 |
| 1:A:1460:LYS:CE | 1:A:1774:GLU:OE1 | 2.62 | 0.41 |
| 1:A:253:ARG:O | 1:A:254:TRP:CD1 | 2.74 | 0.41 |
| 2:H:892:ILE:HD11 | 2:H:903:TRP:CD2 | 2.53 | 0.41 |
| 2:H:615:TYR:CE2 | 2:H:1074:MET:HB3 | 2.56 | 0.41 |
| 2:G:1989:LYS:NZ | 2:G:2037:PRO:HG2 | 2.35 | 0.41 |
| 1:B:444:ASN:CB | 1:B:446:ALA:H | 2.31 | 0.41 |
| 2:H:1589:VAL:HG21 | 2:H:1651:LEU:HD12 | 2.02 | 0.41 |
| 1:A:152:HIS:HD2 | 1:A:163:LEU:CB | 2.32 | 0.41 |
| 2:G:735:GLY:O | 2:G:741:HIS:CD2 | 2.73 | 0.41 |
| 1:C:1431:GLU:O | 1:C:1431:GLU:HG3 | 2.19 | 0.41 |
| 2:G:995:LEU:HB3 | 2:G:1000:ILE:CD1 | 2.50 | 0.41 |
| 2:H:1213:LEU:O | 2:H:1214:LEU:HD23 | 2.19 | 0.41 |
| 2:I:1219:ILE:HB | 2:I:1240:TYR:HB2 | 2.03 | 0.41 |
| 2:I:455:ILE:C | 2:I:455:ILE:HD12 | 2.42 | 0.41 |
| 2:H:753:MET:O | 2:H:757:ILE:HG13 | 2.21 | 0.41 |
| 2:G:1778:GLN:HB2 | 2:G:1779:PRO:HD3 | 2.02 | 0.41 |
| 2:G:1889:VAL:HG22 | 2:G:1977:HIS:O | 2.20 | 0.41 |
| 1:C:1239:HIS:CD2 | 1:C:1241:SER:H | 2.38 | 0.41 |
| 2:H:1815:LEU:O | 2:H:1821:VAL:HG23 | 2.21 | 0.41 |
| 2:G:260:PRO:HD3 | 2:G:289:TRP:CZ2 | 2.54 | 0.41 |
| 2:H:1300:PHE:CB | 2:H:1556:VAL:HG11 | 2.50 | 0.41 |
| 2:G:780:TYR:HB2 | 2:G:799:PHE:CE2 | 2.56 | 0.41 |
| 2:I:827:VAL:HG12 | 2:I:828:PRO:O | 2.20 | 0.41 |
| 2:G:748:THR:CB | 2:G:749:PRO:HD3 | 2.47 | 0.41 |
| 1:A:930:LEU:HD22 | 1:A:933:VAL:CG1 | 2.51 | 0.41 |
| 2:H:827:VAL:HG21 | 2:H:840:THR:CG2 | 2.51 | 0.41 |
| 2:G:1352:HIS:CD2 | 2:G:1410:PHE:CD2 | 3.09 | 0.41 |
| 2:G:1981:LEU:HD12 | 2:G:1981:LEU:N | 2.36 | 0.41 |
| 1:C:32:GLN:HE22 | 1:C:57:ALA:N | 2.19 | 0.41 |
| 2:H:1270:TRP:HZ3 | 2:H:1347:LEU:HD21 | 1.85 | 0.41 |
| 1:B:1418:VAL:N | 1:B:1419:PRO:CD | 2.83 | 0.41 |
| 1:B:1618:LEU:HD23 | 1:B:1621:PHE:HE2 | 1.85 | 0.41 |
| 1:B:1657:HIS:CG | 1:B:1658:PRO:HD2 | 2.55 | 0.41 |
| 1:C:1842:VAL:O | 1:C:1843:ASN:O | 2.39 | 0.41 |
| 2:I:1579:ILE:CD1 | 2:I:1615:MET:SD | 3.09 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:G:1210:ILE:O | 2:G:1210:ILE:HG22 | 2.19 | 0.41 |
| 1:A:612:GLU:O | 1:A:615:SER:HB3 | 2.21 | 0.41 |
| 2:H:1868:GLN:HG3 | 2:H:1898:TYR:HH | 1.83 | 0.41 |
| 2:I:582:LYS:HE2 | 2:I:761:PRO:O | 2.21 | 0.41 |
| 2:I:1503:ILE:HG22 | 2:I:1504:VAL:C | 2.41 | 0.41 |
| 1:C:1705:PRO:HB2 | 1:C:1733:PHE:CD1 | 2.56 | 0.41 |
| 1:C:739:GLN:HB3 | 1:C:794:ILE:HG23 | 2.03 | 0.41 |
| 2:H:804:ARG:NH2 | 2:H:1068:GLU:OE1 | 2.54 | 0.41 |
| 1:C:949:GLU:O | 1:C:953:VAL:HG12 | 2.21 | 0.41 |
| 2:G:258:PHE:N | 2:G:258:PHE:CD1 | 2.87 | 0.41 |
| 1:C:1244:GLY:C | 1:C:1327:CYS:HB2 | 2.41 | 0.41 |
| 1:C:1829:GLY:O | 1:C:1830:GLY:O | 2.39 | 0.41 |
| 2:H:195:LEU:O | 2:H:199:ILE:HG13 | 2.20 | 0.41 |
| 1:C:453:TYR:O | 1:C:457:ASN:HB2 | 2.19 | 0.41 |
| 1:B:1709:GLU:HG3 | 1:B:1709:GLU:H | 1.45 | 0.41 |
| 2:G:1884:TRP:HB3 | 2:G:1885:LEU:H | 1.74 | 0.41 |
| 1:C:683:ALA:HA | 1:C:689:GLY:HA3 | 2.02 | 0.41 |
| 1:A:719:GLN:HG3 | 1:A:720:SER:N | 2.36 | 0.41 |
| 2:I:1514:ASN:HA | 2:I:1515:PRO:HD3 | 1.86 | 0.41 |
| 1:C:1076:VAL:CG1 | 1:C:1081:LYS:HA | 2.50 | 0.41 |
| 2:I:248:HIS:CE1 | 2:I:531:GLY:HA2 | 2.55 | 0.41 |
| 1:A:438:ASN:HD21 | 1:A:698:GLN:HE21 | 1.68 | 0.41 |
| 2:H:425:SER:HA | 2:H:426:PRO:HD3 | 1.78 | 0.41 |
| 1:B:197:THR:HG22 | 1:B:198:PRO:O | 2.21 | 0.41 |
| 1:A:36:LEU:O | 1:A:76:ARG:NH1 | 2.53 | 0.41 |
| 2:G:2049:GLU:O | 2:G:2050:GLN:C | 2.59 | 0.41 |
| 2:G:455:ILE:HD13 | 2:G:457:ILE:O | 2.21 | 0.41 |
| 1:C:1666:THR:HG23 | 1:C:1669:ARG:CB | 2.51 | 0.41 |
| 1:C:427:ASN:HB2 | 1:C:468:LEU:CD2 | 2.51 | 0.41 |
| 2:G:44:PRO:HA | 2:G:53:GLU:OE2 | 2.21 | 0.41 |
| 2:I:1327:ILE:O | 2:I:1331:TRP:HB2 | 2.21 | 0.41 |
| 2:I:827:VAL:HG21 | 2:I:840:THR:CG2 | 2.51 | 0.41 |
| 2:I:754:TYR:CG | 2:I:794:MET:CG | 3.04 | 0.41 |
| 1:B:427:ASN:ND2 | 1:B:610:THR:H | 2.14 | 0.41 |
| 1:B:187:LEU:CD2 | 1:B:201:PRO:HB2 | 2.51 | 0.41 |
| 1:C:294:TYR:CZ | 1:C:298:VAL:HG21 | 2.55 | 0.41 |
| 1:B:504:ASP:O | 1:B:954:ARG:HD3 | 2.21 | 0.41 |
| 2:I:118:LYS:O | 2:I:121:GLU:HB2 | 2.20 | 0.41 |
| 1:C:237:MET:HA | 1:C:238:PRO:HD3 | 1.93 | 0.41 |
| 1:C:644:THR:HG23 | 1:C:648:ASP:N | 2.34 | 0.41 |
| 1:B:82:SER:OG | 1:B:83:LYS:HG3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1063:THR:HG22 | 2:H:1063:THR:O | 2.21 | 0.41 |
| 1:B:32:GLN:HE22 | 1:B:57:ALA:CA | 2.34 | 0.41 |
| 1:C:1019:ILE:HG13 | 1:C:1316:VAL:HG13 | 2.03 | 0.41 |
| 1:A:1705:PRO:HB2 | 1:A:1733:PHE:CD1 | 2.56 | 0.41 |
| 2:H:1949:LYS:O | 2:H:1953:VAL:HG23 | 2.21 | 0.41 |
| 1:A:908:LEU:O | 1:A:913:VAL:HG22 | 2.21 | 0.41 |
| 1:B:1029:PRO:HG2 | 1:B:1581:THR:O | 2.21 | 0.41 |
| 2:I:717:ILE:O | 2:I:720:ALA:HB3 | 2.21 | 0.41 |
| 2:G:339:LEU:HB2 | 2:G:386:LEU:HD22 | 2.03 | 0.41 |
| 2:I:319:LEU:HA | 2:I:319:LEU:HD22 | 1.67 | 0.41 |
| 2:I:2020:GLN:NE2 | 2:I:2020:GLN:HA | 2.36 | 0.41 |
| 1:B:489:VAL:HG22 | 1:B:670:GLY:HA3 | 2.02 | 0.41 |
| 2:H:1387:GLY:HA2 | 2:H:1414:GLY:O | 2.21 | 0.41 |
| 2:G:159:ILE:HG12 | 2:G:512:LEU:HD23 | 2.03 | 0.40 |
| 2:I:2036:GLU:HB2 | 2:I:2037:PRO:CD | 2.47 | 0.40 |
| 2:I:2039:LYS:HA | 2:I:2042:ILE:HG13 | 2.03 | 0.40 |
| 2:H:1227:ARG:CZ | 2:H:1565:VAL:HG12 | 2.51 | 0.40 |
| 2:H:888:ARG:O | 2:H:892:ILE:HB | 2.21 | 0.40 |
| 2:G:1844:ARG:HD2 | 2:G:1848:GLY:O | 2.21 | 0.40 |
| 1:A:197:THR:HG22 | 1:A:198:PRO:O | 2.21 | 0.40 |
| 2:I:1676:MET:HE1 | 2:I:1781:LEU:CD2 | 2.50 | 0.40 |
| 2:I:1889:VAL:HG21 | 2:I:1901:ALA:HB3 | 2.03 | 0.40 |
| 2:H:566:HIS:O | 2:H:567:PRO:C | 2.59 | 0.40 |
| 2:I:247:ALA:O | 2:I:251:VAL:HG13 | 2.21 | 0.40 |
| 2:H:338:MET:HG3 | 2:H:423:VAL:HG21 | 2.02 | 0.40 |
| 1:B:1056:ILE:HG13 | 1:B:1057:MET:N | 2.36 | 0.40 |
| 2:I:846:VAL:CG2 | 2:I:866:LYS:HB2 | 2.51 | 0.40 |
| 1:A:232:LEU:O | 1:A:236:LYS:HB2 | 2.21 | 0.40 |
| 1:A:1418:VAL:N | 1:A:1419:PRO:CD | 2.84 | 0.40 |
| 1:B:483:VAL:O | 1:B:483:VAL:HG12 | 2.21 | 0.40 |
| 1:C:187:LEU:CD2 | 1:C:201:PRO:HB2 | 2.51 | 0.40 |
| 1:B:1557:ILE:HD11 | 1:B:1642:THR:HG21 | 2.03 | 0.40 |
| 2:I:280:ALA:O | 2:I:283:ILE:HG22 | 2.21 | 0.40 |
| 1:B:998:TYR:CD2 | 1:B:1667:GLU:HG3 | 2.56 | 0.40 |
| 2:G:73:GLU:OE2 | 2:G:76:LYS:HD2 | 2.21 | 0.40 |
| 1:A:29:ILE:HG21 | 2:G:1894:GLU:HB2 | 2.04 | 0.40 |
| 1:C:1308:SER:OG | 1:C:1590:ALA:N | 2.54 | 0.40 |
| 2:G:938:TRP:CD1 | 2:G:944:ARG:HG3 | 2.56 | 0.40 |
| 1:A:681:THR:HA | 1:A:706:THR:OG1 | 2.21 | 0.40 |
| 2:G:1343:VAL:HG22 | 2:G:1343:VAL:O | 2.20 | 0.40 |
| 2:I:1880:LYS:HB2 | 2:I:1880:LYS:HE3 | 1.90 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:91:THR:HA | 1:B:92:PRO:HD3 | 1.81 | 0.40 |
| 1:B:933:VAL:HA | 1:B:934:PRO:HD3 | 1.63 | 0.40 |
| 2:G:430:HIS:CE1 | 2:G:431:LEU:HD13 | 2.56 | 0.40 |
| 1:B:989:GLN:NE2 | 2:H:993:GLN:OE1 | 2.53 | 0.40 |
| 2:G:601:THR:HB | 2:G:620:ALA:HB2 | 2.01 | 0.40 |
| 2:G:1227:ARG:NE | 2:G:1565:VAL:HG12 | 2.36 | 0.40 |
| 2:H:638:VAL:HA | 2:H:641:ILE:CG2 | 2.52 | 0.40 |
| 1:C:148:SER:O | 1:C:152:HIS:HB2 | 2.21 | 0.40 |
| 2:I:703:LEU:HD23 | 2:I:705:LEU:HG | 2.04 | 0.40 |
| 2:H:723:HIS:ND1 | 2:H:723:HIS:N | 2.70 | 0.40 |
| 2:G:638:VAL:O | 2:G:641:ILE:HG22 | 2.20 | 0.40 |
| 2:H:1214:LEU:HD11 | 2:H:1220:GLN:NE2 | 2.36 | 0.40 |
| 2:I:543:PHE:CB | 2:I:545:GLN:NE2 | 2.82 | 0.40 |
| 2:H:960:LYS:CE | 2:H:960:LYS:HA | 2.44 | 0.40 |
| 1:A:23:ALA:O | 2:G:1977:HIS:HA | 2.20 | 0.40 |
| 1:A:1665:ILE:HD11 | 1:A:1669:ARG:CG | 2.51 | 0.40 |
| 2:G:1678:MET:HG2 | 2:G:1711:ILE:HG12 | 2.03 | 0.40 |
| 2:I:1889:VAL:HG13 | 2:I:1977:HIS:HB3 | 2.00 | 0.40 |
| 2:H:590:PRO:HA | 2:H:591:PRO:HD3 | 1.81 | 0.40 |
| 1:A:44:VAL:HG13 | 1:A:78:ILE:HG12 | 1.99 | 0.40 |
| 2:G:562:LEU:HD23 | 2:G:562:LEU:HA | 1.85 | 0.40 |
| 2:H:1506:TYR:CZ | 2:H:1515:PRO:HG2 | 2.56 | 0.40 |
| 2:G:827:VAL:HG12 | 2:G:828:PRO:O | 2.21 | 0.40 |
| 2:H:573:LYS:C | 2:H:575:GLY:N | 2.75 | 0.40 |
| 1:A:1021:VAL:HG11 | 1:A:1597:LEU:CD1 | 2.50 | 0.40 |
| 2:I:1339:PHE:N | 2:I:1340:PRO:CD | 2.85 | 0.40 |
| 1:B:1583:HIS:HA | 1:B:1584:PRO:HD3 | 1.84 | 0.40 |
| 1:C:411:GLN:O | 1:C:415:SER:HB2 | 2.21 | 0.40 |
| 2:I:536:ASN:HD21 | 2:I:540:ASP:HB3 | 1.85 | 0.40 |
| 2:I:1091:GLY:O | 2:I:1093:ASP:N | 2.55 | 0.40 |
| 2:G:805:VAL:O | 2:G:805:VAL:HG12 | 2.21 | 0.40 |
| 2:I:816:ASP:HB3 | 2:I:1048:VAL:HG21 | 2.03 | 0.40 |
| 2:G:1940:LEU:HD12 | 2:G:1941:PHE:N | 2.37 | 0.40 |
| 2:I:1359:MET:HB3 | 2:I:1606:ARG:NH2 | 2.36 | 0.40 |
| 1:C:1105:LEU:HA | 1:C:1105:LEU:HD23 | 1.84 | 0.40 |
| 2:I:246:LEU:HA | 2:I:246:LEU:HD12 | 1.79 | 0.40 |
| 1:A:833:PHE:O | 1:A:834:GLY:O | 2.39 | 0.40 |
| 1:B:1829:GLY:O | 1:B:1830:GLY:O | 2.39 | 0.40 |
| 2:H:462:THR:HB | 2:H:482:CYS:SG | 2.61 | 0.40 |
| 2:H:203:LEU:HD12 | 2:H:203:LEU:HA | 1.91 | 0.40 |
| 1:A:1146:HIS:O | 1:A:1146:HIS:HD2 | 2.04 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:1609:THR:O | 2:H:1653:GLY:HA3 | 2.21 | 0.40 |
| 1:A:852:ARG:NH1 | 1:A:852:ARG:CG | 2.73 | 0.40 |
| 2:H:810:GLU:OE2 | 2:H:1070:ILE:N | 2.45 | 0.40 |
| 2:I:612:ASN:HD21 | 2:I:641:ILE:HA | 1.84 | 0.40 |
| 2:G:1875:VAL:HA | 2:G:1878:VAL:CG1 | 2.52 | 0.40 |
| 1:C:1303:GLY:CA | 1:C:1307:THR:HG22 | 2.52 | 0.40 |
| 2:I:1213:LEU:O | 2:I:1214:LEU:HD23 | 2.20 | 0.40 |
| 2:H:912:ARG:HB2 | 2:H:916:THR:HG23 | 2.03 | 0.40 |
| 2:H:1597:ALA:HB1 | 2:H:1657:ILE:HD12 | 2.02 | 0.40 |
| 1:B:1303:GLY:CA | 1:B:1307:THR:HG22 | 2.52 | 0.40 |
| 2:H:560:ASN:O | 2:H:562:LEU:N | 2.54 | 0.40 |
| 2:H:1528:GLU:C | 2:H:1530:LYS:H | 2.17 | 0.40 |
| 2:I:864:LEU:HD13 | 2:I:894:ARG:HB3 | 2.04 | 0.40 |
| 1:B:221:LEU:HD23 | 1:B:221:LEU:HA | 1.94 | 0.40 |
| 2:H:517:HIS:HB2 | 2:H:527:VAL:HG21 | 2.04 | 0.40 |
| 2:H:517:HIS:CE1 | 2:H:540:ASP:O | 2.75 | 0.40 |
| 2:H:1166:VAL:CG1 | 2:H:1167:SER:N | 2.85 | 0.40 |
| 2:G:391:LEU:CD2 | 2:G:394:ARG:NH2 | 2.85 | 0.40 |
| 2:G:582:LYS:HE2 | 2:G:761:PRO:O | 2.22 | 0.40 |
| 2:I:1271:ILE:HG22 | 2:I:1273:GLU:HB2 | 2.04 | 0.40 |
| 2:G:441:LYS:HG2 | 2:G:445:LYS:HE3 | 2.02 | 0.40 |
| 2:G:573:LYS:C | 2:G:575:GLY:N | 2.75 | 0.40 |
| 1:C:43:ARG:O | 2:I:1662:THR:HA | 2.22 | 0.40 |
| 2:I:1855:ILE:HB | 2:I:1907:LEU:HD12 | 2.02 | 0.40 |
| 1:B:293:LYS:O | 1:B:297:ILE:HG13 | 2.20 | 0.40 |
| 2:G:319:LEU:HA | 2:G:319:LEU:HD22 | 1.62 | 0.40 |
| 2:G:1637:LEU:HA | 2:G:1637:LEU:HD23 | 1.77 | 0.40 |
| 2:G:852:GLU:H | 2:G:852:GLU:HG3 | 1.40 | 0.40 |
| 1:B:774:ILE:HA | 1:B:775:PRO:HD3 | 1.74 | 0.40 |
| 1:A:238:PRO:CG | 1:A:283:ALA:HB2 | 2.51 | 0.40 |
| 2:G:248:HIS:CE1 | 2:G:531:GLY:HA2 | 2.56 | 0.40 |
| 1:C:1749:THR:O | 1:C:1874:ASP:HB3 | 2.21 | 0.40 |
| 2:H:607:VAL:HG23 | 2:H:617:ILE:CG2 | 2.51 | 0.40 |
| 2:G:612:ASN:C | 2:G:614:GLY:H | 2.24 | 0.40 |
| 1:B:12:ILE:O | 1:B:16:GLU:HG2 | 2.20 | 0.40 |
| 2:H:1593:ILE:HD13 | 2:H:1626:ILE:CD1 | 2.51 | 0.40 |
| 2:H:1716:ASN:HA | 2:H:1770:LEU:HD11 | 2.04 | 0.40 |
| 2:G:260:PRO:HD3 | 2:G:289:TRP:CD2 | 2.56 | 0.40 |
| 1:A:916:LEU:HD22 | 1:A:922:VAL:HG22 | 2.02 | 0.40 |
| 1:C:655:LEU:HD23 | 1:C:655:LEU:HA | 1.79 | 0.40 |
| 2:H:1281:PRO:O | 2:H:1378:ILE:HG23 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:157:HIS:CE1 | 1:A:269:LEU:HD11 | 2.57 | 0.40 |
| 1:B:509:ILE:HG13 | 1:B:509:ILE:H | 1.50 | 0.40 |
| 2:H:538:ASP:HB2 | 2:H:540:ASP:HB2 | 2.03 | 0.40 |
| 1:C:1639:VAL:HG12 | 1:C:1640:SER:N | 2.35 | 0.40 |
| 2:I:240:LEU:HA | 2:I:240:LEU:HD12 | 1.81 | 0.40 |
| 1:C:406:TRP:CZ3 | 1:C:407:ASN:HB2 | 2.57 | 0.40 |
| 2:I:717:ILE:CG2 | 2:I:760:HIS:CE1 | 3.05 | 0.40 |
| 1:A:1209:ASP:OD1 | 1:A:1210:PRO:HD2 | 2.21 | 0.40 |
| 1:C:1063:HIS:CE1 | 1:C:1067:LEU:CD2 | 3.04 | 0.40 |
| 1:B:1370:THR:HG22 | 1:B:1371:THR:N | 2.36 | 0.40 |
| 1:B:74:LEU:O | 1:B:74:LEU:HD12 | 2.22 | 0.40 |
| 2:I:812:LYS:HA | 2:I:812:LYS:HD3 | 1.82 | 0.40 |
| 1:C:1195:ALA:HB1 | 1:C:1200:ILE:HD12 | 2.03 | 0.40 |
| 1:A:1406:MET:CE | 1:A:1428:THR:HB | 2.52 | 0.40 |
| 2:H:156:LEU:HD23 | 2:H:500:HIS:HB2 | 2.04 | 0.40 |
| 2:I:601:THR:O | 2:I:601:THR:CG2 | 2.68 | 0.40 |
| 2:H:1172:LYS:HZ1 | 2:H:1574:ASN:HA | 1.85 | 0.40 |
| 2:G:2039:LYS:HA | 2:G:2042:ILE:HG13 | 2.03 | 0.40 |
| 2:I:612:ASN:C | 2:I:614:GLY:H | 2.25 | 0.40 |
| 2:G:533:LEU:HG | 2:G:533:LEU:O | 2.21 | 0.40 |
| 2:H:298:LYS:HA | 2:H:448:VAL:CG2 | 2.52 | 0.40 |
| 1:A:427:ASN:HB2 | 1:A:468:LEU:CD2 | 2.51 | 0.40 |
| 2:G:119:THR:HG22 | 2:G:120:LYS:N | 2.36 | 0.40 |
| 2:H:1327:ILE:HA | 2:H:1327:ILE:HD12 | 1.77 | 0.40 |
| 1:B:1577:GLN:NE2 | 1:B:1591:TRP:HB3 | 2.36 | 0.40 |
| 2:I:225:THR:HA | 2:I:226:PRO:HD3 | 1.98 | 0.40 |
| 1:C:413:LEU:HD13 | 1:C:451:MET:HG2 | 2.03 | 0.40 |
| 1:C:187:LEU:HD11 | 1:C:202:GLU:HG3 | 2.03 | 0.40 |
| 2:H:816:ASP:HB3 | 2:H:1048:VAL:CG2 | 2.52 | 0.40 |
| 2:G:606:PHE:HZ | 2:G:805:VAL:CG1 | 2.33 | 0.40 |
| 2:H:233:SER:HA | 2:H:424:ALA:HB3 | 2.03 | 0.40 |
| 2:H:441:LYS:O | 2:H:445:LYS:HG3 | 2.22 | 0.40 |
| 2:H:283:ILE:HD12 | 2:H:283:ILE:HA | 1.89 | 0.40 |
| 1:A:350:LEU:HB2 | 1:A:352:MET:HG2 | 2.03 | 0.40 |
| 1:B:709:ARG:O | 1:B:714:VAL:HG21 | 2.21 | 0.40 |
| 2:G:1830:VAL:HA | 2:G:1991:PHE:HE2 | 1.86 | 0.40 |

All (54) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1784:ASP:CA | 2:G:1087:HIS:CE1[7_655] | 0.16 | 2.04 |
| 1:A:1784:ASP:CG | 2:I:1087:HIS:CE1[7_545] | 0.52 | 1.68 |
| 1:C:1784:ASP:C | 2:G:1087:HIS:NE2[7_655] | 0.54 | 1.66 |
| 1:C:1784:ASP:CB | 2:G:1087:HIS:ND1[7_655] | 0.56 | 1.64 |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:ND1[7_545] | 0.58 | 1.62 |
| 1:B:1480:GLU:OE2 | 2:H:290:GLU:CB[6_555] | 0.74 | 1.46 |
| 1:C:1784:ASP:CB | 2:G:1087:HIS:CG[7_655] | 0.83 | 1.37 |
| 1:A:1784:ASP:CG | 2:I:1087:HIS:NE2[7_545] | 0.91 | 1.29 |
| 1:A:1784:ASP:CB | 2:I:1087:HIS:NE2[7_545] | 0.97 | 1.23 |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:CE1[7_545] | 1.05 | 1.15 |
| 1:C:1784:ASP:CA | 2:G:1087:HIS:ND1[7_655] | 1.19 | 1.01 |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:CG[7_545] | 1.20 | 1.00 |
| 1:C:1784:ASP:O | 2:G:1087:HIS:NE2[7_655] | 1.22 | 0.98 |
| 1:B:1480:GLU:CD | 2:H:290:GLU:CB[6_555] | 1.29 | 0.91 |
| 2:G:77:VAL:CB | 2:I:1929:LYS:CD[6_455] | 1.31 | 0.89 |
| 1:C:1784:ASP:C | 2:G:1087:HIS:CE1[7_655] | 1.38 | 0.82 |
| 1:A:1784:ASP:OD1 | 2:I:1087:HIS:CE1[7_545] | 1.38 | 0.82 |
| 1:C:1784:ASP:CA | 2:G:1087:HIS:NE2[7_655] | 1.42 | 0.78 |
| 1:B:1480:GLU:OE2 | 2:H:290:GLU:CG[6_555] | 1.43 | 0.77 |
| 2:G:77:VAL:CG2 | 2:I:1929:LYS:NZ[6_455] | 1.46 | 0.74 |
| 1:C:1784:ASP:N | 2:G:1087:HIS:CE1[7_655] | 1.46 | 0.74 |
| 1:C:1784:ASP:CG | 2:G:1087:HIS:ND1[7_655] | 1.47 | 0.73 |
| 2:G:77:VAL:CG2 | 2:I:1929:LYS:CE[6_455] | 1.51 | 0.69 |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:NE2[7_545] | 1.60 | 0.60 |
| 1:A:1784:ASP:CG | 2:I:1087:HIS:ND1[7_545] | 1.64 | 0.56 |
| 2:G:79:GLN:OE1 | 2:I:1930:SER:O[6_455] | 1.64 | 0.56 |
| 1:C:1784:ASP:CB | 2:G:1087:HIS:CE1[7_655] | 1.64 | 0.56 |
| 1:A:1784:ASP:OD2 | 2:I:1087:HIS:CD2[7_545] | 1.68 | 0.52 |
| 1:C:1785:THR:N | 2:G:1087:HIS:NE2[7_655] | 1.70 | 0.50 |
| 2:G:77:VAL:CB | 2:I:1929:LYS:CE[6_455] | 1.71 | 0.49 |
| 1:C:1784:ASP:CB | 2:G:1087:HIS:CD2[7_655] | 1.81 | 0.39 |
| 1:B:1480:GLU:OE1 | 2:H:290:GLU:CB[6_555] | 1.83 | 0.37 |
| 1:A:1784:ASP:CB | 2:I:1087:HIS:CE1[7_545] | 1.84 | 0.36 |
| 1:C:1784:ASP:C | 2:G:1087:HIS:CD2[7_655] | 1.86 | 0.34 |
| 2:G:77:VAL:O | 2:I:1929:LYS:CB[6_455] | 1.92 | 0.28 |
| 2:G:77:VAL:O | 2:I:1929:LYS:CA[6_455] | 1.93 | 0.27 |
| 1:A:1784:ASP:CG | 2:I:1087:HIS:CD2[7_545] | 1.94 | 0.26 |
| 2:G:77:VAL:CG1 | 2:I:1929:LYS:CD[6_455] | 1.95 | 0.25 |
| 1:C:1784:ASP:CG | 2:G:1087:HIS:CG[7_655] | 1.97 | 0.23 |
| 2:G:77:VAL:O | 2:I:1929:LYS:CG[6_455] | 1.97 | 0.23 |
| 1:A:1784:ASP:OD1 | 2:I:1087:HIS:NE2[7_545] | 1.98 | 0.22 |
| 1:C:1784:ASP:N | 2:G:1087:HIS:ND1[7_655] | 1.98 | 0.22 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1784:ASP:CB | 2:G:1087:HIS:CB[7_655] | 2.03 | 0.17 |
| 1:C:1784:ASP:OD2 | 2:G:1087:HIS:CB[7_655] | 2.03 | 0.17 |
| 2:H:6:THR:CG2 | 2:I:1935:GLU:OE2[6_455] | 2.05 | 0.15 |
| 2:H:6:THR:CG2 | 2:I:1935:GLU:CD[6_455] | 2.06 | 0.14 |
| 1:C:1784:ASP:OD1 | 2:G:1087:HIS:ND1[7_655] | 2.11 | 0.09 |
| 1:C:1784:ASP:CB | 2:G:1087:HIS:NE2[7_655] | 2.11 | 0.09 |
| 1:C:1784:ASP:O | 2:G:1087:HIS:CD2[7_655] | 2.12 | 0.08 |
| 1:C:1784:ASP:CA | 2:G:1087:HIS:CG[7_655] | 2.13 | 0.07 |
| 2:G:77:VAL:CB | 2:I:1929:LYS:CG[6_455] | 2.15 | 0.05 |
| 1:A:1784:ASP:CB | 2:I:1087:HIS:CD2[7_545] | 2.15 | 0.05 |
| 1:A:852:ARG:NH2 | 1:B:837:GLY:O[7_645] | 2.19 | 0.01 |
| 1:B:1480:GLU:OE1 | 2:H:290:GLU:CA[6_555] | 2.19 | 0.01 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 1736/1887 (92%) | 1614 (93%) | 100 (6%) | 22 (1%) | 15 | 60 |
| 1 | B | 1736/1887 (92%) | 1619 (93%) | 100 (6%) | 17 (1%) | 19 | 65 |
| 1 | C | 1736/1887 (92%) | 1618 (93%) | 96 (6%) | 22 (1%) | 15 | 60 |
| 2 | G | 2029/2051 (99%) | 1825 (90%) | 173 (8%) | 31 (2%) | 13 | 58 |
| 2 | H | 2029/2051 (99%) | 1826 (90%) | 173 (8%) | 30 (2%) | 13 | 58 |
| 2 | I | 2029/2051 (99%) | 1829 (90%) | 174 (9%) | 26 (1%) | 15 | 60 |
| All | All | 11295/11814 (96%) | 10331 (92%) | 816 (7%) | 148 (1%) | 15 | 60 |

All (148) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 488 | PRO |
| 1 | A | 504 | ASP |
| 1 | A | 538 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 605 | LEU |
| 1 | A | 834 | GLY |
| 1 | A | 935 | GLU |
| 1 | A | 1763 | LYS |
| 1 | A | 1830 | GLY |
| 1 | A | 1843 | ASN |
| 1 | B | 504 | ASP |
| 1 | B | 538 | GLU |
| 1 | B | 605 | LEU |
| 1 | B | 834 | GLY |
| 1 | B | 1763 | LYS |
| 1 | B | 1830 | GLY |
| 1 | B | 1843 | ASN |
| 1 | C | 504 | ASP |
| 1 | C | 538 | GLU |
| 1 | C | 605 | LEU |
| 1 | C | 834 | GLY |
| 1 | C | 935 | GLU |
| 1 | C | 1763 | LYS |
| 1 | C | 1830 | GLY |
| 1 | C | 1843 | ASN |
| 2 | G | 521 | ASP |
| 2 | G | 561 | TRP |
| 2 | G | 1177 | SER |
| 2 | G | 1955 | PRO |
| 2 | H | 521 | ASP |
| 2 | H | 561 | TRP |
| 2 | H | 1418 | ASP |
| 2 | H | 1955 | PRO |
| 2 | I | 521 | ASP |
| 2 | I | 1955 | PRO |
| 1 | A | 1252 | GLY |
| 1 | A | 1585 | LYS |
| 1 | A | 1608 | ASN |
| 1 | B | 179 | LYS |
| 1 | B | 1252 | GLY |
| 1 | B | 1585 | LYS |
| 1 | B | 1608 | ASN |
| 1 | C | 1252 | GLY |
| 1 | C | 1585 | LYS |
| 1 | C | 1608 | ASN |
| 2 | G | 203 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 562 | LEU |
| 2 | G | 1044 | VAL |
| 2 | G | 1418 | ASP |
| 2 | G | 1419 | PHE |
| 2 | G | 1722 | GLY |
| 2 | H | 203 | LEU |
| 2 | H | 1044 | VAL |
| 2 | H | 1177 | SER |
| 2 | H | 1420 | GLU |
| 2 | H | 1529 | GLN |
| 2 | H | 1722 | GLY |
| 2 | I | 203 | LEU |
| 2 | I | 1044 | VAL |
| 2 | I | 1177 | SER |
| 2 | I | 1418 | ASP |
| 2 | I | 1722 | GLY |
| 1 | A | 179 | LYS |
| 1 | A | 1749 | THR |
| 1 | B | 1749 | THR |
| 1 | C | 1749 | THR |
| 2 | G | 112 | ASN |
| 2 | G | 139 | LYS |
| 2 | G | 567 | PRO |
| 2 | G | 1101 | GLU |
| 2 | G | 2034 | GLY |
| 2 | H | 112 | ASN |
| 2 | H | 562 | LEU |
| 2 | H | 1101 | GLU |
| 2 | I | 374 | ALA |
| 2 | I | 1092 | ASP |
| 2 | I | 1101 | GLU |
| 2 | I | 2034 | GLY |
| 2 | G | 25 | ALA |
| 2 | G | 26 | SER |
| 2 | G | 374 | ALA |
| 2 | G | 742 | SER |
| 2 | G | 769 | SER |
| 2 | G | 1092 | ASP |
| 2 | G | 1510 | ALA |
| 2 | H | 26 | SER |
| 2 | H | 374 | ALA |
| 2 | H | 567 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 742 | SER |
| 2 | H | 823 | ALA |
| 2 | H | 1510 | ALA |
| 2 | H | 2034 | GLY |
| 2 | I | 26 | SER |
| 2 | I | 112 | ASN |
| 2 | I | 742 | SER |
| 2 | I | 1419 | PHE |
| 1 | A | 485 | ASP |
| 1 | A | 1130 | ASP |
| 1 | A | 1477 | ILE |
| 1 | A | 1536 | LEU |
| 1 | B | 970 | GLY |
| 1 | B | 1477 | ILE |
| 1 | C | 179 | LYS |
| 1 | C | 934 | PRO |
| 1 | C | 1477 | ILE |
| 2 | H | 769 | SER |
| 2 | H | 1092 | ASP |
| 2 | H | 1257 | ASP |
| 2 | I | 25 | ALA |
| 2 | I | 136 | PRO |
| 2 | I | 769 | SER |
| 2 | I | 823 | ALA |
| 2 | I | 1510 | ALA |
| 1 | A | 178 | GLY |
| 1 | A | 970 | GLY |
| 1 | C | 930 | LEU |
| 1 | C | 970 | GLY |
| 1 | C | 1536 | LEU |
| 2 | G | 574 | SER |
| 2 | H | 1419 | PHE |
| 2 | I | 139 | LYS |
| 2 | I | 574 | SER |
| 1 | A | 1543 | GLY |
| 1 | B | 1543 | GLY |
| 1 | C | 1543 | GLY |
| 2 | G | 136 | PRO |
| 2 | G | 335 | PRO |
| 2 | H | 136 | PRO |
| 2 | H | 335 | PRO |
| 2 | H | 1661 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 178 | GLY |
| 2 | G | 1340 | PRO |
| 2 | G | 1956 | ARG |
| 2 | H | 772 | GLY |
| 1 | A | 934 | PRO |
| 1 | C | 178 | GLY |
| 1 | C | 1240 | VAL |
| 2 | G | 772 | GLY |
| 2 | G | 1176 | PRO |
| 2 | G | 1840 | VAL |
| 2 | I | 772 | GLY |
| 1 | B | 726 | GLY |
| 1 | C | 726 | GLY |
| 2 | G | 470 | VAL |
| 2 | H | 470 | VAL |
| 2 | H | 2012 | PRO |
| 2 | I | 335 | PRO |
| 2 | I | 1956 | ARG |
| 2 | I | 1340 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 1460/1566 (93%) | 1308 (90%) | 152 (10%) | 9 | 40 |
| 1 | B | 1460/1566 (93%) | 1312 (90%) | 148 (10%) | 9 | 41 |
| 1 | C | 1460/1566 (93%) | 1310 (90%) | 150 (10%) | 9 | 40 |
| 2 | G | 1772/1789 (99%) | 1563 (88%) | 209 (12%) | 6 | 35 |
| 2 | H | 1772/1789 (99%) | 1560 (88%) | 212 (12%) | 6 | 33 |
| 2 | I | 1772/1789 (99%) | 1561 (88%) | 211 (12%) | 6 | 34 |
| All | All | 9696/10065 (96%) | 8614 (89%) | 1082 (11%) | 7 | 37 |

All (1082) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 14 | LEU |
| 1 | A | 15 | THR |
| 1 | A | 21 | GLN |
| 1 | A | 22 | PHE |
| 1 | A | 145 | VAL |
| 1 | A | 149 | LEU |
| 1 | A | 158 | LYS |
| 1 | A | 165 | SER |
| 1 | A | 171 | THR |
| 1 | A | 202 | GLU |
| 1 | A | 217 | PHE |
| 1 | A | 242 | THR |
| 1 | A | 253 | ARG |
| 1 | A | 328 | LEU |
| 1 | A | 331 | ILE |
| 1 | A | 332 | THR |
| 1 | A | 375 | LEU |
| 1 | A | 378 | LEU |
| 1 | A | 385 | PHE |
| 1 | A | 390 | VAL |
| 1 | A | 392 | THR |
| 1 | A | 400 | ARG |
| 1 | A | 412 | SER |
| 1 | A | 413 | LEU |
| 1 | A | 415 | SER |
| 1 | A | 416 | LEU |
| 1 | A | 428 | VAL |
| 1 | A | 431 | GLU |
| 1 | A | 432 | VAL |
| 1 | A | 435 | GLU |
| 1 | A | 447 | LEU |
| 1 | A | 457 | ASN |
| 1 | A | 460 | GLU |
| 1 | A | 461 | THR |
| 1 | A | 484 | LEU |
| 1 | A | 487 | ASP |
| 1 | A | 490 | TYR |
| 1 | A | 493 | VAL |
| 1 | A | 506 | ASN |
| 1 | A | 509 | ILE |
| 1 | A | 527 | GLN |
| 1 | A | 529 | MET |
| 1 | A | 536 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 599 | MET |
| 1 | A | 600 | ASP |
| 1 | A | 603 | ASP |
| 1 | A | 606 | ASP |
| 1 | A | 607 | LYS |
| 1 | A | 615 | SER |
| 1 | A | 621 | THR |
| 1 | A | 622 | ILE |
| 1 | A | 625 | THR |
| 1 | A | 629 | THR |
| 1 | A | 635 | ILE |
| 1 | A | 644 | THR |
| 1 | A | 648 | ASP |
| 1 | A | 654 | GLN |
| 1 | A | 711 | SER |
| 1 | A | 719 | GLN |
| 1 | A | 728 | LYS |
| 1 | A | 731 | THR |
| 1 | A | 732 | LEU |
| 1 | A | 748 | LEU |
| 1 | A | 749 | ILE |
| 1 | A | 776 | GLU |
| 1 | A | 782 | GLU |
| 1 | A | 793 | ARG |
| 1 | A | 797 | THR |
| 1 | A | 806 | VAL |
| 1 | A | 817 | THR |
| 1 | A | 825 | PRO |
| 1 | A | 852 | ARG |
| 1 | A | 860 | ASN |
| 1 | A | 864 | VAL |
| 1 | A | 873 | ARG |
| 1 | A | 881 | ASN |
| 1 | A | 891 | MET |
| 1 | A | 913 | VAL |
| 1 | A | 930 | LEU |
| 1 | A | 931 | GLN |
| 1 | A | 933 | VAL |
| 1 | A | 935 | GLU |
| 1 | A | 947 | LEU |
| 1 | A | 949 | GLU |
| 1 | A | 953 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 964 | GLU |
| 1 | A | 980 | VAL |
| 1 | A | 1016 | GLU |
| 1 | A | 1020 | VAL |
| 1 | A | 1022 | THR |
| 1 | A | 1047 | LEU |
| 1 | A | 1056 | ILE |
| 1 | A | 1070 | ARG |
| 1 | A | 1087 | LYS |
| 1 | A | 1095 | THR |
| 1 | A | 1101 | SER |
| 1 | A | 1125 | VAL |
| 1 | A | 1127 | VAL |
| 1 | A | 1131 | LEU |
| 1 | A | 1172 | THR |
| 1 | A | 1173 | LEU |
| 1 | A | 1179 | LEU |
| 1 | A | 1184 | LEU |
| 1 | A | 1196 | LYS |
| 1 | A | 1197 | THR |
| 1 | A | 1208 | VAL |
| 1 | A | 1218 | SER |
| 1 | A | 1226 | SER |
| 1 | A | 1229 | THR |
| 1 | A | 1255 | SER |
| 1 | A | 1274 | ILE |
| 1 | A | 1283 | MET |
| 1 | A | 1307 | THR |
| 1 | A | 1327 | CYS |
| 1 | A | 1338 | GLU |
| 1 | A | 1367 | ARG |
| 1 | A | 1372 | THR |
| 1 | A | 1384 | ILE |
| 1 | A | 1385 | GLN |
| 1 | A | 1392 | LEU |
| 1 | A | 1414 | ILE |
| 1 | A | 1426 | LEU |
| 1 | A | 1442 | ASN |
| 1 | A | 1465 | ASN |
| 1 | A | 1479 | SER |
| 1 | A | 1489 | ARG |
| 1 | A | 1502 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1515 | ARG |
| 1 | A | 1522 | LEU |
| 1 | A | 1523 | ARG |
| 1 | A | 1532 | THR |
| 1 | A | 1533 | ILE |
| 1 | A | 1549 | ASN |
| 1 | A | 1556 | THR |
| 1 | A | 1566 | ARG |
| 1 | A | 1580 | LEU |
| 1 | A | 1585 | LYS |
| 1 | A | 1612 | ASP |
| 1 | A | 1625 | LEU |
| 1 | A | 1665 | ILE |
| 1 | A | 1666 | THR |
| 1 | A | 1692 | MET |
| 1 | A | 1693 | ILE |
| 1 | A | 1707 | THR |
| 1 | A | 1709 | GLU |
| 1 | A | 1721 | ARG |
| 1 | A | 1775 | LEU |
| 1 | A | 1782 | GLU |
| 1 | A | 1788 | GLU |
| 1 | A | 1794 | GLN |
| 1 | A | 1841 | ARG |
| 1 | A | 1873 | HIS |
| 1 | B | 14 | LEU |
| 1 | B | 15 | THR |
| 1 | B | 21 | GLN |
| 1 | B | 22 | PHE |
| 1 | B | 145 | VAL |
| 1 | B | 149 | LEU |
| 1 | B | 158 | LYS |
| 1 | B | 165 | SER |
| 1 | B | 171 | THR |
| 1 | B | 202 | GLU |
| 1 | B | 217 | PHE |
| 1 | B | 242 | THR |
| 1 | B | 253 | ARG |
| 1 | B | 300 | VAL |
| 1 | B | 328 | LEU |
| 1 | B | 331 | ILE |
| 1 | B | 332 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 375 | LEU |
| 1 | B | 385 | PHE |
| 1 | B | 390 | VAL |
| 1 | B | 392 | THR |
| 1 | B | 400 | ARG |
| 1 | B | 401 | THR |
| 1 | B | 412 | SER |
| 1 | B | 413 | LEU |
| 1 | B | 415 | SER |
| 1 | B | 416 | LEU |
| 1 | B | 428 | VAL |
| 1 | B | 432 | VAL |
| 1 | B | 435 | GLU |
| 1 | B | 447 | LEU |
| 1 | B | 457 | ASN |
| 1 | B | 460 | GLU |
| 1 | B | 461 | THR |
| 1 | B | 484 | LEU |
| 1 | B | 489 | VAL |
| 1 | B | 493 | VAL |
| 1 | B | 499 | PRO |
| 1 | B | 506 | ASN |
| 1 | B | 509 | ILE |
| 1 | B | 510 | THR |
| 1 | B | 527 | GLN |
| 1 | B | 529 | MET |
| 1 | B | 536 | THR |
| 1 | B | 599 | MET |
| 1 | B | 600 | ASP |
| 1 | B | 603 | ASP |
| 1 | B | 606 | ASP |
| 1 | B | 607 | LYS |
| 1 | B | 615 | SER |
| 1 | B | 621 | THR |
| 1 | B | 622 | ILE |
| 1 | B | 625 | THR |
| 1 | B | 629 | THR |
| 1 | B | 635 | ILE |
| 1 | B | 644 | THR |
| 1 | B | 648 | ASP |
| 1 | B | 711 | SER |
| 1 | B | 719 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 728 | LYS |
| 1 | B | 731 | THR |
| 1 | B | 732 | LEU |
| 1 | B | 748 | LEU |
| 1 | B | 749 | ILE |
| 1 | B | 776 | GLU |
| 1 | B | 782 | GLU |
| 1 | B | 793 | ARG |
| 1 | B | 797 | THR |
| 1 | B | 806 | VAL |
| 1 | B | 852 | ARG |
| 1 | B | 860 | ASN |
| 1 | B | 864 | VAL |
| 1 | B | 873 | ARG |
| 1 | B | 881 | ASN |
| 1 | B | 891 | MET |
| 1 | B | 913 | VAL |
| 1 | B | 930 | LEU |
| 1 | B | 933 | VAL |
| 1 | B | 947 | LEU |
| 1 | B | 949 | GLU |
| 1 | B | 953 | VAL |
| 1 | B | 964 | GLU |
| 1 | B | 980 | VAL |
| 1 | B | 1016 | GLU |
| 1 | B | 1020 | VAL |
| 1 | B | 1047 | LEU |
| 1 | B | 1056 | ILE |
| 1 | B | 1070 | ARG |
| 1 | B | 1078 | SER |
| 1 | B | 1080 | THR |
| 1 | B | 1087 | LYS |
| 1 | B | 1095 | THR |
| 1 | B | 1101 | SER |
| 1 | B | 1125 | VAL |
| 1 | B | 1127 | VAL |
| 1 | B | 1131 | LEU |
| 1 | B | 1172 | THR |
| 1 | B | 1173 | LEU |
| 1 | B | 1179 | LEU |
| 1 | B | 1184 | LEU |
| 1 | B | 1196 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1197 | THR |
| 1 | B | 1208 | VAL |
| 1 | B | 1218 | SER |
| 1 | B | 1229 | THR |
| 1 | B | 1255 | SER |
| 1 | B | 1274 | ILE |
| 1 | B | 1283 | MET |
| 1 | B | 1307 | THR |
| 1 | B | 1327 | CYS |
| 1 | B | 1338 | GLU |
| 1 | B | 1367 | ARG |
| 1 | B | 1372 | THR |
| 1 | B | 1384 | ILE |
| 1 | B | 1385 | GLN |
| 1 | B | 1392 | LEU |
| 1 | B | 1414 | ILE |
| 1 | B | 1426 | LEU |
| 1 | B | 1442 | ASN |
| 1 | B | 1465 | ASN |
| 1 | B | 1479 | SER |
| 1 | B | 1502 | ARG |
| 1 | B | 1515 | ARG |
| 1 | B | 1522 | LEU |
| 1 | B | 1523 | ARG |
| 1 | B | 1532 | THR |
| 1 | B | 1533 | ILE |
| 1 | B | 1549 | ASN |
| 1 | B | 1556 | THR |
| 1 | B | 1566 | ARG |
| 1 | B | 1577 | GLN |
| 1 | B | 1580 | LEU |
| 1 | B | 1585 | LYS |
| 1 | B | 1612 | ASP |
| 1 | B | 1625 | LEU |
| 1 | B | 1665 | ILE |
| 1 | B | 1666 | THR |
| 1 | B | 1692 | MET |
| 1 | B | 1693 | ILE |
| 1 | B | 1707 | THR |
| 1 | B | 1709 | GLU |
| 1 | B | 1721 | ARG |
| 1 | B | 1775 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1782 | GLU |
| 1 | B | 1788 | GLU |
| 1 | B | 1794 | GLN |
| 1 | B | 1841 | ARG |
| 1 | B | 1873 | HIS |
| 1 | C | 14 | LEU |
| 1 | C | 15 | THR |
| 1 | C | 21 | GLN |
| 1 | C | 22 | PHE |
| 1 | C | 145 | VAL |
| 1 | C | 149 | LEU |
| 1 | C | 158 | LYS |
| 1 | C | 165 | SER |
| 1 | C | 171 | THR |
| 1 | C | 202 | GLU |
| 1 | C | 217 | PHE |
| 1 | C | 242 | THR |
| 1 | C | 253 | ARG |
| 1 | C | 328 | LEU |
| 1 | C | 331 | ILE |
| 1 | C | 332 | THR |
| 1 | C | 375 | LEU |
| 1 | C | 378 | LEU |
| 1 | C | 390 | VAL |
| 1 | C | 392 | THR |
| 1 | C | 400 | ARG |
| 1 | C | 412 | SER |
| 1 | C | 413 | LEU |
| 1 | C | 415 | SER |
| 1 | C | 416 | LEU |
| 1 | C | 428 | VAL |
| 1 | C | 431 | GLU |
| 1 | C | 432 | VAL |
| 1 | C | 435 | GLU |
| 1 | C | 447 | LEU |
| 1 | C | 457 | ASN |
| 1 | C | 460 | GLU |
| 1 | C | 461 | THR |
| 1 | C | 484 | LEU |
| 1 | C | 489 | VAL |
| 1 | C | 493 | VAL |
| 1 | C | 506 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 509 | ILE |
| 1 | C | 527 | GLN |
| 1 | C | 529 | MET |
| 1 | C | 536 | THR |
| 1 | C | 599 | MET |
| 1 | C | 600 | ASP |
| 1 | C | 603 | ASP |
| 1 | C | 606 | ASP |
| 1 | C | 607 | LYS |
| 1 | C | 615 | SER |
| 1 | C | 621 | THR |
| 1 | C | 622 | ILE |
| 1 | C | 625 | THR |
| 1 | C | 629 | THR |
| 1 | C | 635 | ILE |
| 1 | C | 644 | THR |
| 1 | C | 648 | ASP |
| 1 | C | 711 | SER |
| 1 | C | 719 | GLN |
| 1 | C | 728 | LYS |
| 1 | C | 731 | THR |
| 1 | C | 732 | LEU |
| 1 | C | 748 | LEU |
| 1 | C | 749 | ILE |
| 1 | C | 776 | GLU |
| 1 | C | 782 | GLU |
| 1 | C | 797 | THR |
| 1 | C | 806 | VAL |
| 1 | C | 824 | LEU |
| 1 | C | 852 | ARG |
| 1 | C | 860 | ASN |
| 1 | C | 864 | VAL |
| 1 | C | 873 | ARG |
| 1 | C | 881 | ASN |
| 1 | C | 891 | MET |
| 1 | C | 913 | VAL |
| 1 | C | 930 | LEU |
| 1 | C | 931 | GLN |
| 1 | C | 933 | VAL |
| 1 | C | 935 | GLU |
| 1 | C | 947 | LEU |
| 1 | C | 949 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 951 | SER |
| 1 | C | 953 | VAL |
| 1 | C | 980 | VAL |
| 1 | C | 1016 | GLU |
| 1 | C | 1020 | VAL |
| 1 | C | 1047 | LEU |
| 1 | C | 1056 | ILE |
| 1 | C | 1070 | ARG |
| 1 | C | 1078 | SER |
| 1 | C | 1087 | LYS |
| 1 | C | 1095 | THR |
| 1 | C | 1101 | SER |
| 1 | C | 1125 | VAL |
| 1 | C | 1127 | VAL |
| 1 | C | 1131 | LEU |
| 1 | C | 1172 | THR |
| 1 | C | 1173 | LEU |
| 1 | C | 1179 | LEU |
| 1 | C | 1184 | LEU |
| 1 | C | 1196 | LYS |
| 1 | C | 1197 | THR |
| 1 | C | 1208 | VAL |
| 1 | C | 1218 | SER |
| 1 | C | 1229 | THR |
| 1 | C | 1255 | SER |
| 1 | C | 1274 | ILE |
| 1 | C | 1283 | MET |
| 1 | C | 1307 | THR |
| 1 | C | 1327 | CYS |
| 1 | C | 1338 | GLU |
| 1 | C | 1367 | ARG |
| 1 | C | 1372 | THR |
| 1 | C | 1384 | ILE |
| 1 | C | 1385 | GLN |
| 1 | C | 1392 | LEU |
| 1 | C | 1414 | ILE |
| 1 | C | 1426 | LEU |
| 1 | C | 1430 | ARG |
| 1 | C | 1432 | HIS |
| 1 | C | 1442 | ASN |
| 1 | C | 1455 | ARG |
| 1 | C | 1465 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 1479 | SER |
| 1 | C | 1489 | ARG |
| 1 | C | 1502 | ARG |
| 1 | C | 1515 | ARG |
| 1 | C | 1522 | LEU |
| 1 | C | 1523 | ARG |
| 1 | C | 1532 | THR |
| 1 | C | 1533 | ILE |
| 1 | C | 1549 | ASN |
| 1 | C | 1556 | THR |
| 1 | C | 1566 | ARG |
| 1 | C | 1577 | GLN |
| 1 | C | 1580 | LEU |
| 1 | C | 1585 | LYS |
| 1 | C | 1612 | ASP |
| 1 | C | 1625 | LEU |
| 1 | C | 1665 | ILE |
| 1 | C | 1666 | THR |
| 1 | C | 1692 | MET |
| 1 | C | 1693 | ILE |
| 1 | C | 1707 | THR |
| 1 | C | 1709 | GLU |
| 1 | C | 1721 | ARG |
| 1 | C | 1775 | LEU |
| 1 | C | 1782 | GLU |
| 1 | C | 1788 | GLU |
| 1 | C | 1794 | GLN |
| 1 | C | 1841 | ARG |
| 1 | C | 1873 | HIS |
| 2 | G | 6 | THR |
| 2 | G | 7 | ARG |
| 2 | G | 45 | THR |
| 2 | G | 46 | GLU |
| 2 | G | 48 | PHE |
| 2 | G | 56 | THR |
| 2 | G | 65 | LEU |
| 2 | G | 84 | LEU |
| 2 | G | 86 | LEU |
| 2 | G | 93 | ASN |
| 2 | G | 99 | ASN |
| 2 | G | 101 | ILE |
| 2 | G | 109 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 117 | VAL |
| 2 | G | 122 | LEU |
| 2 | G | 149 | VAL |
| 2 | G | 153 | ASN |
| 2 | G | 155 | GLN |
| 2 | G | 159 | ILE |
| 2 | G | 173 | LEU |
| 2 | G | 175 | ASP |
| 2 | G | 176 | LEU |
| 2 | G | 178 | GLN |
| 2 | G | 182 | VAL |
| 2 | G | 210 | THR |
| 2 | G | 227 | ASP |
| 2 | G | 236 | ILE |
| 2 | G | 240 | LEU |
| 2 | G | 246 | LEU |
| 2 | G | 281 | VAL |
| 2 | G | 286 | THR |
| 2 | G | 295 | SER |
| 2 | G | 297 | ARG |
| 2 | G | 300 | ILE |
| 2 | G | 303 | LEU |
| 2 | G | 319 | LEU |
| 2 | G | 339 | LEU |
| 2 | G | 340 | SER |
| 2 | G | 342 | SER |
| 2 | G | 344 | LEU |
| 2 | G | 353 | VAL |
| 2 | G | 371 | VAL |
| 2 | G | 376 | ASN |
| 2 | G | 389 | LEU |
| 2 | G | 392 | THR |
| 2 | G | 402 | LEU |
| 2 | G | 418 | ASN |
| 2 | G | 425 | SER |
| 2 | G | 431 | LEU |
| 2 | G | 448 | VAL |
| 2 | G | 455 | ILE |
| 2 | G | 462 | THR |
| 2 | G | 463 | PHE |
| 2 | G | 471 | LEU |
| 2 | G | 476 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 478 | ARG |
| 2 | G | 482 | CYS |
| 2 | G | 492 | THR |
| 2 | G | 499 | THR |
| 2 | G | 539 | ASP |
| 2 | G | 545 | GLN |
| 2 | G | 553 | ASN |
| 2 | G | 562 | LEU |
| 2 | G | 566 | HIS |
| 2 | G | 574 | SER |
| 2 | G | 586 | LEU |
| 2 | G | 587 | ILE |
| 2 | G | 598 | THR |
| 2 | G | 607 | VAL |
| 2 | G | 611 | THR |
| 2 | G | 616 | THR |
| 2 | G | 653 | TYR |
| 2 | G | 665 | LEU |
| 2 | G | 669 | LEU |
| 2 | G | 670 | ARG |
| 2 | G | 676 | ILE |
| 2 | G | 693 | GLU |
| 2 | G | 714 | SER |
| 2 | G | 719 | ILE |
| 2 | G | 723 | HIS |
| 2 | G | 730 | LEU |
| 2 | G | 736 | ARG |
| 2 | G | 741 | HIS |
| 2 | G | 750 | MET |
| 2 | G | 751 | LEU |
| 2 | G | 762 | ASN |
| 2 | G | 767 | PHE |
| 2 | G | 775 | ASP |
| 2 | G | 777 | THR |
| 2 | G | 787 | THR |
| 2 | G | 794 | MET |
| 2 | G | 800 | LEU |
| 2 | G | 810 | GLU |
| 2 | G | 825 | THR |
| 2 | G | 832 | TRP |
| 2 | G | 835 | THR |
| 2 | G | 844 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 852 | GLU |
| 2 | G | 855 | HIS |
| 2 | G | 857 | ILE |
| 2 | G | 869 | ASP |
| 2 | G | 880 | LEU |
| 2 | G | 881 | VAL |
| 2 | G | 892 | ILE |
| 2 | G | 907 | VAL |
| 2 | G | 929 | LEU |
| 2 | G | 945 | THR |
| 2 | G | 952 | ARG |
| 2 | G | 953 | ARG |
| 2 | G | 964 | LEU |
| 2 | G | 971 | SER |
| 2 | G | 993 | GLN |
| 2 | G | 1015 | VAL |
| 2 | G | 1021 | LEU |
| 2 | G | 1024 | ARG |
| 2 | G | 1048 | VAL |
| 2 | G | 1066 | ILE |
| 2 | G | 1070 | ILE |
| 2 | G | 1082 | ILE |
| 2 | G | 1109 | VAL |
| 2 | G | 1123 | ASP |
| 2 | G | 1124 | SER |
| 2 | G | 1145 | SER |
| 2 | G | 1148 | ASN |
| 2 | G | 1160 | THR |
| 2 | G | 1171 | ARG |
| 2 | G | 1189 | THR |
| 2 | G | 1197 | LEU |
| 2 | G | 1211 | LEU |
| 2 | G | 1219 | ILE |
| 2 | G | 1227 | ARG |
| 2 | G | 1260 | GLN |
| 2 | G | 1265 | MET |
| 2 | G | 1284 | VAL |
| 2 | G | 1314 | ARG |
| 2 | G | 1318 | THR |
| 2 | G | 1328 | VAL |
| 2 | G | 1335 | ILE |
| 2 | G | 1348 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 1359 | MET |
| 2 | G | 1360 | ILE |
| 2 | G | 1378 | ILE |
| 2 | G | 1397 | SER |
| 2 | G | 1407 | THR |
| 2 | G | 1408 | SER |
| 2 | G | 1417 | THR |
| 2 | G | 1418 | ASP |
| 2 | G | 1420 | GLU |
| 2 | G | 1424 | GLN |
| 2 | G | 1426 | THR |
| 2 | G | 1434 | HIS |
| 2 | G | 1437 | THR |
| 2 | G | 1441 | ILE |
| 2 | G | 1443 | VAL |
| 2 | G | 1446 | SER |
| 2 | G | 1452 | LEU |
| 2 | G | 1463 | THR |
| 2 | G | 1468 | THR |
| 2 | G | 1470 | THR |
| 2 | G | 1472 | VAL |
| 2 | G | 1473 | THR |
| 2 | G | 1501 | ILE |
| 2 | G | 1511 | SER |
| 2 | G | 1526 | THR |
| 2 | G | 1527 | LEU |
| 2 | G | 1528 | GLU |
| 2 | G | 1533 | LEU |
| 2 | G | 1549 | THR |
| 2 | G | 1563 | ILE |
| 2 | G | 1567 | ARG |
| 2 | G | 1590 | ARG |
| 2 | G | 1602 | SER |
| 2 | G | 1605 | VAL |
| 2 | G | 1609 | THR |
| 2 | G | 1616 | VAL |
| 2 | G | 1624 | THR |
| 2 | G | 1627 | GLN |
| 2 | G | 1632 | ILE |
| 2 | G | 1637 | LEU |
| 2 | G | 1651 | LEU |
| 2 | G | 1672 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 1678 | MET |
| 2 | G | 1680 | LEU |
| 2 | G | 1683 | THR |
| 2 | G | 1712 | ASN |
| 2 | G | 1718 | THR |
| 2 | G | 1757 | GLU |
| 2 | G | 1775 | GLN |
| 2 | G | 1781 | LEU |
| 2 | G | 1784 | MET |
| 2 | G | 1825 | GLU |
| 2 | G | 1831 | VAL |
| 2 | G | 1834 | ARG |
| 2 | G | 1844 | ARG |
| 2 | G | 1847 | LEU |
| 2 | G | 1857 | ILE |
| 2 | G | 1862 | VAL |
| 2 | G | 1886 | VAL |
| 2 | G | 1914 | LEU |
| 2 | G | 1936 | VAL |
| 2 | G | 1937 | GLU |
| 2 | G | 1941 | PHE |
| 2 | G | 1982 | MET |
| 2 | G | 2003 | VAL |
| 2 | G | 2042 | ILE |
| 2 | G | 2044 | ASN |
| 2 | G | 2047 | LYS |
| 2 | G | 2048 | TYR |
| 2 | G | 2050 | GLN |
| 2 | H | 6 | THR |
| 2 | H | 7 | ARG |
| 2 | H | 45 | THR |
| 2 | H | 46 | GLU |
| 2 | H | 48 | PHE |
| 2 | H | 56 | THR |
| 2 | H | 65 | LEU |
| 2 | H | 84 | LEU |
| 2 | H | 86 | LEU |
| 2 | H | 93 | ASN |
| 2 | H | 99 | ASN |
| 2 | H | 101 | ILE |
| 2 | H | 109 | LEU |
| 2 | H | 117 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 122 | LEU |
| 2 | H | 149 | VAL |
| 2 | H | 153 | ASN |
| 2 | H | 155 | GLN |
| 2 | H | 159 | ILE |
| 2 | H | 173 | LEU |
| 2 | H | 176 | LEU |
| 2 | H | 178 | GLN |
| 2 | H | 182 | VAL |
| 2 | H | 186 | ASP |
| 2 | H | 198 | LEU |
| 2 | H | 210 | THR |
| 2 | H | 227 | ASP |
| 2 | H | 236 | ILE |
| 2 | H | 240 | LEU |
| 2 | H | 246 | LEU |
| 2 | H | 281 | VAL |
| 2 | H | 286 | THR |
| 2 | H | 295 | SER |
| 2 | H | 297 | ARG |
| 2 | H | 300 | ILE |
| 2 | H | 317 | THR |
| 2 | H | 319 | LEU |
| 2 | H | 339 | LEU |
| 2 | H | 340 | SER |
| 2 | H | 342 | SER |
| 2 | H | 344 | LEU |
| 2 | H | 353 | VAL |
| 2 | H | 371 | VAL |
| 2 | H | 376 | ASN |
| 2 | H | 389 | LEU |
| 2 | H | 392 | THR |
| 2 | H | 402 | LEU |
| 2 | H | 418 | ASN |
| 2 | H | 425 | SER |
| 2 | H | 431 | LEU |
| 2 | H | 448 | VAL |
| 2 | H | 455 | ILE |
| 2 | H | 462 | THR |
| 2 | H | 463 | PHE |
| 2 | H | 471 | LEU |
| 2 | H | 476 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 478 | ARG |
| 2 | H | 482 | CYS |
| 2 | H | 492 | THR |
| 2 | H | 499 | THR |
| 2 | H | 545 | GLN |
| 2 | H | 553 | ASN |
| 2 | H | 562 | LEU |
| 2 | H | 566 | HIS |
| 2 | H | 572 | ASN |
| 2 | H | 574 | SER |
| 2 | H | 586 | LEU |
| 2 | H | 587 | ILE |
| 2 | H | 598 | THR |
| 2 | H | 607 | VAL |
| 2 | H | 611 | THR |
| 2 | H | 616 | THR |
| 2 | H | 653 | TYR |
| 2 | H | 665 | LEU |
| 2 | H | 669 | LEU |
| 2 | H | 670 | ARG |
| 2 | H | 676 | ILE |
| 2 | H | 693 | GLU |
| 2 | H | 714 | SER |
| 2 | H | 719 | ILE |
| 2 | H | 723 | HIS |
| 2 | H | 730 | LEU |
| 2 | H | 733 | THR |
| 2 | H | 736 | ARG |
| 2 | H | 741 | HIS |
| 2 | H | 751 | LEU |
| 2 | H | 762 | ASN |
| 2 | H | 767 | PHE |
| 2 | H | 775 | ASP |
| 2 | H | 777 | THR |
| 2 | H | 787 | THR |
| 2 | H | 794 | MET |
| 2 | H | 797 | ASP |
| 2 | H | 800 | LEU |
| 2 | H | 810 | GLU |
| 2 | H | 825 | THR |
| 2 | H | 832 | TRP |
| 2 | H | 835 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 844 | VAL |
| 2 | H | 852 | GLU |
| 2 | H | 855 | HIS |
| 2 | H | 857 | ILE |
| 2 | H | 869 | ASP |
| 2 | H | 880 | LEU |
| 2 | H | 881 | VAL |
| 2 | H | 892 | ILE |
| 2 | H | 907 | VAL |
| 2 | H | 929 | LEU |
| 2 | H | 945 | THR |
| 2 | H | 952 | ARG |
| 2 | H | 953 | ARG |
| 2 | H | 964 | LEU |
| 2 | H | 971 | SER |
| 2 | H | 993 | GLN |
| 2 | H | 1015 | VAL |
| 2 | H | 1021 | LEU |
| 2 | H | 1024 | ARG |
| 2 | H | 1048 | VAL |
| 2 | H | 1066 | ILE |
| 2 | H | 1070 | ILE |
| 2 | H | 1082 | ILE |
| 2 | H | 1109 | VAL |
| 2 | H | 1123 | ASP |
| 2 | H | 1145 | SER |
| 2 | H | 1148 | ASN |
| 2 | H | 1160 | THR |
| 2 | H | 1171 | ARG |
| 2 | H | 1189 | THR |
| 2 | H | 1197 | LEU |
| 2 | H | 1211 | LEU |
| 2 | H | 1219 | ILE |
| 2 | H | 1227 | ARG |
| 2 | H | 1260 | GLN |
| 2 | H | 1265 | MET |
| 2 | H | 1284 | VAL |
| 2 | H | 1314 | ARG |
| 2 | H | 1318 | THR |
| 2 | H | 1328 | VAL |
| 2 | H | 1335 | ILE |
| 2 | H | 1348 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 1359 | MET |
| 2 | H | 1360 | ILE |
| 2 | H | 1378 | ILE |
| 2 | H | 1397 | SER |
| 2 | H | 1407 | THR |
| 2 | H | 1408 | SER |
| 2 | H | 1420 | GLU |
| 2 | H | 1422 | THR |
| 2 | H | 1426 | THR |
| 2 | H | 1434 | HIS |
| 2 | H | 1437 | THR |
| 2 | H | 1441 | ILE |
| 2 | H | 1443 | VAL |
| 2 | H | 1446 | SER |
| 2 | H | 1452 | LEU |
| 2 | H | 1463 | THR |
| 2 | H | 1468 | THR |
| 2 | H | 1470 | THR |
| 2 | H | 1472 | VAL |
| 2 | H | 1473 | THR |
| 2 | H | 1501 | ILE |
| 2 | H | 1511 | SER |
| 2 | H | 1526 | THR |
| 2 | H | 1527 | LEU |
| 2 | H | 1528 | GLU |
| 2 | H | 1530 | LYS |
| 2 | H | 1533 | LEU |
| 2 | H | 1549 | THR |
| 2 | H | 1563 | ILE |
| 2 | H | 1567 | ARG |
| 2 | H | 1590 | ARG |
| 2 | H | 1602 | SER |
| 2 | H | 1605 | VAL |
| 2 | H | 1609 | THR |
| 2 | H | 1616 | VAL |
| 2 | H | 1624 | THR |
| 2 | H | 1627 | GLN |
| 2 | H | 1632 | ILE |
| 2 | H | 1637 | LEU |
| 2 | H | 1651 | LEU |
| 2 | H | 1657 | ILE |
| 2 | H | 1661 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 1672 | GLN |
| 2 | H | 1678 | MET |
| 2 | H | 1680 | LEU |
| 2 | H | 1683 | THR |
| 2 | H | 1693 | ARG |
| 2 | H | 1712 | ASN |
| 2 | H | 1718 | THR |
| 2 | H | 1757 | GLU |
| 2 | H | 1775 | GLN |
| 2 | H | 1781 | LEU |
| 2 | H | 1784 | MET |
| 2 | H | 1825 | GLU |
| 2 | H | 1831 | VAL |
| 2 | H | 1834 | ARG |
| 2 | H | 1840 | VAL |
| 2 | H | 1844 | ARG |
| 2 | H | 1847 | LEU |
| 2 | H | 1862 | VAL |
| 2 | H | 1886 | VAL |
| 2 | H | 1914 | LEU |
| 2 | H | 1936 | VAL |
| 2 | H | 1937 | GLU |
| 2 | H | 1982 | MET |
| 2 | H | 2003 | VAL |
| 2 | H | 2038 | ILE |
| 2 | H | 2042 | ILE |
| 2 | H | 2044 | ASN |
| 2 | H | 2047 | LYS |
| 2 | H | 2048 | TYR |
| 2 | H | 2050 | GLN |
| 2 | I | 6 | THR |
| 2 | I | 7 | ARG |
| 2 | I | 45 | THR |
| 2 | I | 46 | GLU |
| 2 | I | 48 | PHE |
| 2 | I | 56 | THR |
| 2 | I | 65 | LEU |
| 2 | I | 84 | LEU |
| 2 | I | 86 | LEU |
| 2 | I | 93 | ASN |
| 2 | I | 99 | ASN |
| 2 | I | 101 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 109 | LEU |
| 2 | I | 117 | VAL |
| 2 | I | 122 | LEU |
| 2 | I | 149 | VAL |
| 2 | I | 153 | ASN |
| 2 | I | 155 | GLN |
| 2 | I | 159 | ILE |
| 2 | I | 173 | LEU |
| 2 | I | 175 | ASP |
| 2 | I | 176 | LEU |
| 2 | I | 178 | GLN |
| 2 | I | 182 | VAL |
| 2 | I | 210 | THR |
| 2 | I | 227 | ASP |
| 2 | I | 236 | ILE |
| 2 | I | 240 | LEU |
| 2 | I | 246 | LEU |
| 2 | I | 281 | VAL |
| 2 | I | 286 | THR |
| 2 | I | 295 | SER |
| 2 | I | 297 | ARG |
| 2 | I | 300 | ILE |
| 2 | I | 303 | LEU |
| 2 | I | 319 | LEU |
| 2 | I | 339 | LEU |
| 2 | I | 340 | SER |
| 2 | I | 342 | SER |
| 2 | I | 344 | LEU |
| 2 | I | 353 | VAL |
| 2 | I | 371 | VAL |
| 2 | I | 376 | ASN |
| 2 | I | 389 | LEU |
| 2 | I | 392 | THR |
| 2 | I | 402 | LEU |
| 2 | I | 418 | ASN |
| 2 | I | 425 | SER |
| 2 | I | 431 | LEU |
| 2 | I | 444 | VAL |
| 2 | I | 448 | VAL |
| 2 | I | 455 | ILE |
| 2 | I | 462 | THR |
| 2 | I | 463 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 471 | LEU |
| 2 | I | 476 | SER |
| 2 | I | 478 | ARG |
| 2 | I | 479 | ILE |
| 2 | I | 482 | CYS |
| 2 | I | 492 | THR |
| 2 | I | 499 | THR |
| 2 | I | 539 | ASP |
| 2 | I | 545 | GLN |
| 2 | I | 553 | ASN |
| 2 | I | 562 | LEU |
| 2 | I | 572 | ASN |
| 2 | I | 574 | SER |
| 2 | I | 586 | LEU |
| 2 | I | 587 | ILE |
| 2 | I | 598 | THR |
| 2 | I | 607 | VAL |
| 2 | I | 611 | THR |
| 2 | I | 616 | THR |
| 2 | I | 653 | TYR |
| 2 | I | 665 | LEU |
| 2 | I | 669 | LEU |
| 2 | I | 670 | ARG |
| 2 | I | 676 | ILE |
| 2 | I | 680 | THR |
| 2 | I | 693 | GLU |
| 2 | I | 714 | SER |
| 2 | I | 719 | ILE |
| 2 | I | 723 | HIS |
| 2 | I | 730 | LEU |
| 2 | I | 733 | THR |
| 2 | I | 736 | ARG |
| 2 | I | 741 | HIS |
| 2 | I | 750 | MET |
| 2 | I | 751 | LEU |
| 2 | I | 762 | ASN |
| 2 | I | 767 | PHE |
| 2 | I | 775 | ASP |
| 2 | I | 777 | THR |
| 2 | I | 787 | THR |
| 2 | I | 794 | MET |
| 2 | I | 800 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 810 | GLU |
| 2 | I | 825 | THR |
| 2 | I | 832 | TRP |
| 2 | I | 835 | THR |
| 2 | I | 844 | VAL |
| 2 | I | 846 | VAL |
| 2 | I | 852 | GLU |
| 2 | I | 855 | HIS |
| 2 | I | 857 | ILE |
| 2 | I | 865 | TRP |
| 2 | I | 869 | ASP |
| 2 | I | 880 | LEU |
| 2 | I | 881 | VAL |
| 2 | I | 892 | ILE |
| 2 | I | 907 | VAL |
| 2 | I | 929 | LEU |
| 2 | I | 945 | THR |
| 2 | I | 952 | ARG |
| 2 | I | 953 | ARG |
| 2 | I | 964 | LEU |
| 2 | I | 971 | SER |
| 2 | I | 993 | GLN |
| 2 | I | 1015 | VAL |
| 2 | I | 1021 | LEU |
| 2 | I | 1024 | ARG |
| 2 | I | 1048 | VAL |
| 2 | I | 1066 | ILE |
| 2 | I | 1070 | ILE |
| 2 | I | 1082 | ILE |
| 2 | I | 1109 | VAL |
| 2 | I | 1123 | ASP |
| 2 | I | 1124 | SER |
| 2 | I | 1145 | SER |
| 2 | I | 1148 | ASN |
| 2 | I | 1160 | THR |
| 2 | I | 1171 | ARG |
| 2 | I | 1189 | THR |
| 2 | I | 1197 | LEU |
| 2 | I | 1211 | LEU |
| 2 | I | 1219 | ILE |
| 2 | I | 1227 | ARG |
| 2 | I | 1260 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 1265 | MET |
| 2 | I | 1284 | VAL |
| 2 | I | 1314 | ARG |
| 2 | I | 1318 | THR |
| 2 | I | 1328 | VAL |
| 2 | I | 1335 | ILE |
| 2 | I | 1348 | LEU |
| 2 | I | 1359 | MET |
| 2 | I | 1360 | ILE |
| 2 | I | 1378 | ILE |
| 2 | I | 1397 | SER |
| 2 | I | 1407 | THR |
| 2 | I | 1408 | SER |
| 2 | I | 1420 | GLU |
| 2 | I | 1421 | ASN |
| 2 | I | 1423 | PHE |
| 2 | I | 1434 | HIS |
| 2 | I | 1437 | THR |
| 2 | I | 1441 | ILE |
| 2 | I | 1443 | VAL |
| 2 | I | 1446 | SER |
| 2 | I | 1452 | LEU |
| 2 | I | 1463 | THR |
| 2 | I | 1468 | THR |
| 2 | I | 1470 | THR |
| 2 | I | 1472 | VAL |
| 2 | I | 1473 | THR |
| 2 | I | 1501 | ILE |
| 2 | I | 1511 | SER |
| 2 | I | 1527 | LEU |
| 2 | I | 1528 | GLU |
| 2 | I | 1533 | LEU |
| 2 | I | 1549 | THR |
| 2 | I | 1563 | ILE |
| 2 | I | 1567 | ARG |
| 2 | I | 1590 | ARG |
| 2 | I | 1602 | SER |
| 2 | I | 1605 | VAL |
| 2 | I | 1609 | THR |
| 2 | I | 1616 | VAL |
| 2 | I | 1624 | THR |
| 2 | I | 1627 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 1632 | ILE |
| 2 | I | 1637 | LEU |
| 2 | I | 1651 | LEU |
| 2 | I | 1672 | GLN |
| 2 | I | 1678 | MET |
| 2 | I | 1680 | LEU |
| 2 | I | 1683 | THR |
| 2 | I | 1712 | ASN |
| 2 | I | 1718 | THR |
| 2 | I | 1757 | GLU |
| 2 | I | 1775 | GLN |
| 2 | I | 1781 | LEU |
| 2 | I | 1784 | MET |
| 2 | I | 1825 | GLU |
| 2 | I | 1831 | VAL |
| 2 | I | 1834 | ARG |
| 2 | I | 1844 | ARG |
| 2 | I | 1847 | LEU |
| 2 | I | 1862 | VAL |
| 2 | I | 1871 | LEU |
| 2 | I | 1886 | VAL |
| 2 | I | 1914 | LEU |
| 2 | I | 1936 | VAL |
| 2 | I | 1937 | GLU |
| 2 | I | 1982 | MET |
| 2 | I | 2003 | VAL |
| 2 | I | 2042 | ILE |
| 2 | I | 2044 | ASN |
| 2 | I | 2047 | LYS |
| 2 | I | 2048 | TYR |
| 2 | I | 2050 | GLN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (294) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 11 | HIS |
| 1 | A | 21 | GLN |
| 1 | A | 32 | GLN |
| 1 | A | 58 | GLN |
| 1 | A | 63 | ASN |
| 1 | A | 157 | HIS |
| 1 | A | 183 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 214 | GLN |
| 1 | A | 271 | ASN |
| 1 | A | 335 | HIS |
| 1 | A | 341 | GLN |
| 1 | A | 344 | GLN |
| 1 | A | 374 | GLN |
| 1 | A | 411 | GLN |
| 1 | A | 427 | ASN |
| 1 | A | 438 | ASN |
| 1 | A | 506 | ASN |
| 1 | A | 527 | GLN |
| 1 | A | 618 | ASN |
| 1 | A | 694 | GLN |
| 1 | A | 738 | ASN |
| 1 | A | 758 | ASN |
| 1 | A | 792 | HIS |
| 1 | A | 860 | ASN |
| 1 | A | 898 | GLN |
| 1 | A | 983 | GLN |
| 1 | A | 987 | ASN |
| 1 | A | 989 | GLN |
| 1 | A | 1000 | GLN |
| 1 | A | 1003 | GLN |
| 1 | A | 1063 | HIS |
| 1 | A | 1064 | ASN |
| 1 | A | 1066 | ASN |
| 1 | A | 1146 | HIS |
| 1 | A | 1239 | HIS |
| 1 | A | 1385 | GLN |
| 1 | A | 1432 | HIS |
| 1 | A | 1433 | HIS |
| 1 | A | 1442 | ASN |
| 1 | A | 1458 | GLN |
| 1 | A | 1482 | GLN |
| 1 | A | 1494 | HIS |
| 1 | A | 1495 | ASN |
| 1 | A | 1505 | GLN |
| 1 | A | 1510 | ASN |
| 1 | A | 1542 | HIS |
| 1 | A | 1549 | ASN |
| 1 | A | 1563 | HIS |
| 1 | A | 1577 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1610 | ASN |
| 1 | A | 1652 | GLN |
| 1 | A | 1690 | ASN |
| 1 | A | 1852 | HIS |
| 1 | B | 11 | HIS |
| 1 | B | 21 | GLN |
| 1 | B | 32 | GLN |
| 1 | B | 58 | GLN |
| 1 | B | 63 | ASN |
| 1 | B | 157 | HIS |
| 1 | B | 183 | GLN |
| 1 | B | 214 | GLN |
| 1 | B | 271 | ASN |
| 1 | B | 335 | HIS |
| 1 | B | 341 | GLN |
| 1 | B | 344 | GLN |
| 1 | B | 374 | GLN |
| 1 | B | 407 | ASN |
| 1 | B | 411 | GLN |
| 1 | B | 427 | ASN |
| 1 | B | 438 | ASN |
| 1 | B | 506 | ASN |
| 1 | B | 527 | GLN |
| 1 | B | 618 | ASN |
| 1 | B | 694 | GLN |
| 1 | B | 738 | ASN |
| 1 | B | 758 | ASN |
| 1 | B | 792 | HIS |
| 1 | B | 898 | GLN |
| 1 | B | 987 | ASN |
| 1 | B | 989 | GLN |
| 1 | B | 1000 | GLN |
| 1 | B | 1003 | GLN |
| 1 | B | 1063 | HIS |
| 1 | B | 1064 | ASN |
| 1 | B | 1066 | ASN |
| 1 | B | 1146 | HIS |
| 1 | B | 1239 | HIS |
| 1 | B | 1385 | GLN |
| 1 | B | 1432 | HIS |
| 1 | B | 1433 | HIS |
| 1 | B | 1442 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1458 | GLN |
| 1 | B | 1482 | GLN |
| 1 | B | 1494 | HIS |
| 1 | B | 1495 | ASN |
| 1 | B | 1505 | GLN |
| 1 | B | 1510 | ASN |
| 1 | B | 1542 | HIS |
| 1 | B | 1549 | ASN |
| 1 | B | 1563 | HIS |
| 1 | B | 1577 | GLN |
| 1 | B | 1610 | ASN |
| 1 | B | 1652 | GLN |
| 1 | B | 1690 | ASN |
| 1 | B | 1794 | GLN |
| 1 | B | 1852 | HIS |
| 1 | C | 11 | HIS |
| 1 | C | 21 | GLN |
| 1 | C | 32 | GLN |
| 1 | C | 58 | GLN |
| 1 | C | 63 | ASN |
| 1 | C | 157 | HIS |
| 1 | C | 183 | GLN |
| 1 | C | 214 | GLN |
| 1 | C | 271 | ASN |
| 1 | C | 335 | HIS |
| 1 | C | 341 | GLN |
| 1 | C | 344 | GLN |
| 1 | C | 374 | GLN |
| 1 | C | 411 | GLN |
| 1 | C | 427 | ASN |
| 1 | C | 438 | ASN |
| 1 | C | 506 | ASN |
| 1 | C | 527 | GLN |
| 1 | C | 618 | ASN |
| 1 | C | 694 | GLN |
| 1 | C | 738 | ASN |
| 1 | C | 758 | ASN |
| 1 | C | 792 | HIS |
| 1 | C | 860 | ASN |
| 1 | C | 898 | GLN |
| 1 | C | 987 | ASN |
| 1 | C | 989 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 1000 | GLN |
| 1 | C | 1003 | GLN |
| 1 | C | 1063 | HIS |
| 1 | C | 1064 | ASN |
| 1 | C | 1066 | ASN |
| 1 | C | 1146 | HIS |
| 1 | C | 1239 | HIS |
| 1 | C | 1385 | GLN |
| 1 | C | 1432 | HIS |
| 1 | C | 1433 | HIS |
| 1 | C | 1442 | ASN |
| 1 | C | 1458 | GLN |
| 1 | C | 1482 | GLN |
| 1 | C | 1495 | ASN |
| 1 | C | 1505 | GLN |
| 1 | C | 1510 | ASN |
| 1 | C | 1542 | HIS |
| 1 | C | 1549 | ASN |
| 1 | C | 1563 | HIS |
| 1 | C | 1577 | GLN |
| 1 | C | 1610 | ASN |
| 1 | C | 1652 | GLN |
| 1 | C | 1690 | ASN |
| 1 | C | 1852 | HIS |
| 2 | G | 34 | GLN |
| 2 | G | 36 | GLN |
| 2 | G | 85 | ASN |
| 2 | G | 102 | HIS |
| 2 | G | 178 | GLN |
| 2 | G | 359 | HIS |
| 2 | G | 376 | ASN |
| 2 | G | 418 | ASN |
| 2 | G | 428 | HIS |
| 2 | G | 440 | ASN |
| 2 | G | 447 | ASN |
| 2 | G | 500 | HIS |
| 2 | G | 517 | HIS |
| 2 | G | 545 | GLN |
| 2 | G | 558 | ASN |
| 2 | G | 572 | ASN |
| 2 | G | 612 | ASN |
| 2 | G | 650 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | G | 718 | ASN |
| 2 | G | 740 | HIS |
| 2 | G | 741 | HIS |
| 2 | G | 747 | HIS |
| 2 | G | 752 | GLN |
| 2 | G | 762 | ASN |
| 2 | G | 855 | HIS |
| 2 | G | 900 | GLN |
| 2 | G | 910 | GLN |
| 2 | G | 1046 | GLN |
| 2 | G | 1148 | ASN |
| 2 | G | 1217 | ASN |
| 2 | G | 1220 | GLN |
| 2 | G | 1260 | GLN |
| 2 | G | 1341 | ASN |
| 2 | G | 1352 | HIS |
| 2 | G | 1355 | ASN |
| 2 | G | 1367 | GLN |
| 2 | G | 1384 | GLN |
| 2 | G | 1595 | ASN |
| 2 | G | 1659 | GLN |
| 2 | G | 1669 | GLN |
| 2 | G | 1672 | GLN |
| 2 | G | 1697 | HIS |
| 2 | G | 1890 | ASN |
| 2 | G | 1896 | GLN |
| 2 | G | 1977 | HIS |
| 2 | G | 2013 | ASN |
| 2 | G | 2020 | GLN |
| 2 | H | 34 | GLN |
| 2 | H | 85 | ASN |
| 2 | H | 102 | HIS |
| 2 | H | 178 | GLN |
| 2 | H | 359 | HIS |
| 2 | H | 376 | ASN |
| 2 | H | 418 | ASN |
| 2 | H | 428 | HIS |
| 2 | H | 440 | ASN |
| 2 | H | 447 | ASN |
| 2 | H | 500 | HIS |
| 2 | H | 517 | HIS |
| 2 | H | 545 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 558 | ASN |
| 2 | H | 572 | ASN |
| 2 | H | 612 | ASN |
| 2 | H | 650 | ASN |
| 2 | H | 718 | ASN |
| 2 | H | 740 | HIS |
| 2 | H | 741 | HIS |
| 2 | H | 747 | HIS |
| 2 | H | 752 | GLN |
| 2 | H | 762 | ASN |
| 2 | H | 900 | GLN |
| 2 | H | 910 | GLN |
| 2 | H | 1039 | HIS |
| 2 | H | 1046 | GLN |
| 2 | H | 1148 | ASN |
| 2 | H | 1217 | ASN |
| 2 | H | 1220 | GLN |
| 2 | H | 1260 | GLN |
| 2 | H | 1341 | ASN |
| 2 | H | 1352 | HIS |
| 2 | H | 1355 | ASN |
| 2 | H | 1367 | GLN |
| 2 | H | 1669 | GLN |
| 2 | H | 1672 | GLN |
| 2 | H | 1697 | HIS |
| 2 | H | 1890 | ASN |
| 2 | H | 1896 | GLN |
| 2 | H | 1977 | HIS |
| 2 | H | 2013 | ASN |
| 2 | H | 2020 | GLN |
| 2 | I | 34 | GLN |
| 2 | I | 36 | GLN |
| 2 | I | 85 | ASN |
| 2 | I | 102 | HIS |
| 2 | I | 178 | GLN |
| 2 | I | 359 | HIS |
| 2 | I | 376 | ASN |
| 2 | I | 418 | ASN |
| 2 | I | 428 | HIS |
| 2 | I | 440 | ASN |
| 2 | I | 447 | ASN |
| 2 | I | 500 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 517 | HIS |
| 2 | I | 545 | GLN |
| 2 | I | 558 | ASN |
| 2 | I | 572 | ASN |
| 2 | I | 612 | ASN |
| 2 | I | 718 | ASN |
| 2 | I | 740 | HIS |
| 2 | I | 741 | HIS |
| 2 | I | 747 | HIS |
| 2 | I | 752 | GLN |
| 2 | I | 762 | ASN |
| 2 | I | 855 | HIS |
| 2 | I | 900 | GLN |
| 2 | I | 910 | GLN |
| 2 | I | 1046 | GLN |
| 2 | I | 1055 | HIS |
| 2 | I | 1148 | ASN |
| 2 | I | 1217 | ASN |
| 2 | I | 1220 | GLN |
| 2 | I | 1260 | GLN |
| 2 | I | 1341 | ASN |
| 2 | I | 1352 | HIS |
| 2 | I | 1355 | ASN |
| 2 | I | 1367 | GLN |
| 2 | I | 1421 | ASN |
| 2 | I | 1595 | ASN |
| 2 | I | 1669 | GLN |
| 2 | I | 1672 | GLN |
| 2 | I | 1697 | HIS |
| 2 | I | 1868 | GLN |
| 2 | I | 1890 | ASN |
| 2 | I | 1896 | GLN |
| 2 | I | 1977 | HIS |
| 2 | I | 2013 | ASN |
| 2 | I | 2020 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | CER | A | 2748 | - | 10,11,15 | 4.07 | 3 (30%) | 9,13,17 | 3.23 | 2 (22%) |
| 3 | CER | B | 2748 | - | 10,11,15 | 4.07 | 3 (30%) | 9,13,17 | 3.11 | 2 (22%) |
| 3 | CER | C | 2748 | - | 10,11,15 | 4.09 | 3 (30%) | 9,13,17 | 3.24 | 2 (22%) |
| 4 | FMN | G | 3051 | - | 32,33,33 | 6.16 | 19 (59%) | 34,50,50 | 1.96 | 6 (17%) |
| 4 | FMN | H | 3051 | - | 32,33,33 | 6.07 | 19 (59%) | 34,50,50 | 1.97 | 6 (17%) |
| 4 | FMN | I | 3051 | - | 32,33,33 | 6.11 | 21 (65%) | 34,50,50 | 1.87 | 6 (17%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | CER | A | 2748 | - | - | 0/12/12/16 | 0/0/0/0 |
| 3 | CER | B | 2748 | - | - | 0/12/12/16 | 0/0/0/0 |
| 3 | CER | C | 2748 | - | - | 0/12/12/16 | 0/0/0/0 |
| 4 | FMN | G | 3051 | - | - | 0/18/18/18 | 0/3/3/3 |
| 4 | FMN | H | 3051 | - | - | 0/18/18/18 | 0/3/3/3 |
| 4 | FMN | I | 3051 | - | - | 0/18/18/18 | 0/3/3/3 |

All (68) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | I | 3051 | FMN | C7M-C7 | 2.12 | 1.55 | 1.51 |
| 4 | I | 3051 | FMN | C8M-C8 | 2.28 | 1.55 | 1.51 |
| 4 | G | 3051 | FMN | P-O3P | 2.92 | 1.64 | 1.54 |
| 3 | A | 2748 | CER | C5-C4 | 3.14 | 1.55 | 1.51 |
| 4 | H | 3051 | FMN | P-O3P | 3.16 | 1.65 | 1.54 |
| 4 | I | 3051 | FMN | P-O3P | 3.20 | 1.65 | 1.54 |
| 3 | C | 2748 | CER | C5-C4 | 3.21 | 1.55 | 1.51 |
| 3 | B | 2748 | CER | C5-C4 | 3.24 | 1.56 | 1.51 |
| 4 | G | 3051 | FMN | P-O2P | 3.25 | 1.66 | 1.54 |
| 4 | H | 3051 | FMN | P-O2P | 3.28 | 1.66 | 1.54 |
| 4 | I | 3051 | FMN | P-O2P | 3.42 | 1.66 | 1.54 |
| 3 | A | 2748 | CER | C1-N1 | 4.37 | 1.47 | 1.32 |
| 3 | B | 2748 | CER | C1-N1 | 4.42 | 1.47 | 1.32 |
| 3 | C | 2748 | CER | C1-N1 | 4.43 | 1.47 | 1.32 |
| 4 | I | 3051 | FMN | C4-C4A | 5.64 | 1.52 | 1.41 |
| 4 | H | 3051 | FMN | C9A-C5A | 5.72 | 1.54 | 1.42 |
| 4 | H | 3051 | FMN | C4-C4A | 5.82 | 1.53 | 1.41 |
| 4 | G | 3051 | FMN | C9A-C5A | 5.97 | 1.55 | 1.42 |
| 4 | G | 3051 | FMN | C4-C4A | 6.04 | 1.53 | 1.41 |
| 4 | H | 3051 | FMN | C8-C7 | 6.21 | 1.57 | 1.41 |
| 4 | I | 3051 | FMN | C9A-C5A | 6.24 | 1.55 | 1.42 |
| 4 | H | 3051 | FMN | C9-C8 | 6.38 | 1.55 | 1.37 |
| 4 | G | 3051 | FMN | C8-C7 | 6.38 | 1.58 | 1.41 |
| 4 | G | 3051 | FMN | C9-C8 | 6.47 | 1.55 | 1.37 |
| 4 | I | 3051 | FMN | C9-C8 | 6.68 | 1.56 | 1.37 |
| 4 | I | 3051 | FMN | C8-C7 | 6.75 | 1.59 | 1.41 |
| 4 | I | 3051 | FMN | C2-N3 | 6.76 | 1.52 | 1.38 |
| 4 | I | 3051 | FMN | C10-N1 | 6.78 | 1.47 | 1.35 |
| 4 | I | 3051 | FMN | O4-C4 | 6.87 | 1.42 | 1.24 |
| 4 | H | 3051 | FMN | C6-C7 | 6.87 | 1.57 | 1.37 |
| 4 | G | 3051 | FMN | C2-N3 | 6.92 | 1.52 | 1.38 |
| 4 | I | 3051 | FMN | C4A-C10 | 6.93 | 1.53 | 1.40 |
| 4 | H | 3051 | FMN | O4-C4 | 7.02 | 1.42 | 1.24 |
| 4 | I | 3051 | FMN | C6-C7 | 7.03 | 1.57 | 1.37 |
| 4 | H | 3051 | FMN | C4A-C10 | 7.09 | 1.53 | 1.40 |
| 4 | I | 3051 | FMN | C2-N1 | 7.09 | 1.52 | 1.38 |
| 4 | G | 3051 | FMN | O4-C4 | 7.11 | 1.42 | 1.24 |
| 4 | H | 3051 | FMN | C10-N1 | 7.14 | 1.47 | 1.35 |
| 4 | H | 3051 | FMN | C2-N1 | 7.15 | 1.53 | 1.38 |
| 4 | G | 3051 | FMN | C6-C7 | 7.20 | 1.57 | 1.37 |
| 4 | G | 3051 | FMN | C10-N1 | 7.24 | 1.48 | 1.35 |
| 4 | H | 3051 | FMN | C2-N3 | 7.31 | 1.53 | 1.38 |
| 4 | G | 3051 | FMN | C2-N1 | 7.32 | 1.53 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | G | 3051 | FMN | C4A-C10 | 7.58 | 1.54 | 1.40 |
| 4 | I | 3051 | FMN | C9A-N10 | 7.68 | 1.49 | 1.38 |
| 4 | H | 3051 | FMN | C9A-N10 | 7.73 | 1.49 | 1.38 |
| 4 | G | 3051 | FMN | C9A-N10 | 8.07 | 1.50 | 1.38 |
| 4 | I | 3051 | FMN | C9-C9A | 8.51 | 1.59 | 1.40 |
| 4 | H | 3051 | FMN | C9-C9A | 8.56 | 1.59 | 1.40 |
| 4 | G | 3051 | FMN | C9-C9A | 8.66 | 1.59 | 1.40 |
| 4 | I | 3051 | FMN | C4-N3 | 9.49 | 1.50 | 1.33 |
| 4 | G | 3051 | FMN | C4-N3 | 9.51 | 1.50 | 1.33 |
| 4 | H | 3051 | FMN | C4-N3 | 9.86 | 1.50 | 1.33 |
| 4 | H | 3051 | FMN | C5A-N5 | 10.04 | 1.51 | 1.35 |
| 4 | G | 3051 | FMN | C5A-N5 | 10.19 | 1.51 | 1.35 |
| 4 | I | 3051 | FMN | C5A-N5 | 10.36 | 1.51 | 1.35 |
| 4 | G | 3051 | FMN | C10-N10 | 10.66 | 1.51 | 1.39 |
| 4 | H | 3051 | FMN | C10-N10 | 10.78 | 1.51 | 1.39 |
| 4 | I | 3051 | FMN | C10-N10 | 10.79 | 1.51 | 1.39 |
| 4 | H | 3051 | FMN | C6-C5A | 10.81 | 1.58 | 1.41 |
| 4 | G | 3051 | FMN | C6-C5A | 11.01 | 1.58 | 1.41 |
| 3 | B | 2748 | CER | O1-C4 | 11.30 | 1.41 | 1.21 |
| 4 | I | 3051 | FMN | C6-C5A | 11.30 | 1.59 | 1.41 |
| 3 | A | 2748 | CER | O1-C4 | 11.34 | 1.41 | 1.21 |
| 4 | H | 3051 | FMN | C4A-N5 | 11.35 | 1.50 | 1.33 |
| 3 | C | 2748 | CER | O1-C4 | 11.35 | 1.41 | 1.21 |
| 4 | I | 3051 | FMN | C4A-N5 | 11.40 | 1.50 | 1.33 |
| 4 | G | 3051 | FMN | C4A-N5 | 11.81 | 1.51 | 1.33 |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | A | 2748 | CER | O1-C4-C3 | -6.71 | 108.66 | 120.03 |
| 3 | C | 2748 | CER | O1-C4-C3 | -6.69 | 108.69 | 120.03 |
| 3 | C | 2748 | CER | O1-C4-C5 | -6.55 | 107.97 | 121.70 |
| 3 | A | 2748 | CER | O1-C4-C5 | -6.51 | 108.06 | 121.70 |
| 3 | B | 2748 | CER | O1-C4-C3 | -6.48 | 109.06 | 120.03 |
| 3 | B | 2748 | CER | O1-C4-C5 | -6.24 | 108.64 | 121.70 |
| 4 | H | 3051 | FMN | N3-C2-N1 | -4.80 | 119.60 | 127.69 |
| 4 | I | 3051 | FMN | N3-C2-N1 | -4.50 | 120.11 | 127.69 |
| 4 | G | 3051 | FMN | N3-C2-N1 | -4.24 | 120.55 | 127.69 |
| 4 | H | 3051 | FMN | C4A-C4-N3 | -4.19 | 118.04 | 123.52 |
| 4 | G | 3051 | FMN | C4A-C4-N3 | -4.15 | 118.10 | 123.52 |
| 4 | I | 3051 | FMN | C4A-C4-N3 | -3.91 | 118.41 | 123.52 |
| 4 | I | 3051 | FMN | C1'-N10-C9A | 2.18 | 121.35 | 118.83 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | H | 3051 | FMN | C1'-N10-C9A | 2.46 | 121.68 | 118.83 |
| 4 | I | 3051 | FMN | C4A-N5-C5A | 2.56 | 119.74 | 116.72 |
| 4 | H | 3051 | FMN | C5A-C9A-N10 | 2.61 | 119.53 | 117.58 |
| 4 | I | 3051 | FMN | C5A-C9A-N10 | 2.69 | 119.59 | 117.58 |
| 4 | G | 3051 | FMN | C1'-N10-C9A | 2.71 | 121.97 | 118.83 |
| 4 | H | 3051 | FMN | C4A-N5-C5A | 2.73 | 119.94 | 116.72 |
| 4 | G | 3051 | FMN | C4A-N5-C5A | 2.83 | 120.06 | 116.72 |
| 4 | G | 3051 | FMN | C5A-C9A-N10 | 3.05 | 119.86 | 117.58 |
| 4 | I | 3051 | FMN | C4-N3-C2 | 7.07 | 121.05 | 115.16 |
| 4 | G | 3051 | FMN | C4-N3-C2 | 7.40 | 121.33 | 115.16 |
| 4 | H | 3051 | FMN | C4-N3-C2 | 7.53 | 121.44 | 115.16 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 32 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 2748 | CER | 3 | 0 |
| 3 | B | 2748 | CER | 4 | 0 |
| 3 | C | 2748 | CER | 4 | 0 |
| 4 | G | 3051 | FMN | 7 | 0 |
| 4 | H | 3051 | FMN | 6 | 0 |
| 4 | I | 3051 | FMN | 8 | 0 |

## 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 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 1750/1887 (92%) | -0.30 | 47 (2%) 58 46 | 95, 134, 347, 457 | 0 |
| 1 | B | 1750/1887 (92%) | -0.34 | 31 (1%) 71 61 | 96, 133, 302, 419 | 0 |
| 1 | C | 1750/1887 (92%) | -0.26 | 64 (3%) 45 34 | 98, 135, 423, 568 | 0 |
| 2 | G | 2033/2051 (99%) | -0.45 | 2 (0%) 95 95 | 131, 169, 218, 267 | 0 |
| 2 | H | 2033/2051 (99%) | -0.36 | 10 (0%) 91 88 | 130, 170, 215, 265 | 0 |
| 2 | I | 2033/2051 (99%) | -0.43 | 6 (0%) 94 92 | 131, 171, 215, 261 | 0 |
| All | All | 11349/11814 (96%) | -0.36 | 160 (1%) 78 68 | 95, 162, 239, 568 | 0 |

All (160) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 1882 | ALA | 10.5 |
| 1 | C | 1831 | GLY | 9.3 |
| 1 | A | 1829 | GLY | 8.0 |
| 1 | C | 1830 | GLY | 7.8 |
| 1 | C | 1870 | SER | 7.7 |
| 1 | C | 1838 | GLU | 7.5 |
| 1 | C | 1850 | GLU | 7.2 |
| 1 | C | 1884 | SER | 7.2 |
| 1 | C | 1832 | ALA | 6.9 |
| 1 | C | 1883 | VAL | 6.2 |
| 1 | A | 1827 | SER | 5.7 |
| 1 | A | 1763 | LYS | 5.3 |
| 1 | A | 1882 | ALA | 5.3 |
| 1 | C | 1872 | SER | 5.2 |
| 1 | C | 1794 | GLN | 5.0 |
| 1 | C | 875 | THR | 5.0 |
| 1 | A | 1881 | VAL | 4.8 |
| 1 | C | 1869 | VAL | 4.8 |
| 1 | A | 1830 | GLY | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 875 | THR | 4.7 |
| 1 | C | 1797 | GLU | 4.5 |
| 1 | C | 1833 | ALA | 4.5 |
| 1 | B | 539 | SER | 4.4 |
| 1 | C | 1766 | ASN | 4.3 |
| 1 | A | 974 | ASP | 4.3 |
| 1 | C | 1857 | LYS | 4.3 |
| 1 | A | 539 | SER | 4.2 |
| 1 | C | 1803 | PRO | 4.1 |
| 1 | C | 1874 | ASP | 4.1 |
| 1 | B | 141 | ALA | 4.1 |
| 1 | A | 875 | THR | 4.1 |
| 1 | C | 1804 | SER | 4.1 |
| 1 | A | 1843 | ASN | 4.0 |
| 1 | C | 1873 | HIS | 4.0 |
| 1 | A | 975 | ALA | 3.9 |
| 1 | C | 1868 | LYS | 3.9 |
| 1 | A | 1762 | GLU | 3.9 |
| 1 | A | 1875 | ASP | 3.8 |
| 1 | C | 1880 | ALA | 3.7 |
| 1 | B | 1833 | ALA | 3.6 |
| 2 | H | 1929 | LYS | 3.6 |
| 1 | B | 1762 | GLU | 3.6 |
| 2 | G | 1956 | ARG | 3.6 |
| 1 | A | 1853 | GLY | 3.6 |
| 1 | C | 540 | GLN | 3.6 |
| 1 | C | 1837 | ILE | 3.6 |
| 1 | B | 599 | MET | 3.5 |
| 1 | A | 1880 | ALA | 3.5 |
| 1 | A | 208 | GLU | 3.5 |
| 1 | C | 1783 | ASN | 3.5 |
| 1 | A | 1866 | ASP | 3.5 |
| 1 | B | 1830 | GLY | 3.5 |
| 1 | C | 200 | LYS | 3.5 |
| 1 | B | 140 | ILE | 3.4 |
| 1 | A | 1826 | LYS | 3.4 |
| 1 | C | 1842 | VAL | 3.4 |
| 1 | A | 1870 | SER | 3.3 |
| 1 | A | 1793 | PRO | 3.3 |
| 1 | B | 1874 | ASP | 3.3 |
| 1 | C | 1765 | SER | 3.3 |
| 2 | H | 1953 | VAL | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 1854 | ASN | 3.3 |
| 2 | H | 1671 | SER | 3.3 |
| 1 | A | 1850 | GLU | 3.3 |
| 2 | I | 1928 | GLN | 3.3 |
| 1 | A | 1831 | GLY | 3.3 |
| 1 | B | 540 | GLN | 3.2 |
| 1 | A | 1770 | GLY | 3.2 |
| 1 | B | 976 | ALA | 3.2 |
| 1 | C | 1816 | LYS | 3.1 |
| 1 | B | 1837 | ILE | 3.0 |
| 1 | A | 1884 | SER | 3.0 |
| 2 | H | 1959 | LYS | 3.0 |
| 1 | B | 1875 | ASP | 3.0 |
| 1 | C | 1793 | PRO | 2.9 |
| 1 | B | 1829 | GLY | 2.9 |
| 1 | B | 1868 | LYS | 2.9 |
| 1 | A | 1883 | VAL | 2.9 |
| 1 | C | 1843 | ASN | 2.9 |
| 2 | H | 1964 | PHE | 2.9 |
| 1 | A | 1873 | HIS | 2.9 |
| 1 | A | 540 | GLN | 2.9 |
| 1 | C | 1875 | ASP | 2.9 |
| 1 | C | 141 | ALA | 2.8 |
| 1 | B | 1836 | ASP | 2.8 |
| 1 | C | 204 | THR | 2.8 |
| 1 | C | 1820 | PHE | 2.7 |
| 1 | B | 1802 | GLN | 2.7 |
| 1 | B | 1883 | VAL | 2.7 |
| 2 | H | 1956 | ARG | 2.7 |
| 1 | C | 202 | GLU | 2.7 |
| 1 | C | 1771 | VAL | 2.7 |
| 1 | B | 219 | GLY | 2.7 |
| 1 | B | 1804 | SER | 2.7 |
| 1 | B | 1850 | GLU | 2.7 |
| 1 | B | 1826 | LYS | 2.7 |
| 1 | B | 1784 | ASP | 2.6 |
| 2 | I | 401 | GLY | 2.6 |
| 1 | A | 1780 | ASN | 2.6 |
| 1 | A | 1476 | GLU | 2.6 |
| 1 | C | 1841 | ARG | 2.6 |
| 1 | B | 600 | ASP | 2.5 |
| 1 | C | 215 | ASP | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 1770 | GLY | 2.5 |
| 1 | C | 539 | SER | 2.5 |
| 1 | A | 1860 | GLU | 2.5 |
| 1 | C | 164 | ASP | 2.5 |
| 1 | C | 1800 | SER | 2.4 |
| 2 | I | 43 | GLU | 2.4 |
| 1 | C | 1840 | VAL | 2.4 |
| 1 | A | 1748 | ASN | 2.4 |
| 1 | C | 203 | GLU | 2.4 |
| 1 | A | 1868 | LYS | 2.4 |
| 1 | C | 1829 | GLY | 2.4 |
| 1 | C | 1812 | THR | 2.4 |
| 2 | H | 2033 | THR | 2.3 |
| 1 | C | 1828 | LEU | 2.3 |
| 1 | C | 1822 | SER | 2.3 |
| 1 | C | 1789 | ARG | 2.3 |
| 1 | C | 1768 | GLY | 2.3 |
| 1 | C | 223 | LYS | 2.3 |
| 1 | B | 195 | GLY | 2.3 |
| 2 | H | 1853 | GLY | 2.3 |
| 2 | I | 1880 | LYS | 2.3 |
| 1 | C | 301 | ASP | 2.3 |
| 1 | A | 1792 | THR | 2.3 |
| 1 | A | 1842 | VAL | 2.3 |
| 1 | A | 1844 | LYS | 2.3 |
| 1 | A | 1885 | THR | 2.2 |
| 1 | A | 1828 | LEU | 2.2 |
| 1 | A | 1874 | ASP | 2.2 |
| 1 | A | 973 | ALA | 2.2 |
| 1 | A | 1838 | GLU | 2.2 |
| 1 | B | 1801 | ALA | 2.2 |
| 1 | C | 1867 | VAL | 2.2 |
| 1 | A | 1782 | GLU | 2.2 |
| 1 | C | 971 | ASN | 2.2 |
| 1 | A | 1836 | ASP | 2.2 |
| 1 | C | 1805 | VAL | 2.2 |
| 1 | C | 1782 | GLU | 2.2 |
| 2 | I | 75 | SER | 2.2 |
| 1 | B | 1831 | GLY | 2.1 |
| 1 | B | 1803 | PRO | 2.1 |
| 1 | C | 1845 | ASN | 2.1 |
| 1 | A | 293 | LYS | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | I | 74 | PRO | 2.1 |
| 1 | C | 1811 | GLY | 2.1 |
| 1 | B | 1886 | LYS | 2.1 |
| 1 | A | 981 | GLU | 2.1 |
| 2 | H | 1739 | GLU | 2.1 |
| 2 | H | 1740 | THR | 2.1 |
| 1 | A | 199 | GLU | 2.1 |
| 1 | C | 1886 | LYS | 2.1 |
| 1 | A | 1872 | SER | 2.0 |
| 1 | C | 1796 | ILE | 2.0 |
| 1 | C | 1802 | GLN | 2.0 |
| 1 | A | 976 | ALA | 2.0 |
| 1 | C | 1885 | THR | 2.0 |
| 1 | B | 1810 | ALA | 2.0 |
| 2 | G | 333 | GLY | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 3 | CER | C | 2748 | 12/16 | 0.90 | 0.34 | 2.51 | 67,131,249,250 | 0 |
| 3 | CER | A | 2748 | 12/16 | 0.84 | 0.30 | 1.87 | 67,131,240,249 | 0 |
| 4 | FMN | H | 3051 | 31/31 | 0.80 | 0.32 | 0.09 | 131,157,181,186 | 0 |
| 4 | FMN | G | 3051 | 31/31 | 0.82 | 0.27 | -0.19 | 135,158,184,203 | 0 |
| 4 | FMN | I | 3051 | 31/31 | 0.82 | 0.26 | -0.23 | 129,161,178,201 | 0 |
| 3 | CER | B | 2748 | 12/16 | 0.91 | 0.20 | -0.50 | 67,131,249,250 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.