# Full wwPDB EM Validation Report ⓘ

Mar 10, 2024 – 11:41 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 6U5W |
| EMDB ID | : | EMD-20658 |
| Title | : | Electron cryomicroscopy structure of C. albicans FAS in the KS-stalled state |
| Authors | : | Lou, J.W.; Mazhab-Jafari, M.T. |
| Deposited on | : | 2019-08-28 |
| Resolution | : | 3.30 Å(reported) |
| Based on initial model | : | 2UV8 |

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

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

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

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

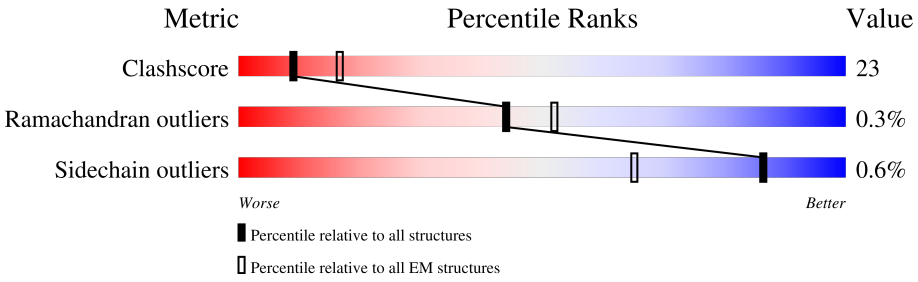
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev70 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1722 | 21% 51% 32% • 17% |
| 2 | B | 2037 | 51% 54% 45% |

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 | NAP | A | 1901 | - | - | X | - |
| 3 | NAP | B | 2102 | - | - | X | - |
| 4 | FMN | B | 2101 | - | - | X | - |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27482 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | A | 1435 | 11309 | 7178 | 1895 | 2190 | 46 | 0 | 0 |

There are 173 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | ? | - | ILE | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |
| A | ? | - | VAL | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | ASN | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | ILE | deletion | UNP P43098 |
| A | ? | - | HIS | deletion | UNP P43098 |
| A | ? | - | VAL | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | VAL | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | GLN | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | VAL | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | ? | - | MET | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | ILE | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | VAL | deletion | UNP P43098 |
| A | ? | - | ASN | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | VAL | deletion | UNP P43098 |
| A | ? | - | GLN | deletion | UNP P43098 |
| A | ? | - | ASN | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | ILE | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | PHE | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | GLN | deletion | UNP P43098 |
| A | ? | - | PHE | deletion | UNP P43098 |
| A | ? | - | GLN | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | PHE | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | GLN | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | ILE | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | ARG | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | MET | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | MET | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | PHE | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | ILE | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | ARG | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | TYR | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | ARG | deletion | UNP P43098 |
| A | ? | - | PHE | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | ARG | deletion | UNP P43098 |
| A | ? | - | GLN | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | VAL | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | MET | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | ASN | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | PRO | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | ASN | deletion | UNP P43098 |
| A | ? | - | ARG | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | GLU | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |
| A | ? | - | THR | deletion | UNP P43098 |
| A | ? | - | PHE | deletion | UNP P43098 |
| A | ? | - | PHE | deletion | UNP P43098 |
| A | ? | - | ASP | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | ILE | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | GLN | deletion | UNP P43098 |
| A | ? | - | LYS | deletion | UNP P43098 |

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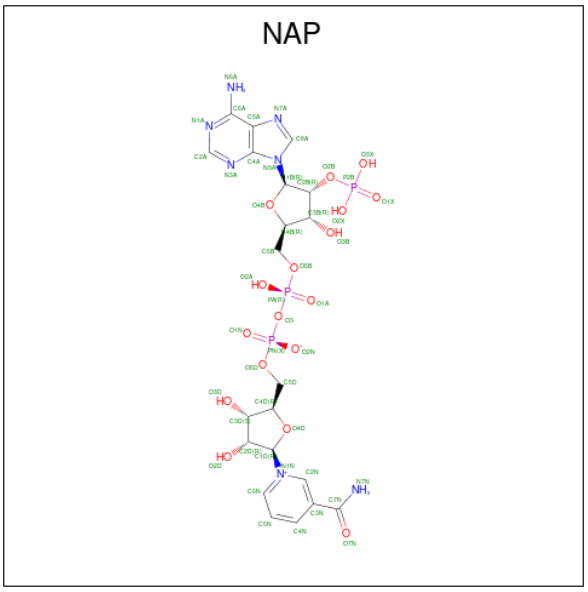
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | ? | - | TYR | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | ALA | deletion | UNP P43098 |
| A | ? | - | GLY | deletion | UNP P43098 |
| A | ? | - | ILE | deletion | UNP P43098 |
| A | ? | - | SER | deletion | UNP P43098 |
| A | ? | - | LEU | deletion | UNP P43098 |
| A | 350 | VAL | SER | conflict | UNP P43098 |
| A | 351 | ASP | ARG | conflict | UNP P43098 |
| A | 353 | ASN | LYS | conflict | UNP P43098 |
| A | 354 | LYS | GLN | conflict | UNP P43098 |
| A | 356 | ALA | LEU | conflict | UNP P43098 |
| A | 813 | THR | PRO | conflict | UNP P43098 |
| A | 1066 | LYS | GLN | conflict | UNP P43098 |
| A | 1123 | VAL | ILE | conflict | UNP P43098 |
| A | 1444 | GLU | LYS | conflict | UNP P43098 |
| A | 1742 | SER | ASN | conflict | UNP P43098 |

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

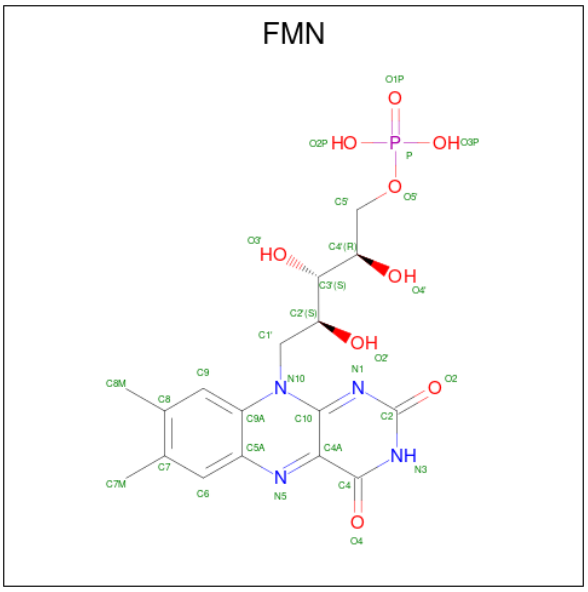
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 2033 | Total | C | N | O | S | 0 | 0 |
| | | | 16046 | 10286 | 2662 | 3044 | 54 | | |

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 3 | A | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |
| 3 | B | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



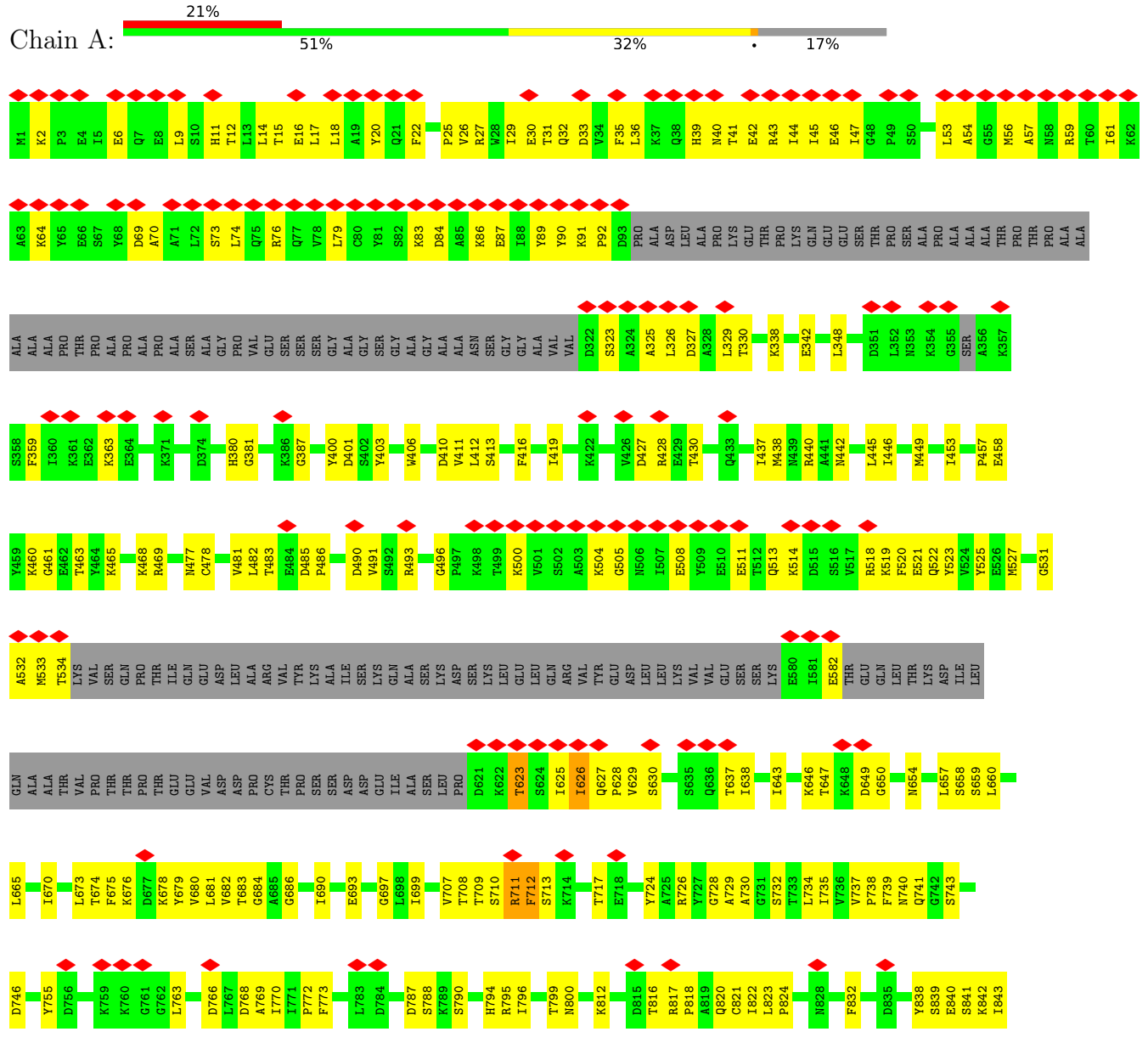

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 4 | B | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

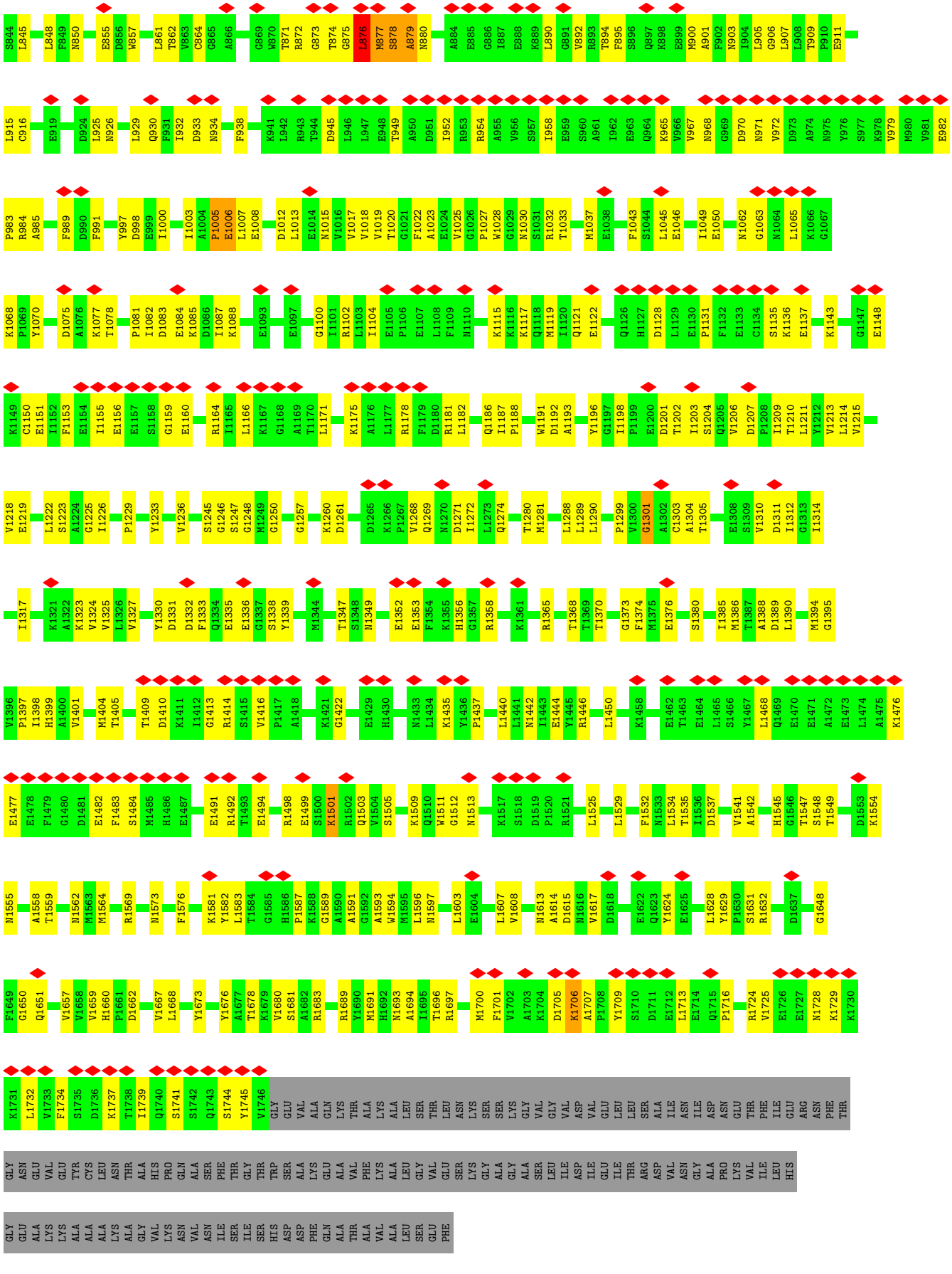
# 3 Residue-property plots (i)

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

- Molecule 1: Fatty acid synthase subunit alpha

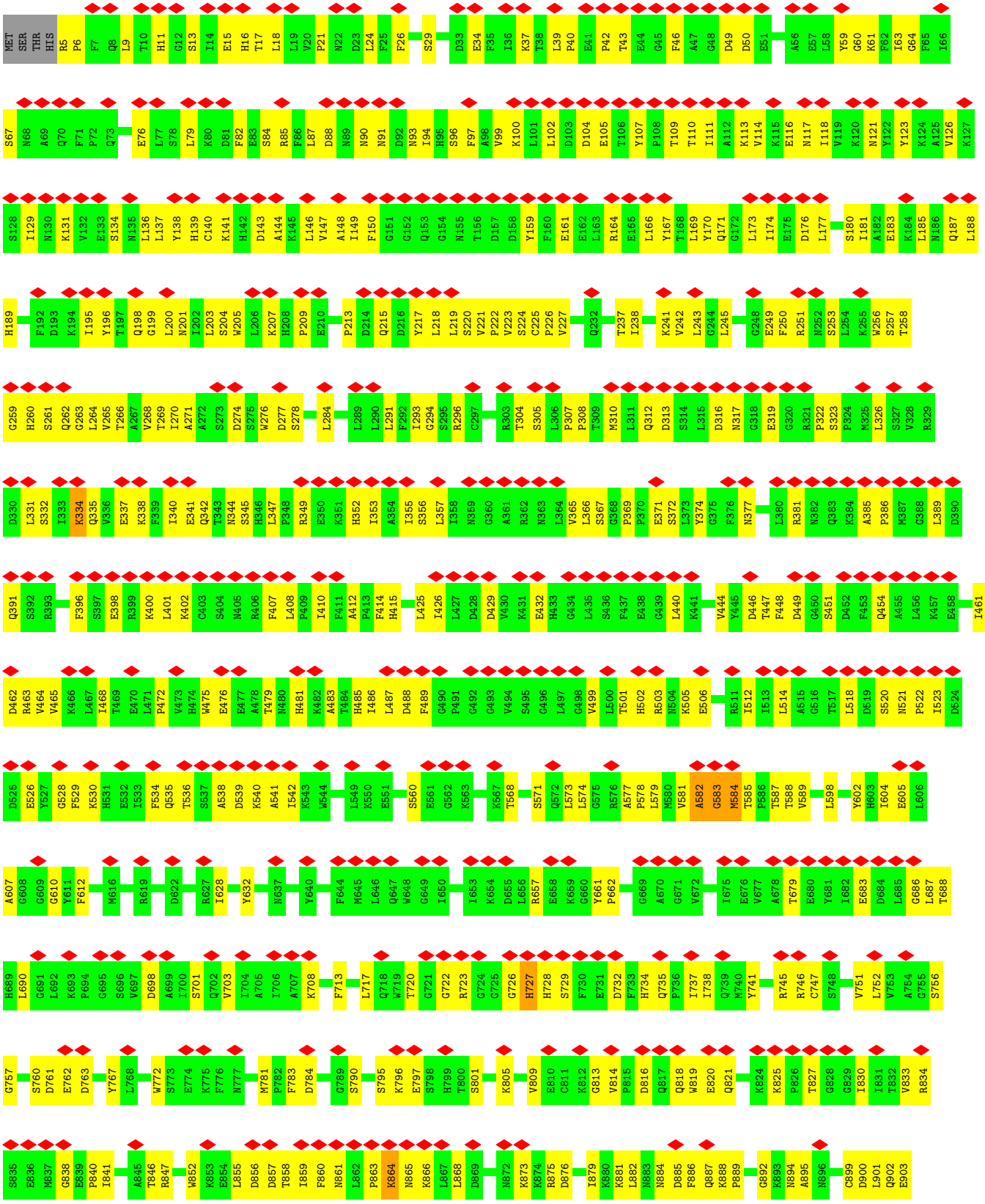
Chain A:

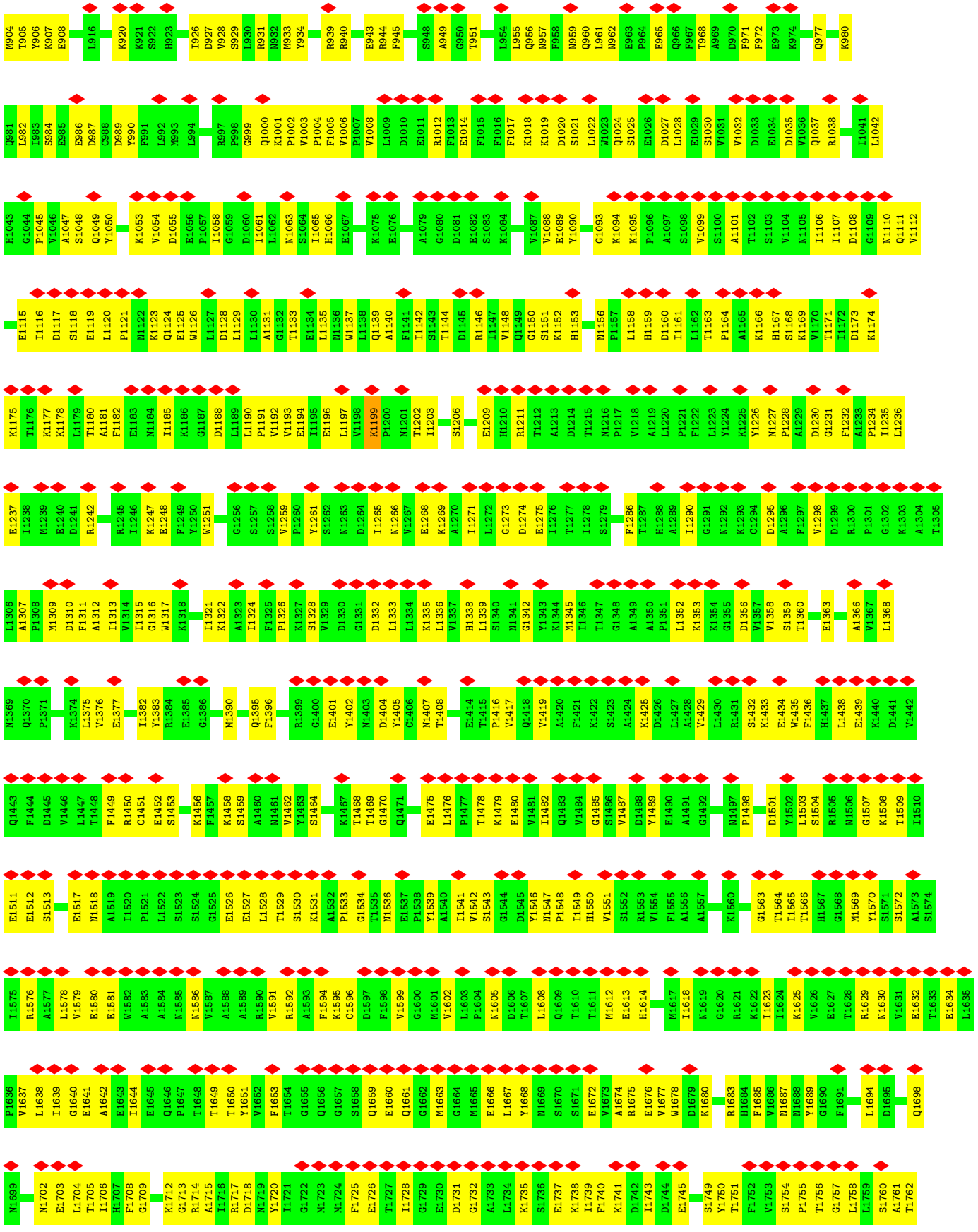


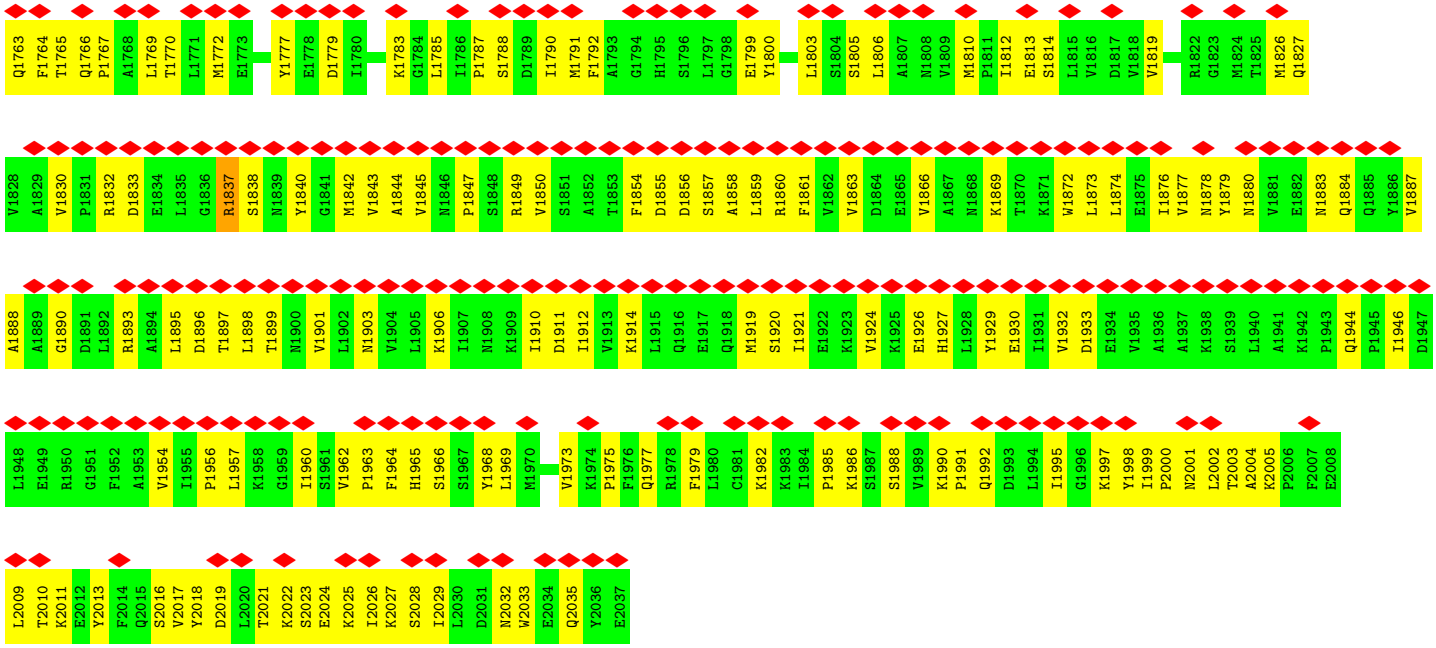

S844 L845 L848 F849 N850 E855 D856 W857 L861 T862 V863 C864 G865 A866 G869 W870 T871 R872 G873 T874 G875 L876 M877 S878 A879 N880 A884 E885 G886 I887 E888 K889 L890 G891 V892 R893 T894 F895 S896 Q897 K898 E899 M900 A901 F902 N903 I904 L905 G906 L907 L908 T909 P910 E911
L915 C916 E919 D924 L925 N926 L929 Q930 F931 I932 D933 N934 F938 K941 L942 R943 T944 D945 L946 L947 E948 T949 A950 D951 I952 R953 R954 A955 V956 S957 I958 E959 S960 A961 I962 E963 Q964 K965 V966 Y967 N968 G969 D970 N971 V972 D973 A974 N975 Y976 S977 K978 V979 M980 V981 E982
P983 R984 A985 F989 D990 F991 Y997 D998 E999 I1000 I1003 A1004 P1005 E1006 L1007 E1008 D1012 L1013 E1014 N1015 V1016 V1017 V1018 V1019 T1020 G1021 F1022 A1023 E1024 V1025 G1026 P1027 W1028 G1029 N1030 S1031 R1032 T1033 M1037 E1038 F1043 S1044 L1045 E1046 I1049 E1050 N1062 G1063 N1064 L1065 K1066 G1067
K1068 P1069 Y1070 D1075 A1076 K1077 T1078 P1081 I1082 D1083 E1084 K1085 D1086 I1087 K1088 E1093 E1097 G1100 I1101 R1102 L1103 I1104 E1105 P1106 E1107 L1108 F1109 N1110 K1115 K1116 K1117 Q1118 M1119 I1120 Q1121 E1122 Q1126 H1127 D1128 L1129 E1130 P1131 F1132 E1133 C1134 S1135 K1136 E1137 K1143 G1147 E1148
K1149 C1150 E1151 I1152 F1153 E1154 I1155 E1156 E1157 S1158 G1159 E1160 R1164 I1165 L1166 K1167 G1168 A1169 T1170 L1171 K1175 A1176 L1177 R1178 F1179 D1180 R1181 L1182 Q1186 I1187 P1188 W1191 D1192 A1193 Y1196 G1197 I1198 P1199 E1200 D1201 T1202 I1203 S1204 Q1205 V1206 D1207 P1208 I1209 T1210 L1211 Y1212 V1213 L1214 V1215
V1218 E1219 L1222 S1223 A1224 G1225 I1226 P1229 Y1233 V1236 S1245 G1246 S1247 G1248 M1249 G1250 G1257 K1260 D1261 D1265 K1266 P1267 V1268 Q1269 N1270 D1271 I1272 L1273 Q1274 T1280 M1281 L1288 L1289 L1290 P1299 V1300 G1301 A1302 C1303 A1304 T1305 E1308 S1309 V1310 D1311 I1312 G1313 I1314
I1317 K1321 A1322 K1323 V1324 V1325 L1326 V1327 Y1330 D1331 D1332 F1333 Q1334 E1335 E1336 G1337 S1338 Y1339 M1344 T1347 S1348 N1349 E1352 E1353 F1354 K1355 H1356 G1357 R1358 K1361 R1365 T1368 T1369 T1370 G1373 F1374 M1375 E1376 S1380 I1385 M1386 T1387 A1388 D1389 L1390 M1394 G1395
V1396 P1397 I1398 H1399 A1400 V1401 M1404 T1405 T1409 D1410 K1411 I1412 G1413 R1414 S1415 V1416 P1417 A1418 K1421 G1422 E1429 H1430 N1433 L1434 K1435 Y1436 P1437 L1440 L1441 N1442 I1443 E1444 Y1445 R1446 L1450 K1458 E1462 T1463 E1464 L1465 S1466 Y1467 L1468 Q1469 E1470 E1471 A1472 E1473 L1474 A1475 K1476
E1477 E1478 F1479 G1480 D1481 E1482 F1483 S1484 M1485 H1486 E1487 E1491 R1492 T1493 E1494 R1498 E1499 S1500 K1501 R1502 Q1503 V1504 S1505 K1509 Q1510 W1511 G1512 N1513 K1517 S1518 D1519 P1520 R1521 L1525 L1529 F1532 N1533 L1534 T1535 I1536 D1537 V1541 A1542 H1545 G1546 T1547 S1548 T1549 D1553 K1554
N1555 A1558 T1559 N1562 M1563 M1564 R1569 N1573 F1576 K1581 Y1582 L1583 T1584 G1585 H1586 P1587 K1588 G1589 A1590 A1591 G1592 A1593 W1594 M1595 L1596 N1597 L1603 E1604 L1607 V1608 N1613 A1614 D1615 N1616 V1617 D1618 E1622 Q1623 Y1624 E1625 L1628 Y1629 P1630 S1631 R1632 D1637 G1648
F1649 G1650 Q1651 V1657 V1658 V1659 H1660 P1661 D1662 V1667 L1668 Y1673 Y1676 A1677 T1678 K1679 V1680 S1681 A1682 R1683 R1689 Y1690 M1691 H1692 N1693 A1694 I1695 T1696 R1697 M1700 F1701 V1702 A1703 K1704 D1705 K1706 A1707 P1708 Y1709 S1710 D1711 E1712 L1713 E1714 Q1715 P1716 R1724 V1725 E1726 E1727 N1728 K1729 K1730
K1731 L1732 V1733 F1734 S1735 D1736 K1737 T1738 I1739 Q1740 S1741 S1742 Q1743 S1744 Y1745 V1746 GLY GLU VAL ALA GLN LYS THR ALA LYS ALA LEU SER THR LEU ASN LYS SER SER LYS GLY VAL GLY VAL ASP VAL GLU LEU LEU SER ALA ILE ASN ILE ASP ASN GLU THR PHE ILE GLU ARG ASN PHE THR
GLY ASN GLU VAL GLU TYR CYS LEU ASN THR ALA HIS PRO GLN ALA SER PHE THR GLY THR TRP SER ALA LYS GLU ALA VAL PHE LYS ALA LEU GLY VAL GLU SER LYS GLY ALA GLY ALA SER LEU ILE ASP ILE GLU THR ARG ASP VAL ASN GLY ALA PRO LYS VAL ILE LEU HIS
GLY GLU ALA LYS LYS ALA ALA GLY VAL LYS ASN VAL ASN ILE SER ILE SER HIS ASP ASP PHE GLN ALA THR ALA VAL ALA LEU SER GLU PHE

• Molecule 2: Fatty acid synthase subunit beta

Chain B:


M904 T905 Y906 K907 E908 L916 K920 K921 S922 H923 I926 D927 V928 S929 L930 R931 N932 M933 Y934 R939 R940 E943 R944 F945 S948 A949 G950 T951 L954 L955 Q956 N957 F958 N959 Q960 L961 N962 E963 P964 E965 Q966 F967 T968 A969 D970 F971 F972 E973 K974 Q977 K980
Q981 L982 I983 S984 E985 E986 D987 C988 D989 Y990 F991 L992 M993 L994 R997 P998 G999 Q1000 K1001 P1002 V1003 P1004 F1005 V1006 P1007 V1008 L1009 D1010 E1011 R1012 F1013 E1014 F1015 F1016 F1017 K1018 K1019 D1020 S1021 L1022 W1023 Q1024 S1025 E1026 D1027 L1028 E1029 S1030 V1031 V1032 D1033 E1034 D1035 V1036 Q1037 R1038 I1041 L1042
H1043 G1044 P1045 V1046 A1047 S1048 Q1049 Y1050 K1053 V1054 D1055 E1056 P1057 I1058 G1059 D1060 I1061 L1062 N1063 S1064 I1065 H1066 E1067 K1075 E1076 A1079 G1080 D1081 E1082 S1083 K1084 V1087 V1088 E1089 Y1090 G1093 K1094 K1095 P1096 A1097 S1098 V1099 S1100 A1101 T1102 S1103 V1104 N1105 I1106 I1107 D1108 G1109 N1110 Q1111 V1112
E1115 I1116 D1117 S1118 E1119 L1120 P1121 N1122 K1123 Q1124 E1125 W1126 L1127 D1128 L1129 L1130 A1131 G1132 T1133 E1134 L1135 N1136 W1137 L1138 Q1139 A1140 F1141 I1142 S1143 T1144 D1145 R1146 I1147 V1148 Q1149 G1150 S1151 K1152 H1153 N1156 P1157 L1158 H1159 D1160 I1161 L1162 T1163 P1164 A1165 K1166 H1167 S1168 K1169 V1170 T1171 I1172 D1173 K1174
K1175 T1176 K1177 K1178 L1179 T1180 A1181 F1182 E1183 N1184 I1185 K1186 G1187 D1188 L1189 L1190 P1191 V1192 V1193 E1194 I1195 E1196 L1197 V1198 K1199 P1200 N1201 T1202 I1203 S1206 E1209 H1210 R1211 T1212 A1213 D1214 T1215 N1216 P1217 V1218 A1219 L1220 P1221 F1222 L1223 Y1224 K1225 Y1226 N1227 P1228 A1229 D1230 G1231 F1232 A1233 P1234 I1235 L1236
E1237 T1238 M1239 E1240 D1241 R1242 R1245 I1246 K1247 E1248 F1249 Y1250 W1251 G1256 S1257 S1258 V1259 P1260 Y1261 S1262 N1263 D1264 I1265 N1266 V1267 E1268 K1269 A1270 I1271 L1272 G1273 D1274 E1275 T1276 T1277 I1278 S1279 F1286 T1287 H1288 A1289 I1290 G1291 N1292 K1293 C1294 D1295 A1296 F1297 V1298 D1299 R1300 P1301 G1302 K1303 A1304 T1305
L1306 A1307 P1308 M1309 D1310 F1311 A1312 I1313 V1314 I1315 G1316 W1317 K1318 I1321 K1322 A1323 I1324 F1325 P1326 K1327 S1328 V1329 D1330 G1331 D1332 L1333 L1334 K1335 L1336 V1337 H1338 L1339 S1340 N1341 G1342 Y1343 K1344 M1345 I1346 T1347 G1348 A1349 A1350 P1351 L1352 K1353 K1354 G1355 D1356 V1357 V1358 S1359 T1360 E1363 A1366 V1367 L1368
N1369 Q1370 P1371 K1374 L1375 V1376 E1377 I1382 Y1383 R1384 E1385 G1386 M1390 Q1395 F1396 R1399 G1400 E1401 Y1402 N1403 D1404 Y1405 C1406 N1407 T1408 E1414 T1415 P1416 V1417 Q1418 V1419 A1420 F1421 K1422 S1423 A1424 K1425 D1426 L1427 A1428 V1429 L1430 R1431 S1432 K1433 E1434 W1435 F1436 H1437 L1438 E1439 K1440 D1441 V1442
Q1443 F1444 D1445 V1446 L1447 T1448 F1449 R1450 C1451 E1452 S1453 K1456 F1457 K1458 S1459 A1460 N1461 V1462 Y1463 S1464 K1467 T1468 T1469 G1470 Q1471 E1475 L1476 P1477 T1478 K1479 E1480 V1481 I1482 Q1483 V1484 G1485 S1486 V1487 D1488 Y1489 E1490 A1491 G1492 N1497 P1498 D1501 Y1502 L1503 S1504 R1505 N1506 G1507 K1508 T1509 I1510
E1511 E1512 S1513 E1517 N1518 A1519 I1520 P1521 L1522 S1523 S1524 G1525 E1526 E1527 L1528 T1529 S1530 K1531 A1532 P1533 G1534 T1535 N1536 E1537 P1538 Y1539 A1540 I1541 V1542 S1543 G1544 D1545 Y1546 N1547 P1548 I1549 H1550 V1551 S1552 R1553 V1554 F1555 A1556 A1557 K1560 G1563 T1564 I1565 T1566 H1567 G1568 M1569 Y1570 S1571 S1572 A1573 S1574
I1575 R1576 A1577 L1578 V1579 E1580 E1581 W1582 A1583 A1584 N1585 N1586 V1587 A1588 A1589 R1590 V1591 R1592 A1593 F1594 K1595 C1596 D1597 F1598 V1599 G1600 M1601 V1602 L1603 P1604 N1605 D1606 T1607 L1608 Q1609 T1610 T1611 M1612 E1613 H1614 M1617 I1618 N1619 G1620 R1621 K1622 I1623 I1624 K1625 V1626 E1627 T1628 R1629 N1630 V1631 E1632 T1633 E1634 L1635
P1636 V1637 L1638 I1639 G1640 E1641 A1642 E1643 I1644 E1645 Q1646 P1647 T1648 T1649 T1650 Y1651 V1652 F1653 T1654 G1655 Q1656 G1657 S1658 Q1659 E1660 Q1661 G1662 M1663 G1664 M1665 E1666 L1667 Y1668 N1669 S1670 S1671 E1672 V1673 A1674 R1675 E1676 V1677 W1678 D1679 K1680 R1683 H1684 F1685 V1686 N1687 N1688 Y1689 G1690 F1691 L1694 D1695 Q1698
N1699 N1702 E1703 L1704 T1705 I1706 H1707 F1708 G1709 K1712 G1713 R1714 A1715 I1716 R1717 D1718 N1719 Y1720 I1721 G1722 M1723 M1724 F1725 E1726 T1727 I1728 G1729 E1730 D1731 G1732 A1733 L1734 K1735 S1736 E1737 K1738 I1739 F1740 K1741 D1742 I1743 D1744 E1745 S1749 Y1750 T1751 F1752 V1753 S1754 P1755 T1756 G1757 L1758 L1759 S1760 A1761 T1762


Q1763 F1764 T1765 Q1766 P1767 A1768 L1769 T1770 L1771 M1772 E1773
Y1777 E1778 D1779 I1780
K1783 G1784 L1785 I1786 P1787 S1788 D1789 I1790 M1791 F1792 A1793 G1794 H1795 S1796 L1797 G1798 E1799 Y1800
L1803 S1804 S1805 L1806 A1807 N1808 V1809 M1810 P1811 I1812 E1813 S1814 L1815 V1816 D1817 V1818 V1819
R1822 G1823 M1824 T1825 M1826 Q1827
V1828 A1829 V1830 P1831 R1832 D1833 E1834 L1835 G1836 R1837 S1838 N1839 Y1840 G1841 M1842 V1843 A1844 V1845 N1846 P1847 S1848 R1849 V1850 S1851 A1852 T1853 F1854 D1855 D1856 S1857 A1858 L1859 R1860 F1861 V1862 V1863 D1864 E1865 V1866 A1867 N1868 K1869 T1870 K1871 W1872 L1873 L1874 E1875 I1876 V1877 N1878 Y1879 N1880 V1881 E1882 N1883 Q1884 Q1885 Y1886 V1887
A1888 A1889 G1890 D1891 L1892 R1893 A1894 L1895 D1896 T1897 L1898 T1899 N1900 V1901 L1902 N1903 V1904 L1905 K1906 I1907 N1908 K1909 I1910 D1911 I1912 V1913 K1914 L1915 Q1916 E1917 Q1918 M1919 S1920 I1921 E1922 K1923 V1924 K1925 E1926 H1927 L1928 Y1929 E1930 I1931 V1932 D1933 E1934 V1935 A1936 A1937 K1938 S1939 L1940 A1941 K1942 P1943 Q1944 P1945 I1946 D1947
L1948 E1949 R1950 G1951 F1952 A1953 V1954 I1955 P1956 L1957 K1958 G1959 I1960 S1961 V1962 P1963 F1964 H1965 S1966 S1967 Y1968 L1969 M1970
V1973 K1974 P1975 F1976 Q1977 R1978 F1979 L1980 C1981 K1982 K1983 I1984 P1985 K1986 S1987 S1988 V1989 K1990 P1991 Q1992 D1993 L1994 I1995 G1996 K1997 Y1998 I1999 P2000 N2001 L2002 T2003 A2004 K2005 P2006 F2007 E2008
L2009 T2010 K2011 E2012 Y2013 F2014 Q2015 S2016 V2017 Y2018 D2019 L2020 T2021 K2022 S2023 E2024 K2025 I2026 K2027 S2028 I2029 L2030 D2031 N2032 W2033 E2034 Q2035 Y2036 E2037

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, D3 | Depositor |
| Number of particles used | 24417 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE; CTFFIND4 within cryoSPARC2 | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 43 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 1.942 | Depositor |
| Minimum map value | -0.817 | Depositor |
| Average map value | 0.012 | Depositor |
| Map value standard deviation | 0.133 | Depositor |
| Recommended contour level | 0.704 | Depositor |
| Map size (Å) | 373.12, 373.12, 373.12 | wwPDB |
| Map dimensions | 352, 352, 352 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.06, 1.06, 1.06 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.54 | 0/11536 | 0.52 | 0/15595 |
| 2 | B | 0.42 | 0/16415 | 0.49 | 1/22269 (0.0%) |
| All | All | 0.47 | 0/27951 | 0.50 | 1/37864 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 2004 | ALA | C-N-CA | -5.59 | 107.73 | 121.70 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 1301 | GLY | Peptide |

## 5.2 Too-close contacts

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 | 11309 | 0 | 11219 | 475 | 0 |
| 2 | B | 16046 | 0 | 16024 | 829 | 0 |
| 3 | A | 48 | 0 | 25 | 34 | 0 |
| 3 | B | 48 | 0 | 25 | 50 | 0 |
| 4 | B | 31 | 0 | 17 | 51 | 0 |
| All | All | 27482 | 0 | 27310 | 1265 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1265) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:584:MET:HE2 | 4:B:2101:FMN:C7 | 1.26 | 1.61 |
| 2:B:584:MET:HB3 | 4:B:2101:FMN:C5A | 1.29 | 1.61 |
| 1:A:712:PHE:CE1 | 1:A:717:THR:HG22 | 1.35 | 1.58 |
| 2:B:727:HIS:ND1 | 3:B:2102:NAP:C4N | 1.79 | 1.45 |
| 2:B:727:HIS:ND1 | 3:B:2102:NAP:C3N | 1.73 | 1.44 |
| 2:B:727:HIS:CE1 | 3:B:2102:NAP:C6N | 2.02 | 1.40 |
| 1:A:712:PHE:CE1 | 1:A:717:THR:CG2 | 2.08 | 1.36 |
| 2:B:727:HIS:CE1 | 3:B:2102:NAP:N1N | 1.90 | 1.36 |
| 2:B:584:MET:HE3 | 4:B:2101:FMN:C9A | 1.56 | 1.34 |
| 2:B:584:MET:HE2 | 4:B:2101:FMN:C6 | 1.57 | 1.33 |
| 1:A:710:SER:OG | 3:A:1901:NAP:C4A | 1.76 | 1.30 |
| 2:B:584:MET:CE | 4:B:2101:FMN:C8 | 2.10 | 1.30 |
| 2:B:584:MET:CB | 4:B:2101:FMN:C5A | 2.13 | 1.27 |
| 2:B:612:PHE:CE2 | 3:B:2102:NAP:N7A | 2.02 | 1.25 |
| 2:B:584:MET:CE | 4:B:2101:FMN:C9 | 2.13 | 1.24 |
| 1:A:877:MET:HE3 | 3:A:1901:NAP:O7N | 1.32 | 1.24 |
| 2:B:727:HIS:CE1 | 3:B:2102:NAP:C2N | 2.20 | 1.23 |
| 2:B:584:MET:HE2 | 4:B:2101:FMN:C8 | 1.67 | 1.22 |
| 2:B:999:GLY:O | 3:B:2102:NAP:H2A | 1.40 | 1.19 |
| 2:B:584:MET:CB | 4:B:2101:FMN:C6 | 2.20 | 1.19 |
| 1:A:877:MET:CE | 3:A:1901:NAP:O7N | 1.90 | 1.18 |
| 2:B:756:SER:HA | 4:B:2101:FMN:C5' | 1.73 | 1.17 |
| 2:B:584:MET:CE | 4:B:2101:FMN:C7 | 2.20 | 1.17 |
| 2:B:727:HIS:CG | 3:B:2102:NAP:C2N | 2.18 | 1.15 |
| 2:B:756:SER:HA | 4:B:2101:FMN:O5' | 1.07 | 1.15 |
| 2:B:584:MET:CB | 4:B:2101:FMN:N5 | 2.10 | 1.13 |
| 2:B:584:MET:CE | 4:B:2101:FMN:C9A | 2.26 | 1.12 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:842:LYS:NZ | 3:A:1901:NAP:O2D | 1.83 | 1.11 |
| 2:B:584:MET:HE1 | 4:B:2101:FMN:C8 | 1.82 | 1.09 |
| 2:B:584:MET:HB3 | 4:B:2101:FMN:C6 | 1.82 | 1.07 |
| 2:B:727:HIS:CD2 | 3:B:2102:NAP:C2N | 2.35 | 1.07 |
| 2:B:727:HIS:ND1 | 3:B:2102:NAP:C2N | 2.10 | 1.07 |
| 2:B:999:GLY:C | 3:B:2102:NAP:H2A | 1.75 | 1.06 |
| 2:B:584:MET:CE | 4:B:2101:FMN:C6 | 2.35 | 1.05 |
| 2:B:727:HIS:ND1 | 3:B:2102:NAP:C5N | 2.19 | 1.05 |
| 2:B:727:HIS:H | 3:B:2102:NAP:H4N | 1.14 | 1.05 |
| 2:B:584:MET:HE3 | 4:B:2101:FMN:C5A | 1.86 | 1.05 |
| 2:B:584:MET:HA | 4:B:2101:FMN:N5 | 1.72 | 1.05 |
| 2:B:756:SER:CA | 4:B:2101:FMN:O5' | 2.03 | 1.04 |
| 2:B:584:MET:HE1 | 4:B:2101:FMN:C9 | 1.84 | 1.03 |
| 1:A:773:PHE:O | 3:A:1901:NAP:O3D | 1.77 | 1.02 |
| 2:B:790:SER:CA | 4:B:2101:FMN:HM83 | 1.88 | 1.02 |
| 2:B:584:MET:CE | 4:B:2101:FMN:C5A | 2.37 | 1.01 |
| 2:B:584:MET:CA | 4:B:2101:FMN:N5 | 2.23 | 1.01 |
| 2:B:727:HIS:CE1 | 3:B:2102:NAP:C5N | 2.43 | 1.01 |
| 2:B:584:MET:HB3 | 4:B:2101:FMN:N5 | 1.74 | 1.00 |
| 2:B:584:MET:HB2 | 4:B:2101:FMN:C6 | 1.95 | 0.97 |
| 1:A:712:PHE:CZ | 1:A:717:THR:HG22 | 1.98 | 0.97 |
| 2:B:584:MET:HA | 4:B:2101:FMN:C4A | 1.95 | 0.97 |
| 2:B:727:HIS:HE1 | 3:B:2102:NAP:C6N | 1.65 | 0.94 |
| 1:A:712:PHE:CZ | 1:A:717:THR:CG2 | 2.51 | 0.93 |
| 2:B:790:SER:HB3 | 4:B:2101:FMN:C8M | 1.99 | 0.93 |
| 2:B:727:HIS:H | 3:B:2102:NAP:C4N | 1.84 | 0.91 |
| 2:B:584:MET:HB2 | 4:B:2101:FMN:H6 | 1.49 | 0.90 |
| 2:B:756:SER:CA | 4:B:2101:FMN:C5' | 2.50 | 0.89 |
| 1:A:873:GLY:O | 1:A:878:SER:HB3 | 1.73 | 0.89 |
| 2:B:727:HIS:NE2 | 3:B:2102:NAP:C2N | 2.35 | 0.88 |
| 2:B:87:LEU:HB3 | 2:B:91:ASN:HA | 1.54 | 0.88 |
| 2:B:391:GLN:HE22 | 2:B:400:LYS:H | 1.17 | 0.88 |
| 2:B:727:HIS:CE1 | 3:B:2102:NAP:H2D | 2.09 | 0.88 |
| 2:B:582:ALA:O | 2:B:605:GLU:HG2 | 1.74 | 0.87 |
| 2:B:727:HIS:N | 3:B:2102:NAP:H4N | 1.88 | 0.87 |
| 2:B:999:GLY:O | 3:B:2102:NAP:C2A | 2.22 | 0.87 |
| 1:A:873:GLY:O | 1:A:878:SER:CB | 2.22 | 0.87 |
| 1:A:712:PHE:CD2 | 1:A:738:PRO:HG3 | 2.11 | 0.86 |
| 1:A:710:SER:OG | 3:A:1901:NAP:C5A | 2.22 | 0.86 |
| 2:B:612:PHE:CE2 | 3:B:2102:NAP:C5A | 2.58 | 0.86 |
| 2:B:727:HIS:HA | 2:B:841:ILE:HD13 | 1.57 | 0.86 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1303:CYS:HB2 | 1:A:1648:GLY:HA2 | 1.58 | 0.85 |
| 1:A:741:GLN:O | 1:A:800:ASN:ND2 | 2.08 | 0.85 |
| 1:A:877:MET:CE | 3:A:1901:NAP:C7N | 2.54 | 0.85 |
| 2:B:1720:TYR:O | 2:B:1738:LYS:NZ | 2.09 | 0.85 |
| 2:B:612:PHE:HE2 | 3:B:2102:NAP:N7A | 1.75 | 0.85 |
| 2:B:727:HIS:HE2 | 3:B:2102:NAP:C2D | 1.89 | 0.85 |
| 1:A:1299:PRO:HG3 | 1:A:1312:ILE:HD12 | 1.60 | 0.84 |
| 1:A:710:SER:OG | 3:A:1901:NAP:N3A | 2.08 | 0.84 |
| 1:A:878:SER:O | 1:A:880:ASN:N | 2.10 | 0.83 |
| 2:B:581:VAL:O | 2:B:582:ALA:O | 1.97 | 0.83 |
| 2:B:727:HIS:NE2 | 3:B:2102:NAP:C2D | 2.42 | 0.83 |
| 2:B:790:SER:HA | 4:B:2101:FMN:HM83 | 1.59 | 0.83 |
| 1:A:1131:PRO:HG3 | 1:A:1164:ARG:HE | 1.44 | 0.82 |
| 1:A:36:LEU:O | 1:A:76:ARG:NH2 | 2.13 | 0.82 |
| 1:A:686:GLY:HA3 | 3:A:1901:NAP:O3B | 1.78 | 0.82 |
| 2:B:612:PHE:CD2 | 3:B:2102:NAP:C5A | 2.63 | 0.82 |
| 2:B:790:SER:CB | 4:B:2101:FMN:C8M | 2.58 | 0.82 |
| 2:B:727:HIS:N | 3:B:2102:NAP:O7N | 1.98 | 0.82 |
| 2:B:347:LEU:O | 2:B:349:ARG:NH1 | 2.13 | 0.81 |
| 1:A:626:ILE:HD12 | 1:A:626:ILE:O | 1.81 | 0.81 |
| 1:A:43:ARG:HB2 | 2:B:1649:THR:HG22 | 1.60 | 0.81 |
| 2:B:727:HIS:NE2 | 3:B:2102:NAP:H2D | 1.97 | 0.80 |
| 1:A:26:VAL:HG23 | 2:B:2001:ASN:HB3 | 1.64 | 0.80 |
| 1:A:842:LYS:NZ | 3:A:1901:NAP:HO2N | 1.79 | 0.79 |
| 2:B:999:GLY:C | 3:B:2102:NAP:C2A | 2.50 | 0.79 |
| 2:B:894:ASN:ND2 | 2:B:903:GLU:O | 2.15 | 0.79 |
| 2:B:585:THR:N | 4:B:2101:FMN:O4 | 2.16 | 0.78 |
| 2:B:1121:PRO:HG2 | 2:B:1126:TRP:HB2 | 1.66 | 0.77 |
| 1:A:795:ARG:HA | 1:A:799:THR:HG22 | 1.66 | 0.77 |
| 1:A:952:ILE:HG22 | 2:B:1425:LYS:HB3 | 1.66 | 0.77 |
| 1:A:1032:ARG:NH1 | 1:A:1050:GLU:OE2 | 2.18 | 0.77 |
| 2:B:984:SER:OG | 2:B:986:GLU:OE1 | 2.02 | 0.76 |
| 2:B:1417:VAL:HA | 2:B:1509:THR:HA | 1.67 | 0.76 |
| 2:B:582:ALA:O | 2:B:605:GLU:CG | 2.33 | 0.75 |
| 2:B:857:ASP:O | 2:B:861:ASN:ND2 | 2.20 | 0.75 |
| 2:B:332:SER:H | 2:B:335:GLN:HE21 | 1.34 | 0.75 |
| 1:A:531:GLY:HA2 | 1:A:534:THR:HA | 1.68 | 0.75 |
| 2:B:790:SER:CB | 4:B:2101:FMN:HM83 | 2.15 | 0.75 |
| 2:B:1020:ASP:N | 3:B:2102:NAP:O1A | 2.19 | 0.75 |
| 2:B:1024:GLN:N | 2:B:1024:GLN:OE1 | 2.21 | 0.74 |
| 1:A:427:ASP:OD1 | 1:A:428:ARG:N | 2.20 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:756:SER:N | 4:B:2101:FMN:O2P | 2.20 | 0.74 |
| 2:B:251:ARG:NH2 | 2:B:274:ASP:OD1 | 2.19 | 0.74 |
| 2:B:727:HIS:NE2 | 3:B:2102:NAP:N1N | 2.31 | 0.74 |
| 2:B:146:LEU:HD22 | 2:B:487:LEU:HD11 | 1.70 | 0.74 |
| 2:B:588:THR:HB | 2:B:607:ALA:HB2 | 1.70 | 0.74 |
| 1:A:876:LEU:HD23 | 3:A:1901:NAP:O2A | 1.87 | 0.74 |
| 2:B:475:TRP:HE1 | 2:B:501:THR:HG22 | 1.54 | 0.73 |
| 1:A:712:PHE:CZ | 1:A:717:THR:HG21 | 2.23 | 0.73 |
| 2:B:1118:SER:HB2 | 2:B:1166:LYS:HB2 | 1.68 | 0.73 |
| 2:B:957:ASN:HD21 | 2:B:959:ASN:HD22 | 1.36 | 0.73 |
| 2:B:920:LYS:HE2 | 2:B:965:GLU:HG2 | 1.70 | 0.73 |
| 2:B:1108:ASP:HB2 | 2:B:1133:THR:HG23 | 1.70 | 0.72 |
| 2:B:847:ARG:NH1 | 2:B:885:ASP:OD1 | 2.21 | 0.72 |
| 2:B:1199:LYS:O | 2:B:1202:THR:OG1 | 2.08 | 0.72 |
| 2:B:1203:ILE:HD11 | 2:B:1226:TYR:HB2 | 1.70 | 0.72 |
| 1:A:712:PHE:HE1 | 1:A:717:THR:HG22 | 0.82 | 0.72 |
| 1:A:876:LEU:N | 3:A:1901:NAP:O1A | 2.21 | 0.72 |
| 1:A:877:MET:HE3 | 3:A:1901:NAP:C7N | 2.18 | 0.71 |
| 2:B:1429:VAL:O | 2:B:1432:SER:OG | 2.07 | 0.71 |
| 1:A:708:THR:HG21 | 1:A:739:PHE:HD2 | 1.55 | 0.71 |
| 2:B:1192:VAL:HG23 | 2:B:1193:VAL:HG23 | 1.71 | 0.71 |
| 2:B:1876:ILE:HA | 2:B:1888:ALA:HA | 1.72 | 0.71 |
| 2:B:727:HIS:CD2 | 3:B:2102:NAP:H2N | 2.24 | 0.71 |
| 2:B:225:CYS:O | 2:B:262:GLN:NE2 | 2.24 | 0.70 |
| 2:B:349:ARG:HA | 2:B:352:HIS:HB2 | 1.72 | 0.70 |
| 2:B:801:SER:HB3 | 2:B:1028:LEU:HD22 | 1.73 | 0.70 |
| 1:A:873:GLY:O | 1:A:878:SER:HB2 | 1.92 | 0.70 |
| 2:B:882:LEU:HD13 | 2:B:1006:VAL:HG11 | 1.74 | 0.70 |
| 2:B:1596:CYS:HA | 2:B:1640:GLY:HA2 | 1.72 | 0.70 |
| 1:A:983:PRO:HD2 | 1:A:1085:LYS:HD2 | 1.73 | 0.70 |
| 2:B:612:PHE:CD2 | 3:B:2102:NAP:C6A | 2.74 | 0.70 |
| 2:B:657:ARG:HH22 | 2:B:1153:HIS:HB2 | 1.56 | 0.70 |
| 2:B:727:HIS:CE1 | 3:B:2102:NAP:C2D | 2.75 | 0.70 |
| 2:B:1158:LEU:HA | 2:B:1161:ILE:HG12 | 1.73 | 0.70 |
| 2:B:1629:ARG:NH2 | 2:B:1634:GLU:OE1 | 2.25 | 0.70 |
| 1:A:27:ARG:HH21 | 2:B:2003:THR:HA | 1.56 | 0.70 |
| 1:A:877:MET:HE2 | 3:A:1901:NAP:C7N | 2.21 | 0.70 |
| 1:A:1446:ARG:NH1 | 1:A:1511:TRP:O | 2.24 | 0.69 |
| 1:A:626:ILE:HG23 | 1:A:627:GLN:N | 2.06 | 0.69 |
| 2:B:1799:GLU:OE2 | 2:B:1998:TYR:OH | 2.10 | 0.69 |
| 1:A:984:ARG:HB2 | 2:B:944:ARG:HA | 1.73 | 0.69 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:673:LEU:HD21 | 1:A:909:THR:HG22 | 1.75 | 0.69 |
| 1:A:710:SER:N | 3:A:1901:NAP:O3X | 2.24 | 0.69 |
| 1:A:712:PHE:HD2 | 1:A:738:PRO:HG3 | 1.56 | 0.69 |
| 1:A:823:LEU:HD21 | 1:A:848:LEU:HD12 | 1.73 | 0.69 |
| 1:A:1476:LYS:NZ | 1:A:1482:GLU:O | 2.26 | 0.69 |
| 2:B:790:SER:N | 4:B:2101:FMN:HM83 | 2.07 | 0.69 |
| 2:B:931:ARG:NH1 | 2:B:962:ASN:OD1 | 2.26 | 0.69 |
| 2:B:1766:GLN:HG3 | 2:B:1819:VAL:HG22 | 1.74 | 0.69 |
| 1:A:787:ASP:O | 1:A:790:SER:OG | 2.10 | 0.69 |
| 1:A:874:THR:O | 1:A:876:LEU:HD12 | 1.93 | 0.69 |
| 1:A:1450:LEU:HD13 | 1:A:1511:TRP:HB2 | 1.73 | 0.69 |
| 2:B:1003:VAL:HG12 | 2:B:1005:PHE:H | 1.58 | 0.69 |
| 2:B:1110:ASN:OD1 | 2:B:1175:LYS:N | 2.26 | 0.69 |
| 1:A:457:PRO:HB2 | 1:A:460:LYS:HG3 | 1.74 | 0.68 |
| 1:A:710:SER:HG | 3:A:1901:NAP:C4A | 1.94 | 0.68 |
| 1:A:770:ILE:HG22 | 1:A:772:PRO:HD3 | 1.75 | 0.68 |
| 1:A:338:LYS:NZ | 1:A:342:GLU:OE2 | 2.26 | 0.68 |
| 1:A:511:GLU:OE2 | 1:A:872:ARG:NH1 | 2.26 | 0.68 |
| 2:B:612:PHE:HD2 | 3:B:2102:NAP:C6A | 2.06 | 0.68 |
| 2:B:1265:ILE:HB | 2:B:1326:PRO:HG3 | 1.75 | 0.68 |
| 2:B:1878:ASN:HB2 | 2:B:1887:VAL:HB | 1.76 | 0.68 |
| 1:A:533:MET:H | 1:A:637:THR:HG23 | 1.58 | 0.68 |
| 2:B:2017:VAL:HG23 | 2:B:2026:ILE:HD12 | 1.75 | 0.68 |
| 2:B:1763:GLN:OE1 | 2:B:1763:GLN:N | 2.25 | 0.68 |
| 1:A:87:GLU:N | 1:A:87:GLU:OE1 | 2.27 | 0.67 |
| 1:A:712:PHE:HE1 | 1:A:717:THR:CG2 | 1.70 | 0.67 |
| 1:A:1247:SER:OG | 1:A:1248:GLY:N | 2.24 | 0.67 |
| 2:B:1854:PHE:HE2 | 2:B:1859:LEU:HB3 | 1.59 | 0.67 |
| 1:A:505:GLY:O | 1:A:954:ARG:NH1 | 2.26 | 0.67 |
| 1:A:1260:LYS:NZ | 1:A:1336:GLU:OE1 | 2.26 | 0.67 |
| 2:B:506:GLU:OE2 | 2:B:746:ARG:NH2 | 2.27 | 0.67 |
| 2:B:560:SER:HB3 | 2:B:1089:GLU:HA | 1.76 | 0.67 |
| 2:B:250:PHE:O | 2:B:253:SER:OG | 2.12 | 0.67 |
| 1:A:1218:VAL:HG11 | 1:A:1701:PHE:HB2 | 1.77 | 0.67 |
| 2:B:1131:ALA:HA | 2:B:1142:ILE:HG21 | 1.74 | 0.67 |
| 1:A:41:THR:O | 1:A:76:ARG:NH1 | 2.27 | 0.67 |
| 2:B:703:VAL:HG11 | 2:B:717:LEU:HD12 | 1.76 | 0.67 |
| 2:B:723:ARG:NH1 | 2:B:756:SER:O | 2.28 | 0.67 |
| 2:B:657:ARG:NH1 | 2:B:661:TYR:O | 2.28 | 0.67 |
| 2:B:331:LEU:HD11 | 2:B:401:LEU:HD23 | 1.75 | 0.67 |
| 1:A:1075:ASP:OD2 | 1:A:1078:THR:N | 2.26 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:722:GLY:O | 2:B:728:HIS:NE2 | 2.28 | 0.66 |
| 2:B:1738:LYS:O | 2:B:1741:LYS:NZ | 2.22 | 0.66 |
| 1:A:657:LEU:HD22 | 1:A:915:LEU:HD11 | 1.76 | 0.66 |
| 2:B:847:ARG:NH2 | 2:B:1035:ASP:OD2 | 2.28 | 0.66 |
| 2:B:1001:LYS:NZ | 2:B:1020:ASP:OD2 | 2.26 | 0.66 |
| 2:B:140:CYS:HB2 | 2:B:143:ASP:HB3 | 1.77 | 0.66 |
| 2:B:727:HIS:ND1 | 2:B:841:ILE:CD1 | 2.59 | 0.66 |
| 2:B:1185:ILE:N | 2:B:1188:ASP:O | 2.24 | 0.66 |
| 1:A:1554:LYS:NZ | 1:A:1624:TYR:OH | 2.28 | 0.66 |
| 2:B:440:LEU:HB2 | 2:B:454:GLN:HG2 | 1.78 | 0.66 |
| 2:B:102:LEU:HD11 | 2:B:111:ILE:HD13 | 1.76 | 0.66 |
| 2:B:900:ASP:OD1 | 2:B:901:LEU:N | 2.26 | 0.66 |
| 2:B:727:HIS:HE2 | 3:B:2102:NAP:H2D | 1.57 | 0.65 |
| 1:A:878:SER:C | 1:A:880:ASN:H | 2.00 | 0.65 |
| 1:A:1494:GLU:OE1 | 1:A:1498:ARG:NH2 | 2.28 | 0.65 |
| 2:B:93:ASN:HD21 | 2:B:535:GLN:HA | 1.60 | 0.65 |
| 2:B:1458:LYS:HB2 | 2:B:1464:SER:HB3 | 1.77 | 0.65 |
| 2:B:1866:VAL:HG11 | 2:B:1898:LEU:HD12 | 1.78 | 0.65 |
| 1:A:22:PHE:HE1 | 2:B:1826:MET:HB3 | 1.60 | 0.65 |
| 1:A:493:ARG:HD3 | 1:A:513:GLN:HG2 | 1.78 | 0.65 |
| 2:B:1307:ALA:HB3 | 2:B:1352:LEU:HB2 | 1.79 | 0.65 |
| 2:B:1893:ARG:HA | 2:B:1946:ILE:HD11 | 1.78 | 0.65 |
| 2:B:1929:TYR:HA | 2:B:1932:VAL:HG12 | 1.77 | 0.65 |
| 1:A:16:GLU:OE2 | 2:B:1977:GLN:NE2 | 2.30 | 0.65 |
| 1:A:1558:ALA:O | 1:A:1562:ASN:ND2 | 2.29 | 0.65 |
| 1:A:59:ARG:NH1 | 2:B:1884:GLN:OE1 | 2.28 | 0.65 |
| 1:A:872:ARG:NE | 1:A:894:THR:OG1 | 2.28 | 0.65 |
| 2:B:263:GLY:O | 2:B:266:THR:OG1 | 2.14 | 0.65 |
| 2:B:745:ARG:NH2 | 2:B:784:ASP:OD1 | 2.28 | 0.65 |
| 1:A:25:PRO:HB3 | 2:B:1877:VAL:HA | 1.79 | 0.65 |
| 2:B:123:TYR:HA | 2:B:126:VAL:HG12 | 1.77 | 0.65 |
| 2:B:1022:LEU:HD12 | 3:B:2102:NAP:O1N | 1.96 | 0.65 |
| 2:B:756:SER:CA | 4:B:2101:FMN:O2P | 2.36 | 0.65 |
| 1:A:40:ASN:HA | 1:A:76:ARG:HH22 | 1.62 | 0.64 |
| 2:B:1843:VAL:HA | 2:B:1956:PRO:HA | 1.80 | 0.64 |
| 2:B:344:ASN:O | 2:B:349:ARG:NH1 | 2.24 | 0.64 |
| 2:B:1345:MET:HB3 | 2:B:1592:ARG:HH21 | 1.61 | 0.64 |
| 1:A:46:GLU:OE1 | 1:A:54:ALA:N | 2.31 | 0.64 |
| 1:A:1117:LYS:NZ | 1:A:1335:GLU:OE2 | 2.29 | 0.64 |
| 2:B:727:HIS:N | 3:B:2102:NAP:C4N | 2.55 | 0.64 |
| 2:B:1111:GLN:HA | 2:B:1173:ASP:HA | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1219:GLU:HA | 1:A:1222:LEU:HD12 | 1.80 | 0.64 |
| 2:B:1093:GLY:O | 2:B:1095:LYS:NZ | 2.25 | 0.64 |
| 1:A:729:ALA:O | 1:A:732:SER:OG | 2.07 | 0.64 |
| 1:A:29:ILE:N | 2:B:1879:TYR:O | 2.31 | 0.64 |
| 2:B:526:GLU:N | 2:B:526:GLU:OE2 | 2.31 | 0.63 |
| 2:B:1019:LYS:HG3 | 3:B:2102:NAP:O5B | 1.99 | 0.63 |
| 1:A:690:ILE:HD11 | 1:A:871:THR:HG21 | 1.79 | 0.63 |
| 2:B:1660:GLU:H | 2:B:1663:MET:HE2 | 1.62 | 0.63 |
| 1:A:32:GLN:HA | 1:A:35:PHE:CE1 | 2.33 | 0.63 |
| 1:A:532:ALA:HB3 | 1:A:638:ILE:H | 1.63 | 0.63 |
| 1:A:647:THR:OG1 | 1:A:649:ASP:OD1 | 2.11 | 0.63 |
| 2:B:293:ILE:HG13 | 2:B:426:ILE:HD13 | 1.79 | 0.63 |
| 2:B:1458:LYS:HB3 | 2:B:1462:VAL:HG23 | 1.79 | 0.63 |
| 1:A:1245:SER:OG | 1:A:1246:GLY:N | 2.32 | 0.63 |
| 2:B:727:HIS:CE1 | 3:B:2102:NAP:C1D | 2.80 | 0.63 |
| 1:A:1207:ASP:O | 1:A:1210:THR:OG1 | 2.17 | 0.63 |
| 1:A:478:CYS:HA | 1:A:481:VAL:HG12 | 1.80 | 0.63 |
| 2:B:1680:LYS:HD2 | 2:B:1812:ILE:HD12 | 1.81 | 0.62 |
| 2:B:296:ARG:HH11 | 2:B:425:LEU:HB3 | 1.65 | 0.62 |
| 2:B:391:GLN:NE2 | 2:B:400:LYS:H | 1.92 | 0.62 |
| 2:B:939:ARG:NH2 | 2:B:955:LEU:O | 2.28 | 0.62 |
| 1:A:968:ASN:HD21 | 1:A:972:VAL:HB | 1.65 | 0.62 |
| 2:B:1706:ILE:O | 2:B:1749:SER:OG | 2.13 | 0.62 |
| 2:B:1837:ARG:NH1 | 2:B:1838:SER:O | 2.32 | 0.62 |
| 2:B:26:PHE:O | 2:B:29:SER:OG | 2.16 | 0.62 |
| 2:B:727:HIS:CE1 | 2:B:841:ILE:CD1 | 2.82 | 0.62 |
| 1:A:911:GLU:N | 1:A:911:GLU:OE1 | 2.32 | 0.62 |
| 2:B:1837:ARG:HH11 | 2:B:1838:SER:H | 1.47 | 0.62 |
| 1:A:1030:ASN:ND2 | 1:A:1050:GLU:OE2 | 2.33 | 0.62 |
| 2:B:1185:ILE:HD11 | 2:B:1190:LEU:HD12 | 1.81 | 0.62 |
| 2:B:1419:VAL:HG12 | 2:B:1507:GLY:HA3 | 1.80 | 0.62 |
| 2:B:1830:VAL:O | 2:B:1832:ARG:NH1 | 2.30 | 0.62 |
| 2:B:2024:GLU:HA | 2:B:2027:LYS:HE2 | 1.82 | 0.62 |
| 1:A:684:GLY:HA2 | 3:A:1901:NAP:H1B | 1.81 | 0.61 |
| 1:A:855:GLU:OE1 | 1:A:857:TRP:NE1 | 2.32 | 0.61 |
| 1:A:985:ALA:O | 2:B:944:ARG:NH1 | 2.31 | 0.61 |
| 1:A:1365:ARG:NH1 | 1:A:1370:THR:O | 2.28 | 0.61 |
| 2:B:107:TYR:CE2 | 2:B:109:THR:HA | 2.35 | 0.61 |
| 1:A:1494:GLU:OE2 | 1:A:1498:ARG:NH1 | 2.33 | 0.61 |
| 2:B:266:THR:O | 2:B:269:THR:OG1 | 2.17 | 0.61 |
| 2:B:801:SER:OG | 2:B:1025:SER:O | 2.15 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1766:GLN:NE2 | 2:B:1819:VAL:O | 2.27 | 0.61 |
| 1:A:86:LYS:HB3 | 1:A:92:PRO:HA | 1.82 | 0.61 |
| 2:B:138:TYR:HD1 | 2:B:144:ALA:HB3 | 1.64 | 0.61 |
| 1:A:1593:ALA:O | 1:A:1597:ASN:ND2 | 2.33 | 0.61 |
| 2:B:46:PHE:O | 2:B:113:LYS:NZ | 2.33 | 0.61 |
| 2:B:486:ILE:HB | 2:B:512:ILE:HD13 | 1.82 | 0.61 |
| 2:B:1019:LYS:HA | 3:B:2102:NAP:O1A | 2.00 | 0.61 |
| 1:A:1018:VAL:HG12 | 1:A:1401:VAL:HG22 | 1.81 | 0.61 |
| 1:A:461:GLY:O | 1:A:465:LYS:NZ | 2.33 | 0.61 |
| 1:A:1143:LYS:NZ | 1:A:1150:CYS:O | 2.31 | 0.61 |
| 2:B:708:LYS:NZ | 2:B:747:CYS:SG | 2.73 | 0.61 |
| 1:A:1368:THR:HG22 | 1:A:1370:THR:H | 1.66 | 0.61 |
| 2:B:1439:GLU:HG3 | 2:B:1485:GLY:HA2 | 1.83 | 0.61 |
| 2:B:1144:THR:HG22 | 2:B:1146:ARG:H | 1.66 | 0.60 |
| 2:B:1725:PHE:HB3 | 2:B:1739:ILE:HD11 | 1.82 | 0.60 |
| 1:A:686:GLY:CA | 3:A:1901:NAP:O3B | 2.49 | 0.60 |
| 2:B:400:LYS:O | 2:B:402:LYS:NZ | 2.32 | 0.60 |
| 2:B:584:MET:CG | 4:B:2101:FMN:C6 | 2.79 | 0.60 |
| 2:B:957:ASN:H | 2:B:960:GLN:NE2 | 2.00 | 0.60 |
| 2:B:331:LEU:HG | 2:B:335:GLN:HG3 | 1.83 | 0.60 |
| 2:B:756:SER:CA | 4:B:2101:FMN:H5'2 | 2.31 | 0.60 |
| 2:B:1581:GLU:HA | 2:B:1586:ASN:H | 1.66 | 0.60 |
| 2:B:1053:LYS:NZ | 2:B:1054:VAL:O | 2.33 | 0.60 |
| 2:B:1124:GLN:CD | 2:B:1124:GLN:H | 2.04 | 0.60 |
| 2:B:1146:ARG:NH1 | 2:B:1232:PHE:O | 2.29 | 0.60 |
| 2:B:1833:ASP:OD1 | 2:B:1837:ARG:N | 2.30 | 0.60 |
| 1:A:493:ARG:HE | 1:A:518:ARG:HG2 | 1.66 | 0.60 |
| 1:A:643:ILE:N | 1:A:658:SER:OG | 2.34 | 0.60 |
| 1:A:892:VAL:HG21 | 1:A:932:ILE:HD11 | 1.84 | 0.60 |
| 2:B:76:GLU:OE1 | 2:B:76:GLU:N | 2.31 | 0.60 |
| 2:B:261:SER:HB2 | 2:B:415:HIS:CE1 | 2.37 | 0.60 |
| 2:B:584:MET:HG3 | 2:B:587:THR:HB | 1.84 | 0.60 |
| 2:B:1117:ASP:HA | 2:B:1167:HIS:H | 1.65 | 0.60 |
| 1:A:440:ARG:HA | 1:A:730:ALA:HB2 | 1.83 | 0.60 |
| 1:A:442:ASN:HB2 | 1:A:445:LEU:HD23 | 1.83 | 0.60 |
| 1:A:525:TYR:CE1 | 1:A:629:VAL:HG22 | 2.37 | 0.60 |
| 1:A:876:LEU:CD2 | 3:A:1901:NAP:PA | 2.77 | 0.60 |
| 2:B:628:ILE:HD12 | 2:B:632:TYR:HB2 | 1.83 | 0.60 |
| 2:B:167:TYR:HA | 2:B:174:ILE:HD11 | 1.84 | 0.59 |
| 2:B:1962:VAL:HG13 | 2:B:1964:PHE:HD1 | 1.68 | 0.59 |
| 2:B:1527:GLU:HG2 | 2:B:1528:LEU:HD22 | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:728:HIS:HB3 | 2:B:840:PRO:HG2 | 1.85 | 0.59 |
| 2:B:855:LEU:HB3 | 2:B:860:PHE:CE2 | 2.38 | 0.59 |
| 1:A:1330:TYR:HB3 | 1:A:1380:SER:HB2 | 1.85 | 0.59 |
| 2:B:391:GLN:HE22 | 2:B:400:LYS:N | 1.96 | 0.59 |
| 1:A:626:ILE:CG2 | 1:A:627:GLN:N | 2.66 | 0.59 |
| 1:A:1525:LEU:HD11 | 1:A:1657:VAL:HG21 | 1.85 | 0.59 |
| 2:B:170:TYR:HB3 | 2:B:173:LEU:HD12 | 1.84 | 0.59 |
| 2:B:767:TYR:HB3 | 2:B:783:PHE:HD2 | 1.67 | 0.59 |
| 2:B:906:TYR:OH | 2:B:987:ASP:OD2 | 2.20 | 0.59 |
| 1:A:1017:VAL:HG21 | 1:A:1314:ILE:HG12 | 1.85 | 0.58 |
| 2:B:1185:ILE:O | 2:B:1188:ASP:N | 2.36 | 0.58 |
| 2:B:1683:ARG:O | 2:B:1687:ASN:ND2 | 2.36 | 0.58 |
| 2:B:446:ASP:OD1 | 2:B:447:THR:N | 2.36 | 0.58 |
| 2:B:1108:ASP:OD2 | 2:B:1133:THR:N | 2.35 | 0.58 |
| 1:A:679:TYR:O | 1:A:768:ASP:N | 2.34 | 0.58 |
| 1:A:755:TYR:OH | 1:A:812:LYS:NZ | 2.36 | 0.58 |
| 2:B:602:TYR:OH | 2:B:1063:ASN:OD1 | 2.15 | 0.58 |
| 2:B:1438:LEU:HA | 2:B:1485:GLY:HA3 | 1.85 | 0.58 |
| 2:B:1899:THR:O | 2:B:1903:ASN:ND2 | 2.36 | 0.58 |
| 2:B:188:LEU:HD23 | 2:B:291:LEU:HD23 | 1.84 | 0.58 |
| 2:B:1309:MET:HG2 | 2:B:1576:ARG:CZ | 2.33 | 0.58 |
| 2:B:1363:GLU:N | 2:B:1363:GLU:OE1 | 2.36 | 0.58 |
| 1:A:1413:GLY:O | 1:A:1414:ARG:NH1 | 2.34 | 0.58 |
| 2:B:583:GLY:HA2 | 2:B:588:THR:HG21 | 1.86 | 0.58 |
| 1:A:411:VAL:HG11 | 1:A:449:MET:HG2 | 1.84 | 0.58 |
| 2:B:136:LEU:HA | 2:B:139:HIS:HB2 | 1.85 | 0.58 |
| 2:B:398:GLU:OE1 | 2:B:398:GLU:N | 2.37 | 0.58 |
| 2:B:319:GLU:OE2 | 2:B:381:ARG:NH2 | 2.35 | 0.58 |
| 2:B:790:SER:HB3 | 4:B:2101:FMN:HM81 | 1.82 | 0.58 |
| 1:A:1028:TRP:O | 1:A:1033:THR:OG1 | 2.19 | 0.58 |
| 2:B:102:LEU:O | 2:B:109:THR:OG1 | 2.17 | 0.58 |
| 2:B:1181:ALA:HB3 | 2:B:1193:VAL:HB | 1.85 | 0.58 |
| 2:B:1595:LYS:O | 2:B:1641:GLU:N | 2.36 | 0.58 |
| 2:B:169:LEU:HD22 | 2:B:170:TYR:CE2 | 2.39 | 0.58 |
| 2:B:215:GLN:O | 2:B:219:LEU:N | 2.35 | 0.58 |
| 2:B:727:HIS:CE1 | 2:B:841:ILE:HD11 | 2.39 | 0.58 |
| 2:B:809:VAL:HG21 | 2:B:1054:VAL:HB | 1.84 | 0.58 |
| 2:B:1019:LYS:HG3 | 3:B:2102:NAP:PA | 2.44 | 0.58 |
| 2:B:881:LYS:HA | 2:B:884:ASN:HB2 | 1.86 | 0.57 |
| 2:B:889:PRO:HG2 | 2:B:1032:VAL:HG11 | 1.84 | 0.57 |
| 2:B:148:ALA:O | 2:B:257:SER:OG | 2.13 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:183:GLU:OE2 | 2:B:187:GLN:NE2 | 2.37 | 0.57 |
| 2:B:1336:LEU:HD11 | 2:B:1396:PHE:HB3 | 1.86 | 0.57 |
| 2:B:181:ILE:HD13 | 2:B:284:LEU:HD23 | 1.86 | 0.57 |
| 2:B:535:GLN:O | 2:B:541:ALA:HB2 | 2.03 | 0.57 |
| 2:B:1106:ILE:HG12 | 2:B:1128:ASP:HB3 | 1.85 | 0.57 |
| 2:B:385:ALA:HB1 | 2:B:389:LEU:HD13 | 1.87 | 0.57 |
| 2:B:1897:THR:O | 2:B:1901:VAL:HG13 | 2.05 | 0.57 |
| 1:A:521:GLU:HG2 | 1:A:670:ILE:HG22 | 1.86 | 0.57 |
| 2:B:726:GLY:O | 2:B:727:HIS:C | 2.38 | 0.57 |
| 2:B:1827:GLN:O | 2:B:1832:ARG:NH2 | 2.33 | 0.57 |
| 1:A:1005:PRO:O | 1:A:1007:LEU:N | 2.38 | 0.57 |
| 2:B:1896:ASP:HA | 2:B:1899:THR:HG22 | 1.87 | 0.57 |
| 2:B:876:ASP:N | 2:B:876:ASP:OD1 | 2.37 | 0.57 |
| 2:B:1014:GLU:HA | 2:B:1017:PHE:HB3 | 1.86 | 0.57 |
| 1:A:438:MET:HB2 | 1:A:481:VAL:HG11 | 1.87 | 0.57 |
| 1:A:1373:GLY:HA2 | 1:A:1549:THR:HG22 | 1.87 | 0.57 |
| 1:A:1404:MET:SD | 1:A:1405:THR:N | 2.77 | 0.57 |
| 1:A:1476:LYS:HZ1 | 1:A:1484:SER:H | 1.52 | 0.57 |
| 2:B:337:GLU:HA | 2:B:340:ILE:HG12 | 1.87 | 0.57 |
| 2:B:185:LEU:O | 2:B:189:HIS:N | 2.38 | 0.57 |
| 2:B:727:HIS:NE2 | 3:B:2102:NAP:C1D | 2.68 | 0.57 |
| 1:A:1389:ASP:OD1 | 1:A:1390:LEU:N | 2.38 | 0.56 |
| 2:B:790:SER:CA | 4:B:2101:FMN:C8M | 2.74 | 0.56 |
| 1:A:766:ASP:OD1 | 1:A:812:LYS:NZ | 2.38 | 0.56 |
| 2:B:1712:LYS:HA | 2:B:1715:ALA:HB3 | 1.85 | 0.56 |
| 1:A:42:GLU:N | 1:A:42:GLU:OE1 | 2.38 | 0.56 |
| 1:A:327:ASP:OD1 | 1:A:327:ASP:N | 2.35 | 0.56 |
| 1:A:766:ASP:HB3 | 1:A:817:ARG:NH1 | 2.20 | 0.56 |
| 2:B:446:ASP:N | 2:B:451:SER:O | 2.34 | 0.56 |
| 2:B:512:ILE:O | 2:B:528:GLY:N | 2.34 | 0.56 |
| 2:B:1019:LYS:HG3 | 3:B:2102:NAP:O1A | 2.04 | 0.56 |
| 2:B:1116:ILE:HD11 | 2:B:1164:PRO:HB3 | 1.86 | 0.56 |
| 2:B:1168:SER:OG | 2:B:1169:LYS:N | 2.38 | 0.56 |
| 2:B:1702:ASN:ND2 | 2:B:1755:PRO:O | 2.38 | 0.56 |
| 1:A:989:PHE:HE1 | 1:A:1032:ARG:HH21 | 1.54 | 0.56 |
| 2:B:161:GLU:OE1 | 2:B:161:GLU:N | 2.39 | 0.56 |
| 1:A:794:HIS:HD2 | 1:A:841:SER:HB3 | 1.71 | 0.56 |
| 2:B:79:LEU:HD21 | 2:B:126:VAL:HG23 | 1.88 | 0.56 |
| 1:A:796:ILE:CD1 | 3:A:1901:NAP:N6A | 2.68 | 0.56 |
| 2:B:1536:ASN:ND2 | 2:B:1550:HIS:O | 2.29 | 0.56 |
| 2:B:1324:ILE:HG22 | 2:B:1376:VAL:HG11 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1511:GLU:OE2 | 2:B:1513:SER:N | 2.33 | 0.56 |
| 2:B:1788:SER:O | 2:B:1997:LYS:NZ | 2.25 | 0.56 |
| 1:A:708:THR:HG23 | 1:A:739:PHE:HB3 | 1.87 | 0.56 |
| 2:B:369:PRO:O | 2:B:372:SER:OG | 2.20 | 0.56 |
| 1:A:710:SER:HB2 | 3:A:1901:NAP:O3X | 2.07 | 0.56 |
| 2:B:138:TYR:CZ | 2:B:141:LYS:HA | 2.41 | 0.56 |
| 2:B:1869:LYS:NZ | 2:B:1933:ASP:OD1 | 2.33 | 0.56 |
| 1:A:401:ASP:O | 1:A:403:TYR:N | 2.38 | 0.55 |
| 2:B:1706:ILE:N | 2:B:1750:TYR:O | 2.38 | 0.55 |
| 2:B:1757:GLY:O | 2:B:1760:SER:OG | 2.20 | 0.55 |
| 2:B:1489:TYR:CE1 | 2:B:1498:PRO:HG2 | 2.41 | 0.55 |
| 2:B:64:GLY:O | 2:B:67:SER:OG | 2.24 | 0.55 |
| 1:A:1012:ASP:OD1 | 1:A:1505:SER:HB3 | 2.06 | 0.55 |
| 2:B:1160:ASP:O | 2:B:1163:THR:OG1 | 2.22 | 0.55 |
| 2:B:1850:VAL:HG23 | 2:B:1906:LYS:HB2 | 1.89 | 0.55 |
| 1:A:839:SER:OG | 1:A:840:GLU:N | 2.39 | 0.55 |
| 2:B:1767:PRO:HG3 | 2:B:1819:VAL:HG13 | 1.87 | 0.55 |
| 1:A:1049:ILE:HG22 | 1:A:1087:ILE:HG21 | 1.87 | 0.55 |
| 2:B:584:MET:HG2 | 2:B:588:THR:OG1 | 2.06 | 0.55 |
| 2:B:589:VAL:HG21 | 2:B:610:GLY:HA3 | 1.87 | 0.55 |
| 2:B:726:GLY:C | 2:B:727:HIS:O | 2.43 | 0.55 |
| 2:B:757:GLY:HA2 | 2:B:1047:ALA:HB2 | 1.87 | 0.55 |
| 2:B:1342:GLY:HA2 | 2:B:1595:LYS:HA | 1.89 | 0.55 |
| 2:B:1548:PRO:HA | 2:B:1551:VAL:HG22 | 1.89 | 0.55 |
| 2:B:1661:GLN:NE2 | 2:B:1698:GLN:O | 2.40 | 0.55 |
| 2:B:107:TYR:OH | 2:B:110:THR:O | 2.25 | 0.55 |
| 2:B:201:ASN:O | 2:B:204:SER:OG | 2.23 | 0.55 |
| 2:B:218:LEU:O | 2:B:224:SER:OG | 2.22 | 0.55 |
| 2:B:860:PHE:CE1 | 2:B:1014:GLU:HB3 | 2.41 | 0.55 |
| 2:B:1960:ILE:HG12 | 2:B:1964:PHE:HE1 | 1.72 | 0.55 |
| 1:A:69:ASP:O | 1:A:73:SER:N | 2.40 | 0.55 |
| 1:A:17:LEU:HD23 | 2:B:2002:LEU:HD23 | 1.89 | 0.55 |
| 1:A:69:ASP:OD1 | 1:A:70:ALA:N | 2.40 | 0.55 |
| 1:A:1012:ASP:HB3 | 1:A:1513:ASN:ND2 | 2.22 | 0.55 |
| 1:A:1198:ILE:HG12 | 1:A:1701:PHE:CD2 | 2.42 | 0.55 |
| 2:B:1668:TYR:CE1 | 2:B:1675:ARG:HG3 | 2.42 | 0.55 |
| 2:B:1726:GLU:OE1 | 2:B:1735:LYS:N | 2.39 | 0.55 |
| 1:A:1607:LEU:HD23 | 1:A:1608:VAL:N | 2.22 | 0.54 |
| 2:B:858:THR:OG1 | 2:B:859:ILE:HD12 | 2.07 | 0.54 |
| 1:A:1214:LEU:O | 1:A:1218:VAL:HG22 | 2.07 | 0.54 |
| 1:A:1349:ASN:O | 1:A:1353:GLU:HG2 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:13:SER:H | 2:B:46:PHE:HZ | 1.55 | 0.54 |
| 2:B:60:GLY:O | 2:B:63:ILE:HG22 | 2.06 | 0.54 |
| 2:B:139:HIS:HA | 2:B:141:LYS:NZ | 2.23 | 0.54 |
| 2:B:1762:THR:HA | 2:B:1765:THR:HG22 | 1.89 | 0.54 |
| 1:A:482:LEU:HG | 1:A:483:THR:HG23 | 1.87 | 0.54 |
| 1:A:1027:PRO:HA | 1:A:1188:PRO:HD3 | 1.87 | 0.54 |
| 2:B:518:LEU:HB2 | 2:B:530:LYS:HE2 | 1.88 | 0.54 |
| 2:B:612:PHE:CD2 | 3:B:2102:NAP:N6A | 2.76 | 0.54 |
| 2:B:863:PRO:HG2 | 2:B:866:LYS:HZ3 | 1.72 | 0.54 |
| 2:B:894:ASN:OD1 | 2:B:895:ALA:N | 2.40 | 0.54 |
| 2:B:1756:THR:OG1 | 2:B:1760:SER:OG | 2.24 | 0.54 |
| 2:B:2010:THR:HG23 | 2:B:2013:TYR:H | 1.72 | 0.54 |
| 2:B:164:ARG:NH1 | 2:B:205:TRP:O | 2.40 | 0.54 |
| 2:B:1531:LYS:NZ | 2:B:1605:ASN:O | 2.27 | 0.54 |
| 1:A:1136:LYS:N | 1:A:1160:GLU:OE2 | 2.41 | 0.54 |
| 1:A:1416:VAL:HG13 | 1:A:1650:GLY:H | 1.71 | 0.54 |
| 1:A:1564:MET:HB3 | 1:A:1569:ARG:HG3 | 1.87 | 0.54 |
| 2:B:902:GLN:N | 2:B:902:GLN:OE1 | 2.39 | 0.54 |
| 2:B:1425:LYS:O | 2:B:1429:VAL:N | 2.38 | 0.54 |
| 2:B:584:MET:HA | 4:B:2101:FMN:C4 | 2.37 | 0.54 |
| 2:B:894:ASN:HB3 | 2:B:899:CYS:SG | 2.48 | 0.54 |
| 2:B:1312:ALA:O | 2:B:1316:GLY:N | 2.39 | 0.54 |
| 2:B:1353:LYS:N | 2:B:1356:ASP:OD2 | 2.26 | 0.54 |
| 2:B:1919:MET:HB2 | 2:B:1924:VAL:HG13 | 1.89 | 0.54 |
| 1:A:1247:SER:OG | 1:A:1250:GLY:N | 2.35 | 0.54 |
| 2:B:386:PRO:HD2 | 2:B:389:LEU:HD12 | 1.89 | 0.54 |
| 2:B:1452:GLU:OE2 | 2:B:1469:THR:OG1 | 2.25 | 0.54 |
| 2:B:1672:GLU:OE1 | 2:B:1675:ARG:NH1 | 2.37 | 0.54 |
| 1:A:33:ASP:OD2 | 1:A:64:LYS:NZ | 2.31 | 0.54 |
| 1:A:458:GLU:O | 1:A:465:LYS:NZ | 2.34 | 0.54 |
| 1:A:1269:GLN:NE2 | 1:A:1271:ASP:OD1 | 2.41 | 0.54 |
| 1:A:1555:ASN:O | 1:A:1559:THR:HG23 | 2.08 | 0.54 |
| 2:B:139:HIS:HA | 2:B:141:LYS:HZ3 | 1.73 | 0.54 |
| 2:B:888:LYS:NZ | 2:B:1019:LYS:O | 2.33 | 0.54 |
| 2:B:927:ASP:OD1 | 2:B:928:VAL:N | 2.40 | 0.54 |
| 2:B:1366:ALA:HB3 | 2:B:1377:GLU:HB2 | 1.90 | 0.54 |
| 2:B:1898:LEU:HA | 2:B:1901:VAL:HG22 | 1.90 | 0.54 |
| 2:B:905:THR:N | 2:B:908:GLU:OE2 | 2.31 | 0.54 |
| 2:B:1295:ASP:OD1 | 2:B:1295:ASP:N | 2.38 | 0.54 |
| 2:B:2011:LYS:HD2 | 2:B:2033:TRP:CD1 | 2.43 | 0.54 |
| 1:A:1545:HIS:O | 1:A:1581:LYS:NZ | 2.40 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:760:SER:OG | 2:B:762:GLU:OE1 | 2.22 | 0.53 |
| 2:B:196:TYR:HB2 | 2:B:217:TYR:OH | 2.08 | 0.53 |
| 2:B:720:THR:HG21 | 4:B:2101:FMN:O3' | 2.09 | 0.53 |
| 2:B:986:GLU:OE1 | 2:B:986:GLU:N | 2.37 | 0.53 |
| 2:B:1743:ILE:HD11 | 2:B:1750:TYR:CG | 2.43 | 0.53 |
| 2:B:1873:LEU:HD12 | 2:B:1890:GLY:HA2 | 1.90 | 0.53 |
| 1:A:35:PHE:HE2 | 1:A:44:ILE:HG12 | 1.72 | 0.53 |
| 2:B:215:GLN:HA | 2:B:218:LEU:HD12 | 1.91 | 0.53 |
| 2:B:1530:SER:OG | 2:B:1531:LYS:N | 2.42 | 0.53 |
| 2:B:1674:ALA:O | 2:B:1677:VAL:HG22 | 2.09 | 0.53 |
| 2:B:1123:LYS:NZ | 2:B:1163:THR:OG1 | 2.40 | 0.53 |
| 2:B:1877:VAL:HB | 2:B:1965:HIS:HB2 | 1.91 | 0.53 |
| 1:A:820:GLN:HA | 1:A:862:THR:HG23 | 1.91 | 0.53 |
| 2:B:855:LEU:HB3 | 2:B:860:PHE:HE2 | 1.74 | 0.53 |
| 1:A:1331:ASP:OD2 | 1:A:1332:ASP:N | 2.40 | 0.53 |
| 1:A:1728:ASN:O | 1:A:1729:LYS:HG2 | 2.09 | 0.53 |
| 2:B:1718:ASP:OD1 | 2:B:1718:ASP:N | 2.41 | 0.53 |
| 1:A:1603:LEU:HD13 | 1:A:1660:HIS:HA | 1.90 | 0.53 |
| 1:A:1668:LEU:HD11 | 1:A:1673:TYR:HB2 | 1.90 | 0.53 |
| 2:B:146:LEU:HD23 | 2:B:485:HIS:HB2 | 1.90 | 0.53 |
| 2:B:929:SER:OG | 2:B:1000:GLN:HG3 | 2.09 | 0.53 |
| 2:B:1436:PHE:CZ | 2:B:1438:LEU:HB3 | 2.44 | 0.53 |
| 2:B:1630:ASN:O | 2:B:1634:GLU:N | 2.37 | 0.53 |
| 1:A:1374:PHE:HB3 | 1:A:1547:THR:O | 2.08 | 0.53 |
| 2:B:129:ILE:O | 2:B:131:LYS:NZ | 2.42 | 0.53 |
| 2:B:374:TYR:HA | 2:B:377:ASN:HD21 | 1.73 | 0.52 |
| 2:B:690:LEU:HB2 | 2:B:713:PHE:HE2 | 1.72 | 0.52 |
| 2:B:1090:TYR:OH | 2:B:1139:GLN:NE2 | 2.33 | 0.52 |
| 2:B:1666:GLU:OE2 | 2:B:1666:GLU:N | 2.36 | 0.52 |
| 2:B:1708:PHE:CG | 2:B:1717:ARG:HB3 | 2.45 | 0.52 |
| 2:B:1979:PHE:HA | 2:B:1982:LYS:HE3 | 1.91 | 0.52 |
| 1:A:1043:PHE:O | 1:A:1088:LYS:NZ | 2.41 | 0.52 |
| 2:B:834:ARG:HB3 | 2:B:838:GLY:HA2 | 1.91 | 0.52 |
| 2:B:389:LEU:HD22 | 2:B:391:GLN:HG3 | 1.90 | 0.52 |
| 2:B:1726:GLU:HB3 | 2:B:1975:PRO:HD3 | 1.92 | 0.52 |
| 1:A:871:THR:HB | 3:A:1901:NAP:O7N | 2.09 | 0.52 |
| 1:A:890:LEU:HD11 | 1:A:938:PHE:CZ | 2.45 | 0.52 |
| 1:A:989:PHE:CZ | 1:A:1223:SER:HA | 2.44 | 0.52 |
| 2:B:414:PHE:HB3 | 2:B:415:HIS:ND1 | 2.24 | 0.52 |
| 2:B:931:ARG:HD3 | 2:B:961:LEU:HB2 | 1.91 | 0.52 |
| 2:B:1434:GLU:N | 2:B:1434:GLU:OE1 | 2.42 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:708:THR:HG21 | 1:A:739:PHE:CD2 | 2.42 | 0.52 |
| 2:B:846:THR:HB | 2:B:1037:GLN:HA | 1.91 | 0.52 |
| 2:B:907:LYS:HG3 | 2:B:972:PHE:CD2 | 2.45 | 0.52 |
| 2:B:218:LEU:HA | 2:B:223:VAL:HG11 | 1.90 | 0.52 |
| 2:B:868:LEU:HD12 | 2:B:868:LEU:H | 1.74 | 0.52 |
| 2:B:1591:VAL:HG12 | 2:B:1644:ILE:HG22 | 1.92 | 0.52 |
| 1:A:504:LYS:HZ3 | 1:A:954:ARG:HH21 | 1.58 | 0.52 |
| 1:A:842:LYS:CE | 3:A:1901:NAP:O2D | 2.58 | 0.52 |
| 1:A:1207:ASP:OD2 | 1:A:1209:ILE:HG22 | 2.10 | 0.52 |
| 1:A:1410:ASP:HB2 | 1:A:1651:GLN:HB3 | 1.92 | 0.52 |
| 2:B:813:GLY:HA2 | 2:B:1048:SER:HB2 | 1.91 | 0.52 |
| 2:B:1401:GLU:OE1 | 2:B:1402:TYR:N | 2.43 | 0.52 |
| 1:A:380:HIS:O | 1:A:788:SER:OG | 2.15 | 0.52 |
| 1:A:626:ILE:O | 1:A:628:PRO:HD3 | 2.09 | 0.52 |
| 2:B:136:LEU:HD11 | 2:B:535:GLN:O | 2.10 | 0.52 |
| 2:B:818:GLN:OE1 | 2:B:821:GLN:NE2 | 2.43 | 0.52 |
| 2:B:1920:SER:OG | 2:B:1921:ILE:N | 2.43 | 0.52 |
| 1:A:1301:GLY:O | 1:A:1304:ALA:N | 2.43 | 0.52 |
| 2:B:1651:TYR:CG | 2:B:1790:ILE:HD11 | 2.45 | 0.52 |
| 1:A:428:ARG:NH2 | 1:A:519:LYS:HD3 | 2.26 | 0.51 |
| 1:A:1117:LYS:HE2 | 1:A:1339:TYR:CD1 | 2.45 | 0.51 |
| 1:A:1225:GLY:O | 1:A:1683:ARG:NH1 | 2.43 | 0.51 |
| 1:A:1271:ASP:OD2 | 1:A:1274:GLN:NE2 | 2.42 | 0.51 |
| 2:B:9:LEU:O | 2:B:17:THR:OG1 | 2.25 | 0.51 |
| 2:B:1375:LEU:HD11 | 2:B:1395:GLN:HE21 | 1.75 | 0.51 |
| 1:A:734:LEU:HD23 | 1:A:735:ILE:N | 2.26 | 0.51 |
| 2:B:662:PRO:HA | 2:B:1153:HIS:HD2 | 1.75 | 0.51 |
| 2:B:1830:VAL:HG22 | 2:B:1968:TYR:HE2 | 1.75 | 0.51 |
| 1:A:1491:GLU:O | 1:A:1494:GLU:HG3 | 2.10 | 0.51 |
| 2:B:861:ASN:OD1 | 2:B:861:ASN:N | 2.43 | 0.51 |
| 1:A:518:ARG:N | 1:A:522:GLN:OE1 | 2.25 | 0.51 |
| 1:A:710:SER:CB | 3:A:1901:NAP:O3X | 2.59 | 0.51 |
| 1:A:796:ILE:HD13 | 3:A:1901:NAP:N6A | 2.25 | 0.51 |
| 2:B:221:VAL:HG12 | 2:B:294:GLY:HA2 | 1.92 | 0.51 |
| 2:B:1209:GLU:OE2 | 2:B:1211:ARG:HG2 | 2.10 | 0.51 |
| 1:A:625:ILE:O | 1:A:625:ILE:HG23 | 2.10 | 0.51 |
| 1:A:945:ASP:O | 1:A:949:THR:HG23 | 2.11 | 0.51 |
| 2:B:93:ASN:HB3 | 2:B:96:SER:OG | 2.10 | 0.51 |
| 2:B:1332:ASP:OD1 | 2:B:1335:LYS:N | 2.34 | 0.51 |
| 2:B:1480:GLU:HG2 | 2:B:1482:ILE:HD11 | 1.92 | 0.51 |
| 2:B:374:TYR:HA | 2:B:377:ASN:ND2 | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:927:ASP:OD2 | 2:B:929:SER:HB3 | 2.10 | 0.51 |
| 2:B:1266:ASN:ND2 | 2:B:1269:LYS:H | 2.08 | 0.51 |
| 2:B:1416:PRO:HB3 | 2:B:1450:ARG:HG2 | 1.92 | 0.51 |
| 2:B:1602:VAL:HG11 | 2:B:1608:LEU:HD21 | 1.92 | 0.51 |
| 2:B:1840:TYR:HE2 | 2:B:1968:TYR:CZ | 2.28 | 0.51 |
| 1:A:1409:THR:HA | 1:A:1651:GLN:O | 2.10 | 0.51 |
| 1:A:979:VAL:N | 2:B:956:GLN:OE1 | 2.29 | 0.51 |
| 2:B:449:ASP:OD2 | 2:B:463:ARG:NH2 | 2.43 | 0.51 |
| 1:A:442:ASN:O | 1:A:446:ILE:HD12 | 2.11 | 0.51 |
| 1:A:646:LYS:NZ | 1:A:850:ASN:OD1 | 2.44 | 0.51 |
| 1:A:984:ARG:HG2 | 2:B:943:GLU:HG2 | 1.91 | 0.51 |
| 1:A:1535:THR:HG22 | 1:A:1537:ASP:H | 1.76 | 0.51 |
| 2:B:220:SER:OG | 2:B:222:PRO:HD2 | 2.10 | 0.51 |
| 2:B:568:THR:H | 2:B:571:SER:HG | 1.59 | 0.51 |
| 1:A:997:TYR:HB2 | 1:A:1673:TYR:HD2 | 1.75 | 0.51 |
| 1:A:1012:ASP:HB3 | 1:A:1513:ASN:HD21 | 1.76 | 0.51 |
| 1:A:1305:THR:HG22 | 1:A:1589:GLY:O | 2.11 | 0.51 |
| 2:B:356:SER:OG | 2:B:365:VAL:O | 2.21 | 0.51 |
| 2:B:1563:GLY:O | 2:B:1565:ILE:N | 2.44 | 0.51 |
| 2:B:1843:VAL:HG12 | 2:B:1956:PRO:HB3 | 1.93 | 0.51 |
| 2:B:265:VAL:O | 2:B:269:THR:HG23 | 2.12 | 0.50 |
| 2:B:761:ASP:HB3 | 2:B:1065:ILE:HA | 1.92 | 0.50 |
| 2:B:1368:LEU:HA | 2:B:1408:THR:OG1 | 2.10 | 0.50 |
| 1:A:1137:GLU:OE1 | 1:A:1137:GLU:N | 2.37 | 0.50 |
| 2:B:1754:SER:HB3 | 2:B:1758:LEU:HD23 | 1.93 | 0.50 |
| 2:B:584:MET:HB2 | 4:B:2101:FMN:N5 | 2.16 | 0.50 |
| 2:B:726:GLY:O | 2:B:727:HIS:O | 2.29 | 0.50 |
| 2:B:833:VAL:HG21 | 2:B:852:TRP:CD1 | 2.46 | 0.50 |
| 2:B:834:ARG:HD2 | 2:B:838:GLY:O | 2.11 | 0.50 |
| 2:B:933:MET:HG3 | 2:B:1000:GLN:HE22 | 1.77 | 0.50 |
| 2:B:1792:PHE:CZ | 2:B:1998:TYR:HB2 | 2.46 | 0.50 |
| 1:A:903:ASN:HB3 | 1:A:925:LEU:HD13 | 1.93 | 0.50 |
| 1:A:1333:PHE:CE1 | 1:A:1338:SER:HB2 | 2.47 | 0.50 |
| 2:B:584:MET:HB2 | 4:B:2101:FMN:C5A | 2.26 | 0.50 |
| 2:B:735:GLN:O | 2:B:738:ILE:HG22 | 2.12 | 0.50 |
| 1:A:327:ASP:O | 1:A:330:THR:OG1 | 2.29 | 0.50 |
| 1:A:675:PHE:HB3 | 1:A:678:LYS:HD2 | 1.93 | 0.50 |
| 1:A:982:GLU:OE2 | 1:A:1085:LYS:HG3 | 2.11 | 0.50 |
| 1:A:1737:LYS:O | 1:A:1741:SER:OG | 2.23 | 0.50 |
| 2:B:166:LEU:HD23 | 2:B:174:ILE:HD13 | 1.94 | 0.50 |
| 2:B:502:HIS:HB2 | 2:B:512:ILE:HG13 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:830:ILE:HD12 | 2:B:1045:PRO:HA | 1.94 | 0.50 |
| 2:B:939:ARG:O | 2:B:943:GLU:HB2 | 2.12 | 0.50 |
| 2:B:2019:ASP:O | 2:B:2022:LYS:NZ | 2.44 | 0.50 |
| 1:A:1075:ASP:OD2 | 1:A:1077:LYS:N | 2.45 | 0.50 |
| 2:B:18:LEU:H | 2:B:18:LEU:HD23 | 1.77 | 0.50 |
| 2:B:1226:TYR:HA | 2:B:1235:ILE:HG12 | 1.94 | 0.50 |
| 2:B:1027:ASP:OD2 | 2:B:1030:SER:N | 2.41 | 0.50 |
| 2:B:1156:ASN:HB3 | 2:B:1159:HIS:HB2 | 1.92 | 0.50 |
| 2:B:1236:LEU:HD23 | 2:B:1236:LEU:H | 1.75 | 0.50 |
| 2:B:1872:TRP:CZ3 | 2:B:1893:ARG:HB3 | 2.47 | 0.50 |
| 1:A:1569:ARG:NH2 | 1:A:1573:ASN:O | 2.32 | 0.50 |
| 2:B:34:GLU:HA | 2:B:37:LYS:HE3 | 1.94 | 0.50 |
| 2:B:261:SER:HB2 | 2:B:415:HIS:HE1 | 1.76 | 0.50 |
| 1:A:400:TYR:HB3 | 1:A:724:TYR:CD2 | 2.47 | 0.50 |
| 1:A:1236:VAL:N | 1:A:1724:ARG:HH12 | 2.09 | 0.50 |
| 2:B:1534:GLY:HA2 | 2:B:1605:ASN:OD1 | 2.12 | 0.50 |
| 2:B:1813:GLU:OE1 | 2:B:1813:GLU:N | 2.41 | 0.50 |
| 1:A:53:LEU:HA | 1:A:56:MET:HB3 | 1.95 | 0.49 |
| 2:B:138:TYR:CE2 | 2:B:141:LYS:HG3 | 2.47 | 0.49 |
| 2:B:534:PHE:O | 2:B:536:THR:HG23 | 2.12 | 0.49 |
| 2:B:756:SER:N | 4:B:2101:FMN:C5' | 2.75 | 0.49 |
| 2:B:1533:PRO:O | 2:B:1605:ASN:N | 2.43 | 0.49 |
| 1:A:1376:GLU:OE1 | 1:A:1376:GLU:N | 2.37 | 0.49 |
| 1:A:1713:LEU:HD22 | 1:A:1739:ILE:HD12 | 1.92 | 0.49 |
| 1:A:787:ASP:N | 1:A:790:SER:OG | 2.46 | 0.49 |
| 1:A:1100:GLY:O | 1:A:1102:ARG:NH1 | 2.45 | 0.49 |
| 2:B:323:SER:HB2 | 2:B:410:ILE:O | 2.12 | 0.49 |
| 2:B:944:ARG:NH2 | 2:B:987:ASP:OD1 | 2.34 | 0.49 |
| 2:B:1847:PRO:HG3 | 2:B:1859:LEU:HD13 | 1.94 | 0.49 |
| 2:B:104:ASP:OD1 | 2:B:105:GLU:N | 2.46 | 0.49 |
| 2:B:342:GLN:O | 2:B:345:SER:OG | 2.30 | 0.49 |
| 2:B:476:GLU:HA | 2:B:479:THR:HG22 | 1.95 | 0.49 |
| 2:B:945:PHE:CE1 | 2:B:977:GLN:HG2 | 2.48 | 0.49 |
| 2:B:1526:GLU:OE2 | 2:B:1529:THR:OG1 | 2.30 | 0.49 |
| 2:B:1709:GLY:N | 2:B:1713:GLY:HA3 | 2.27 | 0.49 |
| 1:A:1614:ALA:HB3 | 1:A:1631:SER:HB2 | 1.94 | 0.49 |
| 2:B:61:LYS:HA | 2:B:121:ASN:ND2 | 2.26 | 0.49 |
| 2:B:741:TYR:CE1 | 2:B:781:MET:HB3 | 2.47 | 0.49 |
| 2:B:1125:GLU:OE1 | 2:B:1125:GLU:N | 2.41 | 0.49 |
| 2:B:1310:ASP:O | 2:B:1313:ILE:HG12 | 2.11 | 0.49 |
| 2:B:1579:VAL:HG12 | 2:B:1612:MET:SD | 2.52 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1738:LYS:HE3 | 2:B:1740:PHE:H | 1.78 | 0.49 |
| 1:A:35:PHE:CD2 | 2:B:1650:THR:HG21 | 2.48 | 0.49 |
| 2:B:169:LEU:HD22 | 2:B:170:TYR:CZ | 2.47 | 0.49 |
| 2:B:271:ALA:HB1 | 2:B:440:LEU:HB3 | 1.95 | 0.49 |
| 2:B:1194:GLU:HB2 | 2:B:1206:SER:HB2 | 1.95 | 0.49 |
| 2:B:1877:VAL:HG23 | 2:B:1878:ASN:OD1 | 2.13 | 0.49 |
| 2:B:2021:THR:HG23 | 2:B:2023:SER:H | 1.77 | 0.49 |
| 1:A:857:TRP:CE3 | 1:A:861:LEU:HB2 | 2.48 | 0.49 |
| 2:B:149:ILE:O | 2:B:488:ASP:HA | 2.13 | 0.49 |
| 2:B:1717:ARG:NH2 | 2:B:1745:GLU:O | 2.43 | 0.49 |
| 1:A:875:GLY:O | 1:A:877:MET:N | 2.46 | 0.49 |
| 1:A:1008:GLU:HA | 1:A:1667:VAL:HA | 1.94 | 0.49 |
| 1:A:1222:LEU:HD13 | 1:A:1691:MET:SD | 2.53 | 0.49 |
| 2:B:989:ASP:OD1 | 2:B:990:TYR:N | 2.46 | 0.49 |
| 2:B:1115:GLU:OE1 | 2:B:1115:GLU:N | 2.45 | 0.49 |
| 2:B:1295:ASP:HA | 2:B:1298:VAL:HG22 | 1.94 | 0.49 |
| 2:B:1968:TYR:HD2 | 2:B:1969:LEU:HD12 | 1.78 | 0.49 |
| 1:A:416:PHE:HA | 1:A:419:ILE:HG12 | 1.95 | 0.49 |
| 1:A:985:ALA:N | 1:A:1084:GLU:OE1 | 2.22 | 0.49 |
| 1:A:1209:ILE:O | 1:A:1213:VAL:HG23 | 2.13 | 0.49 |
| 2:B:322:PRO:HA | 2:B:407:PHE:CG | 2.48 | 0.49 |
| 2:B:813:GLY:HA3 | 2:B:1049:GLN:HB3 | 1.95 | 0.49 |
| 1:A:469:ARG:HB2 | 1:A:469:ARG:CZ | 2.41 | 0.48 |
| 1:A:477:ASN:ND2 | 1:A:582:GLU:OE1 | 2.46 | 0.48 |
| 1:A:824:PRO:HB2 | 3:A:1901:NAP:H1D | 1.95 | 0.48 |
| 1:A:1028:TRP:CE3 | 1:A:1037:MET:HG2 | 2.48 | 0.48 |
| 1:A:1236:VAL:HG23 | 1:A:1323:LYS:HD2 | 1.95 | 0.48 |
| 2:B:304:THR:OG1 | 2:B:305:SER:N | 2.45 | 0.48 |
| 1:A:32:GLN:HA | 1:A:35:PHE:CD1 | 2.48 | 0.48 |
| 1:A:1709:TYR:HA | 1:A:1734:PHE:HB2 | 1.94 | 0.48 |
| 2:B:129:ILE:O | 2:B:131:LYS:N | 2.42 | 0.48 |
| 2:B:1512:GLU:HB3 | 2:B:1618:ILE:HG13 | 1.96 | 0.48 |
| 1:A:965:LYS:HB3 | 1:A:970:ASP:OD1 | 2.13 | 0.48 |
| 1:A:1019:VAL:HG22 | 1:A:1385:ILE:HG22 | 1.96 | 0.48 |
| 2:B:584:MET:CB | 4:B:2101:FMN:H6 | 2.12 | 0.48 |
| 2:B:752:LEU:N | 2:B:784:ASP:OD2 | 2.27 | 0.48 |
| 2:B:1539:TYR:O | 2:B:1543:SER:OG | 2.29 | 0.48 |
| 2:B:1911:ASP:O | 2:B:1914:LYS:HG2 | 2.13 | 0.48 |
| 2:B:1053:LYS:HZ3 | 2:B:1054:VAL:H | 1.61 | 0.48 |
| 1:A:712:PHE:CE1 | 1:A:717:THR:HG21 | 2.29 | 0.48 |
| 1:A:1191:TRP:HZ2 | 1:A:1215:VAL:HG21 | 1.77 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1587:PRO:HG3 | 1:A:1594:TRP:CE3 | 2.49 | 0.48 |
| 2:B:461:ILE:HA | 2:B:464:VAL:HG12 | 1.95 | 0.48 |
| 2:B:1843:VAL:HG13 | 2:B:1895:LEU:HD23 | 1.95 | 0.48 |
| 2:B:429:ASP:O | 2:B:432:GLU:HB2 | 2.13 | 0.48 |
| 1:A:482:LEU:HD12 | 1:A:483:THR:H | 1.78 | 0.48 |
| 1:A:520:PHE:HA | 1:A:523:TYR:HB3 | 1.94 | 0.48 |
| 1:A:1416:VAL:HG13 | 1:A:1650:GLY:N | 2.29 | 0.48 |
| 2:B:243:LEU:HB3 | 2:B:245:LEU:HD23 | 1.95 | 0.48 |
| 2:B:313:ASP:OD1 | 2:B:317:ASN:ND2 | 2.46 | 0.48 |
| 2:B:448:PHE:CE1 | 2:B:472:PRO:HD2 | 2.48 | 0.48 |
| 2:B:612:PHE:CZ | 3:B:2102:NAP:N7A | 2.73 | 0.48 |
| 2:B:767:TYR:HB3 | 2:B:783:PHE:CD2 | 2.48 | 0.48 |
| 2:B:875:ARG:O | 2:B:879:ILE:HG12 | 2.14 | 0.48 |
| 2:B:1792:PHE:CD1 | 2:B:1806:LEU:HD22 | 2.48 | 0.48 |
| 1:A:1233:TYR:OH | 1:A:1290:LEU:O | 2.26 | 0.48 |
| 2:B:167:TYR:OH | 2:B:171:GLN:NE2 | 2.46 | 0.48 |
| 1:A:768:ASP:OD1 | 1:A:817:ARG:NE | 2.45 | 0.48 |
| 1:A:982:GLU:O | 2:B:943:GLU:HG3 | 2.14 | 0.48 |
| 2:B:313:ASP:OD2 | 2:B:374:TYR:OH | 2.30 | 0.48 |
| 1:A:442:ASN:H | 1:A:445:LEU:HB2 | 1.79 | 0.48 |
| 1:A:1201:ASP:O | 1:A:1204:SER:OG | 2.26 | 0.48 |
| 1:A:1203:ILE:HD13 | 1:A:1211:LEU:HD22 | 1.95 | 0.48 |
| 2:B:698:ASP:O | 2:B:701:SER:OG | 2.24 | 0.48 |
| 2:B:797:GLU:CD | 2:B:1058:ILE:H | 2.17 | 0.48 |
| 2:B:1119:GLU:HG2 | 2:B:1120:LEU:H | 1.77 | 0.48 |
| 2:B:1614:HIS:ND1 | 2:B:1623:ILE:O | 2.35 | 0.48 |
| 2:B:2009:LEU:HD23 | 2:B:2009:LEU:H | 1.79 | 0.48 |
| 1:A:22:PHE:CZ | 2:B:1969:LEU:HD23 | 2.49 | 0.47 |
| 1:A:877:MET:O | 1:A:879:ALA:N | 2.47 | 0.47 |
| 1:A:1358:ARG:NH2 | 1:A:1615:ASP:OD2 | 2.33 | 0.47 |
| 2:B:176:ASP:OD2 | 2:B:241:LYS:NZ | 2.47 | 0.47 |
| 2:B:865:ASN:OD1 | 2:B:866:LYS:NZ | 2.47 | 0.47 |
| 2:B:1783:LYS:HB2 | 2:B:1785:LEU:HD23 | 1.95 | 0.47 |
| 2:B:1910:ILE:HA | 2:B:1914:LYS:HD3 | 1.95 | 0.47 |
| 1:A:9:LEU:HD21 | 2:B:2035:GLN:HE22 | 1.79 | 0.47 |
| 1:A:796:ILE:HD11 | 3:A:1901:NAP:N6A | 2.28 | 0.47 |
| 1:A:864:CYS:SG | 1:A:907:LEU:HD13 | 2.54 | 0.47 |
| 1:A:1013:LEU:O | 1:A:1388:ALA:HB3 | 2.14 | 0.47 |
| 1:A:1365:ARG:NH1 | 1:A:1370:THR:HG23 | 2.29 | 0.47 |
| 1:A:1631:SER:O | 1:A:1631:SER:OG | 2.30 | 0.47 |
| 1:A:326:LEU:O | 1:A:329:LEU:HG | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:140:CYS:SG | 2:B:542:ILE:HD13 | 2.54 | 0.47 |
| 2:B:568:THR:HG1 | 2:B:571:SER:H | 1.63 | 0.47 |
| 2:B:1230:ASP:OD1 | 2:B:1232:PHE:N | 2.47 | 0.47 |
| 1:A:29:ILE:HG13 | 2:B:1879:TYR:O | 2.14 | 0.47 |
| 1:A:1716:PRO:HB2 | 1:A:1739:ILE:HD13 | 1.95 | 0.47 |
| 2:B:1227:ASN:N | 2:B:1234:PRO:O | 2.35 | 0.47 |
| 2:B:1449:PHE:CD2 | 2:B:1503:LEU:HD21 | 2.50 | 0.47 |
| 2:B:1456:LYS:O | 2:B:1464:SER:N | 2.47 | 0.47 |
| 2:B:1857:SER:HA | 2:B:1860:ARG:HG2 | 1.95 | 0.47 |
| 1:A:91:LYS:HE2 | 2:B:1518:ASN:HB2 | 1.97 | 0.47 |
| 2:B:147:VAL:HG21 | 2:B:256:TRP:CE2 | 2.49 | 0.47 |
| 2:B:1599:VAL:HG21 | 2:B:1639:ILE:HD13 | 1.96 | 0.47 |
| 1:A:877:MET:C | 1:A:879:ALA:H | 2.18 | 0.47 |
| 1:A:1063:GLY:O | 1:A:1070:TYR:N | 2.41 | 0.47 |
| 1:A:1333:PHE:HE1 | 1:A:1338:SER:HB2 | 1.78 | 0.47 |
| 2:B:539:ASP:N | 2:B:539:ASP:OD1 | 2.47 | 0.47 |
| 2:B:903:GLU:HA | 2:B:982:LEU:HD13 | 1.97 | 0.47 |
| 1:A:821:CYS:SG | 1:A:861:LEU:HD12 | 2.55 | 0.47 |
| 1:A:1005:PRO:HB2 | 1:A:1006:GLU:OE1 | 2.15 | 0.47 |
| 1:A:1046:GLU:H | 1:A:1046:GLU:CD | 2.17 | 0.47 |
| 1:A:1226:ILE:HD11 | 1:A:1394:MET:HE1 | 1.97 | 0.47 |
| 1:A:1332:ASP:OD1 | 1:A:1333:PHE:N | 2.47 | 0.47 |
| 2:B:5:ARG:HG2 | 2:B:6:PRO:O | 2.14 | 0.47 |
| 2:B:177:LEU:O | 2:B:180:SER:OG | 2.30 | 0.47 |
| 2:B:237:THR:HG23 | 2:B:276:TRP:CZ3 | 2.50 | 0.47 |
| 2:B:310:MET:HE1 | 2:B:371:GLU:HA | 1.97 | 0.47 |
| 2:B:679:THR:O | 2:B:683:GLU:HG2 | 2.14 | 0.47 |
| 2:B:790:SER:N | 4:B:2101:FMN:C8M | 2.75 | 0.47 |
| 2:B:1156:ASN:ND2 | 2:B:1159:HIS:HB2 | 2.30 | 0.47 |
| 2:B:1275:GLU:HG2 | 2:B:1359:SER:HB2 | 1.97 | 0.47 |
| 2:B:1501:ASP:O | 2:B:1504:SER:OG | 2.27 | 0.47 |
| 2:B:1728:ILE:HG23 | 2:B:1732:GLY:HA2 | 1.96 | 0.47 |
| 2:B:1856:ASP:N | 2:B:1883:ASN:HD21 | 2.13 | 0.47 |
| 2:B:1893:ARG:HD3 | 2:B:1944:GLN:OE1 | 2.14 | 0.47 |
| 1:A:449:MET:O | 1:A:453:ILE:HG12 | 2.15 | 0.47 |
| 1:A:840:GLU:HA | 1:A:843:ILE:HG22 | 1.97 | 0.47 |
| 2:B:21:PRO:HG2 | 2:B:24:LEU:HD12 | 1.97 | 0.47 |
| 2:B:111:ILE:HD12 | 2:B:114:VAL:HB | 1.97 | 0.47 |
| 2:B:797:GLU:OE1 | 2:B:797:GLU:N | 2.43 | 0.47 |
| 2:B:907:LYS:HA | 2:B:972:PHE:CZ | 2.50 | 0.47 |
| 2:B:1672:GLU:O | 2:B:1676:GLU:HG2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1878:ASN:HB3 | 2:B:1880:ASN:OD1 | 2.15 | 0.47 |
| 2:B:2023:SER:HB3 | 2:B:2026:ILE:HG12 | 1.96 | 0.47 |
| 2:B:198:GLN:OE1 | 2:B:213:PRO:HB3 | 2.15 | 0.47 |
| 2:B:400:LYS:HB2 | 2:B:402:LYS:HZ1 | 1.80 | 0.47 |
| 2:B:1705:THR:HA | 2:B:1751:THR:HA | 1.97 | 0.47 |
| 2:B:1769:LEU:O | 2:B:1772:MET:HG3 | 2.15 | 0.47 |
| 2:B:1861:PHE:CD2 | 2:B:1912:ILE:HG21 | 2.49 | 0.47 |
| 1:A:1498:ARG:NH1 | 1:A:1745:TYR:OH | 2.47 | 0.47 |
| 1:A:1705:ASP:OD2 | 1:A:1706:LYS:N | 2.48 | 0.47 |
| 2:B:222:PRO:HG3 | 2:B:294:GLY:O | 2.14 | 0.47 |
| 2:B:763:ASP:OD1 | 2:B:1050:TYR:OH | 2.26 | 0.47 |
| 2:B:796:LYS:HB2 | 2:B:1055:ASP:O | 2.15 | 0.47 |
| 2:B:899:CYS:SG | 2:B:903:GLU:HG3 | 2.55 | 0.47 |
| 2:B:1118:SER:N | 2:B:1166:LYS:HA | 2.30 | 0.47 |
| 2:B:2005:LYS:NZ | 2:B:2016:SER:OG | 2.48 | 0.47 |
| 1:A:47:ILE:HD12 | 2:B:1653:PHE:HE1 | 1.79 | 0.46 |
| 1:A:654:ASN:ND2 | 1:A:657:LEU:HG | 2.30 | 0.46 |
| 1:A:1181:ARG:NH2 | 1:A:1347:THR:O | 2.35 | 0.46 |
| 1:A:1410:ASP:OD1 | 1:A:1422:GLY:N | 2.42 | 0.46 |
| 2:B:332:SER:OG | 2:B:334:LYS:HG3 | 2.15 | 0.46 |
| 2:B:1166:LYS:HE3 | 2:B:1167:HIS:CE1 | 2.50 | 0.46 |
| 1:A:984:ARG:HH21 | 2:B:940:ARG:CZ | 2.28 | 0.46 |
| 1:A:997:TYR:O | 1:A:1000:ILE:HG22 | 2.16 | 0.46 |
| 1:A:1628:LEU:HD23 | 1:A:1629:TYR:N | 2.31 | 0.46 |
| 2:B:221:VAL:HG21 | 2:B:412:ALA:HB2 | 1.98 | 0.46 |
| 2:B:326:LEU:O | 2:B:366:LEU:N | 2.33 | 0.46 |
| 2:B:538:ALA:HB3 | 2:B:540:LYS:NZ | 2.29 | 0.46 |
| 2:B:1137:TRP:CE2 | 2:B:1197:LEU:HG | 2.51 | 0.46 |
| 1:A:1193:ALA:O | 1:A:1196:TYR:N | 2.37 | 0.46 |
| 2:B:1247:LYS:HA | 2:B:1333:LEU:HD23 | 1.97 | 0.46 |
| 1:A:427:ASP:HB3 | 1:A:430:THR:HG22 | 1.97 | 0.46 |
| 1:A:693:GLU:HB3 | 1:A:901:ALA:HB2 | 1.98 | 0.46 |
| 1:A:1068:LYS:HE2 | 1:A:1068:LYS:HB2 | 1.84 | 0.46 |
| 2:B:164:ARG:HH22 | 2:B:209:PRO:HA | 1.80 | 0.46 |
| 2:B:949:ALA:HB1 | 2:B:951:THR:HG23 | 1.97 | 0.46 |
| 2:B:1018:LYS:O | 2:B:1021:SER:OG | 2.26 | 0.46 |
| 1:A:743:SER:HB3 | 1:A:746:ASP:OD1 | 2.15 | 0.46 |
| 1:A:1678:THR:O | 1:A:1681:SER:OG | 2.25 | 0.46 |
| 2:B:9:LEU:HB2 | 2:B:17:THR:HG23 | 1.98 | 0.46 |
| 2:B:11:HIS:H | 2:B:15:GLU:HG3 | 1.81 | 0.46 |
| 2:B:136:LEU:HD23 | 2:B:136:LEU:H | 1.81 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:573:LEU:HB3 | 2:B:574:LEU:HD12 | 1.98 | 0.46 |
| 2:B:1174:LYS:O | 2:B:1175:LYS:HG2 | 2.15 | 0.46 |
| 1:A:1257:GLY:O | 1:A:1261:ASP:HB2 | 2.15 | 0.46 |
| 1:A:1509:LYS:HA | 1:A:1513:ASN:HB2 | 1.97 | 0.46 |
| 1:A:1744:SER:O | 1:A:1744:SER:OG | 2.29 | 0.46 |
| 2:B:150:PHE:CE1 | 2:B:489:PHE:HD2 | 2.33 | 0.46 |
| 2:B:584:MET:HE2 | 4:B:2101:FMN:C5A | 2.12 | 0.46 |
| 2:B:1211:ARG:HD2 | 2:B:1551:VAL:HB | 1.98 | 0.46 |
| 1:A:500:LYS:NZ | 1:A:508:GLU:OE2 | 2.28 | 0.46 |
| 2:B:136:LEU:HD21 | 2:B:535:GLN:O | 2.15 | 0.46 |
| 1:A:86:LYS:HE3 | 1:A:92:PRO:HA | 1.96 | 0.46 |
| 1:A:1000:ILE:HD12 | 1:A:1003:ILE:HD12 | 1.96 | 0.46 |
| 2:B:59:TYR:CD2 | 2:B:82:PHE:HD1 | 2.34 | 0.46 |
| 2:B:138:TYR:CG | 2:B:138:TYR:O | 2.69 | 0.46 |
| 2:B:198:GLN:HB2 | 2:B:217:TYR:CZ | 2.51 | 0.46 |
| 2:B:1119:GLU:H | 2:B:1119:GLU:CD | 2.19 | 0.46 |
| 1:A:876:LEU:CD2 | 3:A:1901:NAP:O2A | 2.56 | 0.46 |
| 1:A:877:MET:C | 1:A:879:ALA:N | 2.69 | 0.46 |
| 2:B:102:LEU:HD21 | 2:B:111:ILE:HA | 1.97 | 0.46 |
| 2:B:259:GLY:HA3 | 2:B:264:LEU:HA | 1.98 | 0.46 |
| 2:B:797:GLU:OE2 | 2:B:1058:ILE:HG22 | 2.16 | 0.46 |
| 1:A:381:GLY:HA3 | 1:A:788:SER:OG | 2.16 | 0.46 |
| 1:A:490:ASP:OD1 | 1:A:491:VAL:N | 2.49 | 0.46 |
| 1:A:989:PHE:HZ | 1:A:1223:SER:HA | 1.81 | 0.46 |
| 2:B:462:ASP:OD1 | 2:B:462:ASP:N | 2.46 | 0.46 |
| 2:B:1148:VAL:HA | 2:B:1152:LYS:O | 2.15 | 0.46 |
| 1:A:83:LYS:HG3 | 1:A:84:ASP:OD1 | 2.15 | 0.45 |
| 1:A:90:TYR:C | 1:A:92:PRO:HD3 | 2.35 | 0.45 |
| 1:A:1151:GLU:HG3 | 1:A:1166:LEU:HD11 | 1.98 | 0.45 |
| 1:A:1374:PHE:HA | 1:A:1548:SER:OG | 2.15 | 0.45 |
| 2:B:1649:THR:OG1 | 2:B:1787:PRO:HG2 | 2.17 | 0.45 |
| 2:B:1761:ALA:HB3 | 2:B:1764:PHE:HD2 | 1.80 | 0.45 |
| 1:A:496:GLY:HA3 | 1:A:514:LYS:HD3 | 1.98 | 0.45 |
| 1:A:998:ASP:OD1 | 1:A:998:ASP:N | 2.48 | 0.45 |
| 1:A:1121:GLN:NE2 | 1:A:1122:GLU:O | 2.42 | 0.45 |
| 1:A:1713:LEU:C | 1:A:1716:PRO:HD2 | 2.36 | 0.45 |
| 2:B:396:PHE:CD1 | 2:B:732:ASP:HB2 | 2.52 | 0.45 |
| 2:B:461:ILE:O | 2:B:465:VAL:HG22 | 2.15 | 0.45 |
| 2:B:612:PHE:HD2 | 3:B:2102:NAP:N6A | 2.11 | 0.45 |
| 2:B:926:ILE:HD11 | 2:B:1030:SER:HB2 | 1.97 | 0.45 |
| 2:B:1328:SER:HB2 | 2:B:1407:ASN:HB3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1990:LYS:HB3 | 2:B:1992:GLN:HE22 | 1.82 | 0.45 |
| 1:A:47:ILE:HB | 2:B:1653:PHE:CD1 | 2.51 | 0.45 |
| 1:A:649:ASP:OD1 | 1:A:650:GLY:N | 2.50 | 0.45 |
| 1:A:967:VAL:HG22 | 2:B:1498:PRO:HG3 | 1.97 | 0.45 |
| 2:B:94:ILE:HA | 2:B:97:PHE:HB3 | 1.97 | 0.45 |
| 2:B:931:ARG:NH1 | 2:B:959:ASN:HA | 2.31 | 0.45 |
| 2:B:1090:TYR:CE1 | 2:B:1135:LEU:HB3 | 2.52 | 0.45 |
| 2:B:1171:THR:HB | 2:B:1180:THR:HB | 1.98 | 0.45 |
| 1:A:46:GLU:CD | 1:A:53:LEU:H | 2.20 | 0.45 |
| 2:B:84:SER:HA | 2:B:88:ASP:OD1 | 2.16 | 0.45 |
| 2:B:687:LEU:HD23 | 2:B:687:LEU:HA | 1.69 | 0.45 |
| 2:B:940:ARG:HA | 2:B:940:ARG:HD3 | 1.79 | 0.45 |
| 2:B:1311:PHE:O | 2:B:1315:ILE:HG13 | 2.16 | 0.45 |
| 2:B:1517:GLU:OE2 | 2:B:1517:GLU:N | 2.46 | 0.45 |
| 2:B:1547:ASN:HB3 | 2:B:1550:HIS:CD2 | 2.52 | 0.45 |
| 2:B:1745:GLU:N | 2:B:1745:GLU:OE1 | 2.50 | 0.45 |
| 1:A:30:GLU:OE1 | 1:A:30:GLU:N | 2.50 | 0.45 |
| 2:B:999:GLY:CA | 3:B:2102:NAP:H2A | 2.45 | 0.45 |
| 1:A:1229:PRO:HB3 | 1:A:1290:LEU:HD23 | 1.97 | 0.45 |
| 1:A:1317:ILE:HD11 | 1:A:1325:VAL:HG12 | 1.97 | 0.45 |
| 2:B:138:TYR:O | 2:B:141:LYS:HD2 | 2.17 | 0.45 |
| 2:B:356:SER:HB3 | 2:B:367:SER:HB3 | 1.97 | 0.45 |
| 2:B:816:ASP:O | 2:B:819:TRP:HD1 | 1.99 | 0.45 |
| 2:B:1404:ASP:OD1 | 2:B:1407:ASN:ND2 | 2.49 | 0.45 |
| 2:B:1968:TYR:CD2 | 2:B:1969:LEU:HD12 | 2.51 | 0.45 |
| 1:A:709:THR:HA | 3:A:1901:NAP:O1X | 2.16 | 0.45 |
| 1:A:1576:PHE:CD1 | 1:A:1576:PHE:N | 2.83 | 0.45 |
| 2:B:795:SER:O | 2:B:805:LYS:NZ | 2.32 | 0.45 |
| 2:B:1065:ILE:HG13 | 2:B:1066:HIS:N | 2.31 | 0.45 |
| 2:B:1528:LEU:HD12 | 2:B:1578:LEU:HD21 | 1.99 | 0.45 |
| 2:B:2018:TYR:CE1 | 2:B:2027:LYS:HB3 | 2.51 | 0.45 |
| 1:A:323:SER:C | 1:A:325:ALA:H | 2.20 | 0.45 |
| 1:A:678:LYS:HE2 | 1:A:678:LYS:HB2 | 1.82 | 0.45 |
| 1:A:1587:PRO:HG2 | 1:A:1591:ALA:HA | 1.99 | 0.45 |
| 2:B:257:SER:O | 2:B:444:VAL:HA | 2.17 | 0.45 |
| 2:B:479:THR:O | 2:B:505:LYS:NZ | 2.39 | 0.45 |
| 2:B:1230:ASP:OD1 | 2:B:1231:GLY:N | 2.49 | 0.45 |
| 2:B:1475:GLU:OE2 | 2:B:1479:LYS:HA | 2.17 | 0.45 |
| 2:B:1735:LYS:O | 2:B:1737:GLU:N | 2.50 | 0.45 |
| 2:B:1863:VAL:HG12 | 2:B:1898:LEU:CD1 | 2.47 | 0.45 |
| 1:A:14:LEU:HD21 | 2:B:1803:LEU:HD12 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:114:VAL:HA | 2:B:118:ILE:HD13 | 1.98 | 0.45 |
| 2:B:277:ASP:OD1 | 2:B:278:SER:N | 2.50 | 0.45 |
| 2:B:323:SER:OG | 2:B:407:PHE:HB3 | 2.17 | 0.45 |
| 2:B:520:SER:HA | 2:B:521:ASN:HA | 1.72 | 0.45 |
| 1:A:18:LEU:HD22 | 2:B:1800:TYR:CE1 | 2.52 | 0.45 |
| 1:A:493:ARG:HH11 | 1:A:518:ARG:HG2 | 1.82 | 0.45 |
| 1:A:674:THR:HG22 | 1:A:676:LYS:H | 1.82 | 0.45 |
| 1:A:1006:GLU:O | 1:A:1006:GLU:HG2 | 2.18 | 0.45 |
| 1:A:1104:ILE:HA | 1:A:1186:GLN:NE2 | 2.32 | 0.45 |
| 1:A:1155:ILE:O | 1:A:1159:GLY:N | 2.42 | 0.45 |
| 2:B:16:HIS:HE1 | 2:B:85:ARG:HG2 | 1.82 | 0.45 |
| 2:B:312:GLN:NE2 | 2:B:316:ASP:OD2 | 2.49 | 0.45 |
| 2:B:408:LEU:O | 2:B:410:ILE:N | 2.47 | 0.45 |
| 1:A:864:CYS:HB2 | 1:A:916:CYS:SG | 2.57 | 0.44 |
| 1:A:1446:ARG:NH1 | 1:A:1512:GLY:HA2 | 2.32 | 0.44 |
| 2:B:767:TYR:HA | 2:B:772:TRP:CD1 | 2.52 | 0.44 |
| 2:B:977:GLN:H | 2:B:977:GLN:CD | 2.18 | 0.44 |
| 2:B:1226:TYR:CE2 | 2:B:1228:PRO:HG3 | 2.52 | 0.44 |
| 2:B:1602:VAL:HG13 | 2:B:1637:VAL:HG11 | 1.99 | 0.44 |
| 2:B:1876:ILE:HG12 | 2:B:1888:ALA:HB2 | 1.98 | 0.44 |
| 1:A:57:ALA:O | 1:A:61:ILE:HG12 | 2.17 | 0.44 |
| 1:A:735:ILE:HG22 | 1:A:737:VAL:HG23 | 1.99 | 0.44 |
| 1:A:1202:THR:O | 1:A:1206:VAL:HG22 | 2.17 | 0.44 |
| 2:B:905:THR:HA | 2:B:982:LEU:HA | 1.98 | 0.44 |
| 2:B:1767:PRO:HA | 2:B:1770:THR:HG22 | 1.98 | 0.44 |
| 2:B:1860:ARG:HA | 2:B:1863:VAL:HG22 | 1.98 | 0.44 |
| 2:B:1874:LEU:HD13 | 2:B:1895:LEU:HD12 | 1.98 | 0.44 |
| 1:A:359:PHE:CE2 | 1:A:363:LYS:HD3 | 2.53 | 0.44 |
| 2:B:245:LEU:HD12 | 2:B:249:GLU:HG3 | 1.98 | 0.44 |
| 2:B:1150:GLY:O | 2:B:1151:SER:OG | 2.32 | 0.44 |
| 1:A:1446:ARG:HD2 | 1:A:1511:TRP:O | 2.17 | 0.44 |
| 1:A:1676:TYR:CZ | 1:A:1680:VAL:HG21 | 2.51 | 0.44 |
| 1:A:1725:VAL:HG11 | 1:A:1732:LEU:HB3 | 2.00 | 0.44 |
| 2:B:215:GLN:HA | 2:B:218:LEU:HB2 | 2.00 | 0.44 |
| 2:B:296:ARG:NH1 | 2:B:425:LEU:HB3 | 2.31 | 0.44 |
| 2:B:612:PHE:CD2 | 3:B:2102:NAP:N7A | 2.70 | 0.44 |
| 2:B:856:ASP:HA | 2:B:860:PHE:HB2 | 1.98 | 0.44 |
| 2:B:887:GLN:O | 2:B:889:PRO:HD3 | 2.17 | 0.44 |
| 2:B:934:TYR:OH | 2:B:968:THR:HG21 | 2.18 | 0.44 |
| 2:B:977:GLN:HA | 2:B:980:LYS:HG2 | 1.98 | 0.44 |
| 2:B:1685:PHE:O | 2:B:1689:TYR:N | 2.32 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1985:PRO:HG2 | 2:B:1988:SER:OG | 2.17 | 0.44 |
| 1:A:763:LEU:HD23 | 1:A:763:LEU:HA | 1.77 | 0.44 |
| 1:A:1151:GLU:HB3 | 1:A:1153:PHE:CE2 | 2.51 | 0.44 |
| 1:A:1209:ILE:HD11 | 1:A:1330:TYR:HD2 | 1.83 | 0.44 |
| 1:A:1476:LYS:NZ | 1:A:1484:SER:H | 2.16 | 0.44 |
| 2:B:355:ILE:HA | 2:B:366:LEU:HD13 | 1.99 | 0.44 |
| 2:B:945:PHE:HD1 | 2:B:977:GLN:HE21 | 1.65 | 0.44 |
| 2:B:1019:LYS:HD3 | 3:B:2102:NAP:H4B | 1.99 | 0.44 |
| 2:B:1266:ASN:HD21 | 2:B:1268:GLU:HB3 | 1.82 | 0.44 |
| 2:B:1382:ILE:HG22 | 2:B:1390:MET:O | 2.18 | 0.44 |
| 2:B:1725:PHE:CD1 | 2:B:1739:ILE:HG13 | 2.53 | 0.44 |
| 2:B:1863:VAL:HG11 | 2:B:1876:ILE:HG13 | 1.99 | 0.44 |
| 2:B:2029:ILE:HA | 2:B:2032:ASN:OD1 | 2.18 | 0.44 |
| 1:A:387:GLY:O | 1:A:740:ASN:ND2 | 2.48 | 0.44 |
| 1:A:437:ILE:HA | 1:A:440:ARG:HH21 | 1.83 | 0.44 |
| 1:A:681:LEU:HD12 | 1:A:682:VAL:N | 2.32 | 0.44 |
| 1:A:755:TYR:CE1 | 1:A:766:ASP:HA | 2.53 | 0.44 |
| 1:A:820:GLN:NE2 | 1:A:822:ILE:HD11 | 2.33 | 0.44 |
| 1:A:991:PHE:CD2 | 1:A:1397:PRO:HG3 | 2.52 | 0.44 |
| 1:A:1143:LYS:HA | 1:A:1150:CYS:SG | 2.58 | 0.44 |
| 2:B:296:ARG:HA | 2:B:296:ARG:HD3 | 1.74 | 0.44 |
| 2:B:1317:TRP:O | 2:B:1321:ILE:HG12 | 2.18 | 0.44 |
| 1:A:1541:VAL:HG12 | 1:A:1542:ALA:N | 2.33 | 0.44 |
| 2:B:1119:GLU:HG2 | 2:B:1120:LEU:N | 2.33 | 0.44 |
| 2:B:1703:GLU:OE2 | 2:B:1703:GLU:N | 2.50 | 0.44 |
| 2:B:1740:PHE:HB3 | 2:B:1743:ILE:HD13 | 2.00 | 0.44 |
| 1:A:403:TYR:HA | 1:A:406:TRP:HD1 | 1.83 | 0.44 |
| 1:A:630:SER:OG | 1:A:659:SER:HB2 | 2.17 | 0.44 |
| 1:A:707:VAL:HG12 | 1:A:708:THR:N | 2.33 | 0.44 |
| 1:A:954:ARG:O | 1:A:958:ILE:HG12 | 2.18 | 0.44 |
| 1:A:1529:LEU:O | 1:A:1532:PHE:N | 2.40 | 0.44 |
| 2:B:96:SER:HB3 | 2:B:535:GLN:OE1 | 2.18 | 0.44 |
| 2:B:189:HIS:CE1 | 2:B:199:GLY:HA2 | 2.52 | 0.44 |
| 2:B:265:VAL:HA | 2:B:268:VAL:HG12 | 1.99 | 0.44 |
| 2:B:825:LYS:HB2 | 2:B:825:LYS:HE3 | 1.70 | 0.44 |
| 2:B:1985:PRO:O | 2:B:1988:SER:OG | 2.31 | 0.44 |
| 1:A:680:VAL:HG22 | 1:A:769:ALA:HB3 | 2.00 | 0.44 |
| 2:B:266:THR:O | 2:B:270:ILE:HG12 | 2.18 | 0.44 |
| 2:B:756:SER:H | 4:B:2101:FMN:C5' | 2.30 | 0.44 |
| 2:B:907:LYS:HG3 | 2:B:972:PHE:CE2 | 2.53 | 0.44 |
| 2:B:1251:TRP:CE2 | 2:B:1261:TYR:HA | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:89:TYR:OH | 2:B:1779:ASP:OD2 | 2.22 | 0.43 |
| 1:A:1065:LEU:HD23 | 1:A:1081:PRO:HG3 | 2.00 | 0.43 |
| 1:A:1187:ILE:HG23 | 1:A:1188:PRO:HD2 | 2.00 | 0.43 |
| 2:B:42:PRO:HB3 | 2:B:46:PHE:HE1 | 1.83 | 0.43 |
| 2:B:577:ALA:HB1 | 2:B:1066:HIS:CD2 | 2.53 | 0.43 |
| 2:B:1094:LYS:HG3 | 2:B:1095:LYS:N | 2.32 | 0.43 |
| 2:B:1840:TYR:HB3 | 2:B:1963:PRO:HG3 | 2.00 | 0.43 |
| 1:A:39:HIS:ND1 | 2:B:1791:MET:SD | 2.91 | 0.43 |
| 1:A:485:ASP:OD1 | 1:A:486:PRO:HD2 | 2.18 | 0.43 |
| 1:A:979:VAL:O | 2:B:956:GLN:NE2 | 2.46 | 0.43 |
| 1:A:1028:TRP:CZ2 | 1:A:1100:GLY:HA3 | 2.53 | 0.43 |
| 2:B:43:THR:O | 2:B:46:PHE:N | 2.52 | 0.43 |
| 2:B:176:ASP:OD1 | 2:B:176:ASP:N | 2.49 | 0.43 |
| 1:A:876:LEU:HB2 | 1:A:877:MET:H | 1.72 | 0.43 |
| 1:A:984:ARG:HD2 | 1:A:1084:GLU:CD | 2.38 | 0.43 |
| 1:A:984:ARG:N | 2:B:943:GLU:O | 2.48 | 0.43 |
| 1:A:1020:THR:HG21 | 1:A:1386:MET:SD | 2.58 | 0.43 |
| 1:A:1115:LYS:HD3 | 1:A:1182:LEU:HD21 | 2.00 | 0.43 |
| 1:A:1148:GLU:OE2 | 1:A:1148:GLU:N | 2.47 | 0.43 |
| 1:A:1324:VAL:HG22 | 1:A:1386:MET:HG3 | 2.00 | 0.43 |
| 2:B:159:TYR:HE2 | 2:B:227:VAL:HG23 | 1.82 | 0.43 |
| 2:B:1453:SER:HA | 2:B:1468:THR:HA | 1.99 | 0.43 |
| 1:A:1271:ASP:O | 1:A:1274:GLN:HG2 | 2.18 | 0.43 |
| 1:A:1617:VAL:HG11 | 1:A:1629:TYR:HD2 | 1.83 | 0.43 |
| 2:B:96:SER:HA | 2:B:99:VAL:HG22 | 2.00 | 0.43 |
| 2:B:238:ILE:O | 2:B:242:VAL:HG23 | 2.18 | 0.43 |
| 2:B:488:ASP:OD1 | 2:B:514:LEU:HA | 2.18 | 0.43 |
| 2:B:1451:CYS:HA | 2:B:1470:GLY:HA3 | 1.99 | 0.43 |
| 2:B:1459:SER:OG | 2:B:1462:VAL:HG22 | 2.18 | 0.43 |
| 2:B:1678:TRP:HB3 | 2:B:1694:LEU:HD21 | 1.99 | 0.43 |
| 1:A:40:ASN:HB3 | 1:A:74:LEU:HD21 | 2.00 | 0.43 |
| 1:A:832:PHE:HD1 | 1:A:832:PHE:HA | 1.69 | 0.43 |
| 1:A:991:PHE:CE2 | 1:A:1397:PRO:HG3 | 2.54 | 0.43 |
| 1:A:1257:GLY:HA2 | 1:A:1261:ASP:HB2 | 2.01 | 0.43 |
| 1:A:1395:GLY:O | 1:A:1683:ARG:HD2 | 2.18 | 0.43 |
| 1:A:1603:LEU:HD23 | 1:A:1603:LEU:HA | 1.75 | 0.43 |
| 2:B:1926:GLU:O | 2:B:1930:GLU:HG3 | 2.19 | 0.43 |
| 1:A:442:ASN:O | 1:A:445:LEU:N | 2.51 | 0.43 |
| 1:A:878:SER:C | 1:A:880:ASN:N | 2.62 | 0.43 |
| 1:A:933:ASP:OD2 | 1:A:934:ASN:N | 2.51 | 0.43 |
| 1:A:1025:VAL:HG13 | 1:A:1025:VAL:O | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:332:SER:N | 2:B:335:GLN:HE21 | 2.10 | 0.43 |
| 2:B:1182:PHE:HD1 | 2:B:1191:PRO:HA | 1.83 | 0.43 |
| 2:B:1613:GLU:O | 2:B:1625:LYS:N | 2.44 | 0.43 |
| 2:B:1632:GLU:OE1 | 2:B:1632:GLU:N | 2.43 | 0.43 |
| 2:B:1726:GLU:H | 2:B:1975:PRO:HG3 | 1.83 | 0.43 |
| 2:B:1992:GLN:HA | 2:B:1995:ILE:HD12 | 2.00 | 0.43 |
| 1:A:326:LEU:O | 1:A:330:THR:HG23 | 2.19 | 0.43 |
| 1:A:710:SER:OG | 3:A:1901:NAP:C2A | 2.67 | 0.43 |
| 1:A:1015:ASN:HB2 | 1:A:1513:ASN:ND2 | 2.34 | 0.43 |
| 2:B:225:CYS:HB3 | 2:B:226:PRO:HD3 | 2.00 | 0.43 |
| 2:B:579:LEU:HD13 | 2:B:1065:ILE:HD11 | 2.00 | 0.43 |
| 2:B:585:THR:HA | 2:B:607:ALA:HB1 | 1.99 | 0.43 |
| 2:B:1137:TRP:CZ2 | 2:B:1197:LEU:HG | 2.54 | 0.43 |
| 2:B:1704:LEU:HB2 | 2:B:1758:LEU:HD13 | 2.01 | 0.43 |
| 2:B:1990:LYS:HB3 | 2:B:1992:GLN:NE2 | 2.34 | 0.43 |
| 1:A:697:GLY:HA3 | 1:A:905:LEU:HD11 | 2.01 | 0.43 |
| 1:A:1468:LEU:HD11 | 1:A:1492:ARG:CG | 2.49 | 0.43 |
| 2:B:761:ASP:OD1 | 2:B:761:ASP:N | 2.50 | 0.43 |
| 2:B:1547:ASN:HB3 | 2:B:1550:HIS:HD2 | 1.83 | 0.43 |
| 2:B:1569:MET:O | 2:B:1572:SER:OG | 2.23 | 0.43 |
| 2:B:1860:ARG:O | 2:B:1863:VAL:HG22 | 2.19 | 0.43 |
| 1:A:1477:GLU:HG2 | 1:A:1483:PHE:CZ | 2.53 | 0.43 |
| 1:A:1737:LYS:HA | 1:A:1737:LYS:HD2 | 1.78 | 0.43 |
| 2:B:90:ASN:O | 2:B:93:ASN:HB2 | 2.18 | 0.43 |
| 2:B:195:ILE:HG13 | 2:B:196:TYR:CD1 | 2.54 | 0.43 |
| 2:B:1126:TRP:CG | 2:B:1164:PRO:HG3 | 2.53 | 0.43 |
| 2:B:1709:GLY:H | 2:B:1713:GLY:HA3 | 1.84 | 0.43 |
| 2:B:1962:VAL:HA | 2:B:1963:PRO:HD3 | 1.87 | 0.43 |
| 1:A:710:SER:OG | 3:A:1901:NAP:N9A | 2.41 | 0.43 |
| 1:A:1226:ILE:HD13 | 1:A:1226:ILE:HA | 1.88 | 0.43 |
| 1:A:1401:VAL:HB | 1:A:1659:VAL:HG13 | 2.01 | 0.43 |
| 1:A:1525:LEU:HD12 | 1:A:1525:LEU:HA | 1.71 | 0.43 |
| 2:B:818:GLN:HB2 | 2:B:821:GLN:NE2 | 2.34 | 0.43 |
| 2:B:1338:HIS:CE1 | 2:B:1396:PHE:HE1 | 2.36 | 0.43 |
| 2:B:1845:VAL:HG23 | 2:B:1954:VAL:HG22 | 2.00 | 0.43 |
| 2:B:2011:LYS:HB2 | 2:B:2033:TRP:CE2 | 2.53 | 0.43 |
| 1:A:11:HIS:CG | 2:B:1986:LYS:HG3 | 2.54 | 0.42 |
| 1:A:31:THR:HG23 | 2:B:1999:ILE:HG21 | 1.99 | 0.42 |
| 1:A:45:ILE:HD12 | 2:B:1651:TYR:HE1 | 1.84 | 0.42 |
| 1:A:348:LEU:HD23 | 1:A:348:LEU:HA | 1.90 | 0.42 |
| 1:A:699:ILE:HG22 | 1:A:728:GLY:HA2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:877:MET:HE1 | 3:A:1901:NAP:H4N | 2.01 | 0.42 |
| 1:A:1135:SER:OG | 1:A:1136:LYS:N | 2.51 | 0.42 |
| 1:A:1693:ASN:O | 1:A:1696:THR:OG1 | 2.32 | 0.42 |
| 2:B:499:VAL:HG12 | 2:B:503:ARG:NH1 | 2.34 | 0.42 |
| 2:B:522:PRO:HD3 | 2:B:529:PHE:HE2 | 1.84 | 0.42 |
| 2:B:727:HIS:CE1 | 2:B:841:ILE:HD12 | 2.53 | 0.42 |
| 2:B:1088:VAL:HB | 2:B:1135:LEU:HD12 | 2.00 | 0.42 |
| 2:B:1274:ASP:OD1 | 2:B:1274:ASP:N | 2.51 | 0.42 |
| 2:B:1541:ILE:HA | 2:B:1546:TYR:HE1 | 1.84 | 0.42 |
| 1:A:1501:LYS:HE3 | 1:A:1501:LYS:HB3 | 1.91 | 0.42 |
| 2:B:42:PRO:HB3 | 2:B:46:PHE:CE1 | 2.53 | 0.42 |
| 2:B:852:TRP:CD1 | 2:B:852:TRP:C | 2.93 | 0.42 |
| 2:B:1358:VAL:HG13 | 2:B:1383:TYR:O | 2.18 | 0.42 |
| 2:B:1810:MET:HB2 | 2:B:1814:SER:OG | 2.19 | 0.42 |
| 2:B:1842:MET:HE2 | 2:B:1957:LEU:HD12 | 2.01 | 0.42 |
| 1:A:699:ILE:CG2 | 1:A:728:GLY:HA2 | 2.49 | 0.42 |
| 1:A:1018:VAL:HB | 1:A:1398:ILE:HG23 | 2.01 | 0.42 |
| 1:A:1119:MET:O | 1:A:1175:LYS:N | 2.47 | 0.42 |
| 1:A:1693:ASN:OD1 | 1:A:1697:ARG:HD2 | 2.19 | 0.42 |
| 2:B:396:PHE:N | 2:B:820:GLU:OE2 | 2.49 | 0.42 |
| 2:B:1178:LYS:HD3 | 2:B:1196:GLU:HB3 | 2.00 | 0.42 |
| 2:B:1549:ILE:O | 2:B:1564:THR:HA | 2.19 | 0.42 |
| 2:B:1777:TYR:CD2 | 2:B:1805:SER:HB2 | 2.54 | 0.42 |
| 2:B:1849:ARG:O | 2:B:1906:LYS:NZ | 2.27 | 0.42 |
| 2:B:1963:PRO:O | 2:B:1966:SER:OG | 2.26 | 0.42 |
| 1:A:428:ARG:HA | 1:A:428:ARG:HD3 | 1.77 | 0.42 |
| 1:A:1070:TYR:CZ | 1:A:1081:PRO:HB3 | 2.54 | 0.42 |
| 1:A:1694:ALA:HB1 | 1:A:1700:MET:HA | 2.00 | 0.42 |
| 2:B:523:ILE:HD12 | 2:B:523:ILE:HA | 1.87 | 0.42 |
| 2:B:1248:GLU:HG2 | 2:B:1261:TYR:CD2 | 2.54 | 0.42 |
| 2:B:1339:LEU:HD23 | 2:B:1339:LEU:HA | 1.74 | 0.42 |
| 2:B:1878:ASN:CB | 2:B:1887:VAL:HB | 2.48 | 0.42 |
| 1:A:14:LEU:HD11 | 2:B:1803:LEU:HD13 | 2.01 | 0.42 |
| 1:A:665:LEU:HD11 | 1:A:906:GLY:HA3 | 2.01 | 0.42 |
| 1:A:766:ASP:O | 1:A:817:ARG:NH1 | 2.52 | 0.42 |
| 2:B:259:GLY:H | 2:B:264:LEU:HD13 | 1.85 | 0.42 |
| 2:B:728:HIS:CD2 | 2:B:729:SER:H | 2.37 | 0.42 |
| 2:B:885:ASP:O | 2:B:1038:ARG:HA | 2.20 | 0.42 |
| 2:B:1541:ILE:HA | 2:B:1546:TYR:CE1 | 2.55 | 0.42 |
| 2:B:1594:PHE:HD1 | 2:B:1642:ALA:HB2 | 1.85 | 0.42 |
| 1:A:45:ILE:HD12 | 2:B:1651:TYR:CE1 | 2.54 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:683:THR:HB | 1:A:772:PRO:HA | 2.01 | 0.42 |
| 2:B:1638:LEU:HD23 | 2:B:1638:LEU:HA | 1.82 | 0.42 |
| 3:B:2102:NAP:O2N | 3:B:2102:NAP:H3D | 2.19 | 0.42 |
| 1:A:6:GLU:OE1 | 2:B:1991:PRO:HG2 | 2.20 | 0.42 |
| 1:A:816:THR:O | 1:A:818:PRO:HD3 | 2.20 | 0.42 |
| 1:A:857:TRP:HE3 | 1:A:861:LEU:HB2 | 1.85 | 0.42 |
| 1:A:971:ASN:OD1 | 1:A:972:VAL:HG23 | 2.20 | 0.42 |
| 1:A:1128:ASP:HB3 | 1:A:1166:LEU:HA | 2.01 | 0.42 |
| 1:A:1156:GLU:H | 1:A:1156:GLU:CD | 2.21 | 0.42 |
| 2:B:957:ASN:HD21 | 2:B:959:ASN:ND2 | 2.12 | 0.42 |
| 2:B:1273:GLY:N | 2:B:1360:THR:O | 2.48 | 0.42 |
| 2:B:1964:PHE:HD2 | 2:B:1965:HIS:ND1 | 2.18 | 0.42 |
| 1:A:2:LYS:HE2 | 1:A:2:LYS:HB2 | 1.86 | 0.42 |
| 1:A:1198:ILE:HA | 1:A:1701:PHE:CE2 | 2.55 | 0.42 |
| 2:B:717:LEU:N | 2:B:751:VAL:O | 2.38 | 0.42 |
| 2:B:1286:PHE:O | 2:B:1290:ILE:HG12 | 2.20 | 0.42 |
| 2:B:1731:ASP:OD1 | 2:B:1735:LYS:NZ | 2.45 | 0.42 |
| 1:A:20:TYR:CD1 | 2:B:1973:VAL:HG11 | 2.55 | 0.42 |
| 1:A:877:MET:HE2 | 3:A:1901:NAP:C3N | 2.49 | 0.42 |
| 2:B:116:GLU:OE2 | 2:B:117:ASN:ND2 | 2.52 | 0.42 |
| 2:B:136:LEU:CA | 2:B:139:HIS:HB2 | 2.50 | 0.42 |
| 2:B:887:GLN:HB3 | 2:B:1038:ARG:O | 2.20 | 0.42 |
| 2:B:1703:GLU:C | 2:B:1758:LEU:HD11 | 2.39 | 0.42 |
| 2:B:1726:GLU:OE2 | 2:B:1728:ILE:HD13 | 2.19 | 0.42 |
| 1:A:1353:GLU:OE1 | 1:A:1365:ARG:NH2 | 2.52 | 0.42 |
| 1:A:1582:TYR:CZ | 1:A:1583:LEU:HB2 | 2.55 | 0.42 |
| 2:B:16:HIS:CE1 | 2:B:85:ARG:HG2 | 2.55 | 0.42 |
| 2:B:1099:VAL:O | 2:B:1101:ALA:N | 2.48 | 0.42 |
| 2:B:1271:ILE:HD13 | 2:B:1322:LYS:HB3 | 2.02 | 0.42 |
| 2:B:1576:ARG:NH1 | 2:B:1580:GLU:OE1 | 2.53 | 0.42 |
| 1:A:626:ILE:HD12 | 1:A:626:ILE:C | 2.27 | 0.41 |
| 1:A:707:VAL:HG12 | 1:A:708:THR:H | 1.84 | 0.41 |
| 1:A:1499:GLU:O | 1:A:1503:GLN:HG3 | 2.20 | 0.41 |
| 2:B:223:VAL:O | 2:B:226:PRO:HD2 | 2.20 | 0.41 |
| 2:B:571:SER:HB3 | 2:B:578:PRO:HG3 | 2.02 | 0.41 |
| 2:B:598:LEU:HG | 2:B:604:ILE:HD13 | 2.03 | 0.41 |
| 2:B:886:PHE:CG | 2:B:887:GLN:N | 2.88 | 0.41 |
| 2:B:2000:PRO:HG2 | 2:B:2013:TYR:OH | 2.20 | 0.41 |
| 1:A:20:TYR:CE2 | 2:B:2023:SER:HB2 | 2.55 | 0.41 |
| 1:A:523:TYR:O | 1:A:527:MET:HG2 | 2.20 | 0.41 |
| 1:A:985:ALA:HB2 | 1:A:1045:LEU:HD22 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1000:ILE:HD11 | 1:A:1662:ASP:HB3 | 2.02 | 0.41 |
| 1:A:1310:VAL:HA | 1:A:1327:VAL:HG21 | 2.01 | 0.41 |
| 2:B:93:ASN:ND2 | 2:B:534:PHE:O | 2.53 | 0.41 |
| 2:B:261:SER:OG | 2:B:262:GLN:N | 2.53 | 0.41 |
| 2:B:353:ILE:HD11 | 2:B:372:SER:OG | 2.20 | 0.41 |
| 2:B:790:SER:HB3 | 4:B:2101:FMN:HM82 | 1.97 | 0.41 |
| 2:B:1190:LEU:HD23 | 2:B:1190:LEU:HA | 1.82 | 0.41 |
| 2:B:1533:PRO:HG3 | 2:B:1570:TYR:CZ | 2.55 | 0.41 |
| 1:A:1023:ALA:HB1 | 1:A:1219:GLU:HG3 | 2.02 | 0.41 |
| 1:A:1215:VAL:O | 1:A:1219:GLU:HG2 | 2.20 | 0.41 |
| 1:A:1529:LEU:HB3 | 1:A:1534:LEU:HB2 | 2.03 | 0.41 |
| 2:B:726:GLY:HA2 | 2:B:1042:LEU:HD23 | 2.02 | 0.41 |
| 2:B:882:LEU:HA | 2:B:882:LEU:HD23 | 1.81 | 0.41 |
| 1:A:410:ASP:HA | 1:A:413:SER:OG | 2.20 | 0.41 |
| 1:A:1330:TYR:HA | 1:A:1380:SER:HA | 2.03 | 0.41 |
| 1:A:1596:LEU:HD12 | 1:A:1596:LEU:HA | 1.77 | 0.41 |
| 1:A:1706:LYS:HD2 | 1:A:1707:ALA:O | 2.21 | 0.41 |
| 2:B:39:LEU:HA | 2:B:40:PRO:HD3 | 1.95 | 0.41 |
| 2:B:200:LEU:HD12 | 2:B:200:LEU:HA | 1.84 | 0.41 |
| 2:B:203:LEU:HB3 | 2:B:207:LYS:NZ | 2.35 | 0.41 |
| 2:B:734:HIS:HE1 | 2:B:767:TYR:OH | 2.04 | 0.41 |
| 2:B:1061:ILE:H | 2:B:1061:ILE:HG13 | 1.67 | 0.41 |
| 2:B:1433:LYS:HB3 | 2:B:1435:TRP:CE2 | 2.55 | 0.41 |
| 2:B:1962:VAL:HG13 | 2:B:1964:PHE:CD1 | 2.53 | 0.41 |
| 1:A:1192:ASP:OD1 | 1:A:1193:ALA:N | 2.54 | 0.41 |
| 1:A:1280:THR:HG23 | 1:A:1281:MET:SD | 2.60 | 0.41 |
| 1:A:1587:PRO:HB3 | 1:A:1594:TRP:CH2 | 2.55 | 0.41 |
| 2:B:137:LEU:H | 2:B:137:LEU:HD23 | 1.86 | 0.41 |
| 2:B:349:ARG:HE | 2:B:349:ARG:N | 2.19 | 0.41 |
| 2:B:512:ILE:HD13 | 2:B:512:ILE:HA | 1.90 | 0.41 |
| 2:B:814:VAL:HG21 | 2:B:827:THR:HB | 2.01 | 0.41 |
| 2:B:1266:ASN:HD22 | 2:B:1269:LYS:HE2 | 1.86 | 0.41 |
| 2:B:1563:GLY:O | 2:B:1565:ILE:HG23 | 2.20 | 0.41 |
| 2:B:1844:ALA:HA | 2:B:1887:VAL:HA | 2.02 | 0.41 |
| 2:B:1863:VAL:HA | 2:B:1866:VAL:HG12 | 2.03 | 0.41 |
| 2:B:2003:THR:HG22 | 2:B:2005:LYS:HG2 | 2.02 | 0.41 |
| 2:B:2025:LYS:O | 2:B:2028:SER:OG | 2.38 | 0.41 |
| 1:A:845:LEU:HA | 1:A:845:LEU:HD23 | 1.88 | 0.41 |
| 1:A:1062:ASN:OD1 | 1:A:1063:GLY:N | 2.51 | 0.41 |
| 1:A:1311:ASP:HB2 | 1:A:1405:THR:HG22 | 2.03 | 0.41 |
| 1:A:1442:ASN:OD1 | 1:A:1444:GLU:HG2 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:110:THR:O | 2:B:114:VAL:HG23 | 2.20 | 0.41 |
| 2:B:307:PRO:HA | 2:B:308:PRO:HD3 | 1.95 | 0.41 |
| 2:B:892:GLY:HA2 | 2:B:904:MET:SD | 2.61 | 0.41 |
| 2:B:1008:VAL:HG21 | 2:B:1012:ARG:NH2 | 2.36 | 0.41 |
| 2:B:1286:PHE:HA | 2:B:1542:VAL:HG11 | 2.01 | 0.41 |
| 1:A:412:LEU:HD12 | 1:A:412:LEU:HA | 1.83 | 0.41 |
| 1:A:871:THR:HG22 | 1:A:873:GLY:N | 2.35 | 0.41 |
| 1:A:1352:GLU:O | 1:A:1356:HIS:ND1 | 2.48 | 0.41 |
| 2:B:260:HIS:CG | 2:B:261:SER:H | 2.39 | 0.41 |
| 2:B:338:LYS:O | 2:B:341:GLU:HG3 | 2.20 | 0.41 |
| 2:B:1766:GLN:CG | 2:B:1767:PRO:HD3 | 2.50 | 0.41 |
| 1:A:1440:LEU:HD12 | 1:A:1440:LEU:HA | 1.92 | 0.41 |
| 1:A:1446:ARG:HH12 | 1:A:1512:GLY:HA2 | 1.84 | 0.41 |
| 2:B:271:ALA:HB3 | 2:B:440:LEU:HD22 | 2.03 | 0.41 |
| 2:B:1237:GLU:OE2 | 2:B:1242:ARG:NE | 2.52 | 0.41 |
| 2:B:1855:ASP:OD1 | 2:B:1858:ALA:N | 2.54 | 0.41 |
| 1:A:22:PHE:CE1 | 2:B:1826:MET:HB3 | 2.47 | 0.41 |
| 1:A:458:GLU:OE2 | 1:A:468:LYS:HD2 | 2.21 | 0.41 |
| 1:A:895:PHE:HB2 | 1:A:900:MET:HG2 | 2.03 | 0.41 |
| 1:A:1082:ILE:HG22 | 1:A:1083:ASP:O | 2.21 | 0.41 |
| 1:A:1131:PRO:HG3 | 1:A:1164:ARG:NE | 2.24 | 0.41 |
| 1:A:1268:VAL:HG11 | 1:A:1272:ILE:HD13 | 2.02 | 0.41 |
| 1:A:1289:LEU:HA | 1:A:1289:LEU:HD23 | 1.77 | 0.41 |
| 2:B:24:LEU:HD23 | 2:B:24:LEU:HA | 1.93 | 0.41 |
| 2:B:43:THR:O | 2:B:43:THR:OG1 | 2.37 | 0.41 |
| 2:B:475:TRP:O | 2:B:479:THR:HG22 | 2.21 | 0.41 |
| 2:B:521:ASN:CG | 2:B:522:PRO:HD2 | 2.41 | 0.41 |
| 2:B:968:THR:HA | 2:B:971:PHE:HB3 | 2.03 | 0.41 |
| 2:B:1053:LYS:HA | 2:B:1053:LYS:HD2 | 1.86 | 0.41 |
| 2:B:1107:ILE:HD13 | 2:B:1129:LEU:HD21 | 2.01 | 0.41 |
| 2:B:1405:TYR:CD2 | 2:B:1459:SER:HA | 2.55 | 0.41 |
| 2:B:1476:LEU:HB3 | 2:B:1478:THR:HG22 | 2.03 | 0.41 |
| 2:B:1659:GLN:H | 2:B:1659:GLN:CD | 2.24 | 0.41 |
| 1:A:91:LYS:HD2 | 1:A:91:LYS:HA | 1.66 | 0.41 |
| 1:A:1210:THR:HG22 | 1:A:1281:MET:HG3 | 2.02 | 0.41 |
| 1:A:1435:LYS:O | 1:A:1437:PRO:HD3 | 2.20 | 0.41 |
| 1:A:1613:ASN:O | 1:A:1615:ASP:N | 2.53 | 0.41 |
| 2:B:727:HIS:CG | 2:B:841:ILE:CD1 | 3.03 | 0.41 |
| 2:B:864:LYS:HD2 | 2:B:865:ASN:N | 2.36 | 0.41 |
| 2:B:1174:LYS:HG3 | 2:B:1177:LYS:HD2 | 2.03 | 0.41 |
| 2:B:1927:HIS:HA | 2:B:1930:GLU:CD | 2.41 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:930:GLN:OE1 | 1:A:930:GLN:N | 2.35 | 0.40 |
| 1:A:1022:PHE:HE1 | 1:A:1399:HIS:ND1 | 2.19 | 0.40 |
| 1:A:1191:TRP:CZ2 | 1:A:1215:VAL:HG21 | 2.55 | 0.40 |
| 1:A:1236:VAL:HG21 | 1:A:1323:LYS:HB2 | 2.03 | 0.40 |
| 1:A:1468:LEU:HD21 | 1:A:1492:ARG:HB3 | 2.03 | 0.40 |
| 2:B:223:VAL:O | 2:B:227:VAL:HG22 | 2.21 | 0.40 |
| 2:B:258:THR:HA | 2:B:444:VAL:HG13 | 2.03 | 0.40 |
| 2:B:538:ALA:HB3 | 2:B:540:LYS:HZ1 | 1.84 | 0.40 |
| 2:B:737:ILE:HD11 | 2:B:772:TRP:CH2 | 2.56 | 0.40 |
| 2:B:1140:ALA:O | 2:B:1144:THR:N | 2.49 | 0.40 |
| 2:B:1251:TRP:NE1 | 2:B:1259:VAL:HG23 | 2.36 | 0.40 |
| 2:B:1591:VAL:O | 2:B:1592:ARG:HD2 | 2.21 | 0.40 |
| 2:B:1830:VAL:HA | 2:B:1968:TYR:OH | 2.20 | 0.40 |
| 1:A:16:GLU:HG3 | 2:B:2026:ILE:HG23 | 2.03 | 0.40 |
| 1:A:419:ILE:HA | 1:A:463:THR:HB | 2.03 | 0.40 |
| 1:A:713:SER:O | 1:A:717:THR:HG23 | 2.21 | 0.40 |
| 2:B:134:SER:OG | 2:B:136:LEU:HD22 | 2.22 | 0.40 |
| 2:B:481:HIS:ND1 | 2:B:483:ALA:N | 2.68 | 0.40 |
| 2:B:727:HIS:ND1 | 2:B:841:ILE:HD12 | 2.35 | 0.40 |
| 2:B:1002:PRO:HG2 | 2:B:1019:LYS:HG2 | 2.03 | 0.40 |
| 2:B:1112:VAL:N | 2:B:1173:ASP:OD1 | 2.55 | 0.40 |
| 2:B:1512:GLU:OE1 | 2:B:1512:GLU:N | 2.54 | 0.40 |
| 1:A:12:THR:O | 1:A:15:THR:OG1 | 2.36 | 0.40 |
| 1:A:45:ILE:HA | 1:A:79:LEU:O | 2.21 | 0.40 |
| 1:A:485:ASP:CG | 1:A:674:THR:HG21 | 2.41 | 0.40 |
| 1:A:686:GLY:N | 3:A:1901:NAP:O3B | 2.55 | 0.40 |
| 1:A:726:ARG:HH11 | 1:A:1632:ARG:NE | 2.20 | 0.40 |
| 1:A:838:TYR:O | 1:A:841:SER:OG | 2.34 | 0.40 |
| 1:A:1171:LEU:HA | 1:A:1171:LEU:HD23 | 1.69 | 0.40 |
| 2:B:96:SER:HB2 | 2:B:100:LYS:NZ | 2.35 | 0.40 |
| 2:B:1359:SER:OG | 2:B:1360:THR:N | 2.54 | 0.40 |
| 2:B:1874:LEU:HD13 | 2:B:1895:LEU:CD1 | 2.51 | 0.40 |
| 1:A:30:GLU:H | 1:A:30:GLU:CD | 2.23 | 0.40 |
| 1:A:711:ARG:O | 1:A:711:ARG:HG2 | 2.21 | 0.40 |
| 1:A:1288:LEU:HD23 | 1:A:1288:LEU:HA | 1.90 | 0.40 |
| 2:B:147:VAL:O | 2:B:486:ILE:HA | 2.21 | 0.40 |
| 2:B:322:PRO:HA | 2:B:407:PHE:CD2 | 2.56 | 0.40 |
| 2:B:657:ARG:HD3 | 2:B:686:GLY:O | 2.20 | 0.40 |
| 2:B:688:THR:HG21 | 2:B:1232:PHE:HZ | 1.86 | 0.40 |
| 2:B:865:ASN:OD1 | 2:B:865:ASN:N | 2.55 | 0.40 |
| 2:B:1425:LYS:O | 2:B:1429:VAL:HG23 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:926:ASN:OD1 | 1:A:929:LEU:HB2 | 2.21 | 0.40 |
| 2:B:49:ASP:OD2 | 2:B:50:ASP:N | 2.55 | 0.40 |
| 2:B:357:LEU:HB2 | 2:B:365:VAL:HB | 2.04 | 0.40 |
| 2:B:464:VAL:O | 2:B:468:ILE:HG13 | 2.21 | 0.40 |
| 2:B:1003:VAL:HA | 2:B:1004:PRO:HD3 | 1.90 | 0.40 |
| 2:B:1435:TRP:HE3 | 2:B:1487:VAL:HG13 | 1.86 | 0.40 |
| 2:B:1508:LYS:HE3 | 2:B:1508:LYS:HB2 | 1.86 | 0.40 |
| 2:B:1566:THR:HB | 2:B:1602:VAL:HG23 | 2.03 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 1427/1722 (83%) | 1306 (92%) | 115 (8%) | 6 (0%) | 34 | 66 |
| 2 | B | 2031/2037 (100%) | 1860 (92%) | 168 (8%) | 3 (0%) | 51 | 81 |
| All | All | 3458/3759 (92%) | 3166 (92%) | 283 (8%) | 9 (0%) | 44 | 71 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 879 | ALA |
| 2 | B | 582 | ALA |
| 1 | A | 623 | THR |
| 1 | A | 876 | LEU |
| 2 | B | 727 | HIS |
| 1 | A | 878 | SER |
| 1 | A | 1006 | GLU |
| 1 | A | 1005 | PRO |
| 2 | B | 583 | GLY |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 1222/1445 (85%) | 1211 (99%) | 11 (1%) | 78 87 |
| 2 | B | 1780/1784 (100%) | 1772 (100%) | 8 (0%) | 91 95 |
| All | All | 3002/3229 (93%) | 2983 (99%) | 19 (1%) | 86 91 |

All (19) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 623 | THR |
| 1 | A | 626 | ILE |
| 1 | A | 660 | LEU |
| 1 | A | 711 | ARG |
| 1 | A | 712 | PHE |
| 1 | A | 876 | LEU |
| 1 | A | 877 | MET |
| 1 | A | 1178 | ARG |
| 1 | A | 1501 | LYS |
| 1 | A | 1689 | ARG |
| 1 | A | 1706 | LYS |
| 2 | B | 334 | LYS |
| 2 | B | 584 | MET |
| 2 | B | 864 | LYS |
| 2 | B | 873 | LYS |
| 2 | B | 1199 | LYS |
| 2 | B | 1667 | LEU |
| 2 | B | 1714 | ARG |
| 2 | B | 1837 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 473 | GLN |
| 1 | A | 794 | HIS |
| 1 | A | 968 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1064 | ASN |
| 1 | A | 1126 | GLN |
| 1 | A | 1562 | ASN |
| 1 | A | 1597 | ASN |
| 1 | A | 1743 | GLN |
| 2 | B | 16 | HIS |
| 2 | B | 171 | GLN |
| 2 | B | 317 | ASN |
| 2 | B | 335 | GLN |
| 2 | B | 379 | ASN |
| 2 | B | 734 | HIS |
| 2 | B | 818 | GLN |
| 2 | B | 821 | GLN |
| 2 | B | 872 | ASN |
| 2 | B | 884 | ASN |
| 2 | B | 959 | ASN |
| 2 | B | 960 | GLN |
| 2 | B | 1122 | ASN |
| 2 | B | 1153 | HIS |
| 2 | B | 1338 | HIS |
| 2 | B | 1684 | HIS |
| 2 | B | 1688 | ASN |
| 2 | B | 1702 | ASN |
| 2 | B | 1883 | ASN |
| 2 | B | 1965 | HIS |
| 2 | B | 1977 | GLN |
| 2 | B | 2035 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

3 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 | NAP | B | 2102 | - | 45,52,52 | 0.81 | 1 (2%) | 56,80,80 | 1.23 | 4 (7%) |
| 3 | NAP | A | 1901 | - | 45,52,52 | 0.81 | 1 (2%) | 56,80,80 | 1.22 | 4 (7%) |
| 4 | FMN | B | 2101 | - | 33,33,33 | 6.33 | 21 (63%) | 48,50,50 | 1.29 | 5 (10%) |

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 | NAP | B | 2102 | - | - | 6/31/67/67 | 0/5/5/5 |
| 3 | NAP | A | 1901 | - | - | 11/31/67/67 | 0/5/5/5 |
| 4 | FMN | B | 2101 | - | - | 5/18/18/18 | 0/3/3/3 |

All (23) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | B | 2101 | FMN | C6-C7 | 12.63 | 1.58 | 1.39 |
| 4 | B | 2101 | FMN | C9-C9A | 12.27 | 1.59 | 1.39 |
| 4 | B | 2101 | FMN | C6-C5A | 11.98 | 1.58 | 1.40 |
| 4 | B | 2101 | FMN | C9-C8 | 11.14 | 1.55 | 1.39 |
| 4 | B | 2101 | FMN | C4A-N5 | 10.59 | 1.51 | 1.30 |
| 4 | B | 2101 | FMN | O4-C4 | 9.95 | 1.42 | 1.23 |
| 4 | B | 2101 | FMN | O2-C2 | 8.86 | 1.40 | 1.24 |
| 4 | B | 2101 | FMN | C9A-C5A | 8.38 | 1.55 | 1.41 |
| 4 | B | 2101 | FMN | C2-N1 | 7.06 | 1.53 | 1.36 |
| 4 | B | 2101 | FMN | C10-N1 | 7.04 | 1.47 | 1.33 |
| 4 | B | 2101 | FMN | C8-C7 | 6.86 | 1.58 | 1.40 |
| 4 | B | 2101 | FMN | C10-N10 | 6.58 | 1.51 | 1.37 |
| 4 | B | 2101 | FMN | C4-N3 | 6.20 | 1.50 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | B | 2101 | FMN | C5A-N5 | 6.18 | 1.51 | 1.39 |
| 4 | B | 2101 | FMN | C2-N3 | 5.79 | 1.52 | 1.39 |
| 4 | B | 2101 | FMN | C9A-N10 | 5.12 | 1.50 | 1.41 |
| 4 | B | 2101 | FMN | C4A-C10 | 3.64 | 1.54 | 1.44 |
| 4 | B | 2101 | FMN | C1'-C2' | 3.04 | 1.56 | 1.52 |
| 4 | B | 2101 | FMN | P-O2P | 2.93 | 1.66 | 1.54 |
| 4 | B | 2101 | FMN | P-O3P | 2.61 | 1.64 | 1.54 |
| 3 | B | 2102 | NAP | C5A-C4A | 2.47 | 1.47 | 1.40 |
| 3 | A | 1901 | NAP | C5A-C4A | 2.47 | 1.47 | 1.40 |
| 4 | B | 2101 | FMN | C4A-C4 | 2.42 | 1.53 | 1.44 |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | B | 2102 | NAP | PN-O3-PA | -3.57 | 120.58 | 132.83 |
| 3 | A | 1901 | NAP | PN-O3-PA | -3.52 | 120.76 | 132.83 |
| 3 | B | 2102 | NAP | C3D-C2D-C1D | 3.39 | 106.08 | 100.98 |
| 3 | A | 1901 | NAP | C3D-C2D-C1D | 3.38 | 106.06 | 100.98 |
| 3 | B | 2102 | NAP | N3A-C2A-N1A | -3.19 | 123.69 | 128.68 |
| 3 | A | 1901 | NAP | N3A-C2A-N1A | -3.18 | 123.71 | 128.68 |
| 4 | B | 2101 | FMN | C4A-C10-N10 | 2.97 | 120.83 | 116.48 |
| 4 | B | 2101 | FMN | C4'-C3'-C2' | -2.77 | 107.61 | 113.36 |
| 3 | A | 1901 | NAP | C4A-C5A-N7A | -2.72 | 106.56 | 109.40 |
| 4 | B | 2101 | FMN | C10-C4A-N5 | -2.69 | 119.15 | 124.86 |
| 3 | B | 2102 | NAP | C4A-C5A-N7A | -2.69 | 106.60 | 109.40 |
| 4 | B | 2101 | FMN | C4-N3-C2 | -2.34 | 121.31 | 125.64 |
| 4 | B | 2101 | FMN | O2-C2-N1 | -2.05 | 118.44 | 121.83 |

There are no chirality outliers.

All (22) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | A | 1901 | NAP | C5B-O5B-PA-O1A |
| 3 | A | 1901 | NAP | C5D-O5D-PN-O1N |
| 3 | A | 1901 | NAP | C5D-O5D-PN-O2N |
| 3 | B | 2102 | NAP | C5D-O5D-PN-O1N |
| 4 | B | 2101 | FMN | C2'-C3'-C4'-C5' |
| 4 | B | 2101 | FMN | O3'-C3'-C4'-C5' |
| 3 | A | 1901 | NAP | O4B-C4B-C5B-O5B |
| 3 | A | 1901 | NAP | C3B-C4B-C5B-O5B |
| 3 | A | 1901 | NAP | O4D-C4D-C5D-O5D |
| 3 | A | 1901 | NAP | C3D-C4D-C5D-O5D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 4 | B | 2101 | FMN | C2'-C3'-C4'-O4' |
| 4 | B | 2101 | FMN | O3'-C3'-C4'-O4' |
| 3 | A | 1901 | NAP | PA-O3-PN-O5D |
| 3 | B | 2102 | NAP | C5B-O5B-PA-O3 |
| 3 | B | 2102 | NAP | C3B-C4B-C5B-O5B |
| 3 | A | 1901 | NAP | PN-O3-PA-O2A |
| 3 | B | 2102 | NAP | C4D-C5D-O5D-PN |
| 3 | B | 2102 | NAP | PA-O3-PN-O2N |
| 3 | B | 2102 | NAP | O4D-C4D-C5D-O5D |
| 3 | A | 1901 | NAP | C5D-O5D-PN-O3 |
| 3 | A | 1901 | NAP | PN-O3-PA-O1A |
| 4 | B | 2101 | FMN | C4'-C5'-O5'-P |

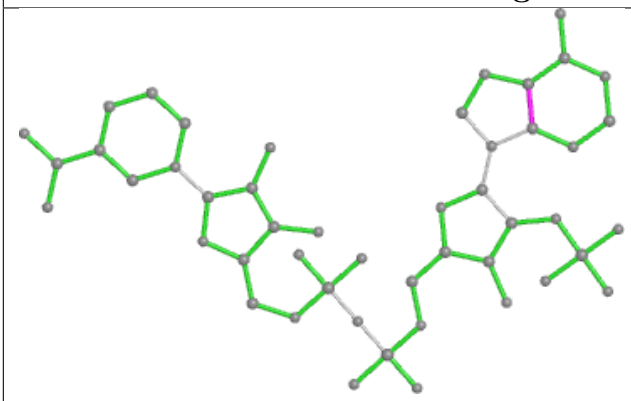
There are no ring outliers.

3 monomers are involved in 135 short contacts:

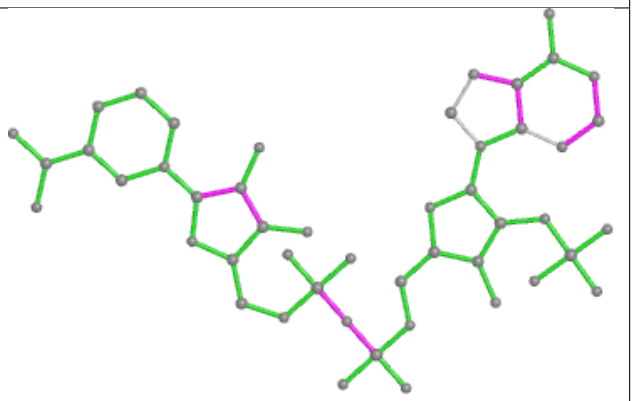
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | B | 2102 | NAP | 50 | 0 |
| 3 | A | 1901 | NAP | 34 | 0 |
| 4 | B | 2101 | FMN | 51 | 0 |

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

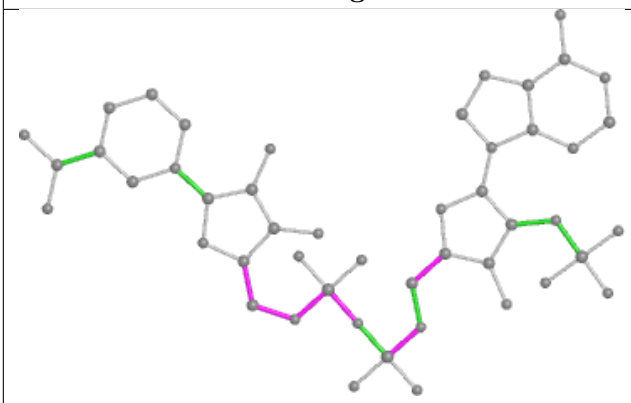
**Ligand NAP B 2102**



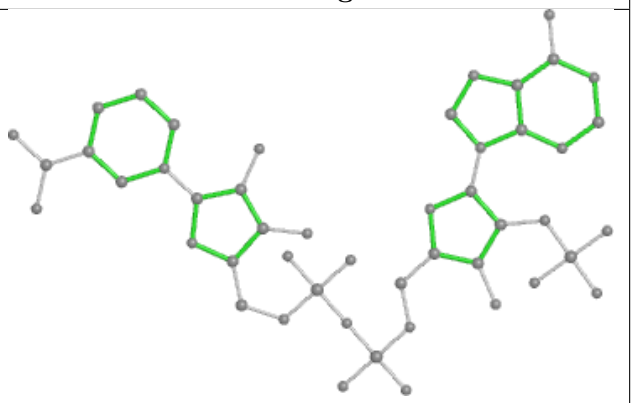
**Bond lengths**



**Bond angles**

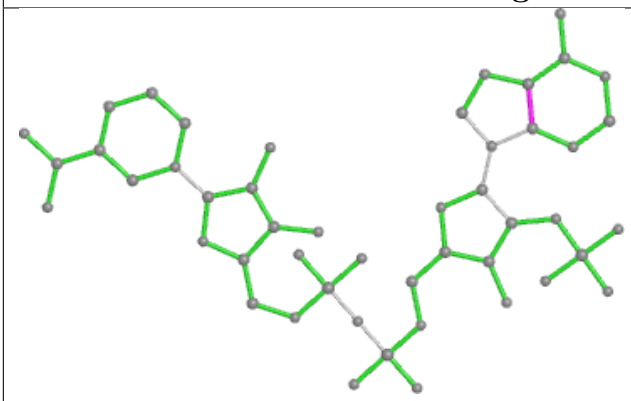


**Torsions**

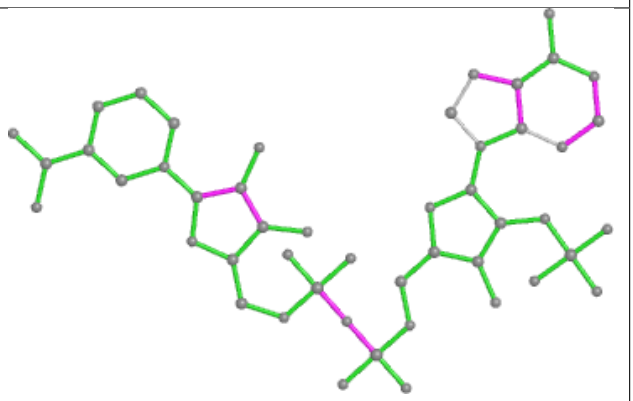


**Rings**

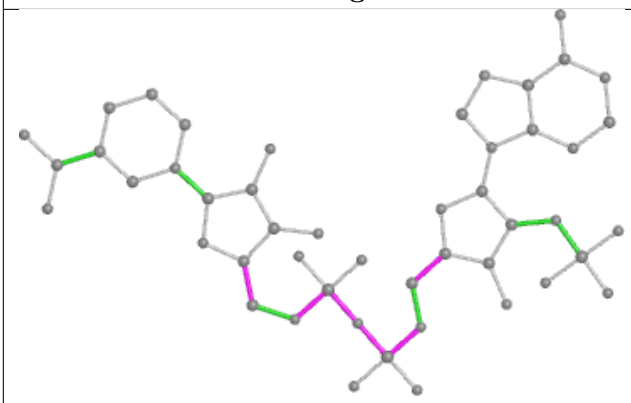
**Ligand NAP A 1901**



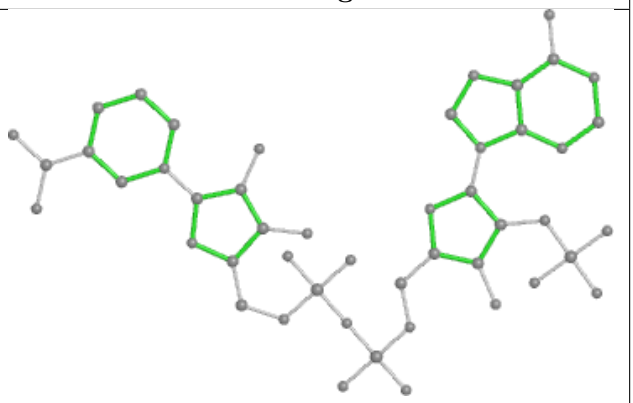
**Bond lengths**



**Bond angles**

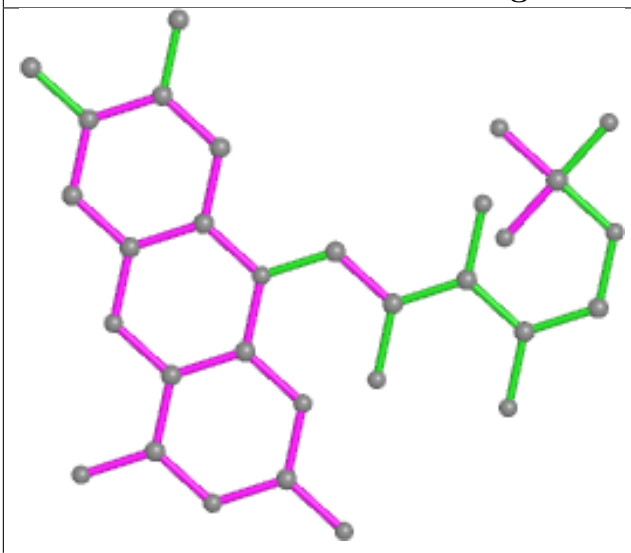


**Torsions**

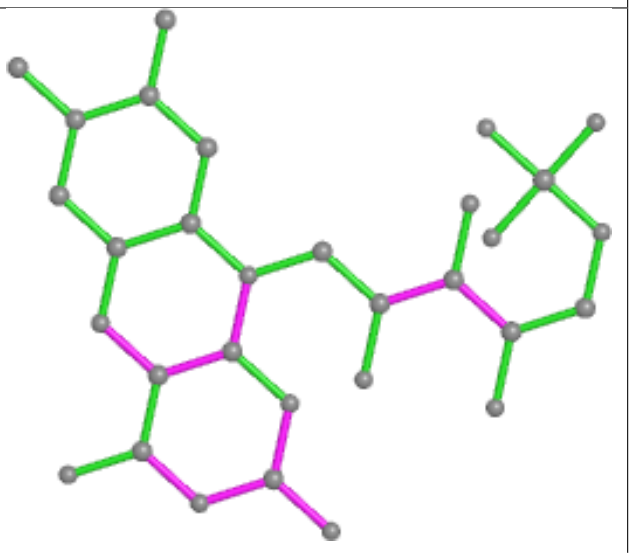


**Rings**

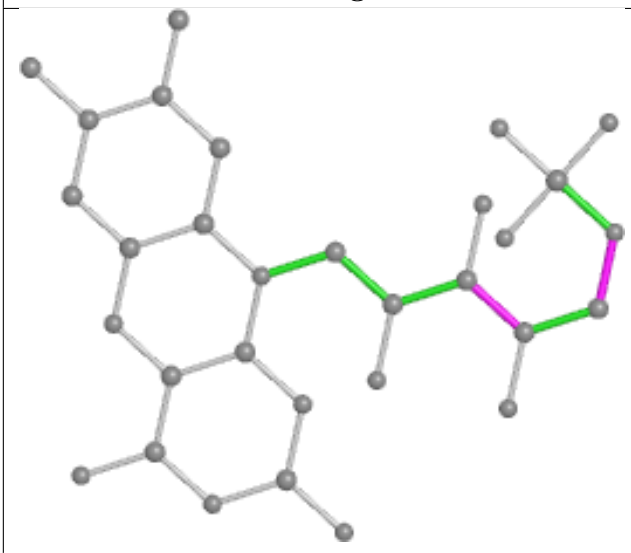
**Ligand FMN B 2101**



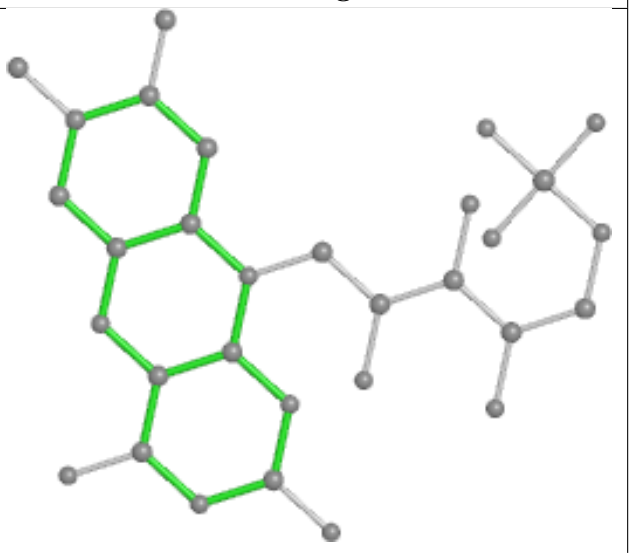
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

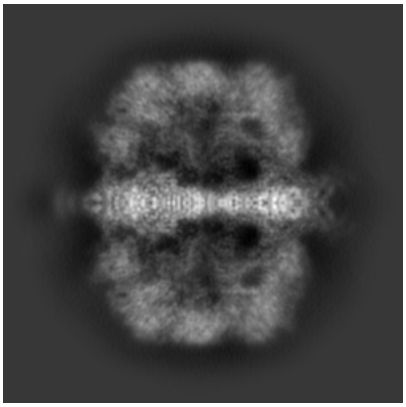
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20658. These allow visual inspection of the internal detail of the map and identification of artifacts.

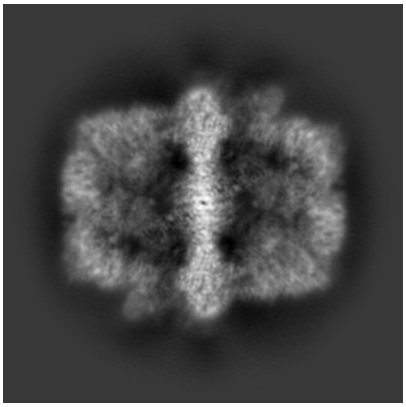
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

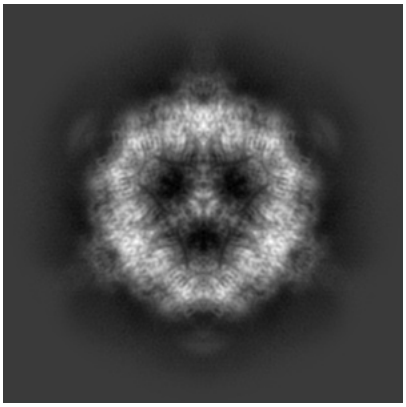
### 6.1.1 Primary map



X



Y

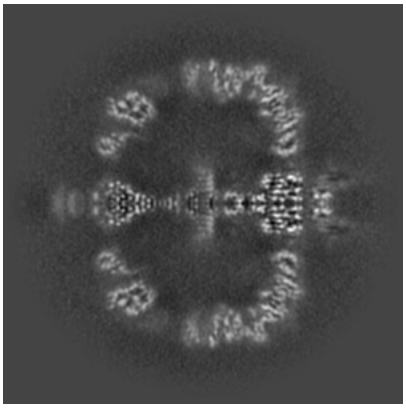


Z

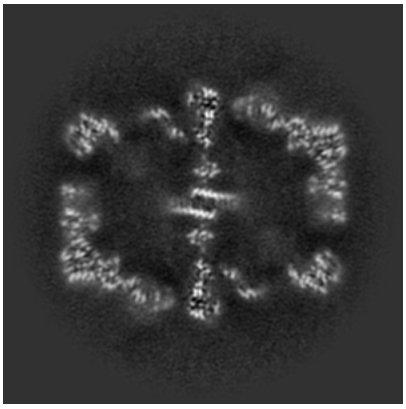
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

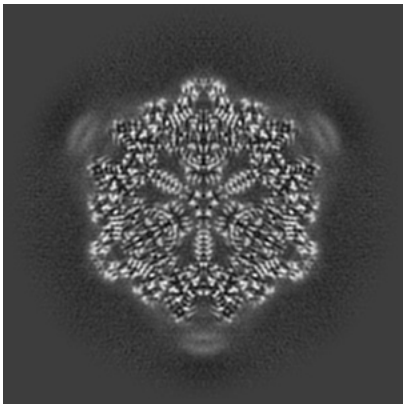
### 6.2.1 Primary map



X Index: 176



Y Index: 176

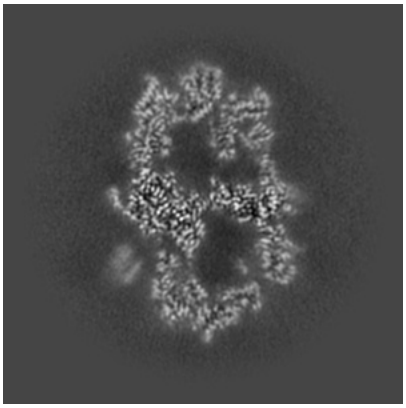


Z Index: 176

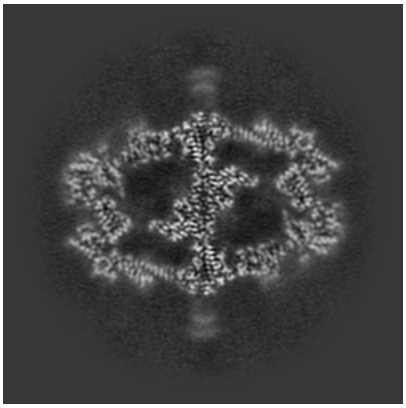
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

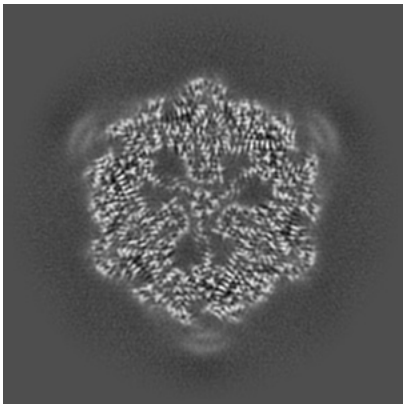
### 6.3.1 Primary map



X Index: 237



Y Index: 231

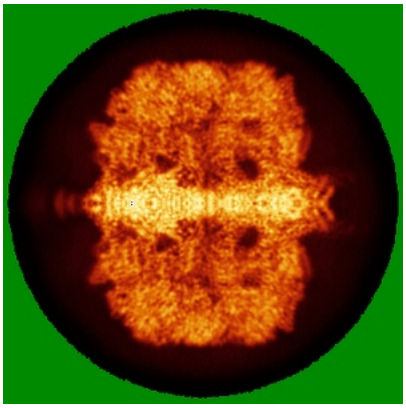


Z Index: 172

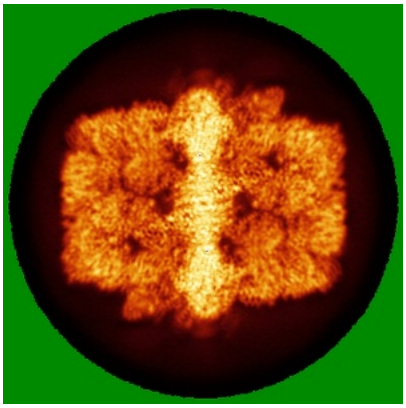
The images above show the largest variance slices of the map in three orthogonal directions.

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

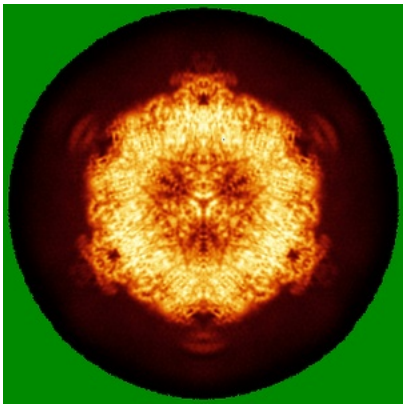
### 6.4.1 Primary map



X



Y

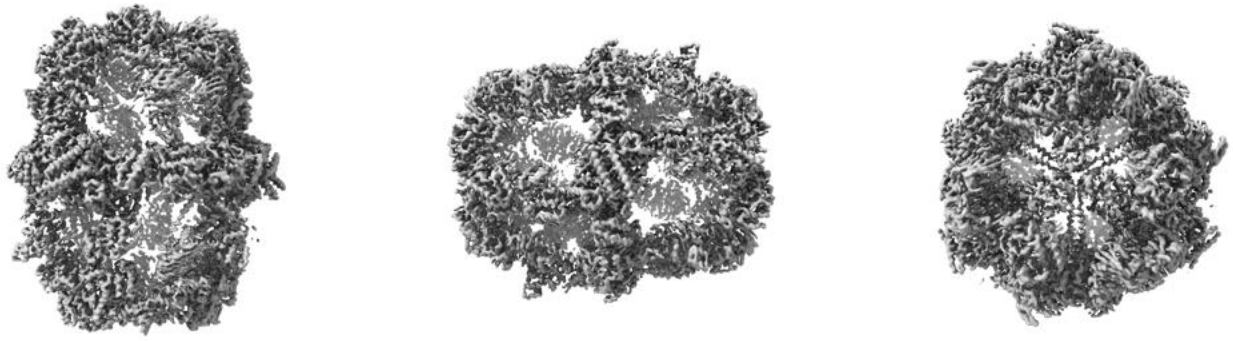


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.704. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

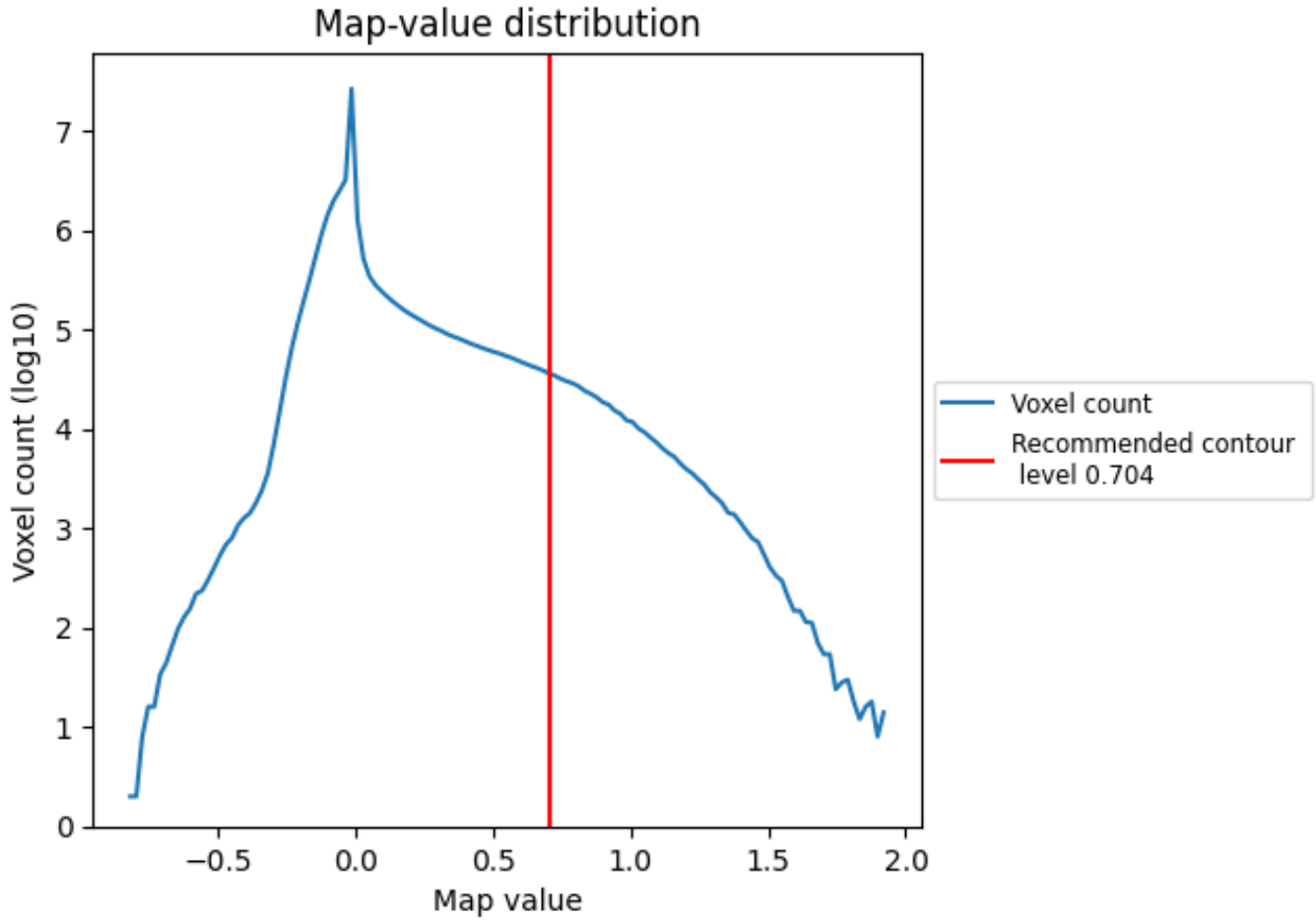
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

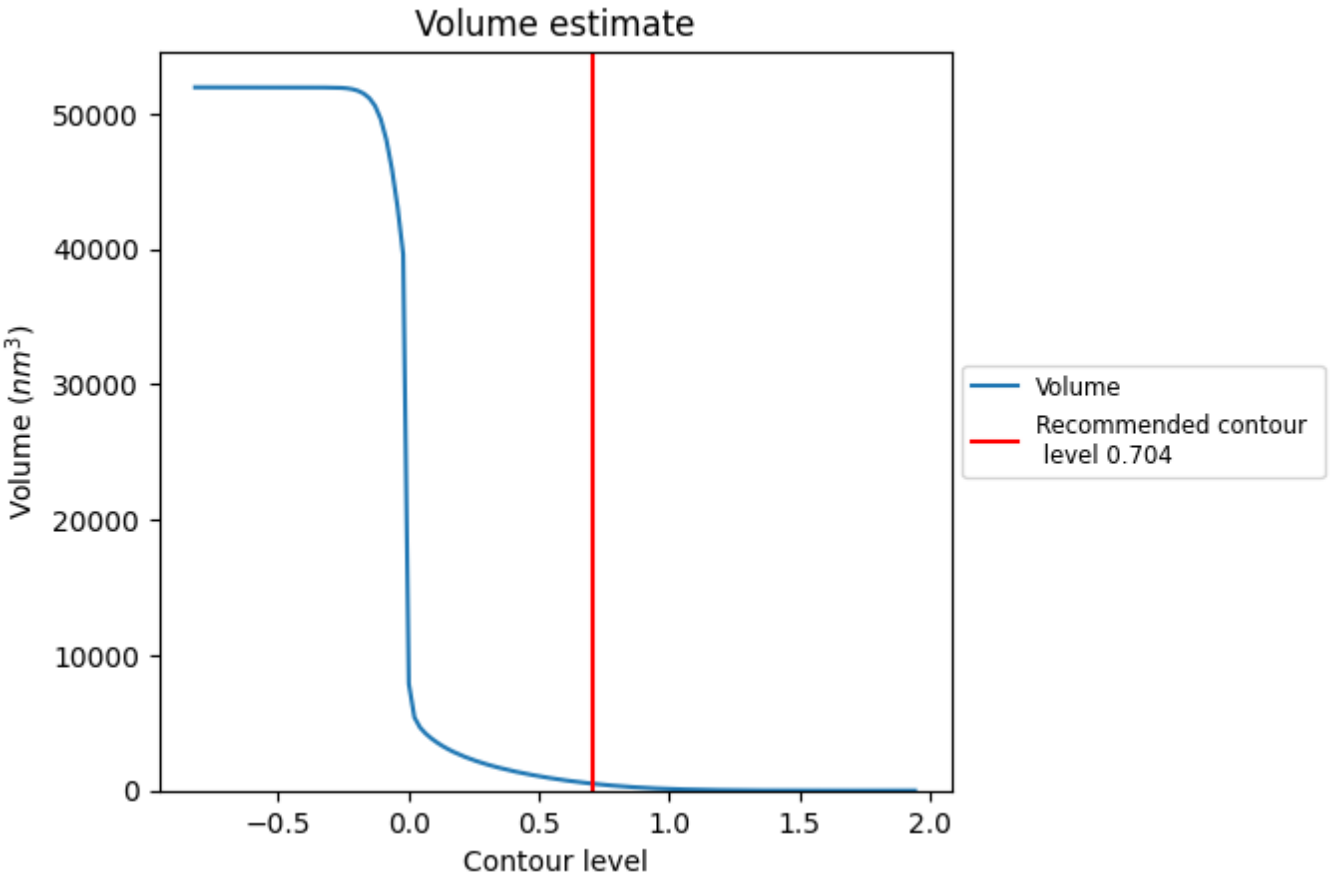
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

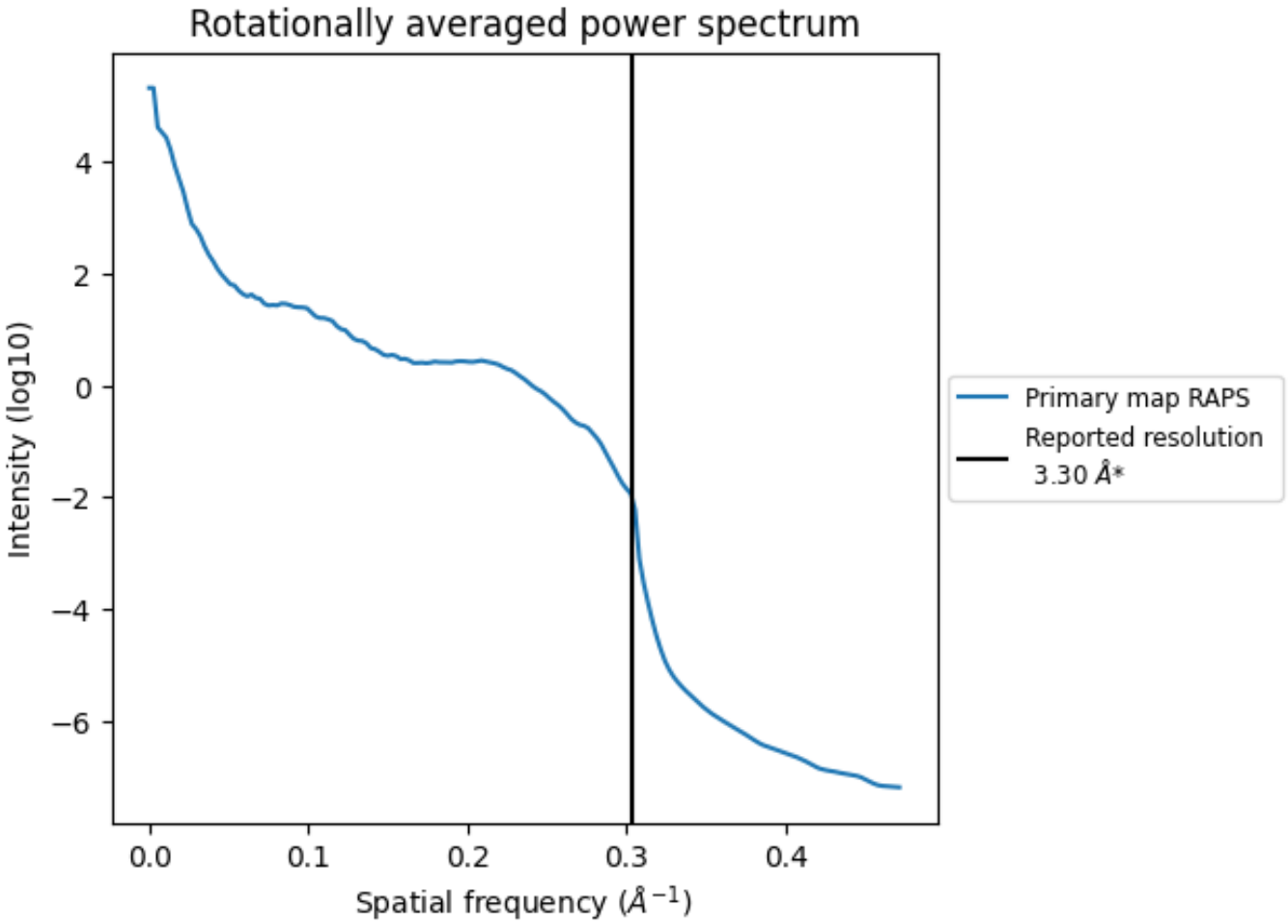
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 513 $nm^3$; this corresponds to an approximate mass of 464 kDa.

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

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.303 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

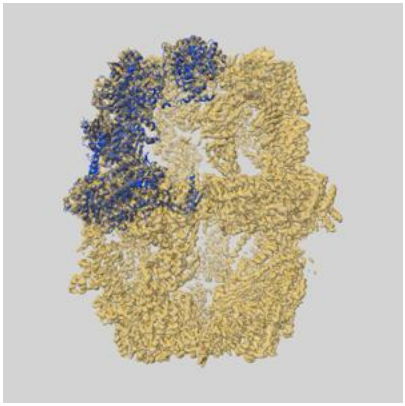
This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit

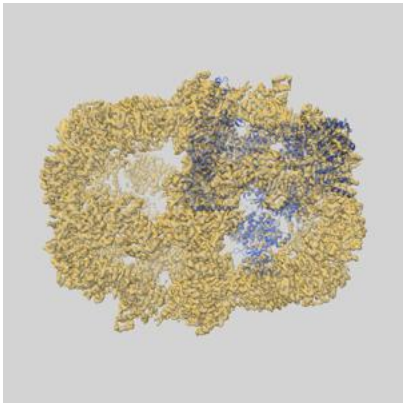
This section contains information regarding the fit between EMDB map EMD-20658 and PDB model 6U5W. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1 Map-model overlays

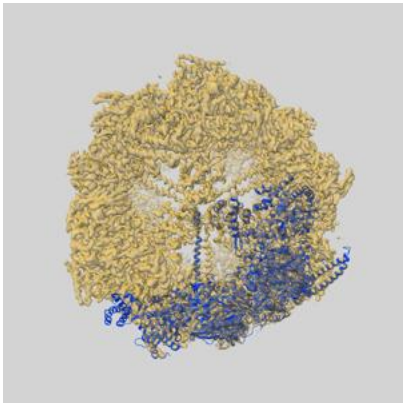
### 9.1.1 Map-model overlay



X

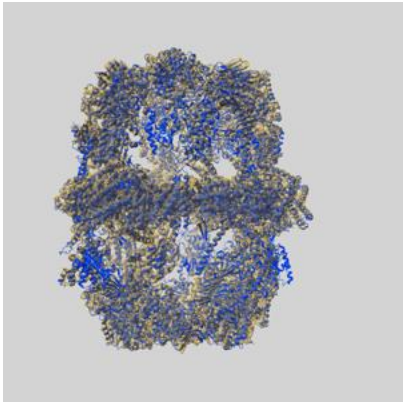


Y

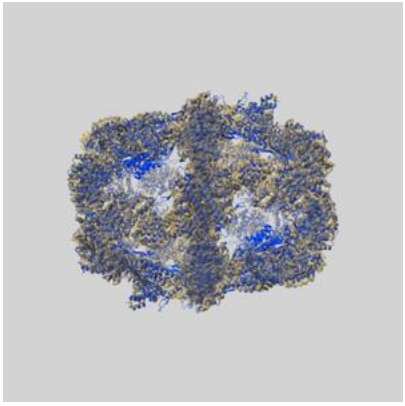


Z

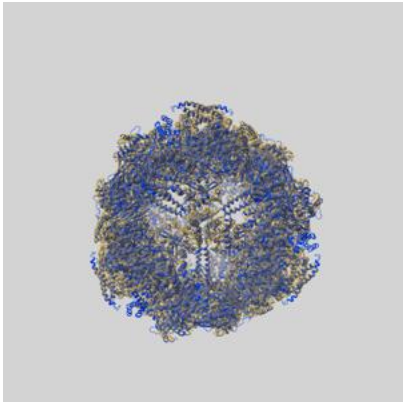
### 9.1.2 Map-model assembly overlay



X



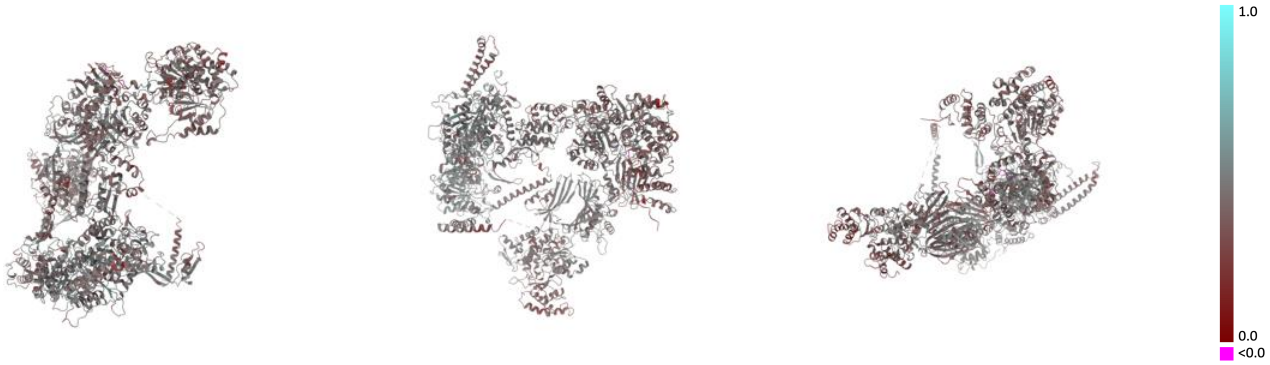
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.704 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

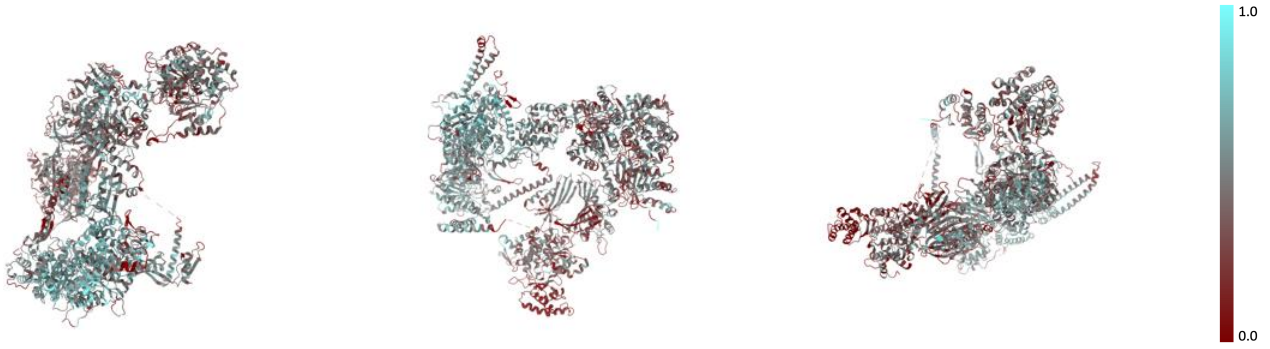
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

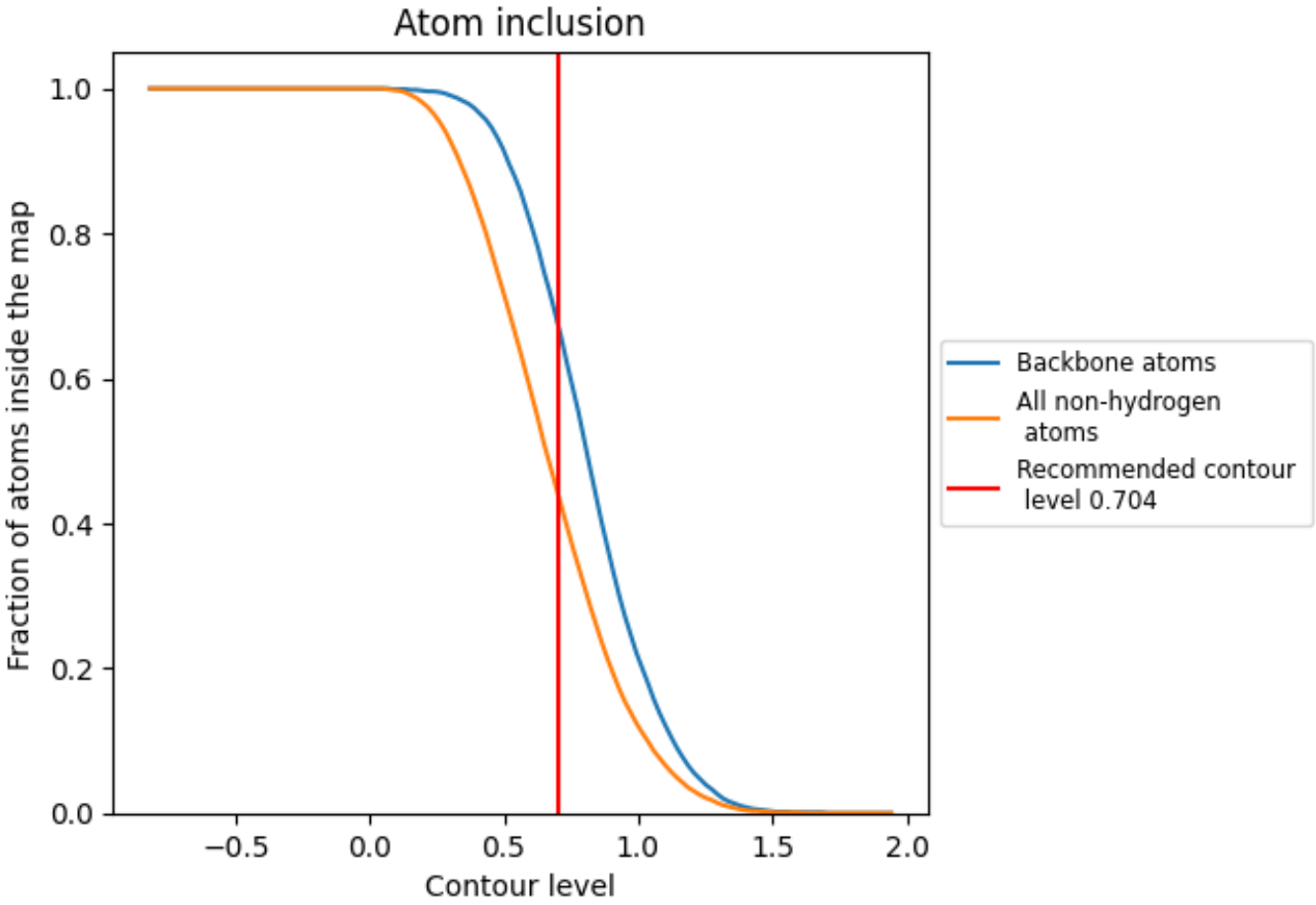
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.704).

## 9.4 Atom inclusion (i)




At the recommended contour level, 67% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.704) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.4360 | 0.4280 |
| A | 0.5230 | 0.4560 |
| B | 0.3760 | 0.4080 |