



## Full wwPDB EM Validation Report ⓘ

Sep 23, 2024 – 10:49 AM EDT

PDB ID : 8VDQ  
EMDB ID : EMD-43155  
Title : Cryogenic electron microscopy model of full-length talin  
Authors : Izard, T.; Rangarajan, E.S.  
Deposited on : 2023-12-17  
Resolution : 5.50 Å (reported)  
Based on initial model : 6r9t

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.dev112  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

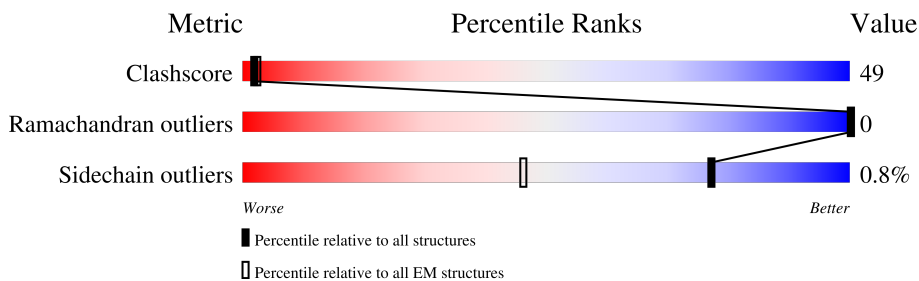
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.50 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<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 210492                      | 15764                       |
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 2804   |                  |

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 16077 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 Green fluorescent protein, Talin-1.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
|     |       |          | Total | C    | N    | O    | S  |         |       |
| 1   | A     | 2192     | 16077 | 9904 | 2874 | 3221 | 78 | 0       | 0     |

There are 33 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -262    | MET      | -      | expression tag | UNP P42212 |
| A     | -261    | HIS      | -      | expression tag | UNP P42212 |
| A     | -260    | HIS      | -      | expression tag | UNP P42212 |
| A     | -259    | HIS      | -      | expression tag | UNP P42212 |
| A     | -258    | HIS      | -      | expression tag | UNP P42212 |
| A     | -257    | HIS      | -      | expression tag | UNP P42212 |
| A     | -256    | HIS      | -      | expression tag | UNP P42212 |
| A     | -255    | HIS      | -      | expression tag | UNP P42212 |
| A     | -254    | HIS      | -      | expression tag | UNP P42212 |
| A     | -253    | HIS      | -      | expression tag | UNP P42212 |
| A     | -252    | HIS      | -      | expression tag | UNP P42212 |
| A     | -251    | MET      | -      | expression tag | UNP P42212 |
| A     | -250    | VAL      | -      | expression tag | UNP P42212 |
| A     | -187    | LEU      | PHE    | conflict       | UNP P42212 |
| A     | -186    | THR      | SER    | conflict       | UNP P42212 |
| A     | -20     | LEU      | HIS    | conflict       | UNP P42212 |
| A     | -12     | GLY      | -      | linker         | UNP P42212 |
| A     | -11     | SER      | -      | linker         | UNP P42212 |
| A     | -10     | LEU      | -      | linker         | UNP P42212 |
| A     | -9      | GLU      | -      | linker         | UNP P42212 |
| A     | -8      | VAL      | -      | linker         | UNP P42212 |
| A     | -7      | LEU      | -      | linker         | UNP P42212 |
| A     | -6      | PHE      | -      | linker         | UNP P42212 |
| A     | -5      | GLN      | -      | linker         | UNP P42212 |
| A     | -4      | GLY      | -      | linker         | UNP P42212 |
| A     | -3      | PRO      | -      | linker         | UNP P42212 |
| A     | -2      | ALA      | -      | linker         | UNP P42212 |
| A     | -1      | ALA      | -      | linker         | UNP P42212 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 0       | ALA      | -      | linker   | UNP P42212 |
| A     | 639     | LEU      | GLN    | conflict | UNP P26039 |
| A     | 673     | ASN      | LYS    | conflict | UNP P26039 |
| A     | 1227    | LEU      | SER    | conflict | UNP P26039 |
| A     | 2349    | VAL      | ALA    | conflict | UNP P26039 |



|       |       |       |       |       |       |       |       |       |       |       |       |      |      |      |      |      |     |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|-----|
| M1407 | M1408 | G1409 | I1410 | S1345 | G1276 | P1204 | L1141 | K1076 | P1009 | A944  | D882  | V808 | A739 | Q670 | R606 | H541 | SER |
| T1408 | L1409 | F1277 | I1410 | Q1348 | Q1276 | G1205 | D1144 | P1077 | I1010 | S945  | S883  | T809 | G740 | L671 | P607 | E542 | GLY |
| I1410 | R1207 | F1278 | P1145 | R1207 | L1079 | Q1206 | P1145 | L1079 | I1011 | A946  | E884  | E310 | R742 | A672 | L608 | H543 | GLN |
| Q1411 | L1350 | F1279 | A1146 | L1208 | E1082 | D1208 | A1146 | T1083 | D1013 | S947  | E885  | I812 | V743 | M811 | L609 | H544 | MET |
| M1412 | T1351 | F1280 | V1147 | M1211 | T1083 | Q1014 | T1147 | T1083 | Q1013 | Q948  | E886  | F813 | V744 | A673 | Q610 | S545 | HIS |
| A1413 | C1353 | E1283 | Q1148 | A1212 | M1084 | A1015 | Q1148 | M1084 | A1015 | Q949  | E887  | S814 | A744 | M812 | A611 | Q546 | ARG |
| K1415 | T1354 | A1284 | A1149 | K1086 | E1085 | S1016 | A1149 | E1085 | A1017 | P950  | Q888  | S815 | V747 | A674 | A612 | V547 | GLY |
| M1416 | Q1355 | V1286 | V1150 | K1086 | L1086 | M1018 | V1150 | K1086 | M1018 | L951  | Q888  | S815 | V747 | A674 | A612 | V547 | GLY |
| G1417 | Q1356 | V1286 | L1152 | C1087 | L1087 | Q1019 | L1152 | C1087 | Q1019 | L952  | R889  | A819 | E748 | A680 | G614 | D548 | HIS |
| M1418 | A1357 | M1288 | D1163 | T1089 | K1089 | L1020 | D1163 | T1089 | L1020 | L953  | R891  | A819 | E748 | A680 | G614 | D548 | HIS |
| E1421 | P1358 | A1289 | T1154 | D1089 | K1089 | Q1022 | T1154 | D1089 | Q1022 | C956  | E893  | M822 | A753 | K685 | S620 | T554 | MET |
| F1422 | G1359 | A1289 | A1155 | D1091 | L1091 | C1023 | A1155 | D1091 | C1023 | X957  | E895  | Q825 | S754 | A686 | E621 | I550 |     |
| I1426 | L1360 | A1292 | S1156 | G1092 | G1092 | A1024 | S1156 | G1092 | A1024 | A958  | E896  | A826 | A756 | A686 | E621 | I550 |     |
| A1427 | E1362 | P1293 | D1157 | N1093 | N1093 | K1025 | D1157 | N1093 | K1025 | Q960  | L897  | R827 | A756 | A686 | E621 | I550 |     |
| T1428 | C1363 | S1294 | V1158 | S1094 | S1094 | M1026 | V1158 | S1094 | M1026 | A960  | R898  | I828 | A756 | A686 | E621 | I550 |     |
| A1429 | L1364 | L1227 | L1159 | T1095 | T1095 | L1027 | L1159 | T1095 | L1027 | E961  | M899  | L829 | A756 | A686 | E621 | I550 |     |
| S1430 | M1365 | P1229 | D1160 | K1096 | K1096 | G1028 | D1160 | K1096 | K1096 | Q963  | A900  | A830 | A756 | A686 | E621 | I550 |     |
| K1431 | A1366 | R1298 | K1161 | A1097 | A1097 | T1029 | K1161 | A1097 | A1097 | P964  | T901  | Q831 | A756 | A686 | E621 | I550 |     |
| K1431 | L1367 | A1299 | A1162 | V1098 | V1098 | A1030 | A1162 | V1098 | V1098 | L966  | N902  | A832 | A756 | A686 | E621 | I550 |     |
| A1432 | R1368 | Q1300 | S1163 | S1099 | S1099 | L1031 | S1163 | S1099 | L1031 | L966  | A903  | T833 | A756 | A686 | E621 | I550 |     |
| L1433 | Q1369 | V1301 | S1164 | A1100 | A1100 | A1032 | S1164 | A1100 | A1032 | Q967  | A904  | S834 | A756 | A686 | E621 | I550 |     |
| C1434 | Q1370 | V1302 | L1165 | A1101 | A1101 | E1033 | L1165 | A1101 | E1033 | Q968  | A905  | D835 | A756 | A686 | E621 | I550 |     |
| G1435 | L1370 | S1303 | L1166 | I1102 | I1102 | L1034 | L1166 | I1102 | L1034 | Q969  | Q906  | L836 | A756 | A686 | E621 | I550 |     |
| F1436 | E1371 | M1304 | E1167 | A1103 | A1103 | R1035 | E1167 | A1103 | R1035 | Q970  | N907  | V837 | A756 | A686 | E621 | I550 |     |
| T1437 | V1372 | N1305 | A1168 | K1104 | K1104 | A1036 | A1168 | K1104 | A1036 | V970  | A908  | M838 | A756 | A686 | E621 | I550 |     |
| E1438 | L1373 | K1306 | A1169 | L1105 | L1105 | A1037 | A1169 | L1105 | A1037 | Q972  | I909  | A839 | A756 | A686 | E621 | I550 |     |
| A1441 | E1375 | G1307 | K1170 | L1106 | L1106 | A1038 | K1170 | L1106 | A1038 | S973  | K910  | I840 | A756 | A686 | E621 | I550 |     |
| Q1442 | L1376 | I1308 | K1171 | G1107 | G1107 | Q1039 | K1171 | G1107 | Q1039 | Q974  | K911  | K841 | A756 | A686 | E621 | I550 |     |
| A1443 | E1377 | S1309 | A1172 | E1108 | E1108 | K1040 | A1172 | E1108 | E1108 | P977  | K912  | K841 | A756 | A686 | E621 | I550 |     |
| A1444 | L1378 | M1310 | S1173 | Q1111 | Q1111 | E1043 | S1173 | Q1111 | E1043 | P980  | L913  | E847 | A756 | A686 | E621 | I550 |     |
| Y1445 | M1379 | K1313 | G1174 | G1112 | G1112 | A1044 | G1174 | G1112 | A1044 | Q980  | Q915  | S848 | A756 | A686 | E621 | I550 |     |
| L1446 | V1381 | K1314 | H1175 | E1113 | E1113 | C1045 | H1175 | E1113 | C1045 | Q981  | Q916  | D849 | A756 | A686 | E621 | I550 |     |
| V1447 | Y1382 | L1315 | P1179 | E1114 | E1114 | G1046 | P1179 | E1114 | G1046 | Q983  | L917  | E851 | A756 | A686 | E621 | I550 |     |
| G1448 | Q1383 | L1316 | E1180 | N1115 | N1115 | P1047 | E1180 | N1115 | P1047 | Q984  | E918  | R852 | A756 | A686 | E621 | I550 |     |
| V1449 | I1384 | L1316 | S1181 | Y1116 | Y1116 | L1048 | S1181 | Y1116 | L1048 | Q985  | H919  | S853 | A756 | A686 | E621 | I550 |     |
| S1450 | I1385 | A1319 | Q1182 | G1118 | G1118 | E1049 | Q1182 | G1118 | E1049 | L986  | A921  | R854 | A756 | A686 | E621 | I550 |     |
| D1451 | D1386 | L1322 | Q1183 | I1119 | I1119 | M1050 | Q1183 | I1119 | M1050 | L987  | K922  | K855 | A756 | A686 | E621 | I550 |     |
| S1454 | M1387 | L1323 | R1184 | T1119 | T1119 | D1051 | R1184 | T1119 | D1051 | Q988  | Q923  | L856 | A756 | A686 | E621 | I550 |     |
| Q1455 | S1388 | T1324 | L1185 | A1120 | A1120 | S1052 | L1185 | A1120 | S1052 | A989  | A924  | L857 | A756 | A686 | E621 | I550 |     |
| A1456 | Y1389 | D1325 | Q1187 | R1122 | R1122 | L1054 | Q1187 | R1122 | L1054 | S990  | A924  | L857 | A756 | A686 | E621 | I550 |     |
| Q1459 | G1391 | S1328 | V1188 | D1123 | D1123 | S1055 | V1188 | D1123 | S1055 | S992  | A926  | A800 | A756 | A686 | E621 | I550 |     |
| G1460 | L1393 | P1329 | A1189 | K1190 | K1190 | V1056 | A1189 | K1190 | V1056 | S992  | S927  | L863 | A756 | A686 | E621 | I550 |     |
| L1461 | D1394 | N1330 | K1191 | N1191 | N1191 | Q1058 | K1191 | N1191 | Q1058 | P996  | T929  | A866 | A756 | A686 | E621 | I550 |     |
| V1462 | S1395 | K1332 | T1192 | L1128 | L1128 | M1059 | T1192 | L1128 | M1059 | K999  | Q930  | T867 | A756 | A686 | E621 | I550 |     |
| E1463 | V1396 | S1333 | V1193 | R1129 | R1129 | D1063 | V1193 | R1129 | D1063 | M1000 | Q930  | A868 | A756 | A686 | E621 | I550 |     |
| P1464 | M1397 | N1333 | Q1194 | S1130 | S1130 | M1000 | Q1194 | S1130 | M1000 | V1001 | T929  | R869 | A756 | A686 | E621 | I550 |     |
| T1465 | E1398 | Q1334 | L1196 | L1131 | L1131 | L1064 | L1196 | L1131 | L1064 | V1001 | T929  | R869 | A756 | A686 | E621 | I550 |     |
| F1467 | M1399 | A1336 | M1197 | A1132 | A1132 | Q1065 | M1197 | A1132 | Q1065 | V1001 | T929  | R869 | A756 | A686 | E621 | I550 |     |
| A1468 | V1402 | A1336 | N1197 | L1133 | L1133 | E1066 | N1197 | L1133 | E1066 | A1002 | H937  | E872 | A756 | A686 | E621 | I550 |     |
| R1469 | G1403 | R1340 | C1199 | A1134 | A1134 | L1067 | C1199 | A1134 | L1067 | A1004 | K1005 | A873 | A756 | A686 | E621 | I550 |     |
| Q1472 | E1404 | A1341 | V1200 | L1136 | L1136 | D1073 | V1200 | L1136 | D1073 | A1006 | K1005 | A873 | A756 | A686 | E621 | I550 |     |
|       | A1406 | V1342 | L1203 | G1137 | G1137 | K1075 | L1203 | G1137 | K1075 | V1008 | A941  | A874 | A756 | A686 | E621 | I550 |     |

|       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Q2268 | L2207 | K2130 | A2066 | G1938 | H1871 | L1743 | V1683 | A1617 | M1554 | M1476 |
| L2269 | S2208 | T2131 | A2067 | C1939 | V1872 | A1744 | S1684 | R1618 | M1555 | A1477 |
| T2270 | S2068 | V2132 | S2068 | S1940 | E1807 | A1745 | Q1685 | A1619 | A1556 |       |
| G2271 | R2210 | K2133 | L2069 | P1941 | E1808 | A1746 | Q1686 |       | S1480 |       |
| S2272 | A2214 | A2134 | G2070 | S1942 | L1810 | G1747 | L1687 | V1622 | Q1557 |       |
| H2273 | D2073 | V2135 | R2005 | D1943 | L1811 | K1751 | A1688 | N1623 | E1483 |       |
| K2274 | P2074 | E2136 | N2006 | Y1944 | T1812 | L1752 | P1624 | R1625 | P1484 |       |
| R2275 | E2075 | D2137 | A2009 | Y1945 | E1880 | L1753 | R1690 | D1626 | A1560 |       |
| S2276 | T2076 | E2138 | E2010 | K1947 | L1814 | L1754 | E1691 | P1627 | A1561 |       |
| V2277 | Q2077 | K2141 | K1948 | L1948 | L1815 | H1755 | G1692 | T1562 | T1487 |       |
| V2278 | Q2077 | L2142 | E1949 | L1882 | L1816 | H1756 | I1693 | Q1490 | Q1490 |       |
| V2279 | T2081 | T2143 | A1949 | G1883 | E1816 | P1756 | S1694 | P1564 | V1491 |       |
| V2280 | L2082 | R2144 | L1950 | P1884 | A1817 | Q1757 | Q1694 | P1564 |       |       |
| E2282 | N2082 | R2145 | I1951 | L1885 | A1818 | Q1758 | E1696 | W1630 |       |       |
| L2283 | A2083 | A2146 | A1952 | L1886 | S1819 | M1759 | A1697 | L1633 | A1494 |       |
| Q2285 | V2084 | L2146 | C1953 | M1887 | S1820 | A1760 | L1698 | L1633 |       |       |
| A2286 | E2084 | E2147 | E1954 | L1888 | G1825 | L1761 | H1699 | H1636 | V1569 |       |
| A2287 | K2086 | A2148 | R1955 | Q1889 | L1762 | H1762 | H1699 | A1499 | V1498 |       |
| E2288 | V2087 | L2149 | R1956 | L1890 | D1763 | Q1764 | T1700 | M1571 | A1599 |       |
| A2289 | A2088 | T2150 | V1957 | S1891 | Q1765 | Q1764 | Q1701 | K1500 | K1500 |       |
| M2290 | K2089 | H2152 | S1988 | D1892 | L1765 | L1765 | M1702 | H1501 | H1501 |       |
| K2291 | A2090 | I2153 | K1960 | G1893 | K1766 | T1704 | V1640 | L1505 | L1505 |       |
| G2292 | L2091 | L2154 | A2023 | Y1893 | S1830 | S1704 | S1641 | R1510 | R1510 |       |
| T2293 | G2092 | R2154 | V2025 | L1895 | L1831 | L1768 | D1642 | P1579 | P1579 |       |
| R2294 | D2093 | Q2155 | S1962 | Q1833 | T1832 | I1644 | S1643 | E1580 | E1580 |       |
| E2295 | L2094 | E2156 | H1963 | A1834 | Q1833 | E1770 | K1645 | F1581 | F1581 |       |
| W2295 | S2096 | L2157 | V1964 | A1834 | A1834 | S1771 | K1646 | S1582 | S1582 |       |
| V2296 | A2097 | A2158 | L1965 | M1836 | A1836 | A1772 | L1647 | S1583 | S1583 |       |
| D2297 | T2098 | F2160 | L1968 | Q1837 | Q1837 | Q1774 | I1648 | R1515 | R1515 |       |
| P2298 | K2099 | K2161 | L1968 | L1838 | L1838 | L1775 | I1648 | V1584 | V1584 |       |
| F2299 | A2100 | C2161 | A1970 | L1838 | L1838 | L1776 | M1651 | T1516 | T1516 |       |
| G2300 | A2101 | P2166 | G1971 | G1841 | G1841 | T1777 | K1654 | Q1587 | Q1587 |       |
| T2301 | G2102 | A2167 | M1972 | P1842 | P1842 | T1778 | A1655 | M1518 | M1518 |       |
| V2302 | K2104 | K2168 | R1973 | A1900 | A1900 | A1779 | L1656 | P1519 | P1519 |       |
| V2303 | V2105 | T2169 | G1974 | E1908 | E1908 | A1781 | G1857 | T1520 | T1520 |       |
| I2304 | G2106 | T2170 | Q1976 | E1910 | E1910 | A1782 | Q1658 | A1592 | A1592 |       |
| E2305 | D2107 | S2170 | A1977 | E1911 | E1911 | A1782 | L1659 | G1592 | G1592 |       |
| N2306 | V2111 | P2172 | I1979 | H1915 | H1915 | P1786 | E1723 | R1593 | R1593 |       |
| E2307 | W2112 | T2172 | T1980 | K1917 | K1917 | A1786 | A1724 | A1594 | A1594 |       |
| E2308 | L2114 | E2173 | S1983 | H1917 | H1917 | Q1788 | S1725 | I1599 | I1599 |       |
| L2309 | K2115 | F2175 | A1984 | R1919 | R1919 | A1789 | Q1726 | T1600 | T1600 |       |
| L2310 | N2116 | R2176 | V1985 | V1920 | V1920 | A1790 | L1727 | L1601 | L1601 |       |
| G2311 | S2117 | R2177 | S1986 | Q1921 | Q1921 | A1791 | A1667 | S1602 | S1602 |       |
| A2314 | A2118 | M2178 | G1987 | E1922 | E1922 | H1791 | L1668 | A1603 | A1603 |       |
| E2315 | K2119 | T2179 | I1988 | L1923 | L1923 | T1792 | K1730 | K1604 | K1604 |       |
| E2316 | L2120 | K2180 | I1989 | L1923 | L1923 | Q1793 | S1670 | L1605 | L1605 |       |
| E2317 | V2120 | I2182 | A1990 | G1924 | G1924 | E1794 | C1671 | M1606 | M1606 |       |
| E2318 | M2121 | S2195 | D1991 | H1925 | H1925 | A1795 | L1672 | L1607 | L1607 |       |
| K2321 | V2122 | C2196 | L1992 | K1862 | K1862 | L1796 | L1672 | E1608 | E1608 |       |
| K2322 | T2123 | R2197 | L1993 | C1927 | C1927 | E1797 | D1674 | S1609 | S1609 |       |
| K2323 | N2124 | Q2198 | A1993 | I1864 | I1864 | E1798 | D1675 | I1543 | I1543 |       |
| E2324 | V2125 | E2199 | T1994 | A1865 | A1865 | A1799 | D1676 | K1544 | K1544 |       |
| Q2325 | T2126 | E2199 | V2061 | A1866 | A1866 | W1800 | Q1677 | A1610 | A1610 |       |
| K2326 | S2127 | I2202 | V2062 | T1867 | T1867 | Q1801 | L1612 | G1611 | G1611 |       |
| K2327 | L2128 | A2205 | K2063 | T1867 | T1867 | M1802 | L1613 | G1612 | G1612 |       |
| Q2267 | L2129 | N2206 | G2065 | Q1869 | Q1869 | M1803 | L1614 | L1614 | L1614 |       |
|       |       |       |       | A1934 | A1934 | M1802 | Q1615 | Q1615 | Q1615 |       |
|       |       |       |       | L1937 | L1937 | M1803 | T1616 | T1616 | T1616 |       |

|       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |       |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |       |       |     |     |  |       |     |     |  |       |     |     |  |       |     |     |  |       |     |     |  |       |     |     |  |       |     |     |
|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|
| K2331 | R2398 | A2466 | TLE | K2332 | M2389 | A2467 | ARG | K2333 | V2400 | S2467 | GLN | E2334 | A2403 | R2469 | GLN | A2335 | T2404 | L2470 | TYR | E2337 | N2405 | V2471 | LYS | S2338 | N2406 | K2472 | PHE | L2339 | L2407 | A2473 | LEU | F2341 | C2408 | A2474 | PRO | E2343 | N2412 | Q2475 | SER | Q2344 | A2413 | K2476 | GLU | I2345 | A2414 | A2477 | LEU | E2346 | V2415 | A2478 | ARG | E2347 | Q2416 | A2479 | ASP | V2349 | G2417 | PHE | GLU | K2350 | H2418 | GLU | GLN | I2352 | A2419 | ASP | ASP | A2353 | S2420 | GLN | HIS | S2357 | Q2421 | ASN | GLU | K2358 | E2422 | GLU | GLU | L2359 | K2423 | THR | THR | L2360 | L2424 | VAL | VAL | K2361 | I2425 | VAL | VAL | A2362 | S2426 | LYS | LYS | A2366 | S2427 | GLU | GLU | Q2367 | A2428 | LYS | LYS | E2369 | K2429 | MET | MET | A2372 | Q2430 | VAL | VAL | Q2373 | V2431 | GLY | GLY | C2374 | A2432 | GLY | GLY | R2375 | T2435 | ILE | ILE | V2376 | A2436 | ALA | ALA | G2377 | Q2437 | ILE | ILE | A2378 | L2438 | ILE | ILE | I2379 | L2439 | ALA | ALA | F2380 | V2440 | ALA | ALA | A2381 | A2441 | GLN | GLN | N2382 | C2442 | GLU | GLU | A2383 | V2444 | GLU | GLU | L2384 | K2445 | MET | MET | D2385 | A2446 | LEU | LEU | D2386 | D2447 | ARG | ARG | C2387 | Q2448 | LYS | LYS | Q2388 | D2449 | ARG | ARG | W2389 | S2450 | LEU | LEU | S2390 | E2451 | LEU | LEU | I2394 | A2452 | GLU | GLU | S2395 | M2453 | ALA | ALA | A2397 | K2454 | ARG | ARG |  | R2455 | LYS | LYS |  | L2456 | LYS | LYS |  | Q2457 | LEU | LEU |  | A2458 | ALA | ALA |  | A2459 | GLN | GLN |  | V2463 | GLN | GLN |
|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-------|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|-------|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|--|-------|-----|-----|



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 8318                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | JEOL CRYO ARM 300                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 48                                      | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 2400                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.816                                   | Depositor |
| Minimum map value                    | -0.325                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.022                                   | Depositor |
| Recommended contour level            | 0.138                                   | Depositor |
| Map size (Å)                         | 368.64, 368.64, 368.64                  | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.44, 1.44, 1.44                        | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | A     | 0.37         | 0/16258 | 0.54        | 0/22030 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 16077 | 0        | 16278    | 1581    | 0            |
| All | All   | 16077 | 0        | 16278    | 1581    | 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 49.

All (1581) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1067:ILE:HG22 | 1:A:1152:LEU:HD21 | 1.25                     | 1.15              |
| 1:A:1213:LEU:HB2  | 1:A:1316:LEU:HD23 | 1.45                     | 0.94              |
| 1:A:1392:CYS:HB3  | 1:A:1442:GLN:HE21 | 1.32                     | 0.93              |
| 1:A:1695:GLN:HB3  | 1:A:1699:HIS:HE1  | 1.33                     | 0.93              |
| 1:A:1850:PHE:HB3  | 1:A:1973:ARG:HD3  | 1.51                     | 0.92              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:240:GLY:HA2   | 1:A:283:HIS:HD2   | 1.36                     | 0.91              |
| 1:A:575:CYS:O     | 1:A:1019:GLN:NE2  | 2.03                     | 0.91              |
| 1:A:1022:GLN:HA   | 1:A:1025:LYS:HD2  | 1.51                     | 0.90              |
| 1:A:1838:LEU:HD12 | 1:A:1901:LYS:HE3  | 1.51                     | 0.89              |
| 1:A:671:LEU:HD22  | 1:A:780:GLU:HB3   | 1.55                     | 0.89              |
| 1:A:1243:ASN:HD21 | 1:A:1354:THR:HG21 | 1.38                     | 0.89              |
| 1:A:339:ARG:O     | 1:A:348:ILE:N     | 2.06                     | 0.87              |
| 1:A:1463:GLU:H    | 1:A:1467:PHE:HE1  | 1.18                     | 0.87              |
| 1:A:684:LEU:HD23  | 1:A:687:LYS:HZ1   | 1.40                     | 0.86              |
| 1:A:388:ILE:HA    | 1:A:391:LEU:HD12  | 1.57                     | 0.86              |
| 1:A:821:GLU:OE1   | 1:A:825:GLN:NE2   | 2.09                     | 0.86              |
| 1:A:720:THR:OG1   | 1:A:721:LYS:NZ    | 2.09                     | 0.85              |
| 1:A:583:ASN:O     | 1:A:586:GLU:N     | 2.10                     | 0.85              |
| 1:A:948:PRO:HG2   | 1:A:950:PRO:HG3   | 1.59                     | 0.84              |
| 1:A:917:LEU:HD23  | 1:A:1037:ALA:HB1  | 1.58                     | 0.84              |
| 1:A:368:LEU:HD11  | 1:A:380:VAL:HG22  | 1.60                     | 0.84              |
| 1:A:1067:ILE:HG22 | 1:A:1152:LEU:CD2  | 2.06                     | 0.83              |
| 1:A:386:GLU:HG3   | 1:A:390:GLN:HE22  | 1.43                     | 0.83              |
| 1:A:1077:LYS:O    | 1:A:1136:ARG:NH1  | 2.08                     | 0.83              |
| 1:A:1849:SER:OG   | 1:A:1973:ARG:NH2  | 2.13                     | 0.82              |
| 1:A:1161:LYS:HB3  | 1:A:1192:VAL:HG12 | 1.62                     | 0.81              |
| 1:A:1433:LEU:HA   | 1:A:1436:PHE:CE1  | 2.15                     | 0.81              |
| 1:A:2097:ALA:O    | 1:A:2101:ALA:N    | 2.14                     | 0.81              |
| 1:A:599:GLU:HA    | 1:A:603:GLY:HA2   | 1.63                     | 0.81              |
| 1:A:2352:ILE:HG12 | 1:A:2466:ALA:HB1  | 1.63                     | 0.81              |
| 1:A:362:SER:HB3   | 1:A:1683:VAL:HG13 | 1.62                     | 0.81              |
| 1:A:1451:ASP:HB3  | 1:A:1454:SER:HB2  | 1.61                     | 0.81              |
| 1:A:310:VAL:HG22  | 1:A:333:THR:HB    | 1.62                     | 0.80              |
| 1:A:556:SER:HB3   | 1:A:735:GLN:HE22  | 1.46                     | 0.80              |
| 1:A:1739:GLU:O    | 1:A:1742:THR:OG1  | 1.99                     | 0.80              |
| 1:A:1785:ASN:HB3  | 1:A:1788:GLN:HG2  | 1.62                     | 0.80              |
| 1:A:708:GLN:NE2   | 1:A:709:CYS:SG    | 2.55                     | 0.80              |
| 1:A:1304:ASN:ND2  | 1:A:1353:CYS:SG   | 2.55                     | 0.80              |
| 1:A:1430:SER:HA   | 1:A:1433:LEU:HD12 | 1.64                     | 0.80              |
| 1:A:1218:ASP:OD1  | 1:A:1221:LYS:NZ   | 2.14                     | 0.79              |
| 1:A:1387:MET:O    | 1:A:1442:GLN:NE2  | 2.15                     | 0.79              |
| 1:A:920:ALA:HB1   | 1:A:1034:LEU:HD23 | 1.64                     | 0.79              |
| 1:A:1067:ILE:CG2  | 1:A:1152:LEU:HD21 | 2.11                     | 0.79              |
| 1:A:1078:PRO:HA   | 1:A:1136:ARG:HH22 | 1.48                     | 0.78              |
| 1:A:1128:LEU:HD13 | 1:A:1131:LEU:HD12 | 1.65                     | 0.78              |
| 1:A:1726:GLN:HG3  | 1:A:1730:LYS:HD2  | 1.66                     | 0.78              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1261:ARG:NH2  | 1:A:1375:GLU:O    | 2.16                     | 0.78              |
| 1:A:361:ALA:HA    | 1:A:366:PHE:HA    | 1.64                     | 0.78              |
| 1:A:1057:VAL:HG11 | 1:A:1163:SER:HB3  | 1.65                     | 0.78              |
| 1:A:1729:HIS:O    | 1:A:1732:SER:OG   | 2.02                     | 0.78              |
| 1:A:517:GLU:HG2   | 1:A:592:LYS:HB3   | 1.64                     | 0.78              |
| 1:A:2259:GLN:HB3  | 1:A:2260:LYS:HD2  | 1.66                     | 0.78              |
| 1:A:2066:ALA:O    | 1:A:2077:GLN:NE2  | 2.17                     | 0.77              |
| 1:A:860:ALA:HA    | 1:A:863:LEU:HD12  | 1.65                     | 0.77              |
| 1:A:1697:ALA:O    | 1:A:1700:THR:OG1  | 2.03                     | 0.77              |
| 1:A:251:ASN:OD1   | 1:A:255:HIS:NE2   | 2.18                     | 0.77              |
| 1:A:906:GLN:HE21  | 1:A:910:LYS:HG2   | 1.49                     | 0.77              |
| 1:A:1031:LEU:HA   | 1:A:1034:LEU:HD12 | 1.67                     | 0.77              |
| 1:A:1468:ALA:O    | 1:A:1472:GLN:NE2  | 2.18                     | 0.77              |
| 1:A:773:ALA:HA    | 1:A:776:GLN:HE21  | 1.49                     | 0.76              |
| 1:A:1434:CYS:O    | 1:A:1437:THR:OG1  | 2.04                     | 0.76              |
| 1:A:932:ILE:O     | 1:A:936:GLN:NE2   | 2.19                     | 0.75              |
| 1:A:1959:GLU:O    | 1:A:1963:HIS:ND1  | 2.18                     | 0.75              |
| 1:A:316:LYS:NZ    | 1:A:325:LEU:O     | 2.19                     | 0.75              |
| 1:A:696:SER:HA    | 1:A:699:GLN:HE22  | 1.50                     | 0.75              |
| 1:A:1892:ASP:OD1  | 1:A:1895:ARG:NH2  | 2.19                     | 0.75              |
| 1:A:1985:VAL:HA   | 1:A:1988:ILE:HD12 | 1.69                     | 0.75              |
| 1:A:582:SER:O     | 1:A:585:THR:OG1   | 2.04                     | 0.75              |
| 1:A:1510:ARG:HH21 | 1:A:1511:LEU:HD23 | 1.51                     | 0.75              |
| 1:A:2160:PHE:CE1  | 1:A:2216:LEU:HB3  | 2.22                     | 0.75              |
| 1:A:1797:GLU:O    | 1:A:1801:GLN:NE2  | 2.20                     | 0.74              |
| 1:A:250:HIS:HD2   | 1:A:253:GLN:HB2   | 1.52                     | 0.74              |
| 1:A:1292:ALA:O    | 1:A:1298:ARG:NH2  | 2.20                     | 0.74              |
| 1:A:259:PHE:O     | 1:A:263:LYS:N     | 2.20                     | 0.74              |
| 1:A:1264:PRO:HA   | 1:A:1267:LEU:HD12 | 1.69                     | 0.74              |
| 1:A:869:LYS:O     | 1:A:889:ARG:NH1   | 2.21                     | 0.74              |
| 1:A:1011:ILE:HG13 | 1:A:1013:ASP:H    | 1.52                     | 0.74              |
| 1:A:1182:GLN:OE1  | 1:A:1183:GLN:NE2  | 2.19                     | 0.74              |
| 1:A:1923:LEU:HD11 | 1:A:1964:VAL:HG11 | 1.69                     | 0.74              |
| 1:A:866:ALA:HB1   | 1:A:897:LEU:HD22  | 1.69                     | 0.74              |
| 1:A:543:ILE:HG23  | 1:A:587:MET:HE1   | 1.68                     | 0.74              |
| 1:A:608:LEU:HG    | 1:A:654:GLN:HG3   | 1.69                     | 0.74              |
| 1:A:1681:ALA:O    | 1:A:1686:GLN:N    | 2.19                     | 0.74              |
| 1:A:1114:GLU:HG3  | 1:A:1116:TYR:H    | 1.51                     | 0.74              |
| 1:A:2021:LYS:HA   | 1:A:2024:LYS:HD2  | 1.70                     | 0.74              |
| 1:A:259:PHE:HA    | 1:A:262:LEU:HB2   | 1.69                     | 0.74              |
| 1:A:391:LEU:HB3   | 1:A:395:TYR:CZ    | 2.23                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:552:ALA:O     | 1:A:735:GLN:NE2   | 2.21                     | 0.73              |
| 1:A:873:ALA:HB2   | 1:A:889:ARG:HH11  | 1.53                     | 0.73              |
| 1:A:354:THR:O     | 1:A:357:LYS:NZ    | 2.21                     | 0.73              |
| 1:A:914:VAL:O     | 1:A:917:LEU:N     | 2.21                     | 0.73              |
| 1:A:821:GLU:O     | 1:A:825:GLN:NE2   | 2.20                     | 0.73              |
| 1:A:585:THR:O     | 1:A:588:SER:OG    | 2.07                     | 0.73              |
| 1:A:490:SER:O     | 1:A:493:GLN:NE2   | 2.21                     | 0.72              |
| 1:A:612:ALA:HA    | 1:A:615:LEU:HD12  | 1.71                     | 0.72              |
| 1:A:1879:PRO:HG3  | 1:A:1941:PRO:HB3  | 1.71                     | 0.72              |
| 1:A:1360:GLN:HG2  | 1:A:1618:ARG:HD2  | 1.71                     | 0.72              |
| 1:A:1900:ALA:O    | 1:A:1904:ALA:N    | 2.21                     | 0.72              |
| 1:A:1778:THR:HB   | 1:A:1796:LEU:HD22 | 1.70                     | 0.72              |
| 1:A:717:VAL:O     | 1:A:720:THR:OG1   | 2.08                     | 0.72              |
| 1:A:834:SER:O     | 1:A:838:ASN:ND2   | 2.23                     | 0.72              |
| 1:A:317:GLU:O     | 1:A:326:VAL:N     | 2.18                     | 0.72              |
| 1:A:802:THR:HA    | 1:A:805:ILE:HD12  | 1.72                     | 0.72              |
| 1:A:1551:THR:OG1  | 1:A:1554:ASN:OD1  | 2.07                     | 0.72              |
| 1:A:1497:ILE:HA   | 1:A:1500:LYS:HE3  | 1.70                     | 0.71              |
| 1:A:1101:ALA:HA   | 1:A:1104:LYS:HE2  | 1.72                     | 0.71              |
| 1:A:1925:HIS:O    | 1:A:1928:SER:OG   | 2.05                     | 0.71              |
| 1:A:1971:GLY:O    | 1:A:1976:GLN:NE2  | 2.23                     | 0.71              |
| 1:A:339:ARG:HE    | 1:A:349:GLN:HB3   | 1.54                     | 0.71              |
| 1:A:705:ALA:O     | 1:A:708:GLN:NE2   | 2.23                     | 0.71              |
| 1:A:1350:ILE:HG21 | 1:A:1365:ASN:HD21 | 1.54                     | 0.71              |
| 1:A:2316:ILE:HD12 | 1:A:2360:VAL:HB   | 1.72                     | 0.71              |
| 1:A:800:GLN:N     | 1:A:800:GLN:OE1   | 2.23                     | 0.71              |
| 1:A:1113:ASN:ND2  | 1:A:1173:SER:O    | 2.24                     | 0.71              |
| 1:A:906:GLN:HG3   | 1:A:910:LYS:HG2   | 1.73                     | 0.71              |
| 1:A:645:GLY:O     | 1:A:648:SER:OG    | 2.09                     | 0.70              |
| 1:A:971:ARG:HH12  | 1:A:974:GLN:HB2   | 1.56                     | 0.70              |
| 1:A:1923:LEU:HD23 | 1:A:1960:LYS:HB3  | 1.73                     | 0.70              |
| 1:A:2134:ALA:O    | 1:A:2141:LYS:NZ   | 2.21                     | 0.70              |
| 1:A:1350:ILE:O    | 1:A:1354:THR:OG1  | 2.08                     | 0.70              |
| 1:A:1853:TYR:O    | 1:A:1856:THR:OG1  | 2.07                     | 0.70              |
| 1:A:2033:LEU:HA   | 1:A:2036:ASN:HB2  | 1.72                     | 0.70              |
| 1:A:837:VAL:HG13  | 1:A:860:ALA:HB1   | 1.74                     | 0.70              |
| 1:A:2326:LEU:O    | 1:A:2350:LYS:NZ   | 2.25                     | 0.70              |
| 1:A:804:THR:O     | 1:A:807:THR:OG1   | 2.09                     | 0.70              |
| 1:A:652:LEU:HD12  | 1:A:725:PRO:HB2   | 1.74                     | 0.70              |
| 1:A:906:GLN:HA    | 1:A:909:ILE:HB    | 1.71                     | 0.70              |
| 1:A:728:SER:O     | 1:A:788:HIS:NE2   | 2.25                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:942:PRO:HG2   | 1:A:945:SER:HA    | 1.73                     | 0.70              |
| 1:A:727:ILE:O     | 1:A:733:GLN:NE2   | 2.15                     | 0.69              |
| 1:A:1768:LEU:HD21 | 1:A:1810:LEU:HD11 | 1.73                     | 0.69              |
| 1:A:1962:SER:HA   | 1:A:1965:LEU:HD12 | 1.73                     | 0.69              |
| 1:A:904:ALA:O     | 1:A:907:ASN:ND2   | 2.25                     | 0.69              |
| 1:A:1530:LYS:NZ   | 1:A:1534:ASN:OD1  | 2.24                     | 0.69              |
| 1:A:1542:THR:HA   | 1:A:1557:GLN:HE22 | 1.57                     | 0.69              |
| 1:A:1316:LEU:HD12 | 1:A:1319:ALA:HB3  | 1.73                     | 0.69              |
| 1:A:1960:LYS:HA   | 1:A:1963:HIS:HD1  | 1.58                     | 0.69              |
| 1:A:2176:ILE:HD11 | 1:A:2284:ILE:HG23 | 1.74                     | 0.69              |
| 1:A:2172:PRO:HB2  | 1:A:2291:LYS:HE3  | 1.74                     | 0.69              |
| 1:A:391:LEU:O     | 1:A:395:TYR:N     | 2.25                     | 0.69              |
| 1:A:652:LEU:HB3   | 1:A:658:SER:HB3   | 1.73                     | 0.69              |
| 1:A:362:SER:OG    | 1:A:365:SER:N     | 2.26                     | 0.69              |
| 1:A:2016:ARG:NE   | 1:A:2136:GLU:OE1  | 2.25                     | 0.69              |
| 1:A:576:ALA:O     | 1:A:580:ILE:HG12  | 1.92                     | 0.69              |
| 1:A:582:SER:HB3   | 1:A:937:HIS:NE2   | 2.08                     | 0.69              |
| 1:A:372:ASP:OD1   | 1:A:1673:ARG:NH2  | 2.26                     | 0.69              |
| 1:A:1785:ASN:ND2  | 1:A:1788:GLN:OE1  | 2.26                     | 0.69              |
| 1:A:1829:ASP:OD2  | 1:A:1833:GLN:NE2  | 2.25                     | 0.69              |
| 1:A:339:ARG:H     | 1:A:347:VAL:HG23  | 1.57                     | 0.68              |
| 1:A:885:GLU:O     | 1:A:888:GLN:NE2   | 2.27                     | 0.68              |
| 1:A:1603:ALA:O    | 1:A:1606:MET:HB2  | 1.93                     | 0.68              |
| 1:A:330:LEU:HD21  | 1:A:380:VAL:HG11  | 1.74                     | 0.68              |
| 1:A:224:LEU:O     | 1:A:268:LYS:NZ    | 2.26                     | 0.68              |
| 1:A:1893:TYR:OH   | 1:A:1920:VAL:O    | 2.06                     | 0.68              |
| 1:A:582:SER:HB3   | 1:A:937:HIS:CD2   | 2.29                     | 0.68              |
| 1:A:1239:GLN:HB2  | 1:A:1354:THR:HG22 | 1.76                     | 0.68              |
| 1:A:1656:PRO:O    | 1:A:1658:GLN:NE2  | 2.27                     | 0.68              |
| 1:A:1887:ASN:O    | 1:A:1890:THR:OG1  | 2.10                     | 0.68              |
| 1:A:2306:GLU:HA   | 1:A:2367:GLN:HE22 | 1.59                     | 0.68              |
| 1:A:543:ILE:HA    | 1:A:546:GLN:HE21  | 1.58                     | 0.68              |
| 1:A:1944:VAL:HA   | 1:A:1947:LYS:HE3  | 1.76                     | 0.68              |
| 1:A:2116:ASN:HA   | 1:A:2119:LYS:HE2  | 1.74                     | 0.68              |
| 1:A:1105:LEU:HD11 | 1:A:1124:VAL:HG11 | 1.74                     | 0.68              |
| 1:A:1874:LYS:O    | 1:A:1878:SER:N    | 2.22                     | 0.68              |
| 1:A:1282:LEU:HD23 | 1:A:1305:LEU:HD12 | 1.76                     | 0.68              |
| 1:A:1760:ALA:O    | 1:A:1764:GLN:NE2  | 2.26                     | 0.68              |
| 1:A:386:GLU:O     | 1:A:390:GLN:NE2   | 2.26                     | 0.67              |
| 1:A:712:SER:HA    | 1:A:715:GLN:NE2   | 2.10                     | 0.67              |
| 1:A:2104:LYS:NZ   | 1:A:2108:ASP:OD1  | 2.26                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:908:ALA:HA    | 1:A:911:LYS:HB2   | 1.76                     | 0.67              |
| 1:A:1827:MET:O    | 1:A:1830:SER:OG   | 2.12                     | 0.67              |
| 1:A:1690:ARG:HB3  | 1:A:1751:LYS:HZ1  | 1.57                     | 0.67              |
| 1:A:1223:LEU:HD11 | 1:A:1286:VAL:HG11 | 1.76                     | 0.67              |
| 1:A:1239:GLN:HA   | 1:A:1288:MET:HE3  | 1.76                     | 0.67              |
| 1:A:1455:GLN:HB3  | 1:A:1587:GLN:HB3  | 1.77                     | 0.67              |
| 1:A:1098:VAL:O    | 1:A:1102:ILE:HG12 | 1.95                     | 0.67              |
| 1:A:2344:GLN:HE22 | 1:A:2473:ALA:HB2  | 1.60                     | 0.67              |
| 1:A:1251:GLN:O    | 1:A:1254:THR:OG1  | 2.09                     | 0.67              |
| 1:A:1699:HIS:HB3  | 1:A:1814:LEU:HD22 | 1.77                     | 0.67              |
| 1:A:1910:GLU:OE1  | 1:A:1910:GLU:N    | 2.24                     | 0.67              |
| 1:A:499:ILE:HG23  | 1:A:623:LEU:HD12  | 1.76                     | 0.67              |
| 1:A:575:CYS:O     | 1:A:578:THR:OG1   | 2.12                     | 0.67              |
| 1:A:1580:GLU:N    | 1:A:1580:GLU:OE1  | 2.26                     | 0.67              |
| 1:A:2020:LEU:HB3  | 1:A:2024:LYS:HZ3  | 1.60                     | 0.67              |
| 1:A:577:VAL:HG21  | 1:A:623:LEU:HD11  | 1.76                     | 0.67              |
| 1:A:551:THR:HG21  | 1:A:726:THR:HG21  | 1.77                     | 0.67              |
| 1:A:1289:ALA:O    | 1:A:1298:ARG:NE   | 2.27                     | 0.67              |
| 1:A:1956:ARG:HB3  | 1:A:1960:LYS:NZ   | 2.10                     | 0.66              |
| 1:A:1100:SER:OG   | 1:A:1574:ALA:O    | 2.13                     | 0.66              |
| 1:A:1461:LEU:O    | 1:A:1515:ARG:NH1  | 2.28                     | 0.66              |
| 1:A:1789:ALA:O    | 1:A:1792:THR:OG1  | 2.13                     | 0.66              |
| 1:A:812:ILE:O     | 1:A:815:SER:N     | 2.29                     | 0.66              |
| 1:A:1460:GLY:HA3  | 1:A:1583:SER:HA   | 1.77                     | 0.66              |
| 1:A:1512:ALA:HA   | 1:A:1515:ARG:HG2  | 1.77                     | 0.66              |
| 1:A:1705:ALA:HB3  | 1:A:1741:LEU:HD12 | 1.77                     | 0.66              |
| 1:A:335:GLU:N     | 1:A:335:GLU:OE1   | 2.29                     | 0.66              |
| 1:A:1880:GLU:OE1  | 1:A:1880:GLU:N    | 2.27                     | 0.66              |
| 1:A:2324:GLU:OE1  | 1:A:2327:LYS:NZ   | 2.23                     | 0.66              |
| 1:A:1082:GLU:HA   | 1:A:1086:LYS:HD3  | 1.78                     | 0.66              |
| 1:A:1413:ASN:O    | 1:A:1417:GLY:N    | 2.26                     | 0.66              |
| 1:A:1523:ARG:O    | 1:A:1527:GLN:NE2  | 2.29                     | 0.65              |
| 1:A:1667:ALA:O    | 1:A:1670:SER:OG   | 2.12                     | 0.65              |
| 1:A:258:GLY:O     | 1:A:262:LEU:N     | 2.26                     | 0.65              |
| 1:A:987:ILE:O     | 1:A:990:SER:OG    | 2.14                     | 0.65              |
| 1:A:1203:LEU:HD23 | 1:A:1206:GLN:HG3  | 1.77                     | 0.65              |
| 1:A:1518:ASN:ND2  | 1:A:1520:THR:OG1  | 2.28                     | 0.65              |
| 1:A:2428:ALA:HB1  | 1:A:2470:LEU:HD13 | 1.77                     | 0.65              |
| 1:A:2256:LEU:O    | 1:A:2260:LYS:N    | 2.27                     | 0.65              |
| 1:A:1660:GLU:OE1  | 1:A:1660:GLU:N    | 2.26                     | 0.65              |
| 1:A:1956:ARG:HB3  | 1:A:1960:LYS:HZ1  | 1.62                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2413:ALA:O    | 1:A:2417:GLY:N    | 2.30                     | 0.65              |
| 1:A:1365:ASN:HA   | 1:A:1368:ARG:HD2  | 1.79                     | 0.65              |
| 1:A:927:SER:HB2   | 1:A:1027:LEU:HD23 | 1.79                     | 0.65              |
| 1:A:1190:LYS:O    | 1:A:1193:THR:OG1  | 2.11                     | 0.65              |
| 1:A:1613:LEU:HB2  | 1:A:1636:HIS:HB3  | 1.77                     | 0.65              |
| 1:A:1389:TYR:O    | 1:A:1393:LEU:HG   | 1.96                     | 0.65              |
| 1:A:2281:THR:HA   | 1:A:2284:ILE:HD12 | 1.79                     | 0.64              |
| 1:A:1758:GLN:HA   | 1:A:1761:LEU:HG   | 1.78                     | 0.64              |
| 1:A:1447:VAL:HG21 | 1:A:1654:LYS:HD2  | 1.78                     | 0.64              |
| 1:A:2087:VAL:HG21 | 1:A:2128:LEU:HD22 | 1.79                     | 0.64              |
| 1:A:2412:ASN:OD1  | 1:A:2413:ALA:N    | 2.30                     | 0.64              |
| 1:A:1035:ARG:NH1  | 1:A:1039:GLN:HB2  | 2.12                     | 0.64              |
| 1:A:2249:GLU:OE2  | 1:A:2272:HIS:ND1  | 2.31                     | 0.64              |
| 1:A:741:ARG:NE    | 1:A:1939:CYS:SG   | 2.71                     | 0.64              |
| 1:A:1129:ARG:O    | 1:A:1133:GLN:NE2  | 2.23                     | 0.64              |
| 1:A:1856:THR:HA   | 1:A:1859:ARG:HH21 | 1.63                     | 0.64              |
| 1:A:882:ASP:O     | 1:A:887:GLN:NE2   | 2.30                     | 0.64              |
| 1:A:1266:ASP:OD1  | 1:A:1269:ARG:NH2  | 2.28                     | 0.64              |
| 1:A:1392:CYS:HB3  | 1:A:1442:GLN:NE2  | 2.10                     | 0.64              |
| 1:A:1695:GLN:O    | 1:A:1699:HIS:ND1  | 2.30                     | 0.64              |
| 1:A:1884:PRO:HA   | 1:A:1887:ASN:HD21 | 1.63                     | 0.64              |
| 1:A:2128:LEU:O    | 1:A:2131:THR:OG1  | 2.15                     | 0.64              |
| 1:A:1162:ALA:HA   | 1:A:1165:LEU:HG   | 1.79                     | 0.64              |
| 1:A:1696:GLU:OE1  | 1:A:1696:GLU:N    | 2.18                     | 0.64              |
| 1:A:1082:GLU:OE2  | 1:A:1136:ARG:NH2  | 2.31                     | 0.64              |
| 1:A:1322:LEU:HD21 | 1:A:1331:LEU:HB3  | 1.79                     | 0.64              |
| 1:A:1405:GLU:O    | 1:A:1408:THR:OG1  | 2.14                     | 0.64              |
| 1:A:1957:VAL:HA   | 1:A:1960:LYS:HE2  | 1.80                     | 0.64              |
| 1:A:2323:LEU:HD21 | 1:A:2349:VAL:HG12 | 1.79                     | 0.64              |
| 1:A:340:VAL:HG22  | 1:A:347:VAL:HA    | 1.79                     | 0.64              |
| 1:A:928:ALA:O     | 1:A:931:THR:OG1   | 2.15                     | 0.64              |
| 1:A:1672:LEU:HA   | 1:A:1675:LEU:HD12 | 1.80                     | 0.64              |
| 1:A:1772:ALA:O    | 1:A:1775:LEU:HG   | 1.97                     | 0.64              |
| 1:A:1011:ILE:HG21 | 1:A:1017:ALA:HB2  | 1.79                     | 0.63              |
| 1:A:1866:VAL:HA   | 1:A:1869:GLN:HE21 | 1.63                     | 0.63              |
| 1:A:1852:ASP:O    | 1:A:1855:THR:OG1  | 2.14                     | 0.63              |
| 1:A:2073:ASP:OD2  | 1:A:2076:THR:OG1  | 2.16                     | 0.63              |
| 1:A:1662:GLU:HA   | 1:A:1665:ILE:HD12 | 1.80                     | 0.63              |
| 1:A:1108:GLU:CD   | 1:A:1117:ALA:HA   | 2.19                     | 0.63              |
| 1:A:1461:LEU:HB2  | 1:A:1515:ARG:HH11 | 1.63                     | 0.63              |
| 1:A:773:ALA:HA    | 1:A:776:GLN:NE2   | 2.12                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1850:PHE:HA   | 1:A:1853:TYR:HD2  | 1.63                     | 0.63              |
| 1:A:1096:LYS:HE2  | 1:A:1579:PRO:HB3  | 1.79                     | 0.63              |
| 1:A:1626:ASP:HB2  | 1:A:1629:ARG:HB2  | 1.80                     | 0.63              |
| 1:A:1695:GLN:HB3  | 1:A:1699:HIS:CE1  | 2.24                     | 0.63              |
| 1:A:2195:SER:O    | 1:A:2197:ARG:NH2  | 2.32                     | 0.63              |
| 1:A:977:PRO:O     | 1:A:983:GLN:NE2   | 2.31                     | 0.63              |
| 1:A:1433:LEU:HA   | 1:A:1436:PHE:HE1  | 1.64                     | 0.63              |
| 1:A:2040:SER:HB3  | 1:A:2043:LYS:NZ   | 2.14                     | 0.63              |
| 1:A:315:VAL:HG21  | 1:A:330:LEU:HG    | 1.81                     | 0.63              |
| 1:A:525:ASP:HB2   | 1:A:528:SER:HB3   | 1.81                     | 0.63              |
| 1:A:2300:ASP:O    | 1:A:2304:ILE:HG12 | 1.99                     | 0.63              |
| 1:A:2318:ALA:O    | 1:A:2321:LYS:HG2  | 1.99                     | 0.63              |
| 1:A:712:SER:HB2   | 1:A:743:VAL:HG12  | 1.80                     | 0.62              |
| 1:A:1035:ARG:HH21 | 1:A:1917:LYS:HD2  | 1.63                     | 0.62              |
| 1:A:1092:GLY:O    | 1:A:1095:THR:OG1  | 2.16                     | 0.62              |
| 1:A:1947:LYS:HA   | 1:A:1950:LEU:HD12 | 1.81                     | 0.62              |
| 1:A:542:GLU:O     | 1:A:546:GLN:HG2   | 1.98                     | 0.62              |
| 1:A:586:GLU:HG2   | 1:A:589:ARG:HH12  | 1.63                     | 0.62              |
| 1:A:1487:THR:OG1  | 1:A:1490:GLN:OE1  | 2.14                     | 0.62              |
| 1:A:1184:ARG:O    | 1:A:1188:VAL:HG22 | 2.00                     | 0.62              |
| 1:A:1729:HIS:O    | 1:A:1733:GLN:NE2  | 2.32                     | 0.62              |
| 1:A:2124:ASN:O    | 1:A:2127:SER:OG   | 2.12                     | 0.62              |
| 1:A:240:GLY:HA2   | 1:A:283:HIS:CD2   | 2.27                     | 0.62              |
| 1:A:702:VAL:HG13  | 1:A:753:ALA:HB1   | 1.81                     | 0.62              |
| 1:A:873:ALA:HB1   | 1:A:890:LEU:HD22  | 1.81                     | 0.62              |
| 1:A:1433:LEU:HD23 | 1:A:1436:PHE:HE1  | 1.63                     | 0.62              |
| 1:A:1919:ARG:HB3  | 1:A:1964:VAL:HG12 | 1.81                     | 0.62              |
| 1:A:2418:HIS:NE2  | 1:A:2423:LYS:HE3  | 2.14                     | 0.62              |
| 1:A:312:PHE:HB3   | 1:A:329:LEU:HD11  | 1.82                     | 0.62              |
| 1:A:797:ARG:NH2   | 1:A:904:ALA:O     | 2.30                     | 0.62              |
| 1:A:1371:GLU:OE1  | 1:A:1374:ARG:NH1  | 2.32                     | 0.62              |
| 1:A:1857:MET:SD   | 1:A:1899:GLN:NE2  | 2.69                     | 0.62              |
| 1:A:1985:VAL:O    | 1:A:1989:ILE:HD12 | 2.00                     | 0.62              |
| 1:A:2282:GLU:O    | 1:A:2285:GLN:HG2  | 2.00                     | 0.62              |
| 1:A:1165:LEU:HA   | 1:A:1168:GLU:CD   | 2.19                     | 0.62              |
| 1:A:1166:ILE:HG22 | 1:A:1170:LYS:HE3  | 1.81                     | 0.62              |
| 1:A:339:ARG:HH21  | 1:A:349:GLN:HB2   | 1.63                     | 0.62              |
| 1:A:910:LYS:O     | 1:A:914:VAL:HG23  | 2.00                     | 0.62              |
| 1:A:1002:ALA:HA   | 1:A:1005:LYS:NZ   | 2.14                     | 0.62              |
| 1:A:1067:ILE:CG2  | 1:A:1152:LEU:CD2  | 2.74                     | 0.62              |
| 1:A:1165:LEU:HD11 | 1:A:1192:VAL:HG11 | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1168:GLU:HA   | 1:A:1171:LYS:HD3  | 1.82                     | 0.62              |
| 1:A:2178:MET:O    | 1:A:2182:ILE:HG12 | 1.99                     | 0.62              |
| 1:A:785:VAL:HG12  | 1:A:786:LYS:HD3   | 1.82                     | 0.62              |
| 1:A:1455:GLN:NE2  | 1:A:1456:ALA:O    | 2.28                     | 0.62              |
| 1:A:1213:LEU:HD11 | 1:A:1313:SER:HA   | 1.81                     | 0.62              |
| 1:A:316:LYS:HG3   | 1:A:325:LEU:HB3   | 1.81                     | 0.61              |
| 1:A:777:ALA:O     | 1:A:781:LEU:HG    | 2.00                     | 0.61              |
| 1:A:815:SER:OG    | 1:A:821:GLU:OE2   | 2.09                     | 0.61              |
| 1:A:1128:LEU:HA   | 1:A:1131:LEU:HD12 | 1.81                     | 0.61              |
| 1:A:1381:VAL:O    | 1:A:1382:GLN:NE2  | 2.33                     | 0.61              |
| 1:A:1641:SER:HA   | 1:A:1644:ILE:HD12 | 1.81                     | 0.61              |
| 1:A:1364:ASP:HA   | 1:A:1367:LEU:HD12 | 1.80                     | 0.61              |
| 1:A:1937:LEU:HD22 | 1:A:1950:LEU:HD11 | 1.81                     | 0.61              |
| 1:A:2205:ALA:O    | 1:A:2208:SER:OG   | 2.15                     | 0.61              |
| 1:A:963:ILE:HA    | 1:A:993:PHE:HE1   | 1.65                     | 0.61              |
| 1:A:627:GLN:O     | 1:A:630:SER:OG    | 2.16                     | 0.61              |
| 1:A:840:ILE:HG23  | 1:A:856:LEU:HB3   | 1.83                     | 0.61              |
| 1:A:1175:HIS:O    | 1:A:1175:HIS:ND1  | 2.34                     | 0.61              |
| 1:A:1330:ASN:O    | 1:A:1333:SER:OG   | 2.16                     | 0.61              |
| 1:A:1885:LEU:O    | 1:A:1888:GLN:HG2  | 2.00                     | 0.61              |
| 1:A:2400:VAL:HG21 | 1:A:2438:LEU:HD22 | 1.83                     | 0.61              |
| 1:A:1252:ALA:O    | 1:A:1256:LEU:HG   | 2.01                     | 0.61              |
| 1:A:1945:TYR:HA   | 1:A:1948:LYS:HE2  | 1.82                     | 0.61              |
| 1:A:606:ARG:HA    | 1:A:609:LEU:HD12  | 1.83                     | 0.61              |
| 1:A:1884:PRO:HA   | 1:A:1887:ASN:ND2  | 2.15                     | 0.61              |
| 1:A:576:ALA:O     | 1:A:579:THR:HG22  | 2.00                     | 0.61              |
| 1:A:1223:LEU:HD12 | 1:A:1227:LEU:HD13 | 1.81                     | 0.61              |
| 1:A:2385:ASP:OD1  | 1:A:2386:ASP:N    | 2.33                     | 0.61              |
| 1:A:2421:GLN:HE22 | 1:A:2474:ALA:HA   | 1.66                     | 0.61              |
| 1:A:495:LEU:HD13  | 1:A:570:TYR:HB3   | 1.82                     | 0.61              |
| 1:A:360:ALA:O     | 1:A:367:THR:N     | 2.30                     | 0.61              |
| 1:A:1538:ASN:O    | 1:A:1542:THR:HG23 | 2.00                     | 0.61              |
| 1:A:1811:THR:O    | 1:A:1815:ASN:ND2  | 2.34                     | 0.61              |
| 1:A:1813:THR:O    | 1:A:1816:GLU:HG2  | 2.00                     | 0.61              |
| 1:A:322:LYS:HB3   | 1:A:324:LYS:NZ    | 2.16                     | 0.60              |
| 1:A:697:GLY:O     | 1:A:700:THR:OG1   | 2.18                     | 0.60              |
| 1:A:1049:GLU:O    | 1:A:1052:SER:OG   | 2.17                     | 0.60              |
| 1:A:1882:LEU:O    | 1:A:1886:ALA:N    | 2.27                     | 0.60              |
| 1:A:553:GLY:O     | 1:A:557:VAL:HG23  | 2.01                     | 0.60              |
| 1:A:1365:ASN:OD1  | 1:A:1368:ARG:NH1  | 2.34                     | 0.60              |
| 1:A:1658:GLN:HB3  | 1:A:1780:LYS:HE2  | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1856:THR:HA   | 1:A:1859:ARG:HE   | 1.67                     | 0.60              |
| 1:A:1943:ASP:OD2  | 1:A:1946:THR:N    | 2.33                     | 0.60              |
| 1:A:2308:GLU:HB2  | 1:A:2394:ILE:HG12 | 1.81                     | 0.60              |
| 1:A:492:GLN:O     | 1:A:496:THR:HG23  | 2.01                     | 0.60              |
| 1:A:734:GLU:O     | 1:A:737:VAL:HG12  | 2.00                     | 0.60              |
| 1:A:805:ILE:O     | 1:A:809:THR:HG23  | 2.00                     | 0.60              |
| 1:A:1108:GLU:O    | 1:A:1112:GLY:N    | 2.25                     | 0.60              |
| 1:A:1735:ALA:HA   | 1:A:1738:PHE:CD1  | 2.36                     | 0.60              |
| 1:A:492:GLN:HG2   | 1:A:628:PRO:HG3   | 1.83                     | 0.60              |
| 1:A:499:ILE:HD13  | 1:A:627:GLN:HG3   | 1.82                     | 0.60              |
| 1:A:954:GLN:OE1   | 1:A:954:GLN:N     | 2.25                     | 0.60              |
| 1:A:1250:ASN:HD21 | 1:A:1368:ARG:HD3  | 1.66                     | 0.60              |
| 1:A:2205:ALA:C    | 1:A:2209:ARG:HE   | 2.05                     | 0.60              |
| 1:A:2396:ALA:O    | 1:A:2400:VAL:HG13 | 2.01                     | 0.60              |
| 1:A:710:ALA:O     | 1:A:713:THR:OG1   | 2.18                     | 0.60              |
| 1:A:1743:LEU:O    | 1:A:1746:VAL:HG22 | 2.02                     | 0.60              |
| 1:A:1991:ASP:O    | 1:A:1994:THR:OG1  | 2.13                     | 0.60              |
| 1:A:2225:HIS:CD2  | 1:A:2227:GLU:HG3  | 2.37                     | 0.60              |
| 1:A:599:GLU:OE1   | 1:A:606:ARG:NH2   | 2.34                     | 0.60              |
| 1:A:1356:GLN:HA   | 1:A:1361:LYS:HE3  | 1.84                     | 0.60              |
| 1:A:514:ASP:OD1   | 1:A:613:LYS:NZ    | 2.34                     | 0.60              |
| 1:A:962:GLN:HG3   | 1:A:993:PHE:CD1   | 2.37                     | 0.60              |
| 1:A:1683:VAL:O    | 1:A:1685:GLN:NE2  | 2.35                     | 0.60              |
| 1:A:2075:GLU:HB3  | 1:A:2206:ASN:HD21 | 1.67                     | 0.60              |
| 1:A:2389:TRP:NE1  | 1:A:2441:ALA:O    | 2.33                     | 0.60              |
| 1:A:835:ASP:HA    | 1:A:838:ASN:HD21  | 1.66                     | 0.60              |
| 1:A:908:ALA:HA    | 1:A:911:LYS:HD2   | 1.83                     | 0.60              |
| 1:A:1693:ILE:HD11 | 1:A:1751:LYS:HE2  | 1.82                     | 0.60              |
| 1:A:1738:PHE:O    | 1:A:1742:THR:HG23 | 2.02                     | 0.60              |
| 1:A:1993:ASP:HA   | 1:A:1996:ILE:HG12 | 1.84                     | 0.60              |
| 1:A:263:LYS:HA    | 1:A:271:VAL:HG11  | 1.83                     | 0.60              |
| 1:A:1085:GLU:OE2  | 1:A:1085:GLU:N    | 2.33                     | 0.59              |
| 1:A:1975:THR:O    | 1:A:1978:CYS:N    | 2.31                     | 0.59              |
| 1:A:2098:THR:HG22 | 1:A:2114:LEU:HD21 | 1.84                     | 0.59              |
| 1:A:2349:VAL:HA   | 1:A:2352:ILE:HD12 | 1.84                     | 0.59              |
| 1:A:1187:GLN:NE2  | 1:A:1188:VAL:HG13 | 2.17                     | 0.59              |
| 1:A:1300:GLN:NE2  | 1:A:1304:ASN:OD1  | 2.34                     | 0.59              |
| 1:A:1604:LYS:O    | 1:A:1607:LEU:N    | 2.35                     | 0.59              |
| 1:A:2094:LEU:HD11 | 1:A:2118:ALA:HA   | 1.84                     | 0.59              |
| 1:A:2366:ALA:HA   | 1:A:2452:ALA:HB1  | 1.84                     | 0.59              |
| 1:A:1303:SER:HA   | 1:A:1306:LYS:HE3  | 1.83                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:529:LYS:HA    | 1:A:532:ARG:HD3   | 1.85                     | 0.59              |
| 1:A:2169:THR:HG21 | 1:A:2225:HIS:HA   | 1.84                     | 0.59              |
| 1:A:321:GLY:H     | 1:A:1770:GLU:CD   | 2.06                     | 0.59              |
| 1:A:589:ARG:O     | 1:A:593:LEU:HG    | 2.02                     | 0.59              |
| 1:A:1247:ALA:HB2  | 1:A:1368:ARG:HH21 | 1.67                     | 0.59              |
| 1:A:1340:ARG:NH1  | 1:A:1372:THR:OG1  | 2.34                     | 0.59              |
| 1:A:1676:ASP:OD2  | 1:A:1766:LYS:NZ   | 2.34                     | 0.59              |
| 1:A:1856:THR:O    | 1:A:1860:THR:HG23 | 2.01                     | 0.59              |
| 1:A:671:LEU:O     | 1:A:675:VAL:HG23  | 2.02                     | 0.59              |
| 1:A:892:GLU:HA    | 1:A:895:GLU:OE2   | 2.02                     | 0.59              |
| 1:A:1105:LEU:O    | 1:A:1108:GLU:HG2  | 2.02                     | 0.59              |
| 1:A:1284:ALA:O    | 1:A:1288:MET:HG2  | 2.02                     | 0.59              |
| 1:A:1624:PRO:O    | 1:A:1630:TRP:NE1  | 2.32                     | 0.59              |
| 1:A:1974:GLY:O    | 1:A:2041:GLN:HG3  | 2.02                     | 0.59              |
| 1:A:2108:ASP:HB3  | 1:A:2111:VAL:HG22 | 1.84                     | 0.59              |
| 1:A:2324:GLU:O    | 1:A:2327:LYS:NZ   | 2.35                     | 0.59              |
| 1:A:685:LYS:HD3   | 1:A:765:ARG:HG3   | 1.85                     | 0.59              |
| 1:A:1591:GLU:OE1  | 1:A:1591:GLU:N    | 2.33                     | 0.59              |
| 1:A:550:ILE:HG23  | 1:A:580:ILE:HG23  | 1.84                     | 0.59              |
| 1:A:1800:VAL:O    | 1:A:1804:THR:HG23 | 2.02                     | 0.59              |
| 1:A:333:THR:HG23  | 1:A:336:CYS:H     | 1.67                     | 0.58              |
| 1:A:1599:ILE:HD12 | 1:A:1599:ILE:H    | 1.66                     | 0.58              |
| 1:A:1690:ARG:HE   | 1:A:1693:ILE:HD13 | 1.67                     | 0.58              |
| 1:A:1833:GLN:HA   | 1:A:1836:ASN:ND2  | 2.18                     | 0.58              |
| 1:A:996:PRO:O     | 1:A:1000:MET:HG2  | 2.03                     | 0.58              |
| 1:A:1410:ILE:HG12 | 1:A:1426:ILE:HB   | 1.85                     | 0.58              |
| 1:A:727:ILE:HG12  | 1:A:784:HIS:HE1   | 1.67                     | 0.58              |
| 1:A:1368:ARG:O    | 1:A:1372:THR:HG23 | 2.02                     | 0.58              |
| 1:A:1747:GLY:O    | 1:A:1751:LYS:HD3  | 2.03                     | 0.58              |
| 1:A:2389:TRP:CE2  | 1:A:2444:VAL:HB   | 2.39                     | 0.58              |
| 1:A:359:TRP:HB2   | 1:A:366:PHE:CZ    | 2.39                     | 0.58              |
| 1:A:658:SER:OG    | 1:A:659:ASP:N     | 2.36                     | 0.58              |
| 1:A:1160:ASP:OD2  | 1:A:1161:LYS:N    | 2.37                     | 0.58              |
| 1:A:1715:PRO:HB2  | 1:A:1730:LYS:HZ1  | 1.68                     | 0.58              |
| 1:A:959:VAL:O     | 1:A:963:ILE:HG23  | 2.03                     | 0.58              |
| 1:A:1412:GLN:HA   | 1:A:1415:LYS:HD2  | 1.86                     | 0.58              |
| 1:A:1491:VAL:HG11 | 1:A:1546:LEU:HD23 | 1.86                     | 0.58              |
| 1:A:1613:LEU:O    | 1:A:1616:THR:OG1  | 2.17                     | 0.58              |
| 1:A:1733:GLN:HA   | 1:A:1736:GLN:NE2  | 2.18                     | 0.58              |
| 1:A:1809:ASP:O    | 1:A:1812:THR:OG1  | 2.20                     | 0.58              |
| 1:A:646:GLN:O     | 1:A:649:GLY:N     | 2.36                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1540:VAL:HG12 | 1:A:1544:LYS:HE2  | 1.84                     | 0.58              |
| 1:A:1800:VAL:HA   | 1:A:1803:MET:HE2  | 1.85                     | 0.58              |
| 1:A:1842:PRO:HG3  | 1:A:1901:LYS:HB3  | 1.85                     | 0.58              |
| 1:A:383:THR:OG1   | 1:A:384:GLU:OE2   | 2.19                     | 0.58              |
| 1:A:1410:ILE:HG23 | 1:A:1422:PHE:HD1  | 1.68                     | 0.58              |
| 1:A:1764:GLN:O    | 1:A:1767:THR:OG1  | 2.20                     | 0.58              |
| 1:A:1886:ALA:O    | 1:A:1890:THR:HG23 | 2.03                     | 0.58              |
| 1:A:2014:ASP:OD1  | 1:A:2015:HIS:N    | 2.32                     | 0.58              |
| 1:A:2123:THR:O    | 1:A:2126:THR:OG1  | 2.18                     | 0.58              |
| 1:A:347:VAL:HG21  | 1:A:350:GLU:HG3   | 1.84                     | 0.58              |
| 1:A:1251:GLN:NE2  | 1:A:1255:GLU:OE2  | 2.37                     | 0.58              |
| 1:A:1447:VAL:HB   | 1:A:1596:MET:CE   | 2.34                     | 0.58              |
| 1:A:1702:MET:HE1  | 1:A:1745:ALA:HA   | 1.85                     | 0.58              |
| 1:A:1791:HIS:CE1  | 1:A:1792:THR:HG23 | 2.39                     | 0.58              |
| 1:A:534:ASN:HB3   | 1:A:968:GLN:HE21  | 1.69                     | 0.58              |
| 1:A:1355:GLN:HG2  | 1:A:1358:PRO:HD2  | 1.86                     | 0.58              |
| 1:A:1427:ALA:O    | 1:A:1430:SER:OG   | 2.18                     | 0.58              |
| 1:A:1673:ARG:O    | 1:A:1677:GLN:NE2  | 2.37                     | 0.58              |
| 1:A:1796:LEU:O    | 1:A:1800:VAL:HG23 | 2.03                     | 0.58              |
| 1:A:2322:LYS:O    | 1:A:2325:GLN:NE2  | 2.37                     | 0.58              |
| 1:A:2359:LEU:HA   | 1:A:2459:ALA:HB1  | 1.85                     | 0.58              |
| 1:A:360:ALA:N     | 1:A:367:THR:OG1   | 2.37                     | 0.57              |
| 1:A:384:GLU:OE2   | 1:A:384:GLU:N     | 2.29                     | 0.57              |
| 1:A:1203:LEU:HD12 | 1:A:1204:PRO:HD2  | 1.87                     | 0.57              |
| 1:A:2101:ALA:HB3  | 1:A:2114:LEU:HD22 | 1.85                     | 0.57              |
| 1:A:2148:ALA:O    | 1:A:2152:HIS:HB2  | 2.03                     | 0.57              |
| 1:A:1237:GLU:O    | 1:A:1241:ARG:HG2  | 2.02                     | 0.57              |
| 1:A:806:LEU:O     | 1:A:809:THR:N     | 2.37                     | 0.57              |
| 1:A:1836:ASN:OD1  | 1:A:1837:GLN:N    | 2.37                     | 0.57              |
| 1:A:1902:PRO:HA   | 1:A:1905:VAL:HG12 | 1.85                     | 0.57              |
| 1:A:716:LEU:O     | 1:A:720:THR:HG23  | 2.05                     | 0.57              |
| 1:A:1134:ALA:O    | 1:A:1138:VAL:HG13 | 2.05                     | 0.57              |
| 1:A:1868:VAL:O    | 1:A:1872:VAL:HG23 | 2.04                     | 0.57              |
| 1:A:2048:ALA:O    | 1:A:2051:SER:OG   | 2.18                     | 0.57              |
| 1:A:2301:PRO:HB3  | 1:A:2387:GLY:HA2  | 1.85                     | 0.57              |
| 1:A:2334:GLU:O    | 1:A:2417:GLY:HA3  | 2.05                     | 0.57              |
| 1:A:1510:ARG:HH12 | 1:A:1514:ALA:HB2  | 1.68                     | 0.57              |
| 1:A:1833:GLN:HA   | 1:A:1836:ASN:HD21 | 1.69                     | 0.57              |
| 1:A:2005:ASN:HA   | 1:A:2070:GLY:HA2  | 1.87                     | 0.57              |
| 1:A:242:GLN:HA    | 1:A:245:ILE:HG12  | 1.87                     | 0.57              |
| 1:A:1016:SER:O    | 1:A:1019:GLN:HB2  | 2.04                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1611:GLY:O    | 1:A:1614:ILE:HG22 | 2.05                     | 0.57              |
| 1:A:1690:ARG:H    | 1:A:1751:LYS:HZ1  | 1.50                     | 0.57              |
| 1:A:1838:LEU:O    | 1:A:1901:LYS:NZ   | 2.27                     | 0.57              |
| 1:A:1860:THR:O    | 1:A:1864:ILE:HG23 | 2.04                     | 0.57              |
| 1:A:696:SER:HA    | 1:A:699:GLN:NE2   | 2.19                     | 0.57              |
| 1:A:1578:ASN:O    | 1:A:1582:SER:OG   | 2.14                     | 0.57              |
| 1:A:2120:VAL:O    | 1:A:2123:THR:OG1  | 2.18                     | 0.57              |
| 1:A:499:ILE:O     | 1:A:502:SER:OG    | 2.19                     | 0.57              |
| 1:A:1850:PHE:HB3  | 1:A:1973:ARG:CD   | 2.31                     | 0.57              |
| 1:A:2006:ARG:NH1  | 1:A:2010:GLU:O    | 2.38                     | 0.57              |
| 1:A:502:SER:O     | 1:A:506:VAL:HG23  | 2.05                     | 0.57              |
| 1:A:1165:LEU:O    | 1:A:1168:GLU:HG2  | 2.05                     | 0.57              |
| 1:A:1253:ALA:HA   | 1:A:1256:LEU:HD12 | 1.87                     | 0.57              |
| 1:A:1669:ASN:HA   | 1:A:1672:LEU:HG   | 1.87                     | 0.57              |
| 1:A:1693:ILE:HD12 | 1:A:1698:LEU:HD21 | 1.87                     | 0.57              |
| 1:A:1713:ILE:HG13 | 1:A:1714:GLU:N    | 2.19                     | 0.57              |
| 1:A:1801:GLN:O    | 1:A:1804:THR:N    | 2.38                     | 0.57              |
| 1:A:1888:GLN:O    | 1:A:1891:SER:OG   | 2.20                     | 0.56              |
| 1:A:2161:CYS:HA   | 1:A:2241:ARG:HH22 | 1.70                     | 0.56              |
| 1:A:938:ALA:O     | 1:A:942:PRO:HD3   | 2.05                     | 0.56              |
| 1:A:1124:VAL:O    | 1:A:1128:LEU:HD23 | 2.04                     | 0.56              |
| 1:A:1386:ASP:OD1  | 1:A:1387:MET:N    | 2.38                     | 0.56              |
| 1:A:2182:ILE:HG13 | 1:A:2215:MET:HG2  | 1.86                     | 0.56              |
| 1:A:2229:ALA:HB3  | 1:A:2232:VAL:HG23 | 1.87                     | 0.56              |
| 1:A:499:ILE:HG21  | 1:A:627:GLN:HE21  | 1.70                     | 0.56              |
| 1:A:546:GLN:HG3   | 1:A:587:MET:HE3   | 1.87                     | 0.56              |
| 1:A:623:LEU:O     | 1:A:627:GLN:NE2   | 2.38                     | 0.56              |
| 1:A:813:PHE:O     | 1:A:1915:HIS:NE2  | 2.38                     | 0.56              |
| 1:A:847:GLU:OE2   | 1:A:849:ASP:N     | 2.37                     | 0.56              |
| 1:A:918:GLU:O     | 1:A:922:LYS:HG2   | 2.04                     | 0.56              |
| 1:A:960:ALA:O     | 1:A:963:ILE:HG12  | 2.05                     | 0.56              |
| 1:A:1680:LEU:O    | 1:A:1684:SER:OG   | 2.22                     | 0.56              |
| 1:A:1919:ARG:O    | 1:A:1923:LEU:HG   | 2.05                     | 0.56              |
| 1:A:550:ILE:O     | 1:A:554:THR:HG23  | 2.05                     | 0.56              |
| 1:A:349:GLN:HG3   | 1:A:351:TRP:CZ2   | 2.41                     | 0.56              |
| 1:A:539:SER:HB2   | 1:A:594:LEU:HD21  | 1.88                     | 0.56              |
| 1:A:2143:THR:HG23 | 1:A:2258:LEU:HD23 | 1.86                     | 0.56              |
| 1:A:223:ILE:O     | 1:A:267:PRO:HG3   | 2.06                     | 0.56              |
| 1:A:1083:THR:O    | 1:A:1086:LYS:HG2  | 2.06                     | 0.56              |
| 1:A:1084:MET:HA   | 1:A:1141:LEU:HD22 | 1.88                     | 0.56              |
| 1:A:1163:SER:HA   | 1:A:1166:ILE:HD12 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1398:GLU:O    | 1:A:1402:VAL:HG23 | 2.05                     | 0.56              |
| 1:A:1410:ILE:HG23 | 1:A:1422:PHE:CD1  | 2.41                     | 0.56              |
| 1:A:322:LYS:HB3   | 1:A:324:LYS:HZ3   | 1.69                     | 0.56              |
| 1:A:604:ASN:HA    | 1:A:606:ARG:NH1   | 2.21                     | 0.56              |
| 1:A:698:LEU:HG    | 1:A:756:ALA:HB1   | 1.88                     | 0.56              |
| 1:A:812:ILE:HD12  | 1:A:822:MET:HG3   | 1.88                     | 0.56              |
| 1:A:825:GLN:O     | 1:A:829:LEU:HB2   | 2.06                     | 0.56              |
| 1:A:1329:PRO:HB2  | 1:A:1382:GLN:HG2  | 1.87                     | 0.56              |
| 1:A:1519:PRO:O    | 1:A:1522:LYS:HG2  | 2.05                     | 0.56              |
| 1:A:1606:MET:HE3  | 1:A:1644:ILE:N    | 2.21                     | 0.56              |
| 1:A:1702:MET:HB2  | 1:A:1814:LEU:HD11 | 1.88                     | 0.56              |
| 1:A:1994:THR:O    | 1:A:1997:MET:HG3  | 2.06                     | 0.56              |
| 1:A:608:LEU:HD12  | 1:A:608:LEU:H     | 1.71                     | 0.56              |
| 1:A:2205:ALA:O    | 1:A:2209:ARG:NE   | 2.37                     | 0.56              |
| 1:A:2473:ALA:HA   | 1:A:2476:LYS:HE2  | 1.87                     | 0.56              |
| 1:A:1252:ALA:O    | 1:A:1255:GLU:HG2  | 2.06                     | 0.56              |
| 1:A:1255:GLU:HA   | 1:A:1258:GLN:CD   | 2.27                     | 0.56              |
| 1:A:1606:MET:HE2  | 1:A:1643:SER:HB2  | 1.86                     | 0.56              |
| 1:A:1850:PHE:CE2  | 1:A:1907:ALA:HB2  | 2.40                     | 0.56              |
| 1:A:2235:ARG:HB3  | 1:A:2239:TYR:CZ   | 2.40                     | 0.56              |
| 1:A:2375:LYS:O    | 1:A:2382:ASN:ND2  | 2.38                     | 0.56              |
| 1:A:1660:GLU:O    | 1:A:1663:THR:OG1  | 2.19                     | 0.55              |
| 1:A:1846:PRO:HB3  | 1:A:1906:ALA:HA   | 1.88                     | 0.55              |
| 1:A:1861:ALA:O    | 1:A:1864:ILE:HG12 | 2.06                     | 0.55              |
| 1:A:311:SER:N     | 1:A:332:ILE:O     | 2.21                     | 0.55              |
| 1:A:579:THR:HB    | 1:A:1019:GLN:HE22 | 1.70                     | 0.55              |
| 1:A:669:MET:HG3   | 1:A:673:ASN:HD21  | 1.72                     | 0.55              |
| 1:A:2048:ALA:O    | 1:A:2052:VAL:HG23 | 2.06                     | 0.55              |
| 1:A:914:VAL:HA    | 1:A:917:LEU:HD12  | 1.87                     | 0.55              |
| 1:A:927:SER:O     | 1:A:931:THR:HG23  | 2.05                     | 0.55              |
| 1:A:1184:ARG:HA   | 1:A:1187:GLN:HE21 | 1.70                     | 0.55              |
| 1:A:1189:ALA:O    | 1:A:1192:VAL:HG22 | 2.06                     | 0.55              |
| 1:A:1284:ALA:O    | 1:A:1287:GLU:HG2  | 2.06                     | 0.55              |
| 1:A:2214:ASP:OD1  | 1:A:2217:ARG:NH2  | 2.35                     | 0.55              |
| 1:A:2359:LEU:HD22 | 1:A:2463:VAL:HG21 | 1.87                     | 0.55              |
| 1:A:498:THR:O     | 1:A:501:SER:OG    | 2.25                     | 0.55              |
| 1:A:1300:GLN:OE1  | 1:A:1304:ASN:ND2  | 2.29                     | 0.55              |
| 1:A:1363:CYS:SG   | 1:A:1618:ARG:HD3  | 2.47                     | 0.55              |
| 1:A:1955:ARG:O    | 1:A:1958:SER:OG   | 2.07                     | 0.55              |
| 1:A:548:ASP:O     | 1:A:551:THR:OG1   | 2.19                     | 0.55              |
| 1:A:1668:LEU:O    | 1:A:1672:LEU:HG   | 2.06                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1961:VAL:O    | 1:A:1965:LEU:HG   | 2.06                     | 0.55              |
| 1:A:1969:GLN:NE2  | 1:A:1976:GLN:OE1  | 2.40                     | 0.55              |
| 1:A:2031:LYS:O    | 1:A:2035:GLN:NE2  | 2.40                     | 0.55              |
| 1:A:2270:THR:HB   | 1:A:2274:LYS:HZ1  | 1.72                     | 0.55              |
| 1:A:2418:HIS:HB3  | 1:A:2424:LEU:HD11 | 1.87                     | 0.55              |
| 1:A:1222:ARG:NH2  | 1:A:1283:GLU:OE2  | 2.39                     | 0.55              |
| 1:A:1383:PRO:HD3  | 1:A:1445:TYR:CZ   | 2.42                     | 0.55              |
| 1:A:1684:SER:HB2  | 1:A:1686:GLN:HE22 | 1.72                     | 0.55              |
| 1:A:1689:PRO:HB3  | 1:A:1751:LYS:HA   | 1.88                     | 0.55              |
| 1:A:1731:VAL:HA   | 1:A:1734:MET:HG2  | 1.87                     | 0.55              |
| 1:A:813:PHE:HE2   | 1:A:894:ALA:HB3   | 1.71                     | 0.55              |
| 1:A:829:LEU:HD22  | 1:A:870:MET:SD    | 2.47                     | 0.55              |
| 1:A:1794:GLU:HA   | 1:A:1797:GLU:CD   | 2.27                     | 0.55              |
| 1:A:267:PRO:HD2   | 1:A:270:TYR:CD2   | 2.42                     | 0.55              |
| 1:A:579:THR:HB    | 1:A:1019:GLN:OE1  | 2.07                     | 0.55              |
| 1:A:854:ARG:HA    | 1:A:857:LEU:HD12  | 1.89                     | 0.55              |
| 1:A:1301:VAL:HG22 | 1:A:1353:CYS:SG   | 2.47                     | 0.55              |
| 1:A:1539:LEU:O    | 1:A:1542:THR:OG1  | 2.17                     | 0.55              |
| 1:A:1892:ASP:HA   | 1:A:1895:ARG:HH21 | 1.72                     | 0.55              |
| 1:A:1084:MET:SD   | 1:A:1084:MET:N    | 2.80                     | 0.55              |
| 1:A:1415:LYS:HA   | 1:A:1625:ARG:HH11 | 1.72                     | 0.55              |
| 1:A:1671:CYS:SG   | 1:A:1742:THR:HG21 | 2.47                     | 0.55              |
| 1:A:1754:SER:HB3  | 1:A:1757:GLN:HB2  | 1.88                     | 0.55              |
| 1:A:2127:SER:O    | 1:A:2131:THR:HG23 | 2.06                     | 0.55              |
| 1:A:1733:GLN:HA   | 1:A:1736:GLN:HE21 | 1.72                     | 0.54              |
| 1:A:2323:LEU:HG   | 1:A:2350:LYS:HG2  | 1.89                     | 0.54              |
| 1:A:1083:THR:H    | 1:A:1086:LYS:HG2  | 1.72                     | 0.54              |
| 1:A:1768:LEU:O    | 1:A:1771:SER:OG   | 2.21                     | 0.54              |
| 1:A:1944:VAL:O    | 1:A:1947:LYS:HG2  | 2.08                     | 0.54              |
| 1:A:969:GLY:HA3   | 1:A:986:LEU:HD13  | 1.89                     | 0.54              |
| 1:A:1755:HIS:HA   | 1:A:1758:GLN:HE21 | 1.72                     | 0.54              |
| 1:A:1887:ASN:OD1  | 1:A:1888:GLN:N    | 2.40                     | 0.54              |
| 1:A:1980:THR:O    | 1:A:1983:SER:OG   | 2.21                     | 0.54              |
| 1:A:670:GLN:HA    | 1:A:673:ASN:HD22  | 1.73                     | 0.54              |
| 1:A:803:ASP:O     | 1:A:807:THR:HG23  | 2.07                     | 0.54              |
| 1:A:951:LEU:HA    | 1:A:954:GLN:NE2   | 2.23                     | 0.54              |
| 1:A:1684:SER:O    | 1:A:1686:GLN:NE2  | 2.40                     | 0.54              |
| 1:A:2087:VAL:O    | 1:A:2091:LEU:HG   | 2.06                     | 0.54              |
| 1:A:2150:THR:HG23 | 1:A:2154:ARG:HH12 | 1.72                     | 0.54              |
| 1:A:2427:SER:O    | 1:A:2431:VAL:HG23 | 2.08                     | 0.54              |
| 1:A:341:ASP:HB3   | 1:A:344:THR:OG1   | 2.08                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:853:SER:O     | 1:A:857:LEU:HG    | 2.08                     | 0.54              |
| 1:A:996:PRO:HA    | 1:A:999:LYS:NZ    | 2.21                     | 0.54              |
| 1:A:1024:ALA:HA   | 1:A:1027:LEU:HD12 | 1.88                     | 0.54              |
| 1:A:1349:LEU:O    | 1:A:1353:CYS:HB2  | 2.06                     | 0.54              |
| 1:A:1377:LEU:HD13 | 1:A:1441:ALA:HB2  | 1.88                     | 0.54              |
| 1:A:1644:ILE:O    | 1:A:1648:ILE:HG12 | 2.08                     | 0.54              |
| 1:A:1690:ARG:H    | 1:A:1751:LYS:NZ   | 2.06                     | 0.54              |
| 1:A:1762:LEU:O    | 1:A:1765:THR:OG1  | 2.18                     | 0.54              |
| 1:A:2379:ILE:HG23 | 1:A:2382:ASN:H    | 1.72                     | 0.54              |
| 1:A:971:ARG:NH1   | 1:A:971:ARG:HA    | 2.22                     | 0.54              |
| 1:A:1388:SER:OG   | 1:A:1389:TYR:N    | 2.38                     | 0.54              |
| 1:A:1717:ALA:O    | 1:A:1721:ARG:HG2  | 2.07                     | 0.54              |
| 1:A:1782:ALA:HB2  | 1:A:1796:LEU:HD21 | 1.90                     | 0.54              |
| 1:A:312:PHE:HA    | 1:A:330:LEU:O     | 2.08                     | 0.54              |
| 1:A:913:LEU:O     | 1:A:917:LEU:HG    | 2.07                     | 0.54              |
| 1:A:1965:LEU:O    | 1:A:1968:LEU:HG   | 2.07                     | 0.54              |
| 1:A:2040:SER:HB3  | 1:A:2043:LYS:HZ3  | 1.70                     | 0.54              |
| 1:A:915:GLN:HA    | 1:A:918:GLU:OE2   | 2.08                     | 0.54              |
| 1:A:1672:LEU:O    | 1:A:1766:LYS:NZ   | 2.40                     | 0.54              |
| 1:A:1960:LYS:HA   | 1:A:1963:HIS:ND1  | 2.23                     | 0.54              |
| 1:A:2247:TYR:O    | 1:A:2251:LEU:HG   | 2.08                     | 0.54              |
| 1:A:2348:ALA:O    | 1:A:2352:ILE:HG13 | 2.08                     | 0.54              |
| 1:A:286:CYS:SG    | 1:A:297:ARG:NH2   | 2.79                     | 0.54              |
| 1:A:525:ASP:O     | 1:A:529:LYS:NZ    | 2.27                     | 0.54              |
| 1:A:1459:GLN:CA   | 1:A:1584:VAL:H    | 2.21                     | 0.54              |
| 1:A:1636:HIS:O    | 1:A:1639:THR:OG1  | 2.24                     | 0.54              |
| 1:A:1754:SER:OG   | 1:A:1757:GLN:OE1  | 2.19                     | 0.54              |
| 1:A:2006:ARG:HH12 | 1:A:2011:THR:HA   | 1.73                     | 0.54              |
| 1:A:910:LYS:NZ    | 1:A:1044:ALA:O    | 2.41                     | 0.54              |
| 1:A:1709:ILE:O    | 1:A:1713:ILE:HG23 | 2.08                     | 0.54              |
| 1:A:2468:ASP:OD1  | 1:A:2472:LYS:NZ   | 2.40                     | 0.54              |
| 1:A:334:LYS:HZ3   | 1:A:395:TYR:HE1   | 1.55                     | 0.53              |
| 1:A:1266:ASP:HA   | 1:A:1269:ARG:HE   | 1.72                     | 0.53              |
| 1:A:1273:ARG:HA   | 1:A:1276:GLN:HE21 | 1.73                     | 0.53              |
| 1:A:1810:LEU:O    | 1:A:1813:THR:OG1  | 2.23                     | 0.53              |
| 1:A:1881:GLU:OE1  | 1:A:1881:GLU:N    | 2.26                     | 0.53              |
| 1:A:1797:GLU:HG2  | 1:A:1798:GLU:N    | 2.24                     | 0.53              |
| 1:A:2390:SER:O    | 1:A:2394:ILE:HG13 | 2.07                     | 0.53              |
| 1:A:2472:LYS:O    | 1:A:2475:GLN:NE2  | 2.41                     | 0.53              |
| 1:A:547:VAL:HA    | 1:A:550:ILE:HD12  | 1.91                     | 0.53              |
| 1:A:1032:ALA:O    | 1:A:1036:THR:HG23 | 2.08                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1172:ALA:HA   | 1:A:1175:HIS:CE1  | 2.44                     | 0.53              |
| 1:A:1850:PHE:HA   | 1:A:1853:TYR:CD2  | 2.44                     | 0.53              |
| 1:A:2403:ALA:HB1  | 1:A:2431:VAL:HG22 | 1.89                     | 0.53              |
| 1:A:2454:LYS:O    | 1:A:2457:GLN:HG2  | 2.08                     | 0.53              |
| 1:A:332:ILE:HG13  | 1:A:337:VAL:HG23  | 1.91                     | 0.53              |
| 1:A:1154:THR:HB   | 1:A:1199:CYS:SG   | 2.48                     | 0.53              |
| 1:A:1188:VAL:O    | 1:A:1192:VAL:HG13 | 2.07                     | 0.53              |
| 1:A:1863:ALA:O    | 1:A:1867:THR:HG23 | 2.08                     | 0.53              |
| 1:A:1873:THR:O    | 1:A:1877:THR:HG23 | 2.08                     | 0.53              |
| 1:A:364:LYS:O     | 1:A:382:THR:N     | 2.36                     | 0.53              |
| 1:A:803:ASP:HA    | 1:A:806:LEU:HD12  | 1.89                     | 0.53              |
| 1:A:1014:GLN:CD   | 1:A:1014:GLN:H    | 2.11                     | 0.53              |
| 1:A:1351:THR:HA   | 1:A:1361:LYS:HZ3  | 1.73                     | 0.53              |
| 1:A:510:GLN:O     | 1:A:513:LEU:HB3   | 2.08                     | 0.53              |
| 1:A:798:TYR:CD1   | 1:A:836:LEU:HD13  | 2.44                     | 0.53              |
| 1:A:802:THR:O     | 1:A:806:LEU:HG    | 2.08                     | 0.53              |
| 1:A:1642:ASP:O    | 1:A:1645:LYS:HG2  | 2.09                     | 0.53              |
| 1:A:1842:PRO:HD3  | 1:A:1901:LYS:HB3  | 1.91                     | 0.53              |
| 1:A:2101:ALA:HB1  | 1:A:2111:VAL:HG12 | 1.90                     | 0.53              |
| 1:A:2327:LYS:H    | 1:A:2329:ARG:NH2  | 2.07                     | 0.53              |
| 1:A:314:LEU:HG    | 1:A:342:GLU:OE1   | 2.09                     | 0.53              |
| 1:A:716:LEU:HD12  | 1:A:743:VAL:HG11  | 1.89                     | 0.53              |
| 1:A:765:ARG:HH21  | 1:A:769:ALA:N     | 2.07                     | 0.53              |
| 1:A:1013:ASP:OD2  | 1:A:1016:SER:N    | 2.36                     | 0.53              |
| 1:A:1148:GLN:O    | 1:A:1151:VAL:HG22 | 2.09                     | 0.53              |
| 1:A:1519:PRO:HA   | 1:A:1522:LYS:HE3  | 1.91                     | 0.53              |
| 1:A:362:SER:N     | 1:A:365:SER:O     | 2.42                     | 0.53              |
| 1:A:521:PRO:O     | 1:A:1077:LYS:HE2  | 2.08                     | 0.53              |
| 1:A:615:LEU:HD11  | 1:A:651:LEU:HD22  | 1.91                     | 0.53              |
| 1:A:808:VAL:HG13  | 1:A:825:GLN:HB3   | 1.91                     | 0.53              |
| 1:A:1911:GLU:OE1  | 1:A:1911:GLU:N    | 2.22                     | 0.53              |
| 1:A:1927:CYS:HA   | 1:A:1930:LEU:HD12 | 1.90                     | 0.53              |
| 1:A:2223:ALA:HB1  | 1:A:2233:ARG:HB2  | 1.90                     | 0.53              |
| 1:A:2337:GLU:HG3  | 1:A:2341:PHE:CE1  | 2.44                     | 0.53              |
| 1:A:518:THR:HG23  | 1:A:520:PRO:HD3   | 1.89                     | 0.53              |
| 1:A:599:GLU:HA    | 1:A:603:GLY:CA    | 2.36                     | 0.53              |
| 1:A:1258:GLN:HG3  | 1:A:1375:GLU:OE1  | 2.09                     | 0.53              |
| 1:A:1384:ILE:HG21 | 1:A:1438:GLU:HB2  | 1.90                     | 0.53              |
| 1:A:1975:THR:HB   | 1:A:1978:CYS:SG   | 2.49                     | 0.53              |
| 1:A:2082:ASN:HA   | 1:A:2085:LYS:HE2  | 1.91                     | 0.53              |
| 1:A:1465:THR:OG1  | 1:A:1469:ARG:NH1  | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1850:PHE:CZ   | 1:A:1907:ALA:HB2  | 2.44                     | 0.53              |
| 1:A:1951:ILE:HG13 | 1:A:1955:ARG:NE   | 2.24                     | 0.53              |
| 1:A:1992:LEU:HD22 | 1:A:2081:ILE:HG23 | 1.90                     | 0.53              |
| 1:A:2019:ILE:HG13 | 1:A:2061:VAL:HG13 | 1.90                     | 0.53              |
| 1:A:604:ASN:O     | 1:A:607:PRO:HD2   | 2.09                     | 0.52              |
| 1:A:1098:VAL:HG11 | 1:A:1131:LEU:HD11 | 1.91                     | 0.52              |
| 1:A:1261:ARG:HH22 | 1:A:1378:GLU:HB2  | 1.73                     | 0.52              |
| 1:A:1559:ARG:HA   | 1:A:1562:THR:HG22 | 1.91                     | 0.52              |
| 1:A:2323:LEU:HD23 | 1:A:2353:ALA:HB2  | 1.91                     | 0.52              |
| 1:A:554:THR:O     | 1:A:558:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:1602:SER:OG   | 1:A:1647:LEU:HG   | 2.09                     | 0.52              |
| 1:A:1773:LEU:HA   | 1:A:1776:LEU:HD12 | 1.90                     | 0.52              |
| 1:A:1805:GLU:HA   | 1:A:1808:GLU:OE2  | 2.10                     | 0.52              |
| 1:A:1818:ALA:HB1  | 1:A:1824:VAL:HG11 | 1.90                     | 0.52              |
| 1:A:804:THR:O     | 1:A:808:VAL:HG23  | 2.09                     | 0.52              |
| 1:A:1497:ILE:O    | 1:A:1500:LYS:HG2  | 2.09                     | 0.52              |
| 1:A:920:ALA:HA    | 1:A:923:GLN:NE2   | 2.25                     | 0.52              |
| 1:A:1518:ASN:HD21 | 1:A:1520:THR:HG1  | 1.53                     | 0.52              |
| 1:A:1651:MET:HA   | 1:A:1654:LYS:HE2  | 1.91                     | 0.52              |
| 1:A:1740:PRO:HA   | 1:A:1743:LEU:HD12 | 1.91                     | 0.52              |
| 1:A:1762:LEU:HD13 | 1:A:1765:THR:HG21 | 1.90                     | 0.52              |
| 1:A:1792:THR:O    | 1:A:1796:LEU:HD23 | 2.10                     | 0.52              |
| 1:A:1084:MET:O    | 1:A:1088:THR:HG23 | 2.09                     | 0.52              |
| 1:A:1518:ASN:ND2  | 1:A:1520:THR:HG1  | 2.08                     | 0.52              |
| 1:A:1789:ALA:HB3  | 1:A:1791:HIS:ND1  | 2.25                     | 0.52              |
| 1:A:1975:THR:HG22 | 1:A:1977:ALA:HB3  | 1.91                     | 0.52              |
| 1:A:515:ASP:O     | 1:A:592:LYS:HE3   | 2.08                     | 0.52              |
| 1:A:1367:LEU:O    | 1:A:1370:LEU:HB3  | 2.09                     | 0.52              |
| 1:A:216:TYR:CE1   | 1:A:295:LYS:HA    | 2.44                     | 0.52              |
| 1:A:220:ARG:HH11  | 1:A:242:GLN:NE2   | 2.07                     | 0.52              |
| 1:A:902:ASN:CB    | 1:A:906:GLN:HB2   | 2.40                     | 0.52              |
| 1:A:2160:PHE:HE1  | 1:A:2216:LEU:HB3  | 1.71                     | 0.52              |
| 1:A:2327:LYS:HB2  | 1:A:2329:ARG:CZ   | 2.39                     | 0.52              |
| 1:A:220:ARG:O     | 1:A:224:LEU:HG    | 2.10                     | 0.52              |
| 1:A:615:LEU:O     | 1:A:619:VAL:HG23  | 2.10                     | 0.52              |
| 1:A:679:ALA:O     | 1:A:683:VAL:HG23  | 2.09                     | 0.52              |
| 1:A:723:VAL:HG21  | 1:A:736:LEU:HD21  | 1.91                     | 0.52              |
| 1:A:950:PRO:HB2   | 1:A:952:LEU:HG    | 1.91                     | 0.52              |
| 1:A:1036:THR:O    | 1:A:1040:LYS:HG2  | 2.09                     | 0.52              |
| 1:A:1304:ASN:HB2  | 1:A:1349:LEU:HD13 | 1.91                     | 0.52              |
| 1:A:208:ASP:OD1   | 1:A:211:GLN:N     | 2.42                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:342:GLU:O     | 1:A:345:LYS:NZ    | 2.28                     | 0.52              |
| 1:A:988:ALA:O     | 1:A:991:GLN:NE2   | 2.42                     | 0.52              |
| 1:A:1297:ASP:O    | 1:A:1301:VAL:HG23 | 2.10                     | 0.52              |
| 1:A:1322:LEU:HD12 | 1:A:1335:LEU:HD13 | 1.92                     | 0.52              |
| 1:A:1381:VAL:HG22 | 1:A:1593:ARG:NH1  | 2.25                     | 0.52              |
| 1:A:2081:ILE:HA   | 1:A:2084:VAL:HG22 | 1.92                     | 0.52              |
| 1:A:2324:GLU:HA   | 1:A:2350:LYS:HZ3  | 1.75                     | 0.52              |
| 1:A:222:ASP:HA    | 1:A:225:ASN:OD1   | 2.09                     | 0.52              |
| 1:A:234:LYS:HE2   | 1:A:301:LEU:HD12  | 1.92                     | 0.52              |
| 1:A:914:VAL:HG12  | 1:A:918:GLU:OE1   | 2.11                     | 0.52              |
| 1:A:1674:ASP:HA   | 1:A:1677:GLN:HE21 | 1.74                     | 0.52              |
| 1:A:296:VAL:O     | 1:A:300:LYS:HG2   | 2.11                     | 0.51              |
| 1:A:1190:LYS:O    | 1:A:1194:GLN:NE2  | 2.43                     | 0.51              |
| 1:A:1257:VAL:HG12 | 1:A:1335:LEU:HD23 | 1.90                     | 0.51              |
| 1:A:500:ASN:O     | 1:A:503:MET:HG2   | 2.10                     | 0.51              |
| 1:A:743:VAL:O     | 1:A:747:VAL:HG23  | 2.11                     | 0.51              |
| 1:A:902:ASN:HB3   | 1:A:906:GLN:HB2   | 1.91                     | 0.51              |
| 1:A:1050:MET:HG2  | 1:A:1170:LYS:HE2  | 1.91                     | 0.51              |
| 1:A:1079:LEU:H    | 1:A:1082:GLU:CD   | 2.13                     | 0.51              |
| 1:A:1841:GLY:HA2  | 1:A:1901:LYS:HD3  | 1.93                     | 0.51              |
| 1:A:2143:THR:OG1  | 1:A:2144:ARG:NH1  | 2.43                     | 0.51              |
| 1:A:1035:ARG:HH12 | 1:A:1039:GLN:HB2  | 1.74                     | 0.51              |
| 1:A:1384:ILE:HG22 | 1:A:1442:GLN:HB3  | 1.91                     | 0.51              |
| 1:A:1659:LEU:O    | 1:A:1663:THR:HG23 | 2.10                     | 0.51              |
| 1:A:1789:ALA:HB3  | 1:A:1791:HIS:CE1  | 2.45                     | 0.51              |
| 1:A:1849:SER:OG   | 1:A:1851:VAL:HG12 | 2.11                     | 0.51              |
| 1:A:267:PRO:HD2   | 1:A:270:TYR:HD2   | 1.76                     | 0.51              |
| 1:A:1208:ASP:O    | 1:A:1212:ALA:N    | 2.35                     | 0.51              |
| 1:A:1459:GLN:HA   | 1:A:1584:VAL:H    | 1.75                     | 0.51              |
| 1:A:1565:LEU:O    | 1:A:1569:VAL:HG23 | 2.10                     | 0.51              |
| 1:A:1943:ASP:OD2  | 1:A:1946:THR:HG23 | 2.10                     | 0.51              |
| 1:A:1978:CYS:HB2  | 1:A:2099:LYS:HD3  | 1.93                     | 0.51              |
| 1:A:786:LYS:HA    | 1:A:789:ALA:HB3   | 1.92                     | 0.51              |
| 1:A:1345:SER:O    | 1:A:1348:GLN:NE2  | 2.43                     | 0.51              |
| 1:A:1675:LEU:HD13 | 1:A:1766:LYS:HD3  | 1.91                     | 0.51              |
| 1:A:1714:GLU:H    | 1:A:1714:GLU:CD   | 2.12                     | 0.51              |
| 1:A:2266:LYS:O    | 1:A:2270:THR:HG23 | 2.10                     | 0.51              |
| 1:A:392:ILE:HD13  | 1:A:395:TYR:HD2   | 1.75                     | 0.51              |
| 1:A:648:SER:O     | 1:A:652:LEU:HG    | 2.10                     | 0.51              |
| 1:A:892:GLU:HA    | 1:A:895:GLU:CD    | 2.30                     | 0.51              |
| 1:A:1891:SER:O    | 1:A:1895:ARG:NE   | 2.43                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:829:LEU:HD21  | 1:A:897:LEU:HG    | 1.92                     | 0.51              |
| 1:A:1961:VAL:O    | 1:A:1964:VAL:HG22 | 2.11                     | 0.51              |
| 1:A:2394:ILE:O    | 1:A:2398:ARG:HG3  | 2.10                     | 0.51              |
| 1:A:727:ILE:HG12  | 1:A:784:HIS:CE1   | 2.46                     | 0.51              |
| 1:A:983:GLN:O     | 1:A:987:ILE:HG13  | 2.11                     | 0.51              |
| 1:A:1606:MET:CE   | 1:A:1643:SER:HB2  | 2.40                     | 0.51              |
| 1:A:1728:GLY:HA2  | 1:A:1731:VAL:HG22 | 1.93                     | 0.51              |
| 1:A:2179:THR:HG22 | 1:A:2215:MET:HE1  | 1.91                     | 0.51              |
| 1:A:2425:ILE:O    | 1:A:2429:LYS:HG3  | 2.10                     | 0.51              |
| 1:A:2475:GLN:NE2  | 1:A:2476:LYS:HG3  | 2.26                     | 0.51              |
| 1:A:245:ILE:HG13  | 1:A:246:GLN:HG3   | 1.92                     | 0.51              |
| 1:A:894:ALA:O     | 1:A:898:ARG:HG3   | 2.10                     | 0.51              |
| 1:A:970:VAL:O     | 1:A:973:SER:OG    | 2.24                     | 0.51              |
| 1:A:1161:LYS:O    | 1:A:1165:LEU:HG   | 2.11                     | 0.51              |
| 1:A:1707:GLN:O    | 1:A:1710:SER:OG   | 2.26                     | 0.51              |
| 1:A:1723:GLU:OE2  | 1:A:1725:SER:HB3  | 2.11                     | 0.51              |
| 1:A:2439:LEU:O    | 1:A:2443:LYS:HG2  | 2.11                     | 0.51              |
| 1:A:729:SER:HB2   | 1:A:731:VAL:HG12  | 1.92                     | 0.51              |
| 1:A:761:GLY:HA2   | 1:A:764:LEU:HD12  | 1.93                     | 0.51              |
| 1:A:867:THR:O     | 1:A:871:VAL:HG23  | 2.11                     | 0.51              |
| 1:A:1101:ALA:O    | 1:A:1105:LEU:HG   | 2.11                     | 0.51              |
| 1:A:2012:PHE:CZ   | 1:A:2016:ARG:HB2  | 2.46                     | 0.51              |
| 1:A:2217:ARG:HD2  | 1:A:2218:ALA:N    | 2.26                     | 0.51              |
| 1:A:2349:VAL:HG13 | 1:A:2407:LEU:HD21 | 1.92                     | 0.51              |
| 1:A:2432:ALA:O    | 1:A:2435:THR:OG1  | 2.27                     | 0.51              |
| 1:A:241:PHE:HB2   | 1:A:298:TYR:HD1   | 1.76                     | 0.50              |
| 1:A:242:GLN:HE21  | 1:A:246:GLN:HE22  | 1.59                     | 0.50              |
| 1:A:621:GLU:OE1   | 1:A:624:ARG:NH2   | 2.44                     | 0.50              |
| 1:A:2250:LEU:O    | 1:A:2254:VAL:HG23 | 2.11                     | 0.50              |
| 1:A:2348:ALA:O    | 1:A:2351:SER:OG   | 2.23                     | 0.50              |
| 1:A:905:ALA:C     | 1:A:907:ASN:H     | 2.14                     | 0.50              |
| 1:A:1193:THR:HA   | 1:A:1196:LEU:HD12 | 1.93                     | 0.50              |
| 1:A:2014:ASP:OD1  | 1:A:2015:HIS:ND1  | 2.44                     | 0.50              |
| 1:A:2125:VAL:O    | 1:A:2129:LEU:HG   | 2.10                     | 0.50              |
| 1:A:2160:PHE:HA   | 1:A:2220:LYS:NZ   | 2.26                     | 0.50              |
| 1:A:579:THR:HB    | 1:A:1019:GLN:NE2  | 2.26                     | 0.50              |
| 1:A:778:LEU:HD22  | 1:A:1945:TYR:CD2  | 2.47                     | 0.50              |
| 1:A:1546:LEU:HD13 | 1:A:1558:CYS:SG   | 2.52                     | 0.50              |
| 1:A:1772:ALA:O    | 1:A:1776:LEU:HG   | 2.10                     | 0.50              |
| 1:A:1793:GLN:NE2  | 1:A:1797:GLU:OE1  | 2.45                     | 0.50              |
| 1:A:2088:ALA:HA   | 1:A:2091:LEU:HD12 | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:307:THR:HG23  | 1:A:308:TYR:CD1   | 2.45                     | 0.50              |
| 1:A:317:GLU:OE2   | 1:A:381:GLN:N     | 2.44                     | 0.50              |
| 1:A:1130:SER:HA   | 1:A:1133:GLN:HG2  | 1.93                     | 0.50              |
| 1:A:1265:GLN:OE1  | 1:A:1265:GLN:N    | 2.43                     | 0.50              |
| 1:A:1713:ILE:O    | 1:A:1716:LEU:HB3  | 2.12                     | 0.50              |
| 1:A:1742:THR:O    | 1:A:1746:VAL:HG13 | 2.11                     | 0.50              |
| 1:A:1976:GLN:NE2  | 1:A:2041:GLN:HE22 | 2.09                     | 0.50              |
| 1:A:2147:GLU:HA   | 1:A:2150:THR:HG22 | 1.92                     | 0.50              |
| 1:A:337:VAL:HG13  | 1:A:351:TRP:HB2   | 1.94                     | 0.50              |
| 1:A:774:VAL:O     | 1:A:778:LEU:HG    | 2.11                     | 0.50              |
| 1:A:929:THR:O     | 1:A:932:ILE:HG12  | 2.11                     | 0.50              |
| 1:A:1105:LEU:HA   | 1:A:1108:GLU:OE2  | 2.12                     | 0.50              |
| 1:A:2261:PRO:O    | 1:A:2266:LYS:NZ   | 2.45                     | 0.50              |
| 1:A:2279:SER:HA   | 1:A:2282:GLU:HG2  | 1.93                     | 0.50              |
| 1:A:250:HIS:O     | 1:A:254:LYS:HG2   | 2.12                     | 0.50              |
| 1:A:1472:GLN:O    | 1:A:1476:MET:HG2  | 2.10                     | 0.50              |
| 1:A:2435:THR:O    | 1:A:2439:LEU:HD23 | 2.11                     | 0.50              |
| 1:A:269:GLU:HA    | 1:A:272:LYS:HE2   | 1.94                     | 0.50              |
| 1:A:336:CYS:HA    | 1:A:352:SER:HA    | 1.93                     | 0.50              |
| 1:A:1168:GLU:OE2  | 1:A:1185:LEU:HD13 | 2.12                     | 0.50              |
| 1:A:1447:VAL:HA   | 1:A:1450:SER:OG   | 2.11                     | 0.50              |
| 1:A:2146:LEU:O    | 1:A:2149:THR:HB   | 2.12                     | 0.50              |
| 1:A:2362:ALA:HB1  | 1:A:2456:LEU:HA   | 1.93                     | 0.50              |
| 1:A:294:ALA:HA    | 1:A:297:ARG:HD3   | 1.93                     | 0.50              |
| 1:A:501:SER:HA    | 1:A:504:GLN:NE2   | 2.26                     | 0.50              |
| 1:A:827:ARG:NH2   | 1:A:828:ILE:HA    | 2.27                     | 0.50              |
| 1:A:1157:ASP:HA   | 1:A:1160:ASP:OD1  | 2.12                     | 0.50              |
| 1:A:1192:VAL:O    | 1:A:1196:LEU:HG   | 2.12                     | 0.50              |
| 1:A:1674:ASP:HA   | 1:A:1677:GLN:NE2  | 2.26                     | 0.50              |
| 1:A:1696:GLU:O    | 1:A:1700:THR:HG23 | 2.12                     | 0.50              |
| 1:A:1997:MET:HE3  | 1:A:2436:ALA:O    | 2.12                     | 0.50              |
| 1:A:984:LEU:HA    | 1:A:987:ILE:HD12  | 1.94                     | 0.50              |
| 1:A:1561:ALA:O    | 1:A:1564:PRO:HD2  | 2.12                     | 0.50              |
| 1:A:2169:THR:HG21 | 1:A:2226:PRO:HD3  | 1.94                     | 0.50              |
| 1:A:322:LYS:HD3   | 1:A:323:ASN:N     | 2.27                     | 0.49              |
| 1:A:578:THR:O     | 1:A:581:SER:OG    | 2.26                     | 0.49              |
| 1:A:1236:GLN:HG2  | 1:A:1237:GLU:H    | 1.77                     | 0.49              |
| 1:A:1404:GLY:O    | 1:A:1408:THR:HG23 | 2.12                     | 0.49              |
| 1:A:1760:ALA:HA   | 1:A:1763:ASP:OD2  | 2.12                     | 0.49              |
| 1:A:1849:SER:HB3  | 1:A:1852:ASP:OD2  | 2.12                     | 0.49              |
| 1:A:1922:GLU:HA   | 1:A:1925:HIS:HD2  | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1991:ASP:O    | 1:A:1995:THR:HG23 | 2.12                     | 0.49              |
| 1:A:2385:ASP:O    | 1:A:2388:GLN:HG3  | 2.11                     | 0.49              |
| 1:A:727:ILE:HG23  | 1:A:784:HIS:CE1   | 2.47                     | 0.49              |
| 1:A:1702:MET:O    | 1:A:1706:VAL:HG12 | 2.11                     | 0.49              |
| 1:A:2018:GLY:O    | 1:A:2022:THR:HG23 | 2.12                     | 0.49              |
| 1:A:2030:THR:O    | 1:A:2034:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:2131:THR:O    | 1:A:2135:VAL:HG23 | 2.12                     | 0.49              |
| 1:A:541:HIS:CE1   | 1:A:925:ALA:HB3   | 2.47                     | 0.49              |
| 1:A:618:ALA:O     | 1:A:622:LEU:HD23  | 2.12                     | 0.49              |
| 1:A:955:SER:HB2   | 1:A:1000:MET:HE2  | 1.93                     | 0.49              |
| 1:A:1372:THR:OG1  | 1:A:1373:VAL:N    | 2.43                     | 0.49              |
| 1:A:1605:THR:O    | 1:A:1609:SER:OG   | 2.15                     | 0.49              |
| 1:A:1995:THR:HA   | 1:A:1998:PHE:HD2  | 1.77                     | 0.49              |
| 1:A:2053:ALA:HB1  | 1:A:2057:ARG:HH12 | 1.77                     | 0.49              |
| 1:A:2425:ILE:C    | 1:A:2429:LYS:HZ3  | 2.15                     | 0.49              |
| 1:A:663:HIS:CE1   | 1:A:664:PHE:HD1   | 2.30                     | 0.49              |
| 1:A:1184:ARG:O    | 1:A:1187:GLN:NE2  | 2.45                     | 0.49              |
| 1:A:1870:GLU:O    | 1:A:1873:THR:OG1  | 2.23                     | 0.49              |
| 1:A:2264:ASP:O    | 1:A:2267:GLN:NE2  | 2.45                     | 0.49              |
| 1:A:1373:VAL:O    | 1:A:1377:LEU:HD23 | 2.13                     | 0.49              |
| 1:A:1705:ALA:O    | 1:A:1709:ILE:HG12 | 2.12                     | 0.49              |
| 1:A:1878:SER:OG   | 1:A:1881:GLU:OE2  | 2.30                     | 0.49              |
| 1:A:2094:LEU:HD21 | 1:A:2118:ALA:N    | 2.28                     | 0.49              |
| 1:A:2328:PRO:HB2  | 1:A:2343:GLU:HG3  | 1.94                     | 0.49              |
| 1:A:733:GLN:HG3   | 1:A:784:HIS:CD2   | 2.48                     | 0.49              |
| 1:A:1771:SER:HB2  | 1:A:1803:MET:SD   | 2.51                     | 0.49              |
| 1:A:1959:GLU:C    | 1:A:1963:HIS:HD1  | 2.16                     | 0.49              |
| 1:A:2095:ILE:O    | 1:A:2098:THR:OG1  | 2.28                     | 0.49              |
| 1:A:2235:ARG:NE   | 1:A:2235:ARG:HA   | 2.26                     | 0.49              |
| 1:A:2334:GLU:HB3  | 1:A:2416:GLN:HA   | 1.94                     | 0.49              |
| 1:A:353:LEU:HD21  | 1:A:399:ILE:HB    | 1.95                     | 0.49              |
| 1:A:575:CYS:HA    | 1:A:1015:ALA:HB1  | 1.95                     | 0.49              |
| 1:A:951:LEU:HD13  | 1:A:954:GLN:NE2   | 2.28                     | 0.49              |
| 1:A:1976:GLN:HE22 | 1:A:2041:GLN:HE22 | 1.60                     | 0.49              |
| 1:A:2246:GLY:O    | 1:A:2250:LEU:HD23 | 2.13                     | 0.49              |
| 1:A:368:LEU:HD13  | 1:A:379:SER:HA    | 1.94                     | 0.49              |
| 1:A:582:SER:HB3   | 1:A:937:HIS:HE2   | 1.76                     | 0.49              |
| 1:A:1073:ASP:HB3  | 1:A:1075:LYS:NZ   | 2.28                     | 0.49              |
| 1:A:1403:LEU:O    | 1:A:1407:MET:HG2  | 2.13                     | 0.49              |
| 1:A:1415:LYS:HG3  | 1:A:1630:TRP:CH2  | 2.47                     | 0.49              |
| 1:A:1483:GLU:HG2  | 1:A:1484:PRO:HD2  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1665:ILE:HG13 | 1:A:1776:LEU:HD13 | 1.95                     | 0.49              |
| 1:A:1761:LEU:O    | 1:A:1765:THR:HG23 | 2.12                     | 0.49              |
| 1:A:2020:LEU:HB3  | 1:A:2024:LYS:NZ   | 2.27                     | 0.49              |
| 1:A:551:THR:O     | 1:A:554:THR:OG1   | 2.23                     | 0.49              |
| 1:A:1404:GLY:O    | 1:A:1407:MET:HB2  | 2.12                     | 0.49              |
| 1:A:1842:PRO:HD3  | 1:A:1901:LYS:HD3  | 1.95                     | 0.49              |
| 1:A:2077:GLN:O    | 1:A:2081:ILE:HG12 | 2.13                     | 0.49              |
| 1:A:699:GLN:O     | 1:A:703:ILE:HG12  | 2.13                     | 0.49              |
| 1:A:2128:LEU:HD12 | 1:A:2131:THR:OG1  | 2.12                     | 0.49              |
| 1:A:801:ALA:O     | 1:A:805:ILE:HG13  | 2.13                     | 0.48              |
| 1:A:1052:SER:O    | 1:A:1055:SER:OG   | 2.25                     | 0.48              |
| 1:A:1707:GLN:O    | 1:A:1711:HIS:ND1  | 2.45                     | 0.48              |
| 1:A:339:ARG:HD3   | 1:A:378:TYR:CE1   | 2.48                     | 0.48              |
| 1:A:1011:ILE:HG13 | 1:A:1013:ASP:N    | 2.25                     | 0.48              |
| 1:A:1349:LEU:HD12 | 1:A:1353:CYS:SG   | 2.53                     | 0.48              |
| 1:A:1698:LEU:HA   | 1:A:1701:GLN:OE1  | 2.13                     | 0.48              |
| 1:A:1773:LEU:HD13 | 1:A:1776:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:1794:GLU:HA   | 1:A:1797:GLU:OE2  | 2.14                     | 0.48              |
| 1:A:2036:ASN:HB3  | 1:A:2044:LEU:HA   | 1.95                     | 0.48              |
| 1:A:2138:GLU:HA   | 1:A:2141:LYS:HE2  | 1.94                     | 0.48              |
| 1:A:2169:THR:HA   | 1:A:2221:GLU:HB3  | 1.94                     | 0.48              |
| 1:A:2238:HIS:HD2  | 1:A:2239:TYR:HD1  | 1.61                     | 0.48              |
| 1:A:509:ALA:O     | 1:A:512:THR:OG1   | 2.29                     | 0.48              |
| 1:A:1127:GLY:O    | 1:A:1130:SER:OG   | 2.27                     | 0.48              |
| 1:A:1477:ALA:O    | 1:A:1480:SER:OG   | 2.29                     | 0.48              |
| 1:A:2116:ASN:O    | 1:A:2120:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:2397:ALA:HA   | 1:A:2400:VAL:HG22 | 1.95                     | 0.48              |
| 1:A:522:LEU:HB2   | 1:A:532:ARG:HD2   | 1.96                     | 0.48              |
| 1:A:1461:LEU:HD22 | 1:A:1516:THR:HG22 | 1.94                     | 0.48              |
| 1:A:1559:ARG:O    | 1:A:1562:THR:HG22 | 2.13                     | 0.48              |
| 1:A:1712:LEU:C    | 1:A:1715:PRO:HD2  | 2.34                     | 0.48              |
| 1:A:1917:LYS:O    | 1:A:1921:GLN:NE2  | 2.46                     | 0.48              |
| 1:A:622:LEU:O     | 1:A:625:SER:OG    | 2.18                     | 0.48              |
| 1:A:811:ASN:O     | 1:A:814:SER:HB2   | 2.13                     | 0.48              |
| 1:A:901:THR:O     | 1:A:905:ALA:HB3   | 2.13                     | 0.48              |
| 1:A:1306:LYS:O    | 1:A:1309:SER:OG   | 2.16                     | 0.48              |
| 1:A:1389:TYR:CE2  | 1:A:1393:LEU:HD11 | 2.48                     | 0.48              |
| 1:A:1996:ILE:O    | 1:A:2000:THR:HG23 | 2.14                     | 0.48              |
| 1:A:578:THR:O     | 1:A:937:HIS:NE2   | 2.47                     | 0.48              |
| 1:A:670:GLN:HA    | 1:A:673:ASN:ND2   | 2.28                     | 0.48              |
| 1:A:885:GLU:HA    | 1:A:888:GLN:HE21  | 1.78                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1919:ARG:NE   | 1:A:1963:HIS:HB3  | 2.29                     | 0.48              |
| 1:A:2202:ILE:O    | 1:A:2206:ASN:ND2  | 2.47                     | 0.48              |
| 1:A:2337:GLU:HG3  | 1:A:2341:PHE:HE1  | 1.79                     | 0.48              |
| 1:A:610:GLN:HA    | 1:A:613:LYS:HD2   | 1.95                     | 0.48              |
| 1:A:1540:VAL:HA   | 1:A:1543:ILE:HD12 | 1.95                     | 0.48              |
| 1:A:1675:LEU:HB2  | 1:A:1766:LYS:HZ3  | 1.78                     | 0.48              |
| 1:A:1943:ASP:O    | 1:A:1946:THR:OG1  | 2.30                     | 0.48              |
| 1:A:1969:GLN:NE2  | 1:A:1969:GLN:O    | 2.46                     | 0.48              |
| 1:A:2339:LEU:HB2  | 1:A:2341:PHE:HD1  | 1.79                     | 0.48              |
| 1:A:241:PHE:O     | 1:A:245:ILE:HG23  | 2.14                     | 0.48              |
| 1:A:303:ARG:HD3   | 1:A:308:TYR:HD2   | 1.78                     | 0.48              |
| 1:A:884:GLU:O     | 1:A:888:GLN:HG3   | 2.14                     | 0.48              |
| 1:A:1100:SER:HB3  | 1:A:1104:LYS:NZ   | 2.29                     | 0.48              |
| 1:A:1144:ASP:OD2  | 1:A:1147:VAL:HG23 | 2.14                     | 0.48              |
| 1:A:1342:VAL:O    | 1:A:1345:SER:OG   | 2.29                     | 0.48              |
| 1:A:1381:VAL:HG22 | 1:A:1593:ARG:HH12 | 1.79                     | 0.48              |
| 1:A:1882:LEU:HD13 | 1:A:1934:ALA:HB1  | 1.95                     | 0.48              |
| 1:A:1885:LEU:O    | 1:A:1889:LEU:HG   | 2.13                     | 0.48              |
| 1:A:2129:LEU:O    | 1:A:2133:LYS:HG2  | 2.13                     | 0.48              |
| 1:A:2208:SER:O    | 1:A:2212:ILE:HG22 | 2.14                     | 0.48              |
| 1:A:2418:HIS:CE1  | 1:A:2423:LYS:HB3  | 2.49                     | 0.48              |
| 1:A:709:CYS:O     | 1:A:713:THR:HG23  | 2.13                     | 0.48              |
| 1:A:1184:ARG:CA   | 1:A:1187:GLN:HE21 | 2.27                     | 0.48              |
| 1:A:316:LYS:CG    | 1:A:325:LEU:HB3   | 2.44                     | 0.48              |
| 1:A:500:ASN:HA    | 1:A:503:MET:HG2   | 1.95                     | 0.48              |
| 1:A:587:MET:O     | 1:A:591:VAL:HG22  | 2.12                     | 0.48              |
| 1:A:1429:ALA:O    | 1:A:1433:LEU:HG   | 2.14                     | 0.48              |
| 1:A:1831:ILE:O    | 1:A:1835:ILE:HG12 | 2.14                     | 0.48              |
| 1:A:2314:ALA:O    | 1:A:2317:GLU:HG3  | 2.13                     | 0.48              |
| 1:A:2343:GLU:O    | 1:A:2347:GLU:HG2  | 2.14                     | 0.48              |
| 1:A:337:VAL:CG1   | 1:A:351:TRP:HB2   | 2.44                     | 0.47              |
| 1:A:524:GLN:C     | 1:A:529:LYS:HZ1   | 2.17                     | 0.47              |
| 1:A:605:GLY:HA2   | 1:A:608:LEU:HD13  | 1.96                     | 0.47              |
| 1:A:713:THR:O     | 1:A:717:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:1536:THR:O    | 1:A:1539:LEU:HB3  | 2.14                     | 0.47              |
| 1:A:1801:GLN:O    | 1:A:1805:GLU:OE1  | 2.32                     | 0.47              |
| 1:A:2098:THR:O    | 1:A:2102:ALA:HB2  | 2.15                     | 0.47              |
| 1:A:2182:ILE:HG13 | 1:A:2215:MET:CG   | 2.43                     | 0.47              |
| 1:A:580:ILE:O     | 1:A:584:LEU:HG    | 2.14                     | 0.47              |
| 1:A:597:LEU:O     | 1:A:600:ASP:HB2   | 2.14                     | 0.47              |
| 1:A:971:ARG:HA    | 1:A:971:ARG:CZ    | 2.43                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1002:ALA:HA   | 1:A:1005:LYS:HZ2  | 1.78                     | 0.47              |
| 1:A:1091:LEU:O    | 1:A:1095:THR:HG23 | 2.14                     | 0.47              |
| 1:A:1695:GLN:O    | 1:A:1698:LEU:HB2  | 2.14                     | 0.47              |
| 1:A:2019:ILE:HA   | 1:A:2022:THR:OG1  | 2.14                     | 0.47              |
| 1:A:313:PHE:HB2   | 1:A:330:LEU:HB2   | 1.95                     | 0.47              |
| 1:A:313:PHE:HD2   | 1:A:330:LEU:HB3   | 1.80                     | 0.47              |
| 1:A:717:VAL:O     | 1:A:721:LYS:HG2   | 2.14                     | 0.47              |
| 1:A:1002:ALA:HA   | 1:A:1005:LYS:HZ3  | 1.79                     | 0.47              |
| 1:A:1029:THR:O    | 1:A:1032:ALA:HB3  | 2.13                     | 0.47              |
| 1:A:1091:LEU:HD21 | 1:A:1200:VAL:HA   | 1.97                     | 0.47              |
| 1:A:1285:GLY:O    | 1:A:1288:MET:HB2  | 2.15                     | 0.47              |
| 1:A:1835:ILE:O    | 1:A:1838:LEU:HB3  | 2.14                     | 0.47              |
| 1:A:2016:ARG:O    | 1:A:2020:LEU:HG   | 2.14                     | 0.47              |
| 1:A:2161:CYS:HA   | 1:A:2241:ARG:NH2  | 2.29                     | 0.47              |
| 1:A:2176:ILE:HA   | 1:A:2179:THR:HG23 | 1.96                     | 0.47              |
| 1:A:243:CYS:HB2   | 1:A:265:PHE:HE2   | 1.80                     | 0.47              |
| 1:A:1252:ALA:HB3  | 1:A:1274:PHE:HD1  | 1.79                     | 0.47              |
| 1:A:1441:ALA:O    | 1:A:1444:ALA:HB3  | 2.15                     | 0.47              |
| 1:A:1636:HIS:O    | 1:A:1640:VAL:HG23 | 2.14                     | 0.47              |
| 1:A:1997:MET:SD   | 1:A:1998:PHE:N    | 2.87                     | 0.47              |
| 1:A:2006:ARG:NE   | 1:A:2010:GLU:OE2  | 2.48                     | 0.47              |
| 1:A:2086:ASP:HA   | 1:A:2089:LYS:HG2  | 1.96                     | 0.47              |
| 1:A:228:HIS:CE1   | 1:A:230:VAL:HB    | 2.48                     | 0.47              |
| 1:A:496:THR:HA    | 1:A:499:ILE:HD12  | 1.97                     | 0.47              |
| 1:A:781:LEU:O     | 1:A:785:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:963:ILE:O     | 1:A:967:VAL:HG23  | 2.14                     | 0.47              |
| 1:A:1380:PRO:HD2  | 1:A:1593:ARG:NH2  | 2.30                     | 0.47              |
| 1:A:2473:ALA:O    | 1:A:2477:ALA:N    | 2.36                     | 0.47              |
| 1:A:587:MET:O     | 1:A:588:SER:C     | 2.53                     | 0.47              |
| 1:A:989:ALA:O     | 1:A:993:PHE:HB2   | 2.14                     | 0.47              |
| 1:A:1350:ILE:HG21 | 1:A:1365:ASN:ND2  | 2.27                     | 0.47              |
| 1:A:1730:LYS:HA   | 1:A:1733:GLN:NE2  | 2.30                     | 0.47              |
| 1:A:2062:VAL:HG21 | 1:A:2084:VAL:HG11 | 1.95                     | 0.47              |
| 1:A:574:GLY:O     | 1:A:578:THR:HG23  | 2.15                     | 0.47              |
| 1:A:597:LEU:HA    | 1:A:600:ASP:OD2   | 2.15                     | 0.47              |
| 1:A:996:PRO:HA    | 1:A:999:LYS:HG2   | 1.96                     | 0.47              |
| 1:A:1189:ALA:O    | 1:A:1193:THR:HG23 | 2.15                     | 0.47              |
| 1:A:1269:ARG:O    | 1:A:1273:ARG:HG3  | 2.14                     | 0.47              |
| 1:A:1614:ILE:HD12 | 1:A:1617:ALA:HB3  | 1.97                     | 0.47              |
| 1:A:1723:GLU:HG2  | 1:A:1724:ALA:N    | 2.29                     | 0.47              |
| 1:A:1893:TYR:CE2  | 1:A:1923:LEU:HB2  | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2160:PHE:CZ   | 1:A:2216:LEU:HB3  | 2.50                     | 0.47              |
| 1:A:2210:ARG:HG3  | 1:A:2211:ALA:N    | 2.29                     | 0.47              |
| 1:A:2282:GLU:HA   | 1:A:2285:GLN:CD   | 2.35                     | 0.47              |
| 1:A:1138:VAL:HA   | 1:A:1141:LEU:HD21 | 1.97                     | 0.47              |
| 1:A:1245:ALA:HB3  | 1:A:1281:PHE:HD1  | 1.79                     | 0.47              |
| 1:A:1310:MET:O    | 1:A:1314:LYS:HD2  | 2.14                     | 0.47              |
| 1:A:1329:PRO:HB2  | 1:A:1382:GLN:CG   | 2.44                     | 0.47              |
| 1:A:1451:ASP:O    | 1:A:1729:HIS:NE2  | 2.32                     | 0.47              |
| 1:A:1668:LEU:HA   | 1:A:1671:CYS:SG   | 2.54                     | 0.47              |
| 1:A:2075:GLU:OE2  | 1:A:2206:ASN:ND2  | 2.44                     | 0.47              |
| 1:A:634:ARG:O     | 1:A:637:LEU:HB3   | 2.15                     | 0.47              |
| 1:A:827:ARG:HH22  | 1:A:831:GLN:HG2   | 1.80                     | 0.47              |
| 1:A:1144:ASP:HB3  | 1:A:1147:VAL:HG23 | 1.97                     | 0.47              |
| 1:A:1459:GLN:N    | 1:A:1584:VAL:HB   | 2.30                     | 0.47              |
| 1:A:611:ALA:O     | 1:A:615:LEU:HG    | 2.15                     | 0.47              |
| 1:A:632:GLU:CD    | 1:A:633:PRO:HD2   | 2.35                     | 0.47              |
| 1:A:814:SER:OG    | 1:A:1919:ARG:NH2  | 2.49                     | 0.47              |
| 1:A:827:ARG:HH21  | 1:A:828:ILE:HG22  | 1.79                     | 0.47              |
| 1:A:1078:PRO:HA   | 1:A:1136:ARG:NH2  | 2.25                     | 0.47              |
| 1:A:1181:SER:O    | 1:A:1185:LEU:HD23 | 2.14                     | 0.47              |
| 1:A:1434:CYS:O    | 1:A:1438:GLU:OE1  | 2.32                     | 0.47              |
| 1:A:2051:SER:O    | 1:A:2055:ILE:HG23 | 2.14                     | 0.47              |
| 1:A:234:LYS:HA    | 1:A:237:GLU:OE1   | 2.15                     | 0.46              |
| 1:A:317:GLU:O     | 1:A:326:VAL:HG12  | 2.15                     | 0.46              |
| 1:A:489:THR:HB    | 1:A:492:GLN:HB2   | 1.96                     | 0.46              |
| 1:A:1033:GLU:O    | 1:A:1036:THR:OG1  | 2.27                     | 0.46              |
| 1:A:1147:VAL:O    | 1:A:1151:VAL:HG13 | 2.14                     | 0.46              |
| 1:A:1259:ALA:C    | 1:A:1262:GLY:H    | 2.18                     | 0.46              |
| 1:A:1673:ARG:HG2  | 1:A:1677:GLN:HE22 | 1.79                     | 0.46              |
| 1:A:1768:LEU:CD2  | 1:A:1810:LEU:HD11 | 2.44                     | 0.46              |
| 1:A:1804:THR:O    | 1:A:1807:VAL:N    | 2.47                     | 0.46              |
| 1:A:1960:LYS:CA   | 1:A:1963:HIS:HD1  | 2.27                     | 0.46              |
| 1:A:2199:GLU:O    | 1:A:2202:ILE:HG12 | 2.15                     | 0.46              |
| 1:A:2310:LEU:HD12 | 1:A:2311:GLY:N    | 2.30                     | 0.46              |
| 1:A:267:PRO:HB2   | 1:A:269:GLU:OE1   | 2.15                     | 0.46              |
| 1:A:584:LEU:O     | 1:A:587:MET:HB2   | 2.15                     | 0.46              |
| 1:A:734:GLU:HA    | 1:A:737:VAL:HG12  | 1.97                     | 0.46              |
| 1:A:882:ASP:C     | 1:A:887:GLN:HE21  | 2.19                     | 0.46              |
| 1:A:1170:LYS:O    | 1:A:1173:SER:OG   | 2.27                     | 0.46              |
| 1:A:1190:LYS:HD3  | 1:A:1194:GLN:HE22 | 1.80                     | 0.46              |
| 1:A:1542:THR:HB   | 1:A:1558:CYS:SG   | 2.55                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2173:GLU:HG2  | 1:A:2296:VAL:HG11 | 1.97                     | 0.46              |
| 1:A:2405:ASN:O    | 1:A:2408:CYS:N    | 2.49                     | 0.46              |
| 1:A:212:LEU:HD13  | 1:A:292:ILE:HD11  | 1.97                     | 0.46              |
| 1:A:358:ARG:HB2   | 1:A:358:ARG:NH1   | 2.30                     | 0.46              |
| 1:A:550:ILE:HG13  | 1:A:583:ASN:HD22  | 1.80                     | 0.46              |
| 1:A:1227:LEU:HD22 | 1:A:1286:VAL:HG21 | 1.97                     | 0.46              |
| 1:A:1714:GLU:HB2  | 1:A:1715:PRO:HD3  | 1.97                     | 0.46              |
| 1:A:2166:PRO:HG3  | 1:A:2224:PHE:HD2  | 1.81                     | 0.46              |
| 1:A:216:TYR:CD1   | 1:A:295:LYS:HA    | 2.51                     | 0.46              |
| 1:A:949:GLN:N     | 1:A:950:PRO:HD3   | 2.30                     | 0.46              |
| 1:A:1135:ALA:HA   | 1:A:1138:VAL:HG22 | 1.98                     | 0.46              |
| 1:A:1261:ARG:CZ   | 1:A:1375:GLU:HG3  | 2.46                     | 0.46              |
| 1:A:1690:ARG:HB3  | 1:A:1751:LYS:NZ   | 2.30                     | 0.46              |
| 1:A:1768:LEU:HD11 | 1:A:1810:LEU:HD11 | 1.98                     | 0.46              |
| 1:A:274:LYS:HB3   | 1:A:274:LYS:HE3   | 1.66                     | 0.46              |
| 1:A:1162:ALA:O    | 1:A:1166:ILE:HG13 | 2.15                     | 0.46              |
| 1:A:1654:LYS:HG2  | 1:A:1656:PRO:HD3  | 1.98                     | 0.46              |
| 1:A:760:ASP:OD2   | 1:A:762:GLN:HB2   | 2.16                     | 0.46              |
| 1:A:867:THR:O     | 1:A:870:MET:HB3   | 2.15                     | 0.46              |
| 1:A:902:ASN:CG    | 1:A:906:GLN:HB2   | 2.35                     | 0.46              |
| 1:A:924:ALA:O     | 1:A:927:SER:OG    | 2.33                     | 0.46              |
| 1:A:950:PRO:CB    | 1:A:952:LEU:HG    | 2.46                     | 0.46              |
| 1:A:1363:CYS:O    | 1:A:1367:LEU:HG   | 2.16                     | 0.46              |
| 1:A:1372:THR:HG1  | 1:A:1373:VAL:H    | 1.63                     | 0.46              |
| 1:A:1520:THR:HB   | 1:A:1524:GLN:HE22 | 1.81                     | 0.46              |
| 1:A:1756:PRO:HB2  | 1:A:1757:GLN:NE2  | 2.31                     | 0.46              |
| 1:A:1944:VAL:O    | 1:A:1948:LYS:HG3  | 2.16                     | 0.46              |
| 1:A:503:MET:O     | 1:A:507:GLN:HG3   | 2.16                     | 0.46              |
| 1:A:536:MET:CE    | 1:A:597:LEU:HB2   | 2.46                     | 0.46              |
| 1:A:733:GLN:HG3   | 1:A:784:HIS:NE2   | 2.31                     | 0.46              |
| 1:A:1454:SER:HA   | 1:A:1589:SER:HB2  | 1.98                     | 0.46              |
| 1:A:1818:ALA:HB1  | 1:A:1824:VAL:HG21 | 1.98                     | 0.46              |
| 1:A:1916:ILE:O    | 1:A:1920:VAL:HG22 | 2.16                     | 0.46              |
| 1:A:2010:GLU:OE2  | 1:A:2068:SER:HA   | 2.15                     | 0.46              |
| 1:A:2467:SER:O    | 1:A:2470:LEU:HG   | 2.16                     | 0.46              |
| 1:A:228:HIS:ND1   | 1:A:230:VAL:HB    | 2.30                     | 0.46              |
| 1:A:322:LYS:HD2   | 1:A:324:LYS:HZ3   | 1.80                     | 0.46              |
| 1:A:621:GLU:OE2   | 1:A:624:ARG:HD2   | 2.16                     | 0.46              |
| 1:A:837:VAL:HA    | 1:A:840:ILE:HD12  | 1.98                     | 0.46              |
| 1:A:1145:PRO:HA   | 1:A:1148:GLN:NE2  | 2.31                     | 0.46              |
| 1:A:1313:SER:OG   | 1:A:1314:LYS:N    | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1369:GLN:O    | 1:A:1372:THR:OG1  | 2.22                     | 0.46              |
| 1:A:1707:GLN:HB3  | 1:A:1711:HIS:CE1  | 2.50                     | 0.46              |
| 1:A:2160:PHE:CD1  | 1:A:2220:LYS:HD3  | 2.51                     | 0.46              |
| 1:A:2318:ALA:HA   | 1:A:2321:LYS:HD3  | 1.98                     | 0.46              |
| 1:A:1413:ASN:HB3  | 1:A:1422:PHE:HB2  | 1.98                     | 0.46              |
| 1:A:1418:ASN:OD1  | 1:A:1418:ASN:N    | 2.49                     | 0.46              |
| 1:A:1651:MET:O    | 1:A:1654:LYS:HB3  | 2.15                     | 0.46              |
| 1:A:1824:VAL:O    | 1:A:1827:MET:HE2  | 2.16                     | 0.46              |
| 1:A:1877:THR:OG1  | 1:A:1878:SER:N    | 2.48                     | 0.46              |
| 1:A:2081:ILE:HG22 | 1:A:2085:LYS:NZ   | 2.31                     | 0.46              |
| 1:A:2091:LEU:O    | 1:A:2095:ILE:HG13 | 2.16                     | 0.46              |
| 1:A:2160:PHE:HA   | 1:A:2220:LYS:HZ1  | 1.80                     | 0.46              |
| 1:A:305:LEU:C     | 1:A:307:THR:H     | 2.19                     | 0.46              |
| 1:A:536:MET:SD    | 1:A:594:LEU:HD23  | 2.55                     | 0.46              |
| 1:A:1106:LEU:HD23 | 1:A:1571:ASN:ND2  | 2.31                     | 0.46              |
| 1:A:1283:GLU:O    | 1:A:1286:VAL:HG12 | 2.14                     | 0.46              |
| 1:A:1959:GLU:O    | 1:A:1962:SER:OG   | 2.21                     | 0.46              |
| 1:A:1983:SER:O    | 1:A:1986:SER:OG   | 2.24                     | 0.46              |
| 1:A:2112:TRP:HA   | 1:A:2115:LYS:HE2  | 1.98                     | 0.46              |
| 1:A:2427:SER:O    | 1:A:2430:GLN:HG3  | 2.16                     | 0.46              |
| 1:A:557:VAL:O     | 1:A:561:THR:HG23  | 2.16                     | 0.45              |
| 1:A:798:TYR:HE1   | 1:A:839:ALA:HB3   | 1.81                     | 0.45              |
| 1:A:883:SER:HB2   | 1:A:885:GLU:CD    | 2.36                     | 0.45              |
| 1:A:1154:THR:O    | 1:A:1158:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:1535:SER:OG   | 1:A:1565:LEU:HD13 | 2.15                     | 0.45              |
| 1:A:1535:SER:HA   | 1:A:1538:ASN:OD1  | 2.16                     | 0.45              |
| 1:A:1642:ASP:O    | 1:A:1646:LYS:HG3  | 2.16                     | 0.45              |
| 1:A:1951:ILE:HG13 | 1:A:1955:ARG:CZ   | 2.46                     | 0.45              |
| 1:A:2021:LYS:O    | 1:A:2025:VAL:HG23 | 2.16                     | 0.45              |
| 1:A:2090:ALA:HA   | 1:A:2093:ASP:OD2  | 2.16                     | 0.45              |
| 1:A:2285:GLN:O    | 1:A:2288:GLU:HG3  | 2.17                     | 0.45              |
| 1:A:303:ARG:HA    | 1:A:308:TYR:CE2   | 2.51                     | 0.45              |
| 1:A:388:ILE:O     | 1:A:391:LEU:HB2   | 2.16                     | 0.45              |
| 1:A:1395:SER:HA   | 1:A:1398:GLU:OE2  | 2.16                     | 0.45              |
| 1:A:1399:ASN:ND2  | 1:A:1432:ALA:O    | 2.40                     | 0.45              |
| 1:A:1619:ALA:HB1  | 1:A:1629:ARG:HD3  | 1.98                     | 0.45              |
| 1:A:1662:GLU:OE2  | 1:A:1780:LYS:HD3  | 2.16                     | 0.45              |
| 1:A:1813:THR:HA   | 1:A:1816:GLU:OE2  | 2.16                     | 0.45              |
| 1:A:1975:THR:H    | 1:A:2099:LYS:HZ2  | 1.64                     | 0.45              |
| 1:A:539:SER:O     | 1:A:543:ILE:HG12  | 2.17                     | 0.45              |
| 1:A:832:ALA:HA    | 1:A:835:ASP:OD2   | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:906:GLN:NE2   | 1:A:910:LYS:HG2   | 2.25                     | 0.45              |
| 1:A:1100:SER:HB3  | 1:A:1104:LYS:HZ3  | 1.81                     | 0.45              |
| 1:A:1882:LEU:HA   | 1:A:1885:LEU:HB2  | 1.97                     | 0.45              |
| 1:A:290:SER:N     | 1:A:293:GLU:OE1   | 2.25                     | 0.45              |
| 1:A:536:MET:HE1   | 1:A:597:LEU:HB2   | 1.99                     | 0.45              |
| 1:A:540:LYS:HZ2   | 1:A:655:ILE:HB    | 1.81                     | 0.45              |
| 1:A:543:ILE:HD13  | 1:A:546:GLN:NE2   | 2.31                     | 0.45              |
| 1:A:583:ASN:O     | 1:A:584:LEU:C     | 2.54                     | 0.45              |
| 1:A:1086:LYS:HA   | 1:A:1089:GLN:OE1  | 2.16                     | 0.45              |
| 1:A:1332:LYS:O    | 1:A:1335:LEU:HB3  | 2.17                     | 0.45              |
| 1:A:1827:MET:SD   | 1:A:1827:MET:N    | 2.90                     | 0.45              |
| 1:A:2031:LYS:O    | 1:A:2034:VAL:HB   | 2.16                     | 0.45              |
| 1:A:2418:HIS:NE2  | 1:A:2423:LYS:HB3  | 2.31                     | 0.45              |
| 1:A:606:ARG:HG3   | 1:A:609:LEU:HD12  | 1.98                     | 0.45              |
| 1:A:1120:ALA:HA   | 1:A:1123:ASP:OD2  | 2.16                     | 0.45              |
| 1:A:1179:PRO:O    | 1:A:1183:GLN:NE2  | 2.49                     | 0.45              |
| 1:A:1187:GLN:HE22 | 1:A:1188:VAL:HG13 | 1.80                     | 0.45              |
| 1:A:1294:SER:HB3  | 1:A:1297:ASP:HB3  | 1.98                     | 0.45              |
| 1:A:1315:LEU:HD13 | 1:A:1342:VAL:HG21 | 1.97                     | 0.45              |
| 1:A:1367:LEU:O    | 1:A:1371:GLU:HG2  | 2.17                     | 0.45              |
| 1:A:281:GLN:NE2   | 1:A:285:ASN:OD1   | 2.48                     | 0.45              |
| 1:A:732:CYS:SG    | 1:A:733:GLN:N     | 2.89                     | 0.45              |
| 1:A:919:HIS:O     | 1:A:923:GLN:OE1   | 2.35                     | 0.45              |
| 1:A:1614:ILE:O    | 1:A:1618:ARG:HG2  | 2.17                     | 0.45              |
| 1:A:1682:ALA:HA   | 1:A:1687:LEU:HD22 | 1.98                     | 0.45              |
| 1:A:1729:HIS:C    | 1:A:1733:GLN:HE22 | 2.20                     | 0.45              |
| 1:A:1757:GLN:O    | 1:A:1761:LEU:HG   | 2.16                     | 0.45              |
| 1:A:1824:VAL:HG12 | 1:A:1826:GLY:H    | 1.82                     | 0.45              |
| 1:A:2264:ASP:HA   | 1:A:2267:GLN:HE21 | 1.82                     | 0.45              |
| 1:A:564:ASP:HB3   | 1:A:567:GLU:OE2   | 2.17                     | 0.45              |
| 1:A:723:VAL:HG21  | 1:A:736:LEU:HD11  | 1.99                     | 0.45              |
| 1:A:730:PRO:HA    | 1:A:733:GLN:OE1   | 2.17                     | 0.45              |
| 1:A:749:GLY:O     | 1:A:752:SER:OG    | 2.32                     | 0.45              |
| 1:A:1029:THR:O    | 1:A:1033:GLU:OE1  | 2.35                     | 0.45              |
| 1:A:1030:ALA:O    | 1:A:1034:LEU:HG   | 2.16                     | 0.45              |
| 1:A:2035:GLN:CD   | 1:A:2035:GLN:H    | 2.20                     | 0.45              |
| 1:A:2060:ASP:HA   | 1:A:2063:LYS:HE2  | 1.99                     | 0.45              |
| 1:A:2442:CYS:HB3  | 1:A:2456:LEU:HD21 | 1.97                     | 0.45              |
| 1:A:534:ASN:HB3   | 1:A:968:GLN:NE2   | 2.31                     | 0.45              |
| 1:A:980:PRO:O     | 1:A:984:LEU:HG    | 2.16                     | 0.45              |
| 1:A:1360:GLN:O    | 1:A:1363:CYS:HB3  | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1809:ASP:O    | 1:A:1813:THR:HG23 | 2.17                     | 0.45              |
| 1:A:2065:GLY:O    | 1:A:2069:LEU:HG   | 2.17                     | 0.45              |
| 1:A:519:LEU:HD11  | 1:A:600:ASP:OD1   | 2.16                     | 0.45              |
| 1:A:685:LYS:NZ    | 1:A:769:ALA:HB2   | 2.32                     | 0.45              |
| 1:A:727:ILE:O     | 1:A:788:HIS:HD2   | 1.99                     | 0.45              |
| 1:A:962:GLN:HG3   | 1:A:993:PHE:CE1   | 2.52                     | 0.45              |
| 1:A:1008:VAL:HB   | 1:A:1009:PRO:HD3  | 1.99                     | 0.45              |
| 1:A:1111:GLN:OE1  | 1:A:1114:GLU:HB2  | 2.17                     | 0.45              |
| 1:A:2152:HIS:O    | 1:A:2155:GLN:HG3  | 2.16                     | 0.45              |
| 1:A:2418:HIS:CE1  | 1:A:2420:SER:O    | 2.70                     | 0.45              |
| 1:A:266:LEU:HB3   | 1:A:270:TYR:HB2   | 1.99                     | 0.45              |
| 1:A:868:ALA:O     | 1:A:871:VAL:N     | 2.50                     | 0.45              |
| 1:A:872:GLU:HG3   | 1:A:875:LYS:NZ    | 2.32                     | 0.45              |
| 1:A:1021:SER:OG   | 1:A:1022:GLN:N    | 2.50                     | 0.45              |
| 1:A:1050:MET:SD   | 1:A:1050:MET:N    | 2.89                     | 0.45              |
| 1:A:1303:SER:O    | 1:A:1306:LYS:HG2  | 2.17                     | 0.45              |
| 1:A:1575:PHE:O    | 1:A:1578:ASN:HB2  | 2.17                     | 0.45              |
| 1:A:2069:LEU:HD12 | 1:A:2077:GLN:HG2  | 1.99                     | 0.45              |
| 1:A:2175:PHE:O    | 1:A:2178:MET:HB2  | 2.17                     | 0.45              |
| 1:A:321:GLY:N     | 1:A:1770:GLU:OE1  | 2.42                     | 0.44              |
| 1:A:554:THR:O     | 1:A:557:VAL:HB    | 2.17                     | 0.44              |
| 1:A:636:ASN:HA    | 1:A:639:LEU:HD12  | 2.00                     | 0.44              |
| 1:A:813:PHE:CZ    | 1:A:891:ARG:HG3   | 2.52                     | 0.44              |
| 1:A:1360:GLN:HG2  | 1:A:1618:ARG:HH21 | 1.81                     | 0.44              |
| 1:A:1407:MET:SD   | 1:A:1637:SER:HB2  | 2.56                     | 0.44              |
| 1:A:2447:ASP:OD1  | 1:A:2447:ASP:N    | 2.48                     | 0.44              |
| 1:A:220:ARG:O     | 1:A:223:ILE:HB    | 2.17                     | 0.44              |
| 1:A:598:LEU:O     | 1:A:603:GLY:N     | 2.33                     | 0.44              |
| 1:A:929:THR:HA    | 1:A:932:ILE:HG12  | 1.99                     | 0.44              |
| 1:A:1808:GLU:O    | 1:A:1812:THR:HG23 | 2.17                     | 0.44              |
| 1:A:1864:ILE:O    | 1:A:1868:VAL:HG13 | 2.17                     | 0.44              |
| 1:A:2217:ARG:O    | 1:A:2221:GLU:OE1  | 2.35                     | 0.44              |
| 1:A:522:LEU:HD22  | 1:A:532:ARG:NH2   | 2.33                     | 0.44              |
| 1:A:708:GLN:O     | 1:A:711:LEU:HB3   | 2.17                     | 0.44              |
| 1:A:812:ILE:HD11  | 1:A:825:GLN:HB2   | 1.98                     | 0.44              |
| 1:A:1243:ASN:ND2  | 1:A:1354:THR:HG21 | 2.20                     | 0.44              |
| 1:A:1596:MET:O    | 1:A:1600:VAL:HG23 | 2.17                     | 0.44              |
| 1:A:1691:GLU:OE1  | 1:A:1691:GLU:N    | 2.41                     | 0.44              |
| 1:A:1755:HIS:HA   | 1:A:1758:GLN:NE2  | 2.32                     | 0.44              |
| 1:A:2173:GLU:O    | 1:A:2176:ILE:HG22 | 2.18                     | 0.44              |
| 1:A:2265:LEU:HD13 | 1:A:2268:GLN:OE1  | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2302:THR:O    | 1:A:2305:ALA:N    | 2.51                     | 0.44              |
| 1:A:583:ASN:OD1   | 1:A:587:MET:HG2   | 2.18                     | 0.44              |
| 1:A:1597:GLU:OE2  | 1:A:1601:ILE:HG13 | 2.17                     | 0.44              |
| 1:A:1612:GLY:O    | 1:A:1616:THR:HG23 | 2.18                     | 0.44              |
| 1:A:2237:LEU:O    | 1:A:2241:ARG:HG2  | 2.17                     | 0.44              |
| 1:A:666:ASP:O     | 1:A:669:MET:HB3   | 2.17                     | 0.44              |
| 1:A:744:ALA:O     | 1:A:747:VAL:HB    | 2.17                     | 0.44              |
| 1:A:782:LEU:O     | 1:A:786:LYS:HE2   | 2.18                     | 0.44              |
| 1:A:806:LEU:O     | 1:A:807:THR:C     | 2.54                     | 0.44              |
| 1:A:829:LEU:O     | 1:A:833:THR:OG1   | 2.22                     | 0.44              |
| 1:A:837:VAL:O     | 1:A:840:ILE:HB    | 2.17                     | 0.44              |
| 1:A:1345:SER:O    | 1:A:1348:GLN:HG3  | 2.18                     | 0.44              |
| 1:A:1390:PHE:HB3  | 1:A:1787:LYS:HE2  | 2.00                     | 0.44              |
| 1:A:1816:GLU:O    | 1:A:1819:SER:OG   | 2.29                     | 0.44              |
| 1:A:1902:PRO:O    | 1:A:1906:ALA:HB2  | 2.17                     | 0.44              |
| 1:A:1995:THR:HA   | 1:A:1998:PHE:CD2  | 2.52                     | 0.44              |
| 1:A:268:LYS:HB3   | 1:A:272:LYS:NZ    | 2.32                     | 0.44              |
| 1:A:635:GLN:HA    | 1:A:638:LEU:HG    | 1.98                     | 0.44              |
| 1:A:1105:LEU:HA   | 1:A:1108:GLU:CD   | 2.38                     | 0.44              |
| 1:A:1145:PRO:HA   | 1:A:1148:GLN:CD   | 2.38                     | 0.44              |
| 1:A:1390:PHE:HB3  | 1:A:1787:LYS:NZ   | 2.33                     | 0.44              |
| 1:A:1851:VAL:O    | 1:A:1855:THR:HG23 | 2.18                     | 0.44              |
| 1:A:682:LEU:HD13  | 1:A:769:ALA:HB3   | 1.99                     | 0.44              |
| 1:A:1310:MET:HB2  | 1:A:1314:LYS:NZ   | 2.33                     | 0.44              |
| 1:A:1426:ILE:HD12 | 1:A:1429:ALA:HB3  | 1.99                     | 0.44              |
| 1:A:1849:SER:HB3  | 1:A:1852:ASP:CG   | 2.38                     | 0.44              |
| 1:A:2105:VAL:HG22 | 1:A:2106:GLY:H    | 1.83                     | 0.44              |
| 1:A:2327:LYS:HB2  | 1:A:2329:ARG:NH1  | 2.33                     | 0.44              |
| 1:A:318:LYS:N     | 1:A:325:LEU:HD13  | 2.33                     | 0.44              |
| 1:A:507:GLN:HA    | 1:A:510:GLN:OE1   | 2.18                     | 0.44              |
| 1:A:1730:LYS:HZ2  | 1:A:1730:LYS:HG2  | 1.72                     | 0.44              |
| 1:A:2418:HIS:CD2  | 1:A:2423:LYS:HE3  | 2.53                     | 0.44              |
| 1:A:238:PHE:HA    | 1:A:241:PHE:CD2   | 2.52                     | 0.44              |
| 1:A:583:ASN:HD21  | 1:A:587:MET:HE3   | 1.83                     | 0.44              |
| 1:A:711:LEU:O     | 1:A:714:SER:N     | 2.51                     | 0.44              |
| 1:A:1627:PRO:HB2  | 1:A:1628:PRO:HD3  | 2.00                     | 0.44              |
| 1:A:1719:ALA:HB1  | 1:A:1727:LEU:HB2  | 2.00                     | 0.44              |
| 1:A:2206:ASN:OD1  | 1:A:2209:ARG:NH1  | 2.51                     | 0.44              |
| 1:A:216:TYR:HD2   | 1:A:220:ARG:HE    | 1.65                     | 0.43              |
| 1:A:733:GLN:HE21  | 1:A:784:HIS:CE1   | 2.36                     | 0.43              |
| 1:A:871:VAL:HG12  | 1:A:875:LYS:NZ    | 2.32                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1336:ALA:O    | 1:A:1340:ARG:HG2  | 2.18                     | 0.43              |
| 1:A:1463:GLU:N    | 1:A:1463:GLU:OE1  | 2.51                     | 0.43              |
| 1:A:1807:VAL:O    | 1:A:1810:LEU:HB2  | 2.18                     | 0.43              |
| 1:A:2053:ALA:O    | 1:A:2057:ARG:HG2  | 2.18                     | 0.43              |
| 1:A:2069:LEU:HB2  | 1:A:2077:GLN:HE21 | 1.82                     | 0.43              |
| 1:A:2242:GLU:HA   | 1:A:2245:ASN:OD1  | 2.18                     | 0.43              |
| 1:A:330:LEU:HD23  | 1:A:330:LEU:HA    | 1.77                     | 0.43              |
| 1:A:365:SER:HB2   | 1:A:381:GLN:OE1   | 2.18                     | 0.43              |
| 1:A:540:LYS:NZ    | 1:A:655:ILE:HB    | 2.33                     | 0.43              |
| 1:A:996:PRO:HA    | 1:A:999:LYS:HZ2   | 1.81                     | 0.43              |
| 1:A:1263:THR:OG1  | 1:A:1266:ASP:OD2  | 2.36                     | 0.43              |
| 1:A:1264:PRO:O    | 1:A:1267:LEU:HB2  | 2.17                     | 0.43              |
| 1:A:1596:MET:O    | 1:A:1599:ILE:N    | 2.51                     | 0.43              |
| 1:A:1896:LEU:HD12 | 1:A:1899:GLN:HE21 | 1.84                     | 0.43              |
| 1:A:1946:THR:HA   | 1:A:1949:GLU:OE1  | 2.18                     | 0.43              |
| 1:A:2175:PHE:O    | 1:A:2179:THR:HG23 | 2.17                     | 0.43              |
| 1:A:2270:THR:O    | 1:A:2273:SER:OG   | 2.17                     | 0.43              |
| 1:A:2377:GLY:HA3  | 1:A:2382:ASN:HD22 | 1.83                     | 0.43              |
| 1:A:655:ILE:HG13  | 1:A:657:GLU:H     | 1.82                     | 0.43              |
| 1:A:814:SER:CB    | 1:A:1963:HIS:HD2  | 2.31                     | 0.43              |
| 1:A:819:ALA:HA    | 1:A:822:MET:HE2   | 2.00                     | 0.43              |
| 1:A:955:SER:O     | 1:A:959:VAL:HG22  | 2.18                     | 0.43              |
| 1:A:1390:PHE:HA   | 1:A:1393:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:1619:ALA:O    | 1:A:1622:VAL:HB   | 2.18                     | 0.43              |
| 1:A:1710:SER:HB3  | 1:A:1807:VAL:HG11 | 2.00                     | 0.43              |
| 1:A:212:LEU:HD11  | 1:A:296:VAL:HG22  | 1.99                     | 0.43              |
| 1:A:777:ALA:HA    | 1:A:780:GLU:OE2   | 2.18                     | 0.43              |
| 1:A:1089:GLN:NE2  | 1:A:1325:ASP:OD1  | 2.50                     | 0.43              |
| 1:A:1156:SER:O    | 1:A:1159:LEU:HG   | 2.18                     | 0.43              |
| 1:A:1268:ALA:O    | 1:A:1271:SER:OG   | 2.34                     | 0.43              |
| 1:A:1702:MET:CB   | 1:A:1814:LEU:HD11 | 2.47                     | 0.43              |
| 1:A:2179:THR:HG22 | 1:A:2215:MET:CE   | 2.48                     | 0.43              |
| 1:A:2425:ILE:HG12 | 1:A:2429:LYS:NZ   | 2.33                     | 0.43              |
| 1:A:1229:PRO:HD3  | 1:A:1286:VAL:HG22 | 2.00                     | 0.43              |
| 1:A:1602:SER:CB   | 1:A:1647:LEU:HG   | 2.49                     | 0.43              |
| 1:A:1798:GLU:O    | 1:A:1802:MET:HG2  | 2.18                     | 0.43              |
| 1:A:1852:ASP:O    | 1:A:1856:THR:HG23 | 2.18                     | 0.43              |
| 1:A:1917:LYS:HB2  | 1:A:1917:LYS:HE2  | 1.84                     | 0.43              |
| 1:A:1920:VAL:HA   | 1:A:1923:LEU:HG   | 1.98                     | 0.43              |
| 1:A:1920:VAL:HA   | 1:A:1923:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:1937:LEU:O    | 1:A:1940:SER:N    | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:966:LEU:HD22  | 1:A:993:PHE:CG    | 2.53                     | 0.43              |
| 1:A:1257:VAL:HG23 | 1:A:1375:GLU:CD   | 2.38                     | 0.43              |
| 1:A:1269:ARG:HD2  | 1:A:1273:ARG:HH22 | 1.84                     | 0.43              |
| 1:A:1465:THR:HB   | 1:A:1469:ARG:HH22 | 1.83                     | 0.43              |
| 1:A:1951:ILE:O    | 1:A:1955:ARG:NE   | 2.34                     | 0.43              |
| 1:A:2006:ARG:NH1  | 1:A:2011:THR:HA   | 2.33                     | 0.43              |
| 1:A:556:SER:HA    | 1:A:559:ASN:ND2   | 2.33                     | 0.43              |
| 1:A:1415:LYS:HA   | 1:A:1625:ARG:NH1  | 2.33                     | 0.43              |
| 1:A:2059:ALA:O    | 1:A:2063:LYS:HG3  | 2.19                     | 0.43              |
| 1:A:734:GLU:O     | 1:A:738:GLU:OE1   | 2.37                     | 0.43              |
| 1:A:747:VAL:O     | 1:A:751:VAL:HG23  | 2.19                     | 0.43              |
| 1:A:825:GLN:HA    | 1:A:828:ILE:HG12  | 1.99                     | 0.43              |
| 1:A:1009:PRO:HG2  | 1:A:1737:TYR:CD1  | 2.54                     | 0.43              |
| 1:A:1269:ARG:HG3  | 1:A:1273:ARG:HH12 | 1.84                     | 0.43              |
| 1:A:1648:ILE:HA   | 1:A:1651:MET:HG2  | 2.01                     | 0.43              |
| 1:A:1648:ILE:O    | 1:A:1651:MET:HG2  | 2.19                     | 0.43              |
| 1:A:2024:LYS:O    | 1:A:2028:GLU:OE1  | 2.37                     | 0.43              |
| 1:A:2033:LEU:HG   | 1:A:2047:ALA:HB1  | 2.01                     | 0.43              |
| 1:A:2055:ILE:HG21 | 1:A:2091:LEU:HD13 | 2.01                     | 0.43              |
| 1:A:2231:ASP:HA   | 1:A:2234:LEU:HD12 | 2.00                     | 0.43              |
| 1:A:574:GLY:HA2   | 1:A:577:VAL:HG12  | 2.01                     | 0.43              |
| 1:A:681:ALA:O     | 1:A:685:LYS:HG3   | 2.19                     | 0.43              |
| 1:A:769:ALA:O     | 1:A:772:THR:OG1   | 2.30                     | 0.43              |
| 1:A:798:TYR:O     | 1:A:802:THR:HG23  | 2.18                     | 0.43              |
| 1:A:1115:ASN:O    | 1:A:1119:ILE:HG12 | 2.19                     | 0.43              |
| 1:A:1383:PRO:HD3  | 1:A:1445:TYR:CE1  | 2.53                     | 0.43              |
| 1:A:1444:ALA:HA   | 1:A:1596:MET:CE   | 2.48                     | 0.43              |
| 1:A:1791:HIS:CG   | 1:A:1792:THR:N    | 2.86                     | 0.43              |
| 1:A:2270:THR:HB   | 1:A:2274:LYS:NZ   | 2.34                     | 0.43              |
| 1:A:2418:HIS:CG   | 1:A:2424:LEU:HD21 | 2.54                     | 0.43              |
| 1:A:2459:ALA:O    | 1:A:2463:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:958:ALA:O     | 1:A:961:GLU:HG3   | 2.19                     | 0.43              |
| 1:A:1240:SER:OG   | 1:A:1241:ARG:NH2  | 2.52                     | 0.43              |
| 1:A:1362:GLU:CD   | 1:A:1365:ASN:HD22 | 2.21                     | 0.43              |
| 1:A:1395:SER:O    | 1:A:1399:ASN:HB2  | 2.19                     | 0.43              |
| 1:A:1672:LEU:HD21 | 1:A:1769:ALA:HB1  | 2.01                     | 0.43              |
| 1:A:1794:GLU:O    | 1:A:1795:ALA:C    | 2.57                     | 0.43              |
| 1:A:2132:VAL:O    | 1:A:2136:GLU:HG2  | 2.19                     | 0.43              |
| 1:A:2308:GLU:HG3  | 1:A:2394:ILE:HA   | 2.01                     | 0.43              |
| 1:A:2318:ALA:O    | 1:A:2322:LYS:HG2  | 2.19                     | 0.43              |
| 1:A:500:ASN:O     | 1:A:501:SER:C     | 2.56                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:608:LEU:HG   | 1:A:654:GLN:CG    | 2.43                     | 0.42              |
| 1:A:640:ALA:HA   | 1:A:643:ASN:OD1   | 2.18                     | 0.42              |
| 1:A:760:ASP:O    | 1:A:763:LEU:HG    | 2.19                     | 0.42              |
| 1:A:821:GLU:HB2  | 1:A:825:GLN:NE2   | 2.34                     | 0.42              |
| 1:A:963:ILE:HA   | 1:A:993:PHE:CE1   | 2.50                     | 0.42              |
| 1:A:1023:CYS:O   | 1:A:1026:ASN:HB2  | 2.19                     | 0.42              |
| 1:A:1148:GLN:HG2 | 1:A:1149:ALA:N    | 2.33                     | 0.42              |
| 1:A:1661:CYS:SG  | 1:A:1780:LYS:HB2  | 2.59                     | 0.42              |
| 1:A:1752:THR:HB  | 1:A:1758:GLN:HB3  | 2.01                     | 0.42              |
| 1:A:1801:GLN:O   | 1:A:1802:MET:C    | 2.57                     | 0.42              |
| 1:A:1850:PHE:HE2 | 1:A:1903:ALA:O    | 2.01                     | 0.42              |
| 1:A:1977:ALA:HA  | 1:A:1980:THR:OG1  | 2.18                     | 0.42              |
| 1:A:2118:ALA:O   | 1:A:2122:VAL:HG23 | 2.18                     | 0.42              |
| 1:A:2177:ARG:HG2 | 1:A:2180:LYS:NZ   | 2.34                     | 0.42              |
| 1:A:253:GLN:HE21 | 1:A:284:LYS:HE3   | 1.84                     | 0.42              |
| 1:A:837:VAL:O    | 1:A:841:LYS:HG2   | 2.20                     | 0.42              |
| 1:A:1026:ASN:O   | 1:A:1029:THR:OG1  | 2.37                     | 0.42              |
| 1:A:1144:ASP:HB3 | 1:A:1147:VAL:CG2  | 2.49                     | 0.42              |
| 1:A:1445:TYR:O   | 1:A:1449:VAL:HG23 | 2.18                     | 0.42              |
| 1:A:339:ARG:N    | 1:A:349:GLN:O     | 2.53                     | 0.42              |
| 1:A:851:GLU:O    | 1:A:854:ARG:HG3   | 2.19                     | 0.42              |
| 1:A:895:GLU:HA   | 1:A:898:ARG:HD3   | 2.00                     | 0.42              |
| 1:A:1014:GLN:O   | 1:A:1017:ALA:HB3  | 2.19                     | 0.42              |
| 1:A:1501:HIS:O   | 1:A:1505:LEU:HG   | 2.19                     | 0.42              |
| 1:A:1662:GLU:HA  | 1:A:1665:ILE:HB   | 1.99                     | 0.42              |
| 1:A:1730:LYS:HA  | 1:A:1733:GLN:HE21 | 1.84                     | 0.42              |
| 1:A:1865:ALA:O   | 1:A:1869:GLN:HG2  | 2.20                     | 0.42              |
| 1:A:2052:VAL:O   | 1:A:2056:THR:OG1  | 2.28                     | 0.42              |
| 1:A:311:SER:O    | 1:A:331:GLY:HA2   | 2.19                     | 0.42              |
| 1:A:343:LYS:HD2  | 1:A:343:LYS:HA    | 1.81                     | 0.42              |
| 1:A:652:LEU:HB3  | 1:A:658:SER:CB    | 2.46                     | 0.42              |
| 1:A:752:SER:HA   | 1:A:755:GLN:CD    | 2.40                     | 0.42              |
| 1:A:840:ILE:CG2  | 1:A:856:LEU:HB3   | 2.48                     | 0.42              |
| 1:A:872:GLU:HG3  | 1:A:875:LYS:HZ1   | 1.84                     | 0.42              |
| 1:A:1563:ALA:HB3 | 1:A:1564:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:2040:SER:OG  | 1:A:2041:GLN:N    | 2.52                     | 0.42              |
| 1:A:2146:LEU:HB3 | 1:A:2255:LEU:HD21 | 2.02                     | 0.42              |
| 1:A:2225:HIS:HD2 | 1:A:2228:VAL:HG23 | 1.84                     | 0.42              |
| 1:A:699:GLN:OE1  | 1:A:699:GLN:N     | 2.51                     | 0.42              |
| 1:A:873:ALA:HB2  | 1:A:889:ARG:NH1   | 2.27                     | 0.42              |
| 1:A:963:ILE:HG13 | 1:A:964:PRO:HD3   | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1054:LEU:HA   | 1:A:1166:ILE:HD13 | 2.01                     | 0.42              |
| 1:A:1073:ASP:HB3  | 1:A:1075:LYS:HZ1  | 1.85                     | 0.42              |
| 1:A:1437:THR:HG22 | 1:A:1607:LEU:HD11 | 2.00                     | 0.42              |
| 1:A:1450:SER:OG   | 1:A:1725:SER:HB2  | 2.20                     | 0.42              |
| 1:A:1459:GLN:C    | 1:A:1584:VAL:H    | 2.22                     | 0.42              |
| 1:A:1596:MET:HA   | 1:A:1599:ILE:HD13 | 2.01                     | 0.42              |
| 1:A:1728:GLY:O    | 1:A:1731:VAL:HG22 | 2.20                     | 0.42              |
| 1:A:1805:GLU:HA   | 1:A:1808:GLU:CD   | 2.39                     | 0.42              |
| 1:A:1915:HIS:CE1  | 1:A:1919:ARG:HH12 | 2.37                     | 0.42              |
| 1:A:1998:PHE:O    | 1:A:2002:GLY:N    | 2.52                     | 0.42              |
| 1:A:2168:LYS:HG3  | 1:A:2169:THR:N    | 2.34                     | 0.42              |
| 1:A:2276:VAL:O    | 1:A:2280:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:500:ASN:O     | 1:A:503:MET:N     | 2.52                     | 0.42              |
| 1:A:597:LEU:O     | 1:A:601:GLU:OE1   | 2.38                     | 0.42              |
| 1:A:740:GLY:HA2   | 1:A:743:VAL:HG22  | 2.00                     | 0.42              |
| 1:A:971:ARG:NH1   | 1:A:974:GLN:HB2   | 2.30                     | 0.42              |
| 1:A:1194:GLN:HA   | 1:A:1197:ASN:OD1  | 2.20                     | 0.42              |
| 1:A:1328:SER:HA   | 1:A:1329:PRO:HD3  | 1.89                     | 0.42              |
| 1:A:1595:ALA:O    | 1:A:1598:PRO:HD2  | 2.19                     | 0.42              |
| 1:A:2055:ILE:O    | 1:A:2058:LEU:HB3  | 2.18                     | 0.42              |
| 1:A:230:VAL:O     | 1:A:345:LYS:HG2   | 2.19                     | 0.42              |
| 1:A:341:ASP:OD1   | 1:A:344:THR:HG23  | 2.20                     | 0.42              |
| 1:A:356:ILE:O     | 1:A:357:LYS:HD3   | 2.19                     | 0.42              |
| 1:A:368:LEU:HB3   | 1:A:370:PHE:CE1   | 2.54                     | 0.42              |
| 1:A:833:THR:O     | 1:A:837:VAL:HG23  | 2.19                     | 0.42              |
| 1:A:912:LYS:O     | 1:A:916:ARG:HG3   | 2.20                     | 0.42              |
| 1:A:1435:GLY:HA2  | 1:A:1438:GLU:OE2  | 2.19                     | 0.42              |
| 1:A:1561:ALA:C    | 1:A:1564:PRO:HD2  | 2.39                     | 0.42              |
| 1:A:1675:LEU:HB2  | 1:A:1766:LYS:NZ   | 2.34                     | 0.42              |
| 1:A:1908:GLU:OE2  | 1:A:1909:ASN:HB2  | 2.18                     | 0.42              |
| 1:A:1930:LEU:HD23 | 1:A:1953:CYS:HB3  | 2.01                     | 0.42              |
| 1:A:2017:GLU:O    | 1:A:2021:LYS:HG2  | 2.20                     | 0.42              |
| 1:A:2032:VAL:HG22 | 1:A:2036:ASN:OD1  | 2.20                     | 0.42              |
| 1:A:2054:THR:HA   | 1:A:2057:ARG:NE   | 2.35                     | 0.42              |
| 1:A:2147:GLU:O    | 1:A:2148:ALA:C    | 2.57                     | 0.42              |
| 1:A:543:ILE:O     | 1:A:547:VAL:HG22  | 2.20                     | 0.42              |
| 1:A:1040:LYS:O    | 1:A:1043:GLU:HG3  | 2.20                     | 0.42              |
| 1:A:1138:VAL:HA   | 1:A:1141:LEU:CD2  | 2.49                     | 0.42              |
| 1:A:1265:GLN:O    | 1:A:1269:ARG:HG2  | 2.20                     | 0.42              |
| 1:A:1360:GLN:HG2  | 1:A:1618:ARG:NH2  | 2.35                     | 0.42              |
| 1:A:2144:ARG:NH2  | 1:A:2147:GLU:OE2  | 2.38                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:212:LEU:CD2   | 1:A:295:LYS:HB3   | 2.49                     | 0.42              |
| 1:A:854:ARG:HD2   | 1:A:855:LYS:N     | 2.34                     | 0.42              |
| 1:A:914:VAL:O     | 1:A:915:GLN:C     | 2.58                     | 0.42              |
| 1:A:955:SER:OG    | 1:A:956:CYS:N     | 2.52                     | 0.42              |
| 1:A:1098:VAL:HG12 | 1:A:1127:GLY:HA3  | 2.00                     | 0.42              |
| 1:A:1555:ARG:O    | 1:A:1559:ARG:HG2  | 2.18                     | 0.42              |
| 1:A:2021:LYS:NZ   | 1:A:2024:LYS:HE2  | 2.35                     | 0.42              |
| 1:A:2328:PRO:CB   | 1:A:2343:GLU:HG3  | 2.50                     | 0.42              |
| 1:A:2451:GLU:HA   | 1:A:2454:LYS:HD2  | 2.02                     | 0.42              |
| 1:A:528:SER:OG    | 1:A:529:LYS:N     | 2.52                     | 0.42              |
| 1:A:528:SER:O     | 1:A:532:ARG:HG3   | 2.20                     | 0.42              |
| 1:A:669:MET:O     | 1:A:673:ASN:ND2   | 2.53                     | 0.42              |
| 1:A:735:GLN:HA    | 1:A:738:GLU:OE2   | 2.20                     | 0.42              |
| 1:A:1269:ARG:HB2  | 1:A:1273:ARG:NH2  | 2.35                     | 0.42              |
| 1:A:1494:ALA:O    | 1:A:1498:VAL:HG22 | 2.19                     | 0.42              |
| 1:A:1563:ALA:HA   | 1:A:1566:LEU:HD12 | 2.02                     | 0.42              |
| 1:A:1713:ILE:O    | 1:A:1717:ALA:N    | 2.47                     | 0.42              |
| 1:A:1771:SER:HB2  | 1:A:1803:MET:HG3  | 2.01                     | 0.42              |
| 1:A:2149:THR:HA   | 1:A:2209:ARG:HD2  | 2.01                     | 0.42              |
| 1:A:751:VAL:O     | 1:A:755:GLN:HG3   | 2.19                     | 0.41              |
| 1:A:796:GLY:N     | 1:A:799:ASP:OD2   | 2.52                     | 0.41              |
| 1:A:819:ALA:HB2   | 1:A:877:ALA:HB1   | 2.02                     | 0.41              |
| 1:A:1249:LEU:HD21 | 1:A:1278:PHE:N    | 2.35                     | 0.41              |
| 1:A:1433:LEU:O    | 1:A:1437:THR:HG23 | 2.20                     | 0.41              |
| 1:A:1613:LEU:HD11 | 1:A:1633:LEU:HG   | 2.02                     | 0.41              |
| 1:A:2420:SER:O    | 1:A:2422:GLU:N    | 2.52                     | 0.41              |
| 1:A:540:LYS:NZ    | 1:A:655:ILE:O     | 2.53                     | 0.41              |
| 1:A:1051:ASP:O    | 1:A:1054:LEU:HB3  | 2.20                     | 0.41              |
| 1:A:1148:GLN:HA   | 1:A:1151:VAL:HG22 | 2.02                     | 0.41              |
| 1:A:1165:LEU:HA   | 1:A:1168:GLU:OE2  | 2.19                     | 0.41              |
| 1:A:1236:GLN:OE1  | 1:A:1236:GLN:N    | 2.48                     | 0.41              |
| 1:A:1252:ALA:HA   | 1:A:1255:GLU:CD   | 2.40                     | 0.41              |
| 1:A:1283:GLU:HA   | 1:A:1286:VAL:HG12 | 2.01                     | 0.41              |
| 1:A:1733:GLN:O    | 1:A:1736:GLN:HG2  | 2.20                     | 0.41              |
| 1:A:1775:LEU:HD12 | 1:A:1776:LEU:N    | 2.35                     | 0.41              |
| 1:A:1804:THR:OG1  | 1:A:1805:GLU:N    | 2.52                     | 0.41              |
| 1:A:1843:MET:SD   | 1:A:1843:MET:N    | 2.93                     | 0.41              |
| 1:A:2369:GLU:OE1  | 1:A:2452:ALA:HB2  | 2.20                     | 0.41              |
| 1:A:303:ARG:HA    | 1:A:308:TYR:CD2   | 2.56                     | 0.41              |
| 1:A:326:VAL:HG11  | 1:A:328:ARG:HE    | 1.85                     | 0.41              |
| 1:A:340:VAL:HG22  | 1:A:347:VAL:CA    | 2.50                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:556:SER:HA    | 1:A:559:ASN:HD22  | 1.85                     | 0.41              |
| 1:A:562:ALA:O     | 1:A:634:ARG:NH1   | 2.51                     | 0.41              |
| 1:A:635:GLN:N     | 1:A:635:GLN:OE1   | 2.53                     | 0.41              |
| 1:A:668:LEU:HG    | 1:A:783:GLN:HG3   | 2.02                     | 0.41              |
| 1:A:711:LEU:O     | 1:A:714:SER:OG    | 2.28                     | 0.41              |
| 1:A:802:THR:O     | 1:A:805:ILE:HB    | 2.21                     | 0.41              |
| 1:A:1307:GLY:HA2  | 1:A:1310:MET:HE3  | 2.03                     | 0.41              |
| 1:A:1601:ILE:HA   | 1:A:1604:LYS:HE2  | 2.02                     | 0.41              |
| 1:A:1668:LEU:O    | 1:A:1671:CYS:HB2  | 2.20                     | 0.41              |
| 1:A:1984:ALA:O    | 1:A:1988:ILE:HG13 | 2.20                     | 0.41              |
| 1:A:2015:HIS:CE1  | 1:A:2068:SER:HB3  | 2.55                     | 0.41              |
| 1:A:2218:ALA:HA   | 1:A:2221:GLU:OE1  | 2.20                     | 0.41              |
| 1:A:2267:GLN:NE2  | 1:A:2268:GLN:HG3  | 2.34                     | 0.41              |
| 1:A:1006:ALA:O    | 1:A:1009:PRO:HD2  | 2.20                     | 0.41              |
| 1:A:1250:ASN:O    | 1:A:1254:THR:HG23 | 2.20                     | 0.41              |
| 1:A:1806:ALA:O    | 1:A:1810:LEU:HG   | 2.20                     | 0.41              |
| 1:A:2149:THR:O    | 1:A:2152:HIS:HB3  | 2.21                     | 0.41              |
| 1:A:243:CYS:HB2   | 1:A:265:PHE:CE2   | 2.55                     | 0.41              |
| 1:A:250:HIS:CE1   | 1:A:254:LYS:HZ1   | 2.38                     | 0.41              |
| 1:A:765:ARG:O     | 1:A:765:ARG:NE    | 2.49                     | 0.41              |
| 1:A:1046:GLY:HA2  | 1:A:1047:PRO:HD3  | 1.90                     | 0.41              |
| 1:A:1084:MET:O    | 1:A:1087:CYS:HB2  | 2.20                     | 0.41              |
| 1:A:1322:LEU:C    | 1:A:1324:THR:N    | 2.74                     | 0.41              |
| 1:A:1436:PHE:CZ   | 1:A:1606:MET:HB3  | 2.56                     | 0.41              |
| 1:A:1444:ALA:HA   | 1:A:1596:MET:SD   | 2.60                     | 0.41              |
| 1:A:1762:LEU:HD13 | 1:A:1762:LEU:HA   | 1.89                     | 0.41              |
| 1:A:1774:GLN:O    | 1:A:1778:THR:HG23 | 2.19                     | 0.41              |
| 1:A:1791:HIS:NE2  | 1:A:1792:THR:HG23 | 2.35                     | 0.41              |
| 1:A:1811:THR:HG22 | 1:A:1815:ASN:ND2  | 2.35                     | 0.41              |
| 1:A:2153:ILE:HA   | 1:A:2156:GLU:OE1  | 2.20                     | 0.41              |
| 1:A:238:PHE:HA    | 1:A:241:PHE:HD2   | 1.86                     | 0.41              |
| 1:A:349:GLN:CD    | 1:A:350:GLU:H     | 2.22                     | 0.41              |
| 1:A:387:GLN:OE1   | 1:A:388:ILE:HD13  | 2.20                     | 0.41              |
| 1:A:574:GLY:O     | 1:A:577:VAL:HG12  | 2.20                     | 0.41              |
| 1:A:1223:LEU:HD22 | 1:A:1283:GLU:OE2  | 2.21                     | 0.41              |
| 1:A:1427:ALA:O    | 1:A:1431:LYS:HG3  | 2.21                     | 0.41              |
| 1:A:1790:ALA:O    | 1:A:1794:GLU:HG3  | 2.21                     | 0.41              |
| 1:A:2152:HIS:O    | 1:A:2156:GLU:OE1  | 2.39                     | 0.41              |
| 1:A:208:ASP:O     | 1:A:212:LEU:N     | 2.47                     | 0.41              |
| 1:A:288:GLN:H     | 1:A:288:GLN:HG3   | 1.71                     | 0.41              |
| 1:A:333:THR:HG1   | 1:A:334:LYS:N     | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:542:GLU:O     | 1:A:545:SER:OG    | 2.28                     | 0.41              |
| 1:A:584:LEU:HD11  | 1:A:619:VAL:HG21  | 2.01                     | 0.41              |
| 1:A:773:ALA:HA    | 1:A:776:GLN:HG2   | 2.03                     | 0.41              |
| 1:A:927:SER:O     | 1:A:930:GLN:HB2   | 2.20                     | 0.41              |
| 1:A:1094:SER:O    | 1:A:1098:VAL:HG22 | 2.20                     | 0.41              |
| 1:A:1121:ALA:O    | 1:A:1124:VAL:HG22 | 2.21                     | 0.41              |
| 1:A:1276:GLN:NE2  | 1:A:1277:ASP:OD1  | 2.54                     | 0.41              |
| 1:A:1322:LEU:O    | 1:A:1325:ASP:N    | 2.49                     | 0.41              |
| 1:A:1345:SER:HA   | 1:A:1348:GLN:HG3  | 2.02                     | 0.41              |
| 1:A:1701:GLN:O    | 1:A:1704:THR:OG1  | 2.33                     | 0.41              |
| 1:A:2043:LYS:HA   | 1:A:2046:GLN:OE1  | 2.20                     | 0.41              |
| 1:A:238:PHE:HD1   | 1:A:241:PHE:CD2   | 2.38                     | 0.41              |
| 1:A:356:ILE:HA    | 1:A:369:ASP:O     | 2.21                     | 0.41              |
| 1:A:899:MET:HA    | 1:A:902:ASN:ND2   | 2.36                     | 0.41              |
| 1:A:906:GLN:CD    | 1:A:909:ILE:HB    | 2.41                     | 0.41              |
| 1:A:1460:GLY:HA3  | 1:A:1582:SER:O    | 2.20                     | 0.41              |
| 1:A:1510:ARG:NH2  | 1:A:1511:LEU:HA   | 2.36                     | 0.41              |
| 1:A:1703:LEU:HG   | 1:A:1707:GLN:OE1  | 2.20                     | 0.41              |
| 1:A:1712:LEU:HD12 | 1:A:1730:LYS:NZ   | 2.35                     | 0.41              |
| 1:A:1838:LEU:HD21 | 1:A:1920:VAL:HG23 | 2.03                     | 0.41              |
| 1:A:1976:GLN:O    | 1:A:1980:THR:HG23 | 2.21                     | 0.41              |
| 1:A:208:ASP:CG    | 1:A:211:GLN:H     | 2.23                     | 0.41              |
| 1:A:358:ARG:HE    | 1:A:1680:LEU:HD22 | 1.86                     | 0.41              |
| 1:A:536:MET:SD    | 1:A:597:LEU:HD22  | 2.61                     | 0.41              |
| 1:A:686:ALA:HA    | 1:A:689:VAL:HG22  | 2.03                     | 0.41              |
| 1:A:724:ALA:N     | 1:A:725:PRO:HD2   | 2.35                     | 0.41              |
| 1:A:735:GLN:HA    | 1:A:738:GLU:CD    | 2.41                     | 0.41              |
| 1:A:1015:ALA:HA   | 1:A:1018:MET:HE2  | 2.01                     | 0.41              |
| 1:A:1054:LEU:O    | 1:A:1055:SER:C    | 2.59                     | 0.41              |
| 1:A:1221:LYS:O    | 1:A:1224:LEU:HB3  | 2.21                     | 0.41              |
| 1:A:1392:CYS:O    | 1:A:1396:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:1604:LYS:O    | 1:A:1608:GLU:OE1  | 2.38                     | 0.41              |
| 1:A:1695:GLN:OE1  | 1:A:1752:THR:HA   | 2.21                     | 0.41              |
| 1:A:1757:GLN:CD   | 1:A:1757:GLN:N    | 2.74                     | 0.41              |
| 1:A:1767:THR:HA   | 1:A:1770:GLU:OE1  | 2.21                     | 0.41              |
| 1:A:1850:PHE:HD2  | 1:A:1906:ALA:HB3  | 1.85                     | 0.41              |
| 1:A:1856:THR:HA   | 1:A:1859:ARG:NH2  | 2.33                     | 0.41              |
| 1:A:1976:GLN:O    | 1:A:1979:ILE:HG22 | 2.21                     | 0.41              |
| 1:A:2043:LYS:HE2  | 1:A:2043:LYS:HB2  | 1.93                     | 0.41              |
| 1:A:2059:ALA:O    | 1:A:2062:VAL:HG12 | 2.21                     | 0.41              |
| 1:A:2081:ILE:HG22 | 1:A:2085:LYS:HZ3  | 1.86                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2152:HIS:CD2  | 1:A:2155:GLN:NE2  | 2.89                     | 0.41              |
| 1:A:2207:LEU:HA   | 1:A:2210:ARG:NE   | 2.36                     | 0.41              |
| 1:A:2249:GLU:OE2  | 1:A:2253:HIS:CE1  | 2.74                     | 0.41              |
| 1:A:2287:ALA:O    | 1:A:2290:MET:HG2  | 2.20                     | 0.41              |
| 1:A:556:SER:O     | 1:A:560:LEU:HG    | 2.21                     | 0.41              |
| 1:A:711:LEU:HD23  | 1:A:715:GLN:HE22  | 1.85                     | 0.41              |
| 1:A:1051:ASP:HA   | 1:A:1170:LYS:HZ1  | 1.86                     | 0.41              |
| 1:A:1421:GLU:H    | 1:A:1421:GLU:CD   | 2.24                     | 0.41              |
| 1:A:1555:ARG:HB3  | 1:A:1559:ARG:NH2  | 2.36                     | 0.41              |
| 1:A:1775:LEU:HD23 | 1:A:1803:MET:SD   | 2.61                     | 0.41              |
| 1:A:1804:THR:O    | 1:A:1808:GLU:OE1  | 2.39                     | 0.41              |
| 1:A:2147:GLU:O    | 1:A:2150:THR:N    | 2.54                     | 0.41              |
| 1:A:2361:LYS:HA   | 1:A:2361:LYS:HE2  | 2.02                     | 0.41              |
| 1:A:227:SER:HB2   | 1:A:312:PHE:HB2   | 2.02                     | 0.40              |
| 1:A:280:PHE:O     | 1:A:283:HIS:HB2   | 2.21                     | 0.40              |
| 1:A:359:TRP:HB2   | 1:A:366:PHE:HZ    | 1.82                     | 0.40              |
| 1:A:916:ARG:O     | 1:A:919:HIS:HB2   | 2.21                     | 0.40              |
| 1:A:1054:LEU:O    | 1:A:1057:VAL:N    | 2.54                     | 0.40              |
| 1:A:1144:ASP:OD2  | 1:A:1146:ALA:HB3  | 2.22                     | 0.40              |
| 1:A:1196:LEU:O    | 1:A:1200:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:1257:VAL:HG12 | 1:A:1335:LEU:CD2  | 2.51                     | 0.40              |
| 1:A:1369:GLN:O    | 1:A:1373:VAL:HG22 | 2.21                     | 0.40              |
| 1:A:1374:ARG:HG2  | 1:A:1378:GLU:OE2  | 2.20                     | 0.40              |
| 1:A:1648:ILE:HA   | 1:A:1651:MET:SD   | 2.61                     | 0.40              |
| 1:A:1798:GLU:HA   | 1:A:1801:GLN:HE21 | 1.86                     | 0.40              |
| 1:A:1830:SER:HA   | 1:A:1833:GLN:OE1  | 2.21                     | 0.40              |
| 1:A:2176:ILE:O    | 1:A:2179:THR:OG1  | 2.21                     | 0.40              |
| 1:A:1027:LEU:O    | 1:A:1031:LEU:HD23 | 2.21                     | 0.40              |
| 1:A:1135:ALA:O    | 1:A:1138:VAL:HG22 | 2.21                     | 0.40              |
| 1:A:1145:PRO:HA   | 1:A:1148:GLN:OE1  | 2.22                     | 0.40              |
| 1:A:1305:LEU:HA   | 1:A:1308:ILE:HD12 | 2.03                     | 0.40              |
| 1:A:1920:VAL:HA   | 1:A:1923:LEU:CD1  | 2.50                     | 0.40              |
| 1:A:2436:ALA:O    | 1:A:2440:VAL:HG23 | 2.22                     | 0.40              |
| 1:A:347:VAL:CG2   | 1:A:350:GLU:HG3   | 2.49                     | 0.40              |
| 1:A:1236:GLN:H    | 1:A:1236:GLN:CD   | 2.23                     | 0.40              |
| 1:A:1260:SER:N    | 1:A:1267:LEU:HD21 | 2.37                     | 0.40              |
| 1:A:1298:ARG:HB2  | 1:A:1298:ARG:HH11 | 1.87                     | 0.40              |
| 1:A:1382:GLN:HA   | 1:A:1445:TYR:CE1  | 2.56                     | 0.40              |
| 1:A:1449:VAL:O    | 1:A:1454:SER:HB3  | 2.22                     | 0.40              |
| 1:A:1611:GLY:O    | 1:A:1615:GLN:OE1  | 2.39                     | 0.40              |
| 1:A:1881:GLU:O    | 1:A:1884:PRO:HG2  | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2249:GLU:OE1  | 1:A:2250:LEU:HD22 | 2.21                     | 0.40              |
| 1:A:2345:ILE:O    | 1:A:2349:VAL:HG23 | 2.22                     | 0.40              |
| 1:A:279:ILE:HG22  | 1:A:283:HIS:CE1   | 2.57                     | 0.40              |
| 1:A:281:GLN:NE2   | 1:A:281:GLN:O     | 2.53                     | 0.40              |
| 1:A:391:LEU:HB3   | 1:A:395:TYR:CE2   | 2.56                     | 0.40              |
| 1:A:885:GLU:CA    | 1:A:888:GLN:HE21  | 2.35                     | 0.40              |
| 1:A:886:GLN:O     | 1:A:890:LEU:HD23  | 2.21                     | 0.40              |
| 1:A:1128:LEU:HD13 | 1:A:1131:LEU:CD1  | 2.42                     | 0.40              |
| 1:A:2246:GLY:HA3  | 1:A:2276:VAL:HG22 | 2.02                     | 0.40              |
| 1:A:2323:LEU:CD2  | 1:A:2349:VAL:HG12 | 2.50                     | 0.40              |
| 1:A:2357:SER:O    | 1:A:2360:VAL:HG12 | 2.21                     | 0.40              |
| 1:A:2369:GLU:HG3  | 1:A:2373:GLN:HE22 | 1.86                     | 0.40              |
| 1:A:622:LEU:HD22  | 1:A:640:ALA:HB1   | 2.03                     | 0.40              |
| 1:A:1004:ALA:O    | 1:A:1008:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:1375:GLU:HA   | 1:A:1378:GLU:CD   | 2.42                     | 0.40              |
| 1:A:1510:ARG:O    | 1:A:1513:SER:OG   | 2.23                     | 0.40              |
| 1:A:1874:LYS:HA   | 1:A:1874:LYS:HD2  | 1.85                     | 0.40              |
| 1:A:2075:GLU:HB3  | 1:A:2206:ASN:ND2  | 2.33                     | 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     | 2188/2804 (78%) | 2040 (93%) | 148 (7%) | 0        | <b>100</b>   <b>100</b> |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

entries.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| 1   | A     | 1677/2215 (76%) | 1664 (99%) | 13 (1%)  | 79 85       |

All (13) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 404  | LYS  |
| 1   | A     | 533  | LYS  |
| 1   | A     | 606  | ARG  |
| 1   | A     | 1035 | ARG  |
| 1   | A     | 1057 | VAL  |
| 1   | A     | 1059 | ASN  |
| 1   | A     | 1063 | ASP  |
| 1   | A     | 1064 | LEU  |
| 1   | A     | 1065 | GLN  |
| 1   | A     | 1122 | ARG  |
| 1   | A     | 1211 | ASN  |
| 1   | A     | 1955 | ARG  |
| 1   | A     | 2177 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 242 | GLN  |
| 1   | A     | 323 | ASN  |
| 1   | A     | 390 | GLN  |
| 1   | A     | 559 | ASN  |
| 1   | A     | 627 | GLN  |
| 1   | A     | 673 | ASN  |
| 1   | A     | 708 | GLN  |
| 1   | A     | 735 | GLN  |
| 1   | A     | 776 | GLN  |
| 1   | A     | 825 | GLN  |
| 1   | A     | 838 | ASN  |
| 1   | A     | 888 | GLN  |
| 1   | A     | 906 | GLN  |
| 1   | A     | 915 | GLN  |
| 1   | A     | 936 | GLN  |
| 1   | A     | 949 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1019 | GLN  |
| 1   | A     | 1187 | GLN  |
| 1   | A     | 1194 | GLN  |
| 1   | A     | 1243 | ASN  |
| 1   | A     | 1276 | GLN  |
| 1   | A     | 1300 | GLN  |
| 1   | A     | 1304 | ASN  |
| 1   | A     | 1356 | GLN  |
| 1   | A     | 1369 | GLN  |
| 1   | A     | 1382 | GLN  |
| 1   | A     | 1412 | GLN  |
| 1   | A     | 1442 | GLN  |
| 1   | A     | 1472 | GLN  |
| 1   | A     | 1527 | GLN  |
| 1   | A     | 1677 | GLN  |
| 1   | A     | 1733 | GLN  |
| 1   | A     | 1736 | GLN  |
| 1   | A     | 1764 | GLN  |
| 1   | A     | 1801 | GLN  |
| 1   | A     | 1869 | GLN  |
| 1   | A     | 1925 | HIS  |
| 1   | A     | 1969 | GLN  |
| 1   | A     | 2041 | GLN  |
| 1   | A     | 2077 | GLN  |
| 1   | A     | 2155 | GLN  |
| 1   | A     | 2267 | GLN  |
| 1   | A     | 2367 | GLN  |
| 1   | A     | 2421 | GLN  |
| 1   | A     | 2475 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

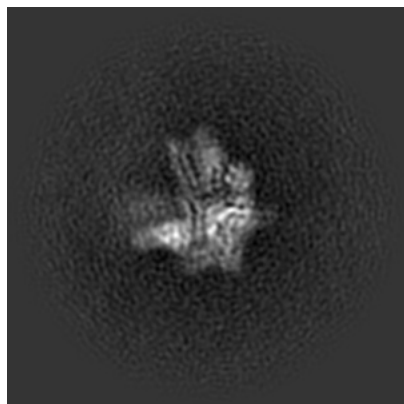
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43155. These allow visual inspection of the internal detail of the map and identification of artifacts.

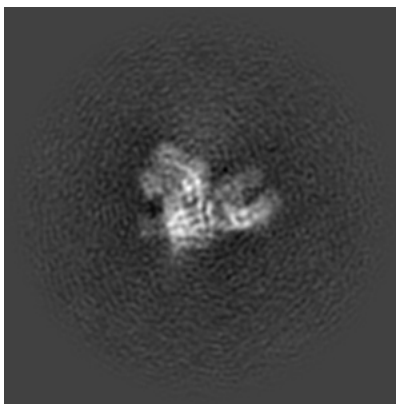
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

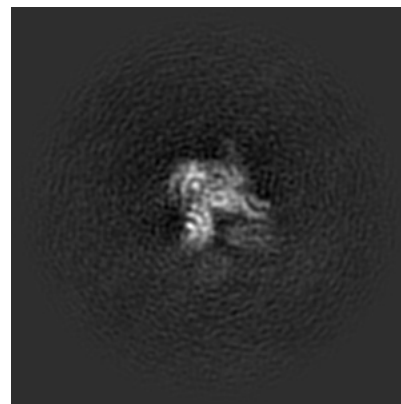
#### 6.1.1 Primary map



X

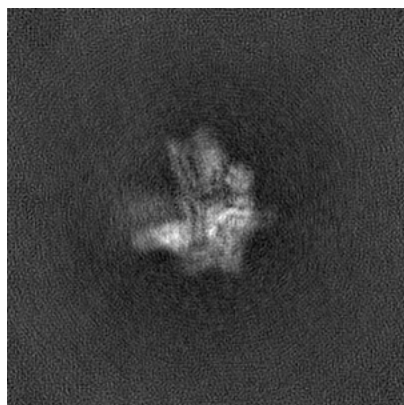


Y

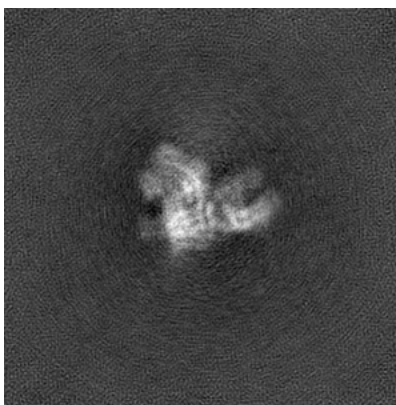


Z

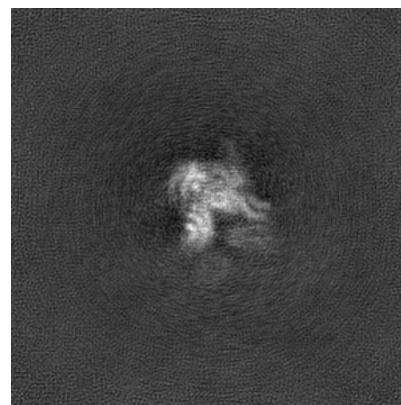
#### 6.1.2 Raw map



X



Y

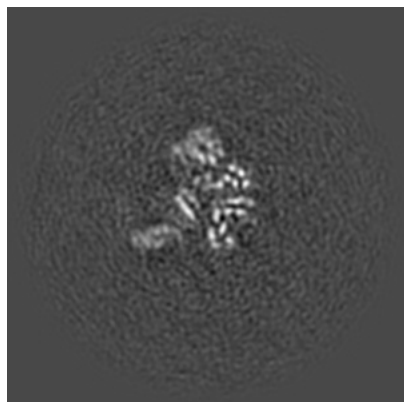


Z

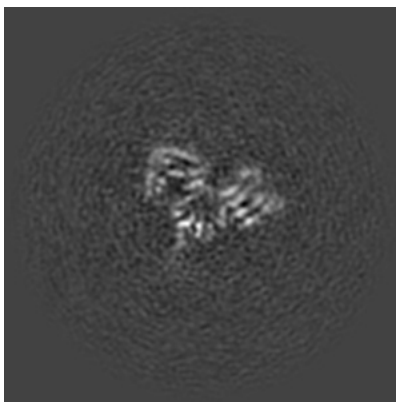
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

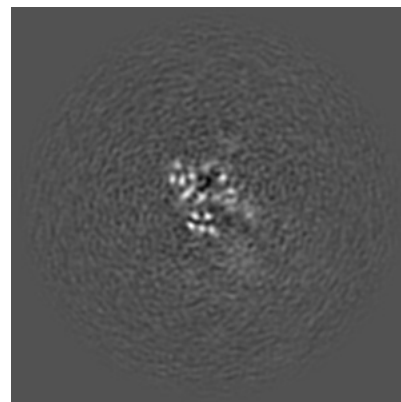
### 6.2.1 Primary map



X Index: 128

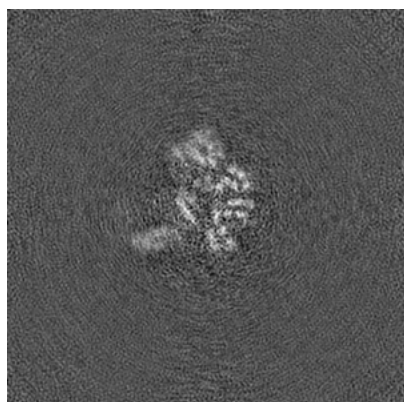


Y Index: 128

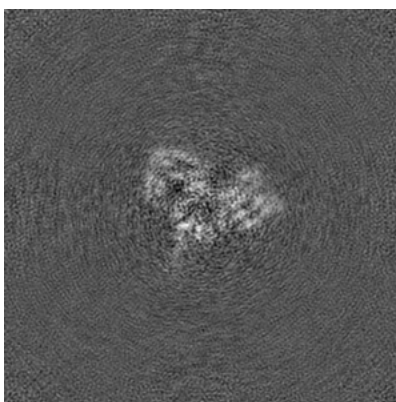


Z Index: 128

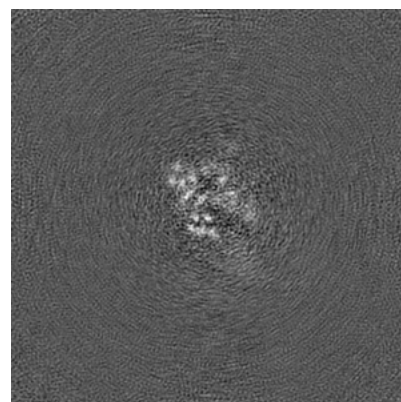
### 6.2.2 Raw map



X Index: 128



Y Index: 128

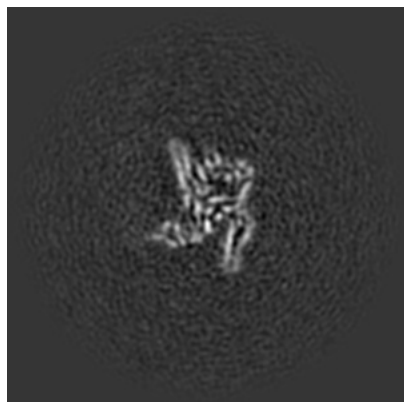


Z Index: 128

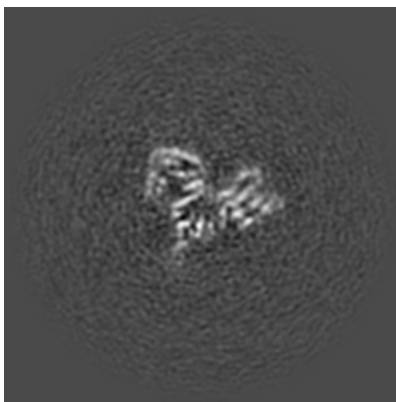
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

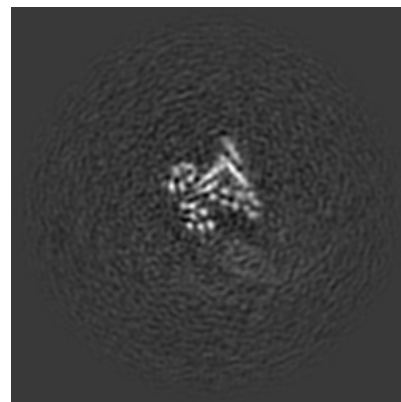
### 6.3.1 Primary map



X Index: 117

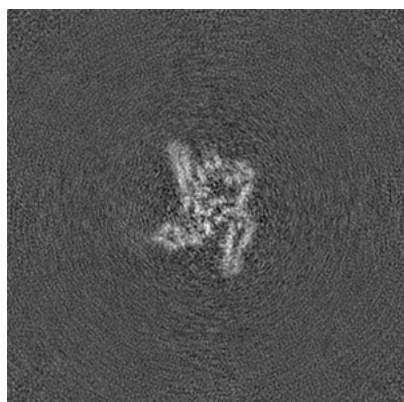


Y Index: 129

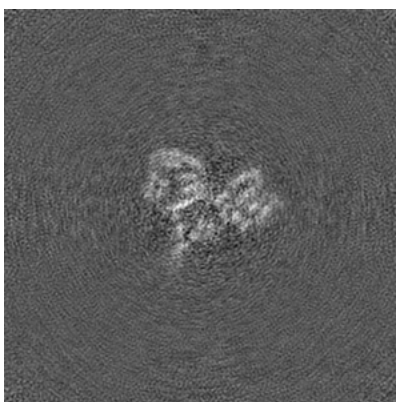


Z Index: 124

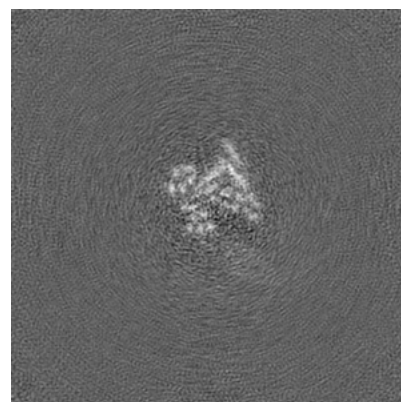
### 6.3.2 Raw map



X Index: 117



Y Index: 130



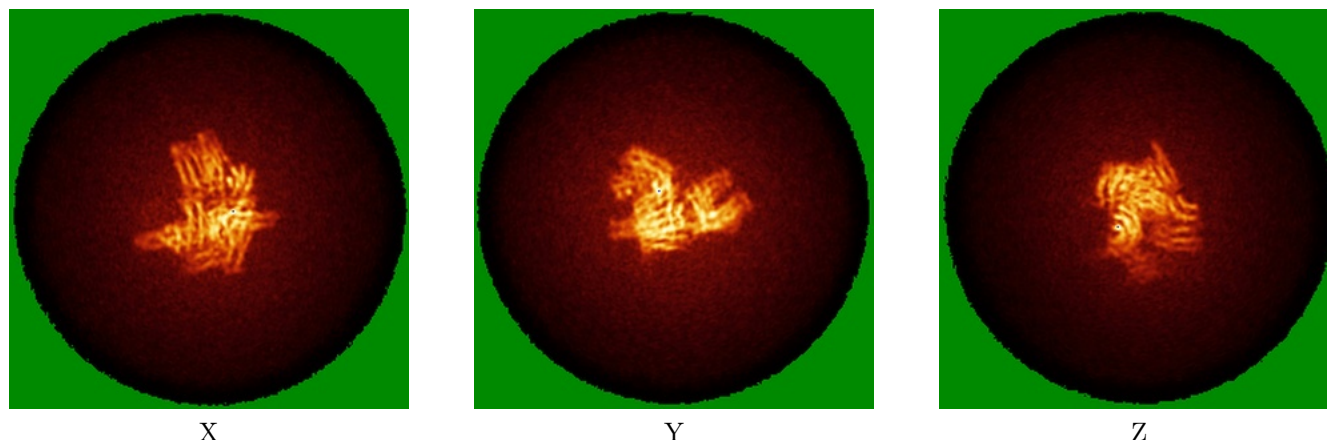
Z Index: 124

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

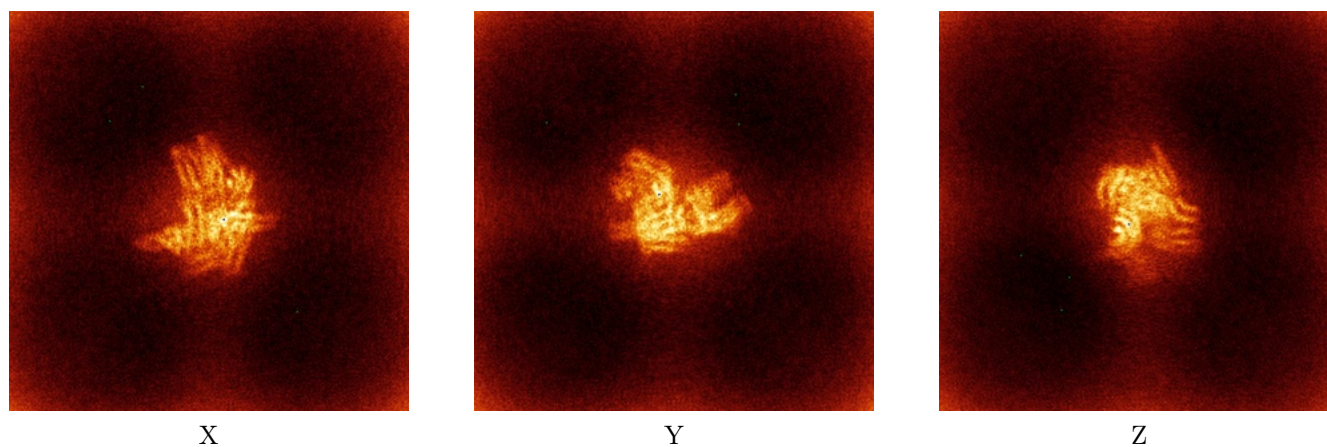


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map

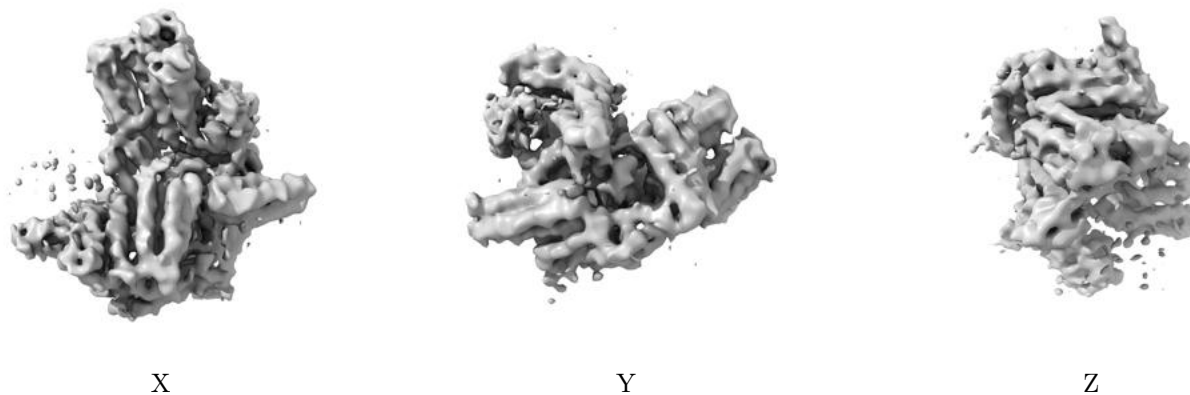


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



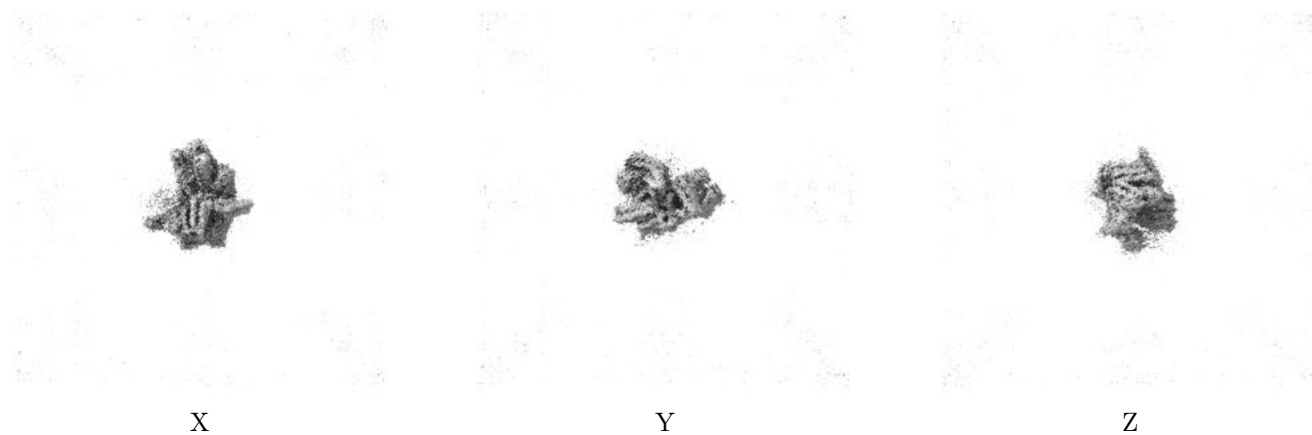
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.138. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

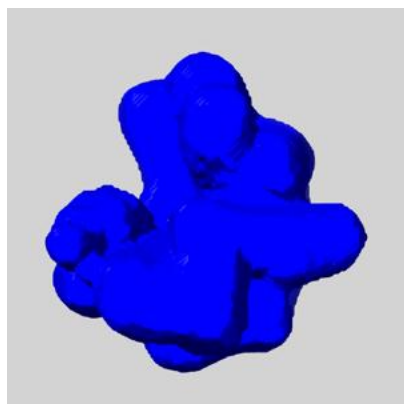
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

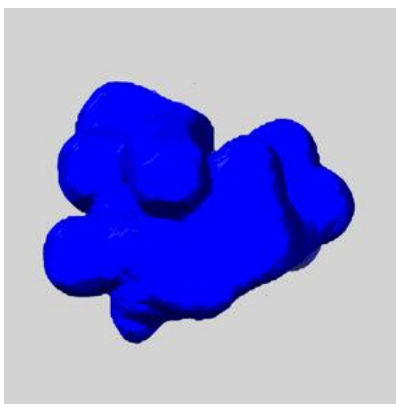
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

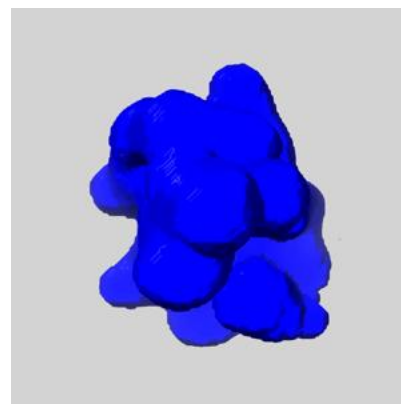
### 6.6.1 emd\_43155\_msk\_1.map [i](#)



X



Y

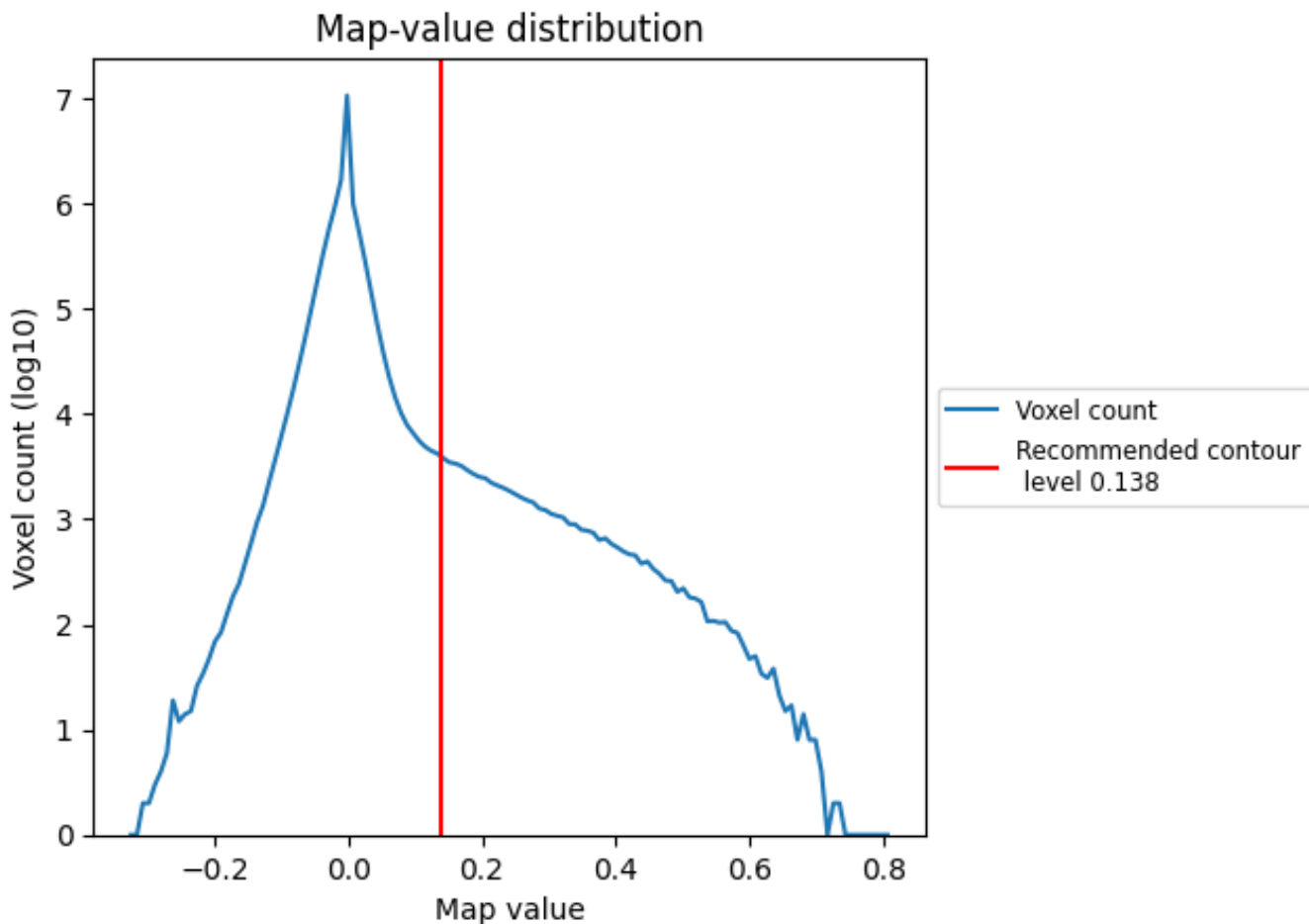


Z

## 7 Map analysis [i](#)

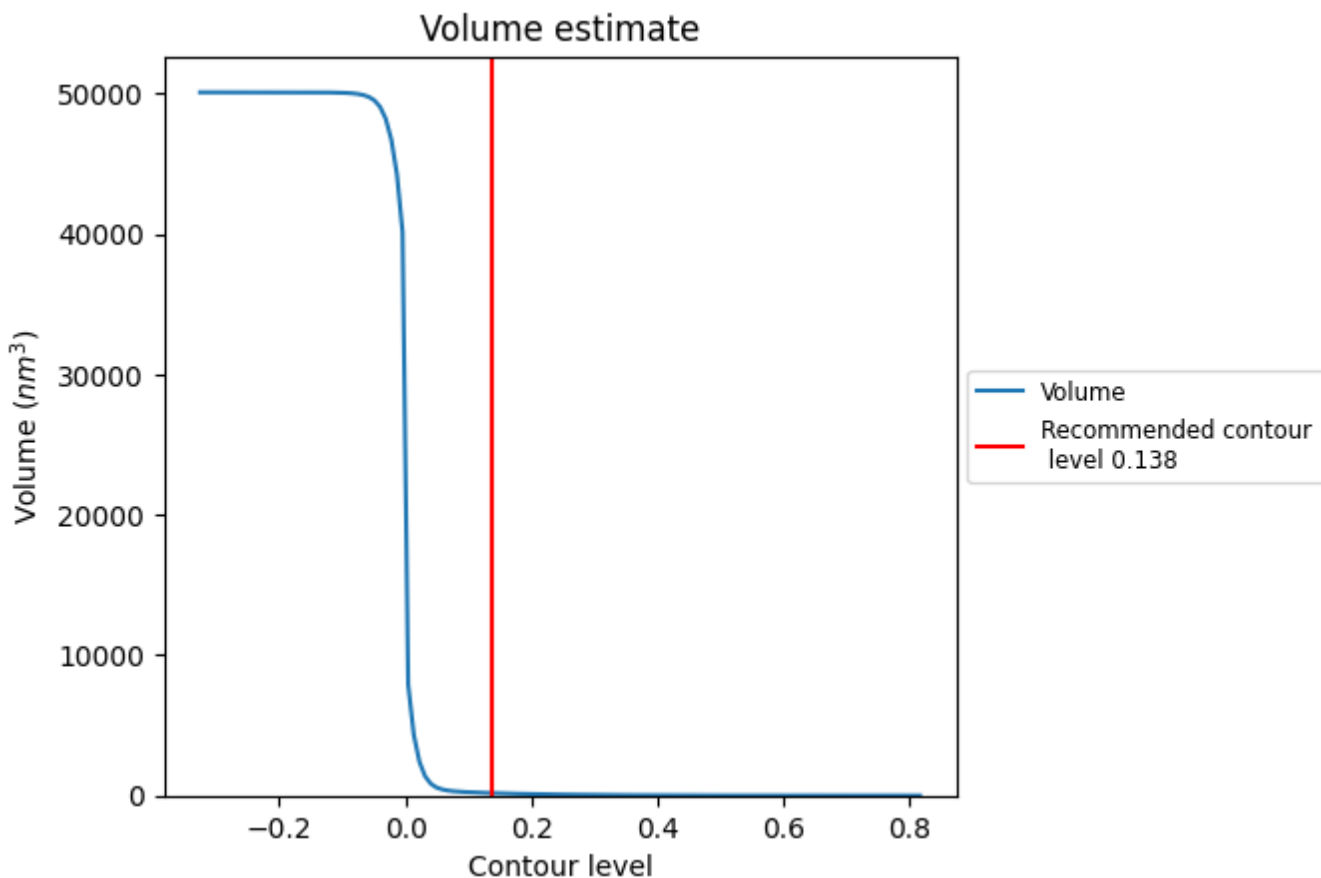
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

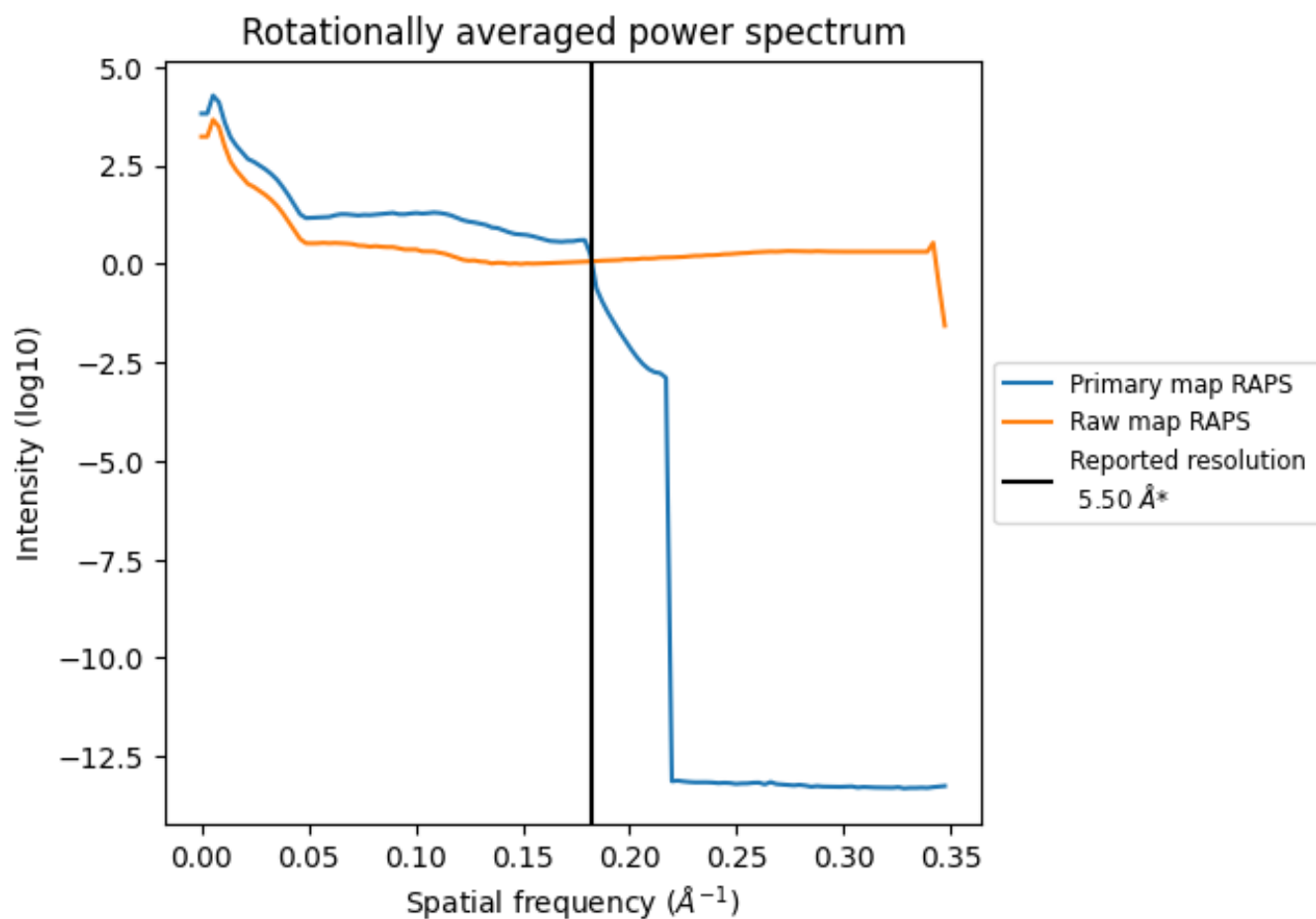
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 174  $\text{nm}^3$ ; this corresponds to an approximate mass of 157 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](#)

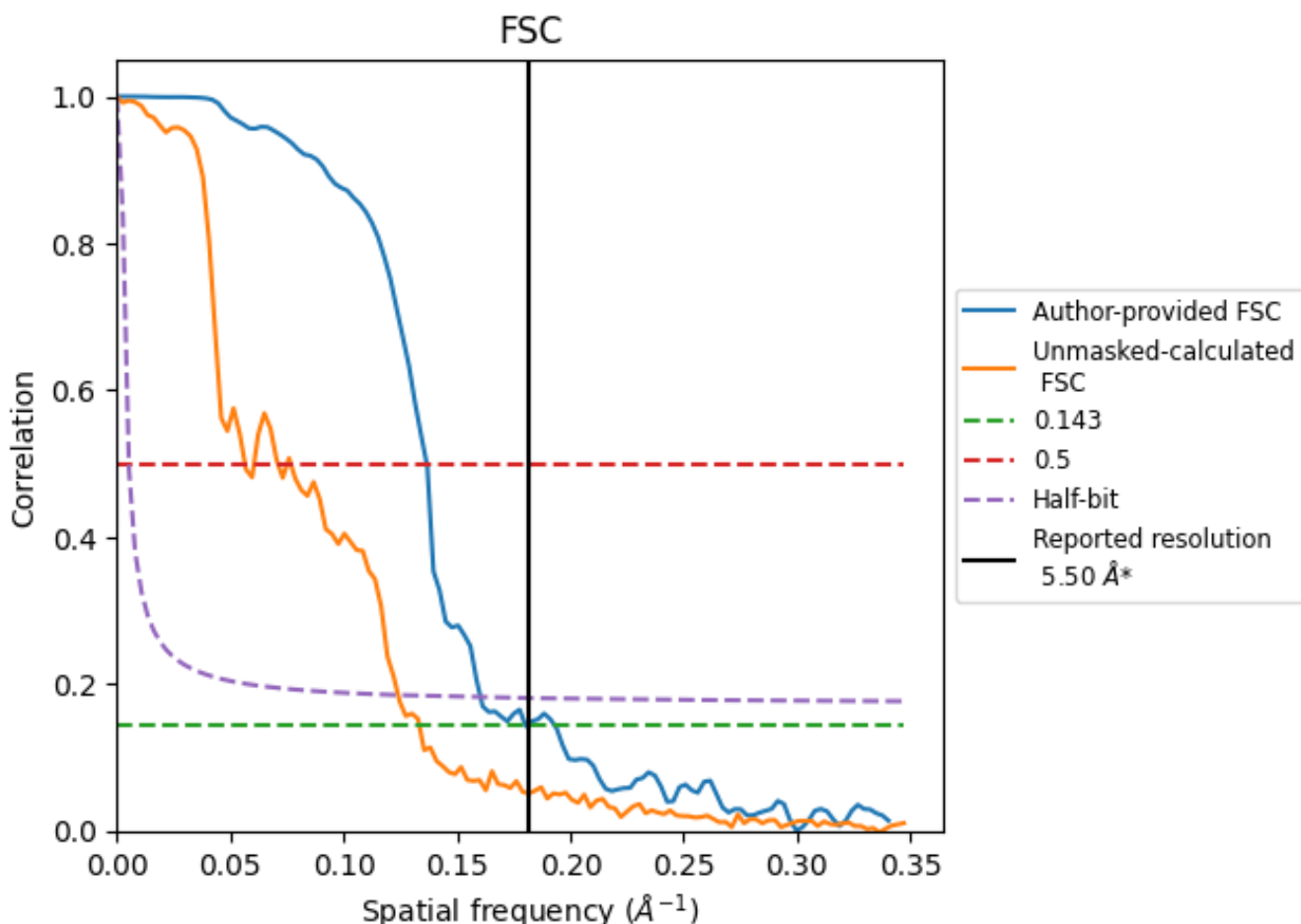


\*Reported resolution corresponds to spatial frequency of 0.182 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.182 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

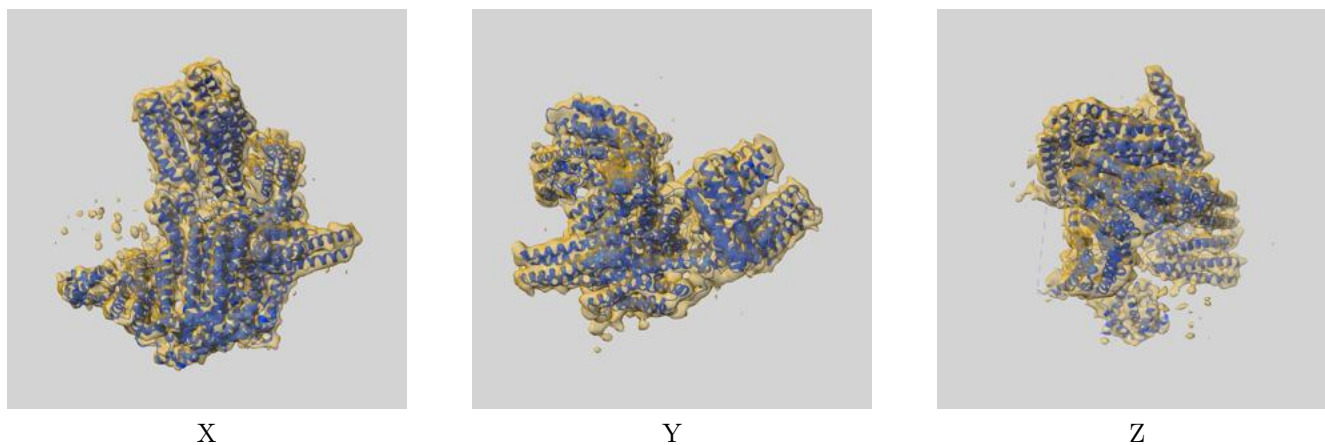
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 5.50                               | -     | -        |
| Author-provided FSC curve | 5.55                               | 7.32  | 6.23     |
| Unmasked-calculated*      | 7.49                               | 17.70 | 8.06     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.49 differs from the reported value 5.5 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43155 and PDB model 8VDQ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

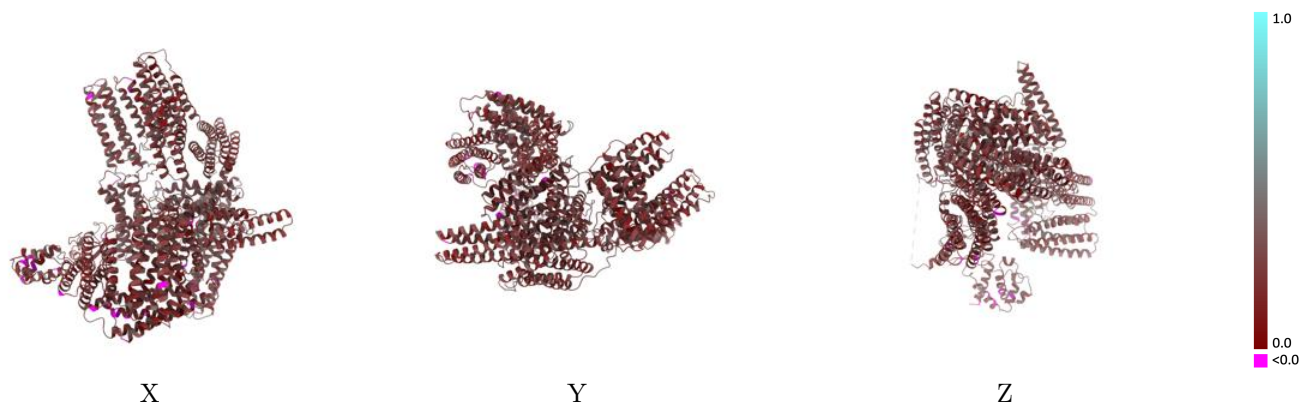
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.138 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.

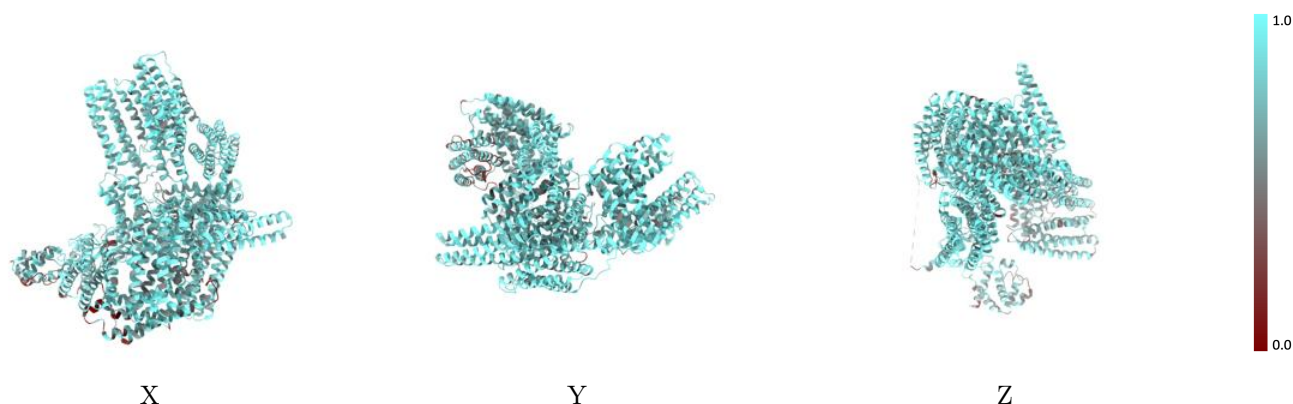


## 9.2 Q-score mapped to coordinate model [i](#)



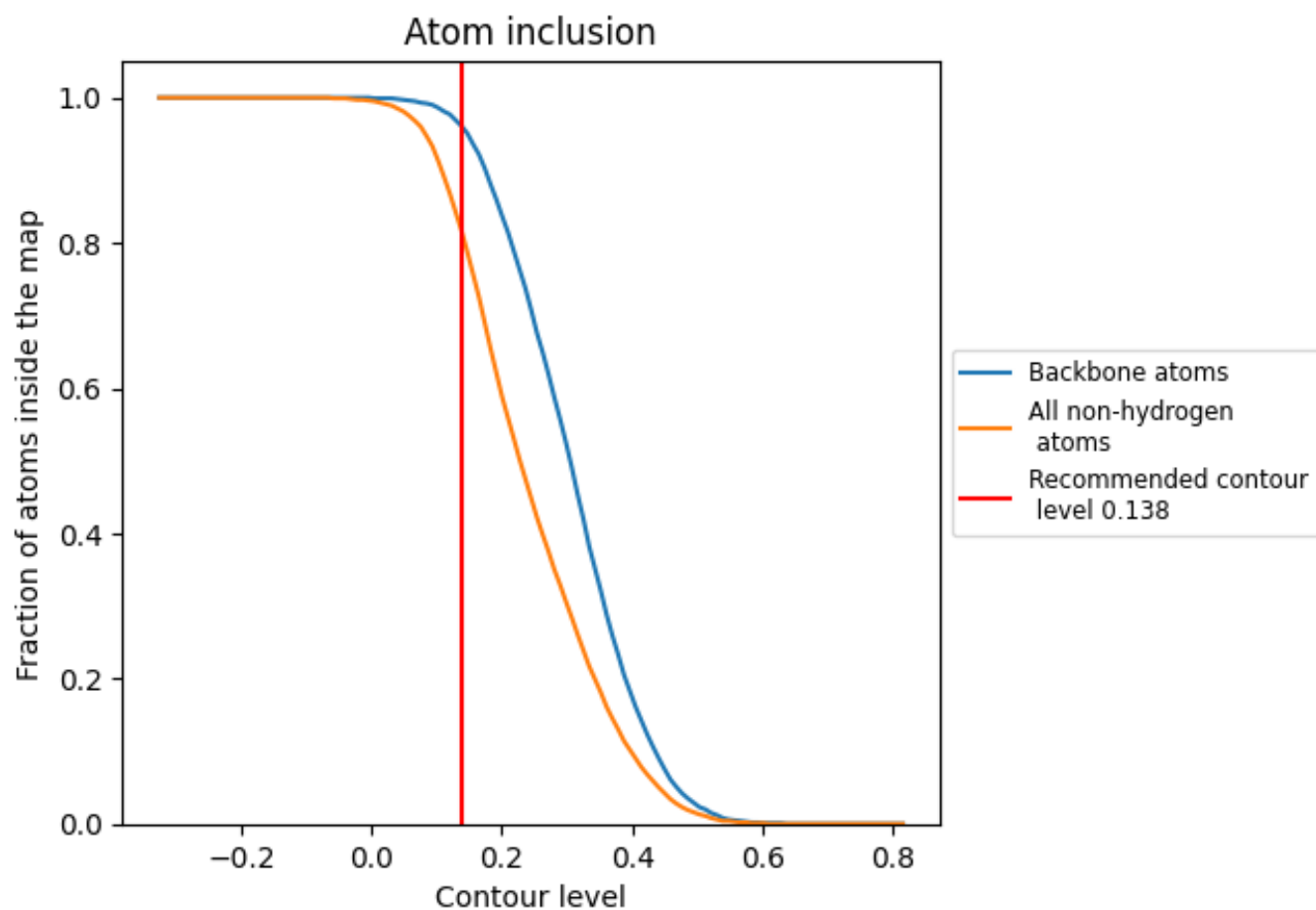
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.138).





## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.138) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8170 |  0.2390 |
| A     |  0.8170 |  0.2390 |

