# Full wwPDB EM Validation Report ⓘ

May 15, 2023 – 05:19 pm BST

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|---|---|---|
| PDB ID | : | 8AUK |
| EMDB ID | : | EMD-15672 |
| Title | : | Cryo-EM structure of human BIRC6 in complex with HTRA2. |
| Authors | : | Ehrmann, J.F.; Grabarczyk, D.B.; Clausen, T. |
| Deposited on | : | 2022-08-25 |
| Resolution | : | 6.20 Å(reported) |
| Based on initial models | : | 7VGE, 8ATU |

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

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

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

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

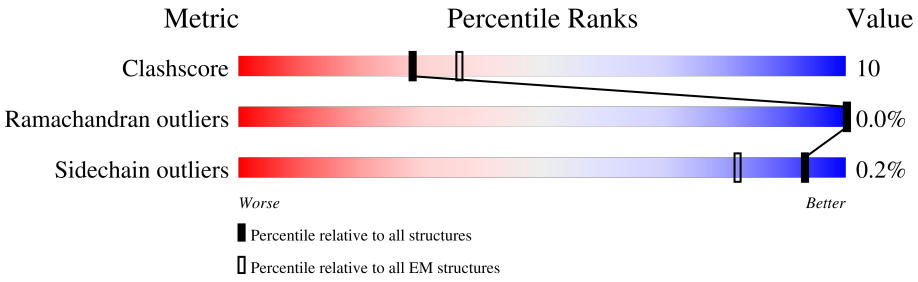
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev50 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.9 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.32.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.20 Å.

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




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

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 4867 | 10% 43% 15% 42% |
| 1 | B | 4867 | 9% 43% 15% 42% |
| 2 | C | 325 | 27% 43% 12% 45% |
| 2 | D | 325 | 29% 43% 13% 43% |
| 2 | E | 325 | 20% 38% 14% 47% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47811 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 Baculoviral IAP repeat-containing protein 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 2832 | Total<br>21902 | C<br>14002 | N<br>3699 | O<br>4050 | S<br>151 | 0 | 0 |
| 1 | B | 2832 | Total<br>21902 | C<br>14002 | N<br>3699 | O<br>4050 | S<br>151 | 0 | 0 |

There are 22 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1332 | VAL | LEU | conflict | UNP Q9NR09 |
| A | 4858 | SER | - | expression tag | UNP Q9NR09 |
| A | 4859 | ALA | - | expression tag | UNP Q9NR09 |
| A | 4860 | TRP | - | expression tag | UNP Q9NR09 |
| A | 4861 | SER | - | expression tag | UNP Q9NR09 |
| A | 4862 | HIS | - | expression tag | UNP Q9NR09 |
| A | 4863 | PRO | - | expression tag | UNP Q9NR09 |
| A | 4864 | GLN | - | expression tag | UNP Q9NR09 |
| A | 4865 | PHE | - | expression tag | UNP Q9NR09 |
| A | 4866 | GLU | - | expression tag | UNP Q9NR09 |
| A | 4867 | LYS | - | expression tag | UNP Q9NR09 |
| B | 1332 | VAL | LEU | conflict | UNP Q9NR09 |
| B | 4858 | SER | - | expression tag | UNP Q9NR09 |
| B | 4859 | ALA | - | expression tag | UNP Q9NR09 |
| B | 4860 | TRP | - | expression tag | UNP Q9NR09 |
| B | 4861 | SER | - | expression tag | UNP Q9NR09 |
| B | 4862 | HIS | - | expression tag | UNP Q9NR09 |
| B | 4863 | PRO | - | expression tag | UNP Q9NR09 |
| B | 4864 | GLN | - | expression tag | UNP Q9NR09 |
| B | 4865 | PHE | - | expression tag | UNP Q9NR09 |
| B | 4866 | GLU | - | expression tag | UNP Q9NR09 |
| B | 4867 | LYS | - | expression tag | UNP Q9NR09 |

- Molecule 2 is a protein called Serine protease HTRA2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | D | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1382 | 873 | 239 | 268 | 2 | | |
| 2 | E | 173 | Total | C | N | O | S | 0 | 0 |
| | | | 1291 | 815 | 223 | 251 | 2 | | |
| 2 | C | 179 | Total | C | N | O | S | 0 | 0 |
| | | | 1332 | 843 | 229 | 258 | 2 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 306 | ALA | SER | engineered mutation | UNP O43464 |
| E | 306 | ALA | SER | engineered mutation | UNP O43464 |
| C | 306 | ALA | SER | engineered mutation | UNP O43464 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

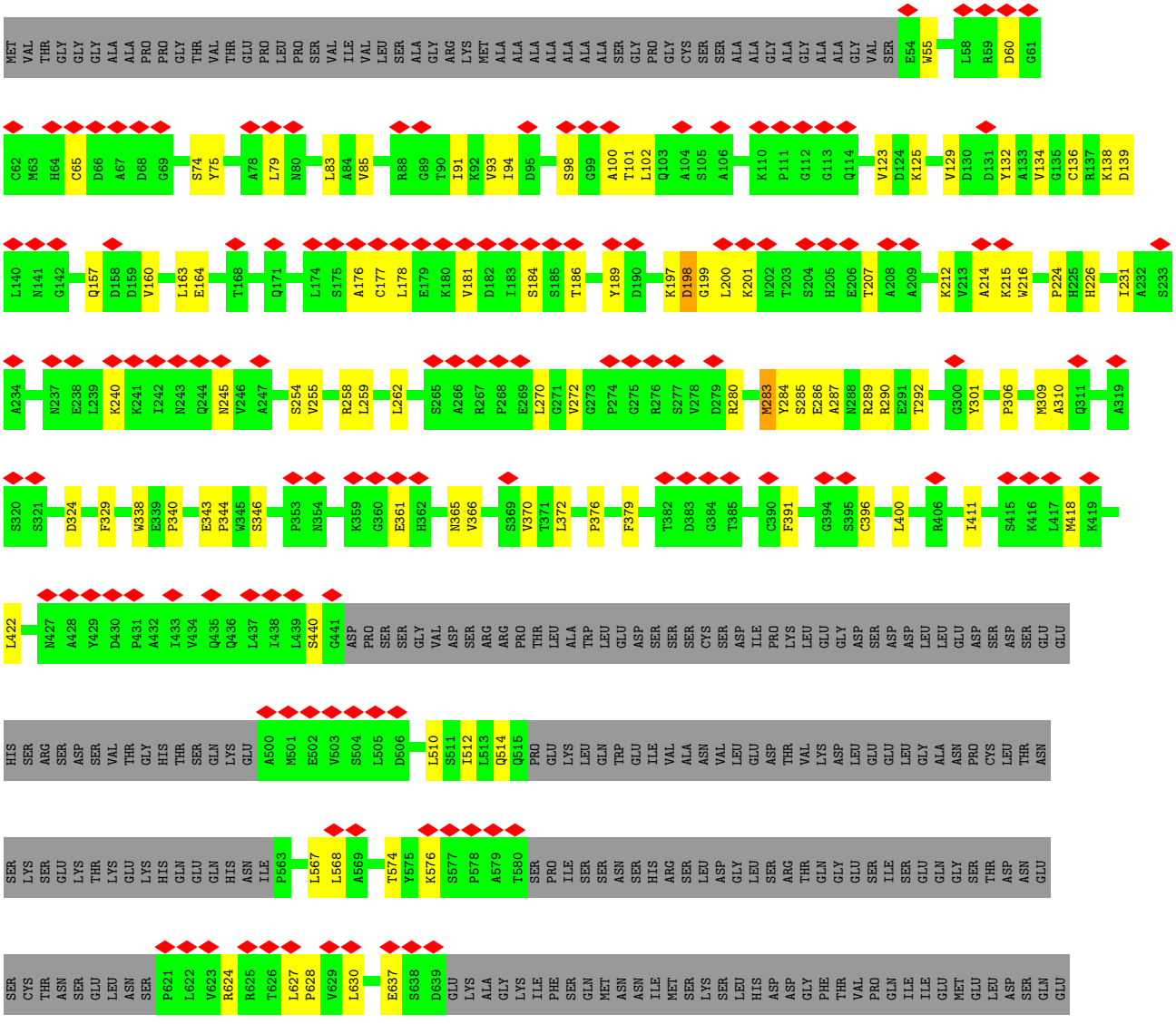
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 3 | B | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

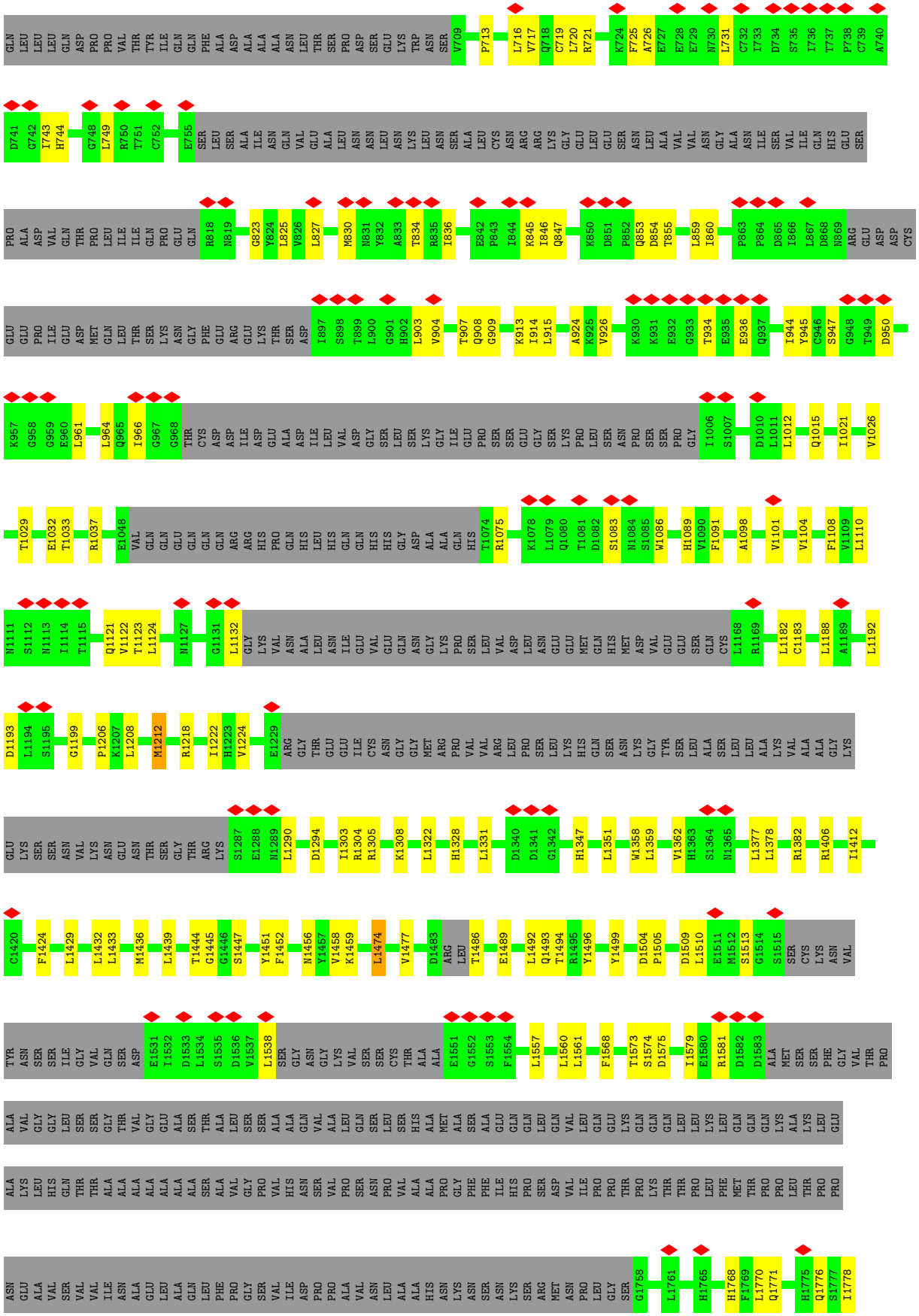
# 3 Residue-property plots (i)

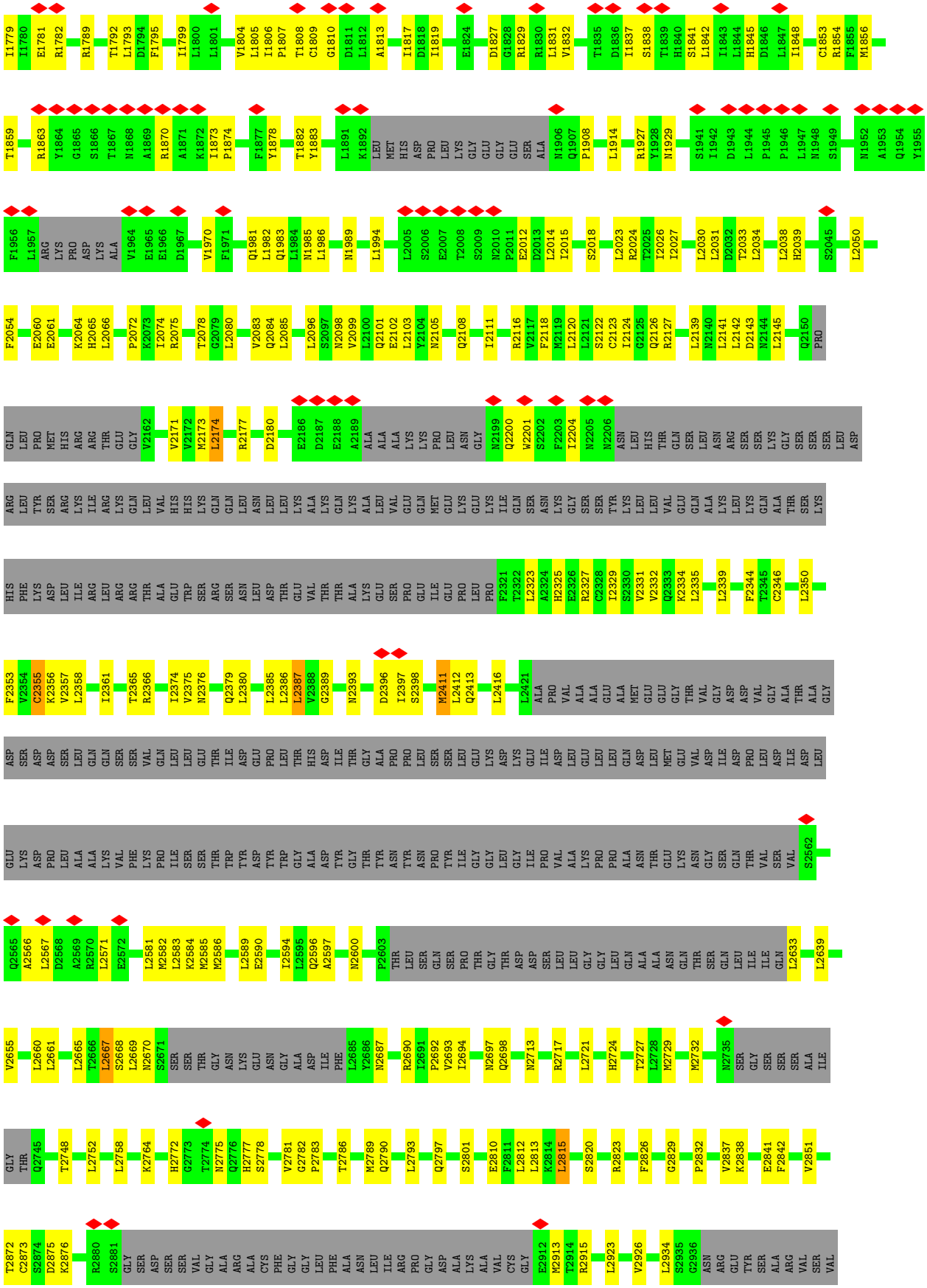
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

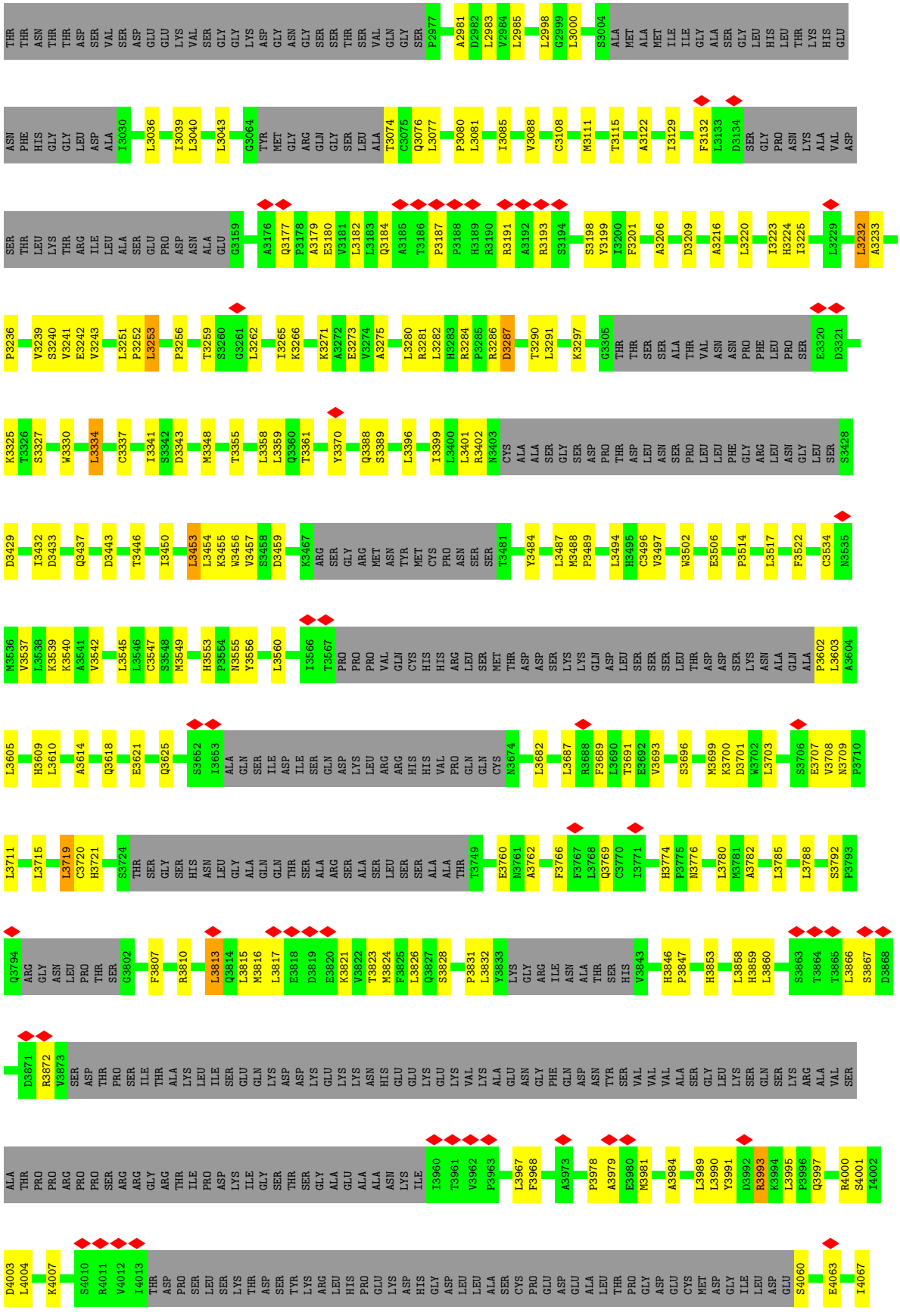
• Molecule 1: Baculoviral IAP repeat-containing protein 6

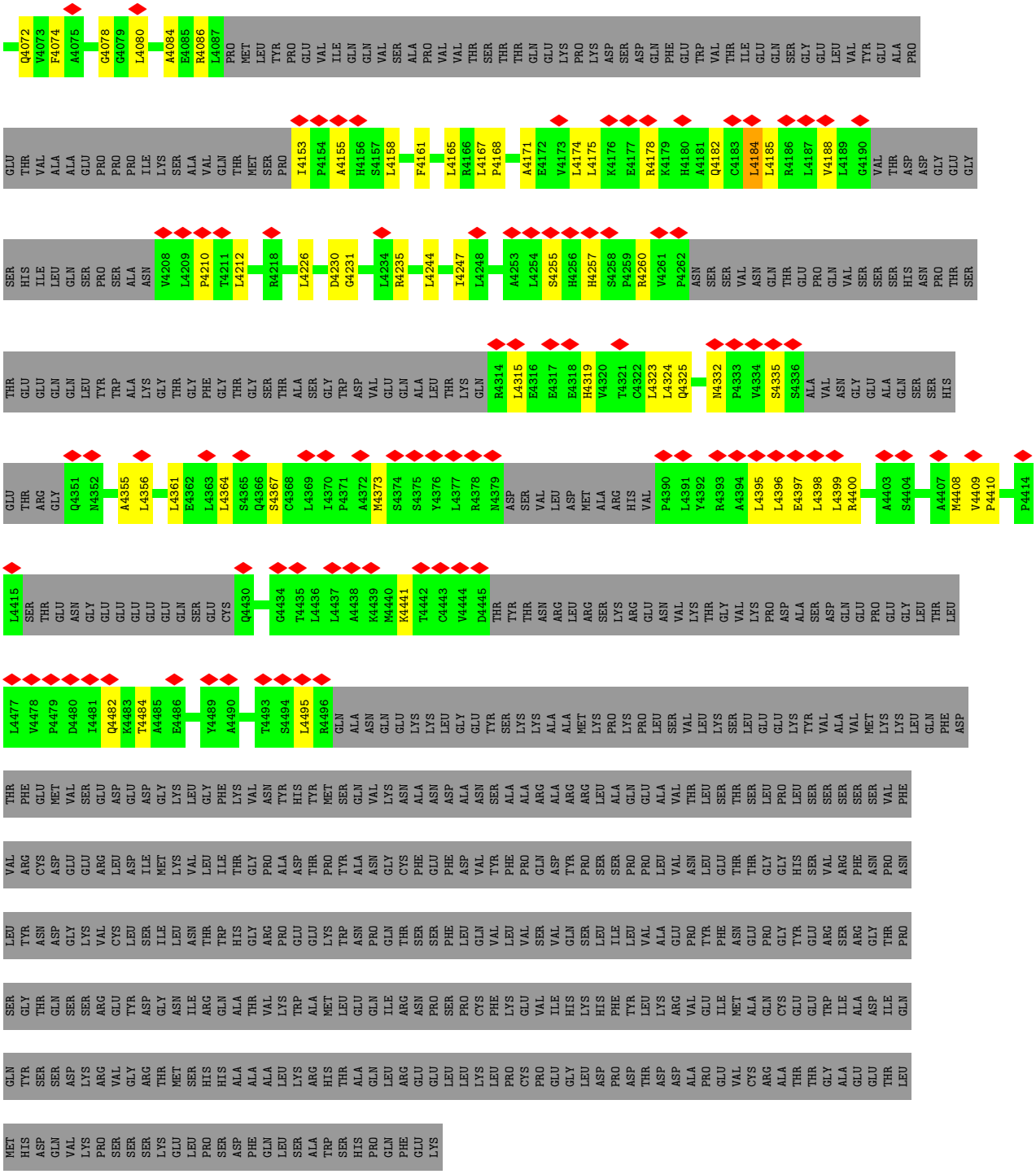
Chain A:


GLN LEU LEU LEU GLN ASP PRO PRO VAL THR TYR ILE GLN GLN PHE ALA ASP ALA ALA ASN LEU THR SER PRO ASP SER GLU LYS TRP ASN SER
V709 P713 L716 V717 Q718 C719 L720 R721 K724 F725 A726 E727 E728 E729 N730 L731 C732 I733 D734 S735 I736 T737 P738 C739 A740
D741 G742 I743 H744 G748 L749 R750 T751 C752 E755 SER LEU SER ALA ILE ASN GLN VAL GLU ALA LEU ASN ASN LEU ASN LYS LEU ASN SER ALA LEU CYS ASN ARG ARG LYS GLY GLU LEU GLU SER ASN LEU ALA VAL VAL ASN GLY ALA ASN ILE SER VAL ILE GLN HIS GLU SER
PRO ALA ASP VAL GLN THR PRO LEU ILE ILE GLN PRO GLU GLN R818 N819 G823 Y824 L825 V826 L827 M830 N831 Y832 A833 T834 R835 I836 E842 P843 I844 K845 I846 Q847 K850 D851 P852 Q853 D854 T855 L859 I860 P863 P864 D865 I866 L867 D868 N869 ARG GLU ASP ASP CYS
GLU GLU PRO ILE GLU ASP MET GLN LEU THR SER LYS ASN GLY PHE GLU ARG GLU LYS THR SER ASP I897 S898 T899 L900 G901 H902 L903 V904 T907 Q908 G909 K913 I914 L915 A924 K925 V926 K930 K931 E932 G933 T934 E935 E936 Q937 I944 Y945 C946 S947 G948 T949 D950
K957 G958 G959 E960 L961 L964 Q965 I966 G967 G968 THR CYS ASP ASP ILE ASP GLU ALA ASP ILE LEU LEU VAL ASP GLY SER LEU SER LYS GLY ILE GLU PRO SER SER GLU GLY SER LYS PRO LEU SER ASN PRO SER SER PRO GLY I1006 S1007 D1010 L1011 L1012 Q1015 I1021 V1026
T1029 E1032 T1033 R1037 E1048 VAL GLN GLN GLU GLN GLN GLN GLN ARG ARG ARG HIS PRO GLN HIS LEU LEU HIS GLN GLN HIS HIS GLY GLY ASP ALA ALA GLN HIS T1074 R1075 K1078 L1079 Q1080 T1081 D1082 S1083 N1084 S1085 W1086 H1089 Y1090 F1091 A1098 V1101 V1104 F1108 V1109 L1110
N1111 S1112 N1113 I1114 T1115 Q1121 V1122 T1123 L1124 N1127 G1131 L1132 GLY LYS VAL ASN ALA LEU ASN ILE GLU VAL GLU GLN ASN GLY LYS PRO SER LEU VAL ASP LEU ASN GLU GLU MET GLN HIS MET ASP VAL GLU GLU SER GLN CYS L1168 R1169 L1182 C1183 L1188 A1189 L1192
D1193 L1194 S1195 G1199 P1206 K1207 L1208 M1212 R1218 I1222 H1223 V1224 E1229 ARG GLY THR GLU GLU ILE CYS ASN GLY GLY MET ARG PRO VAL VAL ARG LEU PRO SER LEU LYS HIS GLN SER ASN LYS GLY TYR SER LEU ALA SER LEU LEU LEU ALA LYS VAL ALA ALA GLY LYS
GLU LYS SER SER ASN VAL LYS ASN GLU ASN THR SER GLY THR ARG LYS S1287 E1288 N1289 L1290 D1294 I1303 R1304 R1305 K1308 L1322 H1328 L1331 D1340 D1341 G1342 H1347 L1351 W1358 L1359 V1362 H1363 S1364 N1365 L1377 L1378 R1382 R1406 I1412
C1420 F1424 L1429 L1432 L1433 M1436 L1439 T1444 G1445 G1446 S1447 Y1451 F1452 N1456 Y1457 V1458 K1459 L1474 V1477 D1483 ARG LEU T1486 E1489 L1492 Q1493 T1494 R1495 Y1496 Y1499 D1504 P1505 D1509 L1510 E1511 M1512 S1513 G1514 S1515 SER CYS LYS ASN VAL
TYR ASN SER SER ILE GLY VAL GLN SER ASP E1531 I1532 D1533 L1534 S1535 D1536 V1537 L1538 SER GLY ASN GLY LYS VAL SER SER CYS THR ALA ALA E1551 G1552 S1553 F1554 L1557 L1560 L1561 F1568 T1573 S1574 D1575 I1579 E1580 R1581 D1582 D1583 ALA MET SER SER PHE GLY VAL THR PRO
ALA VAL GLY GLY LEU SER SER GLY THR VAL GLY GLU ALA SER THR ALA ALA LEU SER SER ALA ALA GLN VAL ALA LEU GLN SER LEU SER HIS ALA MET ALA SER ALA GLU GLN GLN LEU GLN VAL LEU LEU GLN GLU LYS GLN GLN GLN LEU LEU LYS LEU GLN GLN GLN LYS ALA LYS LEU GLU
ALA LYS LEU HIS GLN THR THR ALA ALA ALA ALA ALA ALA SER ALA VAL GLY PRO VAL HIS ASN SER VAL PRO SER ASN PRO VAL ALA ALA PRO GLY PHE PHE ILE HIS PRO SER ASP VAL ILE PRO PRO THR PRO LYS THR THR PRO LEU PHE MET THR PRO PRO LEU THR PRO PRO
ASN GLU ALA VAL SER VAL VAL ILE ASN ALA GLU LEU ALA GLN LEU PHE PRO GLY SER VAL ILE ASP PRO PRO ALA VAL ASN LEU ALA ALA HIS ASN LYS ASN SER ASN LYS SER ARG MET ASN PRO LEU GLY SER G1758 L1761 H1765 H1768 F1769 L1770 Q1771 H1775 Q1776 S1777 I1778

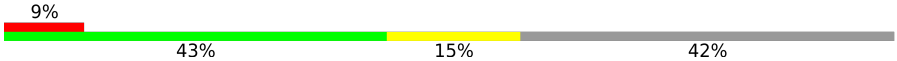


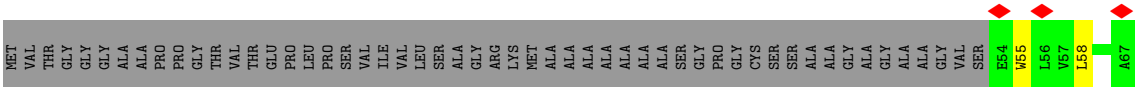


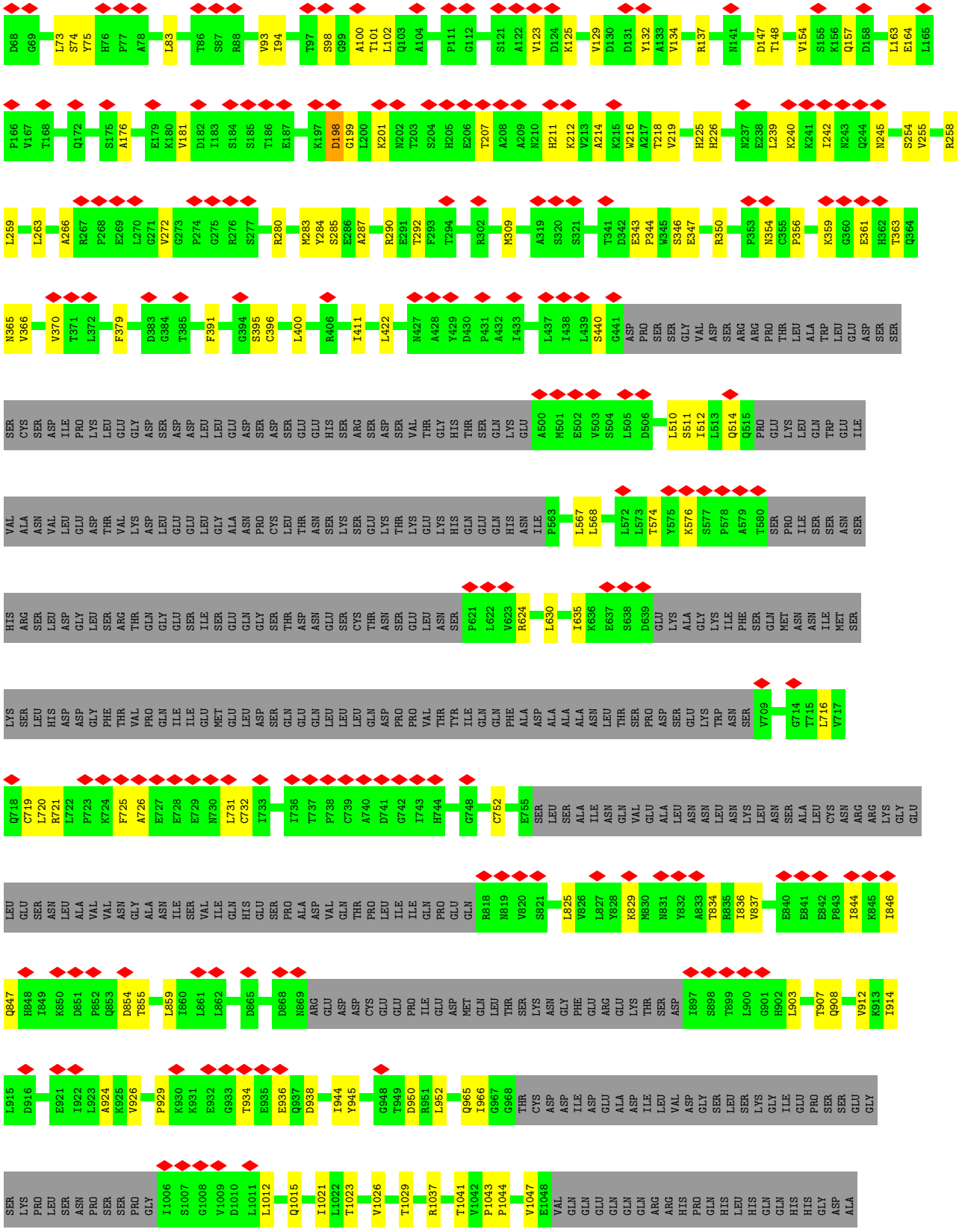


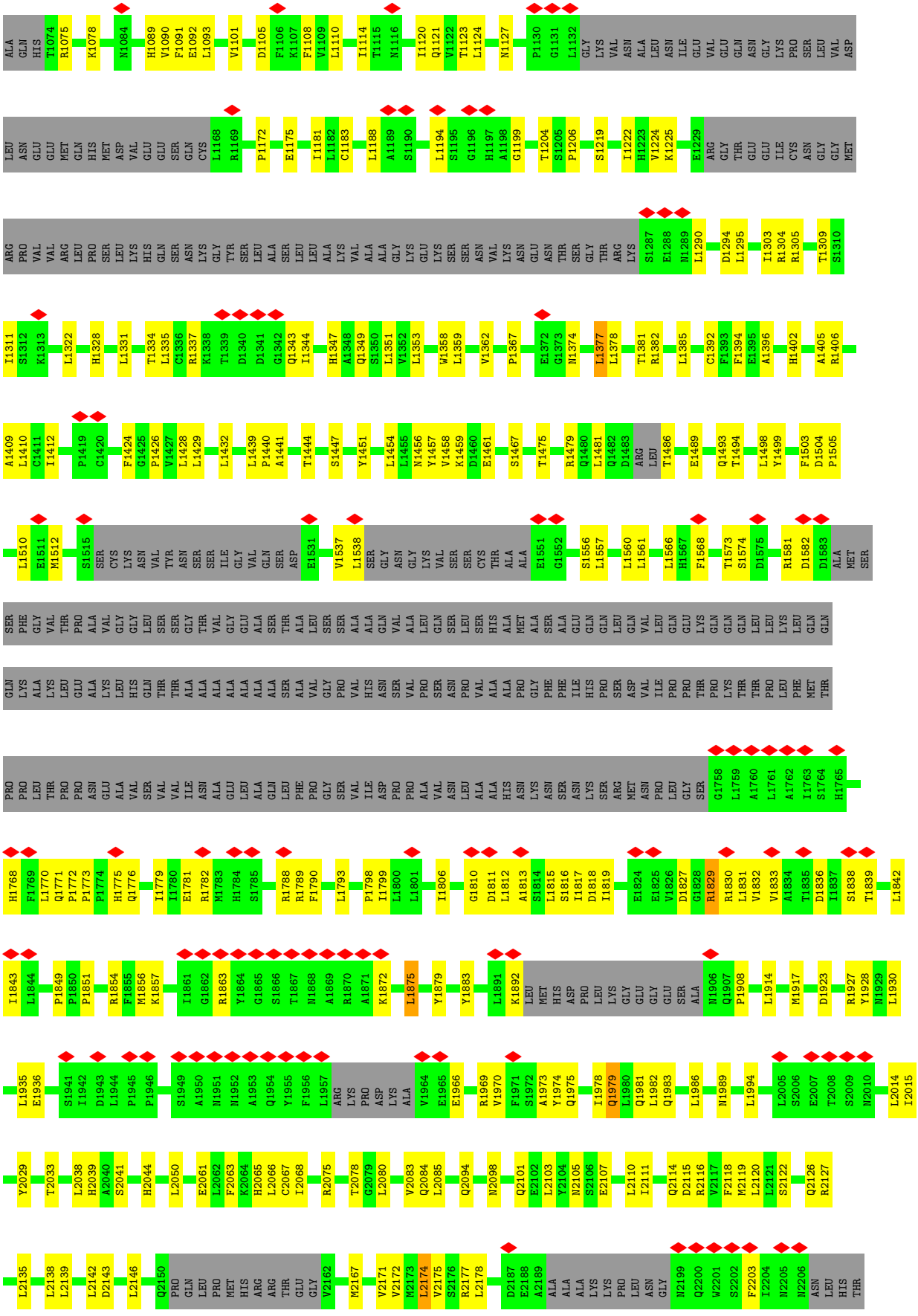
• Molecule 1: Baculoviral IAP repeat-containing protein 6

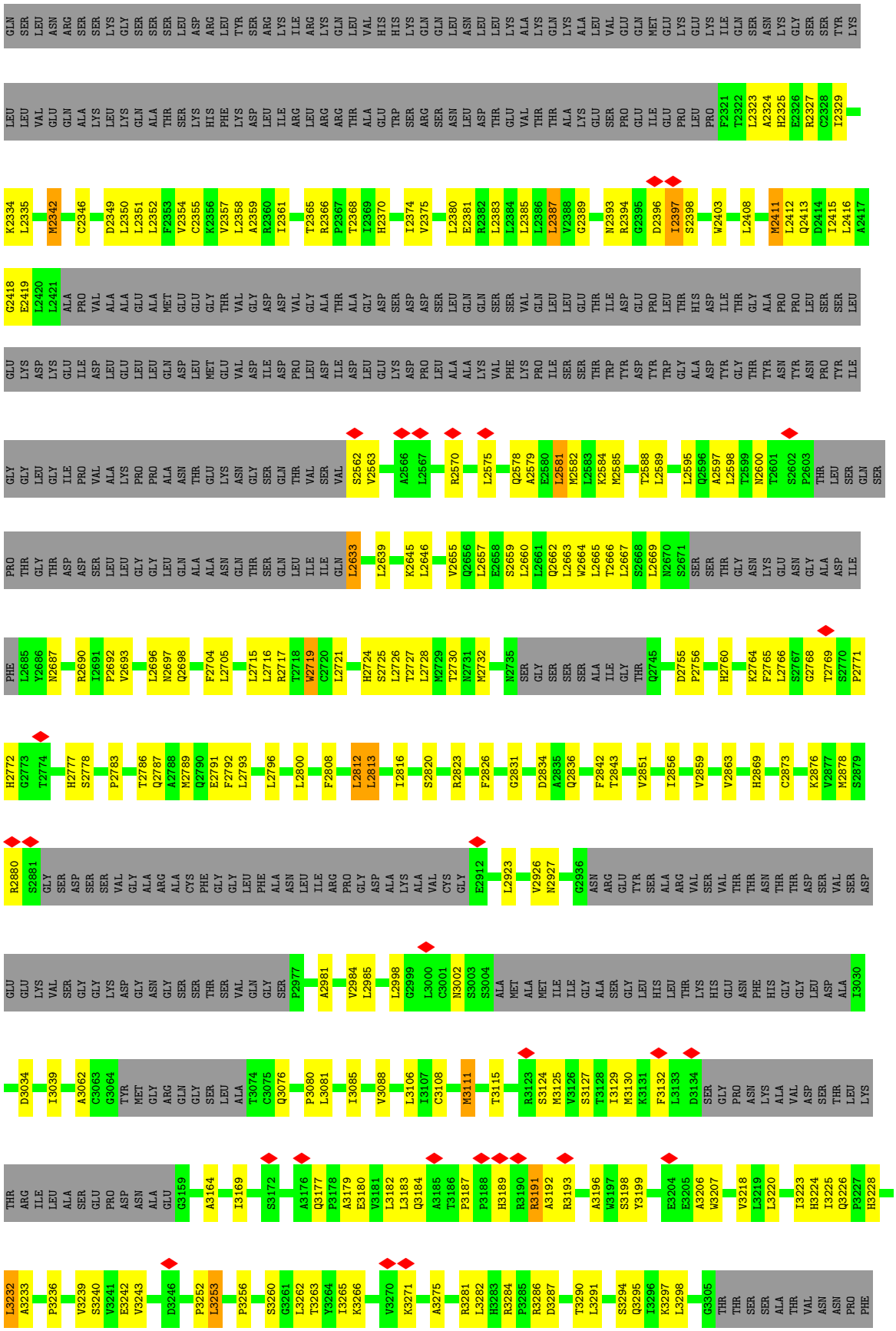
Chain B:

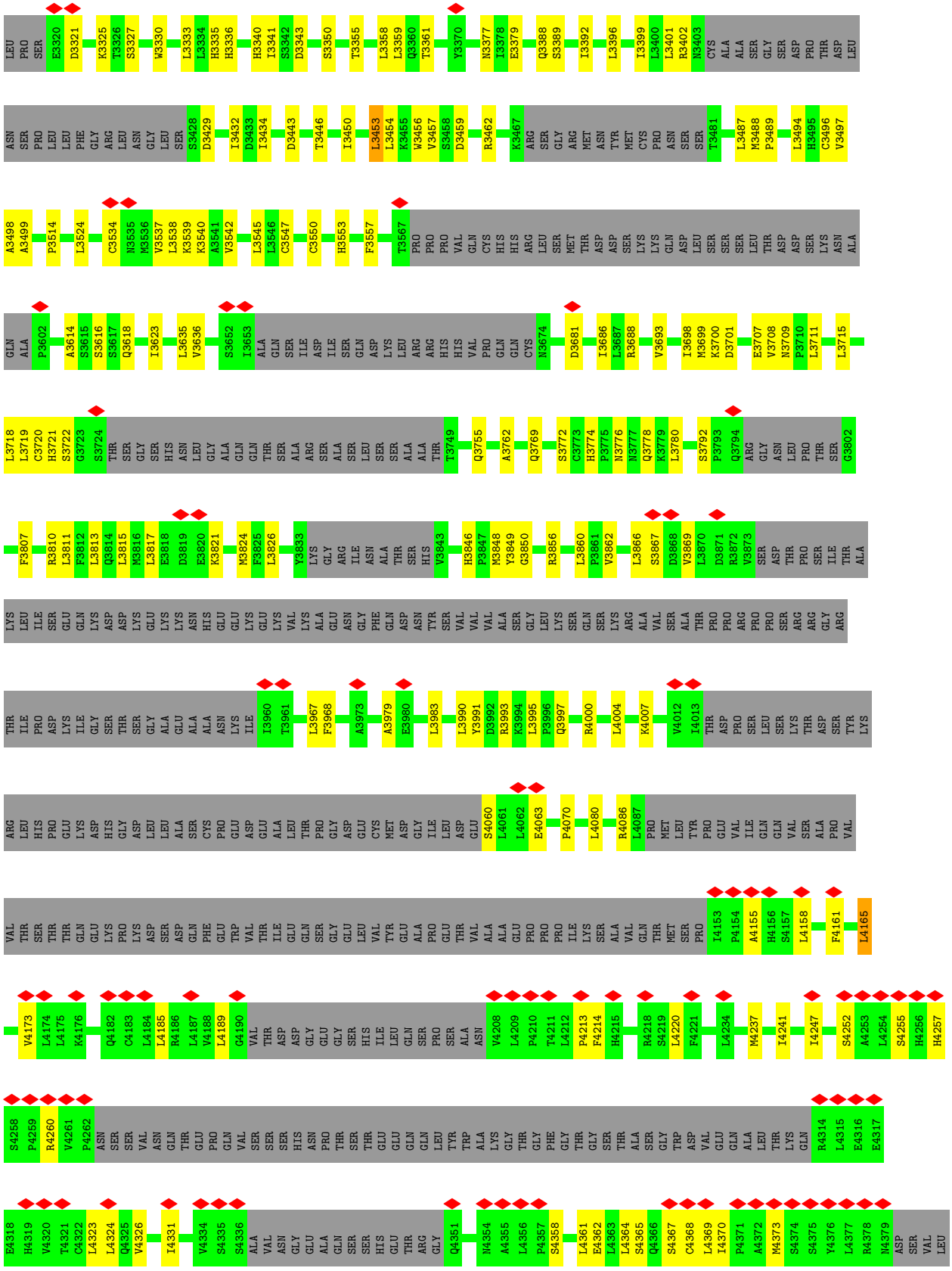


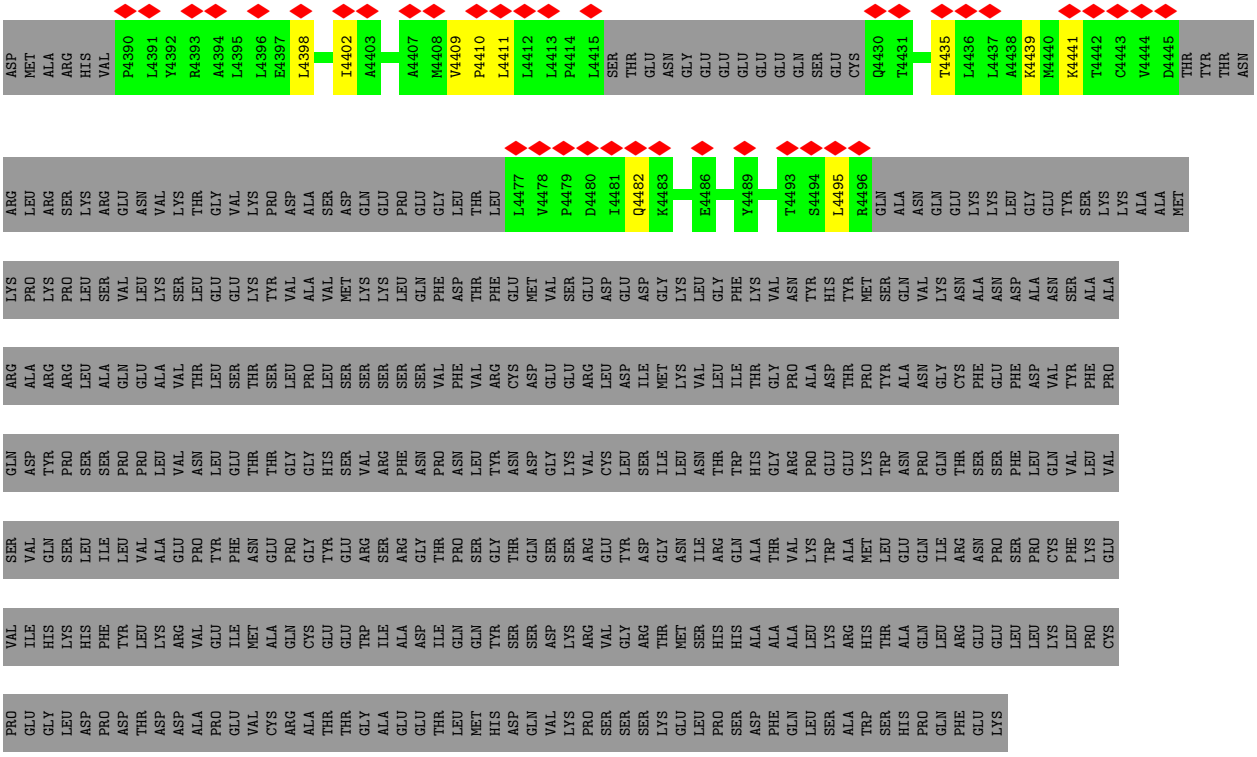






ALA GLN HIS T1074 R1075 K1078 N1084 H1089 V1090 F1091 E1092 L1093 V1101 D1105 F1106 K1107 F1108 V1109 L1110 I1114 T1115 N1116 I1120 Q1121 V1122 T1123 L1124 N1127 P1130 G1131 L1132 GLY LYS VAL ASN ALA LEU ASN ILE GLU VAL GLU GLN ASN GLY LYS PRO SER LEU VAL ASP
LEU ASN GLU GLU MET GLN HIS MET ASP VAL GLU GLU SER GLN CYS L1168 R1169 P1172 E1175 I1181 L1182 C1183 L1188 A1189 S1190 L1194 S1195 G1196 H1197 A1198 G1199 T1204 S1205 P1206 S1219 I1222 H1223 V1224 K1225 E1229 ARG GLY THR GLU GLU ILE CYS ASN GLY GLY MET
ARG PRO VAL VAL ARG LEU PRO SER LEU LYS HIS GLN SER ASN LYS GLY TYR SER LEU ALA SER LEU LEU ALA LYS VAL ALA ALA GLY LYS GLU LYS SER SER ASN VAL LYS ASN GLU ASN THR SER GLY THR ARG LYS S1287 E1288 N1289 L1290 D1294 L1295 I1303 R1304 R1305 T1309 S1310
I1311 S1312 K1313 L1322 H1328 L1331 T1334 L1335 C1336 R1337 K1338 T1339 D1340 D1341 G1342 Q1343 I1344 H1347 A1348 Q1349 S1350 L1351 V1352 L1353 W1358 L1359 V1362 P1367 E1372 G1373 N1374 L1377 L1378 T1381 R1382 L1385 C1392 F1393 F1394 E1395 A1396 H1402 A1405 R1406
A1409 L1410 C1411 I1412 P1419 C1420 F1424 G1425 P1426 V1427 L1428 L1429 L1432 L1439 P1440 A1441 T1444 S1447 Y1451 L1454 L1455 N1456 Y1457 V1458 K1459 D1460 E1461 S1467 T1475 R1479 Q1480 L1481 Q1482 D1483 ARG LEU T1486 E1489 Q1493 T1494 L1498 Y1499 F1503 D1504 P1505
L1510 E1511 M1512 S1515 SER CYS LYS ASN VAL TYR ASN SER SER ILE GLY VAL GLN SER ASP E1531 V1537 L1538 SER GLY ASN GLY LYS VAL SER SER CYS THR ALA ALA E1551 G1552 S1556 L1557 L1560 L1561 L1566 H1567 F1568 T1573 S1574 D1575 R1581 D1582 D1583 ALA MET SER
SER PHE GLY VAL THR PRO GLY VAL GLY GLY LEU SER SER GLY THR VAL GLY GLU ALA SER THR ALA LEU SER SER ALA ALA GLN VAL VAL ALA LEU GLN GLN SER LEU SER HIS ALA MET ALA SER ALA GLU GLN GLN GLN LEU GLN VAL LEU GLN GLU LYS GLN GLN GLN LEU LEU LYS LEU GLN GLN
GLN LYS ALA LYS LEU GLU ALA LYS LEU HIS GLN THR THR ALA ALA ALA ALA ALA ALA ALA SER ALA VAL GLY PRO VAL HIS ASN SER VAL PRO SER ASN PRO VAL ALA ALA PRO GLY PHE PHE ILE HIS PRO SER ASP VAL ILE PRO PRO THR PRO LYS THR THR PRO LEU PHE MET THR
PRO PRO LEU THR PRO PRO ASN GLU ALA VAL SER VAL VAL ILE ASN ALA GLU LEU GLN LEU PHE PRO GLY SER VAL ILE ASP PRO PRO ALA VAL ASN LEU ALA ALA HIS ASN LYS ASN SER ASN LYS SER ARG MET ASN PRO LEU GLY SER G1758 L1759 A1760 L1761 A1762 I1763 S1764 H1765
H1768 F1769 L1770 Q1771 P1772 P1773 P1774 H1775 Q1776 I1779 I1780 E1781 R1782 M1783 H1784 S1785 R1788 R1789 F1790 L1793 P1798 I1799 L1800 L1801 I1806 G1810 D1811 L1812 A1813 S1814 L1815 S1816 I1817 D1818 I1819 E1824 E1825 V1826 D1827 G1828 R1829 R1830 L1831 V1832 V1833 A1834 T1835 D1836 I1837 S1838 T1839 L1842
I1843 L1844 P1849 P1850 P1851 R1854 F1855 M1856 K1857 I1861 G1862 R1863 Y1864 G1865 S1866 T1867 N1868 A1869 R1870 A1871 K1872 L1875 Y1879 Y1883 L1891 K1892 LEU MET HIS ASP PRO LEU LYS GLY GLU GLY GLU SER ALA N1906 Q1907 P1908 L1914 M1917 D1923 R1927 Y1928 N1929 L1930
L1935 E1936 S1941 I1942 D1943 L1944 P1945 P1946 S1949 A1950 N1951 N1952 A1953 Q1954 Y1955 F1956 L1957 ARG LYS PRO ASP LYS ALA V1964 E1965 E1966 R1969 V1970 F1971 S1972 A1973 Y1974 Q1975 I1978 Q1979 L1980 Q1981 L1982 Q1983 L1986 N1989 L1994 L2005 S2006 E2007 T2008 S2009 N2010 L2014 I2015
Y2029 T2033 L2038 H2039 A2040 S2041 H2044 L2050 E2061 L2062 F2063 K2064 H2065 L2066 C2067 I2068 R2075 T2078 G2079 L2080 V2083 Q2084 L2085 Q2094 N2098 Q2101 E2102 L2103 Y2104 N2105 S2106 E2107 L2110 I2111 Q2114 D2115 R2116 V2117 F2118 M2119 L2120 L2121 S2122 Q2126 R2127
L2135 L2138 L2139 L2142 D2143 L2146 Q2150 PRO GLN LEU PRO MET HIS ARG ARG THR GLU GLY V2162 M2167 V2171 V2172 M2173 L2174 V2175 S2176 R2177 L2178 D2187 E2188 A2189 ALA ALA LYS LYS PRO LEU ASN GLY N2199 Q2200 W2201 S2202 F2203 I2204 N2205 N2206 ASN LEU HIS THR

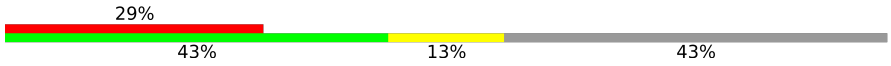


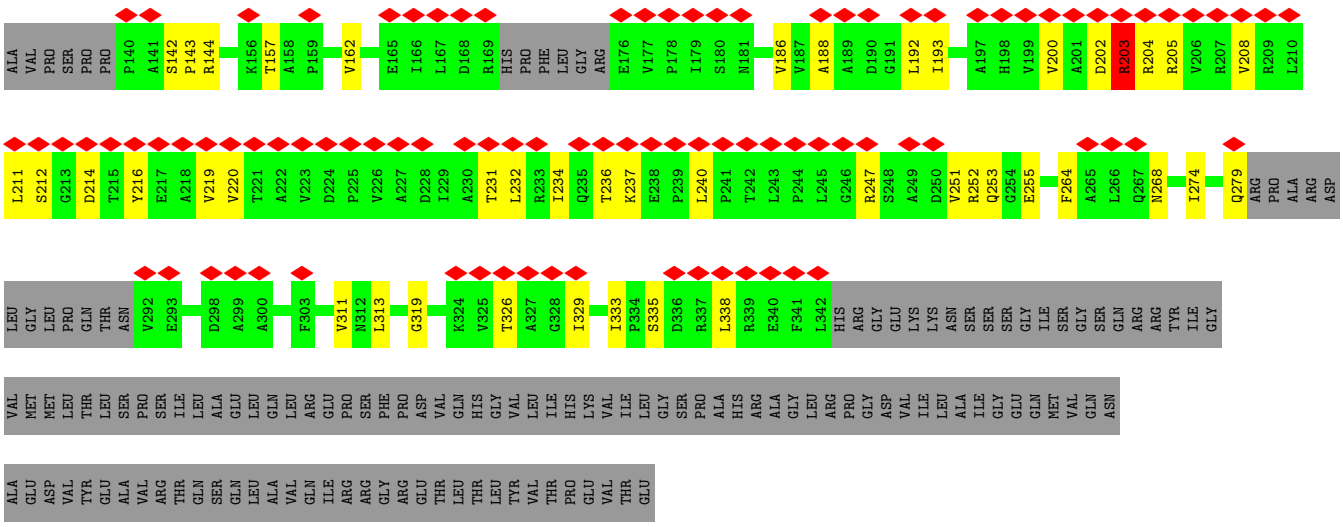




• Molecule 2: Serine protease HTRA2, mitochondrial

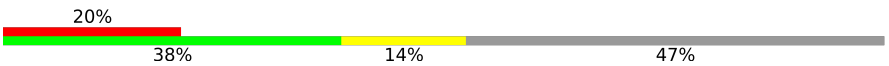
Chain D:

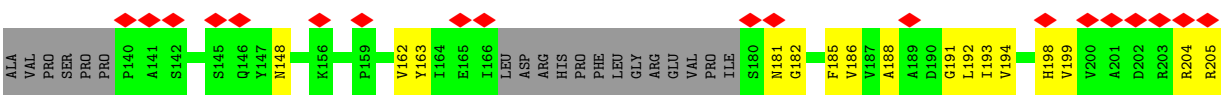


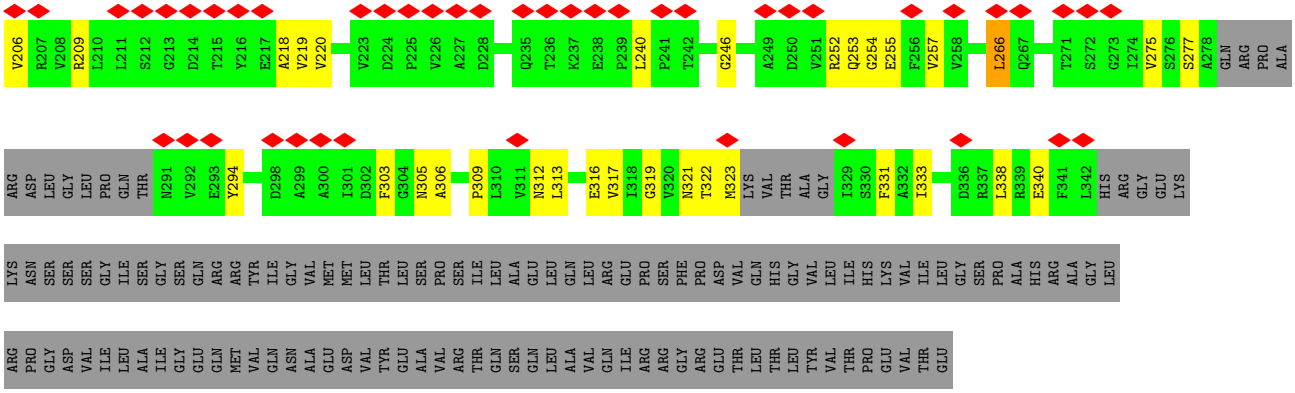



• Molecule 2: Serine protease HTRA2, mitochondrial

Chain E:

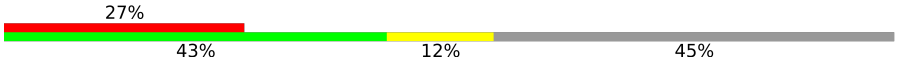


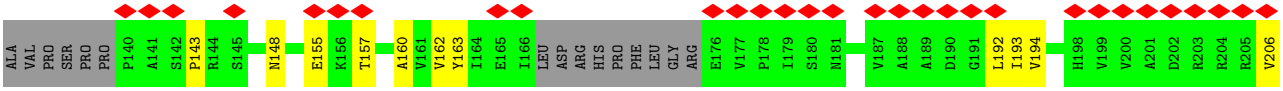



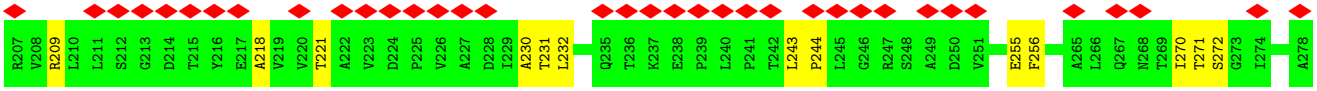



• Molecule 2: Serine protease HTRA2, mitochondrial

Chain C:




# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 15780 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 60 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | Not provided | |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 0.013 | Depositor |
| Minimum map value | -0.003 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.00423 | Depositor |
| Map size (Å) | 425.87997, 425.87997, 425.87997 | wwPDB |
| Map dimensions | 364, 364, 364 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.17, 1.17, 1.17 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.31 | 1/22313 (0.0%) | 0.68 | 33/30313 (0.1%) |
| 1 | B | 0.30 | 0/22313 | 0.67 | 28/30313 (0.1%) |
| 2 | C | 0.36 | 0/1351 | 0.69 | 2/1840 (0.1%) |
| 2 | D | 0.34 | 0/1402 | 0.73 | 1/1911 (0.1%) |
| 2 | E | 0.37 | 0/1309 | 0.70 | 1/1783 (0.1%) |
| All | All | 0.31 | 1/48688 (0.0%) | 0.68 | 65/66160 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | E | 0 | 1 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 2355 | CYS | CB-SG | -5.39 | 1.73 | 1.81 |

All (65) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 3111 | MET | CA-CB-CG | 10.72 | 131.52 | 113.30 |
| 1 | A | 2411 | MET | CB-CG-SD | -8.15 | 87.96 | 112.40 |
| 1 | A | 4399 | LEU | CB-CG-CD2 | -8.03 | 97.35 | 111.00 |
| 1 | A | 2411 | MET | CA-CB-CG | 7.85 | 126.65 | 113.30 |
| 1 | A | 283 | MET | CA-CB-CG | 7.40 | 125.89 | 113.30 |
| 1 | B | 1512 | MET | CA-CB-CG | 7.11 | 125.38 | 113.30 |
| 1 | B | 2732 | MET | CG-SD-CE | 7.02 | 111.43 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 1994 | LEU | CA-CB-CG | -6.74 | 99.80 | 115.30 |
| 1 | B | 3253 | LEU | CA-CB-CG | 6.73 | 130.79 | 115.30 |
| 2 | D | 203 | ARG | CA-CB-CG | 6.47 | 127.64 | 113.40 |
| 1 | A | 3287 | ASP | CB-CG-OD1 | 6.46 | 124.12 | 118.30 |
| 1 | A | 2815 | LEU | CA-CB-CG | 6.27 | 129.71 | 115.30 |
| 1 | A | 1492 | LEU | CA-CB-CG | 6.20 | 129.56 | 115.30 |
| 1 | B | 2387 | LEU | CB-CG-CD2 | 6.19 | 121.52 | 111.00 |
| 1 | A | 1212 | MET | CA-CB-CG | 6.15 | 123.75 | 113.30 |
| 1 | A | 3813 | LEU | CB-CG-CD2 | -6.12 | 100.61 | 111.00 |
| 1 | B | 2813 | LEU | CA-CB-CG | 6.11 | 129.35 | 115.30 |
| 1 | A | 3719 | LEU | CB-CG-CD2 | 6.05 | 121.29 | 111.00 |
| 1 | A | 1982 | LEU | CA-CB-CG | 5.98 | 129.06 | 115.30 |
| 1 | A | 2411 | MET | CG-SD-CE | 5.95 | 109.72 | 100.20 |
| 2 | C | 155 | GLU | CA-CB-CG | 5.92 | 126.42 | 113.40 |
| 1 | A | 830 | MET | CB-CG-SD | -5.85 | 94.86 | 112.40 |
| 1 | A | 2567 | LEU | CA-CB-CG | 5.84 | 128.73 | 115.30 |
| 1 | A | 3251 | LEU | CA-CB-CG | 5.83 | 128.72 | 115.30 |
| 1 | A | 3253 | LEU | CA-CB-CG | 5.79 | 128.61 | 115.30 |
| 1 | A | 2386 | LEU | CA-CB-CG | 5.74 | 128.50 | 115.30 |
| 1 | A | 2633 | LEU | CA-CB-CG | 5.70 | 128.41 | 115.30 |
| 1 | A | 2571 | LEU | CA-CB-CG | 5.67 | 128.35 | 115.30 |
| 1 | A | 3453 | LEU | CA-CB-CG | 5.62 | 128.22 | 115.30 |
| 1 | A | 3682 | LEU | CA-CB-CG | 5.62 | 128.22 | 115.30 |
| 1 | B | 2411 | MET | CG-SD-CE | -5.61 | 91.22 | 100.20 |
| 1 | B | 2589 | LEU | CA-CB-CG | 5.58 | 128.13 | 115.30 |
| 1 | A | 2387 | LEU | CB-CG-CD2 | 5.58 | 120.48 | 111.00 |
| 1 | A | 4184 | LEU | CA-CB-CG | 5.57 | 128.12 | 115.30 |
| 1 | B | 4165 | LEU | CA-CB-CG | 5.57 | 128.12 | 115.30 |
| 1 | B | 198 | ASP | CB-CG-OD1 | 5.55 | 123.29 | 118.30 |
| 1 | A | 2174 | LEU | CA-CB-CG | 5.53 | 128.01 | 115.30 |
| 1 | A | 198 | ASP | CB-CG-OD1 | 5.51 | 123.26 | 118.30 |
| 1 | A | 2667 | LEU | CB-CG-CD1 | -5.43 | 101.77 | 111.00 |
| 1 | B | 2633 | LEU | CA-CB-CG | 5.41 | 127.75 | 115.30 |
| 2 | C | 155 | GLU | N-CA-CB | 5.38 | 120.29 | 110.60 |
| 1 | B | 1979 | GLN | CA-CB-CG | 5.36 | 125.19 | 113.40 |
| 1 | B | 1875 | LEU | CA-CB-CG | 5.34 | 127.58 | 115.30 |
| 1 | B | 3487 | LEU | CA-CB-CG | 5.30 | 127.49 | 115.30 |
| 1 | B | 2174 | LEU | CA-CB-CG | 5.29 | 127.47 | 115.30 |
| 1 | B | 2397 | ILE | CG1-CB-CG2 | -5.23 | 99.89 | 111.40 |
| 1 | A | 3610 | LEU | CA-CB-CG | 5.20 | 127.25 | 115.30 |
| 1 | B | 3034 | ASP | CB-CG-OD1 | 5.18 | 122.97 | 118.30 |
| 1 | A | 3719 | LEU | CA-CB-CG | 5.18 | 127.21 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 3191 | ARG | CB-CG-CD | 5.17 | 125.05 | 111.60 |
| 1 | A | 3232 | LEU | CA-CB-CG | 5.17 | 127.19 | 115.30 |
| 1 | B | 2812 | LEU | CA-CB-CG | 5.15 | 127.15 | 115.30 |
| 1 | B | 3488 | MET | CA-CB-CG | 5.14 | 122.05 | 113.30 |
| 1 | B | 2581 | LEU | CA-CB-CG | 5.12 | 127.07 | 115.30 |
| 1 | B | 3453 | LEU | CA-CB-CG | 5.11 | 127.06 | 115.30 |
| 1 | B | 3232 | LEU | CA-CB-CG | 5.10 | 127.03 | 115.30 |
| 2 | E | 266 | LEU | CB-CG-CD2 | 5.09 | 119.66 | 111.00 |
| 1 | A | 3334 | LEU | CA-CB-CG | 5.09 | 127.00 | 115.30 |
| 1 | A | 1474 | LEU | CA-CB-CG | 5.08 | 126.98 | 115.30 |
| 1 | A | 2385 | LEU | CA-CB-CG | 5.08 | 126.97 | 115.30 |
| 1 | B | 1377 | LEU | CA-CB-CG | 5.06 | 126.94 | 115.30 |
| 1 | B | 2342 | MET | CG-SD-CE | 5.05 | 108.28 | 100.20 |
| 1 | B | 2719 | TRP | CA-CB-CG | 5.04 | 123.27 | 113.70 |
| 1 | B | 2146 | LEU | CA-CB-CG | 5.02 | 126.84 | 115.30 |
| 1 | A | 2355 | CYS | CA-CB-SG | 5.01 | 123.02 | 114.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 2 | E | 340 | GLU | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 21902 | 0 | 22313 | 462 | 0 |
| 1 | B | 21902 | 0 | 22313 | 501 | 0 |
| 2 | C | 1332 | 0 | 1346 | 26 | 0 |
| 2 | D | 1382 | 0 | 1399 | 30 | 0 |
| 2 | E | 1291 | 0 | 1298 | 35 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| All | All | 47811 | 0 | 48669 | 1007 | 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 10.

All (1007) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2359:ALA:HB2 | 1:B:2411:MET:HG3 | 1.66 | 0.77 |
| 1:A:3810:ARG:HA | 1:A:3813:LEU:HD12 | 1.66 | 0.77 |
| 1:B:2075:ARG:HG2 | 1:B:2120:LEU:HD22 | 1.68 | 0.76 |
| 1:B:1556:SER:HB2 | 1:B:1843:ILE:HG21 | 1.67 | 0.75 |
| 1:A:2397:ILE:HD12 | 1:B:3325:LYS:HB2 | 1.69 | 0.75 |
| 1:B:1124:LEU:HB3 | 1:B:1183:CYS:HB3 | 1.67 | 0.74 |
| 1:A:2717:ARG:HH21 | 1:B:3253:LEU:HD13 | 1.53 | 0.73 |
| 1:A:1091:PHE:HB2 | 1:A:1222:ILE:HB | 1.72 | 0.72 |
| 1:B:1378:LEU:HB3 | 1:B:1382:ARG:HH21 | 1.53 | 0.72 |
| 1:B:1923:ASP:OD1 | 1:B:1927:ARG:NH1 | 2.23 | 0.72 |
| 1:B:1806:ILE:HB | 1:B:1842:LEU:HB3 | 1.71 | 0.72 |
| 1:A:98:SER:OG | 1:A:212:LYS:NZ | 2.23 | 0.72 |
| 1:A:1806:ILE:HB | 1:A:1842:LEU:HB3 | 1.72 | 0.71 |
| 1:B:2389:GLY:HA2 | 1:B:2655:VAL:HA | 1.72 | 0.71 |
| 1:A:3224:HIS:HB2 | 1:A:3297:LYS:HG2 | 1.72 | 0.71 |
| 2:C:218:ALA:HB1 | 2:C:232:LEU:HD21 | 1.71 | 0.71 |
| 1:A:2122:SER:O | 1:A:2177:ARG:NH2 | 2.24 | 0.71 |
| 1:B:4370:ILE:HA | 1:B:4373:MET:HE3 | 1.70 | 0.71 |
| 1:B:1557:LEU:HD12 | 1:B:1560:LEU:HD21 | 1.72 | 0.71 |
| 1:B:3709:ASN:HD21 | 1:B:3780:LEU:HD21 | 1.56 | 0.70 |
| 1:B:2692:PRO:HB3 | 1:B:2728:LEU:HD23 | 1.73 | 0.70 |
| 1:A:3817:LEU:HD21 | 1:A:4185:LEU:HD22 | 1.74 | 0.70 |
| 1:A:3709:ASN:HD21 | 1:A:3780:LEU:HD21 | 1.56 | 0.69 |
| 1:A:1439:LEU:HB3 | 1:A:2026:ILE:HD11 | 1.73 | 0.69 |
| 1:B:1782:ARG:O | 1:B:1789:ARG:NH2 | 2.25 | 0.69 |
| 1:A:2099:VAL:O | 1:A:2103:LEU:HB2 | 1.92 | 0.69 |
| 1:A:3325:LYS:HB2 | 1:B:2397:ILE:HD12 | 1.74 | 0.69 |
| 2:E:148:ASN:ND2 | 2:C:255:GLU:OE1 | 2.26 | 0.69 |
| 1:A:4072:GLN:HE21 | 1:A:4178:ARG:HD2 | 1.58 | 0.69 |
| 1:B:2716:LEU:HA | 1:B:2719:TRP:HD1 | 1.58 | 0.69 |
| 1:A:2396:ASP:HA | 1:B:3271:LYS:HE2 | 1.74 | 0.69 |
| 1:A:1853:CYS:SG | 1:A:1854:ARG:N | 2.66 | 0.68 |
| 1:A:1378:LEU:HB3 | 1:A:1382:ARG:HH21 | 1.58 | 0.68 |
| 2:E:253:GLN:HE21 | 2:E:277:SER:HA | 1.58 | 0.68 |
| 1:B:2878:MET:SD | 1:B:2880:ARG:NH1 | 2.66 | 0.68 |
| 1:B:2171:VAL:HA | 1:B:2174:LEU:HD12 | 1.73 | 0.68 |
| 1:A:3700:LYS:NZ | 1:A:3769:GLN:O | 2.28 | 0.67 |
| 1:B:1818:ASP:OD1 | 1:B:1830:ARG:NH1 | 2.27 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:568:LEU:HD11 | 1:B:630:LEU:HB3 | 1.76 | 0.67 |
| 1:A:1101:VAL:HG22 | 1:A:1212:MET:HG2 | 1.76 | 0.67 |
| 1:B:4260:ARG:NH2 | 1:B:4364:LEU:O | 2.26 | 0.67 |
| 1:B:3184:GLN:HB2 | 1:B:3187:PRO:HG3 | 1.77 | 0.67 |
| 1:B:3220:LEU:HD12 | 1:B:3223:ILE:HD11 | 1.76 | 0.67 |
| 1:B:1385:LEU:HD21 | 1:B:1428:LEU:HD23 | 1.77 | 0.66 |
| 1:A:4072:GLN:HB3 | 1:A:4175:LEU:HD22 | 1.77 | 0.66 |
| 2:E:188:ALA:HB3 | 2:E:192:LEU:HB3 | 1.75 | 0.66 |
| 1:A:1098:ALA:HB2 | 1:A:1218:ARG:HE | 1.60 | 0.66 |
| 1:A:1406:ARG:HH21 | 1:A:1848:ILE:HB | 1.60 | 0.66 |
| 1:B:98:SER:OG | 1:B:212:LYS:NZ | 2.28 | 0.66 |
| 1:B:157:GLN:HB3 | 1:B:226:HIS:HB3 | 1.75 | 0.66 |
| 1:B:3700:LYS:NZ | 1:B:3769:GLN:O | 2.28 | 0.66 |
| 1:B:2387:LEU:O | 1:B:2393:ASN:ND2 | 2.29 | 0.66 |
| 1:B:2820:SER:HB3 | 1:B:2826:PHE:HD2 | 1.61 | 0.65 |
| 1:A:1505:PRO:O | 1:A:1985:ASN:ND2 | 2.29 | 0.65 |
| 1:A:3534:CYS:HA | 1:A:3539:LYS:HD2 | 1.78 | 0.65 |
| 1:B:1093:LEU:HD23 | 1:B:1303:ILE:HD11 | 1.77 | 0.65 |
| 1:A:3494:LEU:HD12 | 1:A:3545:LEU:HD11 | 1.78 | 0.65 |
| 1:A:2346:CYS:HB3 | 1:A:2350:LEU:HD11 | 1.78 | 0.65 |
| 1:B:211:HIS:NE2 | 1:B:1044:PRO:O | 2.29 | 0.65 |
| 1:A:1474:LEU:HD21 | 1:A:2034:LEU:HD11 | 1.78 | 0.65 |
| 1:B:3810:ARG:HA | 1:B:3813:LEU:HD12 | 1.78 | 0.65 |
| 1:A:2101:GLN:NE2 | 1:A:2102:GLU:OE1 | 2.30 | 0.65 |
| 1:B:1091:PHE:HB2 | 1:B:1222:ILE:HB | 1.78 | 0.65 |
| 1:B:2335:LEU:HD11 | 1:B:2354:VAL:HB | 1.78 | 0.65 |
| 1:A:2772:HIS:ND1 | 1:B:2873:CYS:O | 2.30 | 0.65 |
| 1:A:1124:LEU:HB3 | 1:A:1183:CYS:HB3 | 1.77 | 0.65 |
| 1:A:60:ASP:HB3 | 1:A:1132:LEU:HD12 | 1.77 | 0.64 |
| 1:A:3826:LEU:HD23 | 1:A:3832:LEU:HD13 | 1.78 | 0.64 |
| 2:D:251:VAL:O | 2:D:279:GLN:NE2 | 2.29 | 0.64 |
| 1:A:1305:ARG:HH22 | 1:A:1308:LYS:HE3 | 1.62 | 0.64 |
| 1:A:2376:ASN:OD1 | 1:A:2379:GLN:NE2 | 2.31 | 0.64 |
| 1:B:3462:ARG:HG3 | 1:B:3524:LEU:HD21 | 1.79 | 0.64 |
| 1:B:4161:PHE:HE1 | 1:B:4213:PRO:HG3 | 1.63 | 0.64 |
| 1:A:568:LEU:HD11 | 1:A:630:LEU:HB3 | 1.79 | 0.64 |
| 1:A:2667:LEU:O | 1:A:2670:ASN:ND2 | 2.31 | 0.64 |
| 1:A:3547:CYS:SG | 1:A:3846:HIS:NE2 | 2.69 | 0.64 |
| 1:A:1771:GLN:OE1 | 1:A:1983:GLN:NE2 | 2.31 | 0.64 |
| 1:A:1494:THR:HG21 | 1:A:2111:ILE:HG22 | 1.78 | 0.64 |
| 1:A:2084:GLN:NE2 | 1:A:2600:ASN:O | 2.31 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1444:THR:HG22 | 1:A:1447:SER:H | 1.61 | 0.64 |
| 1:B:343:GLU:HG2 | 1:B:346:SER:H | 1.63 | 0.64 |
| 2:D:157:THR:HG21 | 2:D:311:VAL:HG11 | 1.79 | 0.64 |
| 1:B:1101:VAL:HA | 1:B:1305:ARG:HE | 1.63 | 0.63 |
| 1:A:3236:PRO:HG3 | 1:A:3282:LEU:HD23 | 1.81 | 0.63 |
| 1:B:254:SER:HB2 | 1:B:370:VAL:HG11 | 1.80 | 0.63 |
| 1:A:3396:LEU:HA | 1:A:3399:ILE:HG12 | 1.81 | 0.63 |
| 1:B:285:SER:HA | 1:B:366:VAL:HB | 1.79 | 0.63 |
| 1:B:1813:ALA:HB2 | 1:B:1863:ARG:HA | 1.80 | 0.63 |
| 1:B:2787:GLN:NE2 | 1:B:2791:GLU:OE2 | 2.31 | 0.63 |
| 1:A:3209:ASP:HB3 | 1:A:3281:ARG:HE | 1.64 | 0.63 |
| 1:A:3989:LEU:HB3 | 1:A:3993:ARG:HH21 | 1.61 | 0.63 |
| 1:B:3225:ILE:HB | 1:B:3265:ILE:HB | 1.81 | 0.62 |
| 1:A:4260:ARG:NH2 | 1:A:4364:LEU:O | 2.32 | 0.62 |
| 2:E:162:VAL:HG21 | 2:E:193:ILE:HD13 | 1.80 | 0.62 |
| 1:A:157:GLN:HB3 | 1:A:226:HIS:HB3 | 1.80 | 0.62 |
| 1:A:178:LEU:HD21 | 1:A:197:LYS:HZ1 | 1.64 | 0.62 |
| 1:A:3867:SER:HB3 | 1:A:3979:ALA:HB1 | 1.81 | 0.62 |
| 1:B:1015:GLN:HG3 | 1:B:1021:ILE:HD13 | 1.81 | 0.62 |
| 1:A:2665:LEU:O | 1:A:2669:LEU:HB2 | 1.99 | 0.62 |
| 1:B:1494:THR:HG21 | 1:B:2111:ILE:HG22 | 1.82 | 0.62 |
| 1:A:1486:THR:OG1 | 1:A:1489:GLU:OE1 | 2.16 | 0.62 |
| 1:B:2342:MET:HG3 | 1:B:2351:LEU:HD21 | 1.82 | 0.62 |
| 1:B:3191:ARG:HD3 | 2:E:266:LEU:HD22 | 1.82 | 0.62 |
| 1:A:827:LEU:HB3 | 1:A:845:LYS:HB3 | 1.81 | 0.62 |
| 1:B:1829:ARG:HH21 | 1:B:1851:PRO:HB2 | 1.64 | 0.62 |
| 1:A:1575:ASP:OD2 | 1:A:1782:ARG:NH2 | 2.33 | 0.62 |
| 1:A:3233:ALA:HB2 | 1:B:3232:LEU:HD21 | 1.80 | 0.62 |
| 1:B:3198:SER:HA | 1:B:3291:LEU:O | 1.99 | 0.62 |
| 1:A:2389:GLY:HA2 | 1:A:2655:VAL:HA | 1.81 | 0.62 |
| 1:A:1206:PRO:HB3 | 1:A:1322:LEU:HD22 | 1.81 | 0.61 |
| 1:B:1561:LEU:HB3 | 1:B:1989:ASN:HD22 | 1.64 | 0.61 |
| 1:B:854:ASP:HA | 1:B:907:THR:HB | 1.82 | 0.61 |
| 1:B:3494:LEU:HD12 | 1:B:3545:LEU:HD11 | 1.82 | 0.61 |
| 1:B:3681:ASP:OD1 | 1:B:3755:GLN:NE2 | 2.33 | 0.61 |
| 1:A:3488:MET:HE3 | 1:B:2107:GLU:HG2 | 1.82 | 0.61 |
| 1:A:2752:LEU:HG | 1:A:2758:LEU:HD22 | 1.83 | 0.61 |
| 1:A:3262:LEU:HD11 | 1:B:3286:ARG:HH21 | 1.65 | 0.61 |
| 1:B:3127:SER:HA | 1:B:3130:MET:HE1 | 1.82 | 0.61 |
| 1:A:3701:ASP:OD1 | 1:A:3774:HIS:NE2 | 2.29 | 0.61 |
| 1:A:75:TYR:HB2 | 1:A:944:ILE:HD12 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1816:SER:HB2 | 1:B:1830:ARG:NH2 | 2.16 | 0.61 |
| 1:A:1510:LEU:HB3 | 1:A:1560:LEU:HB2 | 1.81 | 0.60 |
| 1:B:1456:ASN:HA | 1:B:1459:LYS:HD3 | 1.82 | 0.60 |
| 2:D:200:VAL:HG11 | 2:D:232:LEU:HD11 | 1.82 | 0.60 |
| 1:B:2352:LEU:HD21 | 1:B:2403:TRP:HB3 | 1.83 | 0.60 |
| 1:A:3111:MET:HE3 | 1:A:3334:LEU:HD11 | 1.82 | 0.60 |
| 1:A:3792:SER:O | 1:A:4086:ARG:NH2 | 2.35 | 0.60 |
| 1:A:2781:VAL:HG13 | 1:A:2832:PRO:HB3 | 1.84 | 0.60 |
| 1:A:3179:ALA:HB1 | 1:A:3182:LEU:HD12 | 1.83 | 0.60 |
| 1:B:3688:ARG:HH22 | 1:B:3762:ALA:HA | 1.67 | 0.60 |
| 1:A:177:CYS:HA | 1:A:181:VAL:HB | 1.84 | 0.60 |
| 1:B:55:TRP:HB3 | 1:B:924:ALA:HB2 | 1.84 | 0.60 |
| 1:B:3396:LEU:HA | 1:B:3399:ILE:HG12 | 1.83 | 0.60 |
| 1:A:343:GLU:HG2 | 1:A:346:SER:H | 1.65 | 0.60 |
| 2:E:319:GLY:HA2 | 2:E:333:ILE:O | 2.01 | 0.60 |
| 1:A:3433:ASP:O | 1:A:3437:GLN:NE2 | 2.35 | 0.60 |
| 1:B:1811:ASP:O | 1:B:1863:ARG:NH1 | 2.35 | 0.60 |
| 1:A:3489:PRO:HB2 | 1:A:3494:LEU:HD21 | 1.84 | 0.59 |
| 1:A:1493:GLN:HG2 | 1:A:1499:TYR:HA | 1.85 | 0.59 |
| 1:A:1782:ARG:O | 1:A:1789:ARG:NH2 | 2.35 | 0.59 |
| 1:A:3252:PRO:O | 1:B:2717:ARG:NE | 2.27 | 0.59 |
| 2:D:204:ARG:HD3 | 2:D:219:VAL:HG13 | 1.84 | 0.59 |
| 1:A:2813:LEU:HD12 | 1:A:2851:VAL:HG11 | 1.82 | 0.59 |
| 1:A:1813:ALA:HB2 | 1:A:1863:ARG:HA | 1.85 | 0.59 |
| 1:A:2200:GLN:NE2 | 1:A:2413:GLN:OE1 | 2.36 | 0.59 |
| 1:A:3243:VAL:HG13 | 1:A:3253:LEU:HD21 | 1.85 | 0.59 |
| 1:B:1328:HIS:HA | 1:B:1331:LEU:HD12 | 1.85 | 0.59 |
| 1:B:3867:SER:HB3 | 1:B:3979:ALA:HB1 | 1.84 | 0.59 |
| 2:D:162:VAL:HG21 | 2:D:193:ILE:HD13 | 1.84 | 0.59 |
| 1:A:3220:LEU:HD21 | 1:A:3223:ILE:HD11 | 1.85 | 0.58 |
| 1:B:411:ILE:HD12 | 1:B:422:LEU:HD12 | 1.85 | 0.58 |
| 1:A:3224:HIS:HE1 | 1:A:3266:LYS:HE3 | 1.68 | 0.58 |
| 1:A:3271:LYS:HE2 | 1:B:2396:ASP:HA | 1.83 | 0.58 |
| 1:B:75:TYR:HB2 | 1:B:944:ILE:HD12 | 1.84 | 0.58 |
| 1:B:3402:ARG:NH2 | 1:B:3459:ASP:OD2 | 2.36 | 0.58 |
| 1:B:2412:LEU:HB3 | 1:B:2667:LEU:HD11 | 1.84 | 0.58 |
| 1:A:2139:LEU:HD13 | 1:A:2142:LEU:HD12 | 1.85 | 0.58 |
| 1:A:3815:LEU:HG | 1:A:3816:MET:HE3 | 1.86 | 0.58 |
| 1:B:1475:THR:HB | 1:B:1479:ARG:HH21 | 1.68 | 0.58 |
| 1:B:1568:PHE:HB3 | 1:B:1793:LEU:HD11 | 1.85 | 0.58 |
| 1:B:2323:LEU:HB3 | 1:B:2327:ARG:HH12 | 1.68 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1830:ARG:NH2 | 1:B:1832:VAL:O | 2.36 | 0.58 |
| 2:E:303:PHE:HA | 2:E:306:ALA:HB2 | 1.85 | 0.58 |
| 1:A:1026:VAL:HG21 | 1:A:1351:LEU:HD22 | 1.85 | 0.58 |
| 1:B:2813:LEU:HD11 | 1:B:2856:ILE:HG22 | 1.85 | 0.58 |
| 1:B:2813:LEU:HA | 1:B:2816:ILE:HG12 | 1.85 | 0.58 |
| 1:A:3184:GLN:HB2 | 1:A:3187:PRO:HG3 | 1.86 | 0.58 |
| 1:B:395:SER:HG | 1:B:514:GLN:H | 1.49 | 0.58 |
| 1:B:1504:ASP:O | 1:B:1981:GLN:NE2 | 2.37 | 0.57 |
| 1:B:3220:LEU:HD23 | 1:B:3275:ALA:HB3 | 1.85 | 0.57 |
| 1:A:1561:LEU:HB3 | 1:A:1989:ASN:HD22 | 1.69 | 0.57 |
| 1:A:945:TYR:OH | 1:A:950:ASP:OD1 | 2.22 | 0.57 |
| 1:A:1504:ASP:O | 1:A:1981:GLN:NE2 | 2.35 | 0.57 |
| 1:A:2375:VAL:HG21 | 1:A:2380:LEU:HD13 | 1.85 | 0.57 |
| 1:A:2838:LYS:HA | 1:A:2841:GLU:HG2 | 1.87 | 0.57 |
| 2:C:192:LEU:HD11 | 2:C:231:THR:HB | 1.87 | 0.57 |
| 1:A:3402:ARG:NH2 | 1:A:3459:ASP:OD2 | 2.37 | 0.57 |
| 1:B:2381:GLU:OE2 | 1:B:2645:LYS:NZ | 2.37 | 0.57 |
| 1:A:3236:PRO:O | 1:A:3259:THR:OG1 | 2.20 | 0.57 |
| 1:A:1037:ARG:HH22 | 1:A:1075:ARG:HB3 | 1.69 | 0.57 |
| 2:D:319:GLY:HA2 | 2:D:333:ILE:O | 2.05 | 0.57 |
| 1:A:1538:LEU:HG | 1:A:2126:GLN:HG2 | 1.87 | 0.57 |
| 1:A:3517:LEU:HD13 | 1:A:3549:MET:HG2 | 1.87 | 0.57 |
| 1:B:3062:ALA:HB2 | 1:B:3106:LEU:HD21 | 1.87 | 0.57 |
| 1:A:2180:ASP:OD1 | 1:A:2356:LYS:NZ | 2.36 | 0.57 |
| 1:A:55:TRP:HE1 | 1:A:966:ILE:HG23 | 1.68 | 0.57 |
| 1:A:1804:VAL:HG12 | 1:A:1878:TYR:HD1 | 1.69 | 0.56 |
| 2:D:143:PRO:HB2 | 2:E:313:LEU:HB3 | 1.87 | 0.56 |
| 1:B:2664:TRP:HE3 | 1:B:2665:LEU:HD22 | 1.71 | 0.56 |
| 1:A:280:ARG:HA | 1:A:283:MET:HB3 | 1.87 | 0.56 |
| 1:A:3327:SER:HA | 1:A:3330:TRP:HD1 | 1.70 | 0.56 |
| 1:B:2766:LEU:HD12 | 1:B:2836:GLN:HG3 | 1.87 | 0.56 |
| 2:D:252:ARG:HB2 | 2:D:255:GLU:HG2 | 1.86 | 0.56 |
| 1:B:1412:ILE:HD13 | 1:B:1424:PHE:HB3 | 1.87 | 0.56 |
| 1:B:1836:ASP:OD1 | 1:B:1839:THR:OG1 | 2.23 | 0.56 |
| 1:B:2646:LEU:HB3 | 1:B:2660:LEU:HD11 | 1.87 | 0.56 |
| 1:A:3224:HIS:CE1 | 1:A:3266:LYS:HG2 | 2.40 | 0.56 |
| 1:B:945:TYR:OH | 1:B:950:ASP:OD1 | 2.24 | 0.56 |
| 1:B:3243:VAL:HG13 | 1:B:3253:LEU:HD21 | 1.87 | 0.56 |
| 1:A:3199:TYR:HB3 | 1:A:3291:LEU:HD13 | 1.87 | 0.56 |
| 1:A:3687:LEU:HB3 | 1:A:3762:ALA:HB1 | 1.88 | 0.56 |
| 1:B:3179:ALA:HB1 | 1:B:3182:LEU:HD12 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:207:THR:HA | 1:B:214:ALA:HB2 | 1.87 | 0.56 |
| 2:D:144:ARG:NH2 | 2:E:255:GLU:OE2 | 2.39 | 0.56 |
| 1:B:2769:THR:HG23 | 1:B:2771:PRO:HD3 | 1.88 | 0.56 |
| 2:C:206:VAL:HG13 | 2:C:218:ALA:HB3 | 1.88 | 0.56 |
| 1:B:93:VAL:O | 1:B:102:LEU:N | 2.37 | 0.56 |
| 1:B:1486:THR:OG1 | 1:B:1489:GLU:OE1 | 2.20 | 0.56 |
| 1:B:3450:ILE:HA | 1:B:3453:LEU:HG | 1.88 | 0.56 |
| 2:C:292:VAL:HG22 | 2:C:337:ARG:HH12 | 1.70 | 0.56 |
| 1:A:1089:HIS:HB2 | 1:A:1224:VAL:HB | 1.87 | 0.55 |
| 1:A:1328:HIS:HA | 1:A:1331:LEU:HD12 | 1.87 | 0.55 |
| 1:B:2927:ASN:HB2 | 1:B:3039:ILE:HG12 | 1.87 | 0.55 |
| 1:A:2323:LEU:HD12 | 1:A:2327:ARG:HH12 | 1.71 | 0.55 |
| 1:A:2823:ARG:HH12 | 1:B:2764:LYS:HE3 | 1.72 | 0.55 |
| 1:A:4235:ARG:HD3 | 1:A:4356:LEU:HD21 | 1.88 | 0.55 |
| 1:B:137:ARG:NH2 | 1:B:148:THR:O | 2.40 | 0.55 |
| 1:B:163:LEU:HD11 | 1:B:255:VAL:HG13 | 1.87 | 0.55 |
| 1:B:829:LYS:HD2 | 1:B:844:ILE:HD11 | 1.88 | 0.55 |
| 1:B:4173:VAL:HG11 | 1:B:4220:LEU:HB2 | 1.87 | 0.55 |
| 2:E:185:PHE:HB3 | 2:E:309:PRO:HD3 | 1.88 | 0.55 |
| 1:B:2595:LEU:HD13 | 1:B:2598:LEU:HD21 | 1.87 | 0.55 |
| 2:D:335:SER:HA | 2:D:338:LEU:HD13 | 1.88 | 0.55 |
| 1:B:4155:ALA:HA | 1:B:4158:LEU:HD12 | 1.88 | 0.55 |
| 1:A:285:SER:HA | 1:A:366:VAL:HB | 1.88 | 0.55 |
| 1:A:286:GLU:OE1 | 1:A:289:ARG:NH2 | 2.40 | 0.55 |
| 1:A:440:SER:HA | 1:A:721:ARG:HH22 | 1.71 | 0.55 |
| 1:B:1343:GLN:NE2 | 1:B:1344:ILE:O | 2.39 | 0.55 |
| 1:B:3792:SER:O | 1:B:4086:ARG:NH2 | 2.40 | 0.55 |
| 1:A:2873:CYS:O | 1:B:2772:HIS:ND1 | 2.39 | 0.55 |
| 1:B:3720:CYS:SG | 1:B:3721:HIS:N | 2.79 | 0.55 |
| 1:B:3990:LEU:HA | 1:B:3993:ARG:HG2 | 1.88 | 0.55 |
| 1:A:2139:LEU:HD12 | 1:A:2331:VAL:HG11 | 1.87 | 0.55 |
| 1:B:3453:LEU:HD13 | 1:B:3497:VAL:HG13 | 1.89 | 0.55 |
| 2:D:212:SER:OG | 2:D:214:ASP:OD1 | 2.23 | 0.55 |
| 1:A:411:ILE:HD11 | 1:A:567:LEU:HD22 | 1.88 | 0.55 |
| 1:A:2374:ILE:HG22 | 1:A:2375:VAL:HG13 | 1.88 | 0.55 |
| 1:B:3636:VAL:HG13 | 1:B:3711:LEU:HD12 | 1.89 | 0.55 |
| 1:B:1092:GLU:OE2 | 1:B:1219:SER:OG | 2.26 | 0.54 |
| 1:B:2143:ASP:O | 1:B:2334:LYS:NZ | 2.36 | 0.54 |
| 1:A:1429:LEU:HD13 | 1:A:1458:VAL:HG23 | 1.89 | 0.54 |
| 1:A:2566:ALA:O | 1:A:2584:LYS:NZ | 2.36 | 0.54 |
| 1:A:3453:LEU:HD13 | 1:A:3497:VAL:HG13 | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1510:LEU:HB3 | 1:B:1560:LEU:HB2 | 1.87 | 0.54 |
| 2:D:220:VAL:HA | 2:D:232:LEU:HG | 1.88 | 0.54 |
| 1:A:163:LEU:HD11 | 1:A:255:VAL:HG13 | 1.88 | 0.54 |
| 1:A:1032:GLU:OE2 | 1:A:1305:ARG:NH1 | 2.40 | 0.54 |
| 1:A:4324:LEU:HD22 | 1:A:4398:LEU:HD22 | 1.89 | 0.54 |
| 2:D:202:ASP:O | 2:D:203:ARG:HD3 | 2.07 | 0.54 |
| 1:A:3198:SER:HA | 1:A:3291:LEU:O | 2.07 | 0.54 |
| 1:A:3232:LEU:HD21 | 1:B:3233:ALA:HB2 | 1.89 | 0.54 |
| 1:B:123:VAL:O | 1:B:125:LYS:NZ | 2.37 | 0.54 |
| 1:B:164:GLU:HG2 | 1:B:258:ARG:HH22 | 1.72 | 0.54 |
| 2:D:313:LEU:HB3 | 2:C:143:PRO:HB2 | 1.89 | 0.54 |
| 1:A:2075:ARG:HG2 | 1:A:2120:LEU:HD22 | 1.88 | 0.54 |
| 2:E:163:TYR:HB3 | 2:E:209:ARG:HB3 | 1.88 | 0.54 |
| 1:A:123:VAL:O | 1:A:125:LYS:NZ | 2.36 | 0.54 |
| 1:A:280:ARG:NE | 1:A:329:PHE:O | 2.41 | 0.54 |
| 1:A:3402:ARG:HE | 1:A:3456:TRP:HD1 | 1.54 | 0.54 |
| 1:B:309:MET:HA | 1:B:344:PRO:HB3 | 1.89 | 0.54 |
| 1:A:2143:ASP:O | 1:A:2334:LYS:NZ | 2.35 | 0.54 |
| 1:B:3778:GLN:HG2 | 1:B:4070:PRO:HG3 | 1.89 | 0.54 |
| 1:A:309:MET:HA | 1:A:344:PRO:HB3 | 1.89 | 0.54 |
| 1:A:1568:PHE:HB3 | 1:A:1793:LEU:HD11 | 1.90 | 0.54 |
| 1:A:2039:HIS:HB2 | 1:A:2597:ALA:HB2 | 1.89 | 0.54 |
| 1:A:4325:GLN:NE2 | 1:A:4397:GLU:OE1 | 2.32 | 0.54 |
| 1:B:1788:ARG:HH12 | 1:B:1790:PHE:HB2 | 1.73 | 0.54 |
| 1:B:1883:TYR:HE1 | 1:B:1908:PRO:HG2 | 1.73 | 0.54 |
| 1:B:2727:THR:O | 1:B:2730:THR:OG1 | 2.23 | 0.54 |
| 1:B:4364:LEU:HD11 | 1:B:4369:LEU:HD23 | 1.90 | 0.53 |
| 1:A:3286:ARG:NH1 | 1:B:3260:SER:O | 2.42 | 0.53 |
| 1:A:4361:LEU:HA | 1:A:4408:MET:HE1 | 1.89 | 0.53 |
| 1:B:2105:ASN:HA | 1:B:2167:MET:HE1 | 1.90 | 0.53 |
| 1:B:2687:ASN:HB3 | 1:B:2690:ARG:HG3 | 1.90 | 0.53 |
| 2:D:192:LEU:HD11 | 2:D:231:THR:HB | 1.89 | 0.53 |
| 1:A:245:ASN:ND2 | 1:A:361:GLU:OE1 | 2.41 | 0.53 |
| 1:A:717:VAL:HG11 | 1:A:836:ILE:HG21 | 1.89 | 0.53 |
| 1:A:3180:GLU:O | 1:A:3184:GLN:NE2 | 2.40 | 0.53 |
| 1:B:440:SER:HA | 1:B:721:ARG:HH22 | 1.73 | 0.53 |
| 1:A:2713:ASN:HB2 | 1:B:2869:HIS:CE1 | 2.44 | 0.53 |
| 1:B:1121:GLN:OE1 | 1:B:1123:THR:OG1 | 2.25 | 0.53 |
| 1:B:3224:HIS:HE1 | 1:B:3266:LYS:HE3 | 1.74 | 0.53 |
| 1:A:3450:ILE:HA | 1:A:3453:LEU:HG | 1.91 | 0.53 |
| 1:B:2585:MET:HA | 1:B:2588:THR:HG22 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3866:LEU:HD13 | 1:A:3967:LEU:HD12 | 1.91 | 0.53 |
| 1:A:4332:ASN:ND2 | 1:A:4335:SER:OG | 2.42 | 0.53 |
| 1:A:1452:PHE:O | 1:A:1456:ASN:ND2 | 2.42 | 0.53 |
| 1:B:1849:PRO:O | 1:B:2570:ARG:NH1 | 2.42 | 0.53 |
| 1:B:2084:GLN:NE2 | 1:B:2600:ASN:O | 2.42 | 0.53 |
| 2:E:182:GLY:HA3 | 2:E:199:VAL:HG13 | 1.90 | 0.53 |
| 1:A:576:LYS:HE3 | 1:A:624:ARG:HE | 1.74 | 0.53 |
| 2:D:216:TYR:HD2 | 2:D:234:ILE:HD12 | 1.73 | 0.53 |
| 1:A:1433:LEU:HA | 1:A:1436:MET:HG2 | 1.90 | 0.53 |
| 1:A:2038:LEU:HD21 | 1:A:2085:LEU:HD12 | 1.91 | 0.53 |
| 1:A:3129:ILE:HD12 | 1:A:3132:PHE:HE1 | 1.74 | 0.53 |
| 1:A:3191:ARG:HE | 2:E:331:PHE:HD2 | 1.57 | 0.53 |
| 1:B:4080:LEU:HD12 | 1:B:4165:LEU:HB2 | 1.91 | 0.53 |
| 1:B:1012:LEU:HA | 1:B:1015:GLN:HE22 | 1.74 | 0.53 |
| 1:A:2387:LEU:O | 1:A:2393:ASN:ND2 | 2.35 | 0.52 |
| 1:B:1493:GLN:O | 1:B:2116:ARG:NH2 | 2.41 | 0.52 |
| 1:B:3618:GLN:HE22 | 1:B:3693:VAL:HA | 1.74 | 0.52 |
| 1:B:4158:LEU:HA | 1:B:4161:PHE:CE2 | 2.44 | 0.52 |
| 1:A:164:GLU:HG2 | 1:A:258:ARG:HH22 | 1.73 | 0.52 |
| 2:E:148:ASN:HD21 | 2:C:255:GLU:HA | 1.74 | 0.52 |
| 1:B:245:ASN:ND2 | 1:B:361:GLU:OE1 | 2.42 | 0.52 |
| 2:D:279:GLN:N | 2:D:279:GLN:OE1 | 2.41 | 0.52 |
| 1:A:1771:GLN:HE22 | 1:A:1983:GLN:HG2 | 1.75 | 0.52 |
| 1:A:2655:VAL:HG11 | 1:A:2660:LEU:HD12 | 1.92 | 0.52 |
| 1:A:3537:VAL:HA | 1:A:3540:LYS:HD2 | 1.92 | 0.52 |
| 1:A:3785:LEU:HA | 1:A:3788:LEU:HG | 1.92 | 0.52 |
| 1:A:4441:LYS:HE3 | 1:A:4482:GLN:HG2 | 1.92 | 0.52 |
| 1:B:2359:ALA:HA | 1:B:2415:ILE:HD11 | 1.92 | 0.52 |
| 1:B:2813:LEU:HD13 | 1:B:2851:VAL:HG11 | 1.91 | 0.52 |
| 1:B:272:VAL:HG22 | 1:B:292:THR:HG22 | 1.89 | 0.52 |
| 1:B:3534:CYS:HA | 1:B:3539:LYS:HD3 | 1.92 | 0.52 |
| 1:B:3614:ALA:O | 1:B:3618:GLN:NE2 | 2.36 | 0.52 |
| 1:A:4161:PHE:HD2 | 1:A:4188:VAL:HG21 | 1.75 | 0.52 |
| 1:B:855:THR:HB | 1:B:908:GLN:HB2 | 1.92 | 0.52 |
| 1:B:1331:LEU:O | 1:B:1334:THR:OG1 | 2.19 | 0.52 |
| 1:B:1776:GLN:HE21 | 1:B:1875:LEU:HB2 | 1.73 | 0.52 |
| 1:A:2820:SER:HB3 | 1:A:2826:PHE:HD2 | 1.75 | 0.52 |
| 1:A:3824:MET:HG3 | 1:A:3860:LEU:HD12 | 1.90 | 0.52 |
| 1:B:198:ASP:HA | 1:B:201:LYS:HE3 | 1.91 | 0.52 |
| 1:A:1290:LEU:HD22 | 1:A:1294:ASP:HB3 | 1.92 | 0.52 |
| 1:A:3618:GLN:HE22 | 1:A:3693:VAL:HA | 1.75 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:3811:LEU:HD11 | 1:B:3815:LEU:HD22 | 1.91 | 0.52 |
| 1:B:3967:LEU:HD13 | 1:B:4004:LEU:HD13 | 1.92 | 0.52 |
| 2:E:252:ARG:N | 2:E:255:GLU:OE2 | 2.42 | 0.52 |
| 1:B:2039:HIS:HB2 | 1:B:2597:ALA:HB2 | 1.92 | 0.52 |
| 1:A:716:LEU:HD21 | 1:A:719:CYS:HB2 | 1.92 | 0.51 |
| 1:A:2080:LEU:HA | 1:A:2083:VAL:HG22 | 1.92 | 0.51 |
| 1:B:3206:ALA:O | 1:B:3284:ARG:N | 2.42 | 0.51 |
| 1:A:254:SER:HB2 | 1:A:370:VAL:HG11 | 1.91 | 0.51 |
| 1:B:1290:LEU:HD22 | 1:B:1294:ASP:HB3 | 1.91 | 0.51 |
| 1:B:2380:LEU:HD21 | 1:B:2639:LEU:HD23 | 1.93 | 0.51 |
| 1:A:3287:ASP:OD2 | 1:B:3263:THR:N | 2.42 | 0.51 |
| 1:A:396:CYS:HB3 | 1:A:512:ILE:HG22 | 1.91 | 0.51 |
| 1:A:726:ALA:HA | 1:A:731:LEU:HD12 | 1.92 | 0.51 |
| 1:B:1781:GLU:OE1 | 1:B:1781:GLU:N | 2.43 | 0.51 |
| 1:A:306:PRO:O | 1:A:310:ALA:HB2 | 2.11 | 0.51 |
| 1:A:947:SER:O | 1:A:1218:ARG:NH1 | 2.44 | 0.51 |
| 1:B:55:TRP:HE1 | 1:B:966:ILE:HG23 | 1.75 | 0.51 |
| 1:B:1089:HIS:HB2 | 1:B:1224:VAL:HB | 1.91 | 0.51 |
| 1:A:198:ASP:HA | 1:A:201:LYS:HE3 | 1.92 | 0.51 |
| 1:B:2665:LEU:O | 1:B:2669:LEU:HB2 | 2.11 | 0.51 |
| 1:A:914:ILE:HB | 1:A:924:ALA:HB3 | 1.93 | 0.51 |
| 1:A:2344:PHE:HE2 | 1:B:3115:THR:HA | 1.75 | 0.51 |
| 1:A:3239:VAL:HG22 | 1:A:3282:LEU:HG | 1.93 | 0.51 |
| 1:A:3281:ARG:HH11 | 1:B:2783:PRO:HG2 | 1.75 | 0.51 |
| 1:B:726:ALA:HA | 1:B:731:LEU:HD12 | 1.91 | 0.51 |
| 1:B:3115:THR:HG21 | 1:B:3361:THR:HB | 1.93 | 0.51 |
| 1:A:630:LEU:HD12 | 1:A:720:LEU:HD22 | 1.93 | 0.51 |
| 1:B:859:LEU:HB2 | 1:B:903:LEU:HD11 | 1.93 | 0.51 |
| 1:B:4252:SER:OG | 1:B:4368:CYS:SG | 2.68 | 0.51 |
| 1:A:2693:VAL:HG23 | 1:A:2694:ILE:HD12 | 1.92 | 0.51 |
| 1:B:3327:SER:HA | 1:B:3330:TRP:HD1 | 1.75 | 0.51 |
| 2:E:163:TYR:OH | 2:E:181:ASN:ND2 | 2.43 | 0.51 |
| 1:A:2692:PRO:HG2 | 1:A:2732:MET:SD | 2.51 | 0.51 |
| 1:B:914:ILE:HB | 1:B:924:ALA:HB3 | 1.93 | 0.51 |
| 1:B:1582:ASP:N | 1:B:1775:HIS:O | 2.43 | 0.51 |
| 1:B:3187:PRO:HB2 | 1:B:3189:HIS:CE1 | 2.46 | 0.51 |
| 1:B:4364:LEU:HD23 | 1:B:4411:LEU:HD13 | 1.92 | 0.51 |
| 2:C:162:VAL:HG21 | 2:C:193:ILE:HD13 | 1.93 | 0.51 |
| 1:A:853:GLN:HE21 | 1:A:909:GLY:HA3 | 1.76 | 0.50 |
| 1:A:3076:GLN:OE1 | 1:A:3076:GLN:N | 2.41 | 0.50 |
| 1:B:1503:PHE:HZ | 1:B:1936:GLU:HB2 | 1.76 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1812:LEU:O | 1:B:1838:SER:OG | 2.26 | 0.50 |
| 1:B:1817:ILE:O | 1:B:1830:ARG:NH1 | 2.42 | 0.50 |
| 1:B:2346:CYS:HB3 | 1:B:2350:LEU:HD11 | 1.91 | 0.50 |
| 1:B:2416:LEU:HD21 | 1:B:2693:VAL:HG21 | 1.92 | 0.50 |
| 2:E:205:ARG:HH21 | 2:E:219:VAL:HA | 1.76 | 0.50 |
| 1:A:3388:GLN:OE1 | 1:A:3389:SER:OG | 2.28 | 0.50 |
| 1:A:3821:LYS:HD3 | 1:A:3859:HIS:HB3 | 1.94 | 0.50 |
| 1:A:4175:LEU:HA | 1:A:4178:ARG:HH21 | 1.74 | 0.50 |
| 1:B:396:CYS:HB3 | 1:B:512:ILE:HG22 | 1.92 | 0.50 |
| 1:B:4441:LYS:HE3 | 1:B:4482:GLN:HG2 | 1.93 | 0.50 |
| 1:A:1477:VAL:HB | 1:A:2027:ILE:HD11 | 1.93 | 0.50 |
| 1:A:3984:ALA:HB1 | 1:A:4067:ILE:H | 1.76 | 0.50 |
| 2:D:188:ALA:HB3 | 2:D:192:LEU:HB3 | 1.93 | 0.50 |
| 1:A:1817:ILE:HG23 | 1:A:1831:LEU:HB2 | 1.94 | 0.50 |
| 1:A:2790:GLN:HB2 | 1:A:2838:LYS:HD3 | 1.92 | 0.50 |
| 1:B:239:LEU:HD23 | 1:B:242:ILE:HD11 | 1.94 | 0.50 |
| 1:B:4260:ARG:NH1 | 1:B:4367:SER:O | 2.44 | 0.50 |
| 2:D:236:THR:HG22 | 2:D:237:LYS:H | 1.77 | 0.50 |
| 1:A:1015:GLN:HG3 | 1:A:1021:ILE:HD13 | 1.93 | 0.50 |
| 1:A:1122:VAL:HG22 | 1:A:1224:VAL:HG22 | 1.94 | 0.50 |
| 1:A:2332:VAL:HG13 | 1:A:2358:LEU:HD11 | 1.93 | 0.50 |
| 1:B:280:ARG:HA | 1:B:283:MET:HB3 | 1.94 | 0.50 |
| 1:B:2174:LEU:HA | 1:B:2177:ARG:NH1 | 2.27 | 0.50 |
| 1:B:3701:ASP:OD1 | 1:B:3774:HIS:NE2 | 2.33 | 0.50 |
| 1:B:3711:LEU:HD23 | 1:B:3715:LEU:HD23 | 1.93 | 0.50 |
| 1:A:1778:ILE:HB | 1:A:1873:ILE:HB | 1.94 | 0.50 |
| 1:A:2810:GLU:HG2 | 1:A:2851:VAL:HG13 | 1.93 | 0.50 |
| 1:B:4252:SER:HG | 1:B:4368:CYS:HG | 1.56 | 0.50 |
| 1:A:139:ASP:OD1 | 1:A:139:ASP:N | 2.43 | 0.50 |
| 1:A:207:THR:HA | 1:A:214:ALA:HB2 | 1.94 | 0.50 |
| 1:B:1798:PRO:HD3 | 1:B:1854:ARG:HE | 1.77 | 0.50 |
| 1:B:2135:LEU:HD13 | 1:B:2138:LEU:HD11 | 1.93 | 0.50 |
| 1:B:2349:ASP:N | 1:B:2349:ASP:OD1 | 2.44 | 0.50 |
| 1:B:3076:GLN:OE1 | 1:B:3076:GLN:N | 2.42 | 0.50 |
| 1:B:3189:HIS:NE2 | 1:B:3295:GLN:HB2 | 2.27 | 0.50 |
| 1:B:3454:LEU:HA | 1:B:3457:VAL:HG12 | 1.94 | 0.50 |
| 1:A:4155:ALA:HA | 1:A:4158:LEU:HD12 | 1.92 | 0.50 |
| 1:B:3341:ILE:HG22 | 1:B:3343:ASP:H | 1.77 | 0.50 |
| 2:E:194:VAL:HG21 | 2:E:338:LEU:HD21 | 1.93 | 0.50 |
| 1:A:2412:LEU:HB3 | 1:A:2667:LEU:HD11 | 1.93 | 0.50 |
| 1:A:3967:LEU:HD13 | 1:A:4004:LEU:HD13 | 1.93 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:154:VAL:HG23 | 1:B:263:LEU:HD13 | 1.94 | 0.50 |
| 1:A:93:VAL:O | 1:A:102:LEU:N | 2.43 | 0.49 |
| 1:A:1496:TYR:CZ | 1:A:1970:VAL:HG21 | 2.47 | 0.49 |
| 1:A:1781:GLU:OE1 | 1:A:1781:GLU:N | 2.44 | 0.49 |
| 1:A:1832:VAL:HG21 | 1:A:2566:ALA:HB1 | 1.93 | 0.49 |
| 1:B:2038:LEU:HD21 | 1:B:2085:LEU:HD12 | 1.93 | 0.49 |
| 1:B:2041:SER:O | 1:B:2044:HIS:ND1 | 2.43 | 0.49 |
| 1:B:2080:LEU:HA | 1:B:2083:VAL:HG22 | 1.95 | 0.49 |
| 2:C:157:THR:HG21 | 2:C:311:VAL:HG11 | 1.94 | 0.49 |
| 2:C:296:GLN:HA | 2:C:330:SER:O | 2.12 | 0.49 |
| 1:B:411:ILE:HD11 | 1:B:567:LEU:HD22 | 1.95 | 0.49 |
| 1:B:1377:LEU:O | 1:B:1381:THR:OG1 | 2.22 | 0.49 |
| 1:B:1806:ILE:HG21 | 1:B:1815:LEU:HD21 | 1.94 | 0.49 |
| 1:A:2724:HIS:O | 1:A:2727:THR:OG1 | 2.27 | 0.49 |
| 1:A:2729:MET:SD | 1:A:2748:THR:OG1 | 2.67 | 0.49 |
| 1:A:2764:LYS:HE3 | 1:B:2823:ARG:HH12 | 1.77 | 0.49 |
| 1:A:1121:GLN:OE1 | 1:A:1123:THR:OG1 | 2.30 | 0.49 |
| 1:A:3242:GLU:HG2 | 1:A:3252:PRO:HA | 1.95 | 0.49 |
| 1:B:2355:CYS:HB3 | 1:B:2411:MET:SD | 2.51 | 0.49 |
| 1:B:2582:MET:HA | 1:B:2585:MET:HG3 | 1.94 | 0.49 |
| 1:A:1573:THR:HG22 | 1:A:1574:SER:H | 1.78 | 0.49 |
| 1:A:3614:ALA:HB2 | 1:A:3689:PHE:CD1 | 2.47 | 0.49 |
| 1:B:1194:LEU:HD21 | 1:B:2584:LYS:HG2 | 1.95 | 0.49 |
| 1:A:1012:LEU:HA | 1:A:1015:GLN:HE22 | 1.78 | 0.49 |
| 1:A:1110:LEU:HD21 | 1:A:1188:LEU:HD21 | 1.94 | 0.49 |
| 1:A:2066:LEU:HD22 | 1:A:2078:THR:HG21 | 1.94 | 0.49 |
| 1:B:716:LEU:HD21 | 1:B:719:CYS:HB2 | 1.94 | 0.49 |
| 1:B:1573:THR:HG22 | 1:B:1574:SER:H | 1.78 | 0.49 |
| 1:B:2385:LEU:HD12 | 1:B:2389:GLY:HA3 | 1.94 | 0.49 |
| 1:B:3402:ARG:HE | 1:B:3456:TRP:HD1 | 1.61 | 0.49 |
| 1:B:3550:CYS:HB3 | 1:B:3557:PHE:HB2 | 1.94 | 0.49 |
| 1:B:3698:ILE:HG23 | 1:B:3699:MET:HE2 | 1.95 | 0.49 |
| 1:A:1436:MET:HA | 1:A:1439:LEU:HD23 | 1.94 | 0.49 |
| 1:B:2174:LEU:HD23 | 1:B:2177:ARG:HH12 | 1.78 | 0.49 |
| 1:B:132:TYR:HB3 | 1:B:379:PHE:HE1 | 1.77 | 0.49 |
| 1:B:211:HIS:CE1 | 1:B:1047:VAL:HG12 | 2.48 | 0.49 |
| 1:B:1120:ILE:HG23 | 1:B:1188:LEU:HB2 | 1.95 | 0.49 |
| 1:B:1581:ARG:HA | 1:B:1776:GLN:HA | 1.95 | 0.49 |
| 1:B:1770:LEU:HD13 | 1:B:1986:LEU:HD11 | 1.94 | 0.49 |
| 1:A:2697:ASN:OD1 | 1:A:2698:GLN:N | 2.46 | 0.48 |
| 1:A:3241:VAL:HG12 | 1:A:3280:LEU:HD13 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:147:ASP:OD2 | 1:B:218:THR:OG1 | 2.24 | 0.48 |
| 1:B:567:LEU:HB2 | 1:B:635:ILE:HD11 | 1.95 | 0.48 |
| 1:B:1037:ARG:HH22 | 1:B:1075:ARG:HB3 | 1.78 | 0.48 |
| 1:B:2724:HIS:O | 1:B:2727:THR:OG1 | 2.31 | 0.48 |
| 1:A:132:TYR:HB3 | 1:A:379:PHE:HE1 | 1.77 | 0.48 |
| 1:A:3782:ALA:HA | 1:A:4074:PHE:HD1 | 1.78 | 0.48 |
| 1:B:1402:HIS:CE1 | 1:B:1406:ARG:HD2 | 2.48 | 0.48 |
| 1:B:2800:LEU:HD12 | 1:B:2808:PHE:HB2 | 1.95 | 0.48 |
| 1:B:3239:VAL:HG22 | 1:B:3282:LEU:HG | 1.95 | 0.48 |
| 1:B:3866:LEU:HD13 | 1:B:3967:LEU:HD12 | 1.95 | 0.48 |
| 2:E:323:MET:N | 2:E:323:MET:SD | 2.86 | 0.48 |
| 1:A:1432:LEU:HD22 | 1:A:1451:TYR:HE1 | 1.78 | 0.48 |
| 1:A:1557:LEU:HD12 | 1:A:1845:HIS:HD2 | 1.78 | 0.48 |
| 1:A:2066:LEU:HD21 | 1:A:2074:ILE:HG13 | 1.94 | 0.48 |
| 1:A:2786:THR:HA | 1:A:2789:MET:HG3 | 1.95 | 0.48 |
| 1:A:3823:THR:O | 1:A:4001:SER:HA | 2.13 | 0.48 |
| 1:B:2383:LEU:HD11 | 1:B:2408:LEU:HD11 | 1.93 | 0.48 |
| 1:B:2393:ASN:HA | 1:B:2398:SER:HA | 1.95 | 0.48 |
| 2:E:319:GLY:CA | 2:E:333:ILE:O | 2.61 | 0.48 |
| 1:A:2998:LEU:HD13 | 1:A:3036:LEU:HD22 | 1.96 | 0.48 |
| 1:A:3454:LEU:HA | 1:A:3457:VAL:HG12 | 1.95 | 0.48 |
| 1:A:4260:ARG:NH1 | 1:A:4367:SER:O | 2.47 | 0.48 |
| 1:B:176:ALA:O | 1:B:181:VAL:N | 2.44 | 0.48 |
| 1:B:576:LYS:HE3 | 1:B:624:ARG:HE | 1.78 | 0.48 |
| 1:B:630:LEU:HB2 | 1:B:720:LEU:HB3 | 1.95 | 0.48 |
| 2:D:268:ASN:ND2 | 2:E:277:SER:OG | 2.46 | 0.48 |
| 1:A:1412:ILE:HD13 | 1:A:1424:PHE:HB3 | 1.95 | 0.48 |
| 1:A:3720:CYS:SG | 1:A:3721:HIS:N | 2.86 | 0.48 |
| 1:A:3813:LEU:HD11 | 1:B:1927:ARG:HH21 | 1.78 | 0.48 |
| 1:B:1510:LEU:HD13 | 1:B:1982:LEU:HD11 | 1.95 | 0.48 |
| 1:B:2374:ILE:HG22 | 1:B:2375:VAL:HG13 | 1.96 | 0.48 |
| 1:B:3537:VAL:HA | 1:B:3540:LYS:HD2 | 1.93 | 0.48 |
| 1:A:3707:GLU:HG2 | 1:A:3708:VAL:HG23 | 1.95 | 0.48 |
| 1:B:2370:HIS:ND1 | 1:B:2419:GLU:HG3 | 2.28 | 0.48 |
| 1:A:1807:PRO:HG2 | 1:A:1874:PRO:HB2 | 1.94 | 0.48 |
| 1:A:2998:LEU:HG | 1:A:3081:LEU:HB2 | 1.96 | 0.48 |
| 1:A:3429:ASP:HA | 1:A:3432:ILE:HD12 | 1.94 | 0.48 |
| 1:B:825:LEU:HB2 | 1:B:847:GLN:HB3 | 1.94 | 0.48 |
| 1:B:1023:THR:HA | 1:B:1026:VAL:HG12 | 1.96 | 0.48 |
| 1:A:749:LEU:O | 1:A:823:GLY:HA3 | 2.14 | 0.48 |
| 1:A:725:PHE:HE2 | 1:A:846:ILE:HD13 | 1.78 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1083:SER:HA | 1:A:1086:TRP:HB3 | 1.95 | 0.48 |
| 1:A:2141:LEU:O | 1:A:2145:LEU:HB2 | 2.14 | 0.48 |
| 1:A:2365:THR:O | 1:A:2366:ARG:NH1 | 2.47 | 0.48 |
| 1:A:3605:LEU:HG | 1:A:3609:HIS:HB2 | 1.96 | 0.48 |
| 1:B:2692:PRO:HG3 | 1:B:2728:LEU:HB3 | 1.96 | 0.48 |
| 1:A:1581:ARG:HH11 | 1:A:1776:GLN:HE21 | 1.62 | 0.48 |
| 1:A:2030:LEU:O | 1:A:2033:THR:OG1 | 2.26 | 0.48 |
| 1:A:2120:LEU:O | 1:A:2124:ILE:HG12 | 2.13 | 0.48 |
| 1:A:3484:TYR:HA | 1:A:3487:LEU:HG | 1.96 | 0.48 |
| 1:B:1432:LEU:HD22 | 1:B:1451:TYR:HE1 | 1.78 | 0.48 |
| 1:B:2998:LEU:HG | 1:B:3081:LEU:HB2 | 1.95 | 0.48 |
| 1:B:3429:ASP:HA | 1:B:3432:ILE:HD12 | 1.96 | 0.48 |
| 1:B:4331:ILE:HG21 | 1:B:4402:ILE:HA | 1.96 | 0.48 |
| 1:A:94:ILE:HA | 1:A:101:THR:HA | 1.96 | 0.47 |
| 1:A:129:VAL:HG22 | 1:A:134:VAL:HG22 | 1.95 | 0.47 |
| 1:A:2934:LEU:HD13 | 1:A:2983:LEU:HD11 | 1.95 | 0.47 |
| 1:B:2098:ASN:HD22 | 1:B:2101:GLN:HE21 | 1.62 | 0.47 |
| 1:B:3389:SER:HB2 | 1:B:3392:ILE:HG12 | 1.96 | 0.47 |
| 1:A:289:ARG:O | 1:A:292:THR:OG1 | 2.31 | 0.47 |
| 1:A:1108:PHE:CZ | 1:A:1199:GLY:HA3 | 2.49 | 0.47 |
| 1:A:2201:TRP:CD2 | 1:A:2356:LYS:HG3 | 2.49 | 0.47 |
| 1:A:3262:LEU:HD23 | 1:B:3287:ASP:HB2 | 1.96 | 0.47 |
| 1:A:3522:PHE:CZ | 1:A:3560:LEU:HB2 | 2.49 | 0.47 |
| 1:B:2662:GLN:HB3 | 1:B:2721:LEU:HD21 | 1.95 | 0.47 |
| 1:B:3242:GLU:OE2 | 1:B:3281:ARG:NH1 | 2.47 | 0.47 |
| 2:D:208:VAL:HG11 | 2:D:234:ILE:HG21 | 1.97 | 0.47 |
| 1:A:630:LEU:HB2 | 1:A:720:LEU:HB3 | 1.96 | 0.47 |
| 1:A:3225:ILE:HB | 1:A:3265:ILE:HB | 1.97 | 0.47 |
| 1:B:3124:SER:OG | 1:B:3125:MET:N | 2.47 | 0.47 |
| 1:B:3489:PRO:HB2 | 1:B:3494:LEU:HD21 | 1.96 | 0.47 |
| 1:A:160:VAL:HA | 1:A:224:PRO:HA | 1.95 | 0.47 |
| 1:B:94:ILE:HA | 1:B:101:THR:HA | 1.96 | 0.47 |
| 1:B:1779:ILE:HD11 | 1:B:1872:LYS:HG2 | 1.95 | 0.47 |
| 1:B:3379:GLU:HA | 1:B:3434:ILE:HD11 | 1.97 | 0.47 |
| 1:B:3432:ILE:HG23 | 1:B:3496:CYS:HB2 | 1.95 | 0.47 |
| 1:A:176:ALA:O | 1:A:181:VAL:N | 2.47 | 0.47 |
| 1:A:411:ILE:HD12 | 1:A:422:LEU:HD12 | 1.97 | 0.47 |
| 1:A:1029:THR:HG22 | 1:A:1358:TRP:CE3 | 2.49 | 0.47 |
| 1:A:2014:LEU:O | 1:A:2018:SER:OG | 2.28 | 0.47 |
| 1:A:3191:ARG:NH1 | 2:E:323:MET:O | 2.45 | 0.47 |
| 1:B:356:PRO:HB2 | 1:B:363:THR:HG22 | 1.95 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2777:HIS:CD2 | 1:B:2778:SER:H | 2.33 | 0.47 |
| 1:A:136:CYS:H | 1:A:418:MET:HE2 | 1.80 | 0.47 |
| 1:A:859:LEU:HB2 | 1:A:903:LEU:HD11 | 1.95 | 0.47 |
| 1:A:1779:ILE:HD11 | 1:A:1870:ARG:HE | 1.79 | 0.47 |
| 1:B:725:PHE:HE2 | 1:B:846:ILE:HD13 | 1.79 | 0.47 |
| 1:B:934:THR:HG23 | 1:B:936:GLU:H | 1.80 | 0.47 |
| 1:B:3774:HIS:CE1 | 1:B:3776:ASN:HB2 | 2.50 | 0.47 |
| 1:A:860:ILE:HG13 | 1:A:904:VAL:HB | 1.96 | 0.47 |
| 1:A:1445:GLY:HA3 | 1:A:1509:ASP:HB3 | 1.97 | 0.47 |
| 1:A:2204:ILE:HD12 | 1:A:2356:LYS:HD2 | 1.97 | 0.47 |
| 1:A:4247:ILE:HG13 | 1:A:4323:LEU:HG | 1.96 | 0.47 |
| 1:B:630:LEU:HD12 | 1:B:720:LEU:HD22 | 1.96 | 0.47 |
| 1:B:1047:VAL:O | 1:B:1078:LYS:N | 2.31 | 0.47 |
| 1:B:2719:TRP:HB3 | 1:B:2765:PHE:HE1 | 1.80 | 0.47 |
| 1:B:3236:PRO:HG3 | 1:B:3282:LEU:HD23 | 1.96 | 0.47 |
| 1:B:3538:LEU:O | 1:B:3542:VAL:HG23 | 2.15 | 0.47 |
| 1:B:3817:LEU:HD11 | 1:B:4185:LEU:HD22 | 1.97 | 0.47 |
| 1:A:3358:LEU:HG | 1:A:3359:LEU:HD22 | 1.96 | 0.47 |
| 1:A:2061:GLU:OE2 | 1:A:2065:HIS:NE2 | 2.48 | 0.47 |
| 1:A:3115:THR:HG21 | 1:A:3361:THR:HB | 1.97 | 0.47 |
| 1:B:1335:LEU:HD21 | 1:B:1353:LEU:HD11 | 1.97 | 0.47 |
| 1:B:3443:ASP:OD1 | 1:B:3446:THR:OG1 | 2.25 | 0.47 |
| 1:B:3547:CYS:HB2 | 1:B:3616:SER:HA | 1.97 | 0.47 |
| 1:A:85:VAL:HG22 | 1:A:91:ILE:HG12 | 1.97 | 0.47 |
| 1:A:4003:ASP:OD1 | 1:A:4003:ASP:N | 2.48 | 0.47 |
| 1:B:912:VAL:HB | 1:B:926:VAL:HB | 1.97 | 0.47 |
| 1:B:3108:CYS:HB3 | 1:B:3355:THR:HG21 | 1.97 | 0.47 |
| 1:A:834:THR:HG23 | 1:A:836:ILE:H | 1.79 | 0.46 |
| 1:B:510:LEU:HD22 | 1:B:567:LEU:HD11 | 1.96 | 0.46 |
| 1:B:2413:GLN:NE2 | 1:B:2666:THR:O | 2.42 | 0.46 |
| 2:D:204:ARG:HB2 | 2:D:220:VAL:H | 1.80 | 0.46 |
| 2:E:191:GLY:HA2 | 2:E:240:LEU:HD12 | 1.97 | 0.46 |
| 1:B:1204:THR:HG21 | 1:B:2575:LEU:HD21 | 1.96 | 0.46 |
| 1:B:2655:VAL:HG11 | 1:B:2660:LEU:HD12 | 1.97 | 0.46 |
| 1:B:3707:GLU:HG2 | 1:B:3708:VAL:HG23 | 1.97 | 0.46 |
| 1:A:1827:ASP:OD1 | 1:A:1827:ASP:N | 2.49 | 0.46 |
| 1:A:2393:ASN:HA | 1:A:2398:SER:HA | 1.97 | 0.46 |
| 1:A:2668:SER:HB3 | 1:A:2692:PRO:CB | 2.45 | 0.46 |
| 1:A:1456:ASN:HA | 1:A:1459:LYS:HD3 | 1.98 | 0.46 |
| 1:A:4084:ALA:HB2 | 1:A:4165:LEU:HD11 | 1.97 | 0.46 |
| 1:B:1206:PRO:HB3 | 1:B:1322:LEU:HD13 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1493:GLN:HG2 | 1:B:1499:TYR:HA | 1.98 | 0.46 |
| 1:B:1771:GLN:HE22 | 1:B:1983:GLN:HG2 | 1.79 | 0.46 |
| 1:A:186:THR:HG21 | 1:A:231:ILE:HA | 1.98 | 0.46 |
| 1:A:1810:GLY:HA2 | 1:A:1838:SER:HA | 1.97 | 0.46 |
| 1:A:2793:LEU:HD13 | 1:A:2842:PHE:CD2 | 2.51 | 0.46 |
| 1:A:3828:SER:HB3 | 1:A:3832:LEU:HD21 | 1.97 | 0.46 |
| 1:B:2325:HIS:CE1 | 1:B:2329:ILE:HD11 | 2.50 | 0.46 |
| 1:B:3218:VAL:HG23 | 1:B:3220:LEU:HD22 | 1.98 | 0.46 |
| 1:A:510:LEU:HD22 | 1:A:567:LEU:HD11 | 1.97 | 0.46 |
| 1:A:2096:LEU:HD23 | 1:A:2096:LEU:HA | 1.84 | 0.46 |
| 1:A:4153:ILE:HG23 | 1:A:4210:PRO:HG3 | 1.96 | 0.46 |
| 1:B:287:ALA:HA | 1:B:290:ARG:HE | 1.81 | 0.46 |
| 1:B:1409:ALA:HB1 | 1:B:2582:MET:SD | 2.56 | 0.46 |
| 1:B:1830:ARG:NH2 | 1:B:1833:VAL:HG22 | 2.31 | 0.46 |
| 1:B:1101:VAL:HA | 1:B:1305:ARG:NE | 2.31 | 0.46 |
| 1:A:2355:CYS:SG | 1:A:2411:MET:HG3 | 2.56 | 0.46 |
| 1:A:283:MET:SD | 1:A:289:ARG:HG2 | 2.56 | 0.46 |
| 1:A:855:THR:HB | 1:A:908:GLN:HG2 | 1.98 | 0.46 |
| 1:B:2665:LEU:HD21 | 1:B:2725:SER:HB3 | 1.97 | 0.46 |
| 2:C:271:THR:HG21 | 2:C:300:ALA:O | 2.16 | 0.46 |
| 1:A:324:ASP:OD2 | 1:A:338:TRP:N | 2.47 | 0.46 |
| 1:A:1809:CYS:H | 1:A:1837:ILE:HG22 | 1.80 | 0.46 |
| 1:A:3978:PRO:HD2 | 1:A:3981:MET:SD | 2.56 | 0.46 |
| 1:B:1467:SER:HB2 | 1:B:2050:LEU:HD13 | 1.96 | 0.46 |
| 1:B:2370:HIS:HD2 | 1:B:2633:LEU:HG | 1.81 | 0.46 |
| 1:B:2812:LEU:HD13 | 1:B:2843:THR:HG23 | 1.98 | 0.46 |
| 1:A:1193:ASP:HA | 1:A:2581:LEU:HD11 | 1.98 | 0.45 |
| 1:A:3858:LEU:HD13 | 1:A:3872:ARG:HH22 | 1.80 | 0.45 |
| 2:C:194:VAL:HG21 | 2:C:338:LEU:HD21 | 1.98 | 0.45 |
| 1:A:134:VAL:HG11 | 1:A:400:LEU:HD21 | 1.98 | 0.45 |
| 1:A:934:THR:HG23 | 1:A:936:GLU:H | 1.80 | 0.45 |
| 1:A:2123:CYS:SG | 1:A:2127:ARG:NH2 | 2.89 | 0.45 |
| 1:B:211:HIS:CD2 | 1:B:1044:PRO:HA | 2.51 | 0.45 |
| 1:B:1041:THR:OG1 | 1:B:1092:GLU:HB3 | 2.16 | 0.45 |
| 1:B:1108:PHE:CZ | 1:B:1199:GLY:HA3 | 2.51 | 0.45 |
| 1:B:1410:LEU:HD21 | 1:B:2579:ALA:HB2 | 1.98 | 0.45 |
| 1:B:2387:LEU:HD22 | 1:B:2663:LEU:HD12 | 1.98 | 0.45 |
| 1:B:3129:ILE:HA | 1:B:3132:PHE:CE2 | 2.51 | 0.45 |
| 1:B:3177:GLN:N | 1:B:3177:GLN:OE1 | 2.49 | 0.45 |
| 1:B:3223:ILE:HD12 | 1:B:3298:LEU:HD23 | 1.98 | 0.45 |
| 1:A:2783:PRO:HG3 | 1:B:3207:TRP:CD1 | 2.51 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3831:PRO:HB3 | 1:A:3853:HIS:CE1 | 2.51 | 0.45 |
| 1:B:1105:ASP:OD2 | 1:B:1304:ARG:NH2 | 2.43 | 0.45 |
| 1:B:2115:ASP:OD1 | 1:B:2116:ARG:N | 2.47 | 0.45 |
| 1:B:2335:LEU:HG | 1:B:2358:LEU:HD12 | 1.99 | 0.45 |
| 1:A:2105:ASN:HB2 | 1:A:2108:GLN:HB2 | 1.98 | 0.45 |
| 1:A:2122:SER:OG | 1:A:2177:ARG:NE | 2.49 | 0.45 |
| 1:A:2325:HIS:CE1 | 1:A:2329:ILE:HD11 | 2.50 | 0.45 |
| 1:A:2582:MET:O | 1:A:2586:MET:HG2 | 2.15 | 0.45 |
| 1:A:3036:LEU:HA | 1:A:3039:ILE:HG22 | 1.99 | 0.45 |
| 1:A:3199:TYR:O | 1:A:3290:THR:HA | 2.16 | 0.45 |
| 1:A:4255:SER:O | 1:A:4257:HIS:ND1 | 2.46 | 0.45 |
| 1:B:2068:ILE:HG21 | 1:B:2110:LEU:HD21 | 1.99 | 0.45 |
| 1:B:2578:GLN:HA | 1:B:2581:LEU:HG | 1.98 | 0.45 |
| 1:B:3002:ASN:ND2 | 1:B:3321:ASP:OD2 | 2.49 | 0.45 |
| 1:B:3824:MET:HG3 | 1:B:3860:LEU:HD12 | 1.98 | 0.45 |
| 2:E:186:VAL:HG22 | 2:E:193:ILE:HG12 | 1.99 | 0.45 |
| 1:A:2687:ASN:HB3 | 1:A:2690:ARG:HG3 | 1.98 | 0.45 |
| 1:A:2812:LEU:HA | 1:A:2815:LEU:HG | 1.99 | 0.45 |
| 1:A:3240:SER:HB3 | 1:A:3256:PRO:HG3 | 1.98 | 0.45 |
| 1:B:1810:GLY:HA2 | 1:B:1838:SER:HA | 1.98 | 0.45 |
| 1:A:240:LYS:NZ | 1:A:284:TYR:OH | 2.33 | 0.45 |
| 1:A:2872:THR:HG22 | 1:A:3000:LEU:HD22 | 1.97 | 0.45 |
| 1:B:240:LYS:NZ | 1:B:284:TYR:OH | 2.46 | 0.45 |
| 1:B:1935:LEU:HG | 1:B:1973:ALA:HB1 | 1.97 | 0.45 |
| 1:B:3196:ALA:HB3 | 1:B:3294:SER:HA | 1.99 | 0.45 |
| 2:D:186:VAL:HG22 | 2:D:193:ILE:HG12 | 1.98 | 0.45 |
| 1:A:1770:LEU:HD13 | 1:A:1986:LEU:HD11 | 1.98 | 0.45 |
| 1:A:1819:ILE:HB | 1:A:1853:CYS:SG | 2.56 | 0.45 |
| 1:A:2923:LEU:HA | 1:A:2926:VAL:HG22 | 1.99 | 0.45 |
| 1:B:1440:PRO:HG3 | 1:B:2015:ILE:HG12 | 1.99 | 0.45 |
| 1:B:1788:ARG:NH1 | 1:B:1790:PHE:HB2 | 2.31 | 0.45 |
| 1:B:2719:TRP:HH2 | 1:B:2764:LYS:HB3 | 1.82 | 0.45 |
| 1:A:74:SER:HB2 | 1:A:83:LEU:HB2 | 1.98 | 0.45 |
| 1:A:3085:ILE:HA | 1:A:3088:VAL:HG12 | 1.99 | 0.45 |
| 1:A:3760:GLU:HG3 | 1:A:3810:ARG:HH12 | 1.82 | 0.45 |
| 1:B:1444:THR:HG22 | 1:B:1447:SER:H | 1.81 | 0.45 |
| 1:B:3192:ALA:HB1 | 1:B:3228:HIS:CE1 | 2.51 | 0.45 |
| 1:A:2050:LEU:HD12 | 1:A:2054:PHE:HE2 | 1.82 | 0.45 |
| 1:A:3432:ILE:HG23 | 1:A:3496:CYS:HB2 | 1.99 | 0.45 |
| 1:A:4078:GLY:HA2 | 1:A:4080:LEU:HD23 | 1.99 | 0.45 |
| 1:B:347:GLU:OE1 | 1:B:350:ARG:NH1 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1771:GLN:OE1 | 1:B:1983:GLN:NE2 | 2.50 | 0.45 |
| 1:B:1819:ILE:HG22 | 1:B:1856:MET:HG2 | 1.99 | 0.45 |
| 1:B:3769:GLN:O | 1:B:3772:SER:OG | 2.33 | 0.45 |
| 1:A:2875:ASP:HA | 1:B:2715:LEU:HD11 | 1.99 | 0.45 |
| 1:A:3719:LEU:HD22 | 1:A:3807:PHE:CG | 2.52 | 0.45 |
| 1:A:3774:HIS:CE1 | 1:A:3776:ASN:HB2 | 2.51 | 0.45 |
| 2:C:160:ALA:HB3 | 2:C:243:LEU:HG | 1.98 | 0.45 |
| 1:A:2118:PHE:CZ | 1:A:2173:MET:HG3 | 2.52 | 0.44 |
| 1:A:3216:ALA:HB1 | 1:B:2203:PHE:HA | 1.98 | 0.44 |
| 1:B:74:SER:HB2 | 1:B:83:LEU:HB2 | 1.98 | 0.44 |
| 1:B:2863:VAL:HG11 | 1:B:2926:VAL:HG11 | 2.00 | 0.44 |
| 1:B:2998:LEU:HD11 | 1:B:3080:PRO:HB2 | 1.98 | 0.44 |
| 1:B:4435:THR:O | 1:B:4439:LYS:HG3 | 2.17 | 0.44 |
| 1:A:163:LEU:HD12 | 1:A:259:LEU:HD21 | 1.99 | 0.44 |
| 1:B:134:VAL:HG11 | 1:B:400:LEU:HD21 | 1.99 | 0.44 |
| 1:B:1114:ILE:HD11 | 1:B:1295:LEU:HG | 1.99 | 0.44 |
| 1:B:1827:ASP:OD1 | 1:B:1827:ASP:N | 2.50 | 0.44 |
| 1:B:3177:GLN:HE21 | 1:B:3198:SER:H | 1.65 | 0.44 |
| 1:B:3635:LEU:HB2 | 1:B:3686:ILE:HD11 | 2.00 | 0.44 |
| 1:A:627:LEU:HD12 | 1:A:628:PRO:HD2 | 1.99 | 0.44 |
| 1:A:1792:THR:HA | 1:A:1856:MET:O | 2.18 | 0.44 |
| 1:A:1804:VAL:HG12 | 1:A:1878:TYR:CD1 | 2.51 | 0.44 |
| 1:A:3191:ARG:HE | 2:E:331:PHE:HB2 | 1.82 | 0.44 |
| 1:B:4247:ILE:HG13 | 1:B:4323:LEU:HG | 2.00 | 0.44 |
| 2:C:256:PHE:HB2 | 2:C:313:LEU:HD11 | 1.98 | 0.44 |
| 1:A:65:CYS:SG | 1:A:94:ILE:HD11 | 2.57 | 0.44 |
| 1:B:2029:TYR:O | 1:B:2033:THR:HG23 | 2.18 | 0.44 |
| 2:E:257:VAL:HG12 | 2:E:312:ASN:HA | 1.98 | 0.44 |
| 1:A:391:PHE:HA | 1:A:510:LEU:HD12 | 2.00 | 0.44 |
| 1:A:2876:LYS:HG3 | 1:B:2715:LEU:HG | 1.98 | 0.44 |
| 1:B:574:THR:HG22 | 1:B:624:ARG:HD2 | 1.99 | 0.44 |
| 1:A:2072:PRO:O | 1:A:2116:ARG:NH2 | 2.50 | 0.44 |
| 1:A:2366:ARG:HD3 | 1:A:2366:ARG:HA | 1.80 | 0.44 |
| 1:A:4244:LEU:HA | 1:A:4247:ILE:HG22 | 2.00 | 0.44 |
| 1:B:3242:GLU:HG2 | 1:B:3252:PRO:HA | 2.00 | 0.44 |
| 1:A:1557:LEU:HD22 | 1:A:1805:LEU:HD12 | 1.99 | 0.44 |
| 1:A:2582:MET:HA | 1:A:2585:MET:HG3 | 1.98 | 0.44 |
| 1:A:2717:ARG:HB3 | 1:B:2876:LYS:NZ | 2.33 | 0.44 |
| 1:A:2829:GLY:HA2 | 1:A:2915:ARG:HH12 | 1.82 | 0.44 |
| 1:B:3199:TYR:O | 1:B:3290:THR:HA | 2.18 | 0.44 |
| 1:A:1914:LEU:HD12 | 1:A:1994:LEU:HB3 | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3860:LEU:HD11 | 1:A:3872:ARG:HH21 | 1.83 | 0.44 |
| 1:B:3224:HIS:ND1 | 1:B:3266:LYS:HG2 | 2.33 | 0.44 |
| 2:E:198:HIS:HE1 | 2:E:322:THR:HG23 | 1.83 | 0.44 |
| 1:A:2782:GLY:O | 1:A:2786:THR:HG23 | 2.18 | 0.44 |
| 1:B:514:GLN:HA | 1:B:837:VAL:HG21 | 1.99 | 0.44 |
| 1:B:2094:GLN:NE2 | 1:B:2098:ASN:OD1 | 2.38 | 0.44 |
| 1:B:2139:LEU:HD11 | 1:B:2327:ARG:HD2 | 2.00 | 0.44 |
| 1:B:3388:GLN:OE1 | 1:B:3389:SER:OG | 2.33 | 0.44 |
| 2:E:294:TYR:HB3 | 2:E:331:PHE:HB3 | 2.00 | 0.44 |
| 1:A:306:PRO:O | 1:A:310:ALA:CB | 2.67 | 0.43 |
| 1:A:1795:PHE:HB3 | 1:A:1799:ILE:HD12 | 1.99 | 0.43 |
| 1:A:2998:LEU:HD11 | 1:A:3080:PRO:HB2 | 2.00 | 0.43 |
| 1:A:3696:SER:HB2 | 1:A:3699:MET:HG2 | 1.99 | 0.43 |
| 1:B:3191:ARG:HA | 2:E:303:PHE:CE2 | 2.52 | 0.43 |
| 1:A:1929:ASN:HB3 | 1:B:3810:ARG:NH1 | 2.32 | 0.43 |
| 1:A:2416:LEU:HD11 | 1:A:2639:LEU:HD11 | 2.00 | 0.43 |
| 1:A:2729:MET:HA | 1:A:2732:MET:HG2 | 1.99 | 0.43 |
| 1:A:4335:SER:OG | 1:A:4400:ARG:NH2 | 2.44 | 0.43 |
| 1:B:1538:LEU:HG | 1:B:2126:GLN:HG2 | 2.00 | 0.43 |
| 1:B:2834:ASP:OD1 | 1:B:2834:ASP:N | 2.51 | 0.43 |
| 1:B:4255:SER:O | 1:B:4257:HIS:ND1 | 2.51 | 0.43 |
| 2:C:312:ASN:HD21 | 2:C:316:GLU:HB2 | 1.83 | 0.43 |
| 1:A:287:ALA:HA | 1:A:290:ARG:HE | 1.83 | 0.43 |
| 1:A:2335:LEU:HD22 | 1:A:2358:LEU:HD13 | 1.99 | 0.43 |
| 1:B:3826:LEU:HB2 | 1:B:3856:ARG:HB2 | 2.00 | 0.43 |
| 1:B:3862:VAL:HA | 1:B:3983:LEU:HB2 | 2.00 | 0.43 |
| 2:D:274:ILE:HD13 | 2:C:272:SER:HB3 | 2.00 | 0.43 |
| 1:A:1182:LEU:HD13 | 1:A:1208:LEU:HD12 | 2.00 | 0.43 |
| 1:A:3081:LEU:O | 1:A:3085:ILE:HG12 | 2.18 | 0.43 |
| 1:A:3209:ASP:HB3 | 1:A:3281:ARG:NE | 2.33 | 0.43 |
| 1:A:3691:THR:HG22 | 1:A:3766:PHE:HA | 2.00 | 0.43 |
| 1:B:2116:ARG:HA | 1:B:2119:MET:HE3 | 2.01 | 0.43 |
| 1:B:3335:HIS:CG | 1:B:3377:ASN:HB3 | 2.53 | 0.43 |
| 2:D:236:THR:HG21 | 2:D:240:LEU:HD21 | 2.00 | 0.43 |
| 2:C:337:ARG:O | 2:C:340:GLU:HG3 | 2.19 | 0.43 |
| 1:A:215:LYS:HD2 | 1:A:215:LYS:HA | 1.80 | 0.43 |
| 1:A:2668:SER:HB3 | 1:A:2692:PRO:HB3 | 2.00 | 0.43 |
| 1:A:3621:GLU:O | 1:A:3625:GLN:HG3 | 2.17 | 0.43 |
| 1:B:1029:THR:HG22 | 1:B:1358:TRP:CE3 | 2.54 | 0.43 |
| 1:B:1817:ILE:HG22 | 1:B:1832:VAL:HB | 2.00 | 0.43 |
| 1:B:2365:THR:O | 1:B:2366:ARG:NH1 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2657:LEU:HD11 | 1:B:2704:PHE:HE1 | 1.84 | 0.43 |
| 2:D:234:ILE:HD11 | 2:D:240:LEU:HD11 | 2.01 | 0.43 |
| 1:A:396:CYS:HB2 | 1:A:514:GLN:HB2 | 2.00 | 0.43 |
| 1:A:1808:THR:N | 1:A:1841:SER:OG | 2.52 | 0.43 |
| 1:A:4410:PRO:HA | 1:A:4495:LEU:HD21 | 2.01 | 0.43 |
| 1:B:391:PHE:HA | 1:B:510:LEU:HD12 | 2.00 | 0.43 |
| 1:B:1359:LEU:HA | 1:B:1362:VAL:HG22 | 2.00 | 0.43 |
| 1:B:3081:LEU:O | 1:B:3085:ILE:HG12 | 2.18 | 0.43 |
| 1:B:3199:TYR:HB3 | 1:B:3291:LEU:HB2 | 2.01 | 0.43 |
| 1:B:3866:LEU:HA | 1:B:3869:VAL:HG22 | 2.00 | 0.43 |
| 1:A:1789:ARG:O | 1:A:1859:THR:HA | 2.19 | 0.43 |
| 1:A:2039:HIS:NE2 | 1:A:2596:GLN:OE1 | 2.51 | 0.43 |
| 1:A:4226:LEU:HD22 | 1:A:4355:ALA:HB1 | 2.00 | 0.43 |
| 1:B:1481:LEU:HD11 | 1:B:2065:HIS:O | 2.19 | 0.43 |
| 1:B:1537:VAL:O | 1:B:2127:ARG:NH2 | 2.48 | 0.43 |
| 1:B:1566:LEU:HD22 | 1:B:1799:ILE:HG21 | 2.00 | 0.43 |
| 1:B:2793:LEU:HB3 | 1:B:2842:PHE:CE2 | 2.53 | 0.43 |
| 1:B:3358:LEU:HG | 1:B:3359:LEU:HD22 | 2.01 | 0.43 |
| 1:B:4361:LEU:HA | 1:B:4411:LEU:HD11 | 2.01 | 0.43 |
| 1:A:1347:HIS:O | 1:A:1351:LEU:HG | 2.19 | 0.43 |
| 1:A:2060:GLU:HG2 | 1:A:2064:LYS:NZ | 2.34 | 0.43 |
| 1:A:3206:ALA:O | 1:A:3284:ARG:N | 2.50 | 0.43 |
| 1:A:3711:LEU:HD23 | 1:A:3715:LEU:HD23 | 1.99 | 0.43 |
| 1:A:3817:LEU:HA | 1:A:4182:GLN:HE22 | 1.83 | 0.43 |
| 1:A:4260:ARG:HG2 | 1:A:4367:SER:O | 2.19 | 0.43 |
| 1:B:129:VAL:HG22 | 1:B:134:VAL:HG22 | 2.00 | 0.43 |
| 1:B:199:GLY:HA3 | 1:B:219:VAL:HG13 | 2.01 | 0.43 |
| 1:B:2138:LEU:HD13 | 1:B:2175:VAL:HG12 | 2.01 | 0.43 |
| 1:B:3990:LEU:HB3 | 1:B:3995:LEU:HD22 | 2.01 | 0.43 |
| 1:B:4060:SER:N | 1:B:4063:GLU:OE1 | 2.52 | 0.43 |
| 2:E:254:GLY:H | 2:E:275:VAL:HB | 1.84 | 0.43 |
| 2:C:244:PRO:HG2 | 2:C:316:GLU:HA | 2.00 | 0.43 |
| 1:A:3177:GLN:OE1 | 1:A:3177:GLN:N | 2.52 | 0.43 |
| 1:A:3555:ASN:OD1 | 1:A:3555:ASN:N | 2.52 | 0.43 |
| 1:A:3968:PHE:CE2 | 1:A:4007:LYS:HD2 | 2.54 | 0.43 |
| 1:B:4237:MET:O | 1:B:4241:ILE:HG12 | 2.18 | 0.43 |
| 1:A:200:LEU:HD23 | 1:A:200:LEU:HA | 1.83 | 0.43 |
| 1:A:1359:LEU:HD13 | 1:A:1377:LEU:HD22 | 2.00 | 0.43 |
| 1:A:1477:VAL:HG13 | 1:A:2023:LEU:HD22 | 2.01 | 0.43 |
| 1:A:2171:VAL:HA | 1:A:2174:LEU:HG | 2.00 | 0.43 |
| 1:A:2985:LEU:HG | 1:A:3043:LEU:HD11 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3273:GLU:OE1 | 1:A:3275:ALA:HB2 | 2.19 | 0.43 |
| 1:A:3703:LEU:HD22 | 1:A:3708:VAL:HG11 | 2.00 | 0.43 |
| 1:A:4171:ALA:HA | 1:A:4174:LEU:HB3 | 2.00 | 0.43 |
| 1:B:1121:GLN:HE21 | 1:B:1225:LYS:HB3 | 1.84 | 0.43 |
| 1:A:1015:GLN:HE21 | 1:A:1021:ILE:HG21 | 1.84 | 0.42 |
| 1:A:1883:TYR:OH | 1:A:1908:PRO:O | 2.33 | 0.42 |
| 1:A:3122:ALA:HB2 | 1:A:3370:TYR:CE1 | 2.54 | 0.42 |
| 1:B:396:CYS:HB2 | 1:B:514:GLN:HB2 | 2.01 | 0.42 |
| 1:B:1374:ASN:HA | 1:B:1377:LEU:HG | 2.01 | 0.42 |
| 1:B:1914:LEU:HA | 1:B:1917:MET:HG2 | 1.99 | 0.42 |
| 1:B:2368:THR:HG21 | 1:B:2418:GLY:HA3 | 2.00 | 0.42 |
| 1:B:3164:ALA:HA | 1:B:3298:LEU:HD12 | 2.01 | 0.42 |
| 1:B:3813:LEU:HD23 | 1:B:4189:LEU:HD22 | 2.01 | 0.42 |
| 2:D:255:GLU:OE1 | 2:C:148:ASN:ND2 | 2.52 | 0.42 |
| 1:A:1513:SER:HA | 1:A:1805:LEU:HD11 | 1.99 | 0.42 |
| 1:A:2783:PRO:HG2 | 1:B:3281:ARG:HD3 | 2.00 | 0.42 |
| 1:B:1429:LEU:HD13 | 1:B:1458:VAL:HG23 | 1.99 | 0.42 |
| 1:B:1498:LEU:HD21 | 1:B:1974:TYR:CG | 2.54 | 0.42 |
| 1:B:1498:LEU:HD11 | 1:B:1974:TYR:CD2 | 2.54 | 0.42 |
| 1:B:2981:ALA:HA | 1:B:2984:VAL:HG12 | 2.00 | 0.42 |
| 1:A:79:LEU:HD11 | 1:A:139:ASP:HB3 | 2.01 | 0.42 |
| 1:A:272:VAL:HG21 | 1:A:292:THR:HA | 2.01 | 0.42 |
| 1:A:2012:GLU:HA | 1:A:2015:ILE:HB | 1.99 | 0.42 |
| 1:A:3846:HIS:CG | 1:A:3847:PRO:HD2 | 2.54 | 0.42 |
| 1:B:834:THR:HG23 | 1:B:836:ILE:H | 1.84 | 0.42 |
| 1:B:1172:PRO:HA | 1:B:1175:GLU:HB2 | 2.00 | 0.42 |
| 1:B:1975:GLN:HA | 1:B:1978:ILE:HG22 | 2.01 | 0.42 |
| 1:B:2324:ALA:H | 1:B:2327:ARG:NH2 | 2.16 | 0.42 |
| 1:B:3108:CYS:HA | 1:B:3111:MET:HG2 | 2.00 | 0.42 |
| 1:B:3336:HIS:O | 1:B:3340:HIS:HB2 | 2.19 | 0.42 |
| 1:B:3499:ALA:HB1 | 1:B:3850:GLY:HA2 | 2.00 | 0.42 |
| 1:A:2027:ILE:HG22 | 1:A:2031:LEU:HD23 | 1.99 | 0.42 |
| 1:A:2590:GLU:O | 1:A:2594:ILE:HG12 | 2.19 | 0.42 |
| 1:B:100:ALA:HB3 | 1:B:212:LYS:HZ2 | 1.84 | 0.42 |
| 1:B:1337:ARG:HH21 | 1:B:1349:GLN:HE22 | 1.67 | 0.42 |
| 1:B:2730:THR:HG21 | 1:B:2796:LEU:HD22 | 2.02 | 0.42 |
| 1:B:2786:THR:HA | 1:B:2789:MET:HG3 | 2.01 | 0.42 |
| 1:B:3169:ILE:HD12 | 1:B:3183:LEU:HD21 | 2.00 | 0.42 |
| 1:A:365:ASN:OD1 | 1:A:365:ASN:N | 2.52 | 0.42 |
| 1:A:1033:THR:HA | 1:A:1304:ARG:HG3 | 2.01 | 0.42 |
| 1:A:3108:CYS:HB3 | 1:A:3355:THR:HG21 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3177:GLN:HE21 | 1:A:3198:SER:H | 1.66 | 0.42 |
| 1:B:3085:ILE:HA | 1:B:3088:VAL:HG12 | 2.00 | 0.42 |
| 1:B:3125:MET:O | 1:B:3129:ILE:HG13 | 2.20 | 0.42 |
| 1:A:100:ALA:HB3 | 1:A:212:LYS:HZ1 | 1.85 | 0.42 |
| 1:B:73:LEU:HB3 | 1:B:944:ILE:HD13 | 2.01 | 0.42 |
| 1:B:1412:ILE:HG21 | 1:B:1457:TYR:HE2 | 1.85 | 0.42 |
| 1:B:1966:GLU:O | 1:B:1969:ARG:HG2 | 2.20 | 0.42 |
| 1:B:2066:LEU:HD22 | 1:B:2078:THR:HG21 | 2.02 | 0.42 |
| 1:B:3498:ALA:HB2 | 1:B:3545:LEU:HD23 | 2.02 | 0.42 |
| 2:E:312:ASN:HD21 | 2:E:316:GLU:HB2 | 1.85 | 0.42 |
| 1:A:3201:PHE:CE2 | 1:A:3284:ARG:HA | 2.55 | 0.42 |
| 1:A:3287:ASP:HB3 | 1:B:3262:LEU:HD23 | 2.02 | 0.42 |
| 1:A:3337:CYS:HB3 | 1:A:3348:MET:HE3 | 2.02 | 0.42 |
| 1:A:3502:TRP:O | 1:A:3506:GLU:HG2 | 2.20 | 0.42 |
| 1:A:4409:VAL:HG12 | 1:A:4495:LEU:HD22 | 2.01 | 0.42 |
| 1:B:929:PRO:HG2 | 1:B:938:ASP:HB3 | 2.01 | 0.42 |
| 1:B:1347:HIS:O | 1:B:1351:LEU:HG | 2.20 | 0.42 |
| 1:B:1819:ILE:HG12 | 1:B:1831:LEU:HD21 | 2.01 | 0.42 |
| 1:B:1830:ARG:HH21 | 1:B:1833:VAL:HG22 | 1.84 | 0.42 |
| 1:B:2726:LEU:HB3 | 1:B:2792:PHE:CE1 | 2.55 | 0.42 |
| 1:B:4358:SER:O | 1:B:4361:LEU:HB3 | 2.20 | 0.42 |
| 1:A:1799:ILE:HG23 | 1:A:1882:THR:HA | 2.02 | 0.42 |
| 1:A:2717:ARG:HD2 | 1:B:2876:LYS:HE2 | 2.02 | 0.42 |
| 1:B:1405:ALA:HA | 1:B:1454:LEU:HD11 | 2.00 | 0.42 |
| 1:B:1829:ARG:CZ | 1:B:1892:LYS:HE2 | 2.50 | 0.42 |
| 1:B:2177:ARG:HG3 | 1:B:2178:LEU:N | 2.34 | 0.42 |
| 1:B:2562:SER:OG | 1:B:2563:VAL:N | 2.52 | 0.42 |
| 1:B:2826:PHE:HE1 | 1:B:2836:GLN:HG2 | 1.83 | 0.42 |
| 1:B:2923:LEU:HA | 1:B:2926:VAL:HG22 | 2.01 | 0.42 |
| 1:B:4409:VAL:HG12 | 1:B:4495:LEU:HD22 | 2.01 | 0.42 |
| 2:E:305:ASN:HB2 | 2:E:321:ASN:HD22 | 1.83 | 0.42 |
| 2:C:163:TYR:HB3 | 2:C:209:ARG:HB3 | 2.02 | 0.42 |
| 1:A:102:LEU:HD22 | 1:A:216:TRP:CD1 | 2.55 | 0.42 |
| 1:A:854:ASP:HA | 1:A:907:THR:HB | 2.02 | 0.42 |
| 1:A:1927:ARG:NH2 | 1:B:4189:LEU:O | 2.53 | 0.42 |
| 1:A:3443:ASP:OD1 | 1:A:3446:THR:OG1 | 2.25 | 0.42 |
| 1:B:102:LEU:HD22 | 1:B:216:TRP:CD1 | 2.55 | 0.42 |
| 1:B:225:HIS:NE2 | 1:B:259:LEU:O | 2.49 | 0.42 |
| 1:B:1092:GLU:OE1 | 1:B:1127:ASN:ND2 | 2.53 | 0.42 |
| 1:B:2366:ARG:HA | 1:B:2366:ARG:HD3 | 1.81 | 0.42 |
| 1:B:2411:MET:HE2 | 1:B:2411:MET:HB2 | 1.74 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:2755:ASP:N | 1:B:2755:ASP:OD1 | 2.41 | 0.42 |
| 1:B:2756:PRO:O | 1:B:2760:HIS:ND1 | 2.50 | 0.42 |
| 1:B:3224:HIS:HB2 | 1:B:3297:LYS:HE2 | 2.00 | 0.42 |
| 1:A:825:LEU:HB2 | 1:A:847:GLN:HB3 | 2.02 | 0.42 |
| 1:A:926:VAL:HG21 | 1:A:964:LEU:HD13 | 2.02 | 0.42 |
| 1:B:1309:THR:HG23 | 1:B:1311:ILE:H | 1.85 | 0.42 |
| 1:B:1441:ALA:HB2 | 1:B:2014:LEU:HD13 | 2.02 | 0.42 |
| 1:B:2659:SER:HA | 1:B:2662:GLN:HG2 | 2.02 | 0.42 |
| 1:B:2768:GLY:HA3 | 1:B:2831:GLY:HA2 | 2.02 | 0.42 |
| 1:A:98:SER:HG | 1:A:212:LYS:NZ | 2.17 | 0.41 |
| 1:A:1768:HIS:HA | 1:A:1771:GLN:HG2 | 2.02 | 0.41 |
| 1:A:1883:TYR:HE1 | 1:A:1908:PRO:HG2 | 1.84 | 0.41 |
| 1:A:2586:MET:HA | 1:A:2589:LEU:HG | 2.02 | 0.41 |
| 1:A:4060:SER:N | 1:A:4063:GLU:OE1 | 2.52 | 0.41 |
| 1:B:93:VAL:HG11 | 1:B:216:TRP:CH2 | 2.55 | 0.41 |
| 1:B:1181:ILE:HG23 | 1:B:1367:PRO:HB2 | 2.02 | 0.41 |
| 1:B:2696:LEU:HD23 | 1:B:2696:LEU:HA | 1.84 | 0.41 |
| 1:B:4362:GLU:O | 1:B:4365:SER:OG | 2.31 | 0.41 |
| 1:A:270:LEU:HD12 | 1:A:270:LEU:HA | 1.88 | 0.41 |
| 1:A:3687:LEU:O | 1:A:3691:THR:HG23 | 2.20 | 0.41 |
| 1:B:2114:GLN:O | 1:B:2118:PHE:HB2 | 2.20 | 0.41 |
| 1:B:2139:LEU:HA | 1:B:2142:LEU:HD12 | 2.02 | 0.41 |
| 1:B:2174:LEU:HD23 | 1:B:2177:ARG:HH22 | 1.84 | 0.41 |
| 1:B:2575:LEU:O | 1:B:2578:GLN:NE2 | 2.53 | 0.41 |
| 1:A:961:LEU:HD23 | 1:A:961:LEU:HA | 1.93 | 0.41 |
| 1:A:4167:LEU:HA | 1:A:4168:PRO:HD2 | 1.94 | 0.41 |
| 1:A:4184:LEU:HD11 | 1:A:4212:LEU:HB3 | 2.02 | 0.41 |
| 1:B:1359:LEU:HD13 | 1:B:1377:LEU:HD22 | 2.03 | 0.41 |
| 1:B:1426:PRO:HD3 | 1:B:1461:GLU:HG3 | 2.02 | 0.41 |
| 1:B:1557:LEU:HB3 | 1:B:1560:LEU:HD11 | 2.02 | 0.41 |
| 1:B:1817:ILE:HD12 | 1:B:1857:LYS:O | 2.21 | 0.41 |
| 1:B:2063:PHE:HD1 | 1:B:2067:CYS:HG | 1.67 | 0.41 |
| 1:B:2122:SER:HA | 1:B:2177:ARG:CZ | 2.51 | 0.41 |
| 1:B:2172:VAL:HG23 | 1:B:2357:VAL:HG11 | 2.02 | 0.41 |
| 1:B:3719:LEU:HD13 | 1:B:3807:PHE:HD2 | 1.85 | 0.41 |
| 1:B:3991:TYR:CE1 | 1:B:3997:GLN:HA | 2.55 | 0.41 |
| 1:B:4324:LEU:HG | 1:B:4398:LEU:HD22 | 2.02 | 0.41 |
| 2:E:204:ARG:HG3 | 2:E:220:VAL:HB | 2.01 | 0.41 |
| 2:C:221:THR:H | 2:C:232:LEU:HA | 1.85 | 0.41 |
| 1:A:2204:ILE:HD13 | 1:A:2353:PHE:CZ | 2.56 | 0.41 |
| 1:B:263:LEU:HD23 | 1:B:266:ALA:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1043:PRO:HD3 | 1:B:1090:VAL:O | 2.20 | 0.41 |
| 1:B:1489:GLU:O | 1:B:1493:GLN:HG3 | 2.21 | 0.41 |
| 1:B:2985:LEU:HA | 1:B:2985:LEU:HD23 | 1.73 | 0.41 |
| 1:B:3967:LEU:HD22 | 1:B:4004:LEU:HB3 | 2.03 | 0.41 |
| 1:B:3968:PHE:CE2 | 1:B:4007:LYS:HD2 | 2.55 | 0.41 |
| 1:B:4214:PHE:HB3 | 1:B:4326:VAL:HG21 | 2.02 | 0.41 |
| 1:B:198:ASP:HA | 1:B:201:LYS:HG2 | 2.02 | 0.41 |
| 1:B:2135:LEU:HA | 1:B:2138:LEU:HG | 2.01 | 0.41 |
| 1:B:2859:VAL:O | 1:B:2863:VAL:HG12 | 2.20 | 0.41 |
| 1:A:2339:LEU:HD11 | 1:A:2411:MET:HE1 | 2.02 | 0.41 |
| 1:A:3401:LEU:HD13 | 1:A:3456:TRP:CD2 | 2.56 | 0.41 |
| 1:A:3991:TYR:CE1 | 1:A:3997:GLN:HA | 2.56 | 0.41 |
| 1:B:354:ASN:OD1 | 1:B:359:LYS:NZ | 2.41 | 0.41 |
| 1:B:1568:PHE:HA | 1:B:1793:LEU:HD21 | 2.02 | 0.41 |
| 1:B:2697:ASN:OD1 | 1:B:2698:GLN:N | 2.54 | 0.41 |
| 1:B:3401:LEU:HD13 | 1:B:3456:TRP:CD2 | 2.56 | 0.41 |
| 1:B:4410:PRO:HA | 1:B:4495:LEU:HD21 | 2.02 | 0.41 |
| 1:A:3455:LYS:HE3 | 1:A:3455:LYS:HB3 | 1.93 | 0.41 |
| 1:A:3621:GLU:OE1 | 1:A:3621:GLU:N | 2.47 | 0.41 |
| 1:B:365:ASN:OD1 | 1:B:365:ASN:N | 2.53 | 0.41 |
| 1:B:1966:GLU:O | 1:B:1970:VAL:HG23 | 2.20 | 0.41 |
| 1:B:2705:LEU:HD23 | 1:B:2705:LEU:HA | 1.91 | 0.41 |
| 1:B:3618:GLN:HB2 | 1:B:3846:HIS:NE2 | 2.36 | 0.41 |
| 1:B:3718:LEU:O | 1:B:3722:SER:HB3 | 2.21 | 0.41 |
| 2:C:301:ILE:HD12 | 2:C:330:SER:HB3 | 2.03 | 0.41 |
| 1:A:743:ILE:HG23 | 1:A:744:HIS:CD2 | 2.56 | 0.41 |
| 1:A:1359:LEU:HA | 1:A:1362:VAL:HG22 | 2.02 | 0.41 |
| 1:A:2661:LEU:HB2 | 1:A:2721:LEU:HD23 | 2.02 | 0.41 |
| 1:A:3341:ILE:HG22 | 1:A:3343:ASP:H | 1.86 | 0.41 |
| 1:A:3522:PHE:CE2 | 1:A:3556:TYR:HB3 | 2.56 | 0.41 |
| 1:A:4396:LEU:HB3 | 1:A:4484:THR:HG21 | 2.03 | 0.41 |
| 1:B:58:LEU:HB2 | 1:B:965:GLN:HB3 | 2.02 | 0.41 |
| 1:B:1505:PRO:HB3 | 1:B:1928:TYR:CE2 | 2.56 | 0.41 |
| 1:B:2856:ILE:HA | 1:B:2859:VAL:HG12 | 2.03 | 0.41 |
| 2:C:320:VAL:O | 2:C:332:ALA:HA | 2.21 | 0.41 |
| 1:A:129:VAL:HG21 | 1:A:391:PHE:CG | 2.56 | 0.41 |
| 1:A:138:LYS:HZ2 | 1:A:372:LEU:HB3 | 1.85 | 0.41 |
| 1:A:262:LEU:HA | 1:A:376:PRO:HG3 | 2.03 | 0.41 |
| 1:A:272:VAL:HG22 | 1:A:292:THR:HG22 | 2.02 | 0.41 |
| 1:A:301:TYR:HB3 | 1:A:340:PRO:HA | 2.02 | 0.41 |
| 1:A:913:LYS:HB3 | 1:A:915:LEU:HD11 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1579:ILE:HG12 | 1:A:1778:ILE:HG13 | 2.02 | 0.41 |
| 1:A:2098:ASN:O | 1:A:2101:GLN:HG3 | 2.21 | 0.41 |
| 1:A:2669:LEU:HD12 | 1:A:2669:LEU:HA | 1.93 | 0.41 |
| 1:A:2777:HIS:CD2 | 1:A:2778:SER:H | 2.39 | 0.41 |
| 1:A:2837:VAL:HG11 | 1:A:2913:MET:HE2 | 2.03 | 0.41 |
| 1:A:3040:LEU:HA | 1:A:3040:LEU:HD23 | 1.84 | 0.41 |
| 1:A:4230:ASP:OD1 | 1:A:4231:GLY:N | 2.54 | 0.41 |
| 1:B:1392:CYS:O | 1:B:1396:ALA:HB3 | 2.21 | 0.41 |
| 1:B:1768:HIS:HA | 1:B:1771:GLN:HG2 | 2.03 | 0.41 |
| 1:B:1817:ILE:HD11 | 1:B:1856:MET:SD | 2.61 | 0.41 |
| 1:B:2122:SER:HA | 1:B:2177:ARG:NH2 | 2.35 | 0.41 |
| 1:B:2411:MET:O | 1:B:2415:ILE:HG12 | 2.20 | 0.41 |
| 1:B:2726:LEU:HB3 | 1:B:2792:PHE:HE1 | 1.85 | 0.41 |
| 2:D:211:LEU:HA | 2:D:264:PHE:HE2 | 1.85 | 0.41 |
| 2:D:326:THR:HB | 2:D:329:ILE:HB | 2.02 | 0.41 |
| 1:A:637:GLU:HG2 | 1:A:713:PRO:HG2 | 2.03 | 0.41 |
| 1:A:2797:GLN:O | 1:A:2801:SER:OG | 2.25 | 0.41 |
| 1:A:3074:THR:N | 1:B:2394:ARG:HE | 2.19 | 0.41 |
| 1:A:3602:PRO:HB2 | 1:A:3603:LEU:H | 1.69 | 0.41 |
| 1:A:4319:HIS:O | 1:A:4323:LEU:HD13 | 2.20 | 0.41 |
| 1:B:511:SER:O | 1:B:568:LEU:N | 2.44 | 0.41 |
| 1:B:1110:LEU:HB3 | 1:B:1114:ILE:HD12 | 2.03 | 0.41 |
| 1:B:1394:PHE:HE2 | 1:B:1439:LEU:HA | 1.86 | 0.41 |
| 1:B:2061:GLU:OE2 | 1:B:2065:HIS:NE2 | 2.54 | 0.41 |
| 1:A:198:ASP:OD1 | 1:A:199:GLY:N | 2.54 | 0.40 |
| 1:A:574:THR:HG22 | 1:A:624:ARG:HD2 | 2.02 | 0.40 |
| 1:B:1927:ARG:O | 1:B:1930:LEU:HG | 2.21 | 0.40 |
| 1:B:2357:VAL:O | 1:B:2361:ILE:HG12 | 2.21 | 0.40 |
| 1:B:3180:GLU:O | 1:B:3184:GLN:NE2 | 2.54 | 0.40 |
| 1:A:859:LEU:HA | 1:A:904:VAL:O | 2.21 | 0.40 |
| 1:A:2775:ASN:HB3 | 1:A:2777:HIS:CE1 | 2.56 | 0.40 |
| 1:A:3514:PRO:HB3 | 1:A:3553:HIS:NE2 | 2.35 | 0.40 |
| 1:A:3813:LEU:HD21 | 1:B:1927:ARG:HH21 | 1.86 | 0.40 |
| 1:A:3858:LEU:HD13 | 1:A:3872:ARG:NH2 | 2.37 | 0.40 |
| 1:A:3990:LEU:HB3 | 1:A:3995:LEU:HD22 | 2.04 | 0.40 |
| 1:B:1560:LEU:HD22 | 1:B:1879:TYR:CD2 | 2.56 | 0.40 |
| 2:C:294:TYR:HB3 | 2:C:331:PHE:HB3 | 2.03 | 0.40 |
| 1:A:2583:LEU:HA | 1:A:2586:MET:HG2 | 2.03 | 0.40 |
| 1:A:3077:LEU:HA | 1:A:3081:LEU:HD23 | 2.03 | 0.40 |
| 1:B:732:CYS:HB3 | 1:B:752:CYS:HB2 | 2.03 | 0.40 |
| 1:B:1428:LEU:O | 1:B:1432:LEU:HG | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1772:PRO:HA | 1:B:1773:PRO:HD2 | 1.97 | 0.40 |
| 1:B:2171:VAL:O | 1:B:2175:VAL:HG22 | 2.22 | 0.40 |
| 1:B:3240:SER:HB3 | 1:B:3256:PRO:HG3 | 2.02 | 0.40 |
| 1:B:3623:ILE:HD12 | 1:B:3623:ILE:HA | 1.93 | 0.40 |
| 2:D:253:GLN:NE2 | 2:C:270:ILE:HD13 | 2.36 | 0.40 |
| 2:E:246:GLY:N | 2:E:317:VAL:O | 2.51 | 0.40 |
| 2:C:194:VAL:HA | 2:C:230:ALA:O | 2.22 | 0.40 |
| 1:A:184:SER:HA | 1:A:189:TYR:CD2 | 2.56 | 0.40 |
| 1:A:2981:ALA:HB1 | 1:A:3043:LEU:HD12 | 2.03 | 0.40 |
| 1:A:2985:LEU:HD23 | 1:A:2985:LEU:HA | 1.78 | 0.40 |
| 1:A:3539:LYS:HA | 1:A:3542:VAL:HG22 | 2.03 | 0.40 |
| 1:A:4373:MET:HG3 | 1:A:4395:LEU:HD11 | 2.03 | 0.40 |
| 1:B:1979:GLN:NE2 | 1:B:1983:GLN:HE22 | 2.20 | 0.40 |
| 1:B:3635:LEU:HD13 | 1:B:3686:ILE:HD11 | 2.02 | 0.40 |
| 1:A:1104:VAL:HG23 | 1:A:1303:ILE:HG13 | 2.03 | 0.40 |
| 1:A:1188:LEU:HG | 1:A:1192:LEU:HD21 | 2.04 | 0.40 |
| 1:A:2357:VAL:O | 1:A:2361:ILE:HG12 | 2.21 | 0.40 |
| 1:B:945:TYR:HD1 | 1:B:952:LEU:HD23 | 1.86 | 0.40 |
| 1:B:1328:HIS:CD2 | 1:B:1359:LEU:HD22 | 2.57 | 0.40 |
| 1:B:2103:LEU:HD13 | 1:B:2103:LEU:HA | 1.87 | 0.40 |
| 1:B:3085:ILE:HD12 | 1:B:3333:LEU:HD21 | 2.04 | 0.40 |
| 1:B:3226:GLN:HB2 | 1:B:3295:GLN:H | 1.86 | 0.40 |
| 1:B:3350:SER:HB3 | 1:B:3388:GLN:NE2 | 2.37 | 0.40 |
| 1:B:3514:PRO:HB3 | 1:B:3553:HIS:NE2 | 2.36 | 0.40 |
| 1:B:3848:MET:HG3 | 1:B:3849:TYR:CD1 | 2.57 | 0.40 |
| 2:E:206:VAL:HG23 | 2:E:218:ALA:HB3 | 2.04 | 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 | 2740/4867 (56%) | 2670 (97%) | 69 (2%) | 1 (0%) | 100 | 100 |
| 1 | B | 2740/4867 (56%) | 2670 (97%) | 70 (3%) | 0 | 100 | 100 |
| 2 | C | 171/325 (53%) | 166 (97%) | 5 (3%) | 0 | 100 | 100 |
| 2 | D | 179/325 (55%) | 165 (92%) | 13 (7%) | 1 (1%) | 25 | 66 |
| 2 | E | 165/325 (51%) | 154 (93%) | 11 (7%) | 0 | 100 | 100 |
| All | All | 5995/10709 (56%) | 5825 (97%) | 168 (3%) | 2 (0%) | 100 | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4315 | LEU |
| 2 | D | 142 | SER |

### 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 | 2493/4225 (59%) | 2488 (100%) | 5 (0%) | 93 | 96 |
| 1 | B | 2493/4225 (59%) | 2489 (100%) | 4 (0%) | 93 | 96 |
| 2 | C | 144/269 (54%) | 144 (100%) | 0 | 100 | 100 |
| 2 | D | 150/269 (56%) | 147 (98%) | 3 (2%) | 55 | 74 |
| 2 | E | 140/269 (52%) | 140 (100%) | 0 | 100 | 100 |
| All | All | 5420/9257 (59%) | 5408 (100%) | 12 (0%) | 93 | 96 |

All (12) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1829 | ARG |
| 1 | A | 2024 | ARG |
| 1 | A | 3193 | ARG |
| 1 | A | 3993 | ARG |
| 1 | A | 4000 | ARG |
| 1 | B | 1829 | ARG |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 3193 | ARG |
| 1 | B | 3821 | LYS |
| 1 | B | 4000 | ARG |
| 2 | D | 203 | ARG |
| 2 | D | 205 | ARG |
| 2 | D | 247 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 244 | GLN |
| 1 | A | 744 | HIS |
| 1 | A | 848 | HIS |
| 1 | A | 1376 | ASN |
| 1 | A | 1771 | GLN |
| 1 | A | 1929 | ASN |
| 1 | A | 1983 | GLN |
| 1 | A | 1989 | ASN |
| 1 | A | 2200 | GLN |
| 1 | A | 2325 | HIS |
| 1 | A | 2379 | GLN |
| 1 | A | 2670 | ASN |
| 1 | A | 2931 | GLN |
| 1 | A | 3224 | HIS |
| 1 | A | 3283 | HIS |
| 1 | A | 3335 | HIS |
| 1 | A | 3377 | ASN |
| 1 | A | 3519 | GLN |
| 1 | A | 3697 | HIS |
| 1 | A | 3709 | ASN |
| 1 | A | 3769 | GLN |
| 1 | A | 3814 | GLN |
| 1 | A | 3853 | HIS |
| 1 | A | 4072 | GLN |
| 1 | A | 4332 | ASN |
| 1 | A | 4351 | GLN |
| 1 | B | 1121 | GLN |
| 1 | B | 1323 | GLN |
| 1 | B | 1333 | ASN |
| 1 | B | 1776 | GLN |
| 1 | B | 1913 | HIS |
| 1 | B | 1929 | ASN |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1979 | GLN |
| 1 | B | 1989 | ASN |
| 1 | B | 2101 | GLN |
| 1 | B | 2790 | GLN |
| 1 | B | 3228 | HIS |
| 1 | B | 3609 | HIS |
| 1 | B | 3859 | HIS |
| 1 | B | 4072 | GLN |
| 1 | B | 4245 | HIS |
| 2 | D | 181 | ASN |
| 2 | D | 253 | GLN |
| 2 | E | 146 | GLN |
| 2 | E | 148 | ASN |
| 2 | E | 253 | GLN |
| 2 | E | 321 | ASN |
| 2 | C | 196 | ASN |
| 2 | C | 198 | HIS |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no monosaccharides in this entry.

### 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

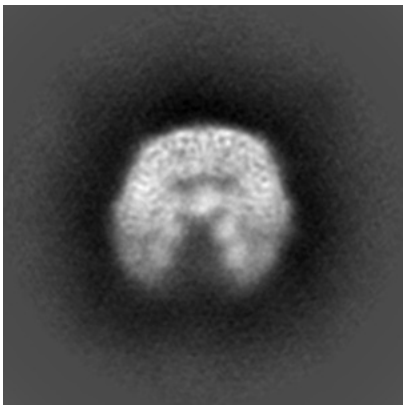
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15672. These allow visual inspection of the internal detail of the map and identification of artifacts.

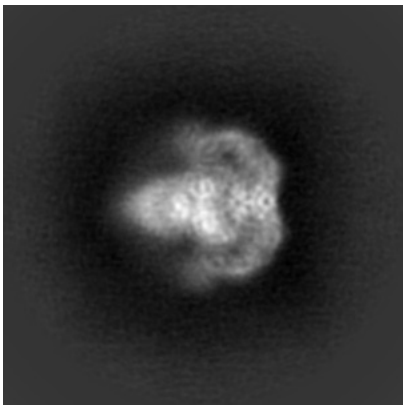
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

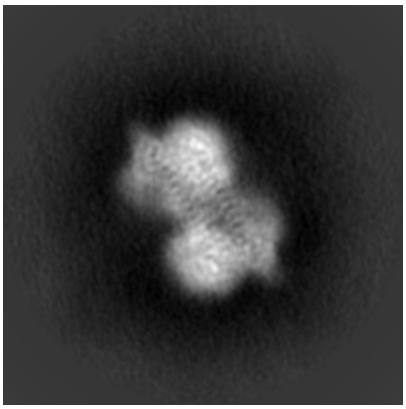
### 6.1.1 Primary map



X

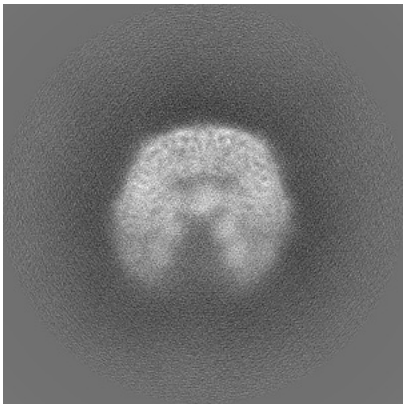


Y

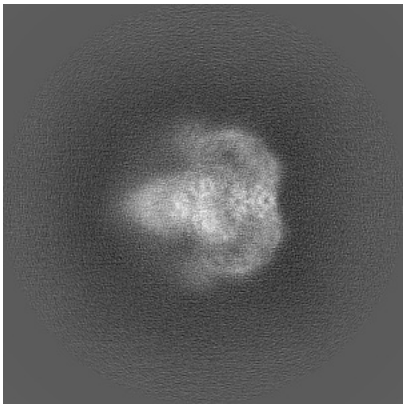


Z

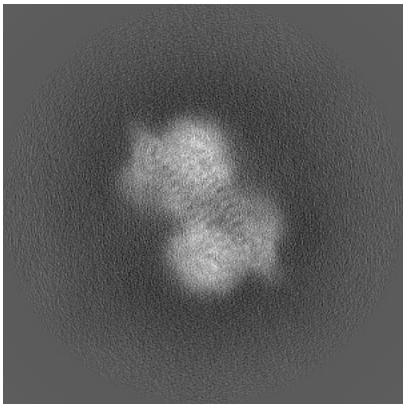
### 6.1.2 Raw map



X



Y

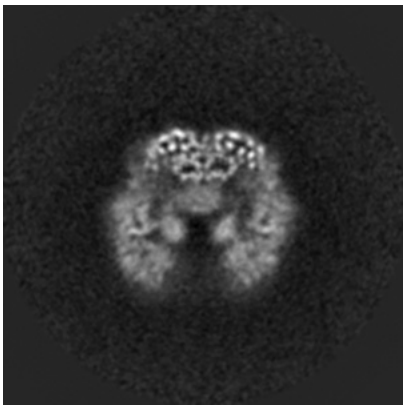


Z

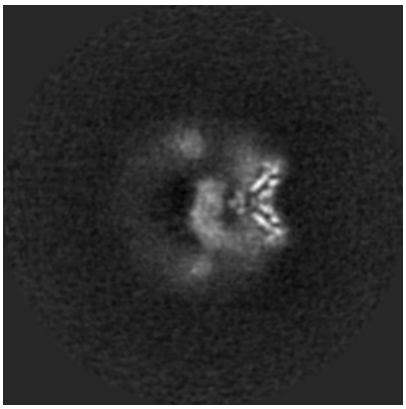
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

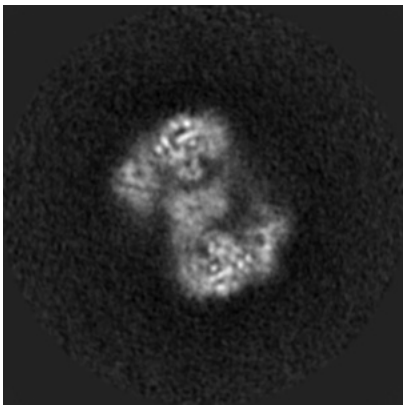
### 6.2.1 Primary map



X Index: 182

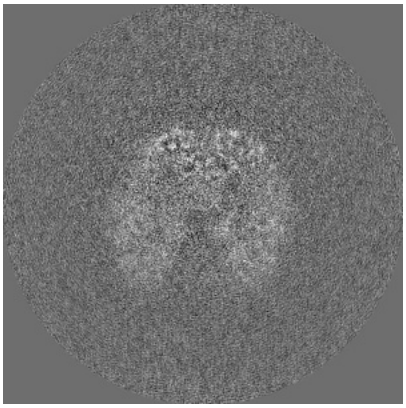


Y Index: 182

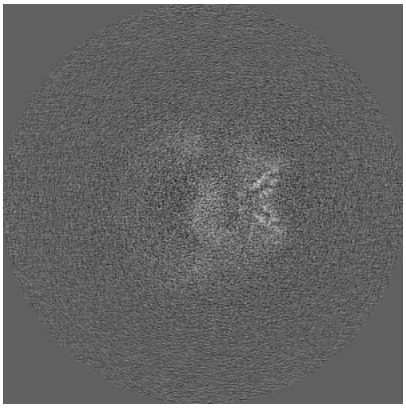


Z Index: 182

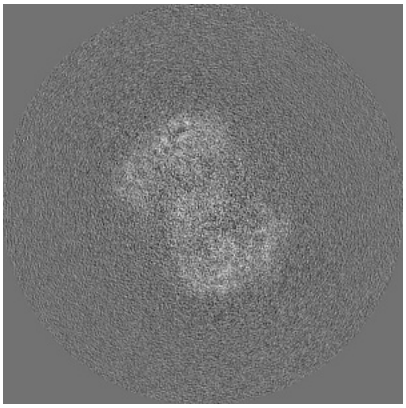
### 6.2.2 Raw map



X Index: 182



Y Index: 182

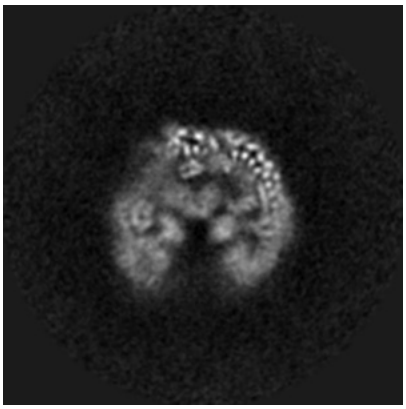


Z Index: 182

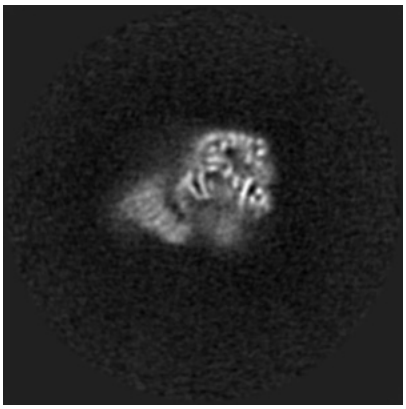
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

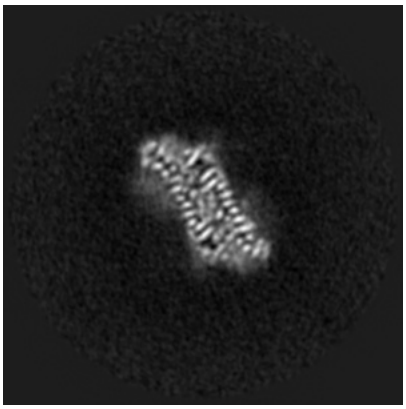
### 6.3.1 Primary map



X Index: 174

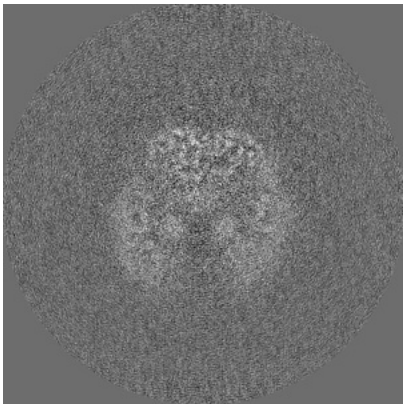


Y Index: 138

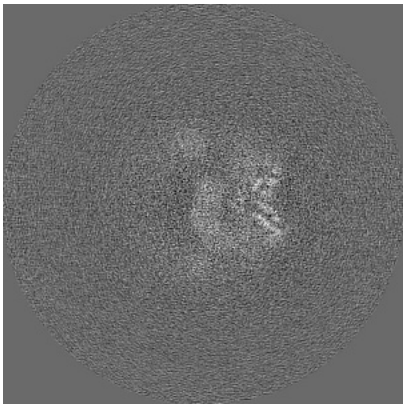


Z Index: 235

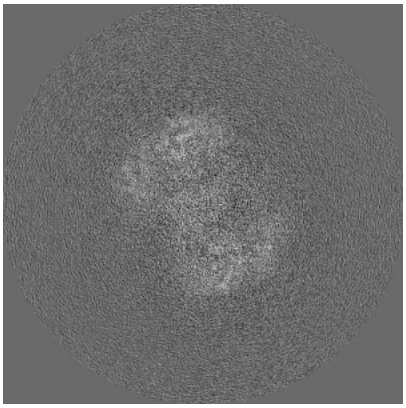
### 6.3.2 Raw map



X Index: 181



Y Index: 181

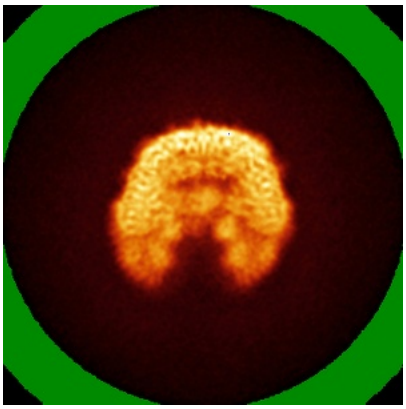


Z Index: 183

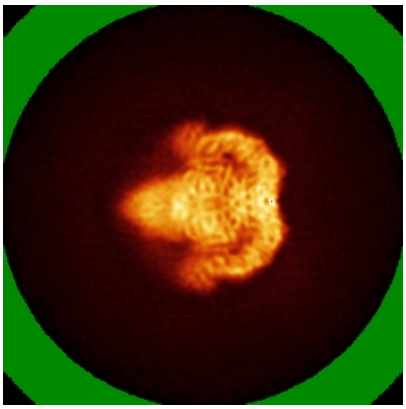
The images above show the largest variance slices of the map in three orthogonal directions.

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

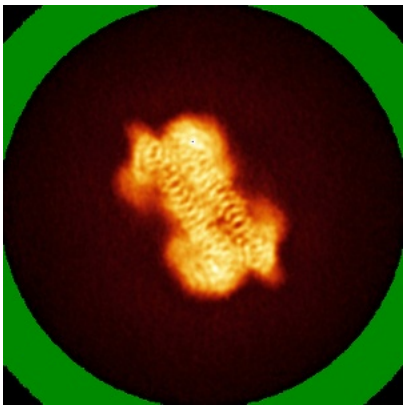
### 6.4.1 Primary map



X

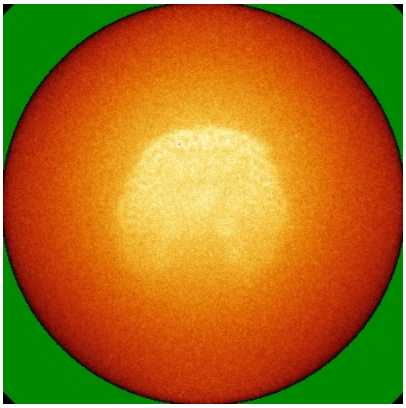


Y

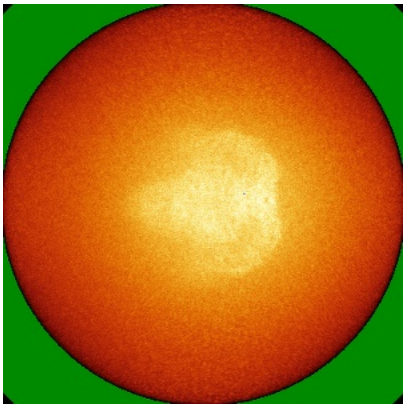


Z

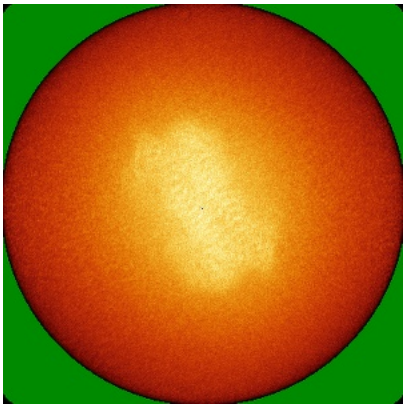
### 6.4.2 Raw map



X



Y

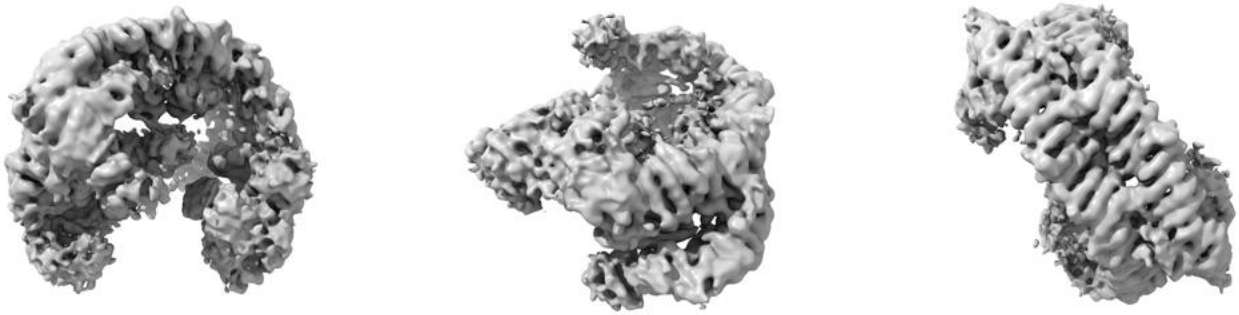


Z

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

## 6.5 Orthogonal surface views (i)

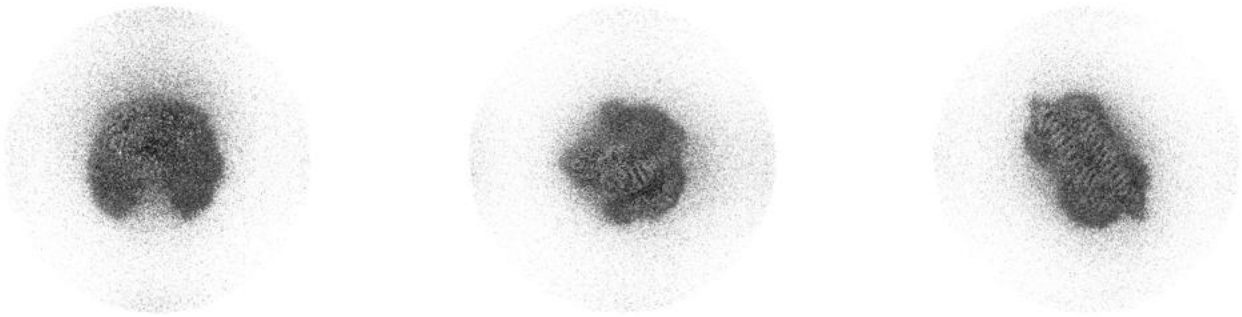
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00423. 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



X Y Z

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.

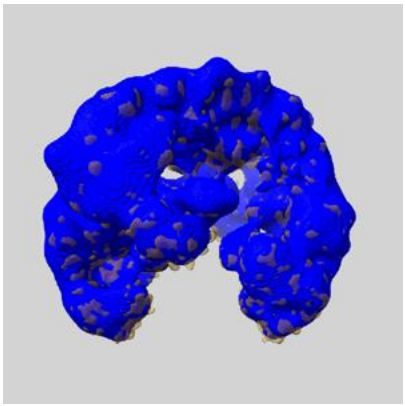
## 6.6 Mask visualisation

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

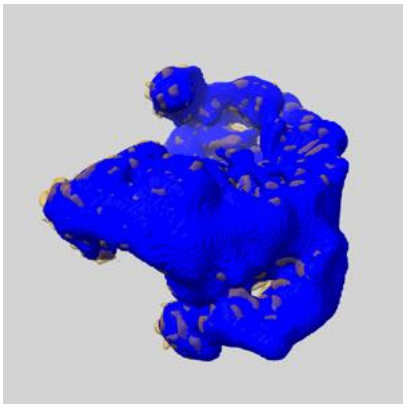
A mask typically either:

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

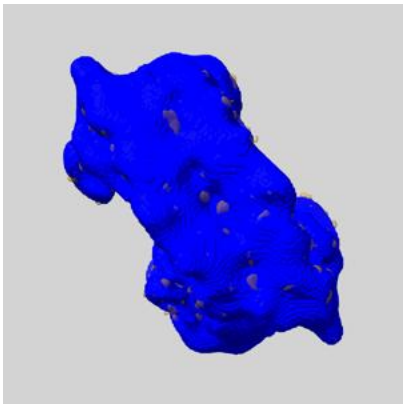
### 6.6.1 emd_15672_msk_1.map



X



Y

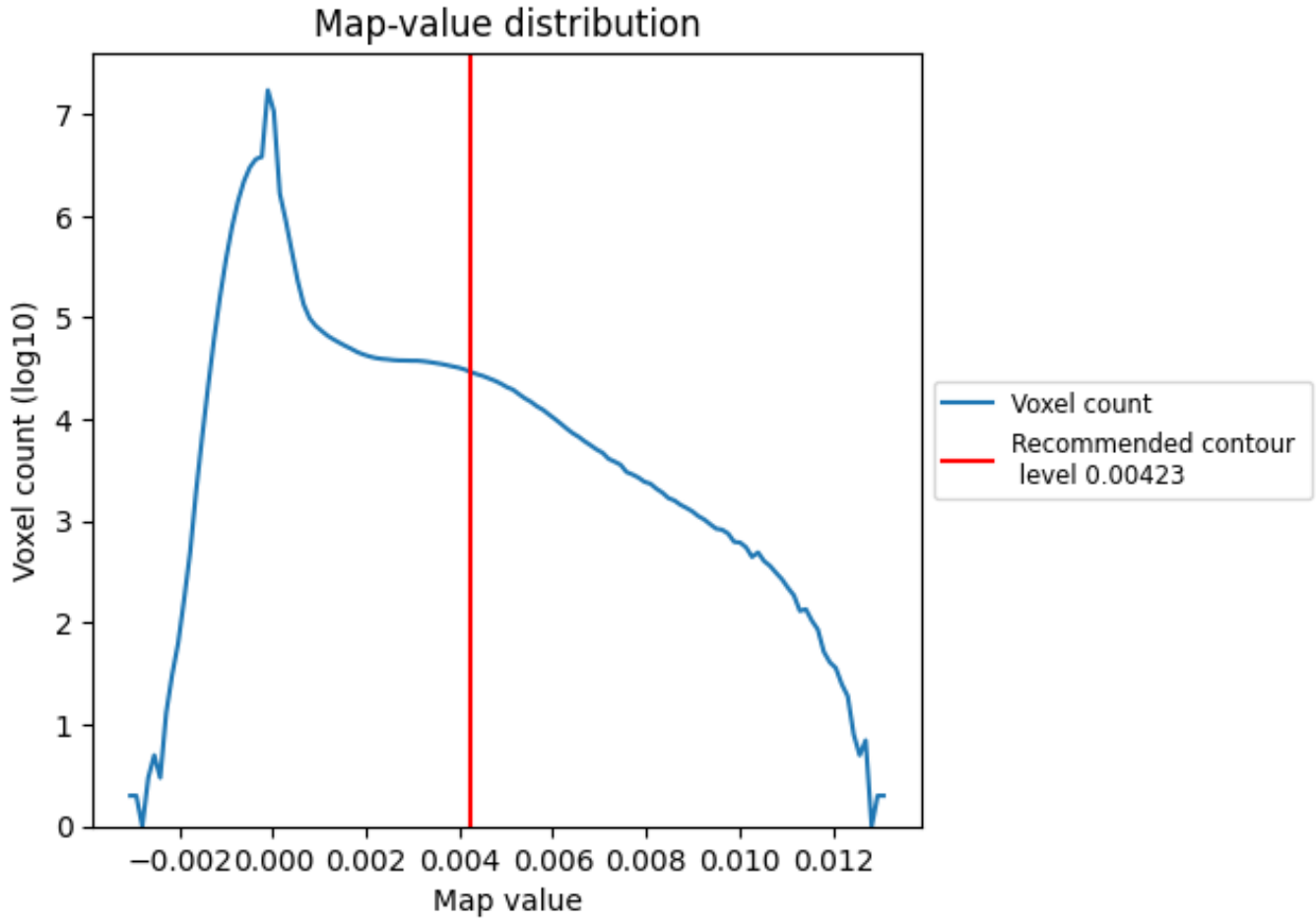


Z

# 7 Map analysis

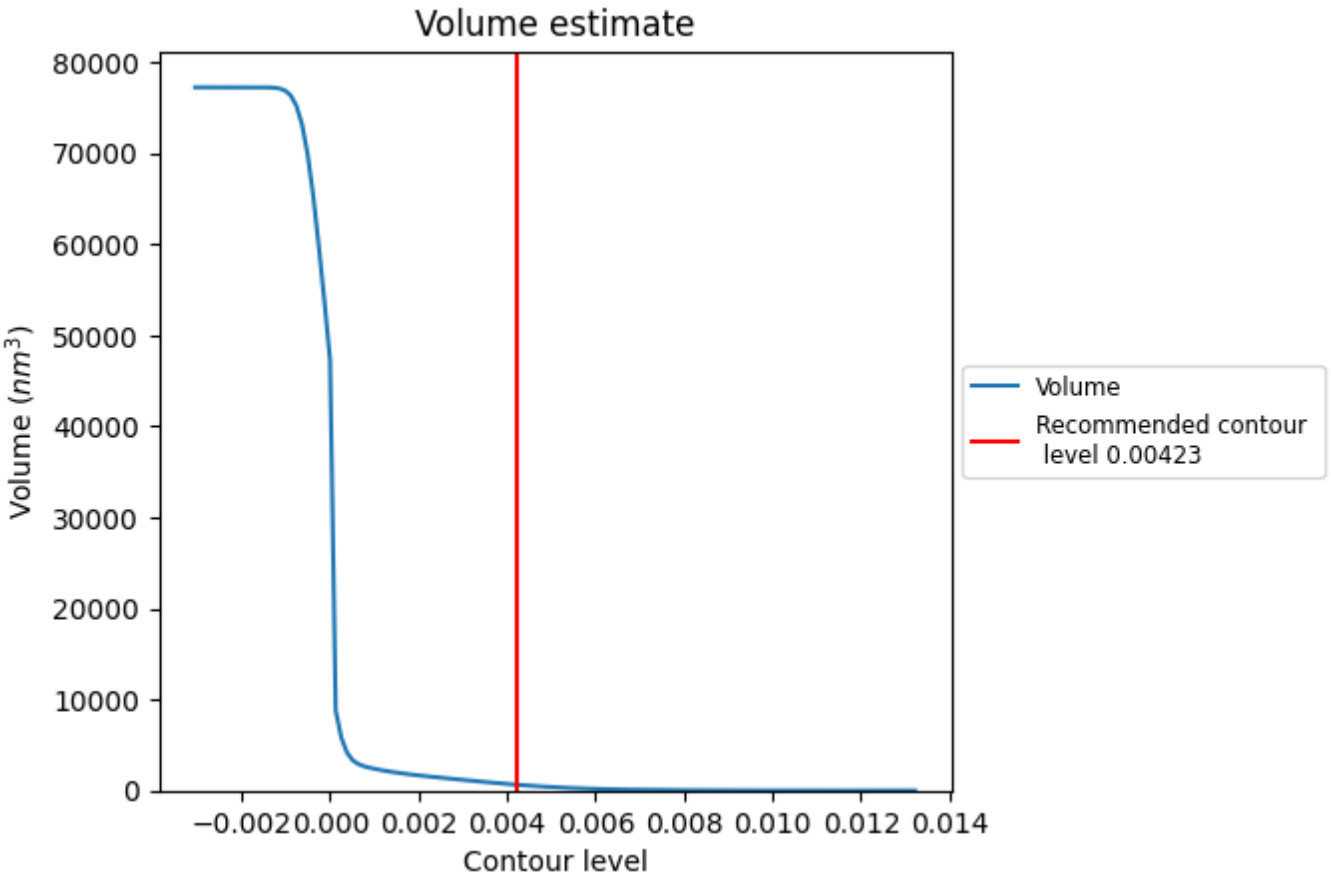
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

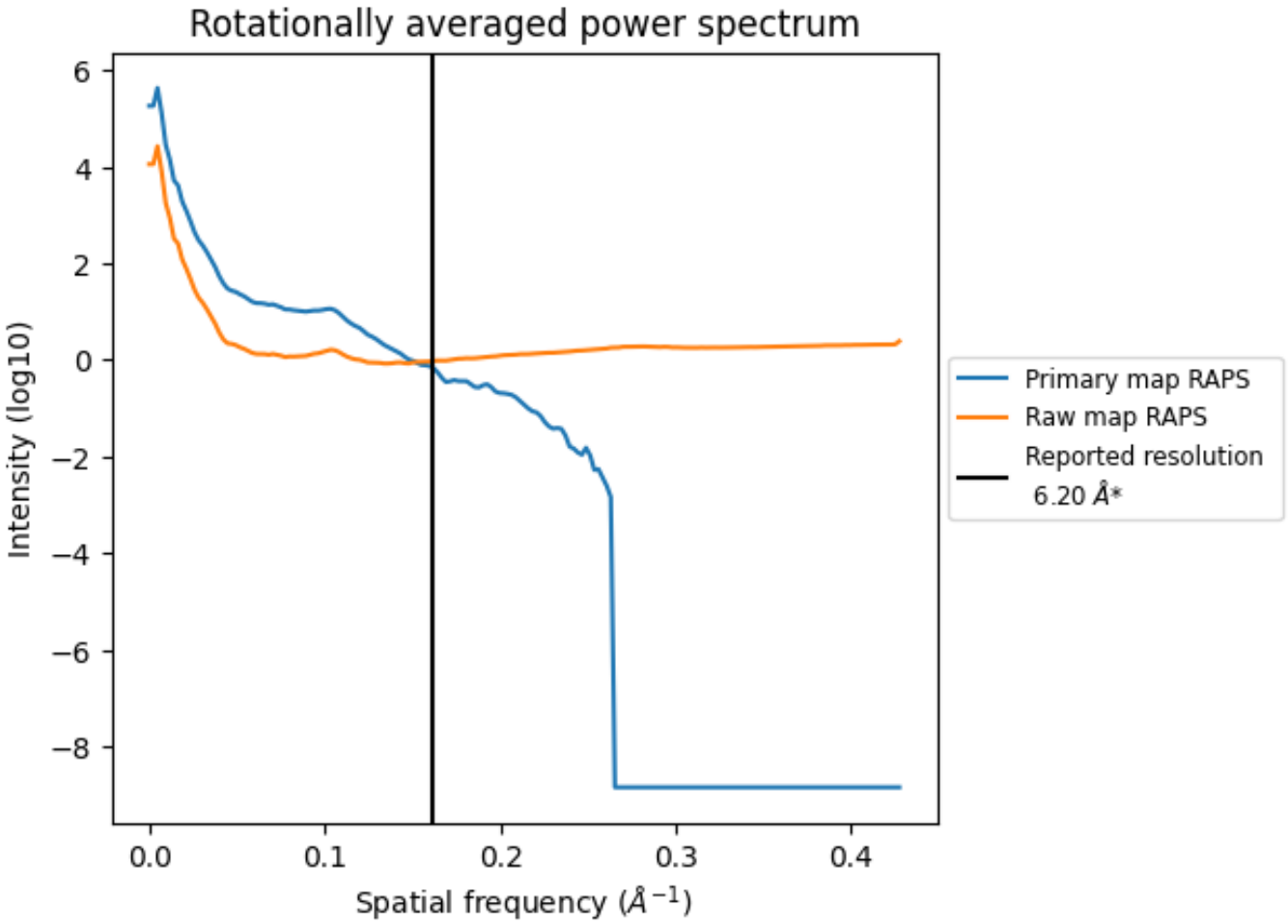
## 7.2 Volume estimate




The volume at the recommended contour level is 634 $nm^3$; this corresponds to an approximate mass of 572 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)

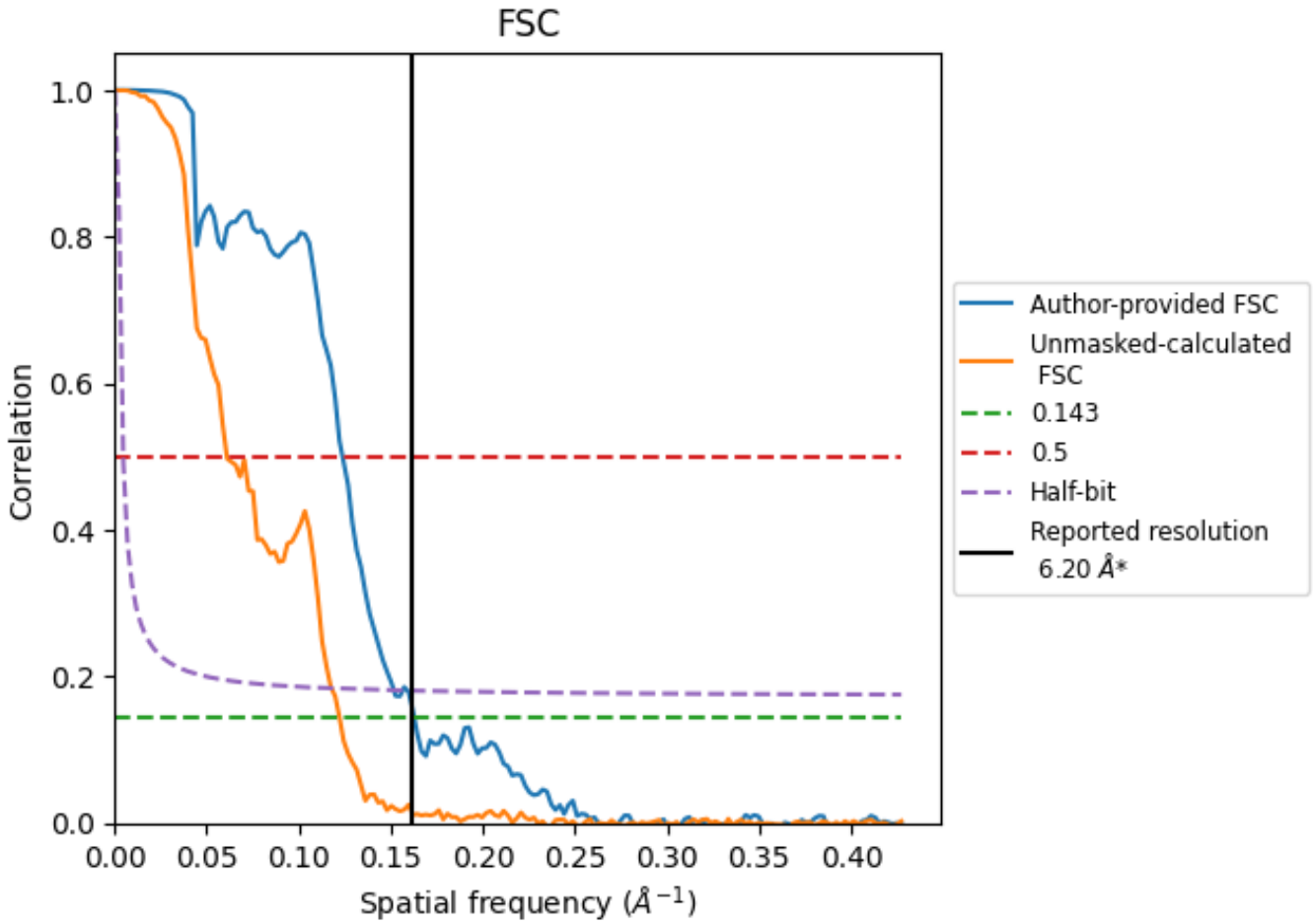



*Reported resolution corresponds to spatial frequency of 0.161 Å$^{-1}$

# 8 Fourier-Shell correlation

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




*Reported resolution corresponds to spatial frequency of 0.161 Å$^{-1}$

## 8.2 Resolution estimates (i)

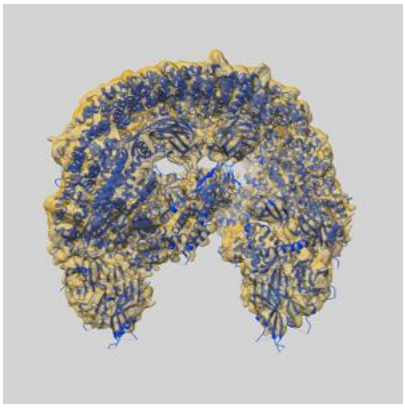
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 6.20 | - | - |
| Author-provided FSC curve | 6.15 | 8.08 | 6.59 |
| Unmasked-calculated* | 8.18 | 16.42 | 8.49 |

*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 8.18 differs from the reported value 6.2 by more than 10 %

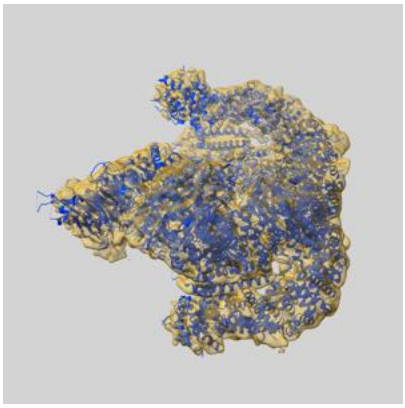
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15672 and PDB model 8AUK. Per-residue inclusion information can be found in section 3 on page 5.

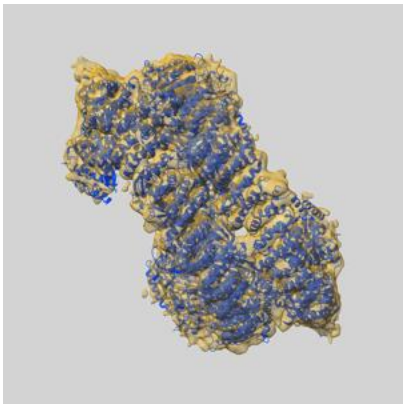
## 9.1 Map-model overlay



X



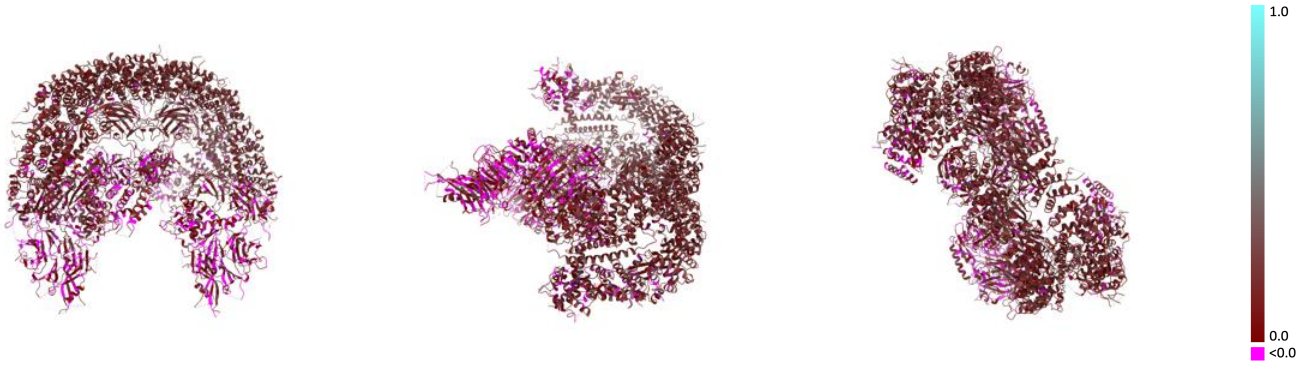
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00423 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

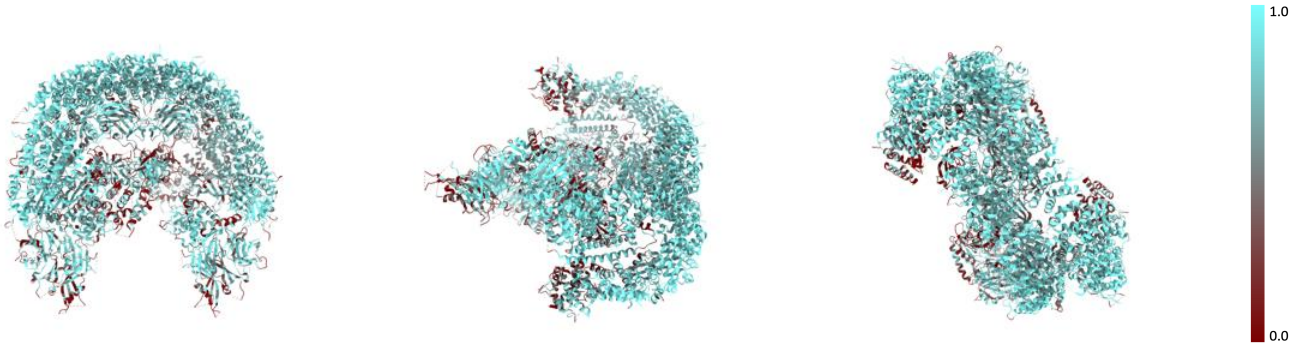
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

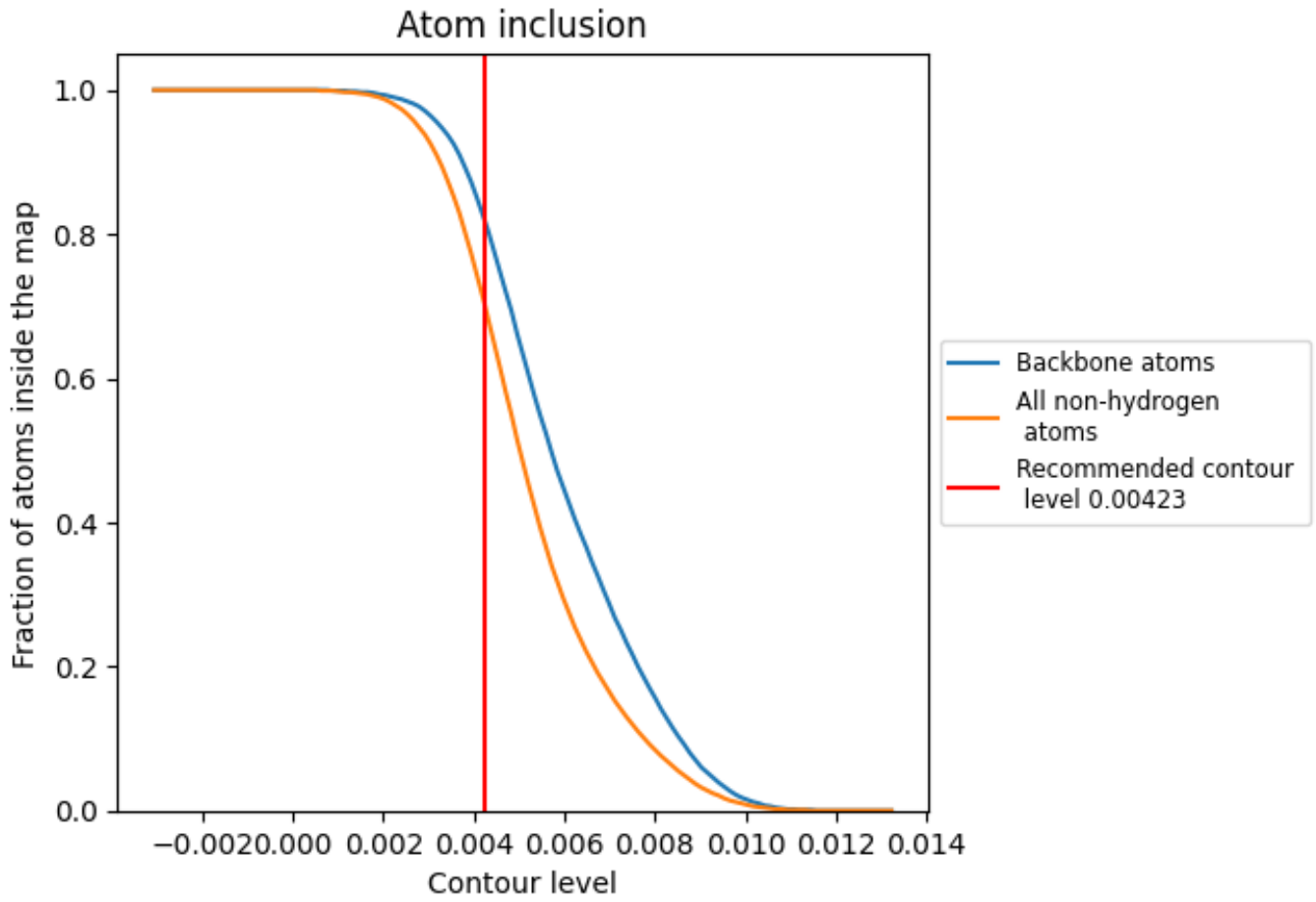
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00423).

## 9.4 Atom inclusion (i)




At the recommended contour level, 82% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.00423) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7050 | 0.1390 |
| A | 0.7200 | 0.1440 |
| B | 0.7310 | 0.1420 |
| C | 0.4560 | 0.0720 |
| D | 0.4480 | 0.0890 |
| E | 0.5370 | 0.1050 |