Full wwPDB EM Validation Report

Mar 3, 2025 – 10:42 AM EST

PDB ID	:	9NJU
EMDB ID	:	EMD-49491
Title	:	Structure of native homodimer of D. discoideum polyketide synthase Pks16
Authors	:	Hoogerbrugge, G.; Keatinge-Clay, A.T.; Marcotte, E.M.
Deposited on	:	2025-02-27
Resolution	:	3.94 Å(reported)

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.

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

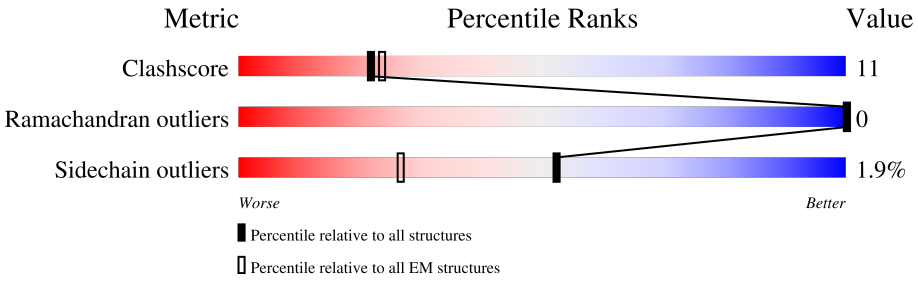
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.94 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	2603	11% 70% 26%
1	B	2603	11% 70% 25%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 39352 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 Probable polyketide synthase 16.

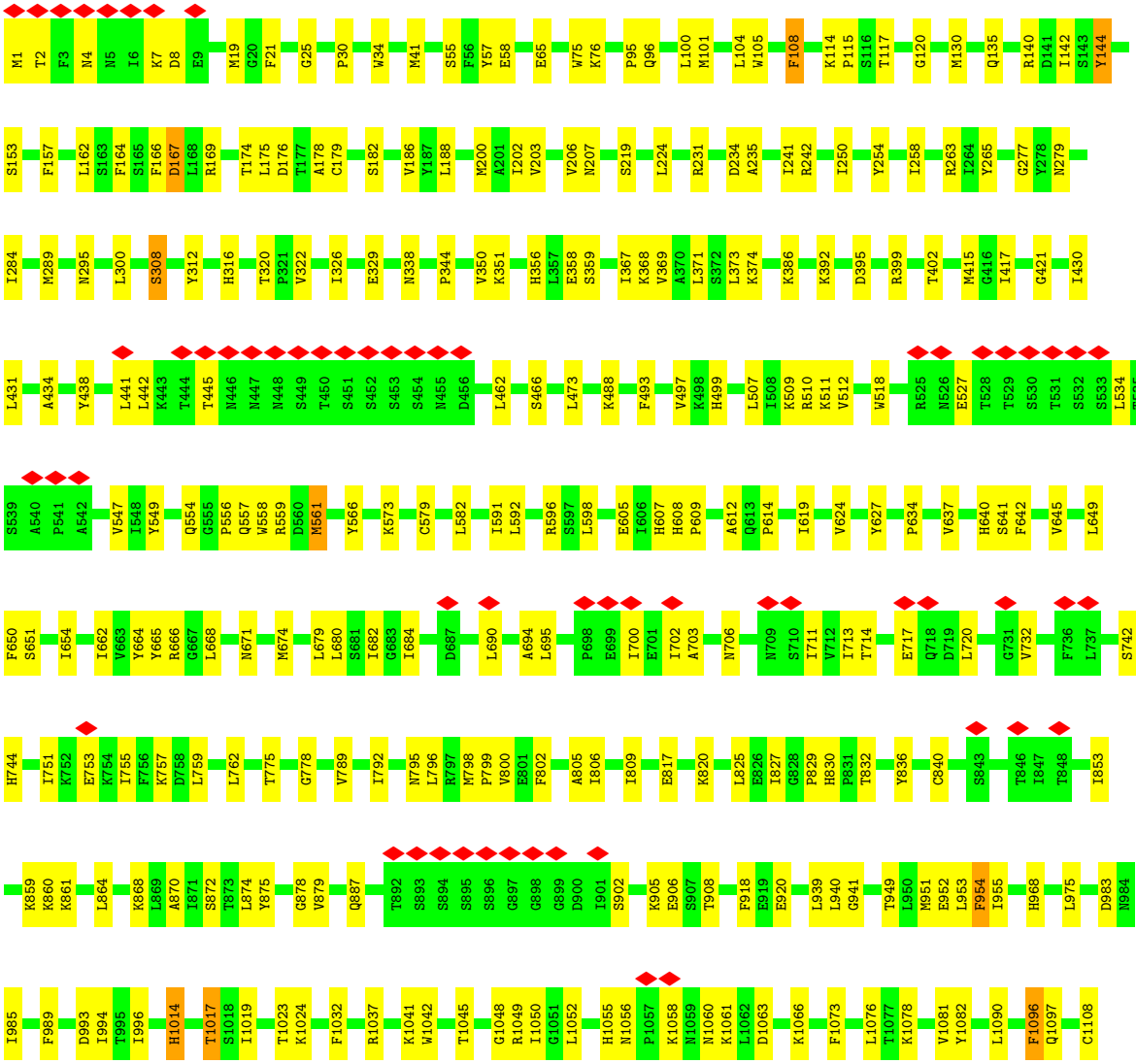
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2496	Total 19676	C 12498	N 3250	O 3862	S 66	0	0
1	B	2496	Total 19676	C 12498	N 3250	O 3862	S 66	0	0

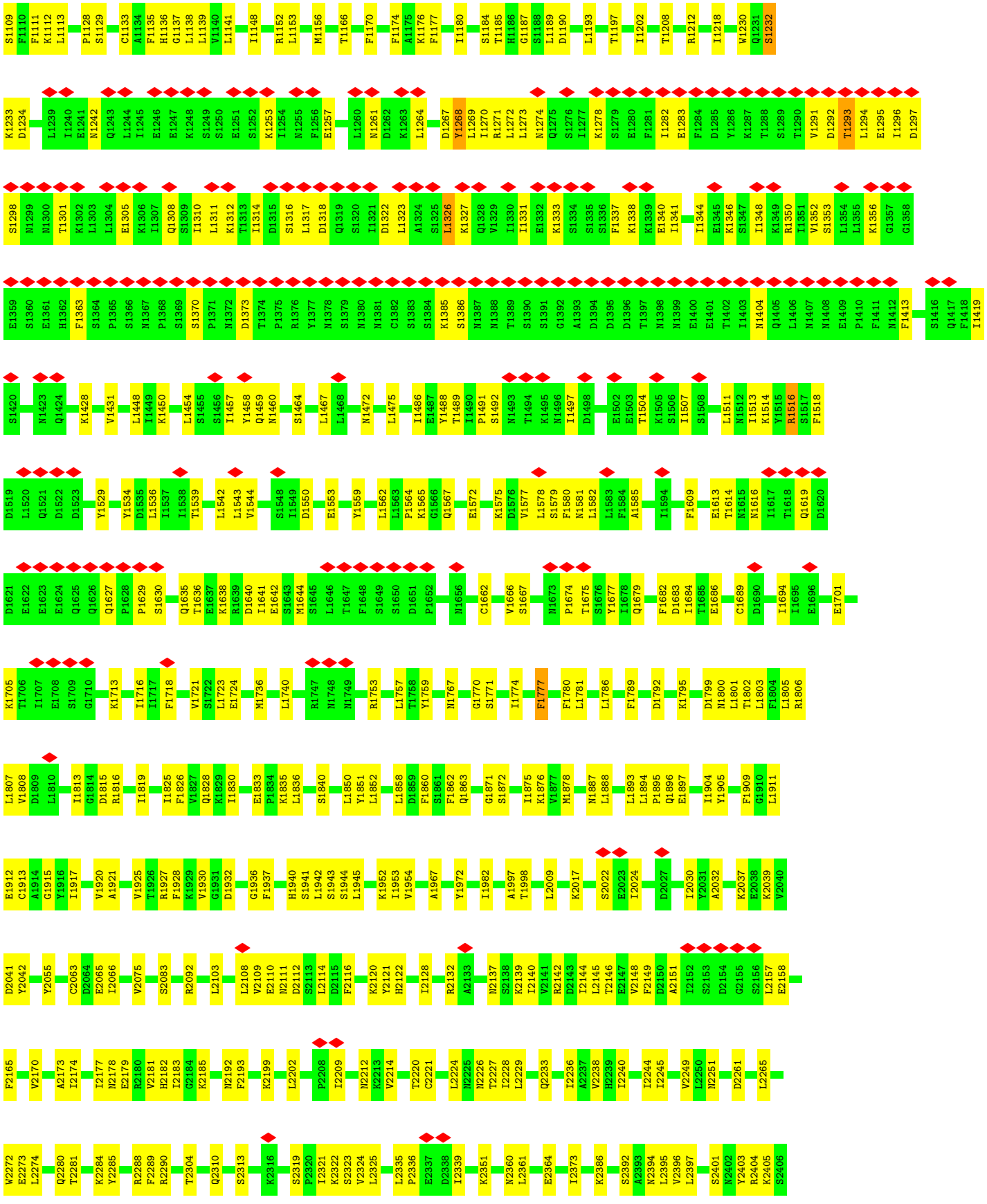
3 Residue-property plots (i)

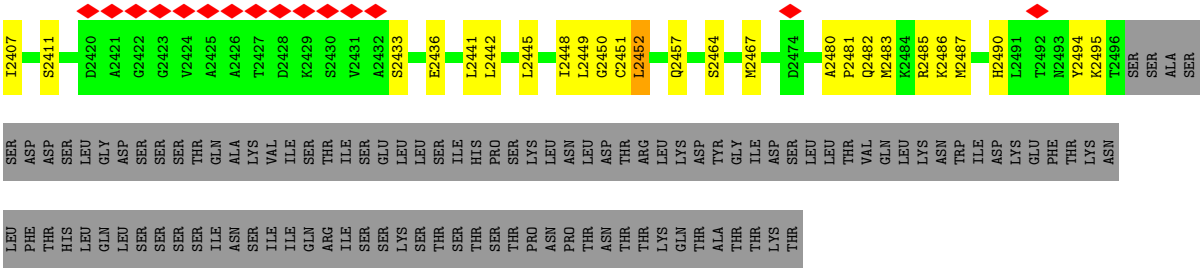
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Probable polyketide synthase 16

Chain A:

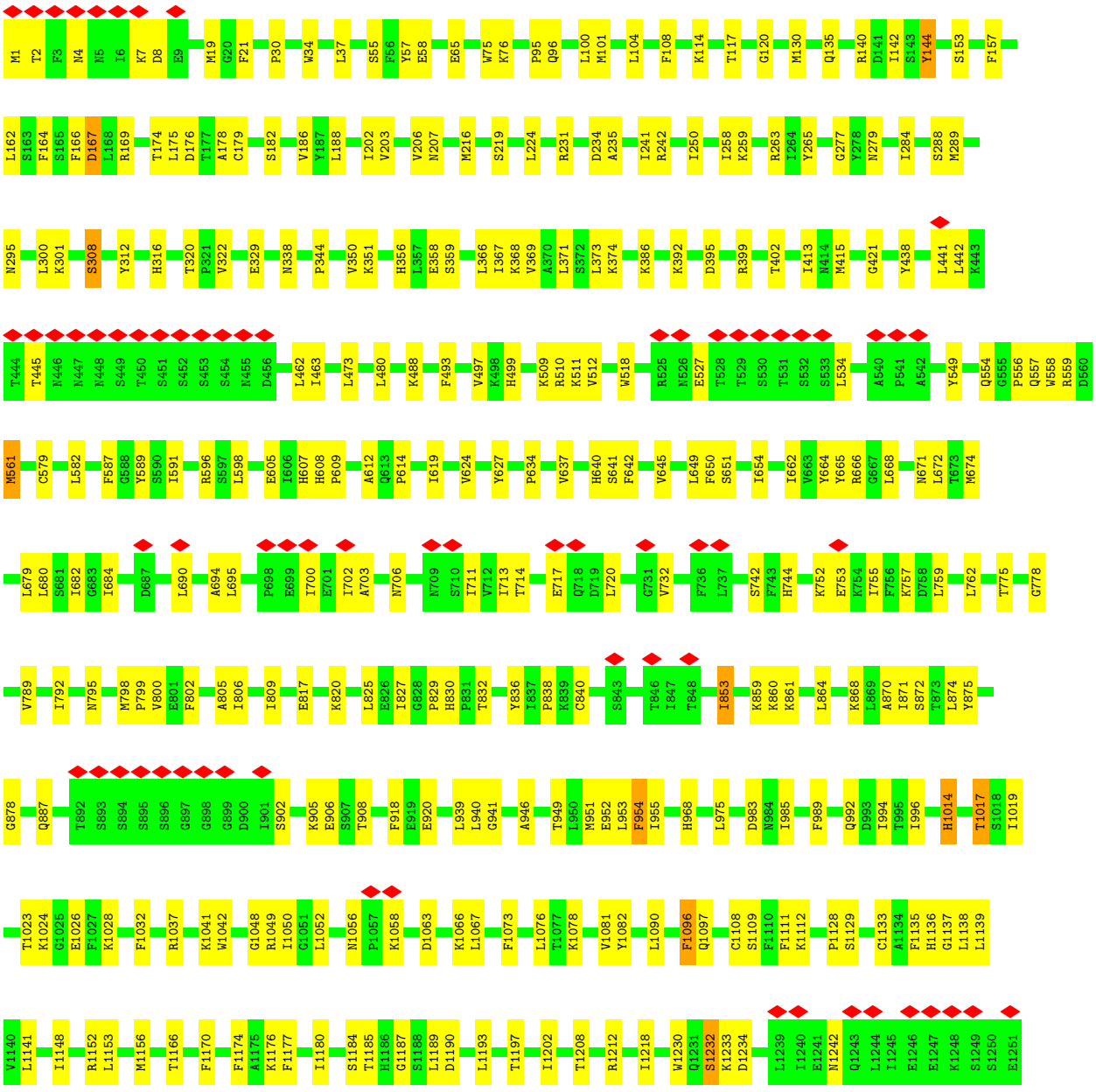


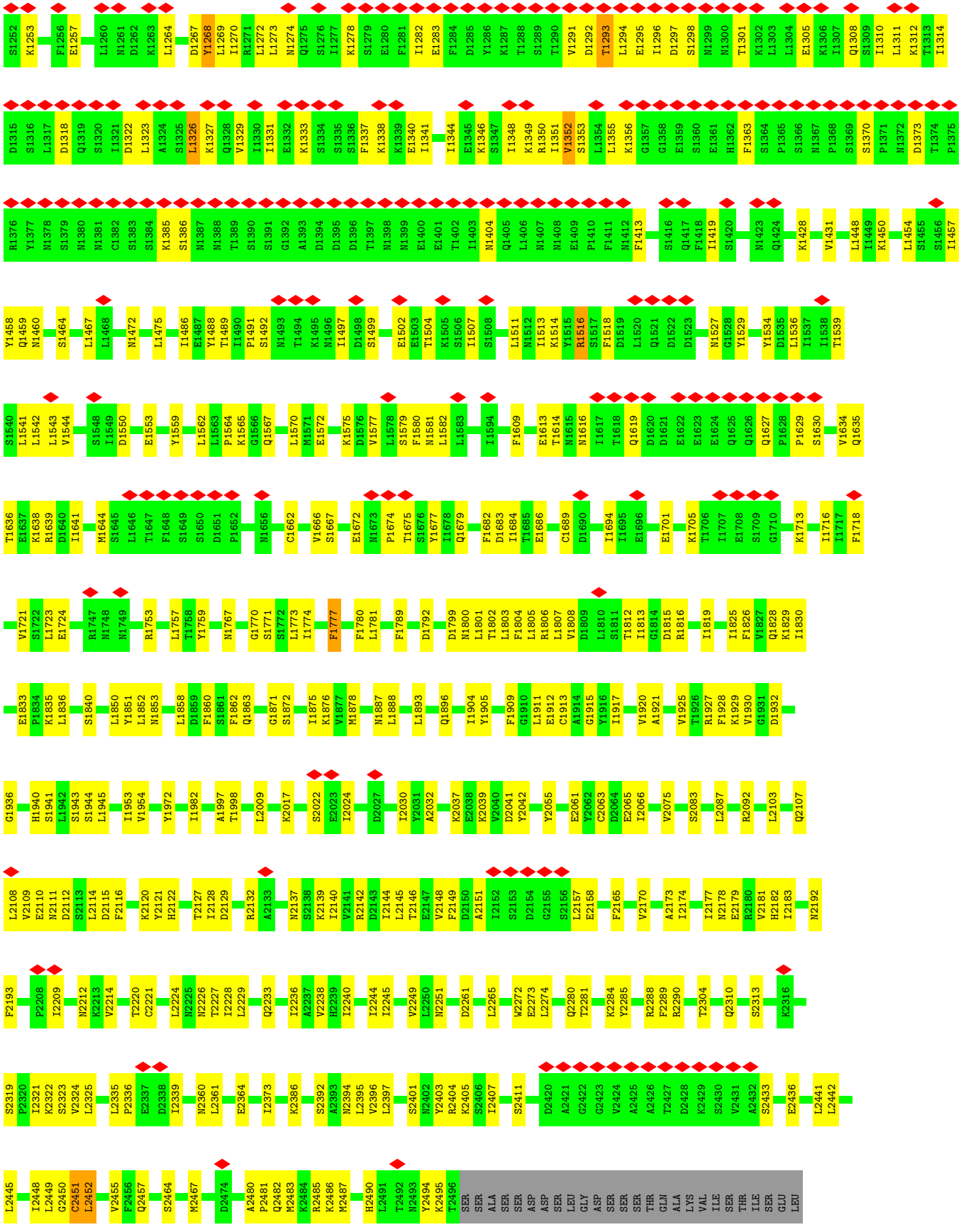

S1109 F1110 F1111 K1112 L1113 P1128 S1129 C1133 A1134 F1135 H1136 G1137 L1138 L1139 V1140 L1141 I1148 R1152 L1153 M1156 T1166 F1170 F1174 A1175 K1176 F1177 I1180 S1184 T1185 H1186 G1187 S1188 L1189 D1190 L1193 T1197 I1202 T1208 R1212 I1218 W1230 Q1231 S1232
K1233 D1234 L1239 I1240 E1241 N1242 Q1243 L1244 I1245 E1246 E1247 K1248 S1249 S1250 E1251 S1252 K1253 I1254 N1255 F1256 E1257 L1260 N1261 D1262 K1263 L1264 D1267 Y1268 L1269 I1270 R1271 L1272 L1273 N1274 Q1275 S1276 I1277 K1278 S1279 E1280 F1281 I1282 E1283 F1284 D1285 Y1286 K1287 T1288 S1289 T1290 V1291 D1292 T1293 L1294 E1295 I1296 D1297
S1298 N1299 N1300 T1301 K1302 L1303 L1304 E1305 K1306 I1307 Q1308 S1309 I1310 L1311 K1312 T1313 I1314 D1315 S1316 L1317 D1318 Q1319 S1320 I1321 D1322 L1323 A1324 S1325 L1326 K1327 Q1328 V1329 I1330 I1331 E1332 K1333 S1334 S1335 S1336 F1337 K1338 K1339 E1340 I1341 I1344 E1345 K1346 S1347 I1348 K1349 R1350 T1351 V1352 S1353 L1354 L1355 K1356 G1357 G1358
E1359 S1360 E1361 H1362 F1363 S1364 P1365 S1366 N1367 P1368 S1369 S1370 P1371 N1372 D1373 T1374 P1375 R1376 Y1377 N1378 S1379 N1380 M1381 C1382 S1383 S1384 K1385 S1386 N1387 N1388 T1389 S1390 S1391 G1392 A1393 D1394 D1395 D1396 T1397 N1398 N1399 E1400 E1401 T1402 I1403 N1404 Q1405 L1406 N1407 N1408 E1409 P1410 F1411 N1412 F1413 S1416 Q1417 F1418 I1419
S1420 N1423 Q1424 K1428 V1431 L1448 I1449 K1450 L1454 S1455 S1456 I1457 Y1458 Q1459 N1460 S1464 L1467 L1468 N1472 L1475 I1486 E1487 Y1488 T1489 I1490 P1491 S1492 N1493 T1494 K1495 N1496 I1497 D1498 E1502 E1503 T1504 K1505 S1506 I1507 S1508 L1511 N1512 I1513 K1514 Y1515 R1516 S1517 F1518
D1519 L1520 Q1521 D1522 D1523 Y1529 Y1534 D1535 L1536 I1537 I1538 T1539 L1542 L1543 V1544 S1548 I1549 D1550 E1553 Y1559 L1562 L1563 P1564 K1565 G1566 Q1567 E1572 K1575 D1576 V1577 L1578 S1579 F1580 N1581 L1582 L1583 F1584 A1585 I1594 F1609 E1613 T1614 N1615 N1616 I1617 T1618 Q1619 D1620
D1621 E1622 E1623 E1624 Q1625 Q1626 Q1627 P1628 P1629 S1630 Q1635 T1636 E1637 K1638 R1639 D1640 I1641 E1642 S1643 M1644 S1645 L1646 T1647 F1648 S1649 S1650 D1651 P1652 N1656 C1662 V1666 S1667 N1673 P1674 T1675 S1676 Y1677 I1678 Q1679 F1682 D1683 I1684 T1685 E1686 C1689 D1690 I1694 I1695 E1696 E1701
K1705 T1706 I1707 E1708 S1709 G1710 K1713 I1716 I1717 F1718 V1721 S1722 L1723 E1724 M1736 L1740 R1747 N1748 N1749 R1753 L1757 T1758 Y1759 N1767 G1770 S1771 I1774 F1777 F1780 L1781 L1786 F1789 D1792 K1795 D1799 N1800 L1801 T1802 L1803 F1804 L1805 R1806
L1807 V1808 D1809 L1810 I1813 G1814 D1815 R1816 I1819 I1825 F1826 V1827 Q1828 K1829 I1830 E1833 P1834 K1835 L1836 S1840 L1850 Y1851 L1852 L1858 D1859 F1860 S1861 F1862 Q1863 G1871 S1872 I1875 K1876 V1877 M1878 N1887 L1888 L1893 L1894 P1895 Q1896 E1897 I1904 Y1905 F1909 G1910 L1911
E1912 C1913 A1914 G1915 Y1916 I1917 V1920 A1921 V1925 T1926 R1927 F1928 K1929 V1930 G1931 D1932 G1936 F1937 H1940 S1941 L1942 S1943 S1944 L1945 K1952 I1953 V1954 A1967 Y1972 I1982 A1997 T1998 L2009 K2017 S2022 E2023 I2024 D2027 I2030 Y2031 A2032 K2037 E2038 K2039 V2040
D2041 Y2042 Y2055 C2063 D2064 E2065 I2066 V2075 S2083 R2092 L2103 L2108 V2109 E2110 N2111 D2112 S2113 L2114 D2115 F2116 K2120 Y2121 H2122 I2128 R2132 A2133 N2137 S2138 K2139 I2140 V2141 R2142 D2143 I2144 L2145 T2146 E2147 V2148 F2149 D2150 A2151 I2152 S2153 D2154 G2155 S2156 L2157 E2158
F2165 V2170 A2173 I2174 I2177 N2178 E2179 R2180 V2181 H2182 I2183 C2184 K2185 N2192 F2193 K2199 L2202 P2208 I2209 W2212 K2213 V2214 T2220 C2221 L2224 W2225 W2226 T2227 I2228 L2229 Q2233 I2236 A2237 V2238 H2239 I2240 I2244 I2245 V2249 L2250 W2251 D2261 L2265
W2272 E2273 L2274 Q2280 T2281 K2284 Y2285 R2288 F2289 R2290 T2304 Q2310 S2313 K2316 S2319 P2320 I2321 K2322 S2323 V2324 L2325 L2335 P2336 E2337 D2338 I2339 K2351 N2360 L2361 E2364 I2373 K2386 S2392 A2393 N2394 L2395 V2396 L2397 S2401 N2402 Y2403 R2404 K2405 S2406



• Molecule 1: Probable polyketide synthase 16

Chain B:




S1252 K1253 F1256 E1257 L1260 N1261 D1262 K1263 L1264 D1267 Y1268 L1269 I1270 R1271 L1272 L1273 N1274 Q1275 S1276 I1277 K1278 S1279 E1280 F1281 I1282 E1283 F1284 D1285 Y1286 K1287 T1288 S1289 T1290 V1291 D1292 T1293 L1294 E1295 I1296 D1297 S1298 N1299 N1300 T1301 K1302 L1303 L1304 E1305 K1306 I1307 Q1308 S1309 I1310 L1311 K1312 T1313 I1314
D1315 S1316 L1317 D1318 Q1319 S1320 I1321 D1322 L1323 A1324 S1325 L1326 K1327 Q1328 V1329 I1330 I1331 E1332 K1333 S1334 S1335 S1336 F1337 K1338 K1339 E1340 I1341 I1344 E1345 K1346 S1347 I1348 K1349 R1350 I1351 V1352 S1353 L1354 L1355 K1356 G1357 G1358 E1359 S1360 E1361 H1362 F1363 S1364 P1365 S1366 N1367 P1368 S1369 S1370 P1371 N1372 D1373 T1374 P1375
R1376 Y1377 N1378 S1379 N1380 N1381 C1382 S1383 S1384 K1385 S1386 N1387 N1388 T1389 S1390 S1391 G1392 A1393 D1394 D1395 D1396 T1397 N1398 N1399 E1400 E1401 T1402 I1403 N1404 Q1405 L1406 N1407 N1408 E1409 P1410 F1411 N1412 F1413 S1416 Q1417 F1418 I1419 S1420 N1423 Q1424 K1428 V1431 L1448 I1449 K1450 L1454 S1455 S1456 I1457
Y1458 Q1459 N1460 S1464 L1467 L1468 N1472 L1475 I1486 E1487 Y1488 T1489 I1490 P1491 S1492 N1493 T1494 K1495 N1496 I1497 D1498 S1499 E1502 E1503 T1504 K1505 S1506 I1507 S1508 L1511 N1512 I1513 K1514 Y1515 R1516 S1517 F1518 D1519 L1520 Q1521 D1522 D1523 N1527 G1528 Y1529 Y1534 D1535 L1536 I1537 I1538 T1539
S1540 L1541 L1542 L1543 V1544 S1548 I1549 D1550 E1553 Y1559 L1562 L1563 P1564 K1565 G1566 Q1567 L1570 M1571 E1572 K1575 D1576 V1577 L1578 S1579 F1580 N1581 L1582 L1583 I1594 F1609 E1613 T1614 N1615 N1616 I1617 T1618 Q1619 D1620 D1621 E1622 E1623 E1624 Q1625 Q1626 Q1627 P1628 P1629 S1630 V1634 Q1635
T1636 E1637 K1638 R1639 D1640 I1641 M1644 S1645 L1646 T1647 F1648 S1649 S1650 D1651 P1652 N1656 C1662 V1666 S1667 E1672 N1673 P1674 T1675 S1676 Y1677 I1678 Q1679 F1682 D1683 I1684 T1685 E1686 C1689 D1690 I1694 I1695 E1696 E1701 K1705 T1706 I1707 E1708 S1709 G1710 K1713 I1716 I1717 F1718
V1721 S1722 L1723 E1724 R1747 N1748 N1749 R1753 L1757 T1758 Y1759 N1767 G1770 S1771 S1772 L1773 I1774 F1777 F1780 L1781 F1789 D1792 D1799 N1800 L1801 T1802 L1803 F1804 L1805 R1806 L1807 V1808 D1809 L1810 S1811 T1812 I1813 G1814 D1815 R1816 I1819 I1825 F1826 V1827 Q1828 K1829 I1830
E1833 P1834 K1835 L1836 S1840 L1850 Y1851 L1852 N1853 L1858 D1859 F1860 S1861 F1862 Q1863 G1871 S1872 I1875 K1876 V1877 M1878 N1887 L1888 L1893 Q1896 I1904 Y1905 F1909 G1910 L1911 E1912 C1913 A1914 G1915 Y1916 I1917 V1920 A1921 V1925 T1926 R1927 F1928 K1929 V1930 G1931 D1932
G1936 H1940 S1941 L1942 S1943 S1944 L1945 I1953 V1954 Y1972 I1982 A1997 T1998 L2009 K2017 S2022 E2023 I2024 D2027 I2030 Y2031 A2032 K2037 E2038 K2039 V2040 D2041 Y2042 Y2055 E2061 Y2062 C2063 D2064 E2065 I2066 V2075 S2083 L2087 R2092 L2103 Q2107
L2108 V2109 E2110 N2111 D2112 S2113 L2114 D2115 F2116 K2120 Y2121 H2122 T2127 I2128 D2129 R2132 A2133 N2137 S2138 K2139 I2140 V2141 R2142 D2143 I2144 L2145 T2146 E2147 V2148 F2149 D2150 A2151 I2152 S2153 D2154 G2155 S2156 L2157 E2158 F2165 V2170 A2173 I2174 I2177 N2178 E2179 R2180 V2181 H2182 I2183 N2192
F2193 P2208 I2209 N2212 K2213 V2214 T2220 C2221 L2224 N2225 N2226 T2227 I2228 L2229 Q2233 I2236 A2237 V2238 H2239 I2240 I2244 I2245 V2249 L2250 N2251 D2261 L2265 W2272 E2273 L2274 Q2280 T2281 K2284 Y2285 R2288 F2289 R2290 T2304 Q2310 S2313 K2316
S2319 P2320 I2321 K2322 S2323 V2324 L2325 L2335 P2336 E2337 D2338 I2339 N2360 L2361 E2364 I2373 K2386 S2392 A2393 N2394 L2395 V2396 L2397 S2401 N2402 Y2403 R2404 K2405 S2406 I2407 S2411 D2420 A2421 G2422 G2423 V2424 A2425 A2426 T2427 D2428 K2429 S2430 V2431 A2432 S2433 E2436 L2441 L2442
L2445 I2448 L2449 G2450 C2451 L2452 V2455 F2456 Q2457 S2464 M2467 D2474 A2480 P2481 Q2482 M2483 K2484 R2485 K2486 M2487 H2490 L2491 T2492 N2493 Y2494 K2495 T2496 SER SER ALA SER SER ASP ASP SER LEU GLY ASP SER SER SER THR GLN ALA LYS VAL ILE SER THR ILE SER GLU LEU

LEU SER ILE HIS PRO SER LYS LEU ASN LEU ASP THR ARG LEU LYS ASP TYR GLY ILE ASP SER LEU LEU THR VAL GLN LEU LYS ASN TRP ILE ASP LYS GLU PHE THR LYS ASN LEU PHE THR HIS LEU GLN LEU SER SER SER ILE ASN SER ILE ILE GLN ARG ILE SER SER LYS

SER THR SER THR SER THR PRO ASN PRO THR ASN THR THR LYS GLN THR ALA THR THR LYS THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5611	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	49.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.444	Depositor
Minimum map value	-0.713	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.239	Depositor
Map size (Å)	447.8464, 447.8464, 447.8464	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7494, 1.7494, 1.7494	Depositor

5 Model quality

5.1 Standard geometry

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	0.29	0/20060	0.48	0/27143
1	B	0.29	0/20060	0.49	0/27143
All	All	0.29	0/40120	0.49	0/54286

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Peptide
1	B	144	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	19676	0	19566	465	0
1	B	19676	0	19566	467	0
All	All	39352	0	39132	894	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 11.

All (894) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:H	1:A:167:ASP:HB3	1.29	0.97
1:B:120:GLY:H	1:B:167:ASP:HB3	1.31	0.93
1:A:179:CYS:HB3	1:A:421:GLY:HA2	1.52	0.90
1:B:179:CYS:HB3	1:B:421:GLY:HA2	1.53	0.90
1:A:1037:ARG:HE	1:B:144:TYR:HB3	1.41	0.86
1:A:144:TYR:HB3	1:B:1037:ARG:HE	1.40	0.85
1:B:2238:VAL:HG11	1:B:2273:GLU:HG3	1.59	0.84
1:A:2122:HIS:HB3	1:B:2132:ARG:HH21	1.43	0.84
1:A:2238:VAL:HG11	1:A:2273:GLU:HG3	1.59	0.84
1:B:1492:SER:HB3	1:B:1497:ILE:HG23	1.60	0.84
1:A:1492:SER:HB3	1:A:1497:ILE:HG23	1.60	0.83
1:A:169:ARG:HH12	1:B:279:ASN:HB2	1.45	0.82
1:A:1454:LEU:HB2	1:A:1539:THR:HG22	1.64	0.78
1:B:1454:LEU:HB2	1:B:1539:THR:HG22	1.65	0.78
1:B:1257:GLU:HG3	1:B:1627:GLN:HB2	1.67	0.77
1:A:1257:GLU:HG3	1:A:1627:GLN:HB2	1.67	0.76
1:A:279:ASN:HB2	1:B:169:ARG:HH12	1.50	0.76
1:B:1272:LEU:HD13	1:B:1348:ILE:HG21	1.68	0.75
1:A:1253:LYS:HE3	1:A:1630:SER:HA	1.69	0.75
1:A:1641:ILE:HA	1:A:1644:MET:HE1	1.69	0.74
1:A:1489:THR:HG22	1:A:1514:LYS:HB2	1.70	0.73
1:B:1253:LYS:HE3	1:B:1630:SER:HA	1.69	0.73
1:B:1489:THR:HG22	1:B:1514:LYS:HB2	1.71	0.72
1:A:642:PHE:HA	1:A:666:ARG:HH12	1.54	0.72
1:A:680:LEU:HD23	1:A:713:ILE:HD11	1.71	0.72
1:A:1272:LEU:HD13	1:A:1348:ILE:HG21	1.69	0.72
1:B:680:LEU:HD23	1:B:713:ILE:HD11	1.70	0.72
1:B:642:PHE:HA	1:B:666:ARG:HH12	1.54	0.72
1:A:104:LEU:HD11	1:A:202:ILE:HD13	1.73	0.71
1:B:100:LEU:HB3	1:B:162:LEU:HD21	1.73	0.71
1:B:104:LEU:HD11	1:B:202:ILE:HD13	1.73	0.70
1:B:207:ASN:HB2	1:B:359:SER:HB3	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1686:GLU:HG3	1:A:1801:LEU:HD23	1.74	0.70
1:B:1686:GLU:HG3	1:B:1801:LEU:HD23	1.73	0.69
1:A:2227:THR:HB	1:A:2321:ILE:HA	1.74	0.69
1:A:100:LEU:HB3	1:A:162:LEU:HD21	1.75	0.69
1:A:1152:ARG:HH12	1:A:2110:GLU:HG3	1.57	0.69
1:A:1616:ASN:HB3	1:A:1629:PRO:HB3	1.75	0.69
1:B:2227:THR:HB	1:B:2321:ILE:HA	1.74	0.69
1:A:775:THR:HB	1:A:800:VAL:HG13	1.75	0.68
1:A:1713:LYS:HE2	1:A:1753:ARG:HH21	1.58	0.68
1:B:775:THR:HB	1:B:800:VAL:HG13	1.76	0.68
1:B:1616:ASN:HB3	1:B:1629:PRO:HB3	1.74	0.68
1:A:344:PRO:HG3	1:A:399:ARG:HE	1.59	0.68
1:B:1713:LYS:HE2	1:B:1753:ARG:HH21	1.58	0.68
1:B:591:ILE:HG21	1:B:614:PRO:HB2	1.75	0.68
1:A:1270:ILE:HG12	1:A:1314:ILE:HG23	1.76	0.68
1:B:637:VAL:HG21	1:B:651:SER:HB3	1.76	0.68
1:A:637:VAL:HG21	1:A:651:SER:HB3	1.75	0.68
1:B:2483:MET:HB3	1:B:2487:MET:HE1	1.76	0.67
1:A:1543:LEU:HG	1:A:1572:GLU:HG3	1.75	0.67
1:B:344:PRO:HG3	1:B:399:ARG:HE	1.60	0.67
1:B:1152:ARG:HH12	1:B:2110:GLU:HG3	1.60	0.67
1:A:591:ILE:HG21	1:A:614:PRO:HB2	1.75	0.67
1:B:1270:ILE:HG12	1:B:1314:ILE:HG23	1.76	0.66
1:A:2116:PHE:CD2	1:B:2107:GLN:HA	2.30	0.66
1:B:1096:PHE:HE1	1:B:1129:SER:HA	1.61	0.66
1:A:1331:ILE:HG12	1:A:1337:PHE:H	1.61	0.66
1:A:2128:ILE:HA	1:B:2122:HIS:CE1	2.30	0.66
1:B:2146:THR:HA	1:B:2149:PHE:HE1	1.62	0.65
1:B:100:LEU:HD21	1:B:206:VAL:HB	1.79	0.65
1:A:2146:THR:HA	1:A:2149:PHE:HE1	1.62	0.64
1:B:902:SER:HA	1:B:905:LYS:HG3	1.79	0.64
1:A:1674:PRO:HB2	1:A:1694:ILE:HD13	1.79	0.64
1:B:1078:LYS:HE2	1:B:1097:GLN:HB3	1.80	0.64
1:A:207:ASN:ND2	1:A:358:GLU:HB3	2.12	0.64
1:B:2229:LEU:HB3	1:B:2324:VAL:HG23	1.79	0.64
1:B:1543:LEU:HG	1:B:1572:GLU:HG3	1.77	0.64
1:A:1096:PHE:HE1	1:A:1129:SER:HA	1.62	0.64
1:A:2229:LEU:HB3	1:A:2324:VAL:HG23	1.80	0.64
1:B:1331:ILE:HG12	1:B:1337:PHE:H	1.62	0.64
1:A:2483:MET:HB3	1:A:2487:MET:HE1	1.80	0.63
1:A:289:MET:HE1	1:A:329:GLU:HG2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:GLN:HE21	1:B:612:ALA:HB3	1.63	0.63
1:A:902:SER:HA	1:A:905:LYS:HG3	1.79	0.63
1:B:968:HIS:HB2	1:B:1096:PHE:HE2	1.63	0.63
1:B:1674:PRO:HB2	1:B:1694:ILE:HD13	1.79	0.63
1:A:100:LEU:HD21	1:A:206:VAL:HB	1.81	0.63
1:A:554:GLN:HE21	1:A:612:ALA:HB3	1.62	0.63
1:B:2392:SER:O	1:B:2396:VAL:HG23	1.99	0.63
1:B:1872:SER:H	1:B:1921:ALA:HB2	1.64	0.62
1:A:1872:SER:H	1:A:1921:ALA:HB2	1.65	0.62
1:A:2392:SER:O	1:A:2396:VAL:HG23	1.99	0.62
1:B:1450:LYS:HD2	1:B:1534:TYR:HA	1.82	0.62
1:A:1078:LYS:HE2	1:A:1097:GLN:HB3	1.80	0.62
1:A:968:HIS:HB2	1:A:1096:PHE:HE2	1.63	0.61
1:B:860:LYS:HB2	1:B:861:LYS:HE2	1.81	0.61
1:B:1920:VAL:HG13	1:B:1930:VAL:HG13	1.81	0.61
1:B:1852:LEU:HB3	1:B:1860:PHE:HD2	1.64	0.61
1:A:806:ILE:HA	1:A:809:ILE:HD12	1.81	0.61
1:A:860:LYS:HB2	1:A:861:LYS:HE2	1.81	0.61
1:A:2116:PHE:CE1	1:B:2114:LEU:HG	2.35	0.61
1:B:242:ARG:HG2	1:B:358:GLU:HB2	1.80	0.61
1:A:1792:ASP:HB3	1:A:1819:ILE:HG12	1.82	0.61
1:B:1457:ILE:HG22	1:B:1492:SER:HA	1.82	0.61
1:A:1852:LEU:HB3	1:A:1860:PHE:HD2	1.66	0.61
1:A:1920:VAL:HG13	1:A:1930:VAL:HG13	1.81	0.61
1:A:649:LEU:HA	1:A:654:ILE:HG12	1.83	0.61
1:A:207:ASN:HB2	1:A:359:SER:HB3	1.83	0.60
1:A:1218:ILE:HG23	1:A:2450:GLY:HA2	1.82	0.60
1:A:1450:LYS:HD2	1:A:1534:TYR:HA	1.82	0.60
1:A:2132:ARG:HH21	1:B:2122:HIS:HB3	1.66	0.60
1:B:175:LEU:HD11	1:B:188:LEU:HD12	1.83	0.60
1:B:789:VAL:HA	1:B:792:ILE:HD12	1.83	0.60
1:A:320:THR:HG22	1:A:322:VAL:H	1.66	0.60
1:A:2233:GLN:HB2	1:A:2274:LEU:HD22	1.83	0.60
1:B:1998:THR:HG21	1:B:2039:LYS:HB3	1.83	0.60
1:A:1457:ILE:HG22	1:A:1492:SER:HA	1.84	0.60
1:B:1218:ILE:HG23	1:B:2450:GLY:HA2	1.82	0.60
1:B:2146:THR:HA	1:B:2149:PHE:CE1	2.36	0.60
1:A:2144:ILE:O	1:A:2148:VAL:HB	2.01	0.60
1:B:649:LEU:HA	1:B:654:ILE:HG12	1.83	0.60
1:B:1273:LEU:HD13	1:B:1310:ILE:HG23	1.83	0.60
1:A:1559:TYR:HA	1:A:1562:LEU:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2146:THR:HA	1:A:2149:PHE:CE1	2.36	0.60
1:B:1667:SER:HB3	1:B:1721:VAL:HG22	1.84	0.60
1:A:1273:LEU:HD13	1:A:1310:ILE:HG23	1.84	0.60
1:A:462:LEU:HD21	1:A:868:LYS:HB3	1.83	0.60
1:B:806:ILE:HA	1:B:809:ILE:HD12	1.81	0.60
1:B:1559:TYR:HA	1:B:1562:LEU:HD12	1.84	0.60
1:A:157:PHE:HE2	1:B:284:ILE:HG21	1.66	0.60
1:B:1675:THR:HG23	1:B:1684:ILE:HD13	1.83	0.60
1:A:284:ILE:HG21	1:B:157:PHE:HE2	1.66	0.60
1:A:175:LEU:HD11	1:A:188:LEU:HD12	1.83	0.59
1:A:1675:THR:HG23	1:A:1684:ILE:HD13	1.84	0.59
1:A:1679:GLN:HG3	1:A:1684:ILE:HG23	1.84	0.59
1:B:527:GLU:HG3	1:B:534:LEU:HD11	1.84	0.59
1:B:320:THR:HG22	1:B:322:VAL:H	1.66	0.59
1:B:1679:GLN:HG3	1:B:1684:ILE:HG23	1.83	0.59
1:A:527:GLU:HG3	1:A:534:LEU:HD11	1.84	0.59
1:A:1667:SER:HB3	1:A:1721:VAL:HG22	1.84	0.59
1:A:1998:THR:HG21	1:A:2039:LYS:HB3	1.83	0.59
1:B:1023:THR:HG22	1:B:1024:LYS:H	1.67	0.59
1:B:2144:ILE:O	1:B:2148:VAL:HB	2.01	0.59
1:B:462:LEU:HD21	1:B:868:LYS:HB3	1.84	0.59
1:B:1565:LYS:H	1:B:1638:LYS:HB3	1.68	0.59
1:A:968:HIS:HB2	1:A:1096:PHE:CE2	2.38	0.59
1:A:2116:PHE:HE1	1:B:2114:LEU:HG	1.66	0.59
1:B:1792:ASP:HB3	1:B:1819:ILE:HG12	1.83	0.59
1:B:2233:GLN:HB2	1:B:2274:LEU:HD22	1.84	0.59
1:A:1023:THR:HG22	1:A:1024:LYS:H	1.67	0.59
1:B:1032:PHE:HB3	1:B:1042:TRP:HB3	1.84	0.59
1:A:462:LEU:H	1:A:887:GLN:HE22	1.51	0.58
1:A:798:MET:HE1	1:A:799:PRO:HD2	1.85	0.58
1:A:1565:LYS:H	1:A:1638:LYS:HB3	1.68	0.58
1:B:671:ASN:O	1:B:674:MET:HG2	2.03	0.58
1:A:789:VAL:HA	1:A:792:ILE:HD12	1.84	0.58
1:A:2249:VAL:HA	1:A:2288:ARG:HH21	1.68	0.58
1:B:968:HIS:HB2	1:B:1096:PHE:CE2	2.38	0.58
1:B:2404:ARG:HE	1:B:2411:SER:HB3	1.69	0.58
1:B:462:LEU:H	1:B:887:GLN:HE22	1.52	0.58
1:B:1807:LEU:HA	1:B:1813:ILE:HD12	1.84	0.58
1:A:994:ILE:HD12	1:A:1052:LEU:HD22	1.86	0.58
1:A:1830:ILE:HD13	1:A:2487:MET:HE2	1.86	0.58
1:A:186:VAL:HA	1:A:203:VAL:HG11	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2017:LYS:HA	1:A:2022:SER:HA	1.86	0.58
1:A:2404:ARG:HE	1:A:2411:SER:HB3	1.69	0.58
1:B:2017:LYS:HA	1:B:2022:SER:HA	1.86	0.58
1:A:207:ASN:HD21	1:A:358:GLU:HB3	1.68	0.57
1:A:2009:LEU:HD13	1:A:2030:ILE:HD13	1.86	0.57
1:A:2037:LYS:HD2	1:A:2041:ASP:OD2	2.04	0.57
1:A:2137:ASN:HA	1:A:2139:LYS:HE2	1.86	0.57
1:B:1613:GLU:HB2	1:B:1635:GLN:HG3	1.86	0.57
1:A:1564:PRO:HB3	1:A:1641:ILE:HB	1.85	0.57
1:B:186:VAL:HA	1:B:203:VAL:HG11	1.84	0.57
1:B:2249:VAL:HA	1:B:2288:ARG:HH21	1.69	0.57
1:A:289:MET:HG3	1:A:326:ILE:HG23	1.86	0.57
1:A:671:ASN:HA	1:A:674:MET:HE2	1.86	0.57
1:A:1613:GLU:HB2	1:A:1635:GLN:HG3	1.87	0.57
1:B:1619:GLN:HG2	1:B:1627:GLN:HE22	1.69	0.57
1:B:2037:LYS:HD2	1:B:2041:ASP:OD2	2.04	0.57
1:B:2336:PRO:HA	1:B:2339:ILE:HD11	1.86	0.57
1:B:2137:ASN:HA	1:B:2139:LYS:HE2	1.87	0.57
1:B:499:HIS:HB2	1:B:908:THR:HG21	1.87	0.57
1:B:1804:PHE:HA	1:B:1807:LEU:HG	1.87	0.57
1:B:2009:LEU:HD13	1:B:2030:ILE:HD13	1.86	0.57
1:A:499:HIS:HB2	1:A:908:THR:HG21	1.87	0.56
1:A:1619:GLN:HG2	1:A:1627:GLN:HE22	1.69	0.56
1:A:1133:CYS:HA	1:A:1136:HIS:CE1	2.40	0.56
1:B:1346:LYS:HE2	1:B:1350:ARG:HG3	1.86	0.56
1:B:1133:CYS:HA	1:B:1136:HIS:CE1	2.40	0.56
1:A:1346:LYS:HE2	1:A:1350:ARG:HG3	1.88	0.56
1:A:1111:PHE:CE1	1:A:1137:GLY:HA3	2.41	0.56
1:A:2336:PRO:HA	1:A:2339:ILE:HD11	1.86	0.56
1:B:1111:PHE:CE1	1:B:1137:GLY:HA3	2.41	0.56
1:B:1888:LEU:HD23	1:B:1893:LEU:HD12	1.88	0.56
1:A:1032:PHE:HB3	1:A:1042:TRP:HB3	1.88	0.56
1:A:142:ILE:HD11	1:B:140:ARG:NH2	2.21	0.56
1:B:1830:ILE:HD13	1:B:2487:MET:HE2	1.88	0.56
1:B:859:LYS:HG3	1:B:860:LYS:HG3	1.88	0.56
1:B:953:LEU:HD21	1:B:955:ILE:HD11	1.89	0.55
1:A:1448:LEU:HD21	1:A:1450:LYS:HE2	1.88	0.55
1:A:1789:PHE:HD1	1:A:1816:ARG:HB3	1.71	0.55
1:B:207:ASN:HD21	1:B:358:GLU:HB3	1.71	0.55
1:A:510:ARG:HD3	1:A:875:TYR:CZ	2.42	0.55
1:A:1667:SER:H	1:A:1677:TYR:HE2	1.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2226:ASN:HB3	1:A:2319:SER:OG	2.07	0.55
1:B:684:ILE:HG22	1:B:732:VAL:HG21	1.88	0.55
1:B:994:ILE:HD12	1:B:1052:LEU:HD22	1.87	0.55
1:B:1564:PRO:HB3	1:B:1641:ILE:HB	1.88	0.55
1:A:438:TYR:HD1	1:A:441:LEU:HD22	1.71	0.55
1:A:1888:LEU:HD23	1:A:1893:LEU:HD12	1.88	0.55
1:A:996:ILE:HD12	1:A:1156:MET:SD	2.47	0.55
1:A:157:PHE:CE2	1:B:284:ILE:HG21	2.42	0.55
1:A:1803:LEU:HD21	1:A:1825:ILE:HD11	1.88	0.55
1:B:798:MET:HE1	1:B:799:PRO:HD2	1.88	0.55
1:A:140:ARG:NH2	1:B:142:ILE:HD11	2.20	0.55
1:A:176:ASP:OD2	1:B:174:THR:HB	2.07	0.55
1:B:1448:LEU:HD21	1:B:1450:LYS:HE2	1.88	0.55
1:B:1789:PHE:HD1	1:B:1816:ARG:HB3	1.72	0.55
1:A:684:ILE:HG22	1:A:732:VAL:HG21	1.88	0.55
1:A:702:ILE:HG21	1:A:711:ILE:HD12	1.89	0.54
1:A:284:ILE:HG21	1:B:157:PHE:CE2	2.42	0.54
1:A:1777:PHE:CE1	1:A:1781:LEU:HD21	2.41	0.54
1:A:1878:MET:HG2	1:A:1915:GLY:HA2	1.89	0.54
1:B:1293:THR:HG22	1:B:1294:LEU:H	1.72	0.54
1:A:864:LEU:O	1:A:868:LYS:HG2	2.06	0.54
1:A:1293:THR:HG22	1:A:1294:LEU:H	1.72	0.54
1:B:473:LEU:HD21	1:B:511:LYS:HB2	1.90	0.54
1:B:510:ARG:HD3	1:B:875:TYR:CZ	2.42	0.54
1:B:662:ILE:HG12	1:B:759:LEU:HD11	1.90	0.54
1:B:2087:LEU:HD21	1:B:2114:LEU:HD21	1.89	0.54
1:B:2109:VAL:HG23	1:B:2112:ASP:HB3	1.87	0.54
1:B:438:TYR:HD1	1:B:441:LEU:HD22	1.72	0.54
1:B:864:LEU:O	1:B:868:LYS:HG2	2.06	0.54
1:A:859:LYS:HG3	1:A:860:LYS:HG3	1.88	0.54
1:A:953:LEU:HD21	1:A:955:ILE:HD11	1.89	0.54
1:A:1909:PHE:N	1:A:1940:HIS:HD1	2.05	0.54
1:B:1486:ILE:HB	1:B:1511:LEU:HD22	1.90	0.54
1:A:242:ARG:HG2	1:A:358:GLU:HB2	1.90	0.54
1:A:778:GLY:HA2	1:A:805:ALA:HB2	1.90	0.54
1:B:778:GLY:HA2	1:B:805:ALA:HB2	1.90	0.54
1:A:174:THR:HB	1:B:176:ASP:OD2	2.07	0.54
1:A:706:ASN:HB3	1:A:836:TYR:CG	2.43	0.54
1:A:870:ALA:O	1:A:874:LEU:HD22	2.06	0.54
1:B:1536:LEU:HD13	1:B:1567:GLN:HB2	1.90	0.54
1:A:473:LEU:HD21	1:A:511:LYS:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1234:ASP:HB3	1:A:1641:ILE:HG21	1.90	0.54
1:B:549:TYR:CG	1:B:634:PRO:HB3	2.43	0.54
1:B:706:ASN:HB3	1:B:836:TYR:CG	2.43	0.54
1:B:1667:SER:H	1:B:1677:TYR:HE2	1.54	0.54
1:A:1536:LEU:HD13	1:A:1567:GLN:HB2	1.90	0.53
1:A:2140:ILE:O	1:A:2144:ILE:HG22	2.08	0.53
1:B:2226:ASN:HB3	1:B:2319:SER:OG	2.07	0.53
1:B:702:ILE:HG21	1:B:711:ILE:HD12	1.88	0.53
1:A:671:ASN:O	1:A:674:MET:HG3	2.08	0.53
1:A:1564:PRO:HG2	1:A:1641:ILE:HD12	1.89	0.53
1:B:1802:THR:HA	1:B:1805:LEU:HD12	1.90	0.53
1:A:549:TYR:CG	1:A:634:PRO:HB3	2.43	0.53
1:B:996:ILE:HD12	1:B:1156:MET:SD	2.47	0.53
1:B:1777:PHE:CE1	1:B:1781:LEU:HD21	2.42	0.53
1:B:1909:PHE:N	1:B:1940:HIS:HD1	2.06	0.53
1:B:2405:LYS:HE2	1:B:2464:SER:HA	1.90	0.53
1:B:864:LEU:HD23	1:B:864:LEU:H	1.74	0.53
1:A:579:CYS:HA	1:A:582:LEU:HD12	1.91	0.53
1:A:1311:LEU:HA	1:A:1314:ILE:HD12	1.91	0.53
1:A:2481:PRO:HD2	1:A:2482:GLN:NE2	2.24	0.53
1:B:2157:LEU:HD12	1:B:2158:GLU:H	1.74	0.53
1:B:2481:PRO:HD2	1:B:2482:GLN:NE2	2.24	0.53
1:A:662:ILE:HG12	1:A:759:LEU:HD11	1.90	0.53
1:B:1917:ILE:HD12	1:B:1932:ASP:HB2	1.91	0.53
1:B:2092:ARG:NH1	1:B:2092:ARG:HB2	2.24	0.53
1:A:556:PRO:HG3	1:A:832:THR:HG21	1.91	0.53
1:A:2092:ARG:HB2	1:A:2092:ARG:NH1	2.24	0.53
1:B:1564:PRO:HG2	1:B:1641:ILE:HD12	1.90	0.53
1:A:130:MET:SD	1:A:178:ALA:HB1	2.49	0.53
1:A:2228:ILE:HG23	1:A:2323:SER:HB2	1.91	0.52
1:B:2394:ASN:HA	1:B:2397:LEU:HD12	1.91	0.52
1:A:130:MET:HG2	1:A:359:SER:HB2	1.91	0.52
1:B:2179:GLU:HB3	1:B:2181:VAL:HG22	1.91	0.52
1:B:2228:ILE:HG23	1:B:2323:SER:HB2	1.91	0.52
1:A:1917:ILE:HD12	1:A:1932:ASP:HB2	1.91	0.52
1:B:1803:LEU:HD21	1:B:1825:ILE:HD11	1.92	0.52
1:B:1835:LYS:HD3	1:B:2209:ILE:HA	1.90	0.52
1:B:2226:ASN:HB2	1:B:2322:LYS:HG3	1.92	0.52
1:A:2405:LYS:HE2	1:A:2464:SER:HA	1.91	0.52
1:B:76:LYS:HB3	1:B:920:GLU:HG3	1.91	0.52
1:A:864:LEU:H	1:A:864:LEU:HD23	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:SER:OG	1:A:1141:LEU:HD21	2.10	0.52
1:B:219:SER:HB3	1:B:224:LEU:HD12	1.92	0.52
1:B:2140:ILE:O	1:B:2144:ILE:HG22	2.08	0.52
1:A:2394:ASN:HA	1:A:2397:LEU:HD12	1.91	0.52
1:B:579:CYS:HA	1:B:582:LEU:HD12	1.91	0.52
1:B:1267:ASP:HB2	1:B:1318:ASP:OD2	2.10	0.52
1:B:1577:VAL:HG12	1:B:1580:PHE:H	1.73	0.52
1:A:182:SER:O	1:A:186:VAL:HG23	2.10	0.52
1:A:1267:ASP:HB2	1:A:1318:ASP:OD2	2.10	0.52
1:B:1875:ILE:HD11	1:B:1953:ILE:HD13	1.92	0.52
1:A:1835:LYS:HD3	1:A:2209:ILE:HA	1.90	0.52
1:A:2109:VAL:HG23	1:A:2112:ASP:HB3	1.91	0.52
1:A:2145:LEU:O	1:A:2148:VAL:HG12	2.10	0.52
1:B:182:SER:O	1:B:186:VAL:HG23	2.10	0.52
1:B:462:LEU:HD21	1:B:868:LYS:HD2	1.92	0.52
1:B:1679:GLN:HG2	1:B:1683:ASP:HA	1.92	0.52
1:A:144:TYR:CG	1:B:1037:ARG:HG2	2.45	0.52
1:A:2157:LEU:HD12	1:A:2158:GLU:H	1.74	0.52
1:B:1323:LEU:HD22	1:B:1327:LYS:HE2	1.92	0.52
1:A:1326:LEU:H	1:A:1326:LEU:HD23	1.75	0.52
1:A:1911:LEU:HB3	1:A:1912:GLU:OE2	2.10	0.52
1:B:1296:ILE:HD12	1:B:1363:PHE:HB2	1.92	0.52
1:A:219:SER:HB3	1:A:224:LEU:HD12	1.92	0.51
1:A:1802:THR:HA	1:A:1805:LEU:HD12	1.91	0.51
1:B:57:TYR:CG	1:B:65:GLU:HB3	2.45	0.51
1:B:1056:ASN:HD21	1:B:1058:LYS:HE2	1.75	0.51
1:B:1833:GLU:HG3	1:B:1836:LEU:HB2	1.92	0.51
1:A:2122:HIS:CD2	1:B:2129:ASP:H	2.28	0.51
1:B:1311:LEU:HA	1:B:1314:ILE:HD12	1.92	0.51
1:A:1305:GLU:O	1:A:1308:GLN:HG3	2.10	0.51
1:A:1486:ILE:HB	1:A:1511:LEU:HD22	1.91	0.51
1:A:1875:ILE:HD11	1:A:1953:ILE:HD13	1.92	0.51
1:A:2226:ASN:HB2	1:A:2322:LYS:HG3	1.92	0.51
1:B:1800:ASN:HB3	1:B:1803:LEU:HB3	1.92	0.51
1:A:488:LYS:HA	1:A:518:TRP:CD1	2.46	0.51
1:A:1353:SER:HB2	1:A:1404:ASN:HD21	1.75	0.51
1:A:1997:ALA:HB2	1:A:2032:ALA:HB1	1.92	0.51
1:A:2179:GLU:HB3	1:A:2181:VAL:HG22	1.91	0.51
1:A:2495:LYS:H	1:A:2495:LYS:HD2	1.75	0.51
1:B:488:LYS:HA	1:B:518:TRP:CD1	2.46	0.51
1:B:1428:LYS:HA	1:B:1431:VAL:HG22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2495:LYS:H	1:B:2495:LYS:HD2	1.75	0.51
1:B:510:ARG:HH12	1:B:878:GLY:HA2	1.76	0.51
1:B:1326:LEU:HD23	1:B:1326:LEU:H	1.74	0.51
1:A:76:LYS:HB3	1:A:920:GLU:HG3	1.91	0.51
1:A:1323:LEU:HD22	1:A:1327:LYS:HE2	1.91	0.51
1:A:1679:GLN:HG2	1:A:1683:ASP:HA	1.92	0.51
1:B:207:ASN:ND2	1:B:358:GLU:HB3	2.25	0.51
1:B:556:PRO:HG3	1:B:832:THR:HG21	1.91	0.51
1:B:1232:SER:HA	1:B:1826:PHE:HA	1.93	0.51
1:B:1565:LYS:N	1:B:1638:LYS:HB3	2.25	0.51
1:A:57:TYR:CG	1:A:65:GLU:HB3	2.45	0.51
1:B:695:LEU:HD23	1:B:695:LEU:H	1.76	0.51
1:B:1828:GLN:HG3	1:B:2486:LYS:HD3	1.93	0.51
1:A:438:TYR:HA	1:A:441:LEU:HB2	1.93	0.51
1:A:817:GLU:O	1:A:820:LYS:HG2	2.11	0.51
1:A:827:ILE:HD12	1:A:827:ILE:H	1.76	0.51
1:A:1833:GLU:HG3	1:A:1836:LEU:HB2	1.92	0.51
1:A:2024:ILE:HG13	1:A:2024:ILE:O	2.11	0.51
1:B:954:PHE:HB3	1:B:1014:HIS:CD2	2.46	0.51
1:A:1803:LEU:O	1:A:1807:LEU:HG	2.11	0.51
1:B:1109:SER:OG	1:B:1141:LEU:HD21	2.10	0.51
1:B:2024:ILE:HG13	1:B:2024:ILE:O	2.11	0.51
1:A:954:PHE:HB3	1:A:1014:HIS:CD2	2.46	0.50
1:A:1565:LYS:N	1:A:1638:LYS:HB3	2.26	0.50
1:B:1559:TYR:CE1	1:B:1638:LYS:HG3	2.46	0.50
1:A:21:PHE:HD2	1:A:367:ILE:HD13	1.77	0.50
1:A:462:LEU:HD21	1:A:868:LYS:HD2	1.93	0.50
1:A:1428:LYS:HA	1:A:1431:VAL:HG22	1.93	0.50
1:A:1056:ASN:HB3	1:B:2061:GLU:HB2	1.93	0.50
1:B:231:ARG:HG2	1:B:234:ASP:HB2	1.93	0.50
1:B:1242:ASN:HD21	1:B:1613:GLU:HA	1.77	0.50
1:B:1349:LYS:O	1:B:1352:VAL:HG12	2.11	0.50
1:B:1927:ARG:HH22	1:B:1954:VAL:HG12	1.77	0.50
1:B:1997:ALA:HB2	1:B:2032:ALA:HB1	1.92	0.50
1:A:1789:PHE:CE2	1:A:1808:VAL:HA	2.46	0.50
1:B:438:TYR:HA	1:B:441:LEU:HB2	1.94	0.50
1:B:817:GLU:O	1:B:820:LYS:HG2	2.12	0.50
1:B:1353:SER:HB2	1:B:1404:ASN:HD21	1.75	0.50
1:B:1518:PHE:HB2	1:B:1529:TYR:OH	2.11	0.50
1:B:1911:LEU:HB3	1:B:1912:GLU:OE2	2.10	0.50
1:B:2145:LEU:O	1:B:2148:VAL:HG12	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1242:ASN:HD21	1:A:1613:GLU:HA	1.77	0.50
1:A:1296:ILE:HD12	1:A:1363:PHE:HB2	1.92	0.50
1:A:1472:ASN:HB2	1:A:1507:ILE:HG23	1.92	0.50
1:A:939:LEU:O	1:A:953:LEU:HD22	2.12	0.50
1:A:1807:LEU:HA	1:A:1813:ILE:HD12	1.94	0.50
1:B:1472:ASN:HB2	1:B:1507:ILE:HG23	1.93	0.50
1:B:2480:ALA:HB1	1:B:2483:MET:HG2	1.92	0.50
1:A:695:LEU:HD23	1:A:695:LEU:H	1.76	0.50
1:B:21:PHE:HD2	1:B:367:ILE:HD13	1.77	0.50
1:B:827:ILE:HD12	1:B:827:ILE:H	1.76	0.50
1:B:939:LEU:O	1:B:953:LEU:HD22	2.12	0.50
1:B:1459:GLN:HG2	1:B:1460:ASN:H	1.77	0.50
1:B:1789:PHE:CE2	1:B:1808:VAL:HA	2.47	0.50
1:A:682:ILE:HD12	1:A:684:ILE:HG12	1.94	0.50
1:A:1559:TYR:CE1	1:A:1638:LYS:HG3	2.46	0.50
1:B:664:TYR:O	1:B:668:LEU:HG	2.12	0.50
1:B:985:ILE:HG21	1:B:996:ILE:HD11	1.94	0.50
1:B:1852:LEU:HB3	1:B:1860:PHE:CD2	2.46	0.50
1:A:985:ILE:HG21	1:A:996:ILE:HD11	1.94	0.49
1:A:1459:GLN:HG2	1:A:1460:ASN:H	1.77	0.49
1:A:1800:ASN:HB3	1:A:1803:LEU:HB3	1.93	0.49
1:A:1828:GLN:HG3	1:A:2486:LYS:HD3	1.94	0.49
1:B:308:SER:OG	1:B:338:ASN:HB3	2.12	0.49
1:B:1076:LEU:HB3	1:B:1081:VAL:HG23	1.94	0.49
1:A:703:ALA:HB1	1:A:744:HIS:HD2	1.78	0.49
1:A:751:ILE:O	1:A:755:ILE:HG12	2.13	0.49
1:A:1840:SER:HB2	1:A:2457:GLN:NE2	2.27	0.49
1:B:554:GLN:HB2	1:B:642:PHE:HB2	1.94	0.49
1:A:1577:VAL:HG12	1:A:1580:PHE:H	1.77	0.49
1:A:510:ARG:HH12	1:A:878:GLY:HA2	1.77	0.49
1:A:759:LEU:HD12	1:A:762:LEU:HD11	1.95	0.49
1:A:1076:LEU:HB3	1:A:1081:VAL:HG23	1.94	0.49
1:A:2236:ILE:O	1:A:2240:ILE:HG12	2.13	0.49
1:B:120:GLY:N	1:B:167:ASP:HB3	2.14	0.49
1:A:1338:LYS:HA	1:A:1341:ILE:HG22	1.95	0.49
1:B:703:ALA:HB1	1:B:744:HIS:HD2	1.77	0.49
1:B:1305:GLU:O	1:B:1308:GLN:HG3	2.12	0.49
1:A:308:SER:OG	1:A:338:ASN:HB3	2.12	0.49
1:A:664:TYR:O	1:A:668:LEU:HG	2.12	0.49
1:A:2480:ALA:HB1	1:A:2483:MET:HG2	1.93	0.49
1:B:759:LEU:HD12	1:B:762:LEU:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HG2	1:A:234:ASP:HB2	1.93	0.49
1:B:682:ILE:HD12	1:B:684:ILE:HG12	1.94	0.49
1:B:2240:ILE:HG22	1:B:2244:ILE:HD11	1.95	0.49
1:A:554:GLN:HB2	1:A:642:PHE:HB2	1.94	0.49
1:B:806:ILE:HB	1:B:840:CYS:SG	2.53	0.49
1:A:2122:HIS:ND1	1:B:2132:ARG:NE	2.61	0.49
1:B:1174:PHE:HZ	1:B:1176:LYS:HD2	1.78	0.49
1:B:1338:LYS:HA	1:B:1341:ILE:HG22	1.95	0.49
1:B:1840:SER:HB2	1:B:2457:GLN:NE2	2.28	0.49
1:A:2261:ASP:OD1	1:A:2290:ARG:HB2	2.12	0.48
1:A:806:ILE:HB	1:A:840:CYS:SG	2.53	0.48
1:A:1516:ARG:HG2	1:A:2494:TYR:HB3	1.94	0.48
1:B:2103:LEU:HD23	1:B:2128:ILE:HB	1.95	0.48
1:A:802:PHE:O	1:A:806:ILE:HG12	2.13	0.48
1:A:1850:LEU:HD13	1:A:1862:PHE:CD2	2.48	0.48
1:B:1063:ASP:HB3	1:B:1066:LYS:HE2	1.96	0.48
1:B:1716:ILE:HA	1:B:1753:ARG:O	2.14	0.48
1:A:1232:SER:HA	1:A:1826:PHE:HA	1.95	0.48
1:B:1575:LYS:HG3	1:B:1581:ASN:ND2	2.28	0.48
1:A:1927:ARG:HH22	1:A:1954:VAL:HG12	1.77	0.48
1:B:2261:ASP:OD1	1:B:2290:ARG:HB2	2.13	0.48
1:A:627:TYR:CE2	1:A:825:LEU:HD21	2.49	0.48
1:A:954:PHE:HB3	1:A:1014:HIS:HD2	1.79	0.48
1:A:1268:TYR:CZ	1:A:1341:ILE:HG13	2.48	0.48
1:B:627:TYR:CE2	1:B:825:LEU:HD21	2.49	0.48
1:B:954:PHE:HB3	1:B:1014:HIS:HD2	1.78	0.48
1:A:1193:LEU:HD12	1:A:1197:THR:HB	1.95	0.48
1:A:2487:MET:HG2	1:A:2490:HIS:CE1	2.49	0.48
1:B:1108:CYS:HB3	1:B:1176:LYS:HE3	1.96	0.48
1:B:1268:TYR:CZ	1:B:1341:ILE:HG13	2.48	0.48
1:B:1850:LEU:HD13	1:B:1862:PHE:CD2	2.48	0.48
1:B:2236:ILE:O	1:B:2240:ILE:HG12	2.14	0.48
1:A:1037:ARG:HG2	1:B:144:TYR:CG	2.48	0.48
1:A:1063:ASP:HB3	1:A:1066:LYS:HE2	1.96	0.48
1:B:1972:TYR:HB3	1:B:2144:ILE:HG12	1.96	0.48
1:A:1174:PHE:HZ	1:A:1176:LYS:HD2	1.78	0.48
1:A:1682:PHE:HB3	1:A:1799:ASP:HA	1.95	0.48
1:B:605:GLU:HA	1:B:608:HIS:CG	2.49	0.48
1:B:1454:LEU:HD11	1:B:1518:PHE:HD1	1.78	0.48
1:A:1544:VAL:HG12	1:A:1585:ALA:HB2	1.94	0.48
1:B:802:PHE:O	1:B:806:ILE:HG12	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:LEU:HD12	1:B:1197:THR:HB	1.95	0.48
1:A:1716:ILE:HA	1:A:1753:ARG:O	2.14	0.47
1:A:2103:LEU:HD23	1:A:2128:ILE:HB	1.96	0.47
1:A:2240:ILE:HG22	1:A:2244:ILE:HD11	1.95	0.47
1:B:130:MET:SD	1:B:178:ALA:HB1	2.53	0.47
1:B:1234:ASP:HB3	1:B:1641:ILE:HG21	1.94	0.47
1:B:1682:PHE:HB3	1:B:1799:ASP:HA	1.95	0.47
1:A:1291:VAL:HG12	1:A:1292:ASP:N	2.29	0.47
1:B:1516:ARG:HG2	1:B:2494:TYR:HB3	1.95	0.47
1:B:2142:ARG:HD3	1:B:2142:ARG:O	2.14	0.47
1:A:1972:TYR:HB3	1:A:2144:ILE:HG12	1.96	0.47
1:B:463:ILE:HD11	1:B:497:VAL:HG22	1.96	0.47
1:B:1639:ARG:NH2	1:B:1644:MET:HG3	2.30	0.47
1:A:512:VAL:HG21	1:A:872:SER:HA	1.95	0.47
1:A:1340:GLU:O	1:A:1344:ILE:HG13	2.15	0.47
1:B:1291:VAL:HG12	1:B:1292:ASP:N	2.29	0.47
1:B:1340:GLU:O	1:B:1344:ILE:HG13	2.15	0.47
1:A:235:ALA:HB3	1:A:386:LYS:HE3	1.97	0.47
1:A:1641:ILE:HA	1:A:1644:MET:CE	2.42	0.47
1:B:1641:ILE:HA	1:B:1644:MET:CE	2.44	0.47
1:B:2335:LEU:HA	1:B:2386:LYS:HB2	1.96	0.47
1:A:169:ARG:HH12	1:B:279:ASN:CB	2.23	0.47
1:A:2310:GLN:HA	1:A:2313:SER:HB3	1.97	0.47
1:B:557:GLN:HE22	1:B:607:HIS:HA	1.79	0.47
1:B:752:LYS:O	1:B:755:ILE:HG13	2.14	0.47
1:B:951:MET:HA	1:B:951:MET:HE3	1.97	0.47
1:A:1082:TYR:CZ	1:A:1097:GLN:HA	2.50	0.47
1:A:1184:SER:HA	1:A:1208:THR:HA	1.97	0.47
1:A:1282:ILE:HG13	1:A:1283:GLU:N	2.29	0.47
1:B:392:LYS:HB3	1:B:395:ASP:HB2	1.96	0.47
1:B:1153:LEU:HD13	1:B:1202:ILE:HD13	1.97	0.47
1:A:493:PHE:O	1:A:497:VAL:HG23	2.15	0.47
1:B:1056:ASN:ND2	1:B:1058:LYS:HE2	2.29	0.47
1:B:2310:GLN:HA	1:B:2313:SER:HB3	1.97	0.47
1:B:2487:MET:HG2	1:B:2490:HIS:CE1	2.50	0.47
1:A:135:GLN:HB2	1:A:153:SER:OG	2.15	0.46
1:A:369:VAL:HG23	1:A:415:MET:CE	2.45	0.46
1:B:512:VAL:HG21	1:B:872:SER:HA	1.96	0.46
1:A:1108:CYS:HB3	1:A:1176:LYS:HE3	1.96	0.46
1:A:1489:THR:HB	1:A:1516:ARG:NE	2.30	0.46
1:B:870:ALA:O	1:B:874:LEU:HD22	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2245:ILE:HD13	1:B:2281:THR:HG21	1.97	0.46
1:B:369:VAL:HG23	1:B:415:MET:CE	2.45	0.46
1:B:1282:ILE:HG13	1:B:1283:GLU:N	2.30	0.46
1:B:1489:THR:HB	1:B:1516:ARG:NE	2.30	0.46
1:A:989:PHE:CE2	1:A:1050:ILE:HD11	2.50	0.46
1:B:1858:LEU:HD13	1:B:2170:VAL:HG12	1.98	0.46
1:A:279:ASN:CB	1:B:169:ARG:HH12	2.24	0.46
1:A:1082:TYR:OH	1:A:1097:GLN:HA	2.16	0.46
1:A:2142:ARG:O	1:A:2142:ARG:HD3	2.15	0.46
1:B:235:ALA:HB3	1:B:386:LYS:HE3	1.97	0.46
1:B:989:PHE:CE2	1:B:1050:ILE:HD11	2.49	0.46
1:B:1082:TYR:CZ	1:B:1097:GLN:HA	2.50	0.46
1:B:1180:ILE:HG23	1:B:1185:THR:HG22	1.97	0.46
1:B:1184:SER:HA	1:B:1208:THR:HA	1.97	0.46
1:B:1853:ASN:HA	1:B:1943:SER:HB2	1.96	0.46
1:B:1878:MET:HG2	1:B:1915:GLY:HA2	1.98	0.46
1:A:1370:SER:O	1:A:1373:ASP:HB2	2.15	0.46
1:B:1370:SER:O	1:B:1373:ASP:HB2	2.15	0.46
1:B:1771:SER:O	1:B:2395:LEU:HD23	2.16	0.46
1:A:1180:ILE:HG23	1:A:1185:THR:HG22	1.97	0.46
1:A:2182:HIS:O	1:A:2183:ILE:HG13	2.16	0.46
1:B:2182:HIS:O	1:B:2183:ILE:HG13	2.16	0.46
1:A:1230:TRP:CZ2	1:A:1828:GLN:HB3	2.51	0.46
1:A:1475:LEU:HD12	1:A:1475:LEU:HA	1.76	0.46
1:A:1852:LEU:HB3	1:A:1860:PHE:CD2	2.48	0.46
1:A:2108:LEU:HD21	1:B:2120:LYS:HD3	1.97	0.46
1:A:2245:ILE:HD13	1:A:2281:THR:HG21	1.98	0.46
1:B:7:LYS:HG2	1:B:8:ASP:N	2.31	0.46
1:B:1082:TYR:OH	1:B:1097:GLN:HA	2.16	0.46
1:B:2142:ARG:O	1:B:2146:THR:HG22	2.16	0.46
1:A:7:LYS:HG2	1:A:8:ASP:N	2.31	0.46
1:B:940:LEU:HD11	1:B:951:MET:HG3	1.97	0.46
1:A:1851:TYR:CE1	1:A:1863:GLN:HB2	2.50	0.46
1:B:1830:ILE:HB	1:B:2487:MET:HG3	1.98	0.46
1:A:1666:VAL:HB	1:A:1677:TYR:HD2	1.82	0.45
1:A:1139:LEU:HD21	1:A:1148:ILE:HG21	1.99	0.45
1:A:1851:TYR:CD2	1:A:1945:LEU:HB2	2.52	0.45
1:A:2403:TYR:O	1:A:2407:ILE:HG12	2.16	0.45
1:B:1156:MET:HB2	1:B:1202:ILE:HG12	1.98	0.45
1:B:1230:TRP:CE2	1:B:1828:GLN:HB3	2.51	0.45
1:A:664:TYR:CZ	1:A:668:LEU:HD11	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1780:PHE:HB3	1:A:1786:LEU:HD23	1.97	0.45
1:A:2116:PHE:HB2	1:B:2112:ASP:O	2.16	0.45
1:A:2142:ARG:O	1:A:2146:THR:HG22	2.16	0.45
1:A:2448:ILE:O	1:A:2452:LEU:HD22	2.17	0.45
1:B:312:TYR:HB3	1:B:415:MET:HG2	1.99	0.45
1:B:1716:ILE:HD13	1:B:1718:PHE:HE1	1.82	0.45
1:B:1777:PHE:HA	1:B:1780:PHE:HD2	1.82	0.45
1:B:2403:TYR:O	1:B:2407:ILE:HG12	2.16	0.45
1:A:1230:TRP:CE2	1:A:1828:GLN:HB3	2.51	0.45
1:A:2401:SER:O	1:A:2405:LYS:HG3	2.17	0.45
1:B:135:GLN:HB2	1:B:153:SER:OG	2.15	0.45
1:B:1067:LEU:HD23	1:B:1067:LEU:HA	1.67	0.45
1:B:1541:LEU:HD22	1:B:1544:VAL:HG21	1.98	0.45
1:A:312:TYR:HB3	1:A:415:MET:HG2	1.98	0.45
1:A:509:LYS:HD3	1:A:509:LYS:HA	1.85	0.45
1:A:805:ALA:O	1:A:809:ILE:HG13	2.17	0.45
1:A:1316:SER:HA	1:A:1317:LEU:HA	1.82	0.45
1:A:1858:LEU:HD13	1:A:2170:VAL:HG12	1.98	0.45
1:A:2335:LEU:HA	1:A:2386:LYS:HB2	1.97	0.45
1:B:1871:GLY:HA2	1:B:1925:VAL:HG23	1.99	0.45
1:B:2325:LEU:HD22	1:B:2373:ILE:HB	1.99	0.45
1:A:1153:LEU:HD13	1:A:1202:ILE:HD13	1.97	0.45
1:A:1852:LEU:HD23	1:A:1852:LEU:HA	1.82	0.45
1:A:1871:GLY:HA2	1:A:1925:VAL:HG23	1.99	0.45
1:A:1771:SER:O	1:A:2395:LEU:HD23	2.16	0.45
1:A:1944:SER:HB3	1:A:2193:PHE:CE2	2.51	0.45
1:B:949:THR:OG1	1:B:1019:ILE:HB	2.17	0.45
1:B:996:ILE:HG12	1:B:1050:ILE:HG22	1.99	0.45
1:B:1230:TRP:CZ2	1:B:1828:GLN:HB3	2.51	0.45
1:B:1666:VAL:HB	1:B:1677:TYR:HD2	1.82	0.45
1:A:1830:ILE:HB	1:A:2487:MET:HG3	1.98	0.45
1:A:2273:GLU:HA	1:A:2273:GLU:OE1	2.16	0.45
1:B:609:PRO:HD2	1:B:674:MET:SD	2.57	0.45
1:B:757:LYS:HA	1:B:757:LYS:HD3	1.84	0.45
1:B:1048:GLY:N	1:B:2111:ASN:HD21	2.13	0.45
1:B:1662:CYS:HB3	1:B:1689:CYS:SG	2.57	0.45
1:A:1640:ASP:O	1:A:1644:MET:HE2	2.17	0.45
1:B:2:THR:HG22	1:B:4:ASN:H	1.81	0.45
1:B:1273:LEU:HB3	1:B:1314:ILE:HD11	1.98	0.45
1:B:1350:ARG:HA	1:B:1350:ARG:HD3	1.87	0.45
1:A:1056:ASN:HD21	1:A:1058:LYS:HE2	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:MET:HB2	1:A:1202:ILE:HG12	1.98	0.45
1:A:1273:LEU:HB3	1:A:1314:ILE:HD11	1.98	0.45
1:A:373:LEU:HA	1:A:373:LEU:HD23	1.77	0.44
1:A:1518:PHE:HB2	1:A:1529:TYR:OH	2.17	0.44
1:A:1716:ILE:HD13	1:A:1718:PHE:HE1	1.81	0.44
1:A:1896:GLN:HE22	1:A:1904:ILE:HB	1.82	0.44
1:B:664:TYR:CZ	1:B:668:LEU:HD11	2.51	0.44
1:B:665:TYR:HD1	1:B:668:LEU:HD12	1.83	0.44
1:B:805:ALA:O	1:B:809:ILE:HG13	2.17	0.44
1:B:1139:LEU:HD21	1:B:1148:ILE:HG21	1.99	0.44
1:B:2401:SER:O	1:B:2405:LYS:HG3	2.17	0.44
1:A:605:GLU:HA	1:A:608:HIS:CG	2.51	0.44
1:A:2433:SER:O	1:A:2436:GLU:HG2	2.17	0.44
1:B:114:LYS:O	1:B:117:THR:HG22	2.18	0.44
1:B:462:LEU:H	1:B:887:GLN:NE2	2.15	0.44
1:B:480:LEU:HA	1:B:480:LEU:HD23	1.75	0.44
1:B:1682:PHE:CD2	1:B:1801:LEU:HD22	2.52	0.44
1:A:104:LEU:HD23	1:A:166:PHE:CE1	2.52	0.44
1:A:1666:VAL:HB	1:A:1677:TYR:CD2	2.52	0.44
1:B:263:ARG:HD3	1:B:906:GLU:HA	1.98	0.44
1:B:2335:LEU:HG	1:B:2386:LYS:HD2	1.99	0.44
1:A:2:THR:HG22	1:A:4:ASN:H	1.82	0.44
1:A:940:LEU:HD11	1:A:951:MET:HG3	1.98	0.44
1:A:949:THR:OG1	1:A:1019:ILE:HB	2.17	0.44
1:A:1269:LEU:O	1:A:1272:LEU:HG	2.16	0.44
1:B:1269:LEU:O	1:B:1272:LEU:HG	2.17	0.44
1:B:1644:MET:H	1:B:1806:ARG:HD3	1.81	0.44
1:B:1666:VAL:HB	1:B:1677:TYR:CD2	2.52	0.44
1:B:2433:SER:O	1:B:2436:GLU:HG2	2.18	0.44
1:A:114:LYS:O	1:A:117:THR:HG22	2.18	0.44
1:A:1177:PHE:HZ	1:A:1180:ILE:HG12	1.83	0.44
1:A:690:LEU:HA	1:A:694:ALA:HB2	2.00	0.44
1:A:2360:ASN:O	1:A:2364:GLU:HG2	2.18	0.44
1:B:624:VAL:HG21	1:B:650:PHE:CZ	2.53	0.44
1:B:642:PHE:O	1:B:645:VAL:HG22	2.17	0.44
1:B:1264:LEU:HB2	1:B:1326:LEU:HD11	1.99	0.44
1:A:624:VAL:HG21	1:A:650:PHE:CZ	2.53	0.44
1:A:1770:GLY:O	1:A:1774:ILE:HG13	2.18	0.44
1:B:509:LYS:HD3	1:B:509:LYS:HA	1.85	0.44
1:B:1076:LEU:HD11	1:B:2272:TRP:CE3	2.53	0.44
1:B:1356:LYS:HE3	1:B:1356:LYS:HB3	1.87	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1936:GLY:HA3	1:B:1953:ILE:HG22	2.00	0.44
1:B:2229:LEU:HD21	1:B:2265:LEU:HD13	2.00	0.44
1:A:1718:PHE:HE2	1:A:1801:LEU:HD11	1.83	0.44
1:A:1736:MET:HE3	1:A:1740:LEU:HD11	2.00	0.44
1:A:1913:CYS:HB2	1:A:1941:SER:OG	2.18	0.44
1:A:2122:HIS:CG	1:B:2132:ARG:HE	2.36	0.44
1:B:373:LEU:HD23	1:B:373:LEU:HA	1.78	0.44
1:B:2249:VAL:HG21	1:B:2285:TYR:CE1	2.53	0.44
1:A:75:TRP:CE3	1:A:95:PRO:HB2	2.53	0.44
1:A:200:MET:HE2	1:A:200:MET:HB2	1.92	0.44
1:A:642:PHE:O	1:A:645:VAL:HG22	2.17	0.44
1:A:1048:GLY:N	1:A:2111:ASN:HD21	2.15	0.44
1:A:1644:MET:H	1:A:1806:ARG:HD3	1.82	0.44
1:A:1662:CYS:HB3	1:A:1689:CYS:SG	2.57	0.44
1:A:1876:LYS:O	1:A:1915:GLY:HA3	2.18	0.44
1:B:55:SER:HA	1:B:58:GLU:OE2	2.18	0.44
1:A:753:GLU:O	1:A:757:LYS:HG2	2.18	0.43
1:A:951:MET:HB2	1:A:1017:THR:OG1	2.18	0.43
1:A:1575:LYS:HG3	1:A:1581:ASN:ND2	2.33	0.43
1:A:1682:PHE:CD2	1:A:1801:LEU:HD22	2.53	0.43
1:B:104:LEU:HD23	1:B:166:PHE:CE1	2.52	0.43
1:B:1718:PHE:HE2	1:B:1801:LEU:HD11	1.83	0.43
1:B:2220:THR:HA	1:B:2251:ASN:OD1	2.18	0.43
1:B:2304:THR:OG1	1:B:2361:LEU:HD11	2.18	0.43
1:A:55:SER:HA	1:A:58:GLU:OE2	2.18	0.43
1:A:263:ARG:HD3	1:A:906:GLU:HA	2.01	0.43
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.81	0.43
1:A:558:TRP:HZ3	1:A:829:PRO:HB2	1.84	0.43
1:A:996:ILE:HG12	1:A:1050:ILE:HG22	2.00	0.43
1:A:2132:ARG:CZ	1:B:2122:HIS:ND1	2.82	0.43
1:B:34:TRP:CE3	1:B:371:LEU:HB3	2.53	0.43
1:B:558:TRP:HZ3	1:B:829:PRO:HB2	1.83	0.43
1:B:587:PHE:HD2	1:B:589:TYR:HH	1.66	0.43
1:B:1177:PHE:HZ	1:B:1180:ILE:HG12	1.83	0.43
1:B:1917:ILE:HG22	1:B:1930:VAL:HA	1.99	0.43
1:B:2055:TYR:CE1	1:B:2065:GLU:HG2	2.52	0.43
1:A:140:ARG:HA	1:A:140:ARG:HD3	1.58	0.43
1:A:1348:ILE:O	1:A:1352:VAL:HG12	2.18	0.43
1:A:1454:LEU:HD11	1:A:1518:PHE:CD2	2.53	0.43
1:A:1264:LEU:HB2	1:A:1326:LEU:HD11	1.99	0.43
1:A:2114:LEU:HB3	1:B:2116:PHE:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:LEU:HA	1:B:445:THR:HG22	1.99	0.43
1:B:690:LEU:HA	1:B:694:ALA:HB2	2.00	0.43
1:B:1850:LEU:HD21	1:B:2214:VAL:HG11	2.01	0.43
1:A:1312:LYS:HE2	1:A:1312:LYS:HB3	1.71	0.43
1:A:2055:TYR:CE1	1:A:2065:GLU:HG2	2.52	0.43
1:B:672:LEU:HD23	1:B:672:LEU:HA	1.83	0.43
1:B:1851:TYR:CD2	1:B:1945:LEU:HB2	2.54	0.43
1:A:2335:LEU:HG	1:A:2386:LYS:HD2	1.99	0.43
1:B:1550:ASP:HB3	1:B:1553:GLU:HG3	2.00	0.43
1:B:2445:LEU:O	1:B:2449:LEU:HG	2.18	0.43
1:A:1037:ARG:HG2	1:B:144:TYR:CD2	2.53	0.43
1:B:242:ARG:HE	1:B:358:GLU:CD	2.21	0.43
1:A:557:GLN:HE22	1:A:607:HIS:HA	1.84	0.43
1:A:561:MET:SD	1:A:619:ILE:HG13	2.59	0.43
1:A:2304:THR:OG1	1:A:2361:LEU:HD11	2.18	0.43
1:B:289:MET:HE1	1:B:329:GLU:HG2	2.00	0.43
1:B:1464:SER:HA	1:B:1467:LEU:HB2	2.01	0.43
1:B:2092:ARG:HB2	1:B:2092:ARG:HH11	1.84	0.43
1:A:25:GLY:HA3	1:A:41:MET:HE2	2.01	0.43
1:A:144:TYR:CD2	1:B:1037:ARG:HG2	2.54	0.43
1:A:351:LYS:HG3	1:A:356:HIS:HA	2.00	0.43
1:A:1264:LEU:HB3	1:A:1322:ASP:OD1	2.19	0.43
1:A:1887:ASN:HD21	1:A:2178:ASN:HB2	1.84	0.43
1:A:2229:LEU:HD21	1:A:2265:LEU:HD13	2.00	0.43
1:B:554:GLN:HB2	1:B:642:PHE:CB	2.48	0.43
1:B:951:MET:HB2	1:B:1017:THR:OG1	2.18	0.43
1:B:1887:ASN:ND2	1:B:2178:ASN:HB2	2.34	0.43
1:A:164:PHE:HA	1:B:277:GLY:HA2	2.00	0.43
1:A:665:TYR:HD1	1:A:668:LEU:HD12	1.83	0.43
1:A:941:GLY:HA3	1:A:952:GLU:O	2.19	0.43
1:A:1274:ASN:O	1:A:1278:LYS:HG3	2.19	0.43
1:A:1550:ASP:HB3	1:A:1553:GLU:HG3	1.99	0.43
1:A:2220:THR:HA	1:A:2251:ASN:OD1	2.18	0.43
1:A:2445:LEU:O	1:A:2449:LEU:HG	2.19	0.43
1:B:753:GLU:O	1:B:757:LYS:HG2	2.19	0.43
1:B:1475:LEU:HD12	1:B:1475:LEU:HA	1.75	0.43
1:B:1829:LYS:HD3	1:B:1829:LYS:HA	1.79	0.43
1:A:34:TRP:CE3	1:A:371:LEU:HB3	2.53	0.42
1:A:392:LYS:HB3	1:A:395:ASP:HB2	2.00	0.42
1:A:1887:ASN:ND2	1:A:2178:ASN:HB2	2.34	0.42
1:A:2249:VAL:HG21	1:A:2285:TYR:CE1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1896:GLN:HE22	1:B:1904:ILE:HB	1.83	0.42
1:A:350:VAL:HB	1:A:368:LYS:HD2	2.02	0.42
1:A:1458:TYR:HD1	1:A:1542:LEU:HD22	1.84	0.42
1:A:1982:ILE:HD11	1:A:2132:ARG:NH1	2.35	0.42
1:B:1026:GLU:CD	1:B:1049:ARG:HD2	2.40	0.42
1:B:1212:ARG:HB2	1:B:1905:TYR:CE2	2.54	0.42
1:B:1385:LYS:HA	1:B:1386:SER:HA	1.57	0.42
1:B:1458:TYR:HD1	1:B:1542:LEU:HD22	1.84	0.42
1:B:1913:CYS:HB2	1:B:1941:SER:OG	2.18	0.42
1:A:1609:PHE:HB3	1:A:1636:THR:OG1	2.19	0.42
1:A:2325:LEU:HD22	1:A:2373:ILE:HB	2.00	0.42
1:B:75:TRP:CE3	1:B:95:PRO:HB2	2.54	0.42
1:B:140:ARG:HA	1:B:140:ARG:HD3	1.58	0.42
1:B:559:ARG:HG3	1:B:598:LEU:HB2	2.01	0.42
1:B:1329:VAL:O	1:B:1333:LYS:HG3	2.18	0.42
1:B:1609:PHE:HB3	1:B:1636:THR:OG1	2.19	0.42
1:B:2441:LEU:HD12	1:B:2442:LEU:H	1.83	0.42
1:B:2448:ILE:O	1:B:2452:LEU:HD22	2.18	0.42
1:A:1076:LEU:HD11	1:A:2272:TRP:CE3	2.53	0.42
1:A:1491:PRO:HA	1:A:1516:ARG:O	2.19	0.42
1:A:1723:LEU:HD21	1:A:1757:LEU:HG	2.01	0.42
1:A:442:LEU:HA	1:A:445:THR:HG22	1.99	0.42
1:A:559:ARG:HG3	1:A:598:LEU:HB2	2.01	0.42
1:A:640:HIS:CG	1:A:641:SER:H	2.38	0.42
1:A:1113:LEU:HD23	1:A:1113:LEU:HA	1.94	0.42
1:A:1212:ARG:HB2	1:A:1905:TYR:CE2	2.54	0.42
1:A:1291:VAL:HG12	1:A:1292:ASP:H	1.84	0.42
1:A:1579:SER:HA	1:A:1582:LEU:HG	2.02	0.42
1:A:1815:ASP:OD2	1:A:2485:ARG:HB2	2.20	0.42
1:A:1936:GLY:HA3	1:A:1953:ILE:HG22	2.01	0.42
1:B:350:VAL:HB	1:B:368:LYS:HD2	2.01	0.42
1:B:561:MET:SD	1:B:619:ILE:HG13	2.59	0.42
1:B:1073:PHE:HE2	1:B:2280:GLN:HA	1.83	0.42
1:B:1312:LYS:HE2	1:B:1312:LYS:HB3	1.71	0.42
1:B:1579:SER:HA	1:B:1582:LEU:HG	2.01	0.42
1:B:2360:ASN:O	1:B:2364:GLU:HG2	2.18	0.42
1:A:265:TYR:HA	1:A:374:LYS:HE2	2.02	0.42
1:A:316:HIS:CG	1:A:316:HIS:O	2.73	0.42
1:A:1724:GLU:H	1:A:1724:GLU:HG2	1.72	0.42
1:B:216:MET:HE2	1:B:216:MET:HB2	1.85	0.42
1:B:351:LYS:HG3	1:B:356:HIS:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1982:ILE:HD11	1:B:2132:ARG:NH1	2.34	0.42
1:A:1640:ASP:OD2	1:A:1642:GLU:HB3	2.19	0.42
1:B:316:HIS:CG	1:B:316:HIS:O	2.73	0.42
1:B:640:HIS:CG	1:B:641:SER:H	2.38	0.42
1:B:838:PRO:HG3	1:B:853:ILE:HD11	2.01	0.42
1:A:96:GLN:HB3	1:A:206:VAL:HG11	2.01	0.42
1:A:608:HIS:HB3	1:A:674:MET:HE1	2.01	0.42
1:A:2441:LEU:HD12	1:A:2442:LEU:H	1.84	0.42
1:B:1135:PHE:N	1:B:1135:PHE:CD1	2.88	0.42
1:B:1189:LEU:HD12	1:B:1190:ASP:N	2.35	0.42
1:B:1264:LEU:HB3	1:B:1322:ASP:OD1	2.19	0.42
1:B:1770:GLY:HA2	1:B:1773:LEU:HD13	2.02	0.42
1:B:1815:ASP:OD2	1:B:2485:ARG:HB2	2.19	0.42
1:A:1049:ARG:NH1	1:B:2115:ASP:HB2	2.35	0.42
1:A:1268:TYR:CE1	1:A:1272:LEU:HD23	2.55	0.42
1:A:1504:THR:HB	1:A:1507:ILE:HD13	2.00	0.42
1:A:1701:GLU:O	1:A:1705:LYS:HG3	2.19	0.42
1:B:21:PHE:CD2	1:B:367:ILE:HD13	2.55	0.42
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.87	0.42
1:B:413:ILE:HD13	1:B:413:ILE:HA	1.87	0.42
1:B:871:ILE:HD13	1:B:871:ILE:HA	1.92	0.42
1:B:1028:LYS:NZ	1:B:2111:ASN:HB3	2.35	0.42
1:B:1291:VAL:HG12	1:B:1292:ASP:H	1.84	0.42
1:B:1295:GLU:HA	1:B:1296:ILE:HA	1.74	0.42
1:B:1504:THR:HB	1:B:1507:ILE:HD13	2.01	0.42
1:B:1887:ASN:HD21	1:B:2178:ASN:HB2	1.84	0.42
1:A:679:LEU:HD21	1:A:742:SER:HA	2.01	0.42
1:A:700:ILE:HG13	1:A:714:THR:O	2.20	0.42
1:A:1135:PHE:N	1:A:1135:PHE:CD1	2.88	0.42
1:A:2092:ARG:HB2	1:A:2092:ARG:HH11	1.84	0.42
1:A:2199:LYS:HA	1:A:2202:LEU:HB2	2.02	0.42
1:B:1770:GLY:O	1:B:1774:ILE:HG13	2.18	0.42
1:A:596:ARG:HA	1:A:596:ARG:HD3	1.88	0.41
1:A:1111:PHE:CZ	1:A:1137:GLY:HA3	2.55	0.41
1:A:1413:PHE:HB3	1:A:1419:ILE:HG12	2.02	0.41
1:B:609:PRO:HA	1:B:612:ALA:HB3	2.02	0.41
1:B:1454:LEU:HD13	1:B:1454:LEU:HA	1.88	0.41
1:B:1836:LEU:HD12	1:B:1836:LEU:HA	1.90	0.41
1:A:101:MET:HG3	1:A:162:LEU:HD23	2.02	0.41
1:B:1268:TYR:CE1	1:B:1272:LEU:HD23	2.54	0.41
1:B:1274:ASN:O	1:B:1278:LYS:HG3	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1413:PHE:HB3	1:B:1419:ILE:HG12	2.02	0.41
1:B:1488:TYR:O	1:B:1513:ILE:HA	2.20	0.41
1:B:1724:GLU:H	1:B:1724:GLU:HG2	1.71	0.41
1:B:1759:TYR:O	1:B:1767:ASN:HB3	2.21	0.41
1:B:2245:ILE:HG23	1:B:2289:PHE:HE2	1.85	0.41
1:A:30:PRO:HB3	1:A:371:LEU:HD21	2.01	0.41
1:A:277:GLY:HA2	1:B:164:PHE:HA	2.02	0.41
1:A:1297:ASP:HA	1:A:1298:SER:HB3	2.02	0.41
1:A:1356:LYS:HE3	1:A:1356:LYS:HB3	1.88	0.41
1:A:1385:LYS:HA	1:A:1386:SER:HA	1.57	0.41
1:A:1888:LEU:HB3	1:A:1894:LEU:HD21	2.03	0.41
1:A:2120:LYS:HD3	1:B:2108:LEU:HD21	2.02	0.41
1:A:2174:ILE:O	1:A:2177:ILE:HG22	2.20	0.41
1:B:188:LEU:HD23	1:B:188:LEU:HA	1.76	0.41
1:B:265:TYR:HA	1:B:374:LYS:HE2	2.02	0.41
1:B:700:ILE:HG13	1:B:714:THR:O	2.20	0.41
1:B:941:GLY:HA3	1:B:952:GLU:O	2.19	0.41
1:B:1297:ASP:HA	1:B:1298:SER:HB3	2.02	0.41
1:B:1454:LEU:HD11	1:B:1518:PHE:CD1	2.55	0.41
1:A:108:PHE:HD1	1:A:108:PHE:HA	1.74	0.41
1:A:434:ALA:HB3	1:A:438:TYR:OH	2.20	0.41
1:A:536:SER:HB3	1:A:538:ILE:HG12	2.03	0.41
1:A:666:ARG:HE	1:A:796:LEU:HD21	1.85	0.41
1:A:1488:TYR:O	1:A:1513:ILE:HA	2.20	0.41
1:A:1917:ILE:HG22	1:A:1930:VAL:HA	2.00	0.41
1:B:30:PRO:HB3	1:B:371:LEU:HD21	2.01	0.41
1:B:241:ILE:O	1:B:356:HIS:HB3	2.21	0.41
1:B:1672:GLU:H	1:B:1672:GLU:HG2	1.61	0.41
1:A:680:LEU:HB3	1:A:720:LEU:HD22	2.03	0.41
1:A:1189:LEU:HD12	1:A:1190:ASP:N	2.35	0.41
1:A:1850:LEU:HD21	1:A:2214:VAL:HG11	2.02	0.41
1:B:700:ILE:HD11	1:B:713:ILE:HB	2.02	0.41
1:B:2066:ILE:HG21	1:B:2075:VAL:HG13	2.03	0.41
1:A:241:ILE:O	1:A:356:HIS:HB3	2.21	0.41
1:A:951:MET:HE3	1:A:951:MET:HA	2.02	0.41
1:A:1073:PHE:HE2	1:A:2280:GLN:HA	1.84	0.41
1:A:2245:ILE:HG23	1:A:2289:PHE:HE2	1.85	0.41
1:B:1112:LYS:HD2	1:B:1170:PHE:CD2	2.55	0.41
1:B:1349:LYS:HD3	1:B:1349:LYS:HA	1.88	0.41
1:B:1701:GLU:O	1:B:1705:LYS:HG3	2.20	0.41
1:B:1777:PHE:O	1:B:1781:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1917:ILE:HD13	1:B:1928:PHE:HB3	2.02	0.41
1:B:1944:SER:HB3	1:B:2193:PHE:CE2	2.56	0.41
1:B:493:PHE:O	1:B:497:VAL:HG23	2.20	0.41
1:B:1253:LYS:HD2	1:B:1627:GLN:HG3	2.02	0.41
1:B:1351:ILE:O	1:B:1355:LEU:HG	2.21	0.41
1:B:1723:LEU:HD21	1:B:1757:LEU:HG	2.01	0.41
1:B:2042:TYR:CD2	1:B:2183:ILE:HD13	2.55	0.41
1:A:430:ILE:HD13	1:A:430:ILE:HA	1.97	0.41
1:A:549:TYR:CD2	1:A:634:PRO:HB3	2.56	0.41
1:A:983:ASP:OD2	1:A:1128:PRO:HG3	2.21	0.41
1:A:1112:LYS:HD2	1:A:1170:PHE:CD2	2.55	0.41
1:A:1759:TYR:O	1:A:1767:ASN:HB3	2.20	0.41
1:A:1917:ILE:HD13	1:A:1928:PHE:HB3	2.01	0.41
1:B:202:ILE:HG12	1:B:250:ILE:HG13	2.03	0.41
1:B:1111:PHE:CZ	1:B:1137:GLY:HA3	2.56	0.41
1:B:1570:LEU:HB3	1:B:1634:VAL:HG23	2.03	0.41
1:B:2151:ALA:HB3	1:B:2157:LEU:HD23	2.02	0.41
1:A:105:TRP:CZ3	1:A:115:PRO:HG2	2.56	0.41
1:A:202:ILE:HG12	1:A:250:ILE:HG13	2.02	0.41
1:A:462:LEU:H	1:A:887:GLN:NE2	2.15	0.41
1:A:554:GLN:HB2	1:A:642:PHE:CB	2.51	0.41
1:A:717:GLU:HA	1:A:720:LEU:HD12	2.03	0.41
1:A:1795:LYS:HD3	1:A:1795:LYS:HA	1.86	0.41
1:A:2042:TYR:CD2	1:A:2183:ILE:HD13	2.55	0.41
1:A:2148:VAL:HG23	1:A:2157:LEU:HD21	2.03	0.41
1:A:2165:PHE:CD2	1:A:2173:ALA:HB2	2.56	0.41
1:B:301:LYS:HE3	1:B:301:LYS:HB3	1.89	0.41
1:B:549:TYR:CD2	1:B:634:PRO:HB3	2.56	0.41
1:B:596:ARG:HA	1:B:596:ARG:HD3	1.89	0.41
1:B:680:LEU:HB3	1:B:720:LEU:HD22	2.03	0.41
1:B:1527:ASN:HB3	1:B:1529:TYR:CE1	2.56	0.41
1:B:2148:VAL:HG23	1:B:2157:LEU:HD21	2.03	0.41
1:B:2284:LYS:HG2	1:B:2285:TYR:CE2	2.56	0.41
1:A:547:VAL:HG13	1:A:879:VAL:HG21	2.02	0.41
1:A:1138:LEU:HD11	1:A:1187:GLY:HA3	2.02	0.41
1:A:1578:LEU:O	1:A:1582:LEU:HG	2.21	0.41
1:A:2284:LYS:HG2	1:A:2285:TYR:CE2	2.56	0.41
1:B:679:LEU:HD21	1:B:742:SER:HA	2.01	0.41
1:A:21:PHE:CD2	1:A:367:ILE:HD13	2.55	0.40
1:A:466:SER:HB2	1:A:507:LEU:H	1.86	0.40
1:A:1108:CYS:HB3	1:A:1176:LYS:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:ARG:CZ	1:A:1322:ASP:HB3	2.52	0.40
1:A:1942:LEU:HD12	1:A:1942:LEU:HA	1.87	0.40
1:B:366:LEU:HD12	1:B:366:LEU:HA	1.91	0.40
1:B:989:PHE:CD1	1:B:1052:LEU:HD11	2.56	0.40
1:B:1929:LYS:HE3	1:B:1929:LYS:HB3	1.90	0.40
1:B:2451:CYS:O	1:B:2455:VAL:HG12	2.22	0.40
1:A:566:TYR:CE1	1:A:573:LYS:HG3	2.56	0.40
1:A:608:HIS:HA	1:A:609:PRO:HD3	1.97	0.40
1:A:2221:CYS:SG	1:A:2224:LEU:HD12	2.61	0.40
1:A:2351:LYS:HB3	1:A:2351:LYS:HE3	1.79	0.40
1:B:96:GLN:HB3	1:B:206:VAL:HG11	2.02	0.40
1:B:101:MET:HG3	1:B:162:LEU:HD23	2.03	0.40
1:B:258:ILE:HG13	1:B:259:LYS:N	2.36	0.40
1:B:1876:LYS:O	1:B:1915:GLY:HA3	2.20	0.40
1:B:1876:LYS:NZ	1:B:1944:SER:HB2	2.36	0.40
1:B:2165:PHE:CD2	1:B:2173:ALA:HB2	2.56	0.40
1:B:2174:ILE:O	1:B:2177:ILE:HG22	2.20	0.40
1:B:2221:CYS:SG	1:B:2224:LEU:HD12	2.62	0.40
1:A:417:ILE:HG12	1:A:431:LEU:HD13	2.04	0.40
1:A:1850:LEU:HD23	1:A:1850:LEU:HA	1.92	0.40
1:A:1967:ALA:HA	1:A:2185:LYS:HG2	2.04	0.40
1:A:2066:ILE:HG21	1:A:2075:VAL:HG13	2.02	0.40
1:A:2122:HIS:HB3	1:B:2132:ARG:NH2	2.23	0.40
1:B:300:LEU:HD23	1:B:300:LEU:HA	1.81	0.40
1:B:717:GLU:HA	1:B:720:LEU:HD12	2.04	0.40
1:B:1138:LEU:HD11	1:B:1187:GLY:HA3	2.03	0.40
1:A:254:TYR:O	1:A:258:ILE:HG22	2.22	0.40
1:A:993:ASP:HB3	1:A:1055:HIS:ND1	2.36	0.40
1:A:1893:LEU:O	1:A:1894:LEU:HD13	2.21	0.40
1:B:992:GLN:O	1:B:994:ILE:HG12	2.22	0.40
1:B:1491:PRO:HA	1:B:1516:ARG:O	2.21	0.40
1:B:1499:SER:HA	1:B:1502:GLU:HG2	2.03	0.40
1:A:1042:TRP:CZ2	1:B:946:ALA:HA	2.57	0.40
1:A:1060:ASN:CG	1:A:1061:LYS:N	2.75	0.40
1:A:1253:LYS:HD2	1:A:1627:GLN:HG3	2.03	0.40
1:A:1295:GLU:HA	1:A:1296:ILE:HA	1.74	0.40
1:A:1464:SER:HA	1:A:1467:LEU:HB2	2.02	0.40
1:A:1819:ILE:HB	1:A:1826:PHE:HB2	2.03	0.40
1:A:1895:PRO:HB2	1:A:1897:GLU:CD	2.42	0.40
1:A:1937:PHE:HB2	1:A:1952:LYS:HB3	2.04	0.40
1:A:2151:ALA:HB3	1:A:2157:LEU:HD23	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:ASP:OD2	1:B:1128:PRO:HG3	2.21	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	2494/2603 (96%)	2334 (94%)	160 (6%)	0	100	100
1	B	2494/2603 (96%)	2333 (94%)	161 (6%)	0	100	100
All	All	4988/5206 (96%)	4667 (94%)	321 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2258/2360 (96%)	2216 (98%)	42 (2%)	52	69
1	B	2258/2360 (96%)	2216 (98%)	42 (2%)	52	69
All	All	4516/4720 (96%)	4432 (98%)	84 (2%)	52	69

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	19	MET
1	A	108	PHE
1	A	167	ASP
1	A	295	ASN
1	A	308	SER
1	A	402	THR
1	A	561	MET
1	A	592	LEU
1	A	795	ASN
1	A	830	HIS
1	A	853	ILE
1	A	918	PHE
1	A	954	PHE
1	A	975	LEU
1	A	1014	HIS
1	A	1017	THR
1	A	1041	LYS
1	A	1045	THR
1	A	1090	LEU
1	A	1096	PHE
1	A	1166	THR
1	A	1232	SER
1	A	1233	LYS
1	A	1261	ASN
1	A	1268	TYR
1	A	1293	THR
1	A	1301	THR
1	A	1326	LEU
1	A	1333	LYS
1	A	1516	ARG
1	A	1614	THR
1	A	1777	PHE
1	A	1943	SER
1	A	2063	CYS
1	A	2083	SER
1	A	2121	TYR
1	A	2192	ASN
1	A	2212	ASN
1	A	2451	CYS
1	A	2452	LEU
1	A	2467	MET
1	B	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	19	MET
1	B	108	PHE
1	B	167	ASP
1	B	288	SER
1	B	295	ASN
1	B	308	SER
1	B	402	THR
1	B	561	MET
1	B	795	ASN
1	B	830	HIS
1	B	853	ILE
1	B	918	PHE
1	B	954	PHE
1	B	975	LEU
1	B	1014	HIS
1	B	1017	THR
1	B	1041	LYS
1	B	1090	LEU
1	B	1096	PHE
1	B	1166	THR
1	B	1232	SER
1	B	1233	LYS
1	B	1268	TYR
1	B	1293	THR
1	B	1301	THR
1	B	1326	LEU
1	B	1352	VAL
1	B	1516	ARG
1	B	1614	THR
1	B	1777	PHE
1	B	1812	THR
1	B	1863	GLN
1	B	2063	CYS
1	B	2083	SER
1	B	2121	TYR
1	B	2127	THR
1	B	2192	ASN
1	B	2212	ASN
1	B	2451	CYS
1	B	2452	LEU
1	B	2467	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	316	HIS
1	A	554	GLN
1	A	607	HIS
1	A	887	GLN
1	A	1014	HIS
1	A	1056	ASN
1	A	1853	ASN
1	A	2111	ASN
1	A	2482	GLN
1	B	207	ASN
1	B	316	HIS
1	B	554	GLN
1	B	607	HIS
1	B	887	GLN
1	B	1014	HIS
1	B	1056	ASN
1	B	1581	ASN
1	B	1853	ASN
1	B	2111	ASN
1	B	2482	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

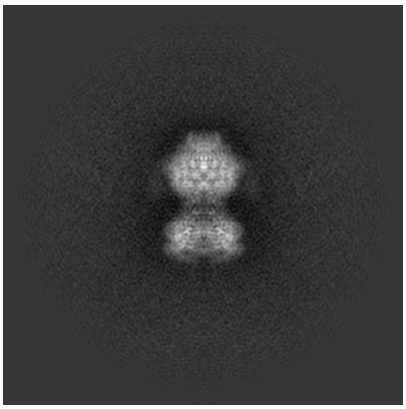
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49491. These allow visual inspection of the internal detail of the map and identification of artifacts.

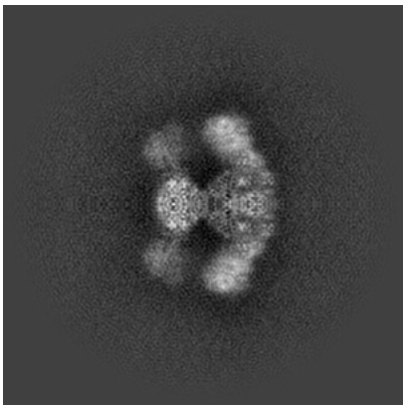
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

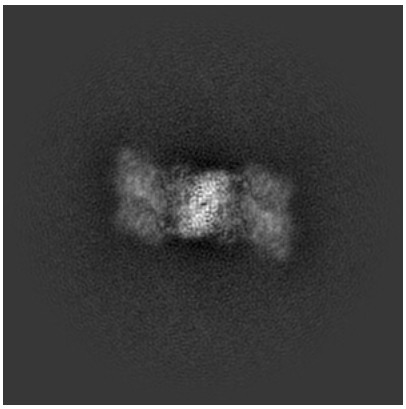
6.1.1 Primary map



X

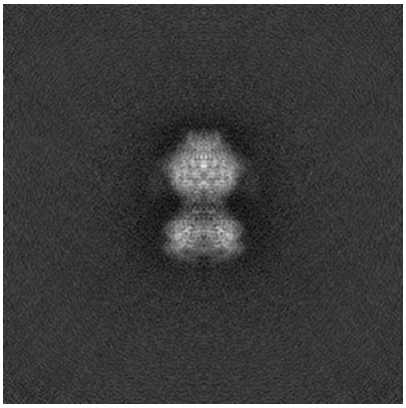


Y

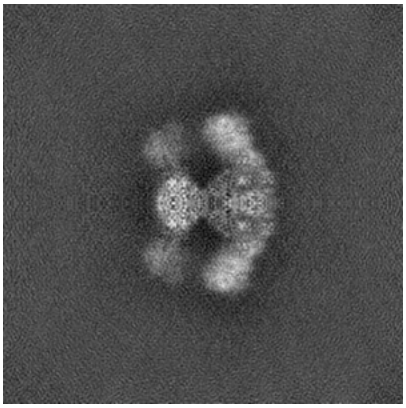


Z

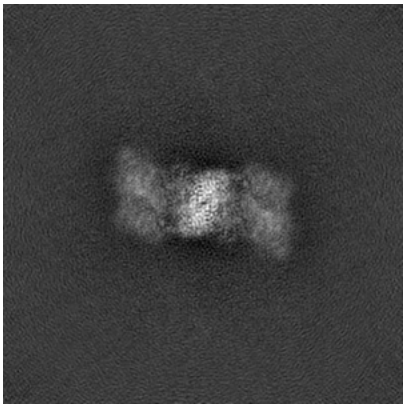
6.1.2 Raw map



X



Y

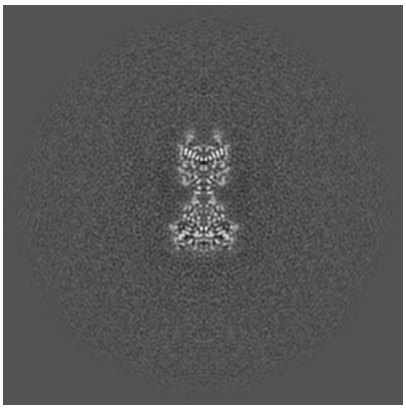


Z

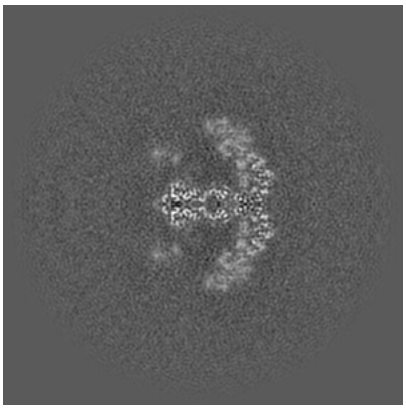
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

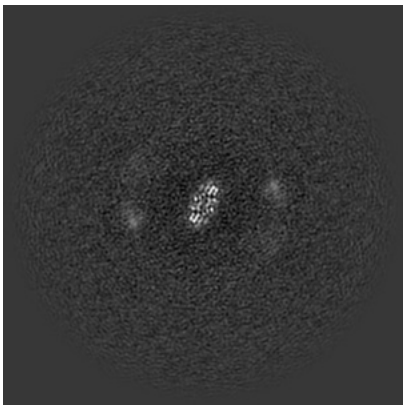
6.2.1 Primary map



X Index: 128



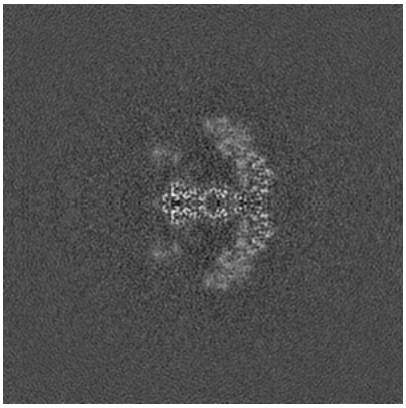
Y Index: 128



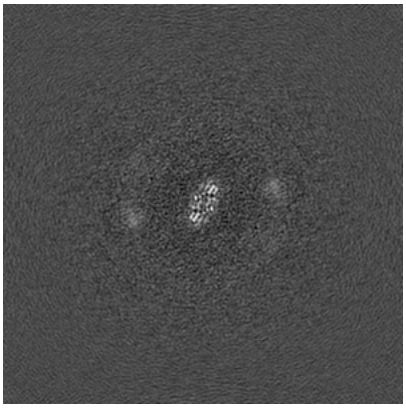
Z Index: 128

6.2.2 Raw map

X Index: 128



Y Index: 128

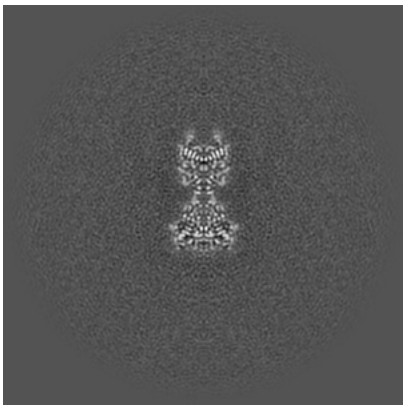


Z Index: 128

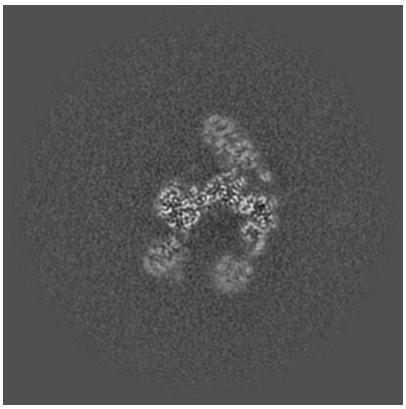
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

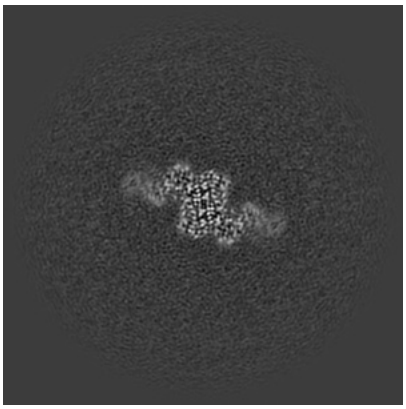
6.3.1 Primary map



X Index: 128



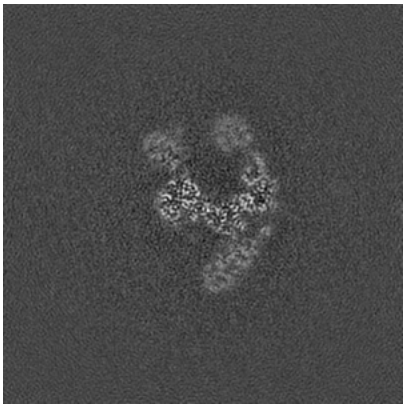
Y Index: 135



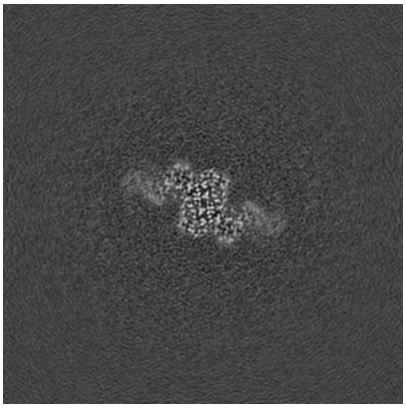
Z Index: 110

6.3.2 Raw map

X Index: 128



Y Index: 121

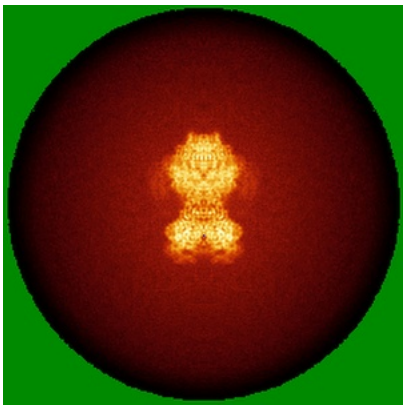


Z Index: 110

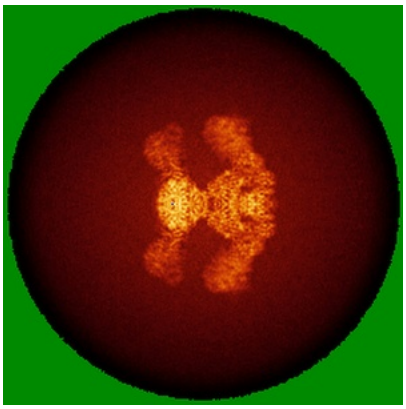
The images above show the largest variance slices of the map in three orthogonal directions.

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

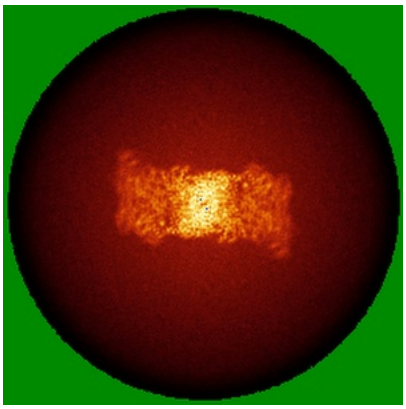
6.4.1 Primary map



X

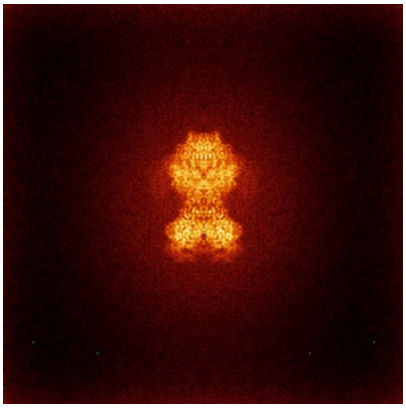


Y

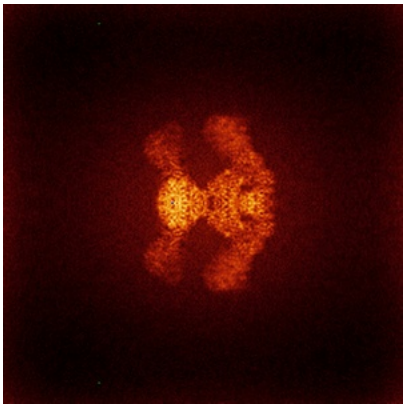


Z

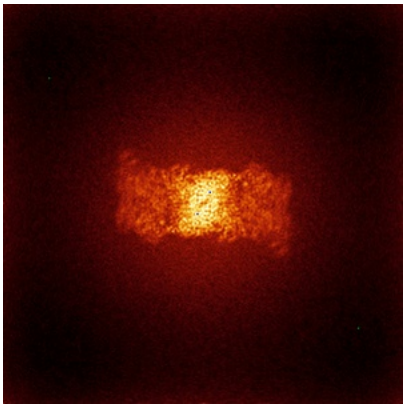
6.4.2 Raw map



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 0.239. 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.

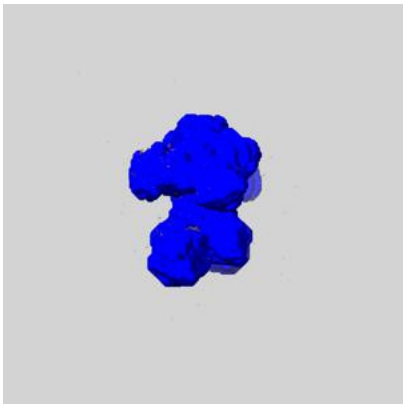
6.6 Mask visualisation (i)

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

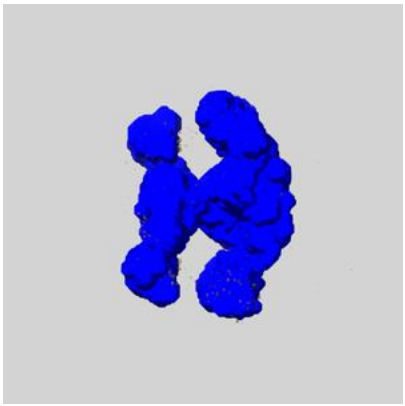
A mask typically either:

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

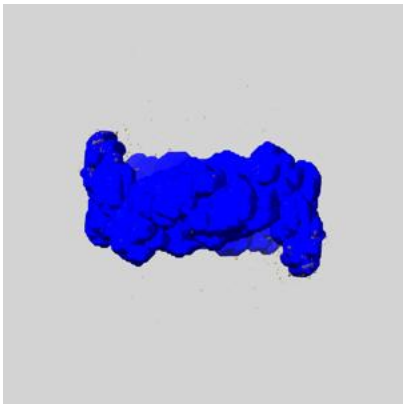
6.6.1 emd_49491_msk_1.map (i)



X



Y

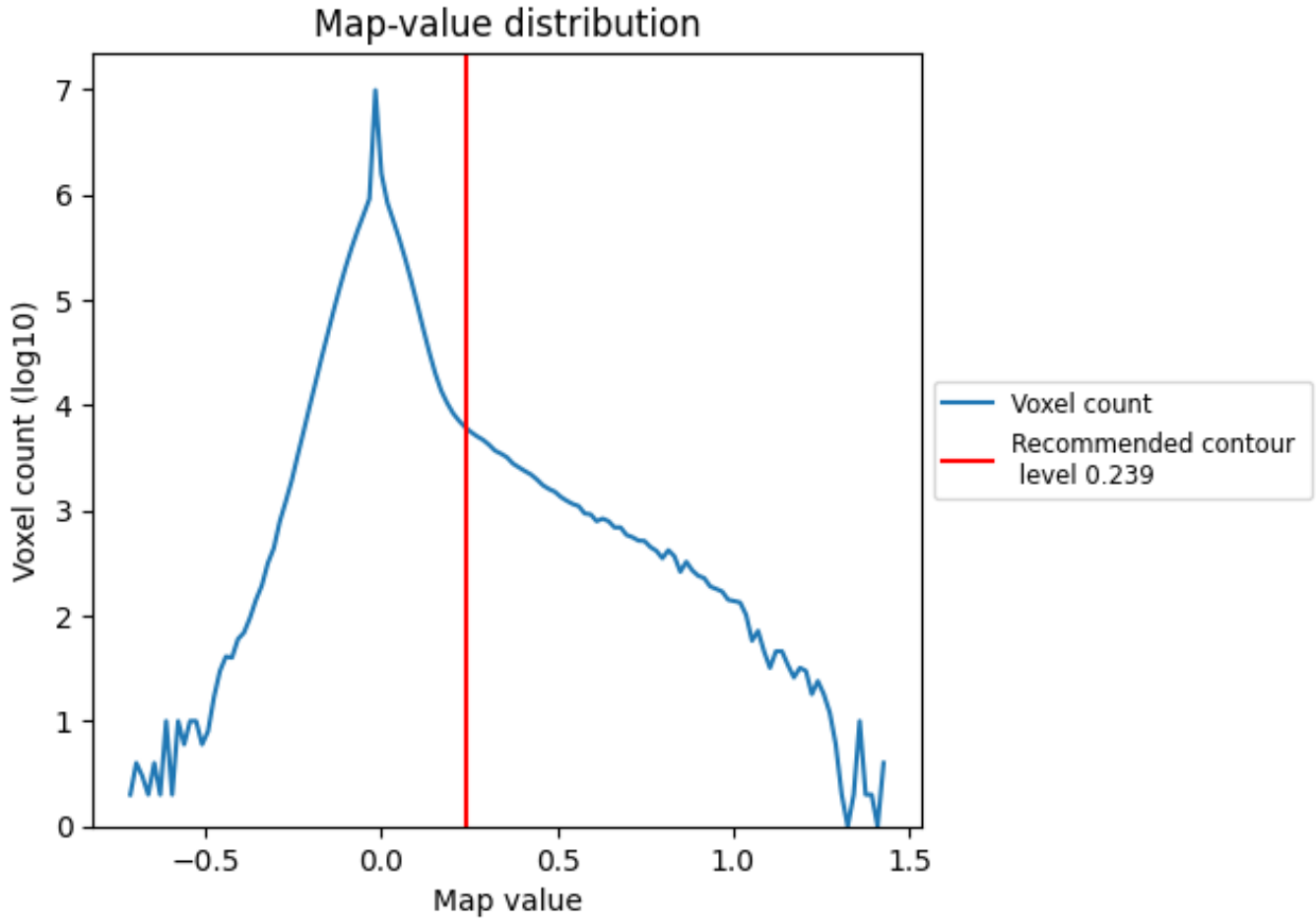


Z

7 Map analysis

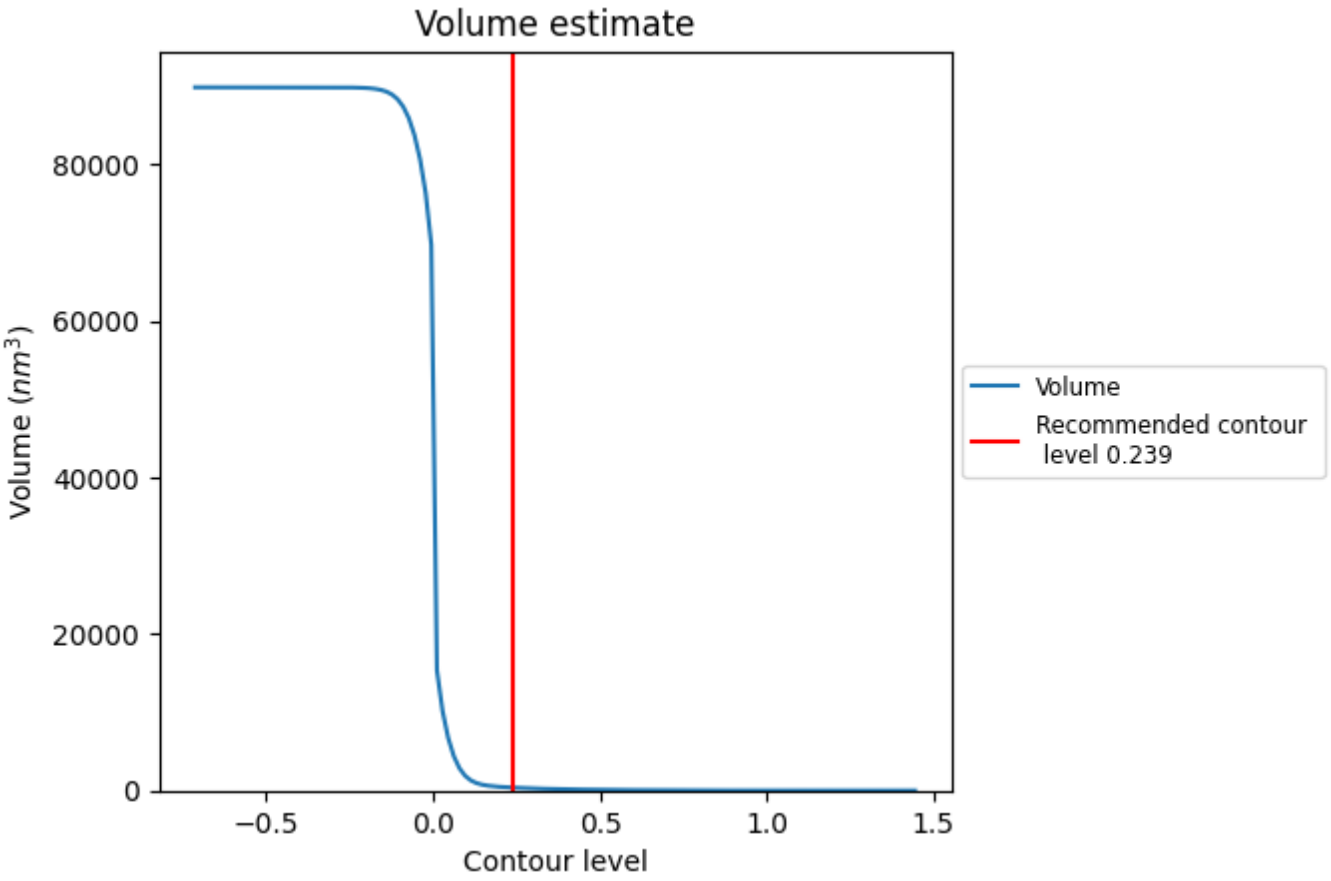
This section contains the results of statistical analysis of the map.

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.

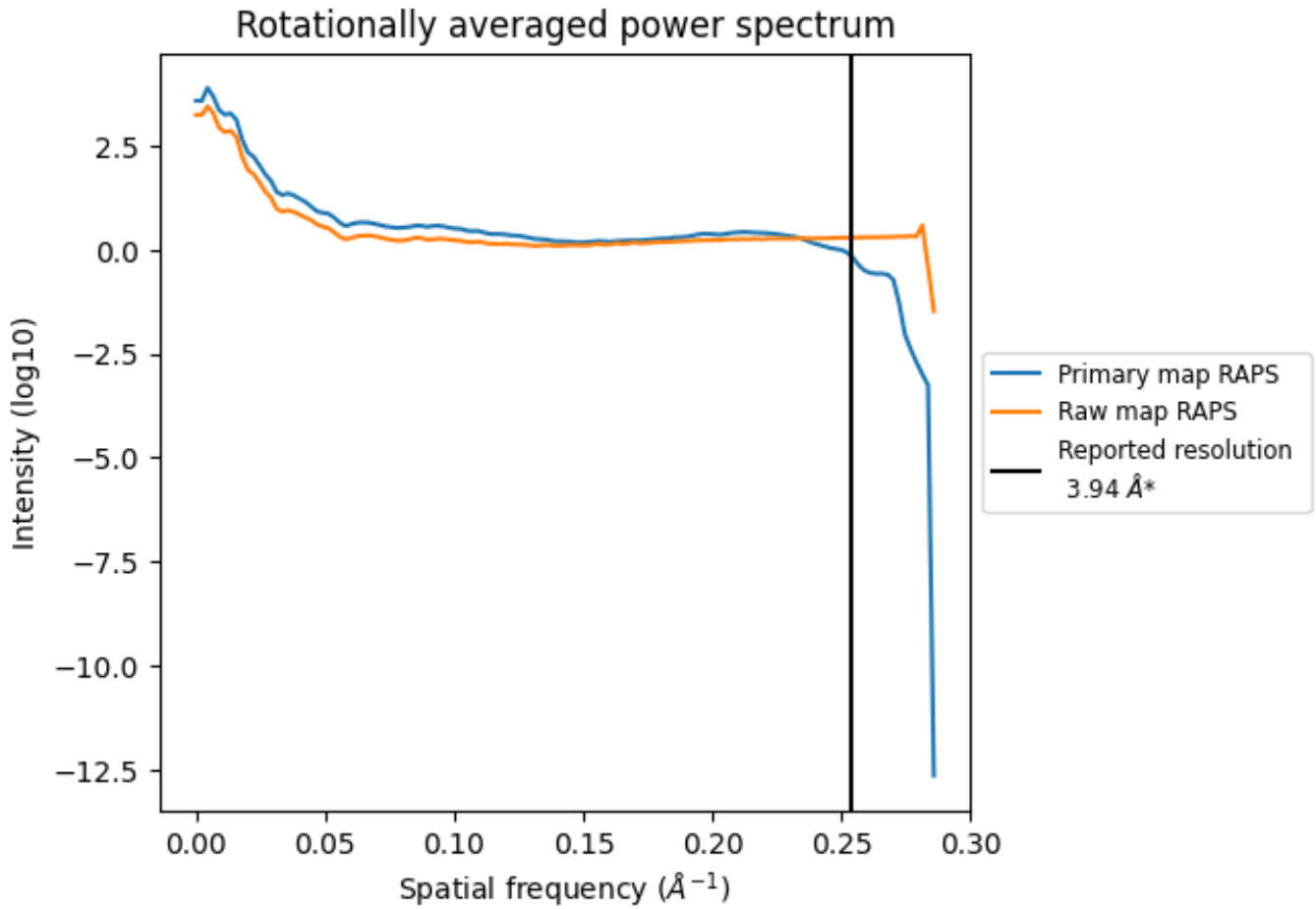
7.2 Volume estimate (i)



The volume at the recommended contour level is 376 nm^3; this corresponds to an approximate mass of 340 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)

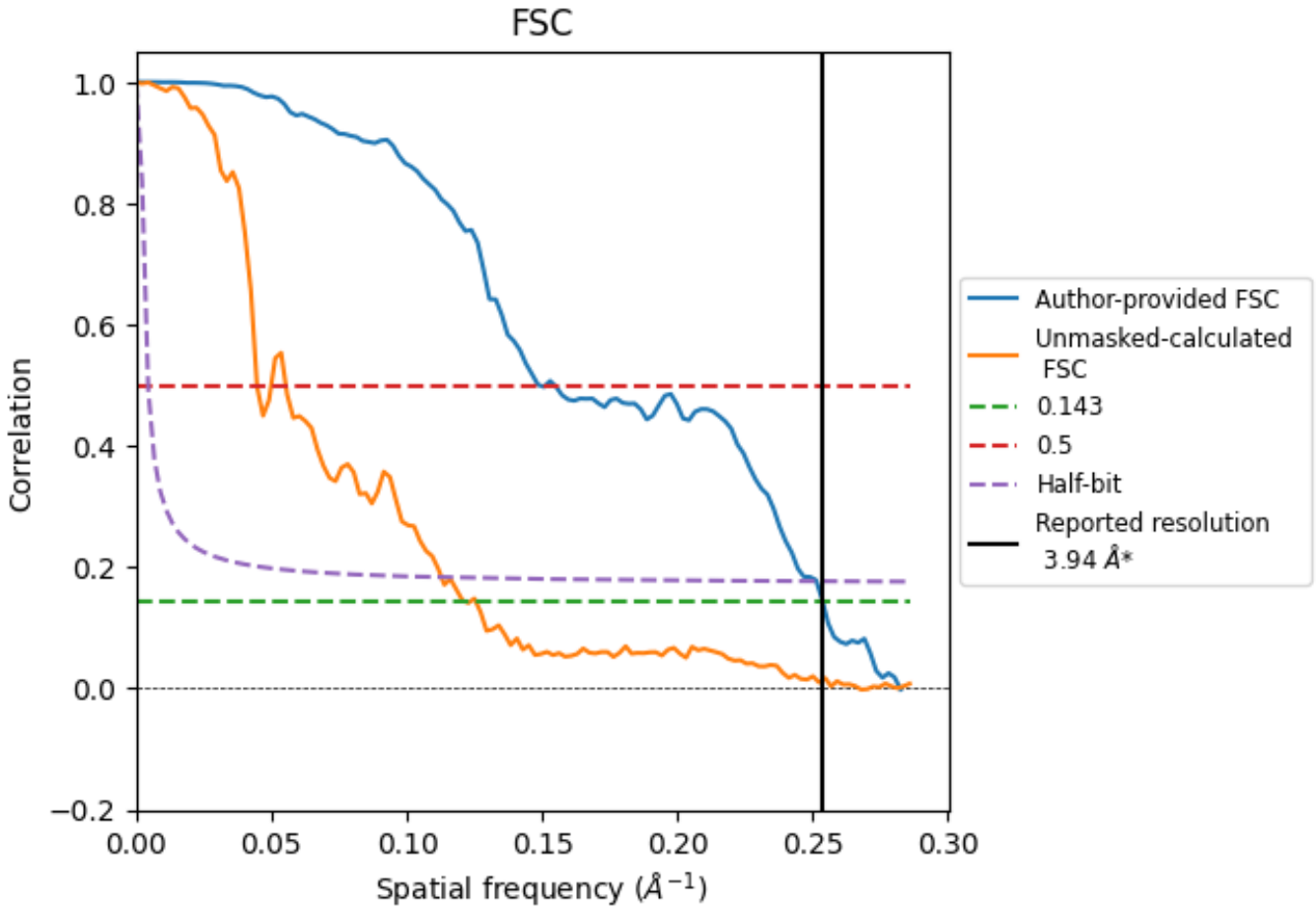


*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

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 0.254 Å^{-1}

8.2 Resolution estimates (i)

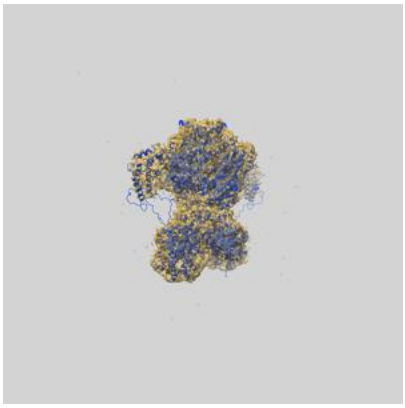
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.94	-	-
Author-provided FSC curve	3.94	6.71	3.98
Unmasked-calculated*	8.22	22.42	8.87

*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 8.22 differs from the reported value 3.94 by more than 10 %

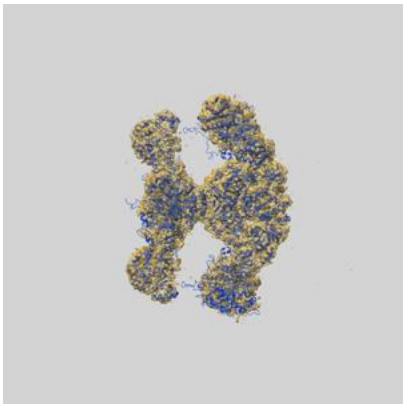
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49491 and PDB model 9NJU. Per-residue inclusion information can be found in section 3 on page 4.

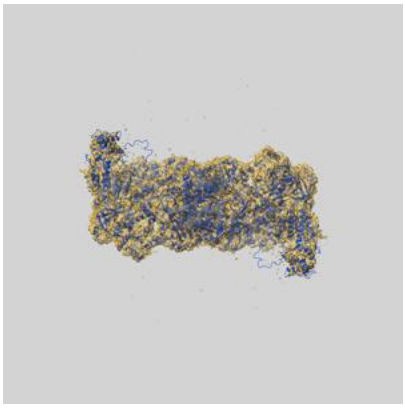
9.1 Map-model overlay



X



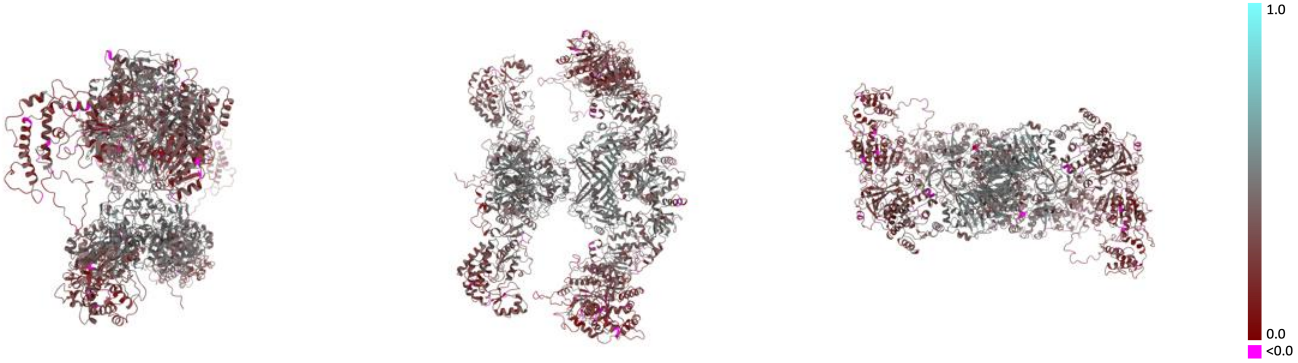
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.239 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.

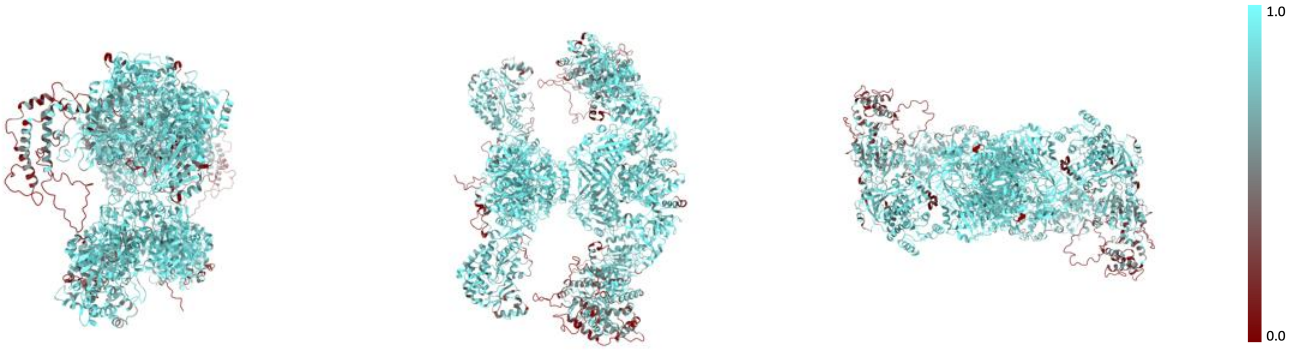
9.2 Q-score mapped to coordinate model (i)



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.

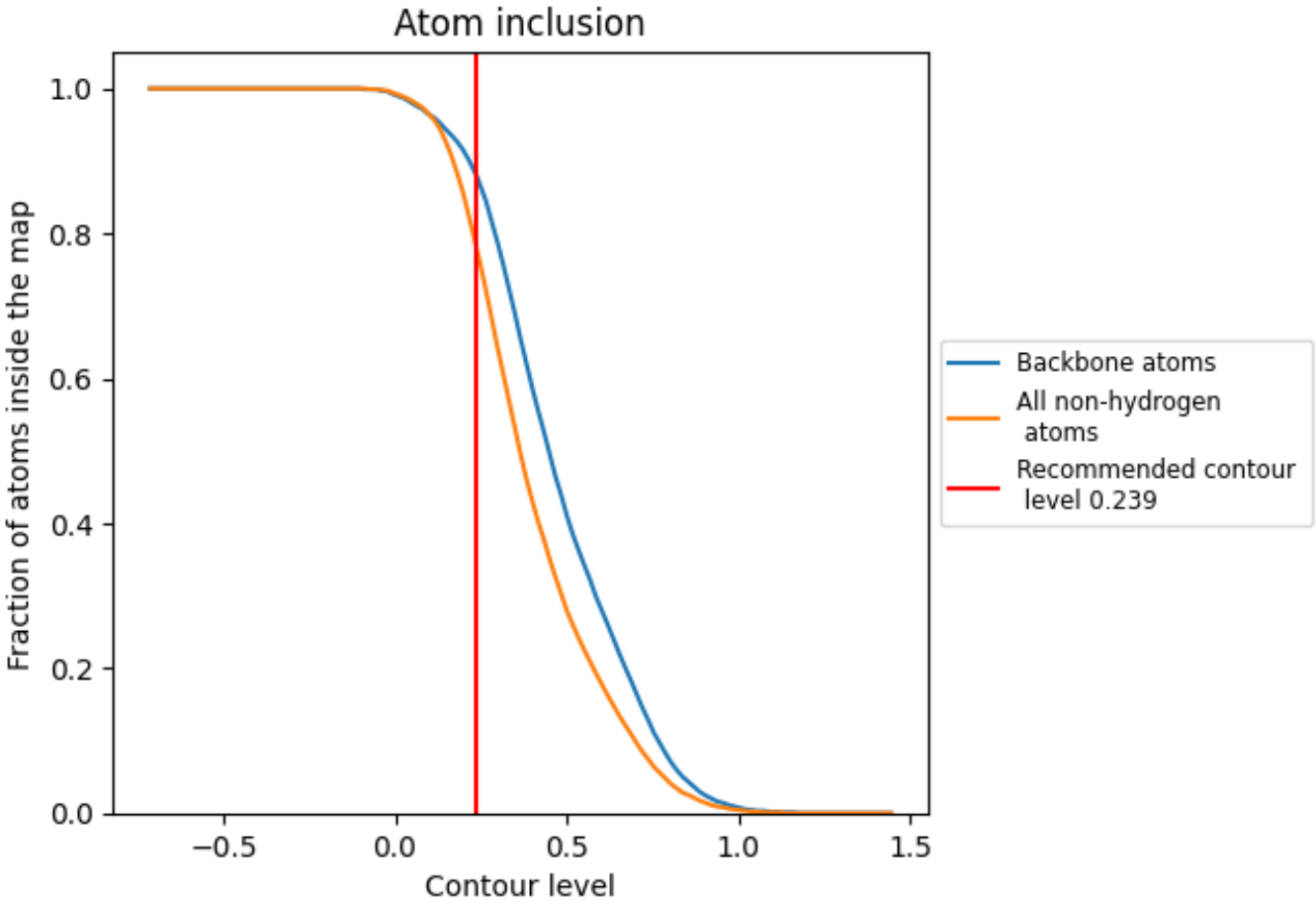
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.239).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.239) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7770	0.3620
A	0.7770	0.3620
B	0.7770	0.3620