Full wwPDB EM Validation Report

May 14, 2025 – 05:38 AM EDT

PDB ID	:	7LI3 / pdb_00007li3
EMDB ID	:	EMD-23359
Title	:	Structure of the LRRK2 G2019S mutant
Authors	:	Myasnikov, A.; Zhu, H.; Hixson, P.; Xie, B.; Yu, K.; Pitre, A.; Peng, J.; Sun, J.
Deposited on	:	2021-01-26
Resolution	:	3.80 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:

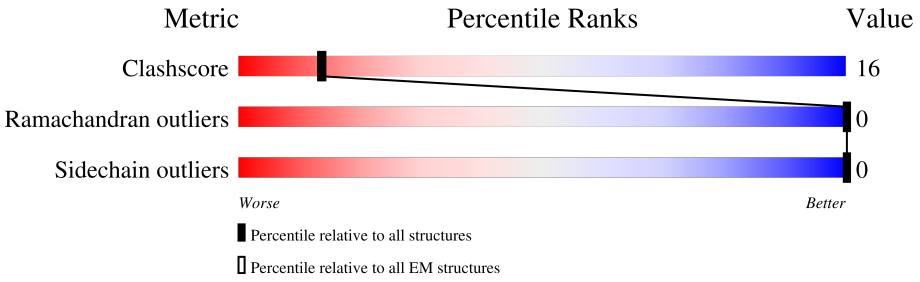
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.80 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	2527	19% 46% 25% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14180 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.

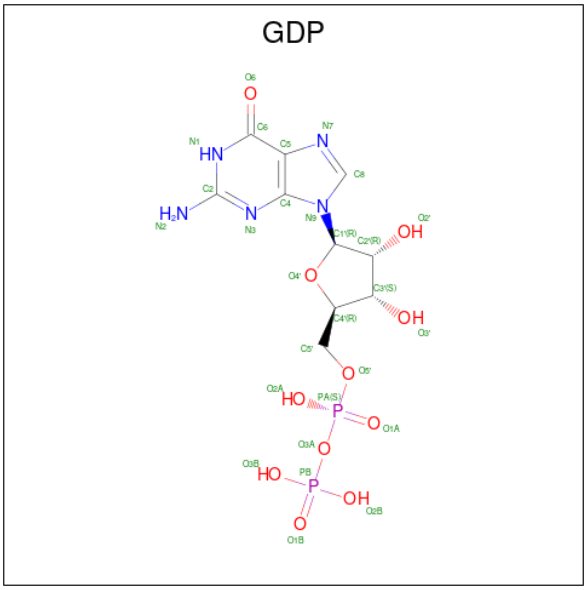
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1795	14121	9030	2435	2566	90	0	0

There are 4 discrepancies between the modelled and reference sequences:

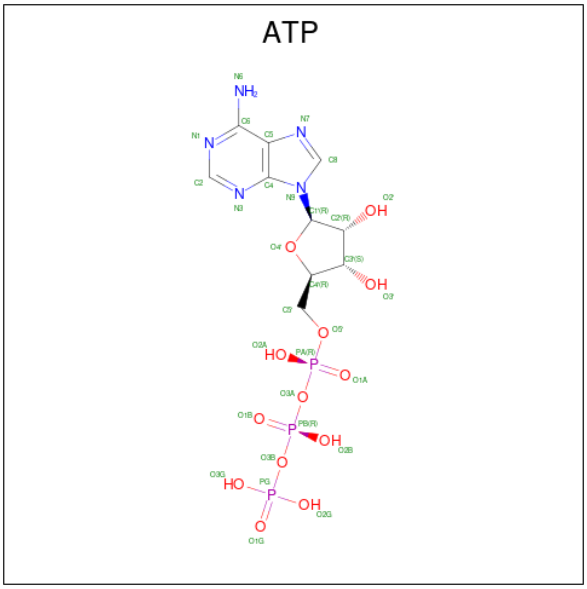
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	HIS	ARG	variant	UNP Q5S007
A	1647	THR	SER	variant	UNP Q5S007
A	2019	SER	GLY	variant	UNP Q5S007
A	2397	THR	MET	variant	UNP Q5S007

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	28	10	5	11	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

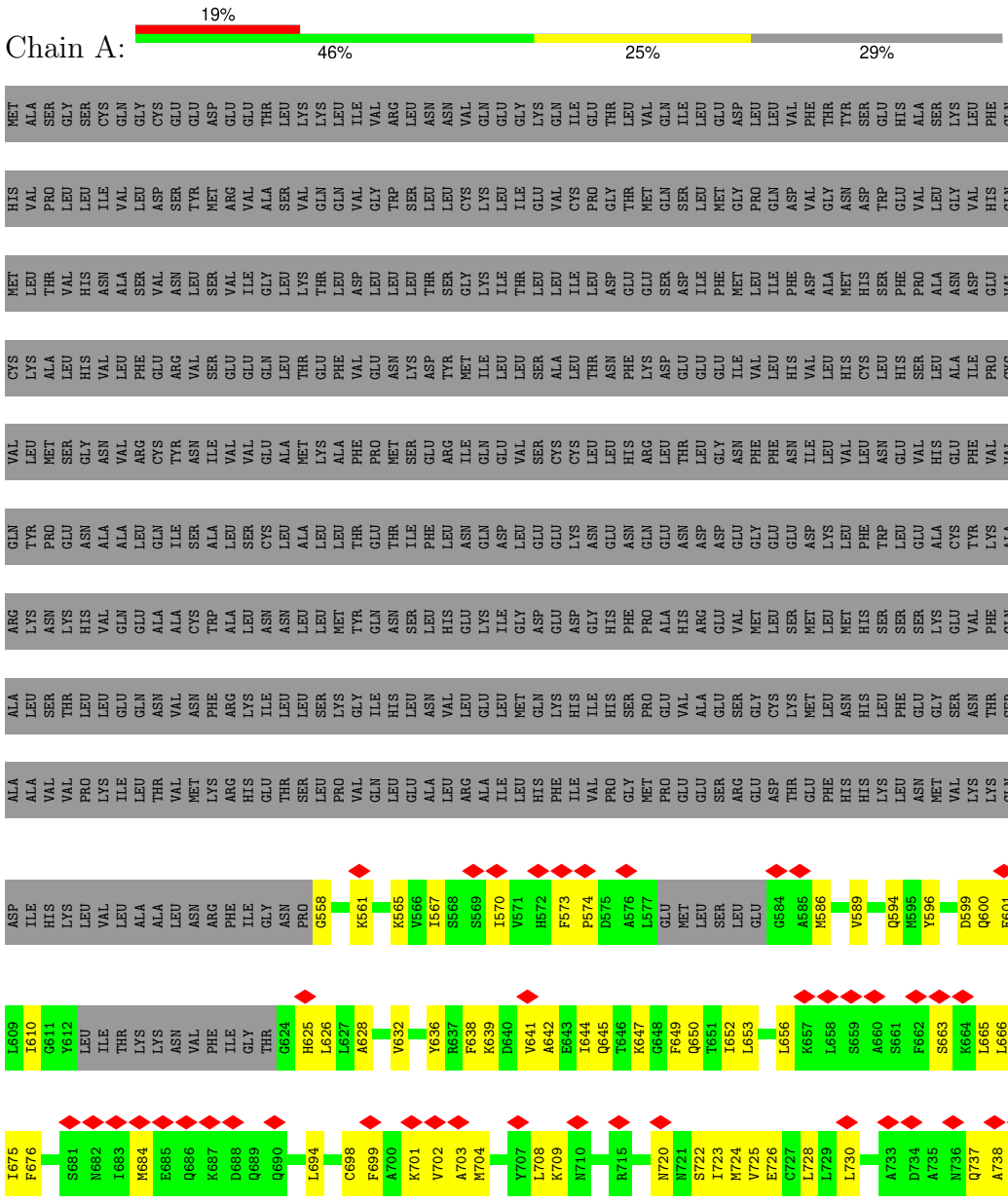


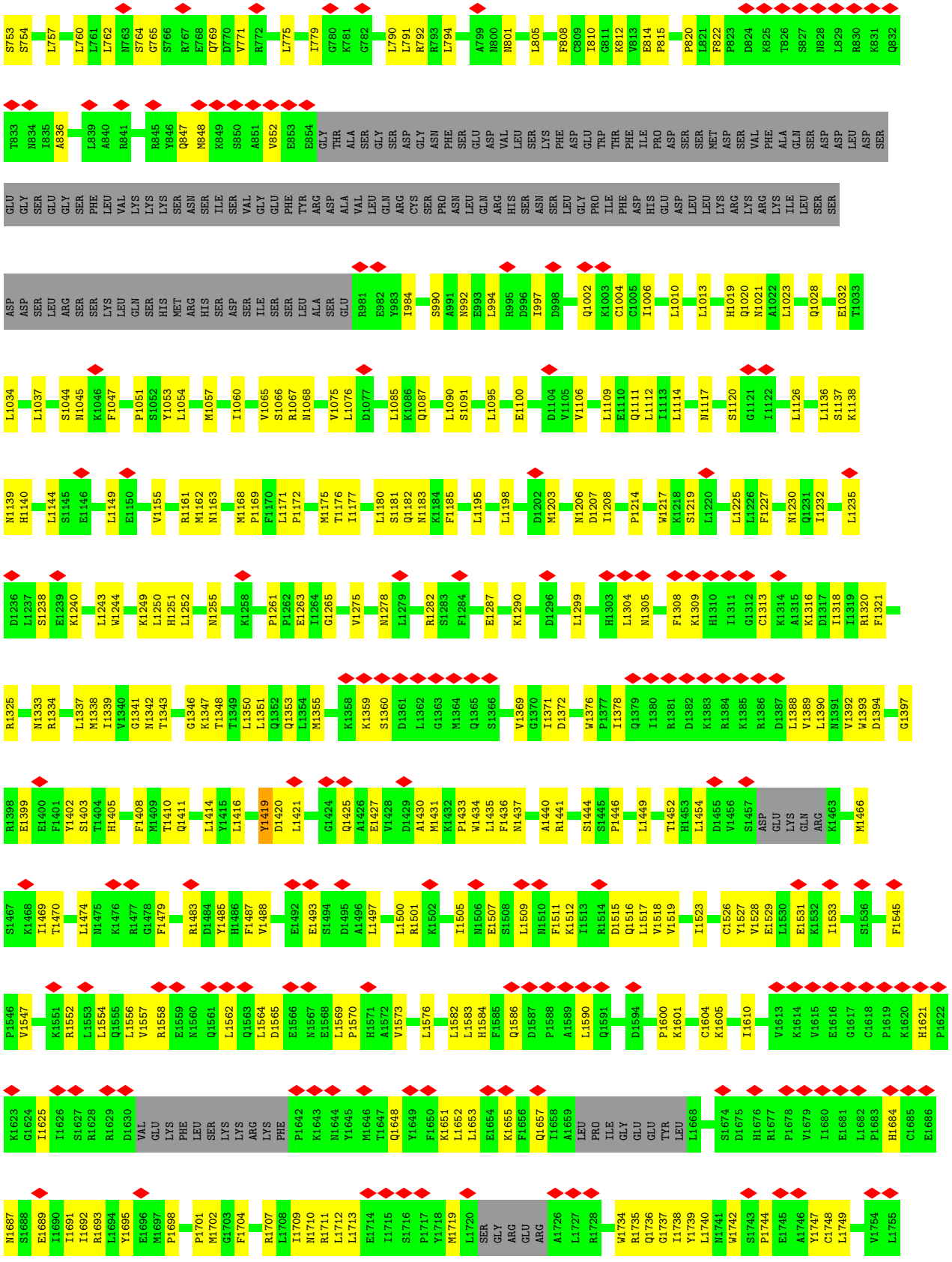
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	31	10	5	13	3	0

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: Leucine-rich repeat serine/threonine-protein kinase 2




S753 S754 L757 L760 L761 L762 N763 S764 G765 S766 R767 E768 Q769 D770 V771 R772 L775 I779 G780 K781 G782 L790 L791 R792 R793 L794 A799 N800 N801 L805 F808 C809 I810 G811 K812 V813 E814 P815 P820 L821 F822 P823 D824 K825 T826 S827 N828 L829 R830 K831 Q832
T833 N834 I835 A836 L839 A840 R841 R845 Y846 Q847 M848 K849 S850 A851 V852 E853 E854 GLY THR ALA SER GLY SER ASP GLY ASN PHE SER GLU ASP VAL LEU SER LYS PHE ASP GLU TRP THR PHE ILE PRO ASP SER SER MET ASP SER VAL PHE ALA GLN SER ASP ASP LEU ASP SER
GLU GLY SER GLU GLY SER PHE LEU VAL LYS LYS LYS SER ASN SER ILE SER VAL GLY GLU PHE TYR ARG ASP ALA VAL LEU GLN ARG CYS SER PRO ASN LEU GLN ARG HIS SER ASN SER LEU GLY PRO ILE PHE ASP HIS GLU ASP LEU LEU LYS ARG LYS ARG LYS ILE LEU SER SER
ASP ASP SER LEU ARG SER SER LYS LEU GLN SER HIS MET ARG HIS SER ASP SER ILE SER SER LEU ALA SER GLU R981 E982 Y983 I984 S990 A991 N992 E993 L994 R995 D996 I997 D998 Q1002 K1003 C1004 C1005 I1006 L1010 L1013 H1019 Q1020 N1021 A1022 L1023 Q1028 E1032 T1033
L1034 L1037 S1044 N1045 K1046 F1047 P1051 S1052 Y1053 L1054 M1057 I1060 V1065 S1066 R1067 N1068 V1075 L1076 D1077 L1085 K1086 Q1087 L1090 S1091 L1095 E1100 D1104 V1105 V1106 L1109 E1110 Q1111 L1112 I1113 L1114 N1117 S1120 G1121 I1122 L1126 L1136 S1137 K1138
N1139 H1140 L1144 S1145 E1146 L1149 E1150 V1155 R1161 M1162 N1163 M1168 P1169 F1170 L1171 P1172 M1175 T1176 I1177 L1180 S1181 Q1182 N1183 K1184 F1185 L1195 L1198 D1202 M1203 N1206 D1207 I1208 P1214 W1217 K1218 S1219 L1220 L1225 L1226 F1227 N1230 Q1231 I1232 L1235
D1236 L1237 S1238 E1239 K1240 L1243 W1244 K1249 L1250 H1251 L1252 N1255 K1258 P1261 P1262 E1263 I1264 G1265 V1275 N1278 L1279 R1282 S1283 F1284 E1287 K1290 D1296 L1299 H1303 L1304 N1305 F1308 K1309 H1310 I1311 G1312 C1313 K1314 A1315 K1316 D1317 I1318 I1319 R1320 F1321
R1325 N1333 R1334 L1337 M1338 I1339 V1340 G1341 N1342 T1343 G1346 K1347 T1348 T1349 L1350 L1351 Q1352 Q1353 L1354 M1355 K1358 K1359 S1360 D1361 L1362 G1363 M1364 Q1365 S1366 V1369 G1370 I1371 D1372 W1376 P1377 I1378 Q1379 I1380 R1381 D1382 K1383 R1384 K1385 R1386 D1387 L1388 V1389 L1390 N1391 V1392 W1393 D1394 G1397
R1398 E1399 E1400 F1401 Y1402 S1403 T1404 H1405 F1408 M1409 T1410 Q1411 L1414 Y1415 L1416 Y1419 D1420 L1421 G1424 Q1425 A1426 E1427 V1428 D1429 A1430 M1431 K1432 P1433 W1434 L1435 F1436 N1437 A1440 R1441 S1444 S1445 P1446 L1449 T1452 H1453 L1454 D1455 Y1456 S1457 ASP GLU LYS GLN ARG K1463 M1466
S1467 K1468 I1469 T1470 L1474 N1475 K1476 R1477 G1478 F1479 R1483 D1484 Y1485 H1486 F1487 V1488 E1492 E1493 S1494 D1495 A1496 L1497 L1500 R1501 K1502 I1505 N1506 E1507 S1508 L1509 N1510 F1511 K1512 I1513 R1514 D1515 Q1516 L1517 V1518 V1519 I1523 C1526 Y1527 V1528 E1529 L1530 E1531 K1532 I1533 S1536 F1545
P1546 V1547 K1551 R1552 L1553 L1554 Q1555 L1556 V1557 R1558 E1559 N1560 Q1561 L1562 Q1563 L1564 D1565 E1566 N1567 E1568 L1569 P1570 H1571 A1572 V1573 L1576 L1582 L1583 H1584 F1585 Q1586 D1587 P1588 A1589 L1590 Q1591 D1594 P1600 K1601 C1604 K1605 I1610 V1613 K1614 V1615 E1616 G1617 C1618 P1619 K1620 H1621 P1622
K1623 G1624 I1625 I1626 S1627 R1628 R1629 D1630 VAL GLU LYS PHE LEU SER LYS LYS ARG LYS PHE P1642 K1643 N1644 Y1645 M1646 T1647 Q1648 Y1649 F1650 K1651 L1652 L1653 E1654 K1655 F1656 Q1657 I1658 A1659 LEU PRO ILE GLY GLU GLU TYR LEU L1668 S1674 D1675 H1676 R1677 P1678 V1679 I1680 E1681 L1682 P1683 H1684 C1685 E1686
N1687 S1688 E1689 I1690 I1691 I1692 R1693 L1694 Y1695 E1696 M1697 P1698 P1701 M1702 G1703 F1704 R1707 L1708 I1709 N1710 R1711 L1712 L1713 E1714 I1715 S1716 P1717 Y1718 M1719 L1720 SER GLY ARG GLU ARG A1726 L1727 R1728 W1734 R1735 Q1736 G1737 I1738 Y1739 L1740 N1741 W1742 S1743 P1744 E1745 A1746 Y1747 C1748 L1749 V1754 L1755


D1756 N1757 H1758 P1759 E1760 L1763 K1764 I1765 T1766 V1767 P1768 S1769 C1770 R1771 C1774 I1775 L1776 L1777 G1778 Q1779 V1780 V1781 D1782 H1783 I1784 L1787 M1788 E1789 E1790 W1791 F1792 L1795 L1796 E1797 I1798 D1799 I1800 C1801 G1802 E1803 G1804 E1805 T1806 Y1814 S1815 F1816 N1817 D1818 G1819 E1820 E1821 H1822 Q1823 K1824 I1825
D1829 L1830 M1831 K1832 E1836 G1837 D1838 L1839 L1840 V1841 N1842 P1843 D1844 Q1845 P1846 R1847 L1848 T1849 I1850 P1851 I1852 S1853 Q1854 I1855 A1856 P1857 D1858 L1859 I1860 L1861 A1862 D1863 L1864 P1865 R1866 N1867 I1868 M1869 L1870 N1871 N1872 D1873 E1876 Q1879 A1880 P1881 E1882 F1883 L1884 L1885 G1886 D1887 G1888 S1889 F1890
Y1894 E1899 G1900 E1901 V1905 K1910 H1911 T1912 R1915 R1918 Q1919 V1922 V1923 L1924 C1925 H1926 L1927 H1928 L1932 L1935 I1940 R1941 P1942 R1943 M1944 L1945 V1946 M1947 E1948 D1956 R1957 L1958 L1959 Q1960 Q1961 D1962 K1963 A1964 S1965 L1966 T1967 R1968 T1969 L1970 Q1971 D1980 H1986
M1989 I1990 I1991 Y1992 R1993 D1994 L1995 K1996 P1997 H1998 L2001 N2008 A2016 D2017 Q2022 Y2023 R2026 M2027 GLY ILE LYS T2031 S2032 E2033 G2037 F2038 R2039 A2040 P2041 E2042 V2043 A2044 R2045 G2046 N2047 V2048 I2049 Y2050 N2051 Q2052 Q2053 S2058 L2063 Y2064 D2065 T2069 G2070 G2071 R2072 I2073 V2074
E2075 G2076 L2077 K2078 F2079 P2080 N2081 E2082 F2083 D2084 E2085 L2086 E2087 I2088 Q2089 G2090 K2091 P2095 V2096 K2097 E2098 A2102 L2110 K2116 Q2120 E2121 R2122 S2125 A2126 Q2127 V2128 F2129 D2130 I2131 L2132 N2133 L2146 N2149 V2150 I2151 V2152 E2153 C2154 M2155 T2158 H2159 H2160 N2161 S2162 R2163 N2164
W2168 L2169 G2172 H2173 T2174 D2175 R2176 G2177 Q2178 L2179 S2180 F2181 L2182 D2183 T2186 T2190 S2191 E2192 E2193 V2194 A2195 D2196 S2197 R2198 I2199 A2203 L2204 V2205 H2206 L2207 P2208 V2209 E2210 K2211 E2212 S2213 V2216 S2217 G2218 T2219 Q2220 S2221 G2222 T2223 L2224 I2227 N2228 T2229 E2230 D2231 G2232 K2233 K2234
R2235 H2236 T2237 L2238 E2239 K2240 M2241 T2242 L2248 Y2249 C2250 N2251 S2252 F2253 S2254 K2255 Q2256 S2257 K2258 Q2259 K2260 N2261 F2262 L2263 L2264 V2265 G2266 T2267 A2268 D2269 G2270 K2271 L2272 A2273 I2274 F2275 E2276 D2277 K2278 T2279 V2280 K2281 L2282 K2283 G2284 A2285 A2286 P2287 L2288 K2289 I2290 L2291 N2292 I2293 G2294 N2295 V2296 S2297 T2298
P2299 L2300 M2301 C2302 L2303 S2304 E2305 S2306 T2307 N2308 S2309 T2310 E2311 R2312 N2313 V2314 M2315 W2316 N2328 D2329 F2330 T2331 I2332 Q2333 K2334 L2335 T2338 R2339 T2340 S2341 Q2342 L2343 F2344 S2345 Y2346 A2347 A2348 F2349 S2350 D2351 S2352 N2353 I2354 I2355 T2356 V2357 V2358 V2359 D2360 T2361 A2362 L2363 Y2364 I2365 A2366 K2367 Q2368
V2373 W2376 D2377 K2378 K2379 T2380 E2381 K2382 L2383 C2384 G2385 L2386 C2389 V2390 H2391 F2392 L2393 R2394 E2395 V2396 T2397 V2398 K2399 E2400 N2401 K2402 E2403 S2404 K2405 H2406 K2407 M2408 S2409 Y2410 S2411 G2412 R2413 L2417 C2418 L2419 Q2420 K2421 N2422 T2423 A2424 L2425 W2426 I2427 G2430 G2431 G2432 H2433 I2434 L2435 L2436 L2437
D2438 L2439 S2440 T2441 R2442 R2443 L2444 I2445 I2448 Y2449 N2450 N2453 S2454 V2455 R2456 Q2462 L2463 G2464 S2465 L2466 K2467 N2468 V2472 L2473 N2476 R2477 K2478 N2479 T2480 E2481 G2482 T2483 Q2484 K2485 Q2486 K2487 E2488 I2489 Q2490 S2491 C2492 I2498 H2502 Q2505 I2511 R2514 E2519 K2520 M2521
R2522 R2523 T2524 S2525 V2526 E2527

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81046	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 ($e^-/Å^2$)	81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.960	Depositor
Minimum map value	-0.909	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.19	0/14386	0.42	1/19457 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	644	ILE	N-CA-C	-5.16	105.80	113.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1419	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	14121	0	14407	450	0
2	A	28	0	12	1	0
3	A	31	0	12	2	0
All	All	14180	0	14431	450	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 16.

All (450) 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:2462:GLN:HB2	1:A:2467:LYS:HD2	1.62	0.79
1:A:1075:VAL:HG12	1:A:1100:GLU:HG3	1.67	0.76
1:A:1403:SER:O	1:A:1707:ARG:NH1	2.19	0.76
1:A:1869:MET:HE3	1:A:1870:LEU:H	1.50	0.76
1:A:2110:LEU:HD11	1:A:2128:VAL:HG23	1.67	0.76
1:A:1526:CYS:HB3	1:A:1564:LEU:HD11	1.70	0.73
1:A:1402:TYR:HA	1:A:1405:HIS:HD2	1.54	0.73
1:A:1034:LEU:HD11	1:A:1037:LEU:HD22	1.70	0.73
1:A:558:GLY:N	1:A:596:TYR:HH	1.87	0.73
1:A:1935:LEU:HD11	1:A:1945:LEU:HD11	1.71	0.72
1:A:726:GLU:HB2	1:A:760:LEU:HD13	1.72	0.72
1:A:2265:VAL:HB	1:A:2273:ALA:HB3	1.70	0.72
1:A:1693:ARG:NH1	1:A:1829:ASP:OD2	2.23	0.71
1:A:2476:ASN:ND2	1:A:2492:CYS:SG	2.63	0.71
1:A:1341:GLY:HA3	1:A:1347:LYS:HD2	1.73	0.70
1:A:2227:ILE:HD13	1:A:2235:ARG:HB3	1.73	0.69
1:A:2287:PRO:HB2	1:A:2290:ILE:HD11	1.73	0.69
1:A:990:SER:O	1:A:1021:ASN:ND2	2.25	0.69
1:A:1968:ARG:NH2	1:A:1971:GLN:OE1	2.24	0.69
1:A:1701:PRO:HG2	1:A:1704:PHE:HB2	1.74	0.69
1:A:2413:ARG:H	1:A:2430:GLY:H	1.41	0.69
1:A:625:HIS:HB3	1:A:665:LEU:HD23	1.74	0.68
1:A:1512:LYS:HG2	1:A:1515:ASP:HA	1.75	0.68
1:A:2146:LEU:O	1:A:2490:GLN:NE2	2.27	0.68
1:A:1282:ARG:O	1:A:1305:ASN:ND2	2.27	0.68
1:A:2197:SER:HB2	1:A:2220:GLN:HG3	1.76	0.67
1:A:808:PHE:O	1:A:992:ASN:ND2	2.28	0.66
1:A:1557:VAL:HG12	1:A:1562:LEU:HD12	1.77	0.66
1:A:1832:LYS:HZ2	1:A:1859:LEU:HD12	1.61	0.65
1:A:2116:LYS:O	1:A:2122:ARG:NH2	2.26	0.65
1:A:2301:MET:HE1	1:A:2368:GLN:HE21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:LEU:HA	1:A:1519:VAL:HG11	1.79	0.65
1:A:1433:PRO:O	1:A:1437:ASN:ND2	2.30	0.64
1:A:771:VAL:HG13	1:A:790:LEU:HD22	1.80	0.64
1:A:1275:VAL:O	1:A:1278:ASN:ND2	2.31	0.64
1:A:1992:TYR:OH	1:A:2016:ALA:O	2.13	0.64
1:A:1816:PHE:HA	1:A:1850:ILE:HD11	1.80	0.63
1:A:2228:ASN:HD22	1:A:2234:LYS:HD2	1.61	0.63
1:A:638:PHE:O	1:A:645:GLN:NE2	2.31	0.63
1:A:801:ASN:HB3	1:A:984:ILE:HA	1.81	0.63
1:A:2248:LEU:HD23	1:A:2263:LEU:HD21	1.80	0.63
1:A:1991:ILE:HD11	1:A:1993:ARG:HE	1.64	0.63
1:A:2043:VAL:HA	1:A:2050:TYR:HE1	1.64	0.62
1:A:1778:GLY:O	1:A:1918:ARG:NH1	2.31	0.62
1:A:558:GLY:O	1:A:561:LYS:NZ	2.33	0.62
1:A:663:SER:HA	1:A:666:LEU:HD12	1.80	0.62
1:A:1168:MET:HE3	1:A:1171:LEU:HD21	1.81	0.62
1:A:1610:ILE:HG21	1:A:1653:LEU:HD21	1.82	0.62
1:A:2177:GLY:HA3	1:A:2195:ALA:HB3	1.80	0.62
1:A:762:LEU:HD11	1:A:790:LEU:HD23	1.82	0.61
1:A:1493:GLU:OE2	1:A:1501:ARG:NH2	2.21	0.61
1:A:1420:ASP:H	1:A:1452:THR:HG22	1.65	0.61
1:A:810:ILE:H	1:A:992:ASN:HD22	1.49	0.61
1:A:1693:ARG:NH2	1:A:1858:ASP:OD1	2.33	0.61
1:A:1905:VAL:HG12	1:A:1946:VAL:HG22	1.82	0.61
1:A:1959:LEU:HD13	1:A:2070:GLY:HA3	1.83	0.61
1:A:1343:THR:H	1:A:1397:GLY:HA3	1.65	0.60
1:A:1590:LEU:HD22	1:A:1655:LYS:HG3	1.82	0.60
1:A:720:ASN:HD21	1:A:754:SER:HB3	1.65	0.60
1:A:2302:CYS:SG	1:A:2303:LEU:N	2.75	0.60
1:A:1171:LEU:HD13	1:A:1175:MET:HE3	1.82	0.60
1:A:1028:GLN:NE2	1:A:1032:GLU:OE2	2.34	0.60
1:A:1863:ASP:OD2	1:A:1918:ARG:NH2	2.35	0.60
1:A:1437:ASN:OD1	1:A:1702:MET:N	2.34	0.59
1:A:2125:SER:HA	1:A:2128:VAL:HG12	1.85	0.59
1:A:1287:GLU:O	1:A:1290:LYS:NZ	2.35	0.59
1:A:704:MET:SD	1:A:847:GLN:NE2	2.71	0.59
1:A:992:ASN:O	1:A:1021:ASN:ND2	2.36	0.59
1:A:1020:GLN:HA	1:A:1044:SER:HB2	1.85	0.59
1:A:1948:GLU:O	3:A:2602:ATP:N6	2.32	0.59
1:A:1176:THR:HG22	1:A:1177:ILE:HG13	1.85	0.58
1:A:1692:ILE:HG12	1:A:1766:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2304:SER:OG	1:A:2305:GLU:N	2.36	0.58
1:A:2151:ILE:O	1:A:2172:GLY:N	2.36	0.58
1:A:2363:LEU:HB3	1:A:2376:TRP:HB2	1.86	0.58
1:A:2232:GLY:O	1:A:2235:ARG:NH2	2.26	0.58
1:A:667:VAL:HG11	1:A:708:LEU:HD22	1.86	0.58
1:A:2417:LEU:HD12	1:A:2425:LEU:HD11	1.86	0.57
1:A:567:ILE:HA	1:A:570:ILE:HG22	1.86	0.57
1:A:1435:LEU:HD13	1:A:1474:LEU:HD11	1.85	0.57
1:A:1832:LYS:HZ1	1:A:1852:ILE:HG23	1.68	0.57
1:A:1235:LEU:HD23	1:A:1261:PRO:HD2	1.87	0.57
1:A:1940:ILE:HG22	1:A:1941:ARG:H	1.70	0.57
1:A:594:GLN:HE22	1:A:626:LEU:HD11	1.69	0.57
1:A:1316:LYS:HG3	1:A:1320:ARG:HH12	1.69	0.57
1:A:2152:VAL:HG11	1:A:2169:LEU:HD23	1.87	0.57
1:A:2521:MET:O	1:A:2524:THR:OG1	2.22	0.57
1:A:1181:SER:OG	1:A:1182:GLN:OE1	2.16	0.57
1:A:1346:GLY:H	1:A:1452:THR:HG21	1.69	0.57
1:A:1214:PRO:HA	1:A:1217:TRP:HD1	1.69	0.57
1:A:2254:SER:N	1:A:2312:ARG:HH12	2.03	0.57
1:A:1240:LYS:HD2	1:A:1243:LEU:HD11	1.87	0.56
1:A:2213:SER:O	1:A:2229:THR:OG1	2.22	0.56
1:A:1023:LEU:HB2	1:A:1045:ASN:HD22	1.70	0.56
1:A:1529:GLU:O	1:A:1533:ILE:HG12	2.05	0.56
1:A:1840:LEU:HD13	1:A:1849:THR:HG21	1.88	0.56
1:A:1956:ASP:OD1	1:A:1957:ARG:N	2.38	0.56
1:A:2133:ASN:ND2	1:A:2511:ILE:HG13	2.21	0.56
1:A:2355:ILE:N	1:A:2366:ALA:O	2.31	0.56
1:A:1993:ARG:NH2	1:A:2023:TYR:OH	2.34	0.56
1:A:1299:LEU:HD11	1:A:1318:ILE:HD11	1.88	0.56
1:A:812:LYS:NZ	1:A:814:GLU:OE2	2.39	0.56
1:A:1782:ASP:HB2	1:A:1918:ARG:HH11	1.70	0.56
1:A:2205:VAL:HG11	1:A:2263:LEU:HD12	1.88	0.56
1:A:2338:THR:HG22	1:A:2376:TRP:CE2	2.40	0.56
1:A:672:ASP:HA	1:A:675:ILE:HG22	1.88	0.56
1:A:1161:ARG:O	1:A:1163:ASN:ND2	2.38	0.56
1:A:1531:GLU:HB2	1:A:1576:LEU:HD11	1.88	0.56
1:A:1836:GLU:O	1:A:1941:ARG:NH1	2.35	0.56
1:A:2173:HIS:CD2	1:A:2174:THR:HG23	2.41	0.56
1:A:2455:VAL:HG13	1:A:2472:VAL:HG13	1.88	0.55
1:A:1333:ASN:HB3	1:A:1388:LEU:HA	1.87	0.55
1:A:1207:ASP:OD1	1:A:1207:ASP:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1684:HIS:HB3	1:A:1689:GLU:HG3	1.87	0.55
1:A:2153:GLU:HB3	1:A:2456:ARG:HH21	1.70	0.55
1:A:1227:PHE:O	1:A:1230:ASN:ND2	2.40	0.55
1:A:2390:VAL:HA	1:A:2393:LEU:HB2	1.89	0.55
1:A:628:ALA:O	1:A:632:VAL:HG22	2.06	0.55
1:A:1446:PRO:HD3	1:A:1511:PHE:CE1	2.41	0.55
1:A:1342:ASN:ND2	1:A:1427:GLU:OE2	2.40	0.55
1:A:675:ILE:HD11	1:A:699:PHE:HB2	1.89	0.54
1:A:1087:GLN:OE1	1:A:1111:GLN:NE2	2.38	0.54
1:A:1339:ILE:HD11	1:A:1351:LEU:HD13	1.89	0.54
1:A:1888:GLY:HA3	3:A:2602:ATP:H4'	1.89	0.54
1:A:2080:PRO:HA	1:A:2083:PHE:HB3	1.89	0.54
1:A:2438:ASP:HB2	1:A:2445:ILE:HD11	1.89	0.54
1:A:1980:ASP:OD2	1:A:2514:ARG:NH1	2.34	0.54
1:A:1149:LEU:HD22	1:A:1155:VAL:HG21	1.90	0.54
1:A:2159:HIS:HB2	1:A:2462:GLN:HE21	1.73	0.54
1:A:848:MET:O	1:A:852:VAL:HG22	2.08	0.54
1:A:1454:LEU:HD11	1:A:1487:PHE:HB3	1.90	0.54
1:A:1371:ILE:HD12	1:A:1393:TRP:CE3	2.43	0.54
1:A:1788:MET:HG3	1:A:1796:LEU:HD22	1.90	0.54
1:A:753:SER:HB2	1:A:757:LEU:HD23	1.88	0.54
1:A:1512:LYS:HA	1:A:1517:LEU:H	1.72	0.54
1:A:775:LEU:O	1:A:779:ILE:HG12	2.08	0.54
1:A:1411:GLN:OE1	1:A:1444:SER:OG	2.26	0.54
1:A:2468:ASN:HB3	1:A:2498:ILE:HG21	1.88	0.54
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	1.90	0.53
1:A:2236:HIS:NE2	1:A:2280:VAL:O	2.41	0.53
1:A:1923:VAL:HA	1:A:1926:HIS:HE1	1.72	0.53
1:A:2438:ASP:HB3	1:A:2442:ARG:O	2.08	0.53
1:A:1434:TRP:CZ3	1:A:1702:MET:HE1	2.42	0.53
1:A:1709:ILE:HA	1:A:1738:ILE:HD11	1.91	0.53
1:A:1378:ILE:HD13	1:A:1505:ILE:HD11	1.91	0.53
1:A:701:LYS:HA	1:A:704:MET:HG2	1.90	0.53
1:A:1371:ILE:HD12	1:A:1393:TRP:HE3	1.74	0.53
1:A:1832:LYS:HE2	1:A:1852:ILE:HG12	1.91	0.53
1:A:2039:ARG:NH1	1:A:2084:ASP:OD1	2.41	0.53
1:A:1249:LYS:HE3	1:A:1251:HIS:HE1	1.73	0.52
1:A:1779:GLN:O	1:A:1783:HIS:ND1	2.28	0.52
1:A:650:GLN:HG3	1:A:694:LEU:HD21	1.90	0.52
1:A:1648:GLN:HA	1:A:1651:LYS:HB2	1.92	0.52
1:A:2276:GLU:HB3	1:A:2279:THR:HG22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2477:ARG:HB3	1:A:2489:ILE:HD13	1.90	0.52
1:A:698:CYS:O	1:A:702:VAL:HG23	2.09	0.52
1:A:2223:THR:HA	1:A:2240:LYS:HG3	1.92	0.52
1:A:586:MET:HA	1:A:589:VAL:HG12	1.91	0.52
1:A:2065:ASP:OD2	1:A:2072:ARG:NH2	2.34	0.52
1:A:599:ASP:O	1:A:603:GLN:HG2	2.10	0.52
1:A:738:ALA:HB3	1:A:743:SER:HA	1.90	0.52
1:A:1912:THR:O	1:A:1943:ARG:NH2	2.42	0.52
1:A:2363:LEU:O	1:A:2376:TRP:N	2.38	0.52
1:A:2051:ASN:OD1	1:A:2052:GLN:N	2.37	0.52
1:A:1149:LEU:HB3	1:A:1172:PRO:HD3	1.93	0.51
1:A:2178:GLN:NE2	1:A:2191:SER:HB2	2.25	0.51
1:A:2389:CYS:SG	1:A:2390:VAL:N	2.83	0.51
1:A:1735:ARG:HG2	1:A:1736:GLN:HG3	1.92	0.51
1:A:2267:THR:HG22	1:A:2268:ALA:H	1.74	0.51
1:A:1789:GLU:OE2	1:A:1915:ARG:NH1	2.43	0.51
1:A:2022:GLN:HE21	1:A:2026:ARG:HH11	1.58	0.51
1:A:2043:VAL:HA	1:A:2050:TYR:CE1	2.45	0.51
1:A:1195:LEU:O	1:A:1219:SER:HB3	2.11	0.51
1:A:1305:ASN:ND2	1:A:1516:GLN:HE22	2.08	0.51
1:A:1334:ARG:HG3	1:A:1389:VAL:O	2.11	0.51
1:A:1932:LEU:HD22	1:A:2017:ASP:HB3	1.92	0.51
1:A:2043:VAL:HG22	1:A:2050:TYR:CD1	2.46	0.51
1:A:2350:SER:O	1:A:2367:LYS:NZ	2.38	0.51
1:A:1023:LEU:HB2	1:A:1045:ASN:ND2	2.25	0.51
1:A:1351:LEU:HD11	1:A:1392:VAL:HG21	1.93	0.50
1:A:1788:MET:SD	1:A:1795:LEU:HD12	2.51	0.50
1:A:1601:LYS:HA	1:A:1604:CYS:SG	2.51	0.50
1:A:1734:TRP:CZ2	1:A:1737:GLY:HA3	2.46	0.50
1:A:2168:TRP:HZ2	1:A:2229:THR:HG23	1.74	0.50
1:A:1734:TRP:CD1	1:A:1736:GLN:H	2.29	0.50
1:A:1252:LEU:O	1:A:1255:ASN:ND2	2.45	0.50
1:A:1488:VAL:HG11	1:A:1500:LEU:HD22	1.92	0.50
1:A:2276:GLU:OE1	1:A:2279:THR:N	2.45	0.50
1:A:600:GLN:HG2	1:A:638:PHE:CE1	2.46	0.50
1:A:792:ARG:NH1	1:A:820:PRO:O	2.37	0.50
1:A:1185:PHE:HD2	1:A:1203:MET:HE3	1.76	0.50
1:A:1523:ILE:HD11	1:A:1528:VAL:HG23	1.94	0.50
1:A:1816:PHE:CE1	1:A:1843:PRO:HD3	2.47	0.50
1:A:2261:ASN:N	1:A:2277:ASP:OD2	2.39	0.50
1:A:2397:THR:HB	1:A:2401:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2085:GLU:O	1:A:2088:ILE:HG22	2.11	0.49
1:A:1057:MET:SD	1:A:1060:ILE:HD12	2.52	0.49
1:A:1997:PRO:HG2	1:A:2073:ILE:HD11	1.93	0.49
1:A:2519:GLU:O	1:A:2523:ARG:HG2	2.12	0.49
1:A:1337:LEU:HD12	1:A:1414:LEU:O	2.12	0.49
1:A:1347:LYS:HD3	2:A:2601:GDP:O3B	2.13	0.49
1:A:1885:LEU:HD12	1:A:1894:TYR:CZ	2.47	0.49
1:A:676:PHE:CD1	1:A:724:MET:HG2	2.48	0.49
1:A:743:SER:OG	1:A:744:LEU:N	2.46	0.49
1:A:1309:LYS:N	1:A:1313:CYS:SG	2.86	0.49
1:A:2377:ASP:HB2	1:A:2384:CYS:SG	2.52	0.49
1:A:2441:THR:O	1:A:2443:ARG:NH2	2.41	0.49
1:A:1051:PRO:HB3	1:A:1053:TYR:CE2	2.48	0.49
1:A:1183:ASN:N	1:A:1206:ASN:HD21	2.11	0.49
1:A:1214:PRO:HB3	1:A:1244:TRP:CD1	2.48	0.49
1:A:2363:LEU:N	1:A:2376:TRP:O	2.31	0.49
1:A:2379:LYS:HG3	1:A:2380:THR:H	1.78	0.49
1:A:1925:CYS:O	1:A:1928:HIS:NE2	2.44	0.49
1:A:742:SER:O	1:A:747:GLN:NE2	2.36	0.49
1:A:2155:MET:HE3	1:A:2473:LEU:HB2	1.95	0.49
1:A:2365:ILE:O	1:A:2373:VAL:HG23	2.13	0.49
1:A:1923:VAL:HA	1:A:1926:HIS:CE1	2.48	0.48
1:A:725:VAL:HG11	1:A:757:LEU:HD13	1.95	0.48
1:A:2022:GLN:HE21	1:A:2026:ARG:NH1	2.11	0.48
1:A:1217:TRP:NE1	1:A:1244:TRP:HZ2	2.11	0.48
1:A:1419:TYR:O	1:A:1427:GLU:HG2	2.14	0.48
1:A:1863:ASP:OD1	1:A:1863:ASP:N	2.44	0.48
1:A:1996:LYS:NZ	1:A:1998:HIS:HB3	2.29	0.48
1:A:672:ASP:HB2	1:A:676:PHE:CE2	2.49	0.48
1:A:2306:SER:OG	1:A:2314:VAL:O	2.29	0.48
1:A:2332:ILE:HD13	1:A:2335:LEU:HD13	1.96	0.48
1:A:2423:THR:HG21	1:A:2502:HIS:CE1	2.49	0.48
1:A:636:TYR:O	1:A:639:LYS:HG3	2.14	0.47
1:A:737:GLN:N	1:A:737:GLN:OE1	2.47	0.47
1:A:1002:GLN:HB2	1:A:1004:CYS:SG	2.54	0.47
1:A:1583:LEU:HD11	1:A:1600:PRO:HB3	1.97	0.47
1:A:2224:LEU:HB3	1:A:2238:LEU:HB2	1.94	0.47
1:A:665:LEU:O	1:A:669:HIS:ND1	2.45	0.47
1:A:2064:TYR:CD2	1:A:2095:PRO:HG3	2.48	0.47
1:A:2484:GLN:N	1:A:2484:GLN:OE1	2.48	0.47
1:A:1342:ASN:OD1	1:A:1342:ASN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2178:GLN:HE21	1:A:2191:SER:HB2	1.79	0.47
1:A:1095:LEU:HD12	1:A:1117:ASN:ND2	2.30	0.47
1:A:1554:LEU:O	1:A:1558:ARG:HG3	2.14	0.47
1:A:2254:SER:H	1:A:2312:ARG:HH12	1.63	0.47
1:A:1120:SER:HA	1:A:1140:HIS:O	2.14	0.47
1:A:1698:PRO:HA	1:A:1760:GLU:OE1	2.15	0.47
1:A:1584:HIS:CE1	1:A:1586:GLN:HG2	2.50	0.47
1:A:1316:LYS:HG3	1:A:1320:ARG:NH1	2.29	0.47
1:A:2276:GLU:CD	1:A:2278:LYS:H	2.22	0.47
1:A:1427:GLU:O	1:A:1431:MET:N	2.49	0.46
1:A:649:PHE:HA	1:A:652:ILE:HD12	1.97	0.46
1:A:1701:PRO:HB2	1:A:1792:PHE:CE2	2.50	0.46
1:A:1858:ASP:OD1	1:A:1858:ASP:N	2.48	0.46
1:A:2153:GLU:HB3	1:A:2456:ARG:NH2	2.30	0.46
1:A:573:PHE:HB2	1:A:574:PRO:HD3	1.97	0.46
1:A:2079:PHE:O	1:A:2083:PHE:N	2.47	0.46
1:A:2053:GLN:NE2	1:A:2122:ARG:O	2.48	0.46
1:A:1321:PHE:HE1	1:A:1527:TYR:HE2	1.63	0.46
1:A:1942:PRO:HD2	1:A:1944:MET:HE3	1.98	0.46
1:A:1968:ARG:HH11	1:A:2102:ALA:HB3	1.80	0.46
1:A:2255:LYS:HB3	1:A:2312:ARG:HH11	1.81	0.46
1:A:2267:THR:HG22	1:A:2268:ALA:N	2.31	0.46
1:A:1957:ARG:O	1:A:1961:GLN:HG2	2.16	0.46
1:A:2413:ARG:O	1:A:2430:GLY:N	2.49	0.46
1:A:608:SER:HB3	1:A:647:LYS:HD3	1.97	0.46
1:A:1339:ILE:HB	1:A:1394:ASP:HA	1.98	0.46
1:A:2427:ILE:HB	1:A:2435:LEU:HB2	1.97	0.46
1:A:791:LEU:HD22	1:A:805:LEU:HD21	1.97	0.46
1:A:1137:SER:HB2	1:A:1161:ARG:HB2	1.98	0.46
1:A:1180:LEU:HB3	1:A:1183:ASN:HD22	1.80	0.46
1:A:1350:LEU:HD12	1:A:1488:VAL:HG21	1.98	0.46
1:A:1545:PHE:CE2	1:A:1547:VAL:HB	2.51	0.46
1:A:1966:LEU:HD12	1:A:2069:THR:HG22	1.98	0.46
1:A:1719:MET:H	1:A:1719:MET:HE2	1.81	0.46
1:A:2437:LEU:HA	1:A:2443:ARG:O	2.15	0.46
1:A:2522:ARG:HH21	1:A:2523:ARG:HD3	1.81	0.46
1:A:703:ALA:HB1	1:A:709:LYS:HG2	1.97	0.46
1:A:1861:LEU:HD12	1:A:1864:LEU:HD12	1.97	0.46
1:A:2146:LEU:HB2	1:A:2491:SER:O	2.16	0.46
1:A:2206:HIS:HA	1:A:2213:SER:HA	1.98	0.46
1:A:2274:ILE:O	1:A:2288:LEU:N	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1832:LYS:NZ	1:A:1859:LEU:HD12	2.28	0.45
1:A:2040:ALA:HB3	1:A:2043:VAL:HG23	1.98	0.45
1:A:2203:ALA:O	1:A:2216:VAL:HG12	2.16	0.45
1:A:1684:HIS:HE1	1:A:1744:PRO:HB2	1.81	0.45
1:A:1707:ARG:HB3	1:A:1787:LEU:HD11	1.98	0.45
1:A:1935:LEU:HD11	1:A:1945:LEU:CD1	2.45	0.45
1:A:2078:LYS:HG3	1:A:2079:PHE:CD2	2.52	0.45
1:A:726:GLU:O	1:A:730:LEU:HG	2.16	0.45
1:A:1265:GLY:HA3	1:A:1290:LYS:NZ	2.31	0.45
1:A:1740:LEU:H	1:A:1740:LEU:HD23	1.81	0.45
1:A:2306:SER:HA	1:A:2359:VAL:HB	1.97	0.45
1:A:1149:LEU:HA	1:A:1149:LEU:HD23	1.82	0.45
1:A:1692:ILE:HA	1:A:1765:ILE:O	2.17	0.45
1:A:2279:THR:HA	1:A:2282:LEU:HD23	1.99	0.45
1:A:1739:TYR:HB2	1:A:1749:LEU:HD13	1.98	0.45
1:A:1841:VAL:O	1:A:1849:THR:OG1	2.22	0.45
1:A:1171:LEU:HD12	1:A:1195:LEU:HD11	1.98	0.45
1:A:1446:PRO:HB3	1:A:1483:ARG:HG3	1.99	0.45
1:A:1687:ASN:OD1	1:A:1815:SER:OG	2.24	0.45
1:A:1337:LEU:HB2	1:A:1390:LEU:HD13	1.99	0.45
1:A:1425:GLN:HG3	1:A:1469:ILE:HG21	1.99	0.45
1:A:1436:PHE:CZ	1:A:1795:LEU:HD21	2.51	0.45
1:A:2001:LEU:HD11	1:A:2016:ALA:HB2	1.99	0.45
1:A:1195:LEU:HD12	1:A:1198:LEU:HD12	1.98	0.45
1:A:1689:GLU:O	1:A:1769:SER:N	2.34	0.45
1:A:1867:ASN:OD1	1:A:1868:ILE:HG23	2.17	0.45
1:A:2390:VAL:HB	1:A:2394:ARG:HG3	1.97	0.45
1:A:641:VAL:HG13	1:A:642:ALA:H	1.81	0.45
1:A:1085:LEU:HD23	1:A:1106:VAL:HG11	1.97	0.45
1:A:1304:LEU:HB2	1:A:1308:PHE:HE2	1.82	0.44
1:A:1621:HIS:HB3	1:A:1625:ILE:HG23	1.99	0.44
1:A:1926:HIS:HA	1:A:1928:HIS:HD2	1.82	0.44
1:A:1308:PHE:HD1	1:A:1309:LYS:HG2	1.80	0.44
1:A:822:PHE:CD1	1:A:984:ILE:HD11	2.53	0.44
1:A:1371:ILE:HD13	1:A:1408:PHE:CD2	2.52	0.44
1:A:1803:GLU:HG2	1:A:1804:GLY:N	2.33	0.44
1:A:2181:PHE:HB3	1:A:2190:THR:HB	1.98	0.44
1:A:601:GLU:HG2	1:A:602:ILE:HG23	2.00	0.44
1:A:2488:GLU:N	1:A:2488:GLU:OE2	2.50	0.44
1:A:990:SER:HB3	1:A:1019:HIS:CE1	2.52	0.44
1:A:1126:LEU:HD23	1:A:1126:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1958:LEU:HD12	1:A:1962:ASP:HB2	2.00	0.44
1:A:1995:LEU:HB3	1:A:2058:SER:OG	2.18	0.44
1:A:2127:GLN:O	1:A:2131:ILE:HG12	2.17	0.44
1:A:2295:ASN:H	1:A:2298:THR:HB	1.83	0.44
1:A:2395:GLU:OE1	1:A:2395:GLU:N	2.50	0.44
1:A:1935:LEU:HA	1:A:1935:LEU:HD12	1.69	0.44
1:A:558:GLY:HA2	1:A:596:TYR:HE2	1.81	0.43
1:A:1090:LEU:HB2	1:A:1114:LEU:HD23	1.99	0.43
1:A:1434:TRP:CE3	1:A:1702:MET:HE1	2.53	0.43
1:A:1781:VAL:HA	1:A:1784:ILE:HG22	2.00	0.43
1:A:1348:THR:HG22	1:A:1394:ASP:OD2	2.17	0.43
1:A:1369:VAL:O	1:A:1605:LYS:NZ	2.51	0.43
1:A:1376:TRP:HE1	1:A:1392:VAL:HG13	1.83	0.43
1:A:2205:VAL:HG12	1:A:2250:CYS:SG	2.58	0.43
1:A:2252:SER:O	1:A:2252:SER:OG	2.34	0.43
1:A:2502:HIS:HA	1:A:2505:GLN:HE21	1.83	0.43
1:A:1709:ILE:O	1:A:1713:LEU:HB2	2.19	0.43
1:A:764:SER:OG	1:A:765:GLY:N	2.51	0.43
1:A:1321:PHE:CE2	1:A:1325:ARG:HD2	2.54	0.43
1:A:1371:ILE:HG12	1:A:1604:CYS:HB2	1.99	0.43
1:A:1483:ARG:NE	1:A:1507:GLU:OE2	2.33	0.43
1:A:2254:SER:HB2	1:A:2258:LYS:O	2.19	0.43
1:A:653:LEU:HD23	1:A:653:LEU:HA	1.80	0.43
1:A:684:MET:SD	1:A:684:MET:N	2.90	0.43
1:A:699:PHE:HZ	1:A:728:LEU:HD21	1.84	0.43
1:A:1449:LEU:O	1:A:1485:TYR:HA	2.18	0.43
1:A:745:ILE:HD12	1:A:745:ILE:H	1.84	0.43
1:A:1466:MET:O	1:A:1469:ILE:HG22	2.19	0.43
1:A:2442:ARG:HA	1:A:2442:ARG:HD2	1.86	0.43
1:A:794:LEU:HA	1:A:794:LEU:HD23	1.79	0.43
1:A:1047:PHE:HB2	1:A:1068:ASN:HB3	2.00	0.43
1:A:1109:LEU:HD21	1:A:1112:LEU:HB2	2.01	0.43
1:A:1183:ASN:H	1:A:1206:ASN:HD21	1.66	0.43
1:A:1832:LYS:NZ	1:A:1852:ILE:HG23	2.33	0.43
1:A:1865:PRO:O	1:A:1868:ILE:HG12	2.19	0.43
1:A:1076:LEU:HD23	1:A:1076:LEU:HA	1.87	0.43
1:A:1225:LEU:HB3	1:A:1227:PHE:HE2	1.84	0.43
1:A:1341:GLY:O	1:A:1434:TRP:NE1	2.52	0.43
1:A:1353:GLN:HB3	1:A:1497:LEU:HD21	2.01	0.43
1:A:1470:THR:O	1:A:1474:LEU:HB3	2.18	0.43
1:A:1742:TRP:CZ3	1:A:1776:LEU:HD11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1427:GLU:HA	1:A:1430:ALA:HB3	2.00	0.43
1:A:2216:VAL:HG11	1:A:2248:LEU:HD22	2.00	0.43
1:A:652:ILE:O	1:A:656:LEU:HG	2.19	0.42
1:A:992:ASN:O	1:A:994:LEU:N	2.51	0.42
1:A:1054:LEU:O	1:A:1057:MET:HG3	2.19	0.42
1:A:1066:SER:HB2	1:A:1091:SER:OG	2.19	0.42
1:A:1337:LEU:HB3	1:A:1392:VAL:HG12	2.01	0.42
1:A:1552:ARG:O	1:A:1556:LEU:HG	2.18	0.42
1:A:2219:THR:HG22	1:A:2223:THR:O	2.19	0.42
1:A:822:PHE:HE2	1:A:1006:ILE:HB	1.85	0.42
1:A:1657:GLN:HB3	1:A:1710:ASN:CG	2.44	0.42
1:A:1840:LEU:HD23	1:A:1851:PRO:HA	2.00	0.42
1:A:2453:ASN:HD22	1:A:2477:ARG:H	1.66	0.42
1:A:1832:LYS:NZ	1:A:1856:ALA:HB3	2.33	0.42
1:A:2302:CYS:SG	1:A:2356:THR:HA	2.60	0.42
1:A:728:LEU:HD23	1:A:728:LEU:HA	1.78	0.42
1:A:1431:MET:HE3	1:A:1431:MET:HB3	1.87	0.42
1:A:1711:ARG:NH1	1:A:1790:GLU:OE1	2.51	0.42
1:A:722:SER:HA	1:A:725:VAL:HG12	2.01	0.42
1:A:1355:MET:HG2	1:A:1376:TRP:CD2	2.54	0.42
1:A:606:GLY:O	1:A:610:ILE:HG12	2.19	0.42
1:A:1013:LEU:HD12	1:A:1013:LEU:HA	1.79	0.42
1:A:1359:LYS:HG3	1:A:1360:SER:N	2.35	0.42
1:A:1739:TYR:HA	1:A:1748:CYS:O	2.20	0.42
1:A:723:ILE:HD12	1:A:836:ALA:HB2	2.01	0.42
1:A:1045:ASN:O	1:A:1068:ASN:ND2	2.50	0.42
1:A:1138:LYS:HA	1:A:1162:MET:HB2	2.02	0.42
1:A:1180:LEU:HB3	1:A:1183:ASN:ND2	2.35	0.42
1:A:1250:LEU:HG	1:A:1252:LEU:HD23	2.01	0.42
1:A:1940:ILE:HG22	1:A:1941:ARG:N	2.33	0.42
1:A:1986:HIS:ND1	1:A:2052:GLN:HB2	2.35	0.42
1:A:2151:ILE:HB	1:A:2173:HIS:N	2.34	0.42
1:A:2293:ILE:HD12	1:A:2332:ILE:HD11	2.02	0.42
1:A:1010:LEU:HD22	1:A:1013:LEU:HD22	2.02	0.41
1:A:1441:ARG:NH2	1:A:1791:TRP:O	2.53	0.41
1:A:1474:LEU:HD12	1:A:1479:PHE:CD2	2.55	0.41
1:A:1573:VAL:HG23	1:A:1582:LEU:HD11	2.00	0.41
1:A:815:PRO:HG3	1:A:1004:CYS:SG	2.60	0.41
1:A:1065:VAL:HG23	1:A:1090:LEU:HD23	2.02	0.41
1:A:2301:MET:HE1	1:A:2368:GLN:NE2	2.33	0.41
1:A:769:GLN:CD	1:A:769:GLN:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:LEU:HD12	1:A:1479:PHE:HD2	1.85	0.41
1:A:1565:ASP:OD1	1:A:1565:ASP:N	2.45	0.41
1:A:2110:LEU:HD13	1:A:2131:ILE:HD11	2.02	0.41
1:A:1339:ILE:HG12	1:A:1416:LEU:HD12	2.02	0.41
1:A:1691:ILE:HG13	1:A:1769:SER:HB3	2.02	0.41
1:A:1747:TYR:CE1	1:A:1768:PRO:HD3	2.55	0.41
1:A:1238:SER:HA	1:A:1263:GLU:HG2	2.01	0.41
1:A:1372:ASP:HB2	1:A:1605:LYS:NZ	2.34	0.41
1:A:2228:ASN:OD1	1:A:2229:THR:N	2.49	0.41
1:A:1045:ASN:HB2	1:A:1068:ASN:HD21	1.85	0.41
1:A:1512:LYS:HG3	1:A:1517:LEU:H	1.85	0.41
1:A:1569:LEU:N	1:A:1570:PRO:HD2	2.35	0.41
1:A:2289:LYS:HG2	1:A:2291:LEU:HD11	2.03	0.41
1:A:1419:TYR:HD2	1:A:1421:LEU:HD13	1.86	0.41
1:A:1440:ALA:HB1	1:A:1792:PHE:HB3	2.02	0.41
1:A:1687:ASN:HB3	1:A:1819:GLY:HA2	2.03	0.41
1:A:1712:LEU:HD22	1:A:1780:VAL:HG22	2.03	0.41
1:A:2064:TYR:CE2	1:A:2095:PRO:HG3	2.55	0.41
1:A:561:LYS:O	1:A:565:LYS:HG3	2.20	0.41
1:A:665:LEU:HA	1:A:668:HIS:HB3	2.02	0.41
1:A:997:ILE:HB	1:A:1023:LEU:HD21	2.03	0.41
1:A:1044:SER:H	1:A:1067:ARG:HB2	1.84	0.41
1:A:1263:GLU:OE2	1:A:1263:GLU:N	2.51	0.41
1:A:1338:MET:HE1	1:A:1410:THR:H	1.85	0.41
1:A:1355:MET:HG2	1:A:1376:TRP:CG	2.55	0.41
1:A:1511:PHE:HD2	1:A:1518:VAL:HG11	1.86	0.41
1:A:1652:LEU:HA	1:A:1655:LYS:HB2	2.03	0.41
1:A:2168:TRP:H	1:A:2168:TRP:CD1	2.39	0.41
1:A:2168:TRP:HB3	1:A:2179:LEU:HD21	2.03	0.41
1:A:2363:LEU:HD12	1:A:2363:LEU:HA	1.87	0.41
1:A:2378:LYS:H	1:A:2378:LYS:HG2	1.61	0.41
1:A:2434:ILE:CG2	1:A:2448:ILE:HB	2.51	0.41
1:A:1136:LEU:O	1:A:1139:ASN:ND2	2.54	0.41
1:A:1230:ASN:HD22	1:A:1232:ILE:HD11	1.85	0.41
1:A:1376:TRP:CH2	1:A:1378:ILE:HD11	2.56	0.41
1:A:790:LEU:HD23	1:A:790:LEU:HA	1.90	0.40
1:A:1399:GLU:HA	1:A:1402:TYR:CE1	2.56	0.40
1:A:1695:TYR:OH	1:A:1781:VAL:HG23	2.22	0.40
1:A:1919:GLN:O	1:A:1922:VAL:HG12	2.20	0.40
1:A:1144:LEU:HB2	1:A:1169:PRO:HG3	2.03	0.40
1:A:1208:ILE:HD12	1:A:1230:ASN:ND2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:ILE:HD12	1:A:1527:TYR:HB2	2.03	0.40
1:A:2307:THR:HG23	1:A:2308:ASN:OD1	2.21	0.40
1:A:604:CYS:HB2	1:A:647:LYS:HD2	2.03	0.40
1:A:1814:TYR:O	1:A:1825:ILE:N	2.48	0.40
1:A:1967:THR:C	1:A:1969:THR:H	2.29	0.40
1:A:2063:LEU:HD23	1:A:2063:LEU:HA	1.89	0.40
1:A:2433:HIS:CD2	1:A:2449:TYR:HB3	2.56	0.40
1:A:1774:CYS:O	1:A:1775:ILE:C	2.64	0.40
1:A:2037:GLY:HA3	1:A:2083:PHE:CE2	2.57	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	1777/2527 (70%)	1563 (88%)	214 (12%)	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	1577/2282 (69%)	1577 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	GLN
1	A	689	GLN
1	A	693	ASN
1	A	720	ASN
1	A	785	GLN
1	A	992	ASN
1	A	1019	HIS
1	A	1021	ASN
1	A	1028	GLN
1	A	1062	ASN
1	A	1068	ASN
1	A	1163	ASN
1	A	1206	ASN
1	A	1216	HIS
1	A	1230	ASN
1	A	1251	HIS
1	A	1254	HIS
1	A	1305	ASN
1	A	1323	GLN
1	A	1405	HIS
1	A	1411	GLN
1	A	1475	ASN
1	A	1486	HIS
1	A	1516	GLN
1	A	1521	GLN
1	A	1571	HIS
1	A	1586	GLN
1	A	1621	HIS
1	A	1684	HIS
1	A	1758	HIS
1	A	1919	GLN
1	A	1926	HIS
1	A	1972	HIS
1	A	2022	GLN
1	A	2081	ASN
1	A	2127	GLN
1	A	2133	ASN
1	A	2149	ASN
1	A	2173	HIS

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Mol	Chain	Res	Type
1	A	2178	GLN
1	A	2368	GLN
1	A	2401	ASN
1	A	2433	HIS
1	A	2462	GLN
1	A	2468	ASN
1	A	2476	ASN
1	A	2502	HIS
1	A	2505	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GDP	A	2601	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	3 (10%)
3	ATP	A	2602	-	28,33,33	0.88	0	34,52,52	1.19	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	2601	-	-	6/12/32/32	0/3/3/3
3	ATP	A	2602	-	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2601	GDP	C6-N1	-2.50	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2602	ATP	N3-C2-N1	-3.62	123.76	128.67
2	A	2601	GDP	C8-N7-C5	2.86	107.41	102.55
3	A	2602	ATP	C4-C5-N7	-2.43	106.77	109.34
2	A	2601	GDP	C5-C6-N1	2.27	118.39	114.07
2	A	2601	GDP	O4'-C1'-N9	2.11	111.54	108.75

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	PA-O3A-PB-O2B
2	A	2601	GDP	PA-O3A-PB-O3B
2	A	2601	GDP	C5'-O5'-PA-O3A
2	A	2601	GDP	C5'-O5'-PA-O1A
2	A	2601	GDP	O4'-C4'-C5'-O5'
2	A	2601	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

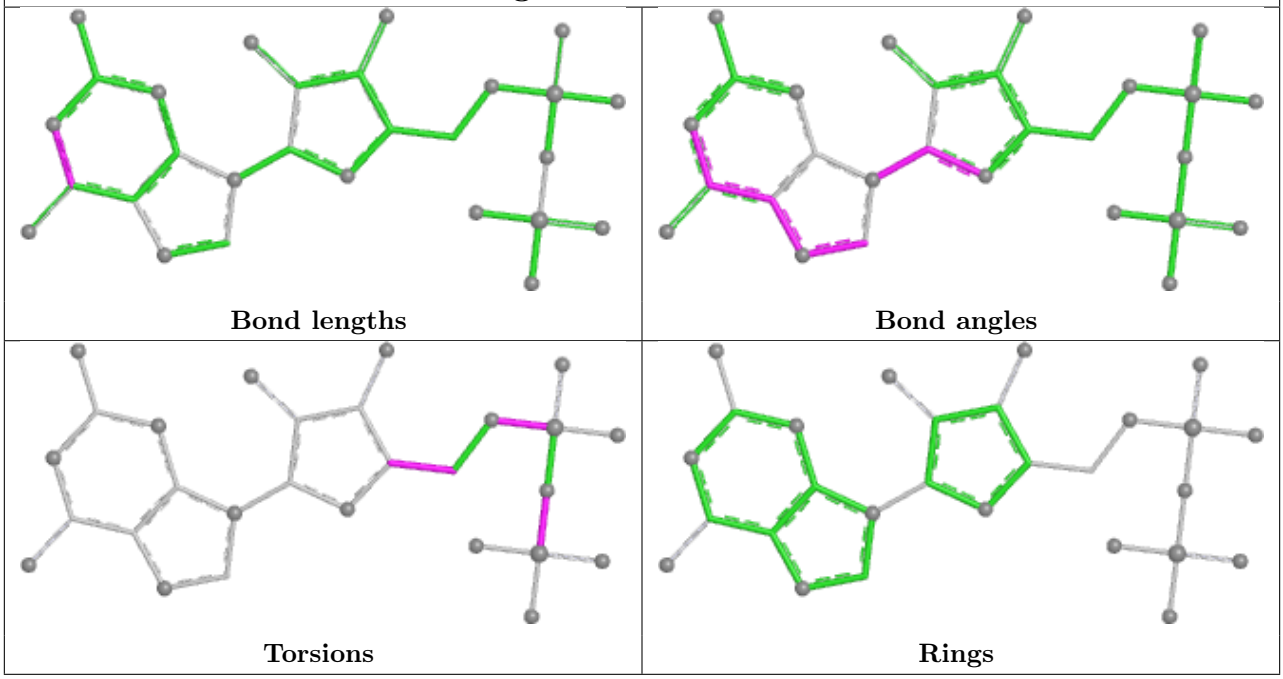
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	GDP	1	0
3	A	2602	ATP	2	0

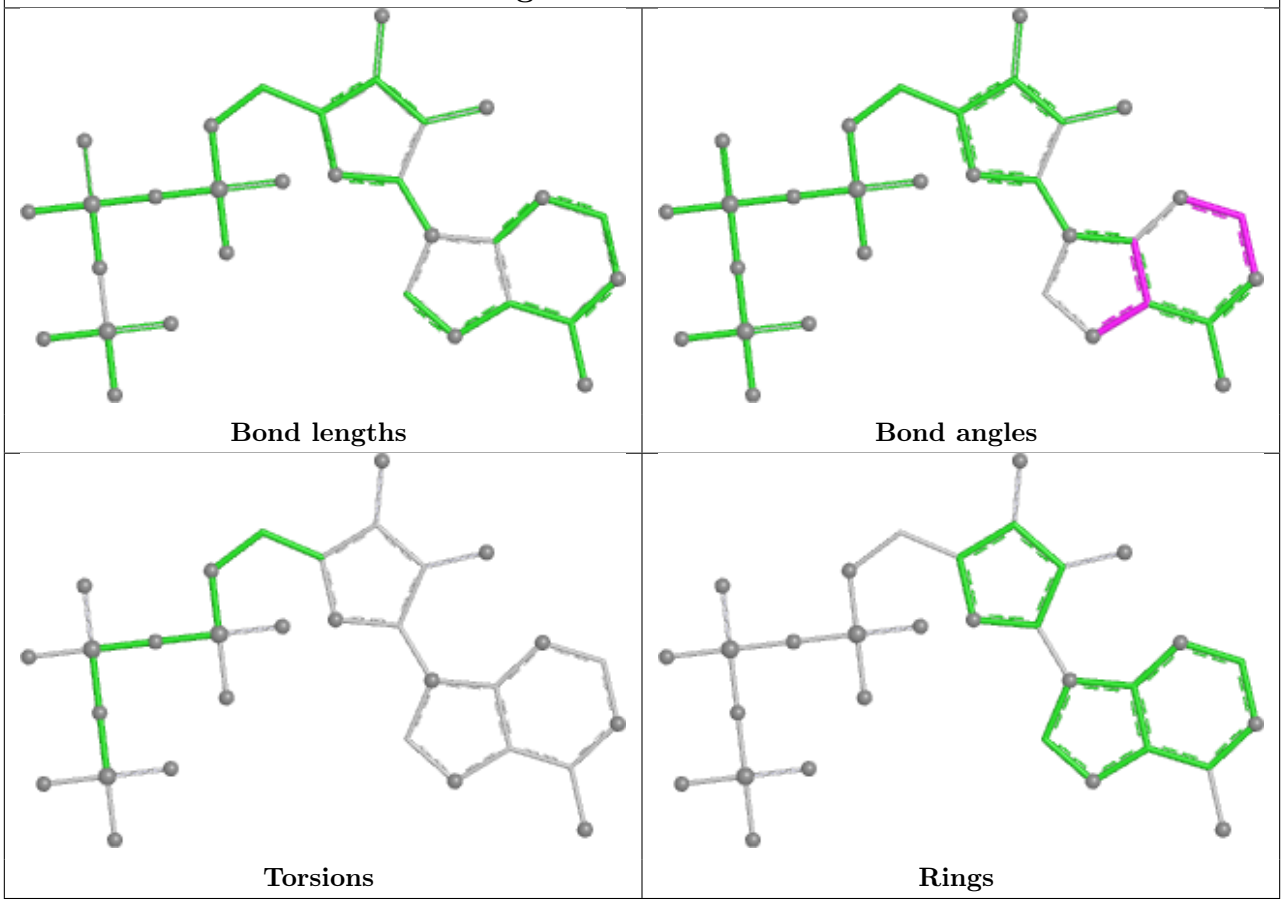
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP A 2601



Ligand ATP A 2602



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.

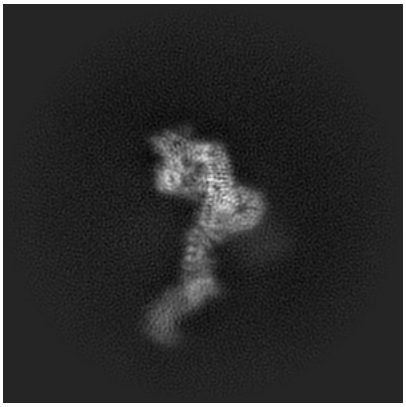
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23359. These allow visual inspection of the internal detail of the map and identification of artifacts.

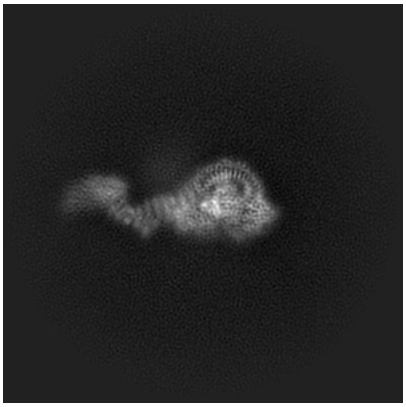
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

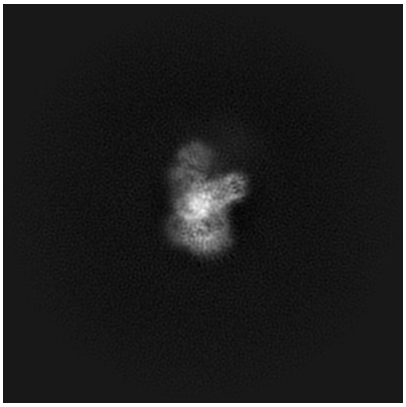
6.1.1 Primary map



X



Y

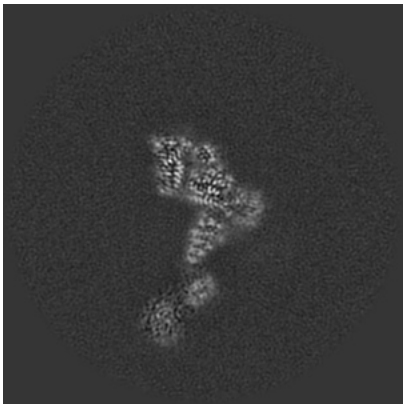


Z

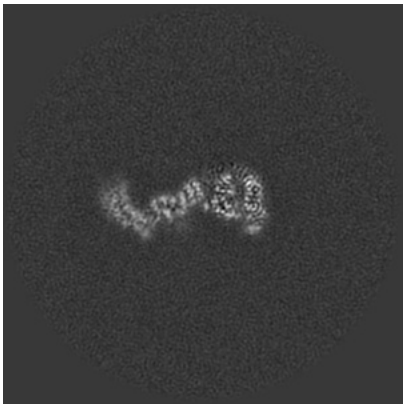
The images above show the map projected in three orthogonal directions.

6.2 Central slices

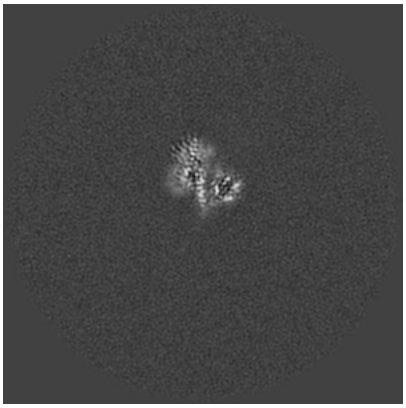
6.2.1 Primary map



X Index: 256



Y Index: 256



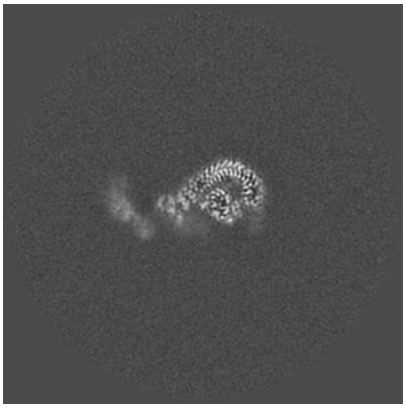
Z Index: 256

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

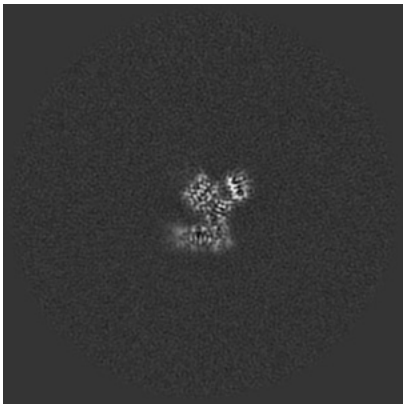
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 246



Y Index: 266

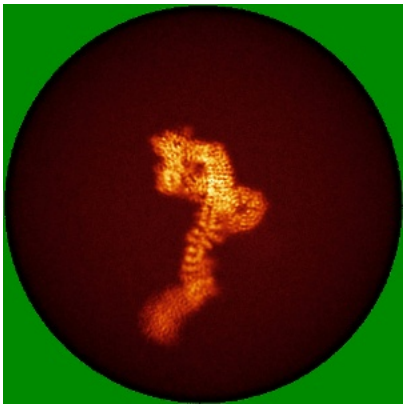


Z Index: 285

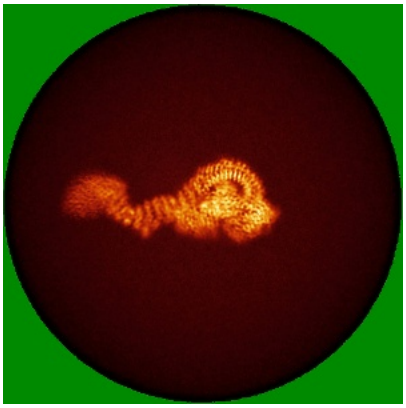
The images above show the largest variance slices of the map in three orthogonal directions.

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

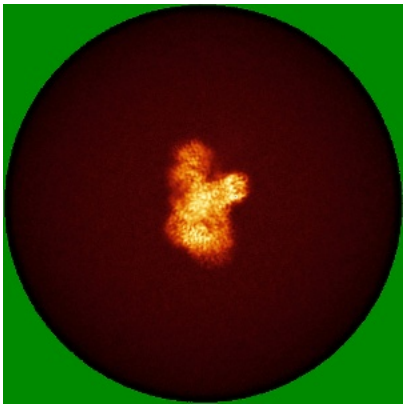
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

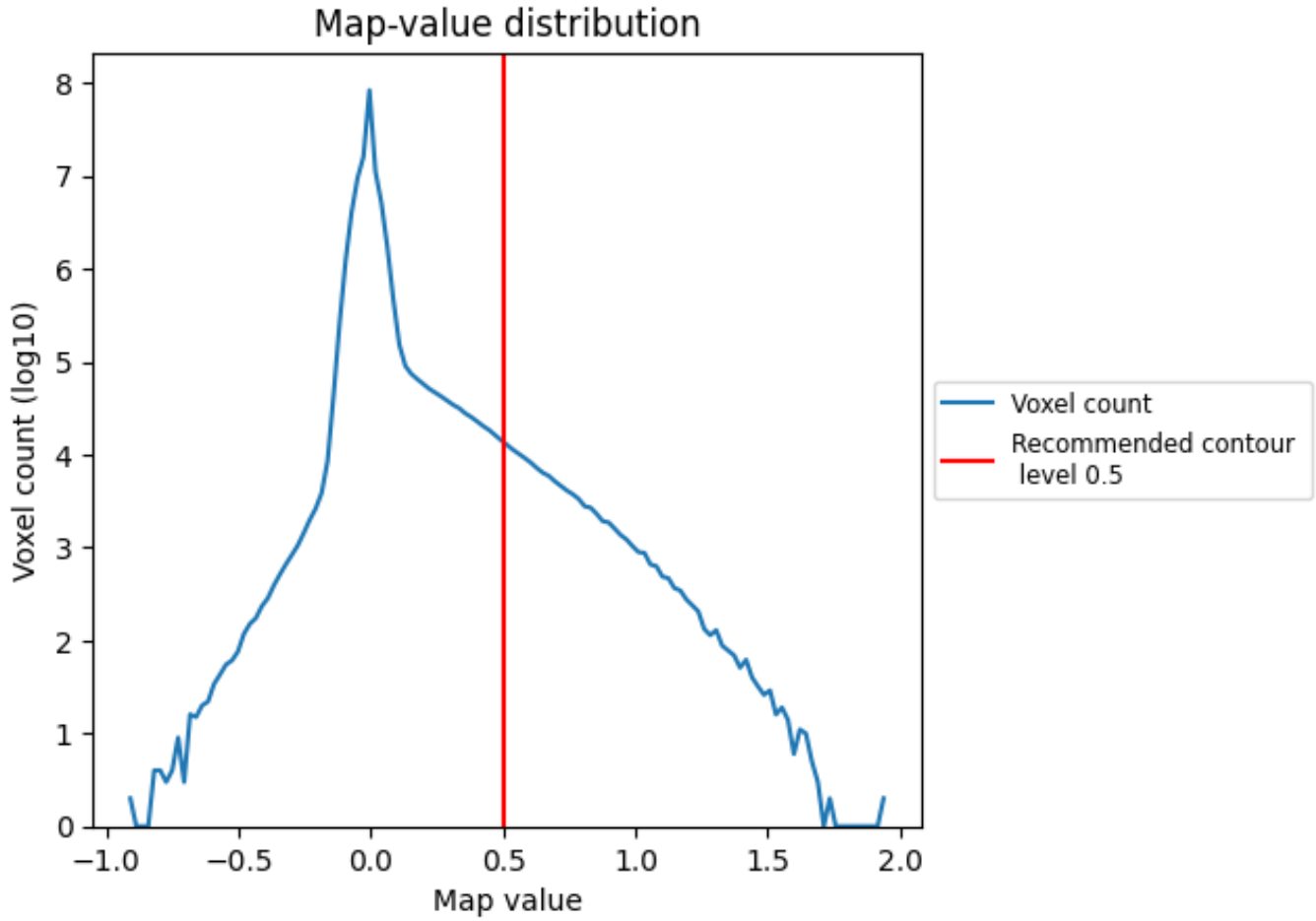
6.6 Mask visualisation (i)

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

7 Map analysis

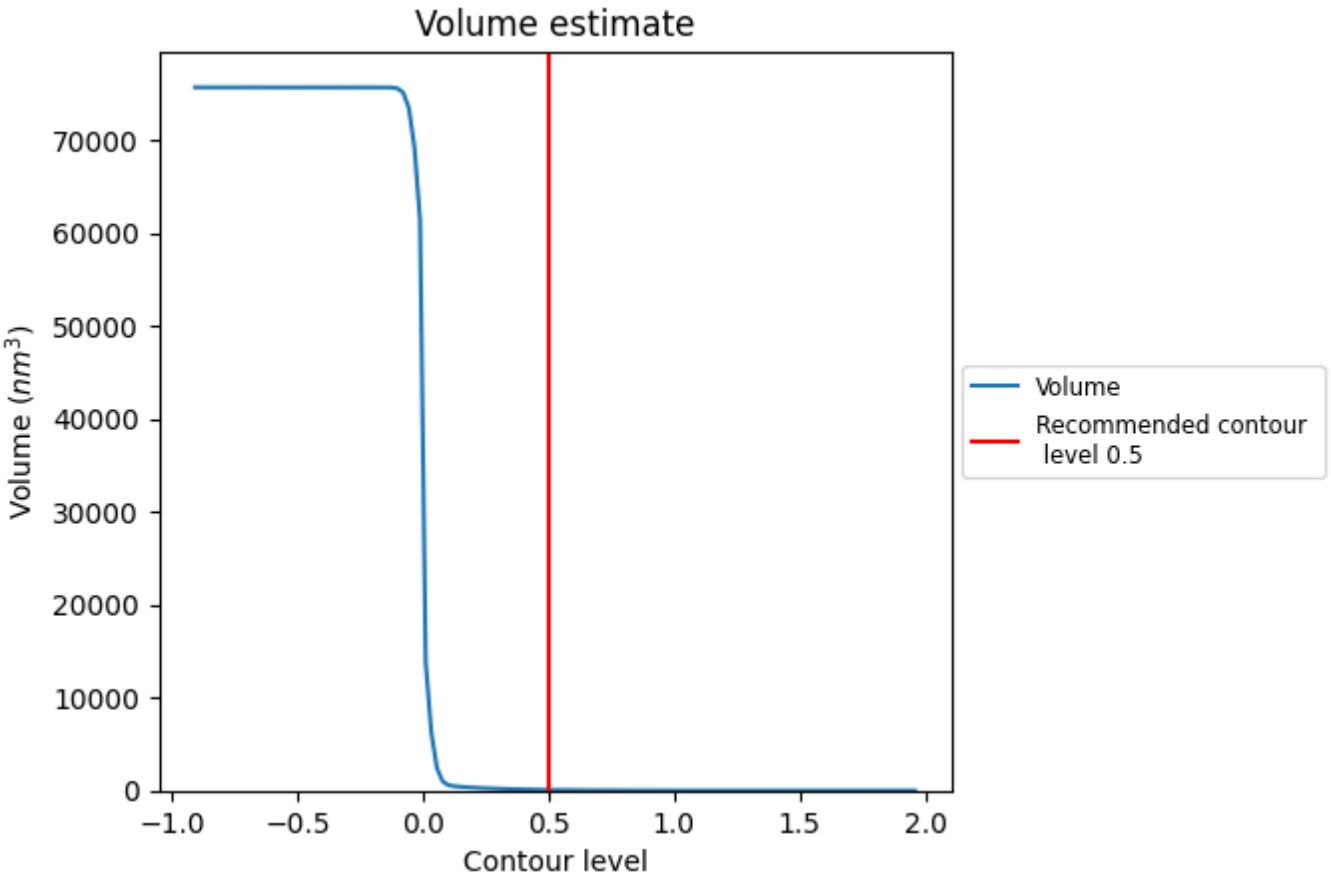
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

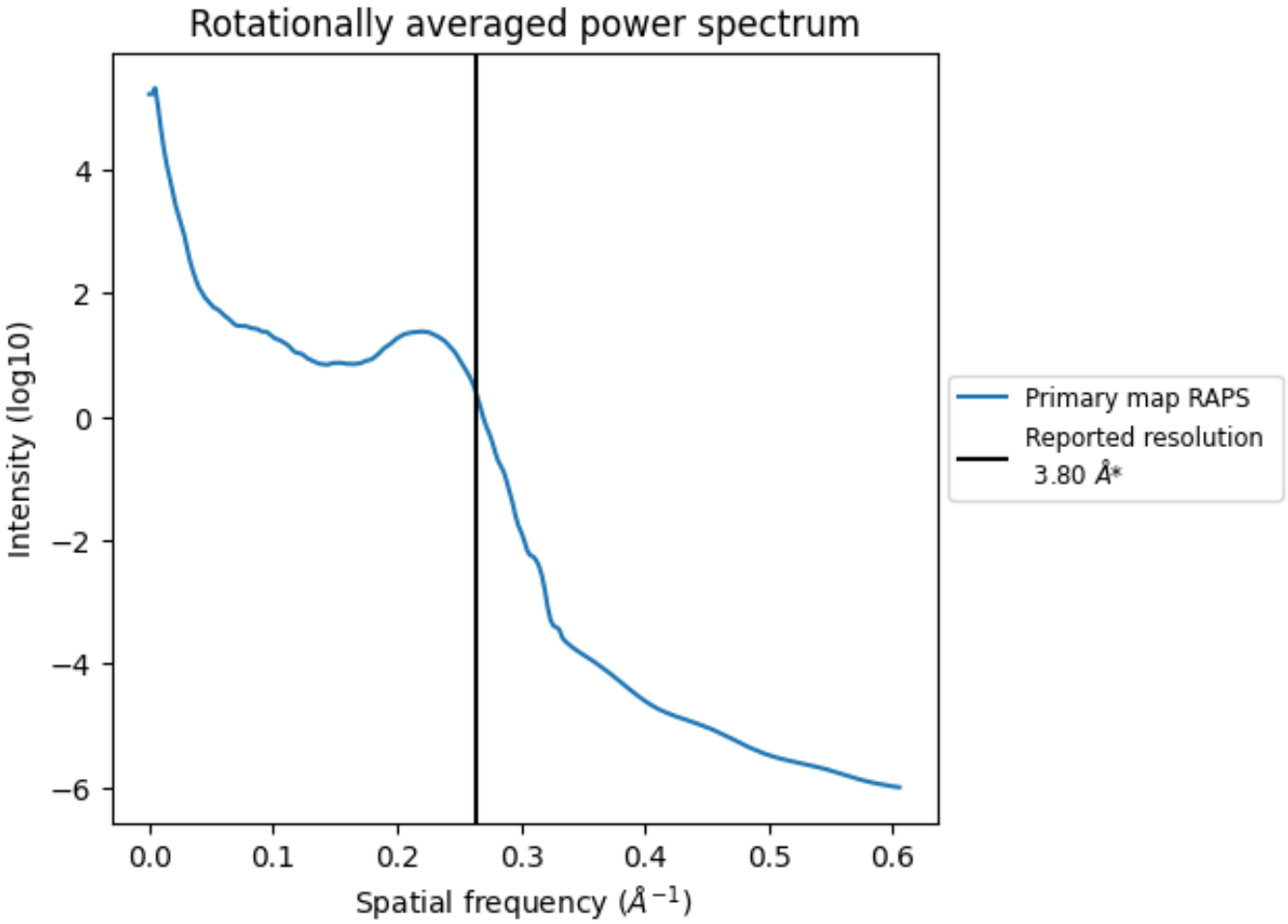
7.2 Volume estimate (i)



The volume at the recommended contour level is 70 nm^3; this corresponds to an approximate mass of 63 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 0.263 Å^{-1}

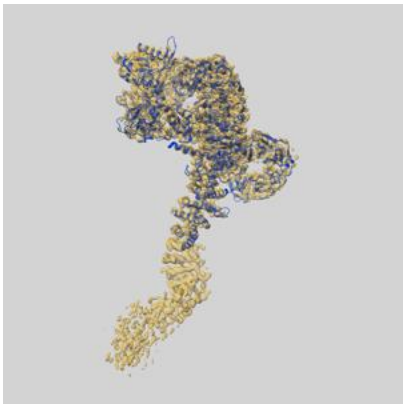
8 Fourier-Shell correlation (i)

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

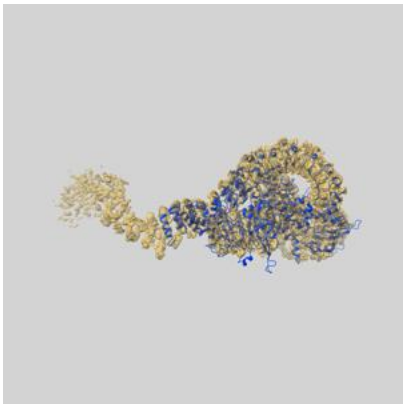
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23359 and PDB model 7LI3. Per-residue inclusion information can be found in section 3 on page 5.

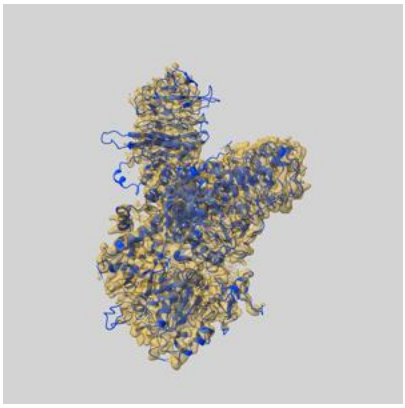
9.1 Map-model overlay



X



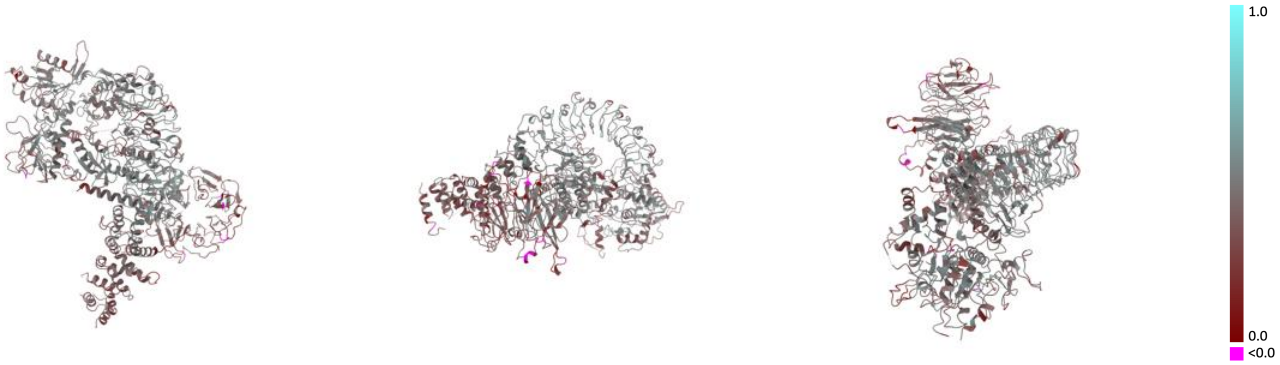
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

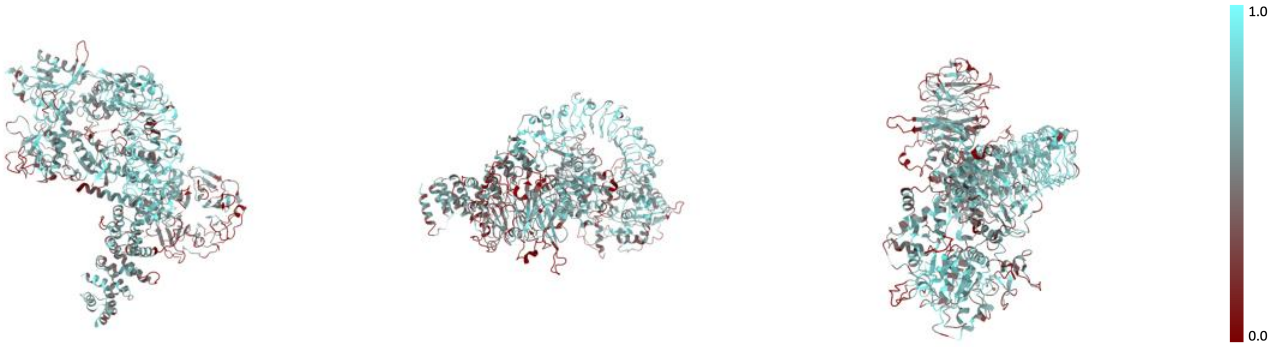
9.2 Q-score mapped to coordinate model (i)



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.

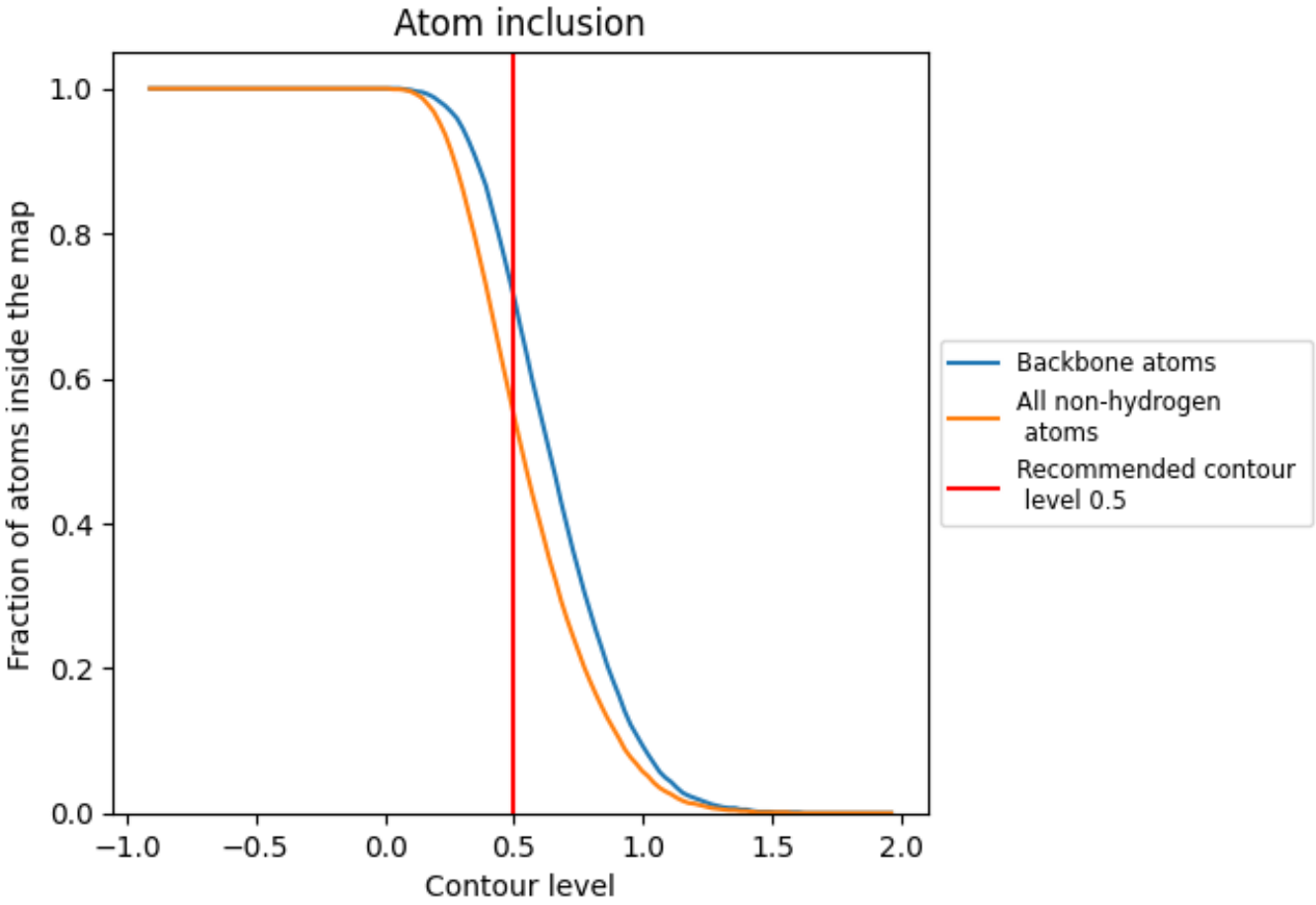
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5470	0.4020
A	0.5470	0.4020