# wwPDB EM Validation Summary Report

May 13, 2025 – 09:53 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 7LI4 / pdb_00007li4 |
| EMDB ID | : | EMD-23360 |
| Title | : | Structure of LRRK2 after symmetry expansion |
| Authors | : | Myasnikov, A.; Zhu, H.; Hixson, P.; Xie, B.; Yu, K.; Pitre, A.; Peng, J.; Sun, J. |
| Deposited on | : | 2021-01-26 |
| Resolution | : | 3.10 Å(reported) |

This is a wwPDB EM Validation Summary 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:

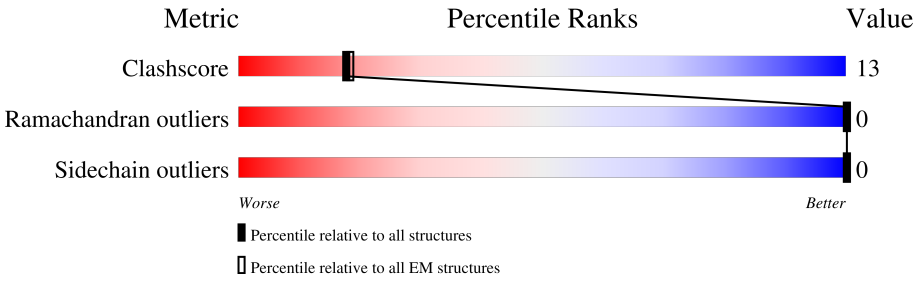
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev118 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0rc1 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 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 3.10 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 | 7% 52% 19% 29% |

# 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14169 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.

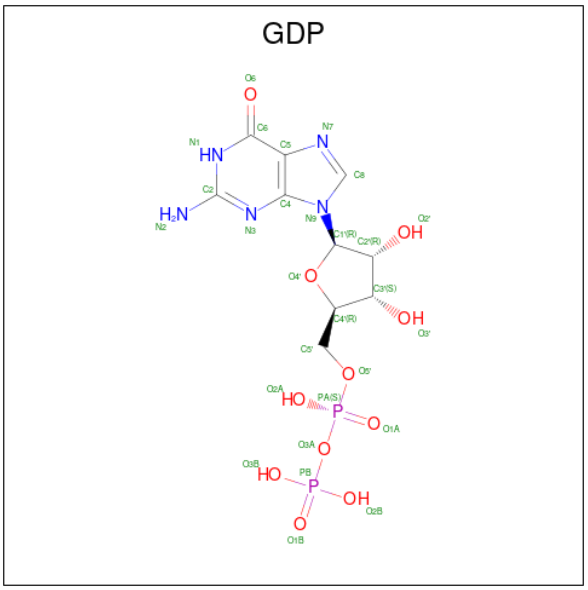
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 1795 | Total | C | N | O | S | 0 | 0 |
| | | | 14110 | 9023 | 2433 | 2563 | 91 | | |

There are 3 discrepancies between the modelled and reference sequences:

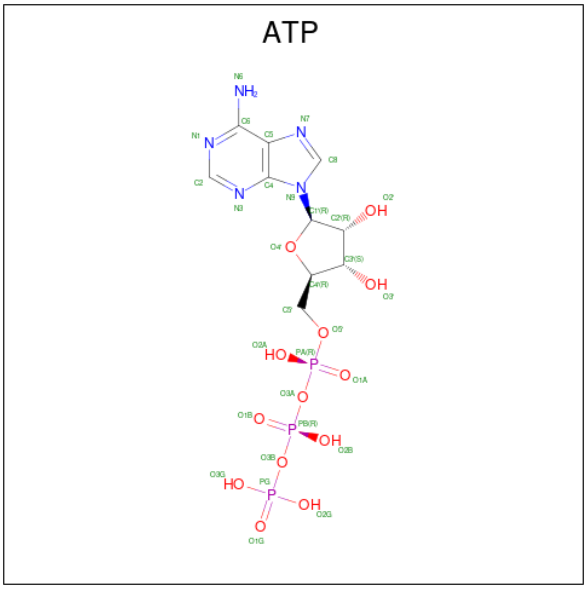
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 50 | HIS | ARG | variant | UNP Q5S007 |
| A | 1647 | THR | SER | variant | UNP Q5S007 |
| A | 2397 | THR | MET | variant | UNP Q5S007 |

- 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 |
|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

- 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).

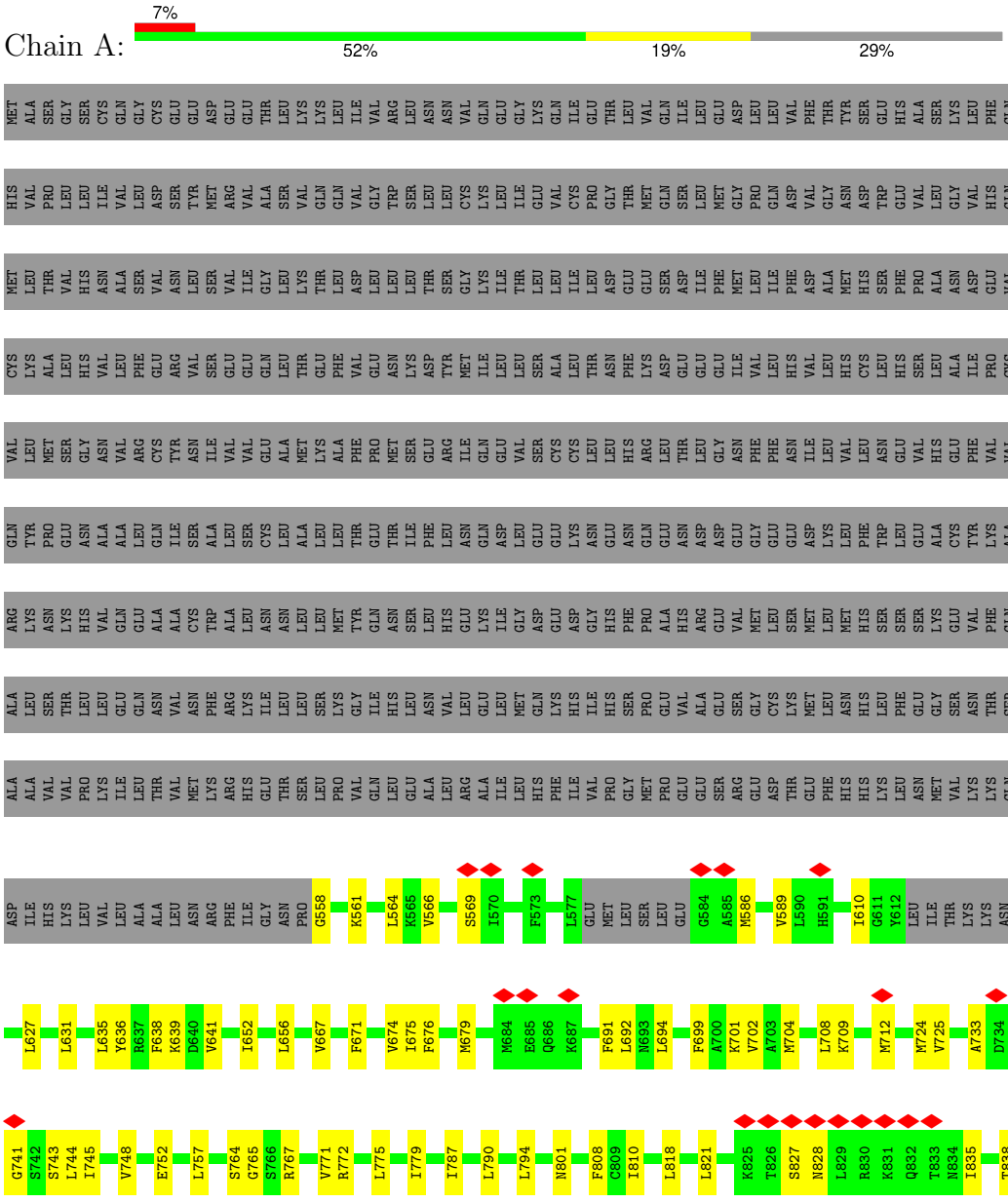


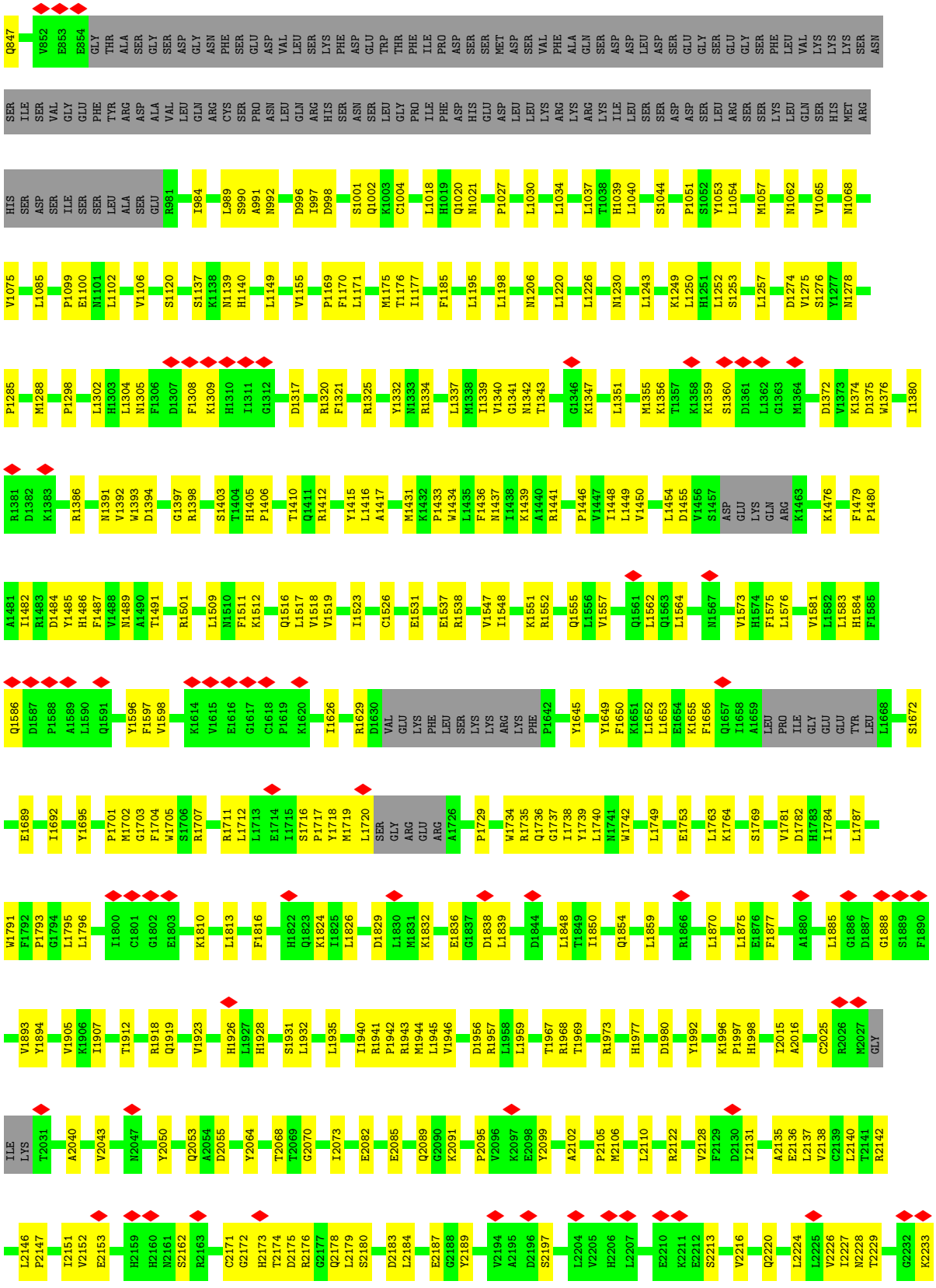

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 3 | A | 1 | 31 | 10 | 5 | 13 | 3 | 0 |

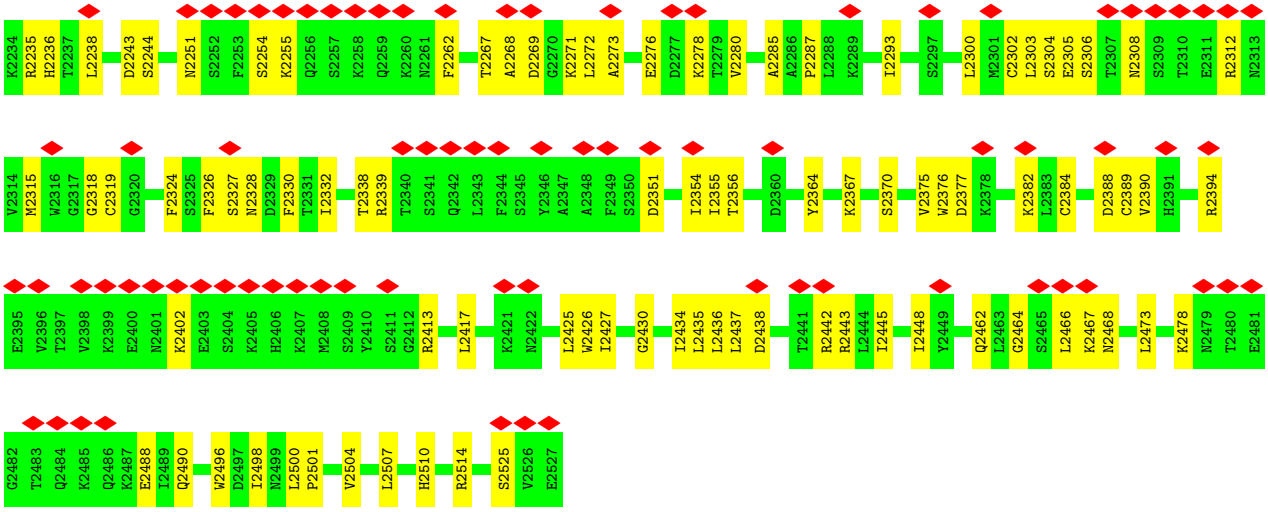
# 3 Residue-property plots (i)

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




Q847 V852 E853 E854 GLY THR ALA SER GLY SER ASP GLY ASN PHE SER GLU ASP VAL LEU LEU SER LYS PHE ASP GLU TRP THR PHE ILE PRO ASP SER SER MET ASP SER VAL PHE ALA GLN SER 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 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 I984 L989 S990 A991 N992 D996 I997 D998 S1001 Q1002 K1003 C1004 L1018 H1019 Q1020 N1021 P1027 L1030 L1034 L1037 T1038 H1039 L1040 S1044 P1051 S1052 Y1053 L1054 M1057 N1062 V1065 N1068
V1075 L1085 P1099 E1100 N1101 L1102 V1106 S1120 S1137 K1138 N1139 H1140 L1149 V1155 P1169 F1170 L1171 M1175 T1176 I1177 F1185 L1195 L1198 N1206 L1220 L1226 N1230 L1243 K1249 L1250 H1251 L1252 S1253 L1257 D1274 V1275 S1276 Y1277 N1278
P1285 M1288 P1298 L1302 H1303 L1304 N1305 F1306 D1307 F1308 K1309 H1310 I1311 G1312 D1317 R1320 F1321 R1325 Y1332 N1333 R1334 L1337 M1338 I1339 V1340 G1341 N1342 T1343 G1346 K1347 L1351 M1355 K1356 T1357 K1358 K1359 S1360 D1361 L1362 G1363 M1364 D1372 V1373 K1374 D1375 W1376 I1380
R1381 D1382 K1383 R1386 N1391 V1392 W1393 D1394 G1397 R1398 S1403 T1404 H1405 P1406 T1410 Q1411 R1412 Y1415 L1416 A1417 M1431 K1432 P1433 W1434 L1435 F1436 N1437 I1438 K1439 A1440 R1441 P1446 V1447 I1448 L1449 V1450 L1454 D1455 V1456 S1457 ASP GLU LYS GLN ARG K1463 K1476 F1479 P1480
A1481 I1482 R1483 D1484 Y1485 H1486 F1487 V1488 N1489 A1490 T1491 R1501 L1509 N1510 F1511 K1512 Q1516 L1517 V1518 V1519 I1523 C1526 E1531 E1537 R1538 V1547 I1548 K1551 R1552 Q1555 L1556 V1557 Q1561 L1562 Q1563 L1564 N1567 V1573 H1574 F1575 L1576 V1581 L1582 L1583 H1584 F1585
Q1586 D1587 P1588 A1589 L1590 Q1591 Y1596 F1597 V1598 K1614 V1615 E1616 G1617 C1618 P1619 K1620 I1626 R1629 D1630 VAL GLU LYS PHE LEU SER LYS LYS ARG LYS PHE P1642 Y1645 Y1649 F1650 K1651 L1652 L1653 E1654 K1655 F1656 Q1657 I1658 A1659 LEU PRO ILE GLY GLU GLU TYR LEU L1668 S1672
E1689 I1692 Y1695 P1701 M1702 G1703 F1704 W1705 S1706 R1707 R1711 L1712 L1713 E1714 I1715 S1716 P1717 Y1718 M1719 L1720 SER GLY ARG GLU ARG A1726 P1729 W1734 R1735 Q1736 G1737 I1738 Y1739 L1740 N1741 W1742 L1749 E1753 L1763 K1764 S1769 V1781 D1782 H1783 I1784 L1787
W1791 F1792 P1793 G1794 L1795 L1796 I1800 C1801 G1802 E1803 K1810 L1813 F1816 H1822 Q1823 K1824 L1825 L1826 D1829 L1830 M1831 K1832 E1836 G1837 D1838 L1839 D1844 L1848 T1849 I1850 Q1854 L1859 R1866 L1870 L1875 E1876 F1877 A1880 L1885 G1886 D1887 G1888 S1889 F1890
V1893 Y1894 V1905 K1906 I1907 T1912 R1918 Q1919 V1923 H1926 L1927 H1928 S1931 L1932 L1935 I1940 R1941 P1942 R1943 M1944 L1945 V1946 D1956 R1957 L1958 L1959 T1967 R1968 T1969 R1973 H1977 D1980 Y1992 K1996 P1997 H1998 I2015 A2016 C2025 R2026 M2027 GLY
ILE LYS T2031 A2040 V2043 N2047 Y2050 Q2053 A2054 D2055 Y2064 T2068 T2069 G2070 I2073 E2082 E2085 Q2089 G2090 K2091 P2095 V2096 K2097 E2098 Y2099 A2102 P2105 M2106 L2110 R2122 V2128 F2129 D2130 I2131 A2135 E2136 L2137 V2138 C2139 L2140 T2141 R2142
L2146 P2147 I2151 V2152 E2153 H2159 H2160 N2161 S2162 R2163 C2171 G2172 H2173 T2174 D2175 R2176 G2177 Q2178 L2179 S2180 D2183 L2184 E2187 G2188 Y2189 V2194 A2195 D2196 S2197 L2204 V2205 H2206 L2207 E2210 K2211 E2212 S2213 V2216 Q2220 L2224 L2225 V2226 I2227 N2228 T2229 G2232 K2233


K2234 R2235 H2236 T2237 L2238 D2243 S2244 N2251 S2252 P2253 S2254 K2255 Q2256 S2257 K2258 Q2259 K2260 N2261 F2262 T2267 A2268 D2269 G2270 K2271 L2272 A2273 E2276 D2277 K2278 T2279 V2280 A2285 A2286 P2287 L2288 K2289 I2293 S2297 L2300 M2301 C2302 L2303 S2304 E2305 S2306 T2307 N2308 S2309 T2310 E2311 R2312 W2313
V2314 M2315 W2316 G2317 G2318 C2319 G2320 F2324 S2325 F2326 S2327 N2328 D2329 F2330 T2331 I2332 T2338 R2339 T2340 S2341 Q2342 L2343 F2344 S2345 Y2346 A2347 A2348 F2349 S2350 D2351 I2354 I2355 T2356 D2360 Y2364 K2367 S2370 V2375 W2376 D2377 K2378 K2382 L2383 C2384 D2388 C2389 V2390 H2391 R2394
E2395 V2396 T2397 V2398 K2399 E2400 N2401 K2402 E2403 S2404 K2405 H2406 K2407 M2408 S2409 Y2410 S2411 G2412 R2413 L2417 K2421 N2422 L2425 W2426 I2427 G2430 I2434 L2435 L2436 L2437 D2438 T2441 R2442 R2443 L2444 I2445 I2448 Y2449 Q2462 L2463 G2464 S2465 L2466 K2467 N2468 L2473 K2478 N2479 T2480 E2481
G2482 T2483 Q2484 K2485 Q2486 K2487 E2488 I2489 Q2490 W2496 D2497 I2498 N2499 L2500 P2501 V2504 L2507 H2510 R2514 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 | 231875 | 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 | 0.068 | Depositor |
| Minimum map value | -0.046 | Depositor |
| Average map value | 0.000 | Depositor |
| Map value standard deviation | 0.001 | Depositor |
| Recommended contour level | 0.009 | 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: ATP, GDP

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 | 0.21 | 0/14375 | 0.45 | 6/19443 (0.0%) |

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1171 | LEU | CA-C-N | -6.87 | 113.31 | 120.38 |
| 1 | A | 1171 | LEU | C-N-CA | -6.87 | 113.31 | 120.38 |
| 1 | A | 1342 | ASN | N-CA-C | 5.95 | 117.14 | 107.32 |
| 1 | A | 1372 | ASP | N-CA-C | 5.40 | 118.85 | 111.39 |
| 1 | A | 741 | GLY | N-CA-C | -5.40 | 106.25 | 112.73 |

There are no chirality outliers.

There are no planarity outliers.

## 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 | 14110 | 0 | 14392 | 377 | 0 |
| 2 | A | 28 | 0 | 12 | 0 | 0 |
| 3 | A | 31 | 0 | 12 | 2 | 0 |
| All | All | 14169 | 0 | 14416 | 377 | 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 13.

The worst 5 of 377 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:2106:MET:CB | 1:A:2137:LEU:CD1 | 1.77 | 1.59 |
| 1:A:2106:MET:HB3 | 1:A:2137:LEU:CD1 | 1.11 | 1.54 |
| 1:A:2136:GLU:CD | 1:A:2448:ILE:CG2 | 1.95 | 1.40 |
| 1:A:2106:MET:CB | 1:A:2137:LEU:HD12 | 1.35 | 1.39 |
| 1:A:2136:GLU:CD | 1:A:2448:ILE:HG23 | 1.51 | 1.32 |

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%) | 1561 (88%) | 216 (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 | 1575/2281 (69%) | 1575 (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. 5 of 21 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1871 | ASN |
| 1 | A | 2133 | ASN |
| 1 | A | 2462 | GLN |
| 1 | A | 2160 | HIS |
| 1 | A | 2053 | 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 | 1.00 | 1 (4%) | 30,47,47 | 1.12 | 2 (6%) |
| 3 | ATP | A | 2602 | - | 28,33,33 | 0.91 | 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 | - | - | 5/12/32/32 | 0/3/3/3 |
| 3 | ATP | A | 2602 | - | - | 1/18/38/38 | 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 | -2.42 | 1.34 | 1.37 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | A | 2602 | ATP | N3-C2-N1 | -3.59 | 123.79 | 128.67 |
| 2 | A | 2601 | GDP | C8-N7-C5 | 2.66 | 107.08 | 102.55 |
| 3 | A | 2602 | ATP | C4-C5-N7 | -2.55 | 106.65 | 109.34 |
| 2 | A | 2601 | GDP | C5-C6-N1 | 2.27 | 118.40 | 114.07 |

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 2601 | GDP | C5'-O5'-PA-O3A |
| 2 | A | 2601 | GDP | C5'-O5'-PA-O1A |
| 3 | A | 2602 | ATP | C5'-O5'-PA-O2A |
| 2 | A | 2601 | GDP | C3'-C4'-C5'-O5' |
| 2 | A | 2601 | GDP | O4'-C4'-C5'-O5' |

There are no ring outliers.

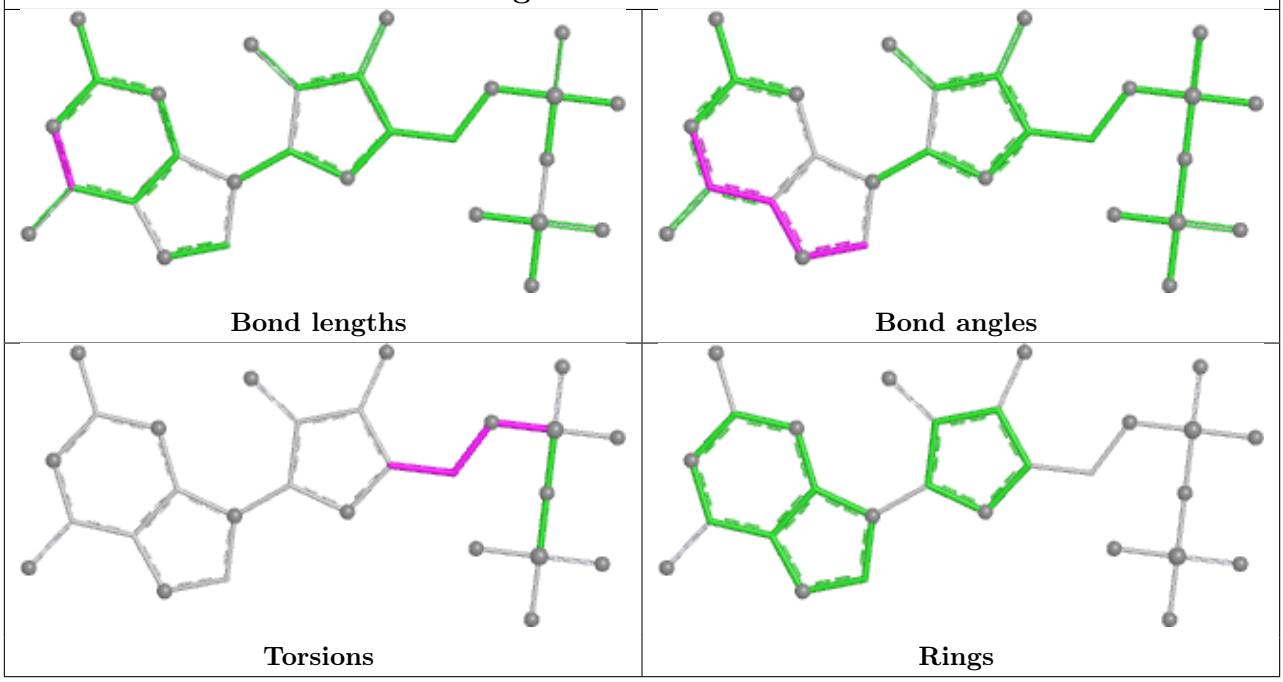
1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 2602 | ATP | 2 | 0 |

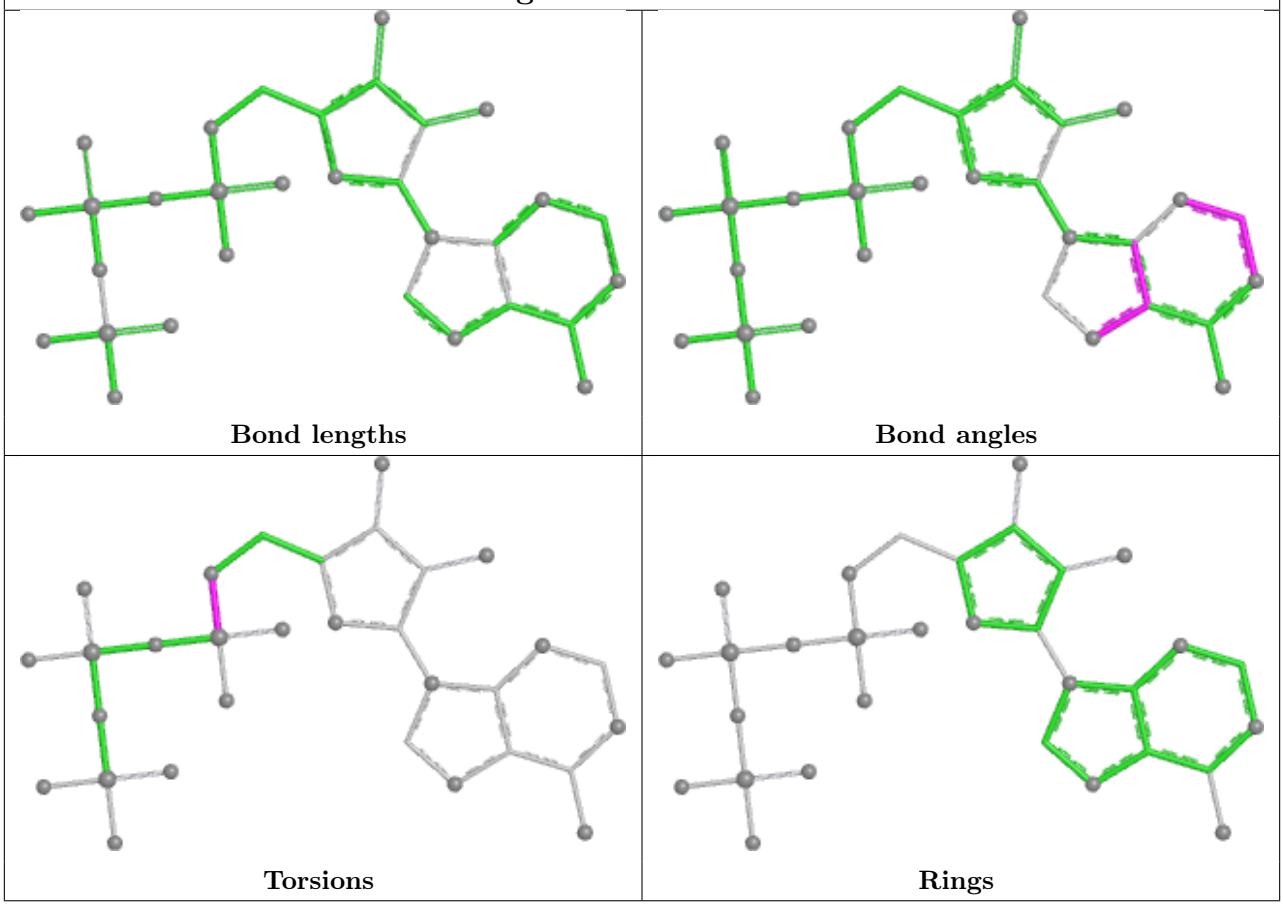
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

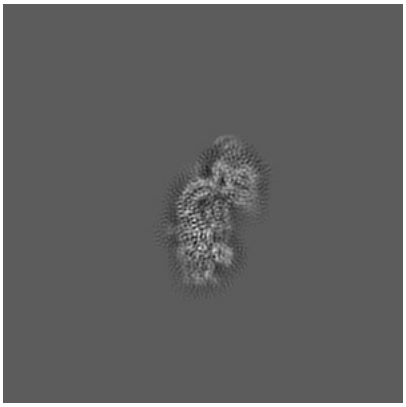
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23360. These allow visual inspection of the internal detail of the map and identification of artifacts.

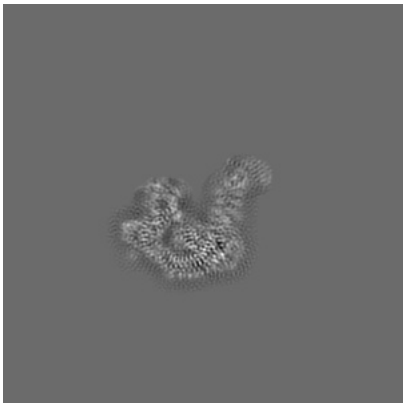
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

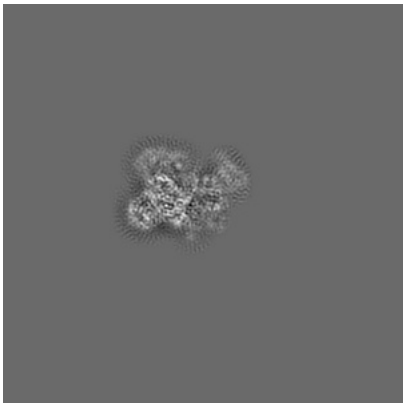
### 6.1.1 Primary map



X



Y

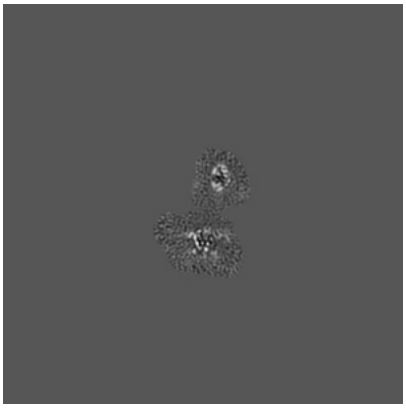


Z

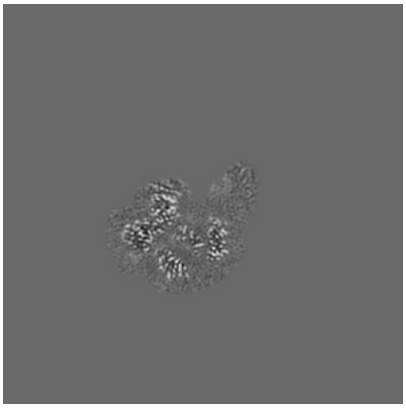
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

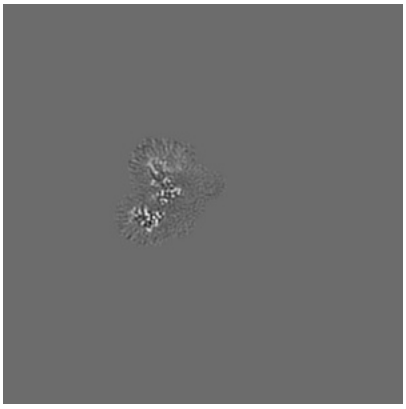
### 6.2.1 Primary map



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: 200

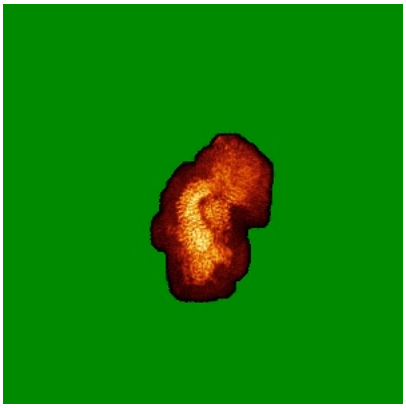
Y Index: 250

Z Index: 268

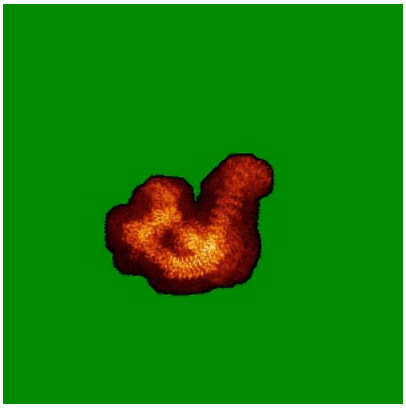
The images above show the largest variance slices of the map in three orthogonal directions.

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

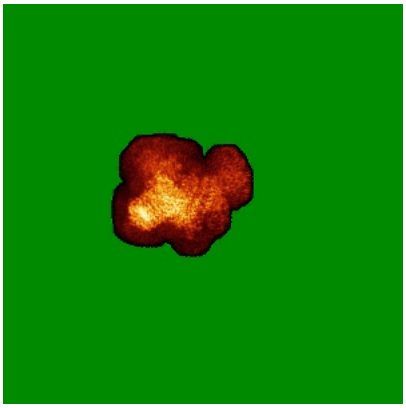
### 6.4.1 Primary map



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 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

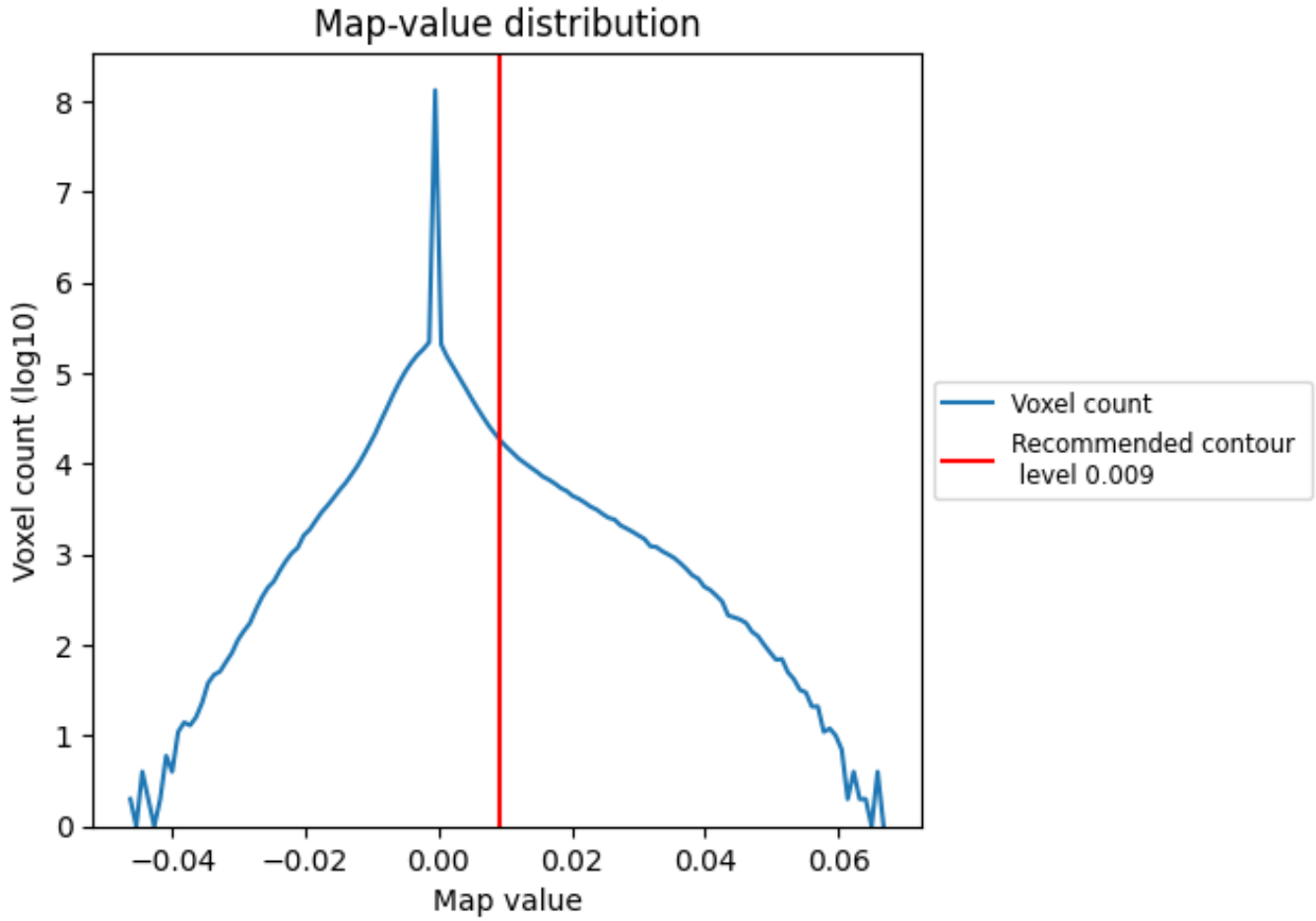
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

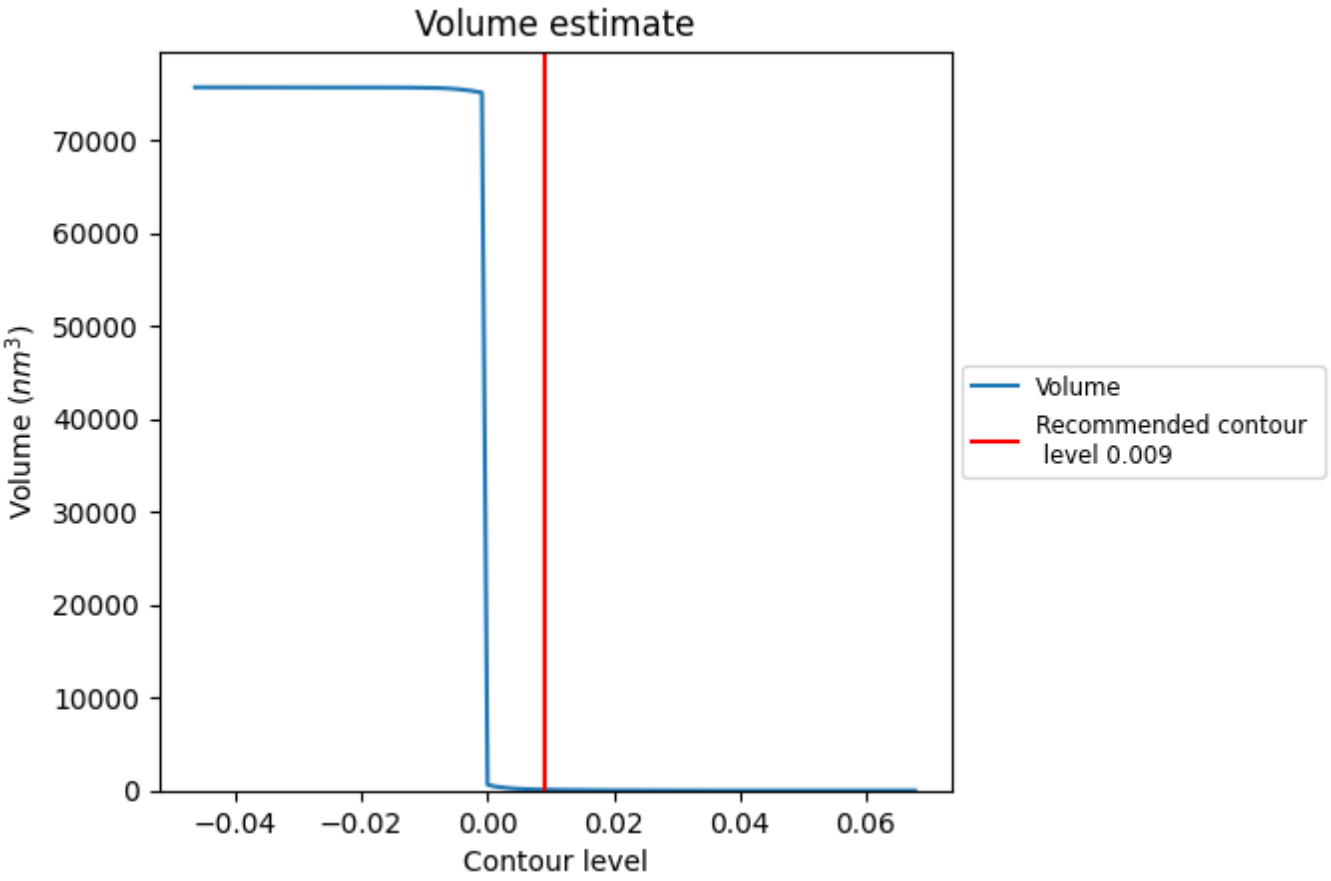
This section contains the results of statistical analysis of the map.

## 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.

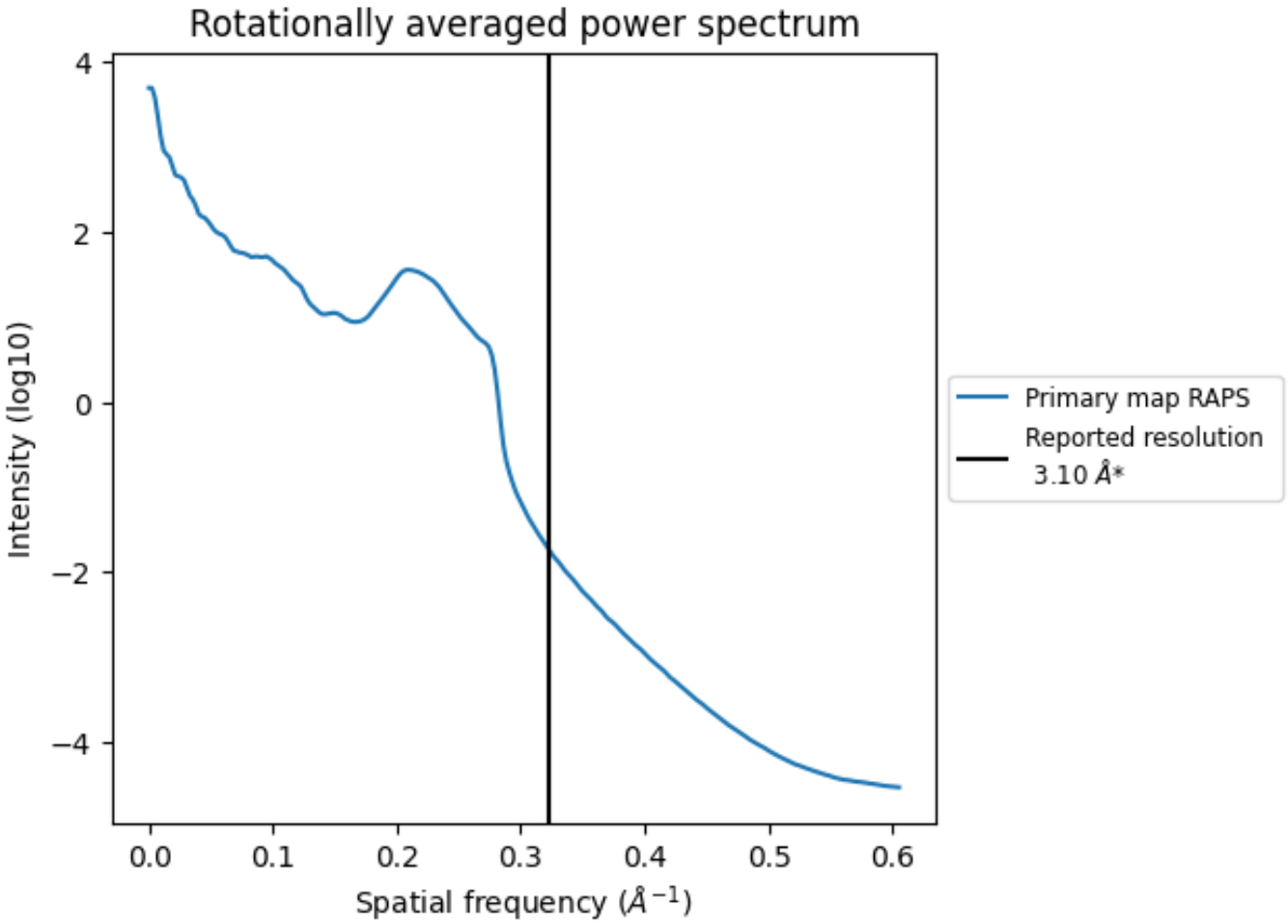
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 96 $nm^3$; this corresponds to an approximate mass of 86 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 0.323 Å$^{-1}$

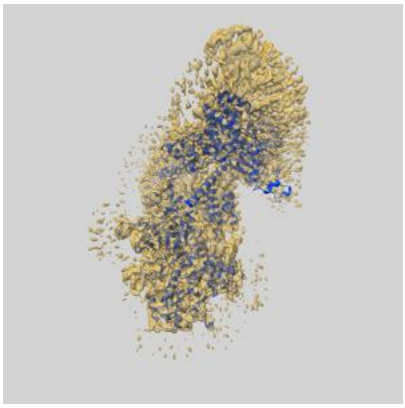
# 8 Fourier-Shell correlation (i)

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

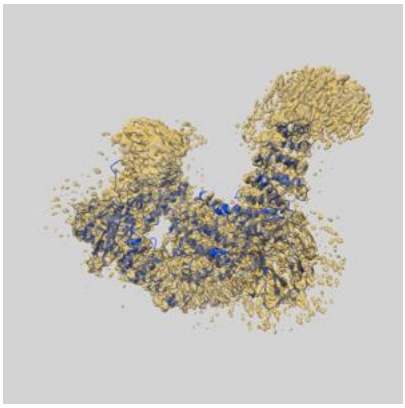
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23360 and PDB model 7LI4. Per-residue inclusion information can be found in section 3 on page 5.

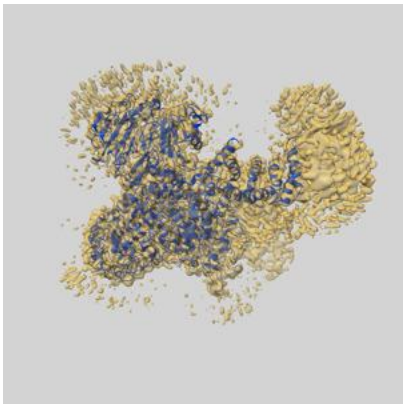
## 9.1 Map-model overlay



X



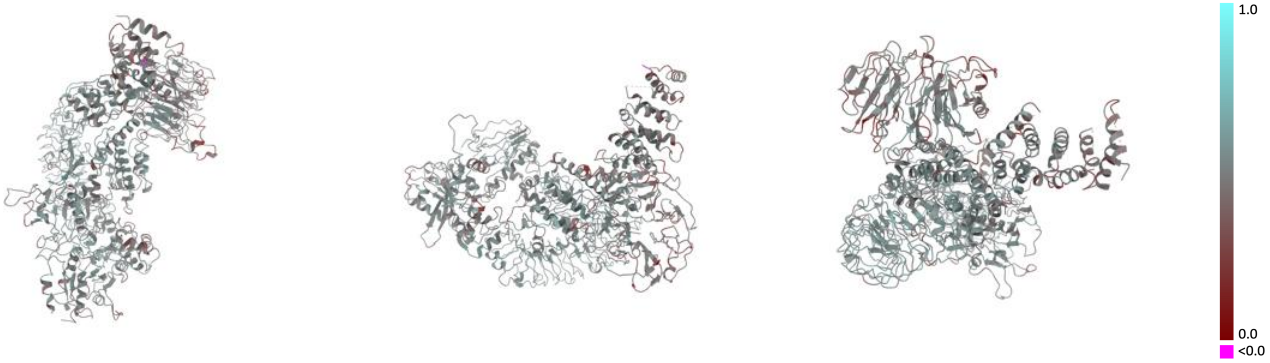
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

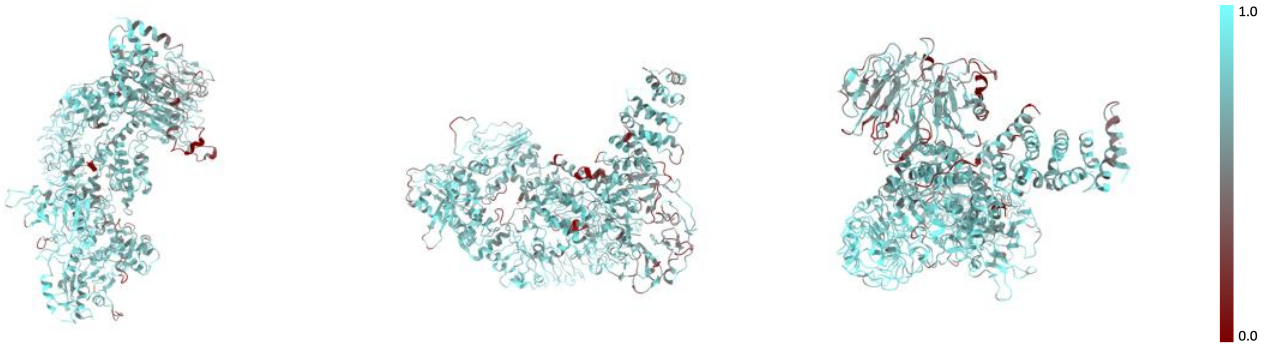
## 9.2 Q-score mapped to coordinate model (i)




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.

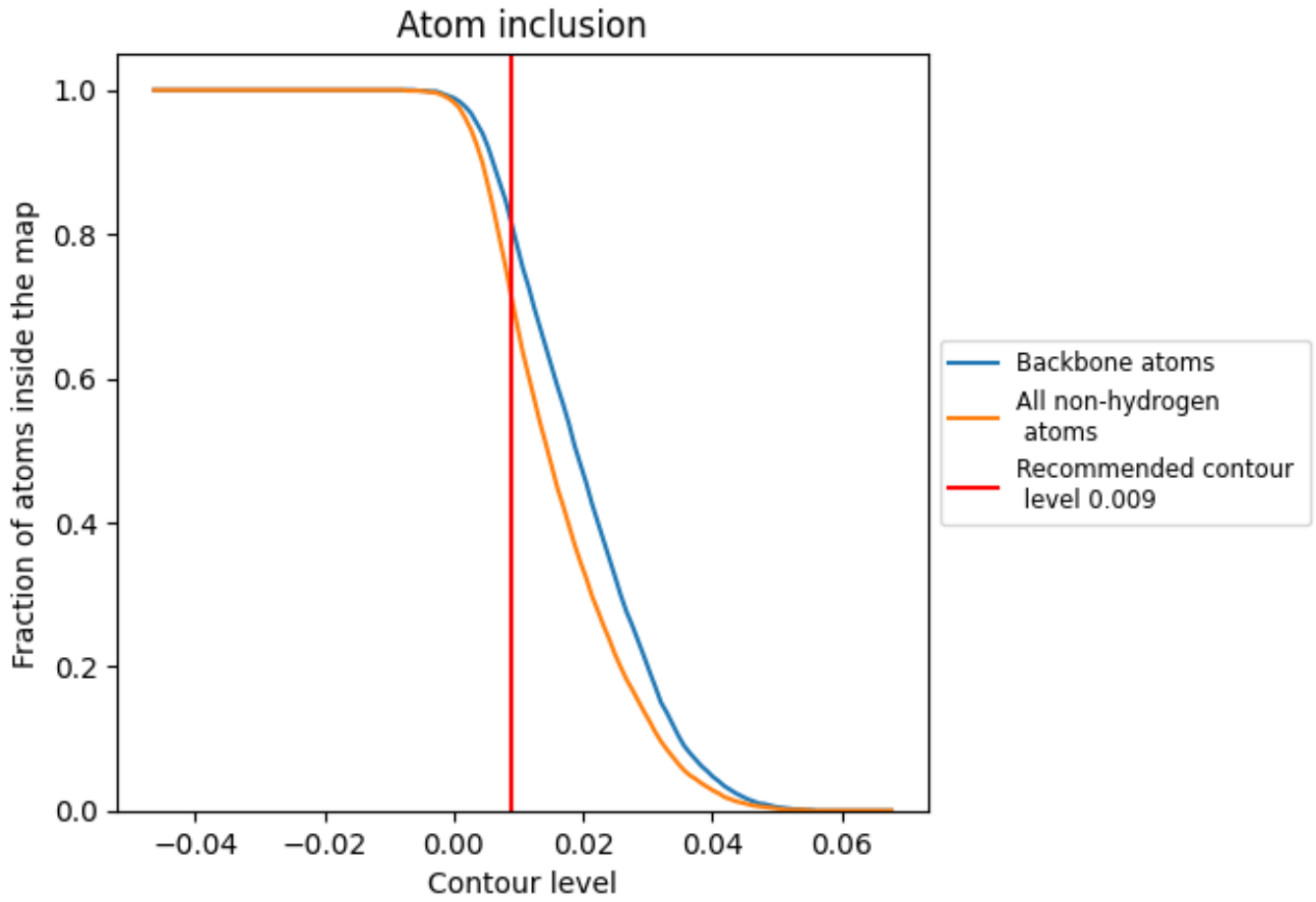
## 9.3 Atom inclusion mapped to coordinate model (i)




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 (0.009).

## 9.4 Atom inclusion (i)




At the recommended contour level, 81% of all backbone atoms, 71% 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 (0.009) and Q-score for the entire model and for each chain.


| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.7100 | 0.4910 |
| A | 0.7100 | 0.4910 |