Full wwPDB EM Validation Report ⓘ

Jan 24, 2024 – 04:26 PM EST

PDB ID	:	8U8A
EMDB ID	:	EMD-42019
Title	:	Cryo-EM structure of LRRK2 bound to type II inhibitor ponatinib
Authors	:	Zhu, H.; Sun, J.
Deposited on	:	2023-09-16
Resolution	:	3.40 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:

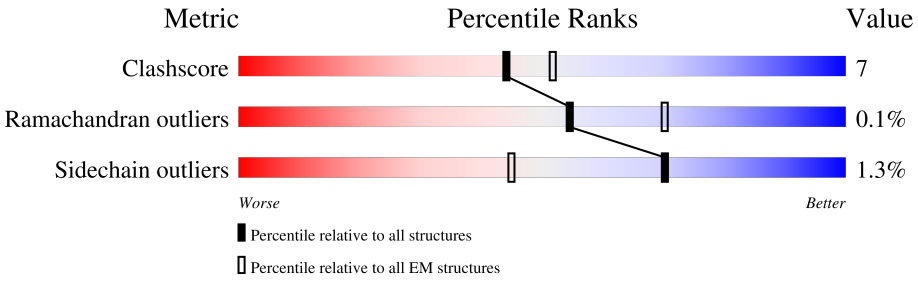
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	B	2527	23% 56% 11% 33%
1	C	2527	22% 57% 11% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24428 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.

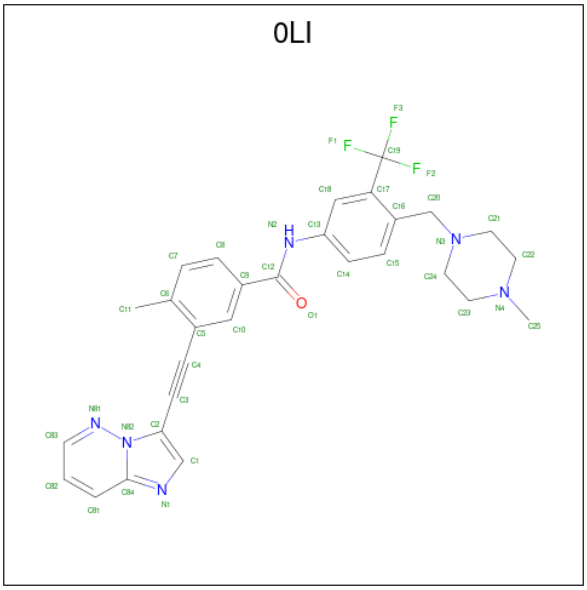
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1705	Total	C	N	O	S	0	0
			12147	7832	2080	2163	72		
1	C	1705	Total	C	N	O	S	0	0
			12147	7832	2080	2163	72		

There are 6 discrepancies between the modelled and reference sequences:

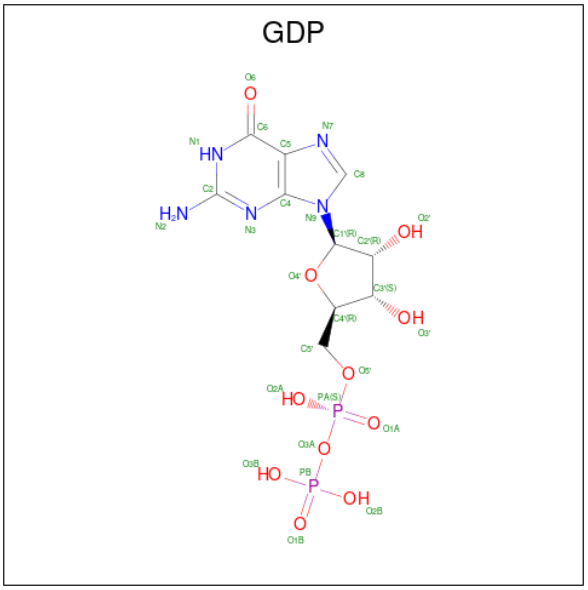
Chain	Residue	Modelled	Actual	Comment	Reference
B	50	HIS	ARG	conflict	UNP Q5S007
B	1647	THR	SER	conflict	UNP Q5S007
B	2397	THR	MET	conflict	UNP Q5S007
C	50	HIS	ARG	conflict	UNP Q5S007
C	1647	THR	SER	conflict	UNP Q5S007
C	2397	THR	MET	conflict	UNP Q5S007

- Molecule 2 is 3-(imidazo[1,2-b]pyridazin-3-ylethynyl)-4-methyl-N-{4-[(4-methylpiperazin-1-yl)methyl]-3-(trifluoromethyl)phenyl}benzam ide (three-letter code: 0LI) (formula: $C_{29}H_{27}F_3N_6O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	F	N	O	0
			39	29	3	6	1	
2	C	1	Total	C	F	N	O	0
			39	29	3	6	1	

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



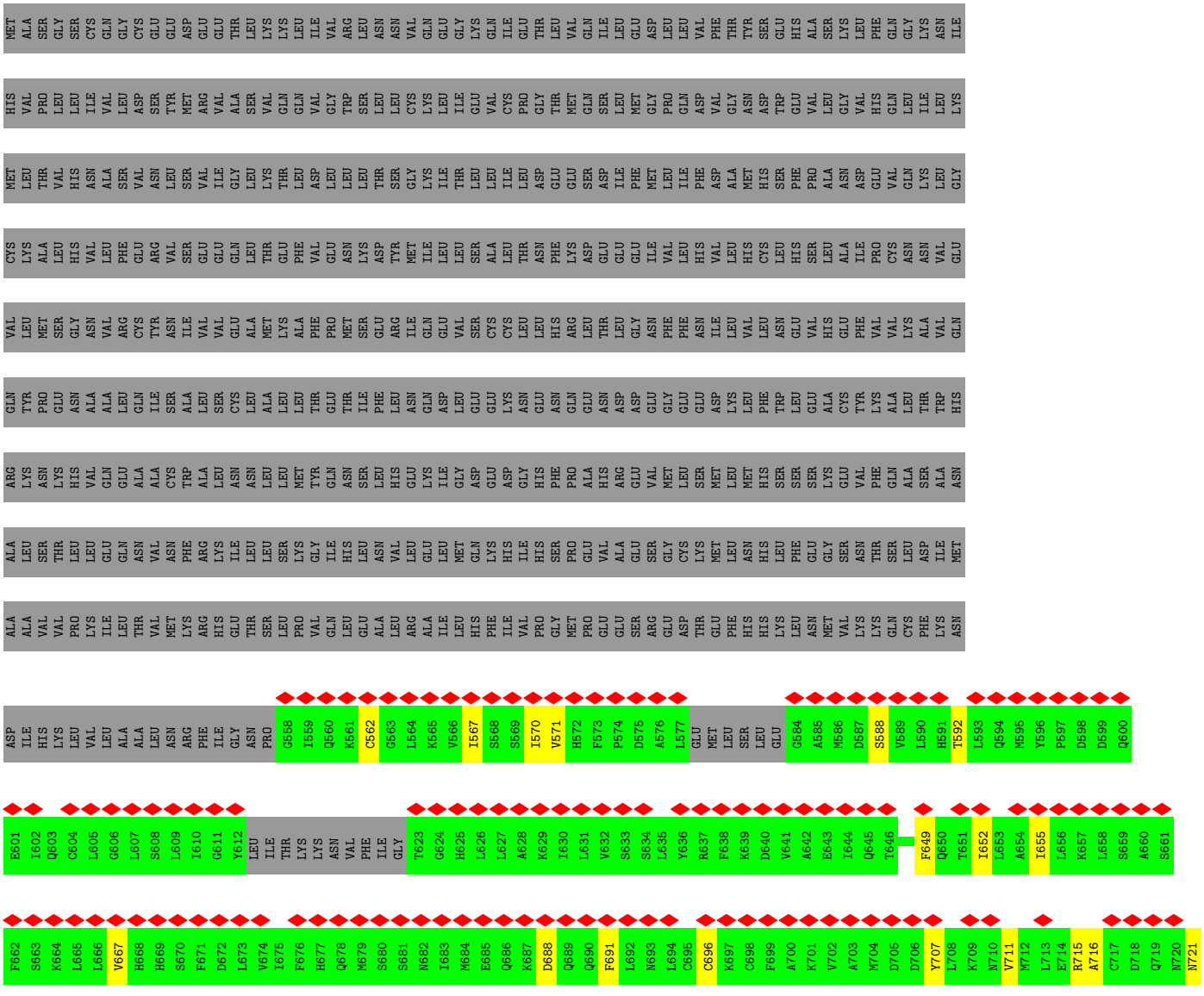
Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
3	C	1	Total	C	N	O	P	0
			28	10	5	11	2	

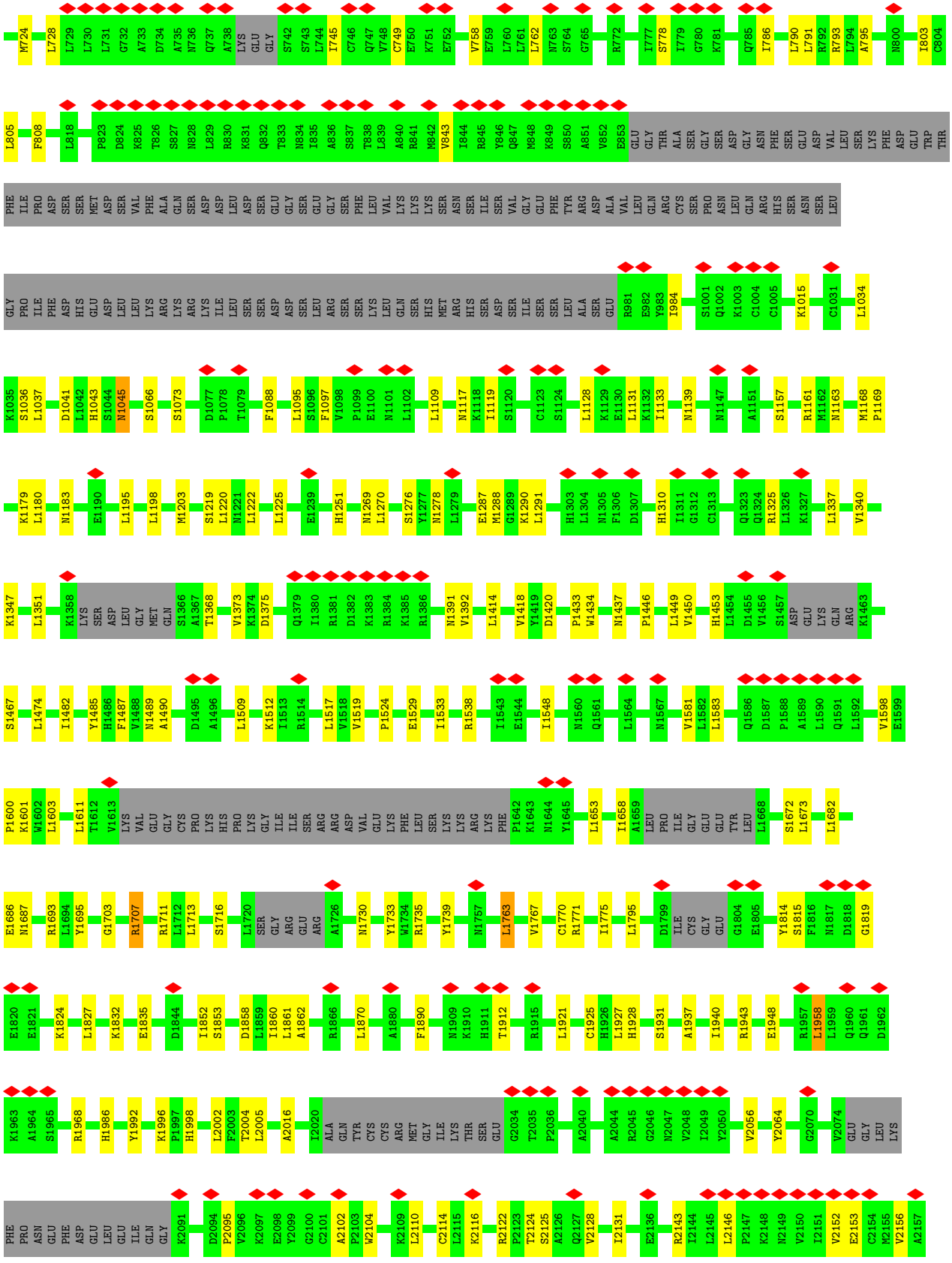
3 Residue-property plots (i)

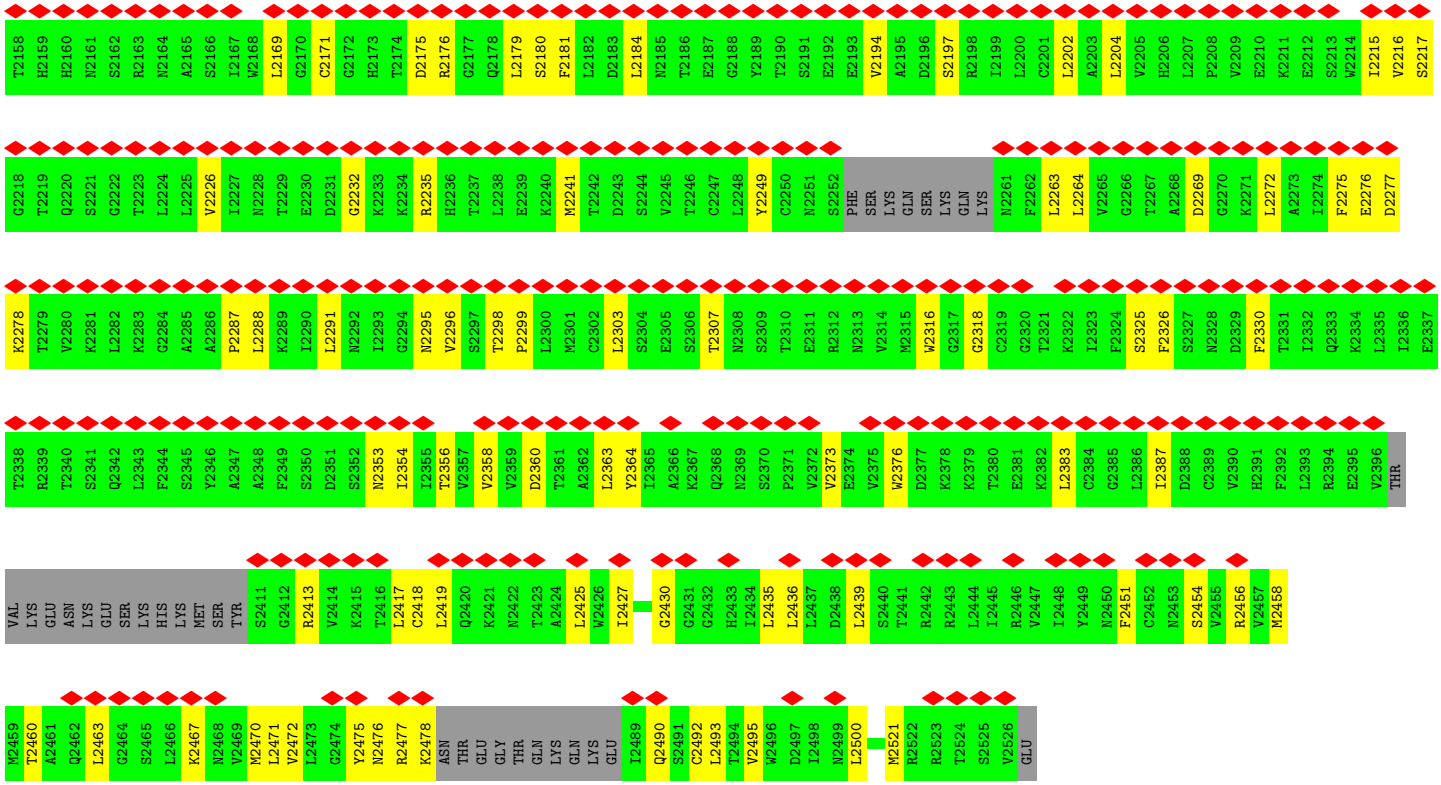
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain B:

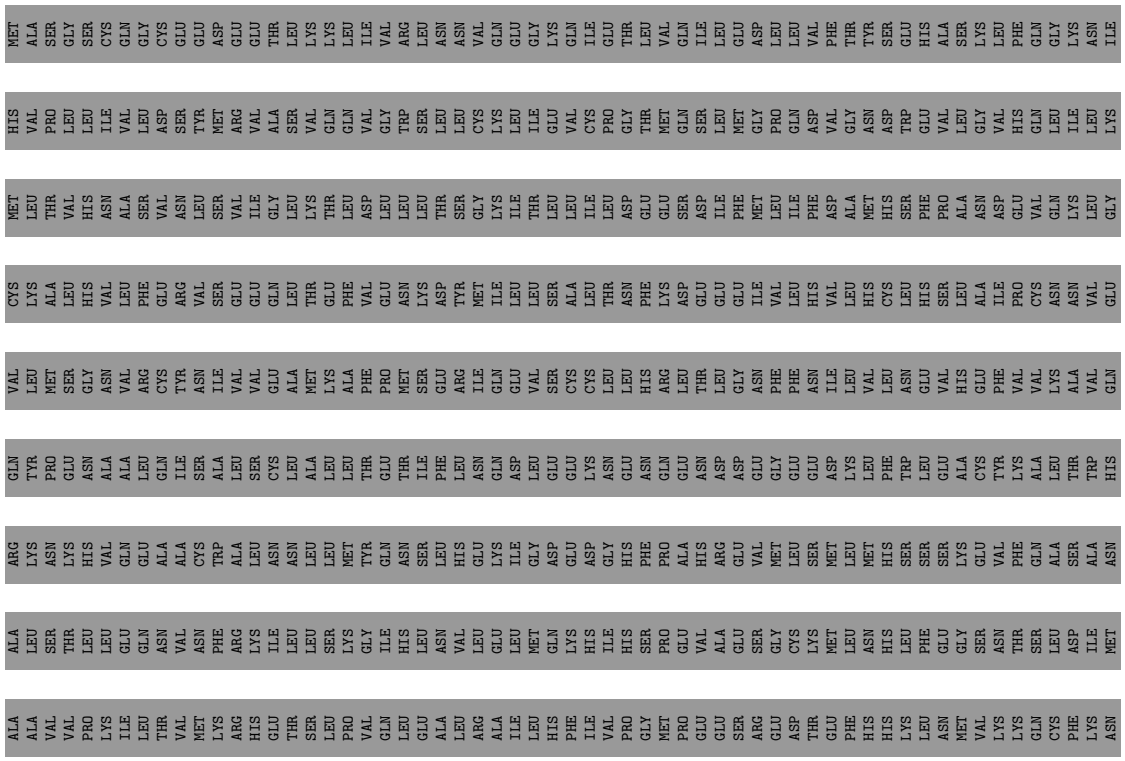


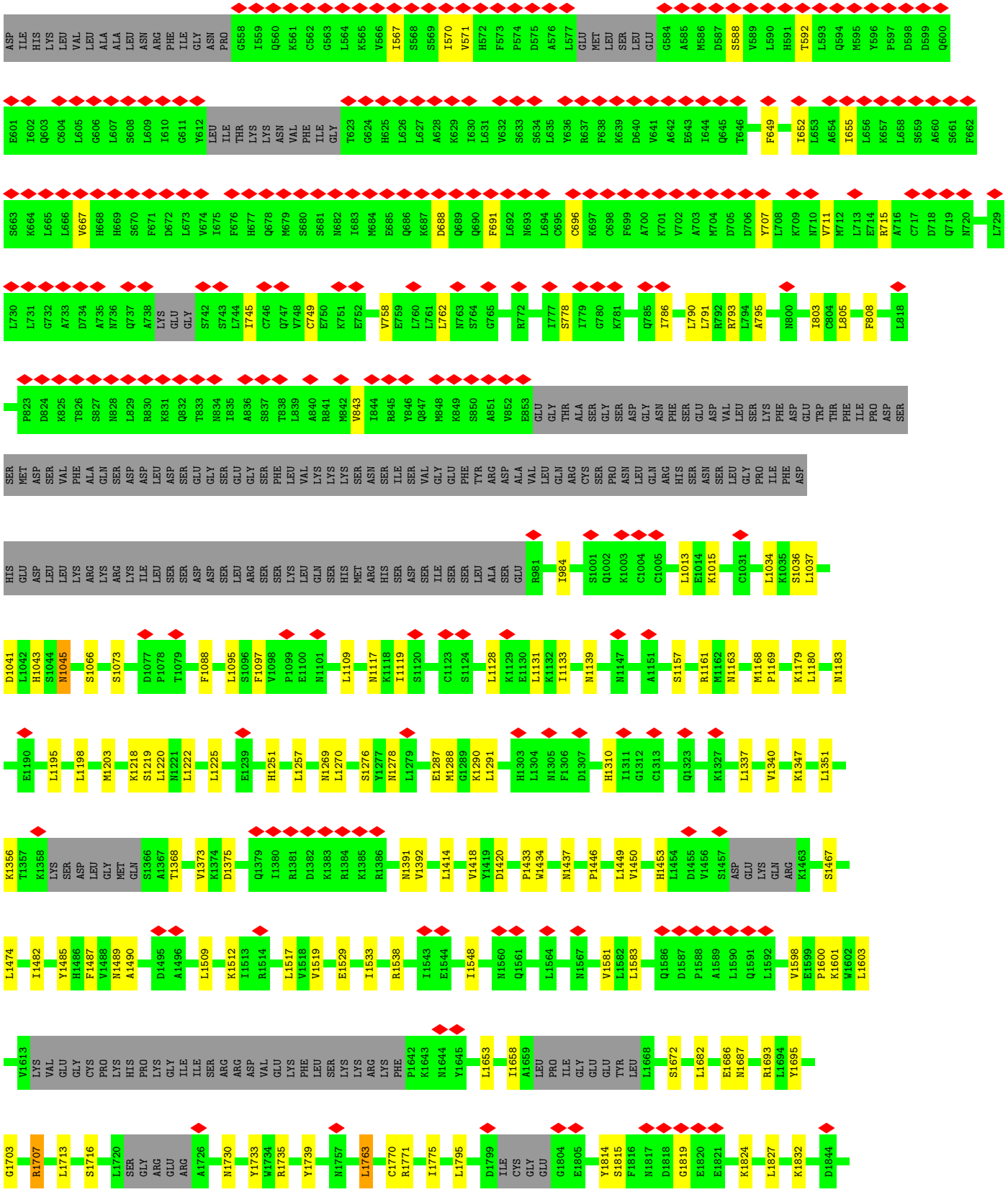

M724 L728 L729 L730 L731 G732 A733 D734 A735 N736 Q737 A738 LYS GLU GLY S742 S743 L744 I745 C746 Q747 V748 C749 E750 K751 E752 V758 E759 L760 L761 L762 N763 S764 G765 R772 I777 S778 I779 G780 K781 Q785 I786 L790 L791 R792 R793 L794 A795 N800 I803 C804
L805 F808 L818 F823 D824 K825 T826 S827 N828 L829 R830 K831 Q832 T833 N834 I835 A836 S837 T838 L839 A840 R841 M842 V843 I844 R845 Y846 Q847 M848 K849 S850 A851 V852 E853 GLU 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 SER GLU LEU ARG SER SER PHE SER LYS LEU GLN SER HIS MET ARG HIS SER ASP SER ILE SER SER LEU ALA SER GLU R981 E982 Y983 I984 S1001 Q1002 K1003 C1004 C1005 K1015 C1031 L1034
K1035 S1036 L1037 D1041 L1042 H1043 S1044 N1045 S1066 S1073 D1077 P1078 T1079 F1088 L1095 S1096 F1097 V1098 P1099 E1100 N1101 L1102 L1109 N1117 K1118 I1119 S1120 C1123 S1124 L1128 K1129 E1130 L1131 K1132 I1133 N1139 N1147 A1151 S1157 R1161 M1162 N1163 M1168 P1169
K1179 L1180 N1183 E1190 L1195 L1198 M1203 S1219 L1220 N1221 L1222 L1225 E1239 H1251 N1269 L1270 S1276 Y1277 N1278 L1279 E1287 M1288 G1289 K1290 L1291 H1303 L1304 N1305 F1306 D1307 H1310 I1311 G1312 C1313 Q1323 Q1324 R1325 L1326 K1327 L1337 V1340
K1347 L1351 K1358 LYS SER ASP LEU GLY MET GLN S1366 A1367 T1368 V1373 K1374 D1375 Q1379 I1380 R1381 D1382 K1383 R1384 K1385 R1386 N1391 V1392 L1414 V1418 Y1419 D1420 P1433 W1434 N1437 P1446 L1449 V1450 H1453 L1454 D1455 V1456 S1457 ASP GLU LYS GLN ARG K1463
S1467 L1474 I1482 Y1485 H1486 F1487 V1488 N1489 A1490 D1495 A1496 L1509 K1512 I1513 R1514 L1517 V1518 V1519 P1524 E1529 I1533 R1538 I1543 E1544 I1548 N1560 Q1561 L1564 N1567 V1581 L1582 L1583 Q1586 D1587 P1588 A1589 L1590 Q1591 L1592 V1598 E1599
P1600 K1601 W1602 L1603 L1611 T1612 Y1613 LYS VAL GLU GLY CYS PRO LYS HIS PRO LYS GLY ILE ILE SER ARG ARG ASP VAL GLU GLY LYS PHE LEU SER LYS LYS ARG LYS PHE P1642 K1643 N1644 Y1645 L1653 I1658 A1659 LEU PRO ILE GLY GLU GLU TYR LEU L1668 S1672 L1673 L1682
E1686 N1687 R1693 L1694 Y1695 G1703 R1707 R1711 L1712 L1713 S1716 L1720 SER GLY ARG GLU ARG A1726 N1730 Y1733 W1734 R1735 Y1739 N1757 L1763 V1767 C1770 R1771 I1775 L1795 D1799 ILE CYS GLY GLU G1804 E1805 Y1814 S1815 F1816 N1817 D1818 G1819
E1820 E1821 K1824 L1827 K1832 E1835 D1844 I1852 S1853 D1858 L1859 I1860 L1861 A1862 R1866 L1870 A1880 F1890 N1909 K1910 H1911 T1912 R1915 L1921 C1925 H1926 L1927 H1928 S1931 A1937 I1940 R1943 E1948 R1957 L1958 L1959 Q1960 Q1961 D1962
K1963 A1964 S1965 R1968 H1986 Y1992 K1996 P1997 H1998 L2002 F2003 T2004 L2005 A2016 I2020 ALA GLN TYR CYS CYS ARG MET GLY ILE LYS THR SER GLU G2034 T2035 P2036 A2040 A2044 R2045 G2046 N2047 V2048 I2049 Y2050 V2056 Y2064 G2070 V2074 GLU GLY LEU LYS
PHE PRO ASN GLU PHE ASP GLU LEU GLU ILE GLN GLY K2091 D2094 P2095 V2096 K2097 E2098 Y2099 G2100 C2101 A2102 P2103 W2104 K2109 L2110 C2114 L2115 K2116 R2122 P2123 T2124 S2125 A2126 Q2127 V2128 I2131 E2136 R2143 I2144 L2145 L2146 P2147 K2148 N2149 V2150 I2151 V2152 E2153 C2154 M2155 V2156 A2157

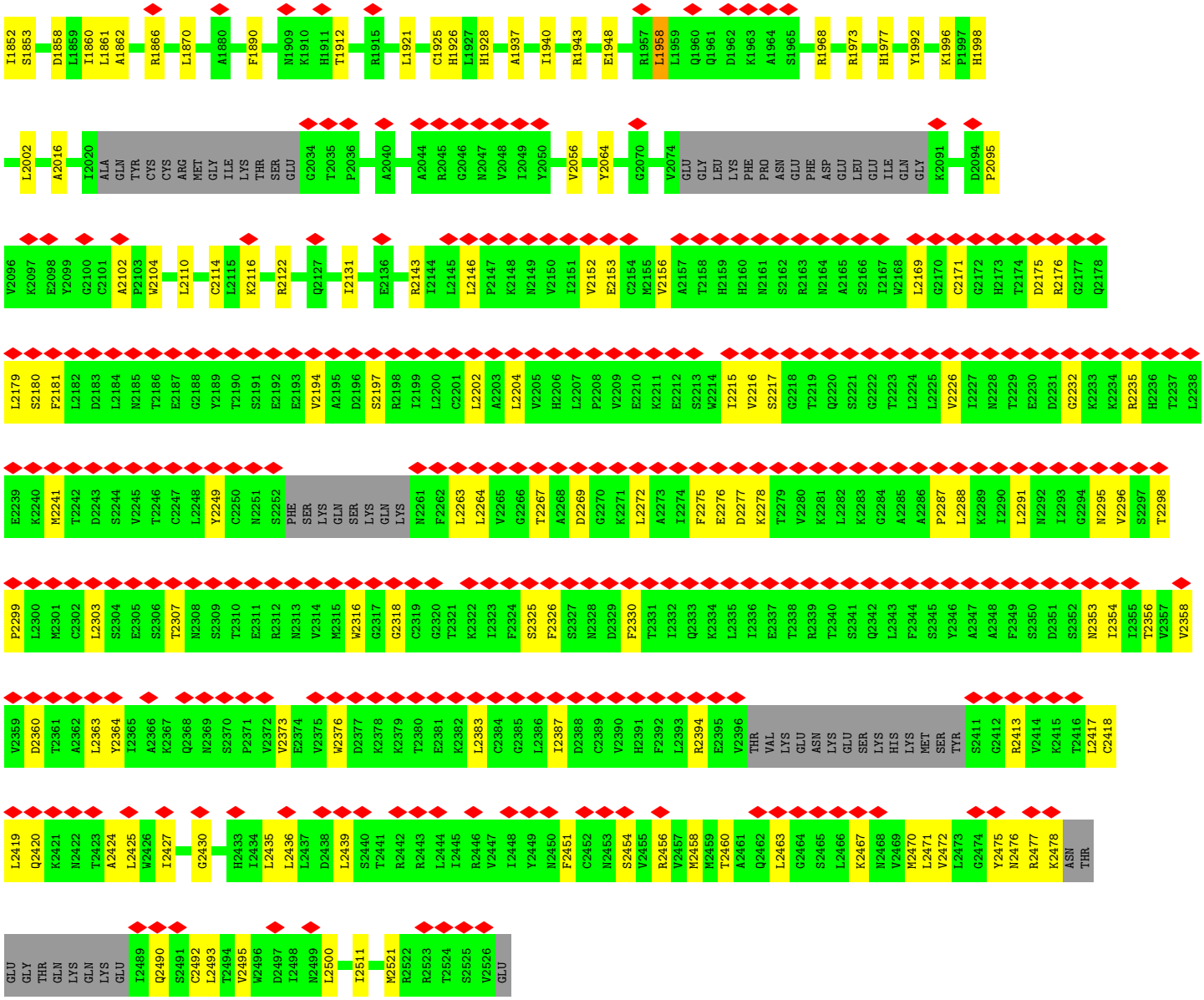


• Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

Chain C:




ASP ILE HIS LYS LEU VAL LEU ALA ALA LEU ASN ARG PHE ILE GLY ASN PRO G558 I559 Q560 K561 C562 G563 L564 K565 V566 I567 S568 S569 I570 V571 H572 F573 P574 D575 A576 L577 GLU MET LEU SER LEU GLU G584 A585 M586 D587 S588 V589 L590 H591 T592 L593 Q594 M595 Y596 P597 D598 D599 Q600
E601 I602 Q603 C604 L605 G606 L607 S608 L609 I610 G611 Y612 LEU ILE THR LYS LYS ASN VAL PHE ILE GLY T623 G624 H625 L626 L627 A628 K629 I630 L631 V632 S633 S634 L635 Y636 R637 F638 K639 D640 V641 A642 E643 I644 Q645 T646 F649 I652 L653 A654 I655 L656 K657 L658 S659 A660 S661 F662
S663 K664 L665 L666 V667 H668 H669 S670 F671 D672 L673 V674 I675 F676 H677 Q678 M679 S680 S681 N682 I683 M684 E685 Q686 K687 D688 Q689 Q690 F691 L692 N693 L694 C695 C696 K697 C698 F699 A700 K701 V702 A703 M704 D705 D706 Y707 L708 K709 N710 V711 M712 L713 E714 R715 A716 C717 D718 Q719 N720 L729
L730 L731 G732 A733 D734 A735 N736 Q737 A738 LYS GLU GLY S742 S743 L744 I745 C746 Q747 V748 C749 E750 K751 E752 V758 E759 L760 L761 L762 N763 S764 G765 R772 I777 S778 I779 G780 K781 Q785 I786 L790 L791 R792 R793 L794 A795 N800 I803 C804 L805 F808 L818
P823 D824 K825 T826 S827 N828 L829 R830 K831 Q832 T833 N834 I835 A836 S837 T838 L839 A840 R841 M842 V843 I844 R845 Y846 Q847 M848 K849 S850 A851 V852 E853 GLU 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 I984 S1001 Q1002 K1003 C1004 C1005 L1013 E1014 K1015 C1031 L1034 K1035 S1036 L1037
D1041 L1042 H1043 S1044 N1045 S1066 S1073 D1077 P1078 T1079 F1088 L1095 S1096 F1097 V1098 P1099 E1100 N1101 L1109 N1117 K1118 I1119 S1120 C1123 S1124 L1128 K1129 E1130 L1131 K1132 I1133 N1139 N1147 A1151 S1157 R1161 M1162 N1163 M1168 P1169 K1179 L1180 N1183
E1190 L1195 L1198 M1203 K1218 S1219 L1220 N1221 L1222 L1225 E1239 H1251 L1257 N1269 L1270 S1276 Y1277 N1278 L1279 E1287 M1288 G1289 K1290 L1291 H1303 L1304 N1305 F1306 D1307 H1310 I1311 G1312 C1313 Q1323 K1327 L1337 V1340 K1347 L1351
K1356 T1357 K1358 LYS SER ASP LEU GLY MET GLN S1366 A1367 T1368 V1373 K1374 D1375 Q1379 I1380 R1381 D1382 K1383 R1384 K1385 R1386 N1391 V1392 L1414 V1418 Y1419 D1420 P1433 W1434 N1437 P1446 L1449 V1450 H1453 L1454 D1455 V1456 S1457 ASP GLU LYS GLN ARG K1463 S1467
L1474 I1482 Y1485 H1486 F1487 V1488 N1489 A1490 D1495 A1496 L1509 K1512 I1513 R1514 L1517 V1518 V1519 E1529 I1533 R1538 L1543 E1544 I1548 N1560 Q1561 L1564 N1567 V1581 L1582 L1583 Q1586 D1587 P1588 A1589 L1590 Q1591 L1592 V1598 E1599 P1600 K1601 W1602 L1603
V1613 LYS VAL GLU GLY CYS PRO LYS HIS PRO LYS GLY ILE ILE SER ARG ARG ASP VAL GLU LYS PHE LEU SER LYS LYS ARG LYS PHE P1642 K1643 N1644 Y1645 L1653 I1658 A1659 LEU PRO ILE GLY GLU GLU TYR LEU L1668 S1672 L1682 E1686 N1687 R1693 L1694 Y1695
G1703 R1707 L1713 S1716 L1720 SER GLY ARG GLU ARG A1726 N1730 Y1733 W1734 R1735 Y1739 N1757 L1763 C1770 R1771 I1775 L1795 D1799 ILE CYS GLY GLU G1804 E1805 Y1814 S1815 F1816 N1817 D1818 G1819 E1820 E1821 K1824 L1827 K1832 D1844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L2002 A2016 I2020 ALA GLN TYR CYS CYS ARG MET GLY ILE LYS THR SER GLU G2034 T2035 P2036 A2040 A2044 R2045 G2046 N2047 V2048 I2049 Y2050 V2056 Y2064 G2070 V2074 GLU GLY LEU LYS PHE PRO ASN GLU PHE ASP GLU LEU GLU ILE GLN GLY K2091 D2094 P2095
V2096 K2097 E2098 Y2099 G2100 C2101 A2102 P2103 W2104 L2110 C2114 L2115 K2116 R2122 Q2127 I2131 E2136 R2143 I2144 L2145 L2146 P2147 K2148 N2149 V2150 I2151 V2152 E2153 C2154 M2155 V2156 A2157 T2158 H2159 H2160 N2161 S2162 R2163 N2164 A2165 S2166 I2167 W2168 L2169 G2170 C2171 G2172 H2173 T2174 D2175 R2176 G2177 Q2178
L2179 S2180 F2181 L2182 D2183 L2184 N2185 T2186 E2187 G2188 Y2189 T2190 S2191 E2192 E2193 V2194 A2195 D2196 S2197 R2198 I2199 L2200 C2201 L2202 A2203 L2204 V2205 H2206 L2207 P2208 V2209 E2210 K2211 E2212 S2213 W2214 I2215 V2216 S2217 G2218 T2219 Q2220 S2221 G2222 T2223 L2224 L2225 V2226 I2227 N2228 T2229 E2230 D2231 G2232 K2233 K2234 R2235 H2236 T2237 L2238
E2239 K2240 M2241 T2242 D2243 S2244 V2245 T2246 C2247 L2248 Y2249 C2250 N2251 S2252 PHE SER LYS GLN SER LYS GLN LYS 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 G2317 G2318 C2319 G2320 T2321 K2322 I2323 F2324 S2325 F2326 S2327 N2328 D2329 F2330 T2331 I2332 Q2333 K2334 L2335 I2336 E2337 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 N2369 S2370 P2371 V2372 V2373 E2374 V2375 W2376 D2377 K2378 K2379 T2380 E2381 K2382 L2383 C2384 G2385 L2386 I2387 D2388 C2389 V2390 H2391 F2392 L2393 R2394 E2395 V2396 THR VAL LYS GLU ASN LYS GLU SER LYS HIS LYS MET SER TYR S2411 G2412 R2413 V2414 K2415 T2416 L2417 C2418
L2419 Q2420 K2421 N2422 T2423 A2424 L2425 W2426 I2427 G2430 H2433 I2434 L2435 L2436 L2437 D2438 L2439 S2440 T2441 R2442 R2443 L2444 I2445 R2446 V2447 I2448 Y2449 N2450 F2451 C2452 N2453 S2454 V2455 R2456 V2457 M2458 W2459 T2460 A2461 Q2462 L2463 G2464 S2465 L2466 K2467 N2468 V2469 M2470 L2471 V2472 L2473 G2474 Y2475 N2476 R2477 K2478 ASN THR
GLU GLY THR GLN LYS GLN LYS GLU I2489 Q2490 S2491 C2492 L2493 T2494 V2495 W2496 D2497 I2498 N2499 L2500 I2511 M2521 R2522 R2523 T2524 S2525 V2526 GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	68.11	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.068	Depositor
Minimum map value	-2.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	498.04803, 498.04803, 498.04803	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.297, 1.297, 1.297	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, 0LI

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	B	0.39	1/12370 (0.0%)	0.55	2/16909 (0.0%)
1	C	0.38	0/12370	0.54	1/16909 (0.0%)
All	All	0.39	1/24740 (0.0%)	0.54	3/33818 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1767	VAL	CB-CG1	-5.15	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1763	LEU	CA-CB-CG	5.33	127.57	115.30
1	B	1763	LEU	CA-CB-CG	5.33	127.57	115.30
1	B	1767	VAL	CG1-CB-CG2	-5.07	102.79	110.90

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	B	12147	0	11499	167	0
1	C	12147	0	11499	163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	39	0	27	2	0
2	C	39	0	27	2	0
3	B	28	0	12	1	0
3	C	28	0	12	1	0
All	All	24428	0	23076	328	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 7.

All (328) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1912:THR:O	1:B:1943:ARG:NH1	2.20	0.73
1:C:2116:LYS:O	1:C:2122:ARG:NH1	2.21	0.73
1:B:2116:LYS:O	1:B:2122:ARG:NH1	2.21	0.73
1:B:2110:LEU:HD13	1:B:2131:ILE:HD11	1.70	0.72
1:C:2110:LEU:HD13	1:C:2131:ILE:HD11	1.71	0.72
1:C:1912:THR:O	1:C:1943:ARG:NH1	2.19	0.71
1:C:2146:LEU:O	1:C:2490:GLN:NE2	2.24	0.71
1:B:2146:LEU:O	1:B:2490:GLN:NE2	2.24	0.70
1:B:2318:GLY:HA3	1:B:2354:ILE:HG21	1.75	0.68
1:C:1161:ARG:O	1:C:1163:ASN:ND2	2.27	0.68
1:B:1161:ARG:O	1:B:1163:ASN:ND2	2.27	0.68
1:C:2318:GLY:HA3	1:C:2354:ILE:HG21	1.75	0.67
1:B:2156:VAL:HG12	1:B:2202:LEU:HD13	1.76	0.67
1:C:2156:VAL:HG12	1:C:2202:LEU:HD13	1.76	0.67
1:B:2427:ILE:HB	1:B:2435:LEU:HB2	1.78	0.66
1:C:2427:ILE:HB	1:C:2435:LEU:HB2	1.78	0.66
1:C:688:ASP:HB3	1:C:691:PHE:HB3	1.80	0.64
1:B:1928:HIS:HB3	1:B:2521:MET:HG2	1.80	0.64
1:B:1730:ASN:ND2	1:C:1739:TYR:OH	2.31	0.64
1:B:1739:TYR:OH	1:C:1730:ASN:ND2	2.32	0.63
1:C:1034:LEU:HD13	1:C:1037:LEU:HD11	1.80	0.63
1:B:1368:THR:OG1	3:B:2602:GDP:O3B	2.17	0.63
1:B:2356:THR:HG21	1:B:2417:LEU:HB2	1.80	0.63
1:B:1034:LEU:HD13	1:B:1037:LEU:HD11	1.80	0.63
1:C:2356:THR:HG21	1:C:2417:LEU:HB2	1.80	0.62
1:B:688:ASP:HB3	1:B:691:PHE:HB3	1.83	0.61
1:B:1583:LEU:HG	1:B:1600:PRO:HB3	1.83	0.61
1:C:1653:LEU:HG	1:C:1658:ILE:HB	1.82	0.61
1:B:2413:ARG:O	1:B:2430:GLY:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1928:HIS:HB3	1:C:2521:MET:HG2	1.81	0.61
1:C:2413:ARG:O	1:C:2430:GLY:N	2.33	0.61
1:C:1583:LEU:HG	1:C:1600:PRO:HB3	1.83	0.60
1:B:1815:SER:HB3	1:B:1824:LYS:HG2	1.84	0.59
1:C:1368:THR:OG1	3:C:2602:GDP:O3B	2.17	0.59
1:C:1548:ILE:HD12	1:C:1598:VAL:HG21	1.85	0.59
1:B:1653:LEU:HG	1:B:1658:ILE:HB	1.83	0.59
1:C:1815:SER:HB3	1:C:1824:LYS:HG2	1.84	0.59
1:C:1222:LEU:HD22	1:C:1225:LEU:HD11	1.85	0.58
1:B:1128:LEU:HD12	1:B:1131:LEU:HD13	1.85	0.58
1:B:1222:LEU:HD22	1:B:1225:LEU:HD11	1.85	0.58
1:B:2232:GLY:O	1:B:2235:ARG:NH1	2.36	0.58
1:C:2232:GLY:O	1:C:2235:ARG:NH1	2.36	0.58
1:C:1128:LEU:HD12	1:C:1131:LEU:HD13	1.84	0.57
1:C:2152:VAL:HA	1:C:2171:CYS:HB3	1.86	0.57
1:B:2152:VAL:HA	1:B:2171:CYS:HB3	1.85	0.56
1:B:1548:ILE:HD12	1:B:1598:VAL:HG21	1.86	0.56
1:B:1420:ASP:OD1	1:B:1453:HIS:ND1	2.39	0.56
1:B:1512:LYS:HA	1:B:1517:LEU:H	1.70	0.56
1:B:2477:ARG:NH1	1:B:2478:LYS:O	2.39	0.56
1:C:1420:ASP:OD1	1:C:1453:HIS:ND1	2.39	0.56
1:C:1351:LEU:HD21	1:C:1392:VAL:HG21	1.88	0.56
1:C:2476:ASN:HB3	1:C:2490:GLN:HB3	1.87	0.56
1:C:2263:LEU:HB3	1:C:2275:PHE:HB2	1.88	0.55
1:C:2477:ARG:NH1	1:C:2478:LYS:O	2.39	0.55
1:B:1351:LEU:HD21	1:B:1392:VAL:HG21	1.88	0.55
1:B:2476:ASN:N	1:B:2490:GLN:O	2.40	0.55
1:C:2476:ASN:N	1:C:2490:GLN:O	2.40	0.55
1:B:2263:LEU:HB3	1:B:2275:PHE:HB2	1.88	0.55
1:B:2476:ASN:HB3	1:B:2490:GLN:HB3	1.87	0.55
1:B:1041:ASP:OD1	1:B:1043:HIS:ND1	2.39	0.55
1:C:1041:ASP:OD1	1:C:1043:HIS:ND1	2.39	0.55
1:C:1861:LEU:HG	1:C:1940:ILE:HD11	1.89	0.54
1:B:2179:LEU:HD23	1:B:2194:VAL:H	1.72	0.54
1:B:2463:LEU:HD12	1:B:2467:LYS:HE2	1.90	0.54
1:B:1687:ASN:HB2	1:B:1819:GLY:HA2	1.90	0.54
1:B:1861:LEU:HG	1:B:1940:ILE:HD11	1.89	0.54
1:C:1687:ASN:HB2	1:C:1819:GLY:HA2	1.90	0.54
1:C:1512:LYS:HA	1:C:1517:LEU:H	1.71	0.53
1:C:2463:LEU:HD12	1:C:2467:LYS:HE2	1.90	0.53
1:C:1034:LEU:HB3	1:C:1037:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:VAL:HG11	1:B:786:ILE:HD12	1.90	0.53
1:B:1034:LEU:HB3	1:B:1037:LEU:HG	1.90	0.53
1:B:1814:TYR:HE2	1:B:1827:LEU:HB2	1.74	0.53
1:C:1814:TYR:HE2	1:C:1827:LEU:HB2	1.74	0.53
1:C:2179:LEU:HD23	1:C:2194:VAL:H	1.72	0.53
1:B:1695:TYR:HB2	1:B:1763:LEU:HB3	1.92	0.52
1:C:1973:ARG:O	1:C:1977:HIS:ND1	2.26	0.52
1:B:1921:LEU:O	1:B:1925:CYS:HB2	2.10	0.52
1:B:1509:LEU:HA	1:B:1519:VAL:HG21	1.92	0.52
1:B:1703:GLY:O	1:B:1707:ARG:HD2	2.10	0.51
1:C:1695:TYR:HB2	1:C:1763:LEU:HB3	1.92	0.51
1:B:2276:GLU:HG2	1:B:2288:LEU:HD23	1.93	0.51
1:C:2358:VAL:HB	1:C:2364:TYR:HB2	1.92	0.51
1:C:758:VAL:HG11	1:C:786:ILE:HD12	1.92	0.51
1:C:2307:THR:HG21	1:C:2419:LEU:HD22	1.92	0.51
1:B:1414:LEU:HG	1:B:1446:PRO:HG2	1.92	0.51
1:B:1716:SER:O	1:B:1716:SER:OG	2.29	0.51
1:B:1996:LYS:HE3	1:B:1998:HIS:HB3	1.93	0.51
1:C:2276:GLU:HG2	1:C:2288:LEU:HD23	1.93	0.51
1:C:1414:LEU:HG	1:C:1446:PRO:HG2	1.92	0.51
1:C:1509:LEU:HA	1:C:1519:VAL:HG21	1.91	0.51
1:B:1375:ASP:N	1:B:1375:ASP:OD1	2.43	0.51
1:B:2307:THR:HG21	1:B:2419:LEU:HD22	1.92	0.51
1:B:2425:LEU:HB2	1:B:2439:LEU:HD21	1.93	0.51
1:B:2358:VAL:HB	1:B:2364:TYR:HB2	1.92	0.50
1:C:1827:LEU:HD23	1:C:1832:LYS:HZ3	1.76	0.50
1:C:1703:GLY:O	1:C:1707:ARG:HD2	2.11	0.50
1:C:1716:SER:O	1:C:1716:SER:OG	2.29	0.50
1:C:2420:GLN:HE21	1:C:2424:ALA:HB3	1.75	0.50
1:B:652:ILE:HA	1:B:655:ILE:HG22	1.93	0.50
1:B:1133:ILE:HG12	1:B:1157:SER:HB3	1.94	0.50
1:B:2436:LEU:HD21	1:B:2500:LEU:HD22	1.94	0.50
1:C:1996:LYS:HE3	1:C:1998:HIS:HB3	1.93	0.50
1:C:2425:LEU:HB2	1:C:2439:LEU:HD21	1.93	0.50
1:C:2454:SER:HB2	1:C:2475:TYR:HB2	1.93	0.50
1:B:1036:SER:O	1:B:1036:SER:OG	2.26	0.49
1:B:2418:CYS:SG	1:B:2419:LEU:N	2.85	0.49
1:C:1133:ILE:HG12	1:C:1157:SER:HB3	1.94	0.49
1:C:2176:ARG:HA	1:C:2197:SER:HA	1.94	0.49
1:C:2418:CYS:SG	1:C:2419:LEU:N	2.86	0.49
1:C:2436:LEU:HD21	1:C:2500:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2216:VAL:HG12	1:B:2226:VAL:HG22	1.95	0.49
1:C:2373:VAL:HB	1:C:2387:ILE:HB	1.94	0.49
1:B:1711:ARG:HE	1:B:1711:ARG:HB2	1.46	0.49
1:C:1036:SER:O	1:C:1036:SER:OG	2.26	0.49
1:B:696:CYS:HB3	1:B:843:VAL:HG12	1.95	0.48
1:B:2152:VAL:HG11	1:B:2169:LEU:HD23	1.95	0.48
1:C:762:LEU:HD11	1:C:790:LEU:HD23	1.95	0.48
1:C:1270:LEU:HD12	1:C:1291:LEU:HD13	1.94	0.48
1:C:2152:VAL:HG11	1:C:2169:LEU:HD23	1.95	0.48
1:B:1270:LEU:HD12	1:B:1291:LEU:HD13	1.94	0.48
1:B:2176:ARG:HA	1:B:2197:SER:HA	1.94	0.48
1:B:2373:VAL:HB	1:B:2387:ILE:HB	1.94	0.48
1:B:2454:SER:HB2	1:B:2475:TYR:HB2	1.95	0.48
1:C:696:CYS:HB3	1:C:843:VAL:HG12	1.96	0.48
1:C:2216:VAL:HG12	1:C:2226:VAL:HG22	1.94	0.48
1:B:1713:LEU:HD12	1:B:1733:TYR:OH	2.14	0.48
1:C:1375:ASP:OD1	1:C:1375:ASP:N	2.43	0.47
1:B:1948:GLU:O	2:B:2601:0LI:H1	2.14	0.47
1:B:1968:ARG:HD2	1:B:2104:TRP:CE2	2.49	0.47
1:C:1713:LEU:HD12	1:C:1733:TYR:OH	2.14	0.47
1:B:762:LEU:HD11	1:B:790:LEU:HD23	1.96	0.47
1:B:1583:LEU:HD12	1:B:1603:LEU:HD23	1.97	0.47
1:B:1287:GLU:O	1:B:1290:LYS:NZ	2.45	0.47
1:C:1073:SER:HB3	1:C:1097:PHE:HD2	1.79	0.47
1:C:1095:LEU:HB2	1:C:1117:ASN:HD22	1.80	0.47
1:B:1073:SER:HB3	1:B:1097:PHE:HD2	1.79	0.47
1:B:1827:LEU:HD23	1:B:1832:LYS:HZ3	1.80	0.47
1:B:1931:SER:O	1:B:1931:SER:OG	2.33	0.47
1:B:1986:HIS:HD1	1:B:2125:SER:HG	1.62	0.47
1:C:2269:ASP:HA	1:C:2296:VAL:HA	1.97	0.47
1:B:1337:LEU:O	1:B:1392:VAL:HA	2.15	0.46
1:B:1968:ARG:NH2	1:B:2102:ALA:HB3	2.30	0.46
1:C:667:VAL:O	1:C:715:ARG:NH1	2.48	0.46
1:C:2417:LEU:HG	1:C:2427:ILE:HD13	1.98	0.46
1:C:1583:LEU:HD12	1:C:1603:LEU:HD23	1.97	0.46
1:C:1968:ARG:NH2	1:C:2102:ALA:HB3	2.30	0.46
1:B:1095:LEU:HB2	1:B:1117:ASN:HD22	1.80	0.46
1:B:1375:ASP:HA	1:B:1391:ASN:HA	1.98	0.46
1:B:1693:ARG:NH2	1:B:1858:ASP:OD1	2.48	0.46
1:B:2460:THR:HG22	1:B:2470:MET:HE2	1.96	0.46
1:C:795:ALA:HB2	1:C:808:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1890:PHE:CD2	2:C:2601:0LI:H83	2.51	0.46
1:B:1890:PHE:CD2	2:B:2601:0LI:H83	2.50	0.46
1:B:2269:ASP:HA	1:B:2296:VAL:HA	1.97	0.46
1:B:2417:LEU:HG	1:B:2427:ILE:HD13	1.98	0.46
1:C:1449:LEU:HD12	1:C:1482:ILE:HG21	1.98	0.46
1:C:1693:ARG:NH2	1:C:1858:ASP:OD1	2.48	0.46
1:C:2471:LEU:HG	1:C:2495:VAL:HG22	1.98	0.46
1:B:1832:LYS:HA	1:B:1835:GLU:HB2	1.98	0.46
1:B:1852:ILE:HB	1:B:1860:ILE:HD12	1.98	0.45
1:B:567:ILE:O	1:B:571:VAL:HG13	2.16	0.45
1:B:791:LEU:HD22	1:B:805:LEU:HD21	1.99	0.45
1:B:1771:ARG:O	1:B:1775:ILE:HG13	2.15	0.45
1:B:2471:LEU:HG	1:B:2495:VAL:HG22	1.98	0.45
1:C:1337:LEU:O	1:C:1392:VAL:HA	2.15	0.45
1:B:1449:LEU:HD12	1:B:1482:ILE:HG21	1.98	0.45
1:B:1672:SER:H	1:B:1735:ARG:HH12	1.64	0.45
1:B:2143:ARG:NH2	1:B:2451:PHE:O	2.49	0.45
1:C:791:LEU:HD22	1:C:805:LEU:HD21	1.99	0.45
1:C:1968:ARG:HD2	1:C:2104:TRP:CE2	2.51	0.45
1:B:795:ALA:HB2	1:B:808:PHE:HE2	1.81	0.45
1:B:1538:ARG:NH2	1:B:1581:VAL:O	2.49	0.45
1:C:2143:ARG:NH2	1:C:2451:PHE:O	2.50	0.45
1:C:1489:ASN:OD1	1:C:1490:ALA:N	2.50	0.45
1:C:1474:LEU:HD23	1:C:1474:LEU:HA	1.78	0.45
1:C:1852:ILE:HB	1:C:1860:ILE:HD12	1.98	0.45
1:C:2460:THR:HG22	1:C:2470:MET:HE2	1.98	0.45
1:B:1860:ILE:O	1:B:1862:ALA:N	2.50	0.45
1:C:1866:ARG:NH1	1:C:1925:CYS:SG	2.90	0.45
1:B:2204:LEU:HD12	1:B:2215:ILE:HG13	1.99	0.45
1:C:1948:GLU:O	2:C:2601:0LI:H1	2.16	0.45
1:C:2299:PRO:HD2	1:C:2353:ASN:ND2	2.32	0.45
1:B:707:TYR:O	1:B:711:VAL:HG23	2.17	0.44
1:B:1276:SER:O	1:B:1278:ASN:ND2	2.50	0.44
1:C:649:PHE:HA	1:C:652:ILE:HG12	1.99	0.44
1:C:1375:ASP:HA	1:C:1391:ASN:HA	1.98	0.44
1:B:2299:PRO:HD2	1:B:2353:ASN:ND2	2.32	0.44
1:C:1045:ASN:N	1:C:1045:ASN:HD22	2.15	0.44
1:B:1489:ASN:OD1	1:B:1490:ALA:N	2.50	0.44
1:B:2153:GLU:HG2	1:B:2456:ARG:HH21	1.83	0.44
1:C:2202:LEU:HD23	1:C:2217:SER:HB3	1.99	0.44
1:B:2249:TYR:HD2	1:B:2264:LEU:HD12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1276:SER:O	1:C:1278:ASN:ND2	2.50	0.44
1:C:1538:ARG:NH2	1:C:1581:VAL:O	2.49	0.44
1:C:1219:SER:OG	1:C:1220:LEU:N	2.50	0.44
1:C:2267:THR:OG1	1:C:2269:ASP:OD1	2.23	0.44
1:B:1673:LEU:HD23	1:B:1673:LEU:HA	1.84	0.44
1:B:1795:LEU:HD23	1:B:1795:LEU:HA	1.81	0.44
1:B:2064:TYR:CE2	1:B:2095:PRO:HG3	2.53	0.44
1:C:1672:SER:H	1:C:1735:ARG:HH12	1.64	0.44
1:C:1795:LEU:HD23	1:C:1795:LEU:HA	1.81	0.44
1:C:1467:SER:HB2	1:C:1487:PHE:HZ	1.83	0.44
1:C:2204:LEU:HD12	1:C:2215:ILE:HG13	1.99	0.44
1:C:2249:TYR:HD2	1:C:2264:LEU:HD12	1.83	0.44
1:B:1992:TYR:OH	1:B:2016:ALA:O	2.36	0.43
1:C:1015:LYS:HE3	1:C:1015:LYS:HB2	1.70	0.43
1:C:1771:ARG:O	1:C:1775:ILE:HG13	2.18	0.43
1:C:2326:PHE:HD2	1:C:2330:PHE:HA	1.83	0.43
1:B:749:CYS:SG	1:B:778:SER:HB2	2.59	0.43
1:B:2180:SER:OG	1:B:2181:PHE:N	2.51	0.43
1:B:2202:LEU:HD23	1:B:2217:SER:HB3	1.99	0.43
1:C:1433:PRO:O	1:C:1437:ASN:ND2	2.51	0.43
1:C:1921:LEU:O	1:C:1925:CYS:HB2	2.18	0.43
1:C:2180:SER:OG	1:C:2181:PHE:N	2.50	0.43
1:C:2264:LEU:HD13	1:C:2303:LEU:HD22	2.00	0.43
1:B:588:SER:O	1:B:592:THR:HG23	2.17	0.43
1:B:649:PHE:HA	1:B:652:ILE:HG12	2.01	0.43
1:B:667:VAL:O	1:B:715:ARG:NH1	2.52	0.43
1:C:1373:VAL:HB	1:C:1601:LYS:HB3	2.00	0.43
1:C:1968:ARG:HH21	1:C:2102:ALA:HB3	1.82	0.43
1:B:567:ILE:HA	1:B:570:ILE:HG22	1.99	0.43
1:B:2326:PHE:HD2	1:B:2330:PHE:HA	1.83	0.43
1:C:567:ILE:O	1:C:571:VAL:HG13	2.18	0.43
1:C:1682:LEU:HD23	1:C:1682:LEU:HA	1.83	0.43
1:C:2153:GLU:HG2	1:C:2456:ARG:HH21	1.83	0.43
1:B:1015:LYS:HB2	1:B:1015:LYS:HE3	1.69	0.43
1:B:2363:LEU:N	1:B:2376:TRP:O	2.51	0.43
1:C:1218:LYS:HB3	1:C:1218:LYS:HE2	1.70	0.43
1:B:1045:ASN:HD22	1:B:1045:ASN:N	2.15	0.43
1:B:1219:SER:OG	1:B:1220:LEU:N	2.50	0.43
1:C:749:CYS:SG	1:C:778:SER:HB2	2.59	0.43
1:C:1287:GLU:O	1:C:1290:LYS:NZ	2.45	0.43
1:C:2458:MET:HG3	1:C:2472:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2264:LEU:HD13	1:B:2303:LEU:HD22	2.00	0.43
1:C:1860:ILE:O	1:C:1862:ALA:N	2.50	0.43
1:C:2269:ASP:OD1	1:C:2269:ASP:N	2.47	0.43
1:B:1373:VAL:HB	1:B:1601:LYS:HB3	2.01	0.43
1:B:745:ILE:HD11	1:B:758:VAL:HG23	2.01	0.42
1:B:2307:THR:OG1	1:B:2360:ASP:OD1	2.36	0.42
1:B:2458:MET:HG3	1:B:2472:VAL:HG22	2.01	0.42
1:C:2272:LEU:N	1:C:2291:LEU:O	2.47	0.42
1:C:2316:TRP:CD2	1:C:2325:SER:HB3	2.54	0.42
1:B:2316:TRP:CD2	1:B:2325:SER:HB3	2.54	0.42
1:C:1161:ARG:HH21	1:C:1179:LYS:HD2	1.84	0.42
1:C:2471:LEU:HD23	1:C:2493:LEU:HD21	2.01	0.42
1:C:2511:ILE:HD12	1:C:2511:ILE:HA	1.93	0.42
1:B:724:MET:O	1:B:728:LEU:HG	2.20	0.42
1:B:1117:ASN:OD1	1:B:1117:ASN:N	2.50	0.42
1:B:1161:ARG:HH21	1:B:1179:LYS:HD2	1.83	0.42
1:B:1180:LEU:O	1:B:1203:MET:HA	2.20	0.42
1:C:652:ILE:HA	1:C:655:ILE:HG22	2.00	0.42
1:C:1958:LEU:HA	1:C:1958:LEU:HD23	1.79	0.42
1:C:2307:THR:OG1	1:C:2360:ASP:OD1	2.36	0.42
1:C:2376:TRP:CD1	1:C:2383:LEU:HA	2.55	0.42
1:B:1347:LYS:HG3	1:B:1418:VAL:HG21	2.01	0.42
1:B:2275:PHE:CE1	1:B:2287:PRO:HB3	2.55	0.42
1:B:2291:LEU:HD23	1:B:2291:LEU:HA	1.87	0.42
1:C:2064:TYR:CE2	1:C:2095:PRO:HG3	2.54	0.42
1:B:1611:LEU:HD23	1:B:1611:LEU:HA	1.86	0.42
1:C:1870:LEU:HB3	1:C:1937:ALA:HB1	2.02	0.42
1:B:1529:GLU:O	1:B:1533:ILE:HG23	2.19	0.42
1:C:803:ILE:HG12	1:C:984:ILE:HG21	2.01	0.42
1:C:2275:PHE:CE1	1:C:2287:PRO:HB3	2.55	0.42
1:B:2275:PHE:HE1	1:B:2287:PRO:HB3	1.84	0.42
1:B:803:ILE:HG12	1:B:984:ILE:HG21	2.00	0.41
1:C:2394:ARG:HA	1:C:2394:ARG:HD3	1.87	0.41
1:B:1418:VAL:HA	1:B:1450:VAL:O	2.20	0.41
1:C:1347:LYS:HG3	1:C:1418:VAL:HG21	2.02	0.41
1:C:1356:LYS:HE3	1:C:1356:LYS:HB2	1.95	0.41
1:C:1992:TYR:OH	1:C:2016:ALA:O	2.36	0.41
1:C:2175:ASP:O	1:C:2197:SER:HA	2.20	0.41
1:B:716:ALA:HB1	1:B:721:ASN:HD21	1.84	0.41
1:B:1340:VAL:HG13	1:B:1434:TRP:CE3	2.55	0.41
1:B:1467:SER:HB2	1:B:1487:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1180:LEU:O	1:C:1203:MET:HA	2.19	0.41
1:B:1109:LEU:HB3	1:B:1128:LEU:HD13	2.01	0.41
1:B:1119:ILE:HB	1:B:1139:ASN:HD22	1.85	0.41
1:B:1433:PRO:O	1:B:1437:ASN:ND2	2.53	0.41
1:B:1682:LEU:HD23	1:B:1682:LEU:HA	1.84	0.41
1:B:1958:LEU:HD12	1:B:2002:LEU:HD12	2.01	0.41
1:C:745:ILE:HD11	1:C:758:VAL:HG23	2.03	0.41
1:C:1109:LEU:HB3	1:C:1128:LEU:HD13	2.01	0.41
1:B:1168:MET:SD	1:B:1169:PRO:HD2	2.60	0.41
1:B:1870:LEU:HB3	1:B:1937:ALA:HB1	2.02	0.41
1:C:588:SER:O	1:C:592:THR:HG23	2.20	0.41
1:C:707:TYR:O	1:C:711:VAL:HG23	2.21	0.41
1:C:2295:ASN:H	1:C:2298:THR:HG23	1.85	0.41
1:C:2363:LEU:N	1:C:2376:TRP:O	2.51	0.41
1:B:2376:TRP:CD1	1:B:2383:LEU:HA	2.55	0.41
1:C:2291:LEU:HD23	1:C:2291:LEU:HA	1.87	0.41
1:B:1325:ARG:HG3	1:B:1524:PRO:HG3	2.03	0.41
1:B:2175:ASP:O	1:B:2197:SER:HA	2.21	0.41
1:B:2295:ASN:H	1:B:2298:THR:HG23	1.85	0.41
1:B:2471:LEU:HD23	1:B:2493:LEU:HD21	2.01	0.41
1:C:1340:VAL:HG13	1:C:1434:TRP:CE3	2.55	0.41
1:B:1927:LEU:HD23	1:B:1927:LEU:HA	1.87	0.41
1:B:2110:LEU:HD11	1:B:2128:VAL:HG13	2.02	0.41
1:C:1013:LEU:HD12	1:C:1013:LEU:HA	1.87	0.41
1:C:1168:MET:SD	1:C:1169:PRO:HD2	2.61	0.41
1:C:1958:LEU:HD12	1:C:2002:LEU:HD12	2.03	0.41
1:B:1474:LEU:HA	1:B:1474:LEU:HD23	1.78	0.41
1:B:2124:THR:O	1:B:2128:VAL:HG23	2.21	0.41
1:C:1119:ILE:HB	1:C:1139:ASN:HD22	1.85	0.41
1:C:1183:ASN:N	1:C:1183:ASN:OD1	2.54	0.41
1:C:1418:VAL:HA	1:C:1450:VAL:O	2.20	0.41
1:C:1529:GLU:O	1:C:1533:ILE:HG23	2.21	0.41
1:B:1195:LEU:HD12	1:B:1198:LEU:HD13	2.03	0.40
1:B:1860:ILE:HA	1:B:1940:ILE:CD1	2.51	0.40
1:B:2269:ASP:OD1	1:B:2269:ASP:N	2.47	0.40
1:C:567:ILE:HA	1:C:570:ILE:HG22	2.03	0.40
1:C:2056:VAL:HG12	1:C:2114:CYS:HB2	2.02	0.40
1:C:2179:LEU:HD13	1:C:2179:LEU:HA	1.88	0.40
1:C:2277:ASP:OD1	1:C:2278:LYS:N	2.54	0.40
1:B:2056:VAL:HG12	1:B:2114:CYS:HB2	2.03	0.40
1:C:1117:ASN:N	1:C:1117:ASN:OD1	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1926:HIS:HA	1:C:1928:HIS:NE2	2.37	0.40
1:B:2184:LEU:HA	1:B:2184:LEU:HD23	1.81	0.40
1:B:2277:ASP:OD1	1:B:2278:LYS:N	2.54	0.40
1:C:1195:LEU:HD12	1:C:1198:LEU:HD13	2.02	0.40
1:B:2272:LEU:N	1:B:2291:LEU:O	2.47	0.40
1:C:1257:LEU:HD23	1:C:1257:LEU:HA	1.91	0.40
1:C:2275:PHE:HE1	1:C:2287:PRO:HB3	1.85	0.40
1:B:1183:ASN:OD1	1:B:1183:ASN:N	2.54	0.40
1:B:1771:ARG:NH1	1:B:1862:ALA:O	2.55	0.40
1:B:1958:LEU:HD23	1:B:1958:LEU:HA	1.77	0.40
1:B:1986:HIS:CE1	1:B:2125:SER:HG	2.39	0.40
1:B:2004:THR:OG1	1:B:2005:LEU:N	2.54	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	B	1673/2527 (66%)	1557 (93%)	115 (7%)	1 (0%)	51 82
1	C	1673/2527 (66%)	1557 (93%)	115 (7%)	1 (0%)	51 82
All	All	3346/5054 (66%)	3114 (93%)	230 (7%)	2 (0%)	54 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1686	GLU
1	C	1686	GLU

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	B	1171/2281 (51%)	1155 (99%)	16 (1%)	67 83
1	C	1171/2281 (51%)	1156 (99%)	15 (1%)	69 84
All	All	2342/4562 (51%)	2311 (99%)	31 (1%)	70 84

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	562	CYS
1	B	793	ARG
1	B	1045	ASN
1	B	1066	SER
1	B	1088	PHE
1	B	1251	HIS
1	B	1269	ASN
1	B	1288	MET
1	B	1310	HIS
1	B	1485	TYR
1	B	1707	ARG
1	B	1770	CYS
1	B	1853	SER
1	B	1958	LEU
1	B	2241	MET
1	B	2492	CYS
1	C	793	ARG
1	C	1045	ASN
1	C	1066	SER
1	C	1088	PHE
1	C	1251	HIS
1	C	1269	ASN
1	C	1288	MET
1	C	1310	HIS
1	C	1485	TYR
1	C	1707	ARG
1	C	1770	CYS

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Mol	Chain	Res	Type
1	C	1853	SER
1	C	1958	LEU
1	C	2241	MET
1	C	2492	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	721	ASN
1	B	1730	ASN
1	C	721	ASN
1	C	1730	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	0LI	B	2601	-	40,43,43	1.65	10 (25%)	51,62,62	1.03	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GDP	B	2602	-	24,30,30	1.05	1 (4%)	30,47,47	1.43	6 (20%)
2	0LI	C	2601	-	40,43,43	1.67	10 (25%)	51,62,62	1.06	1 (1%)
3	GDP	C	2602	-	24,30,30	1.06	1 (4%)	30,47,47	1.43	6 (20%)

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	0LI	B	2601	-	-	4/20/33/33	0/5/5/5
3	GDP	B	2602	-	-	4/12/32/32	0/3/3/3
2	0LI	C	2601	-	-	3/20/33/33	0/5/5/5
3	GDP	C	2602	-	-	4/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2601	0LI	C16-C17	4.63	1.46	1.40
2	C	2601	0LI	C16-C17	4.59	1.46	1.40
2	C	2601	0LI	C15-C16	3.16	1.45	1.39
2	B	2601	0LI	C15-C16	3.14	1.44	1.39
3	C	2602	GDP	C6-N1	-3.10	1.33	1.37
3	B	2602	GDP	C6-N1	-3.10	1.33	1.37
2	C	2601	0LI	C8-C9	3.07	1.44	1.39
2	B	2601	0LI	C8-C9	2.94	1.44	1.39
2	C	2601	0LI	C5-C6	2.83	1.45	1.40
2	C	2601	0LI	C14-C15	2.63	1.43	1.38
2	B	2601	0LI	C14-C15	2.59	1.43	1.38
2	B	2601	0LI	C18-C13	2.58	1.43	1.39
2	C	2601	0LI	C18-C13	2.56	1.43	1.39
2	B	2601	0LI	C5-C6	2.45	1.45	1.40
2	B	2601	0LI	C84-N1	-2.36	1.31	1.33
2	C	2601	0LI	C8-C7	2.29	1.42	1.38
2	B	2601	0LI	C8-C7	2.21	1.42	1.38
2	C	2601	0LI	C2-C3	-2.20	1.39	1.43
2	B	2601	0LI	C2-C3	-2.17	1.39	1.43
2	C	2601	0LI	C84-N1	-2.17	1.31	1.33
2	B	2601	0LI	C20-C16	2.08	1.54	1.51
2	C	2601	0LI	C20-C16	2.00	1.54	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2602	GDP	PA-O3A-PB	-4.15	118.60	132.83
3	B	2602	GDP	PA-O3A-PB	-4.12	118.67	132.83
2	C	2601	0LI	C19-C17-C16	3.71	125.38	121.22
2	B	2601	0LI	C19-C17-C16	3.66	125.32	121.22
3	C	2602	GDP	C3'-C2'-C1'	2.63	104.93	100.98
3	B	2602	GDP	C3'-C2'-C1'	2.61	104.91	100.98
3	C	2602	GDP	C5-C6-N1	2.52	118.40	113.95
3	B	2602	GDP	C5-C6-N1	2.50	118.36	113.95
3	C	2602	GDP	C8-N7-C5	2.34	107.46	102.99
3	B	2602	GDP	C8-N7-C5	2.32	107.40	102.99
3	B	2602	GDP	O2B-PB-O3A	2.30	112.33	104.64
3	C	2602	GDP	O2B-PB-O3A	2.27	112.26	104.64
3	B	2602	GDP	O6-C6-C5	-2.06	120.35	124.37
3	C	2602	GDP	O6-C6-C5	-2.05	120.36	124.37

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2602	GDP	C5'-O5'-PA-O1A
3	B	2602	GDP	O4'-C4'-C5'-O5'
3	B	2602	GDP	C3'-C4'-C5'-O5'
3	C	2602	GDP	C5'-O5'-PA-O1A
3	C	2602	GDP	O4'-C4'-C5'-O5'
3	C	2602	GDP	C3'-C4'-C5'-O5'
2	C	2601	0LI	C3-C4-C5-C6
2	B	2601	0LI	C3-C4-C5-C6
2	B	2601	0LI	C3-C4-C5-C10
2	C	2601	0LI	C3-C4-C5-C10
2	B	2601	0LI	C14-C13-N2-C12
2	C	2601	0LI	C14-C13-N2-C12
3	B	2602	GDP	C5'-O5'-PA-O3A
3	C	2602	GDP	C5'-O5'-PA-O3A
2	B	2601	0LI	C18-C13-N2-C12

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2601	0LI	2	0

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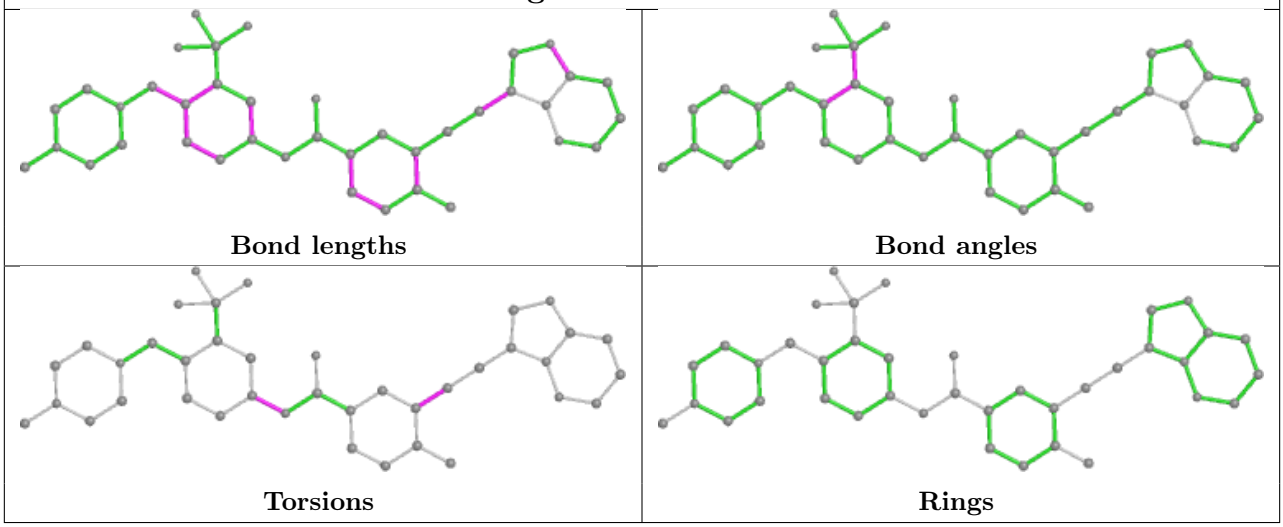
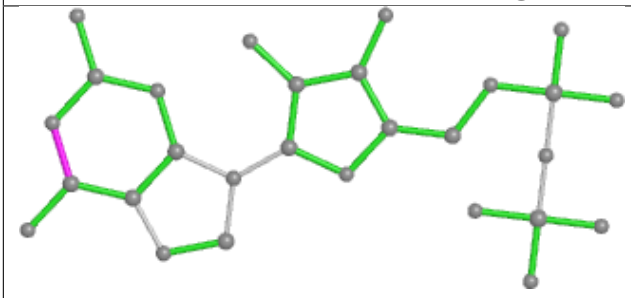
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2602	GDP	1	0
2	C	2601	0LI	2	0
3	C	2602	GDP	1	0

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.

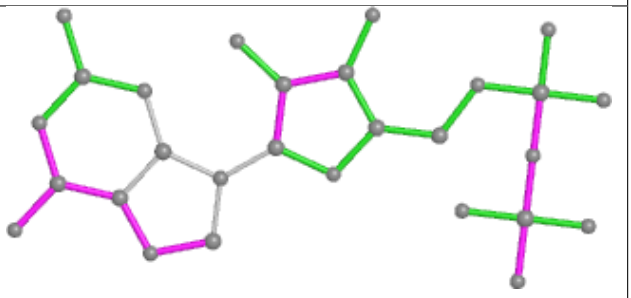
Ligand 0LI B 2601



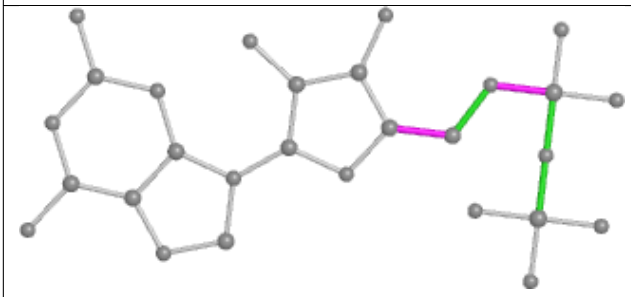
Ligand GDP B 2602



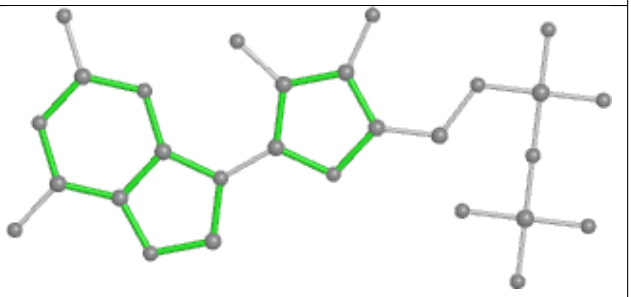
Bond lengths



Bond angles

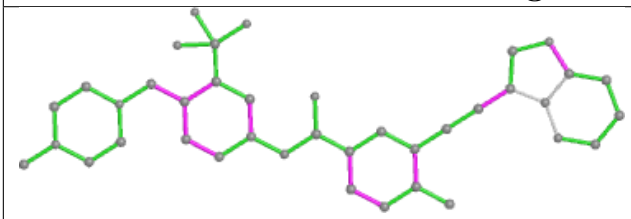


Torsions

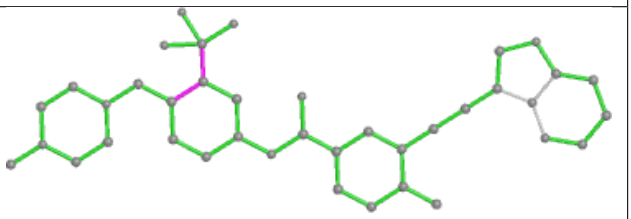


Rings

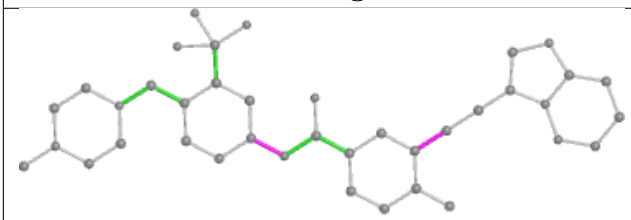
Ligand 0LI C 2601



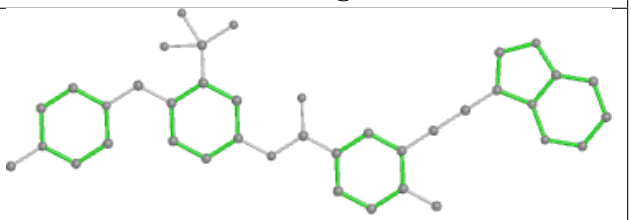
Bond lengths



Bond angles

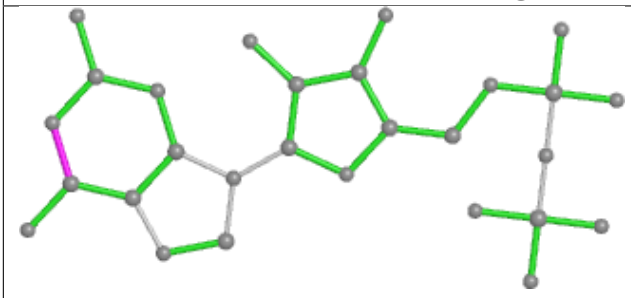


Torsions

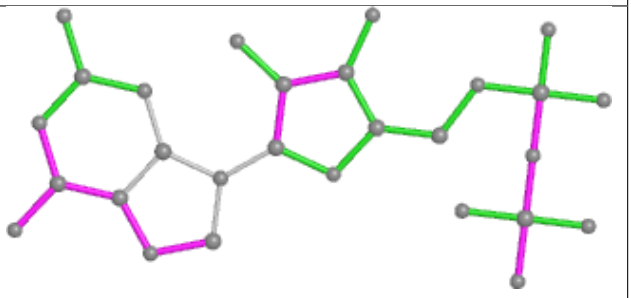


Rings

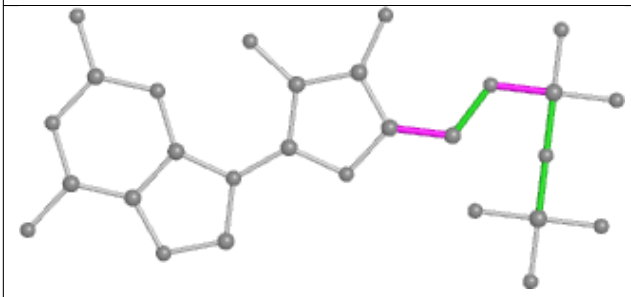
Ligand GDP C 2602



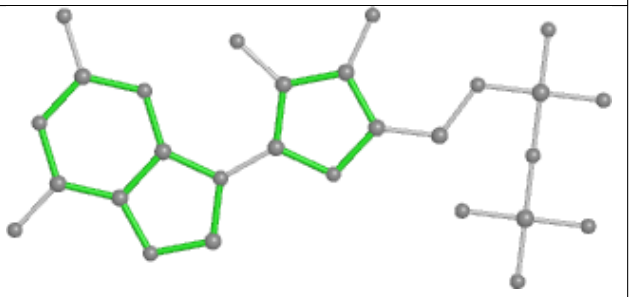
Bond lengths



Bond angles



Torsions



Rings

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.

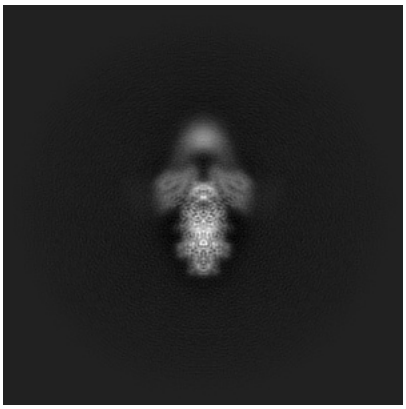
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42019. These allow visual inspection of the internal detail of the map and identification of artifacts.

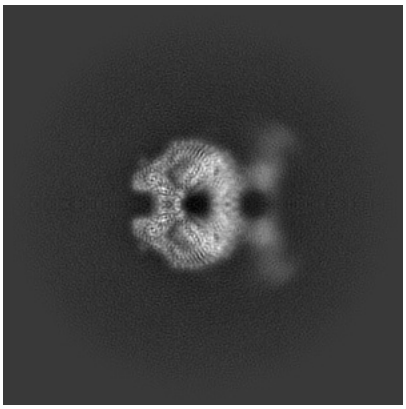
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

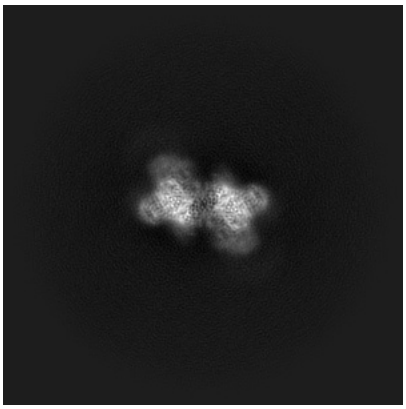
6.1.1 Primary map



X

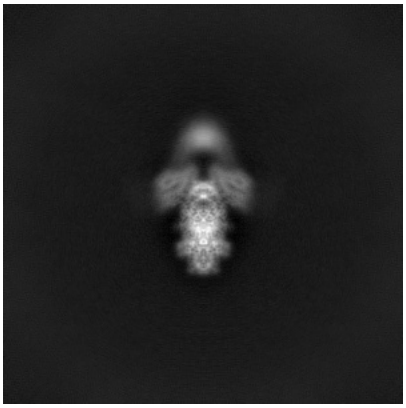


Y

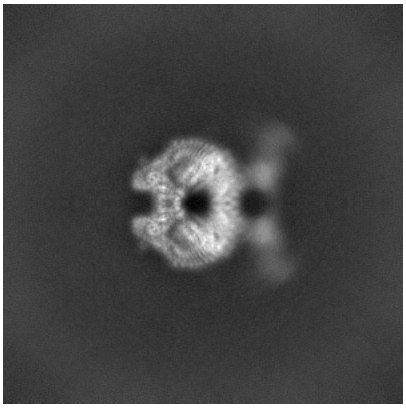


Z

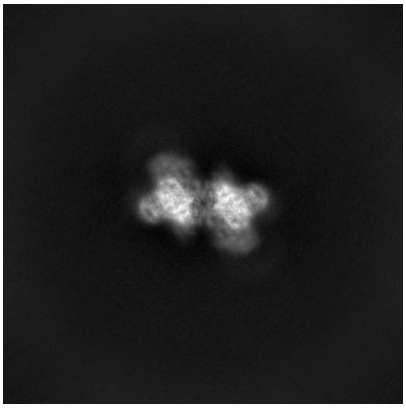
6.1.2 Raw map



X



Y

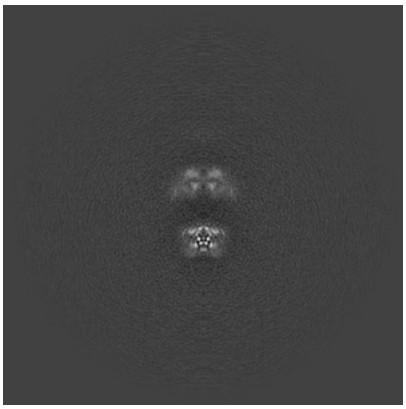


Z

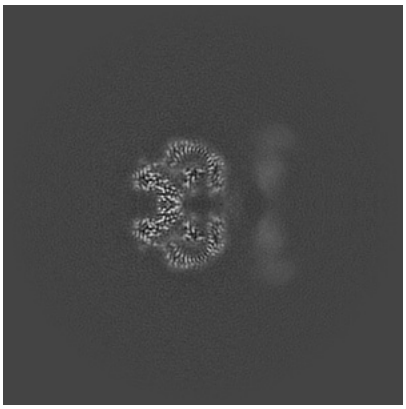
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

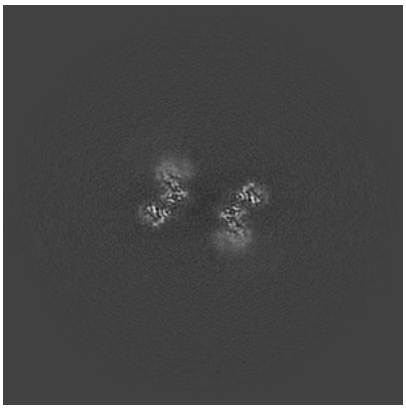
6.2.1 Primary map



X Index: 192

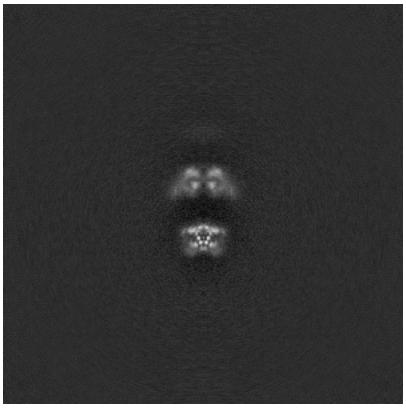


Y Index: 192

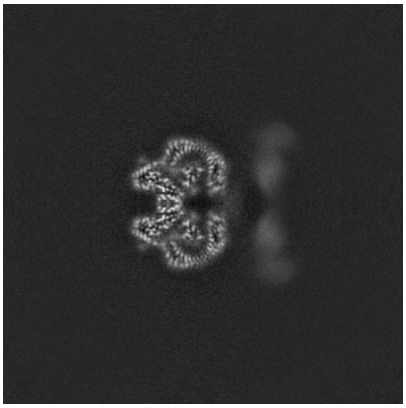


Z Index: 192

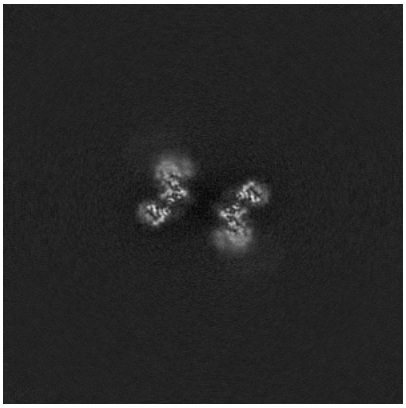
6.2.2 Raw map



X Index: 192



Y Index: 192

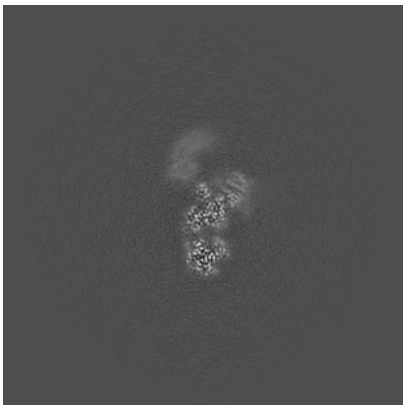


Z Index: 192

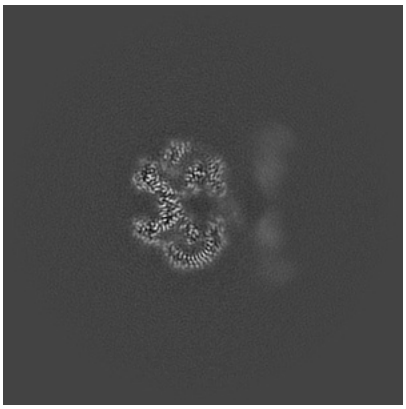
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

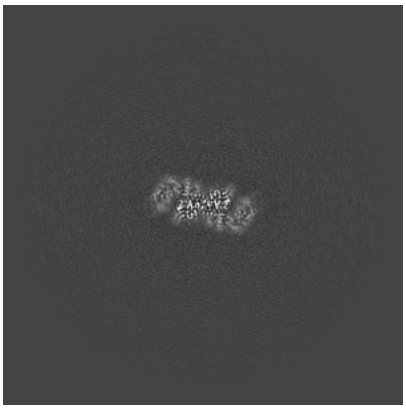
6.3.1 Primary map



X Index: 168



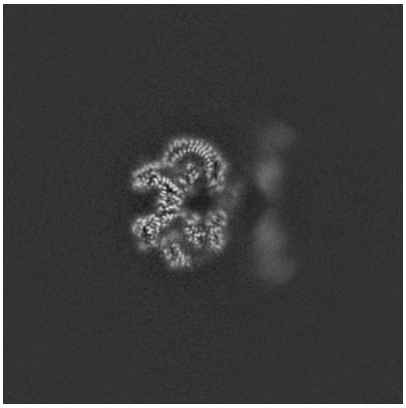
Y Index: 189



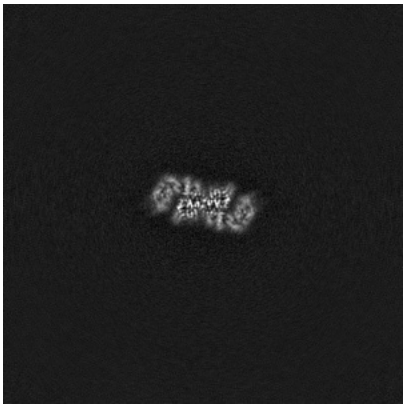
Z Index: 154

6.3.2 Raw map

X Index: 168



Y Index: 195

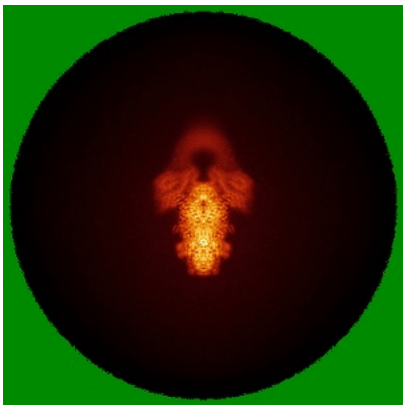


Z Index: 154

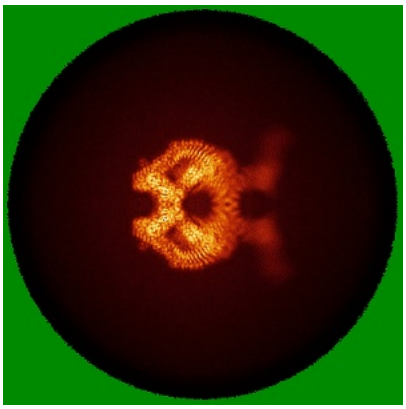
The images above show the largest variance slices of the map in three orthogonal directions.

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

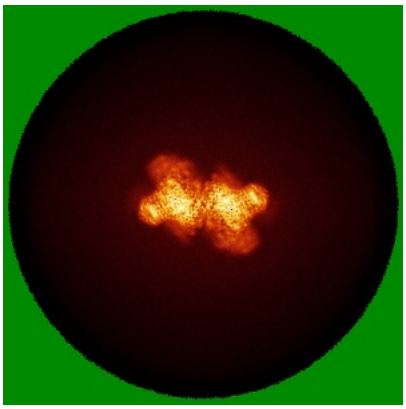
6.4.1 Primary map



X

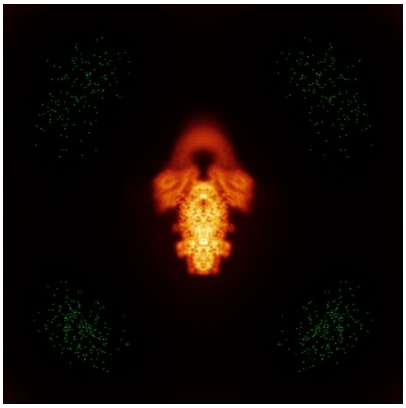


Y

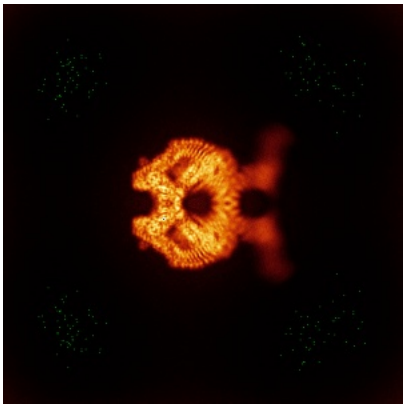


Z

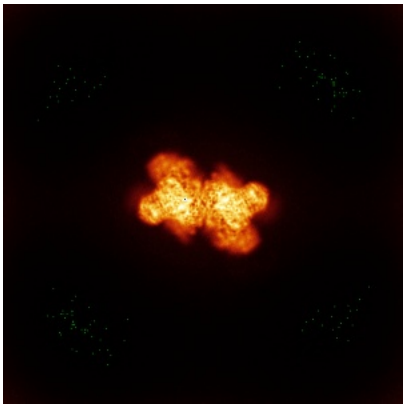
6.4.2 Raw map



X



Y

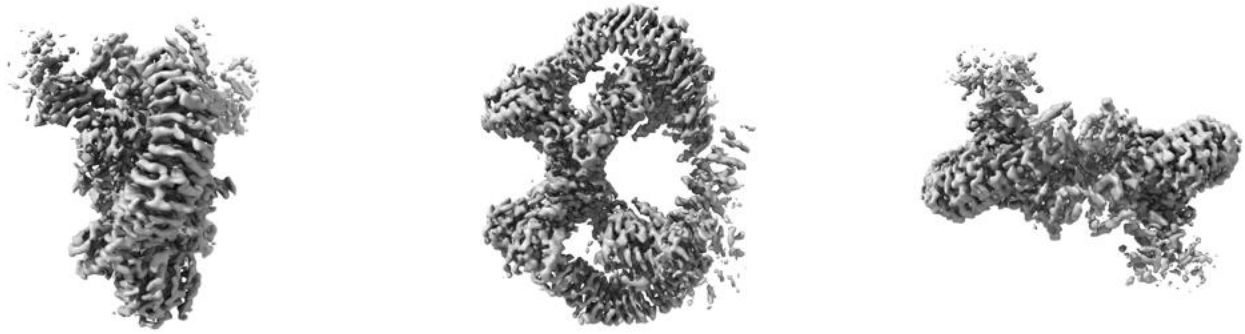


Z

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)

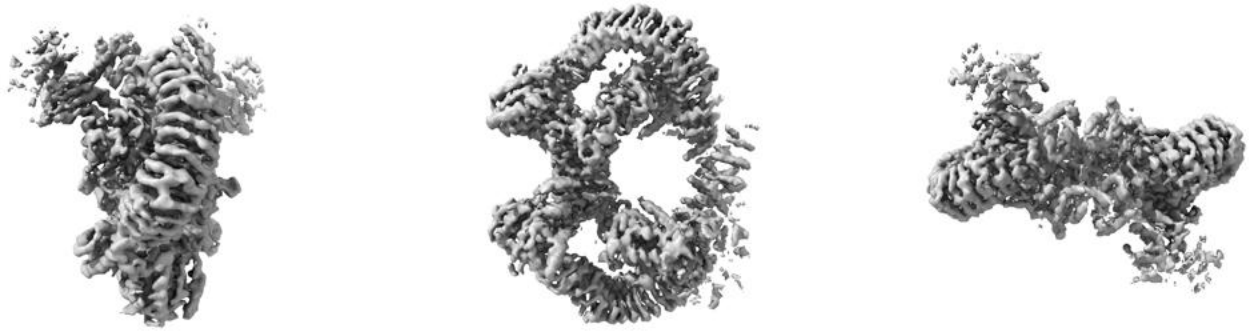
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

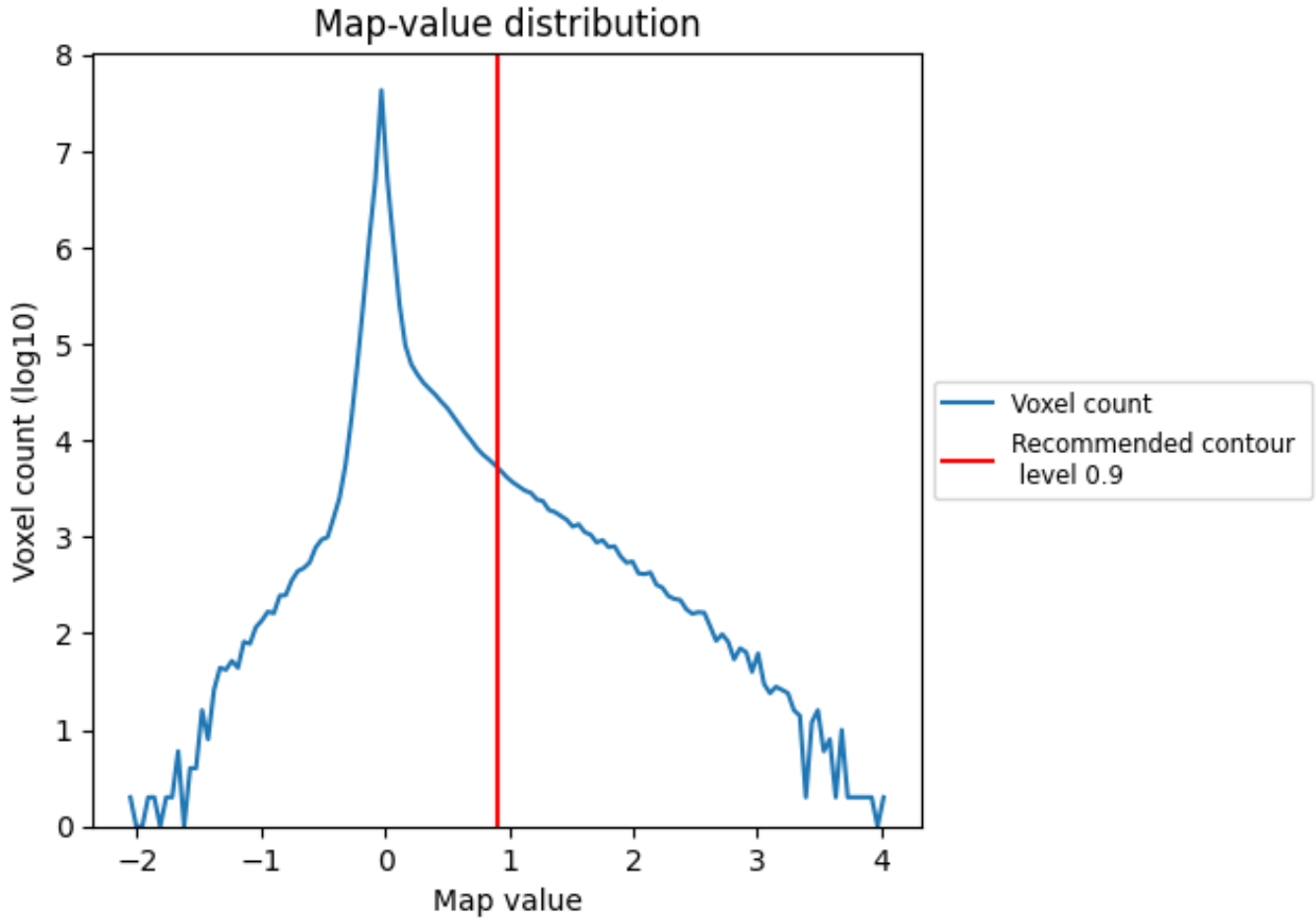
6.6 Mask visualisation (i)

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

7 Map analysis

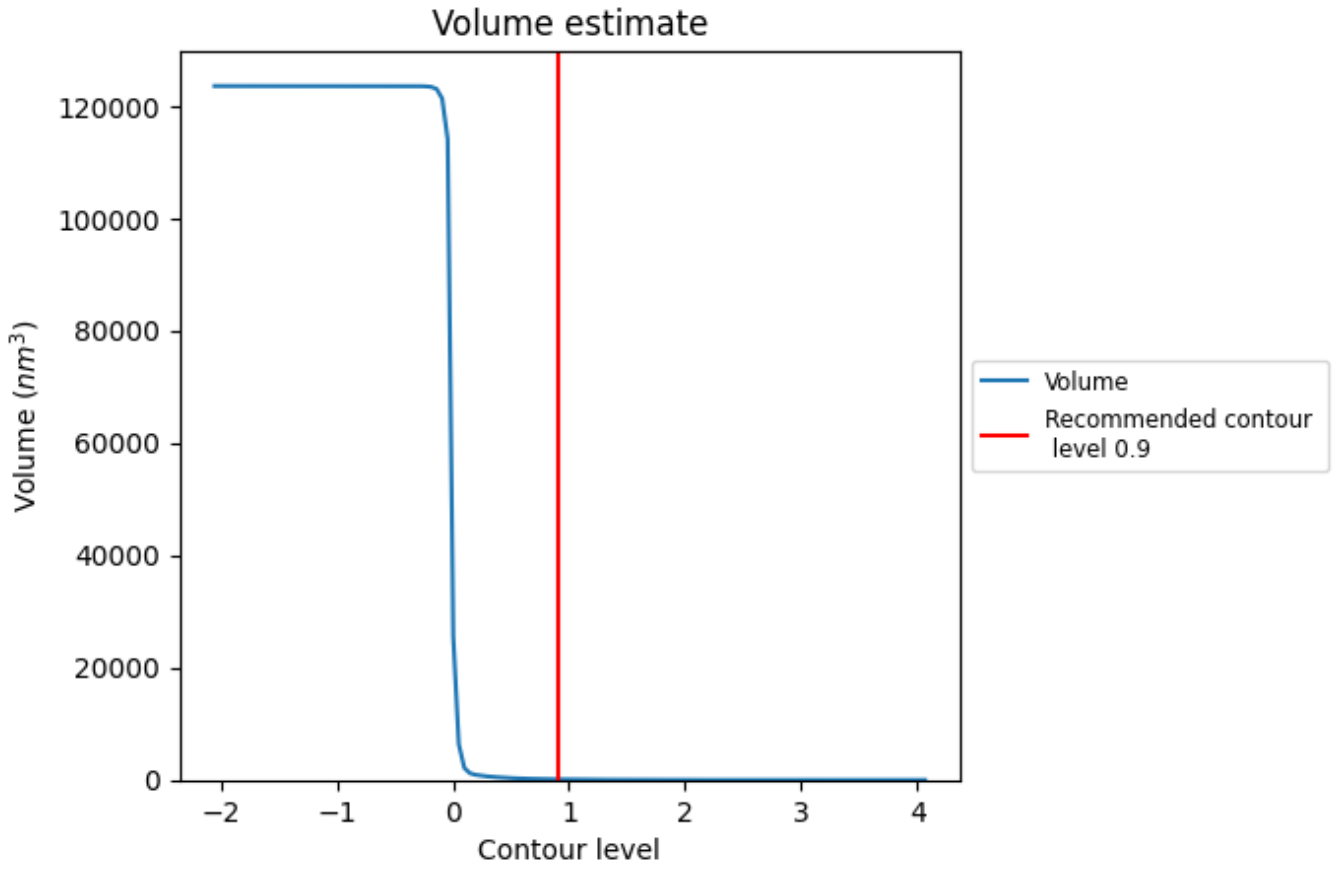
This section contains the results of statistical analysis of the map.

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.

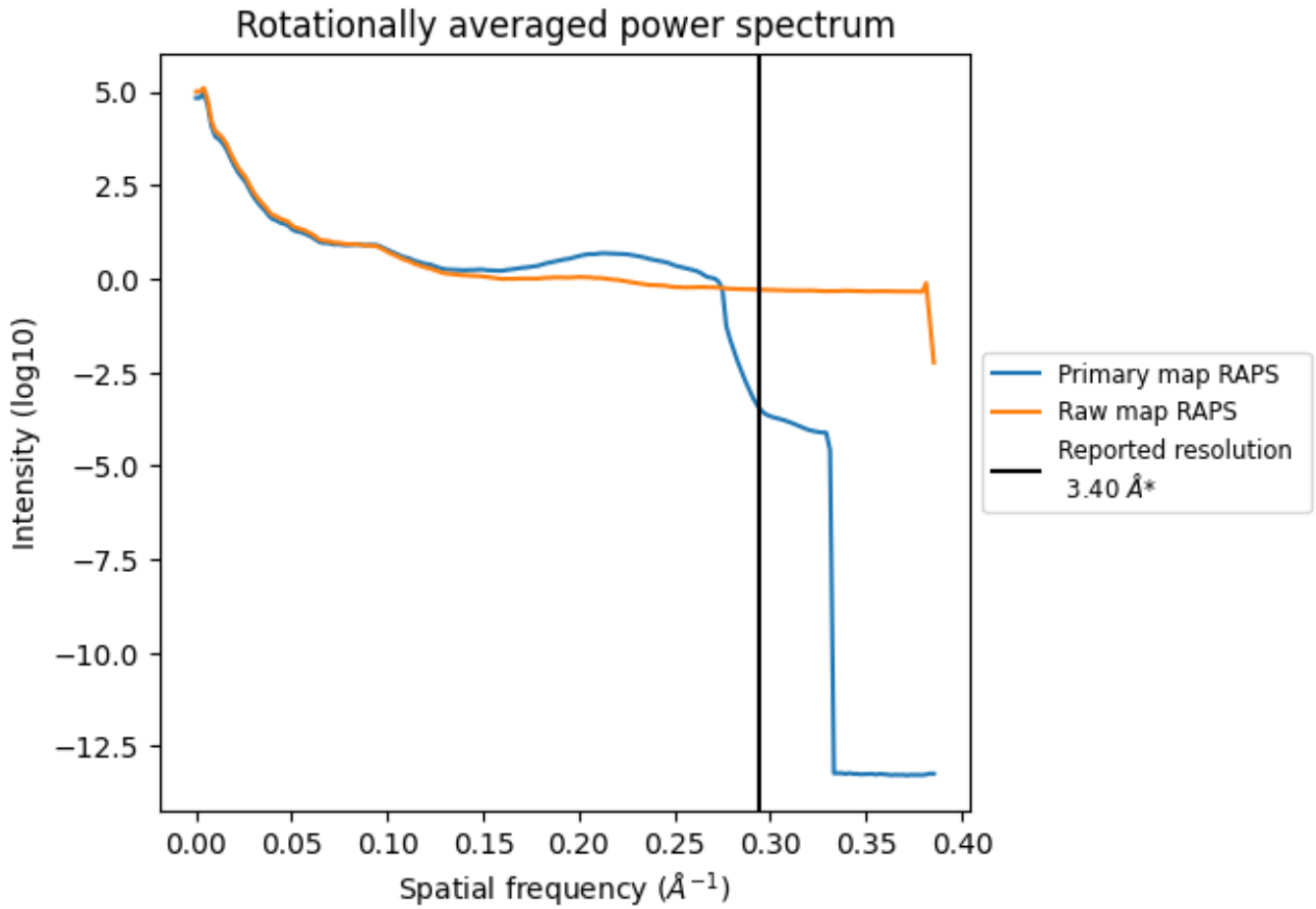
7.2 Volume estimate



The volume at the recommended contour level is 113 nm^3; this corresponds to an approximate mass of 102 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)

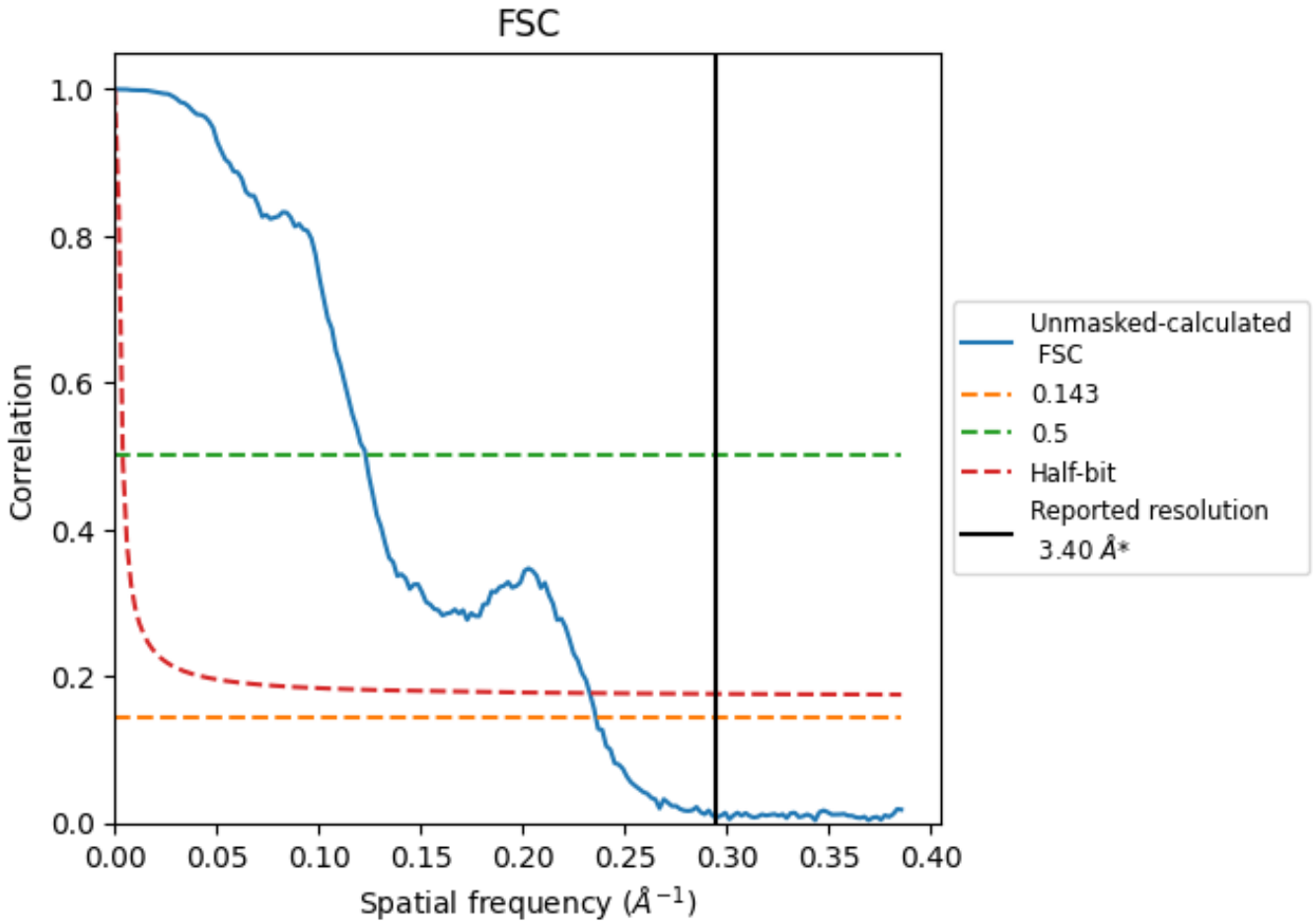


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

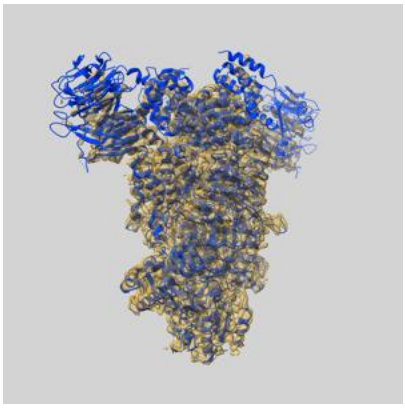
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	8.14	4.30

*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 4.24 differs from the reported value 3.4 by more than 10 %

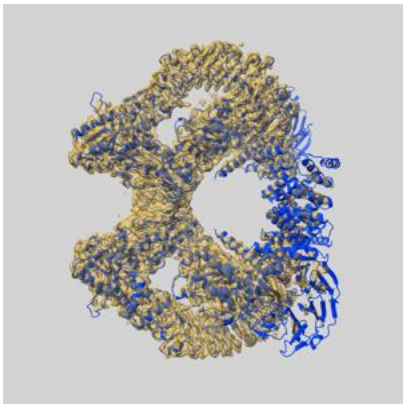
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42019 and PDB model 8U8A. Per-residue inclusion information can be found in section 3 on page 5.

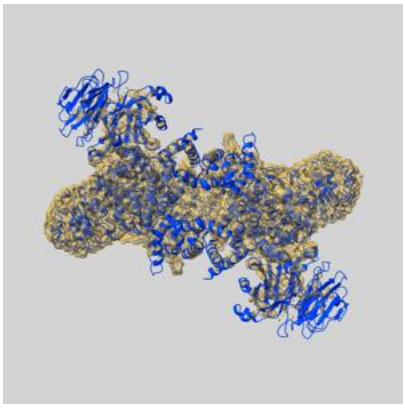
9.1 Map-model overlay



X



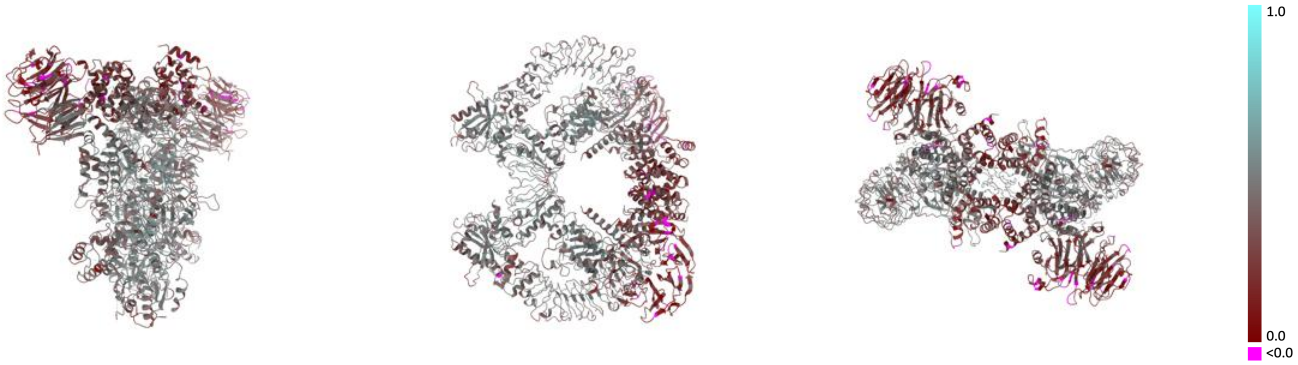
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

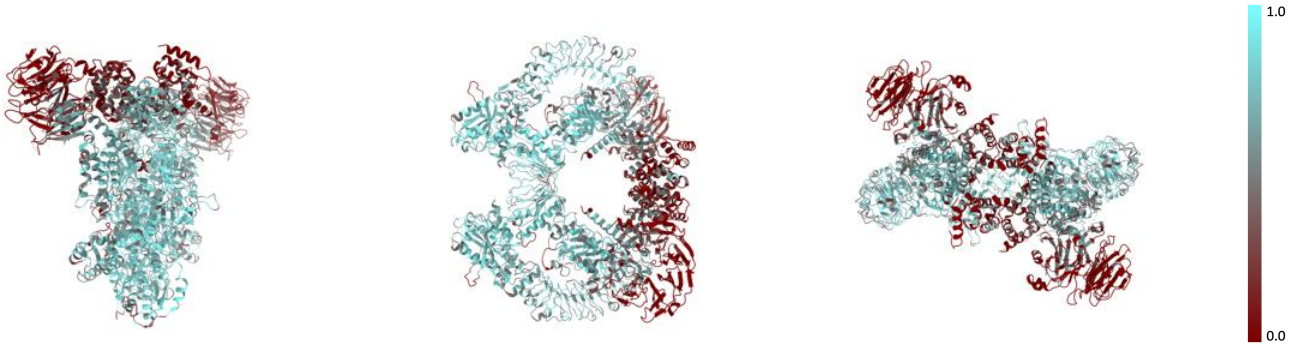
9.2 Q-score mapped to coordinate model (i)



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.

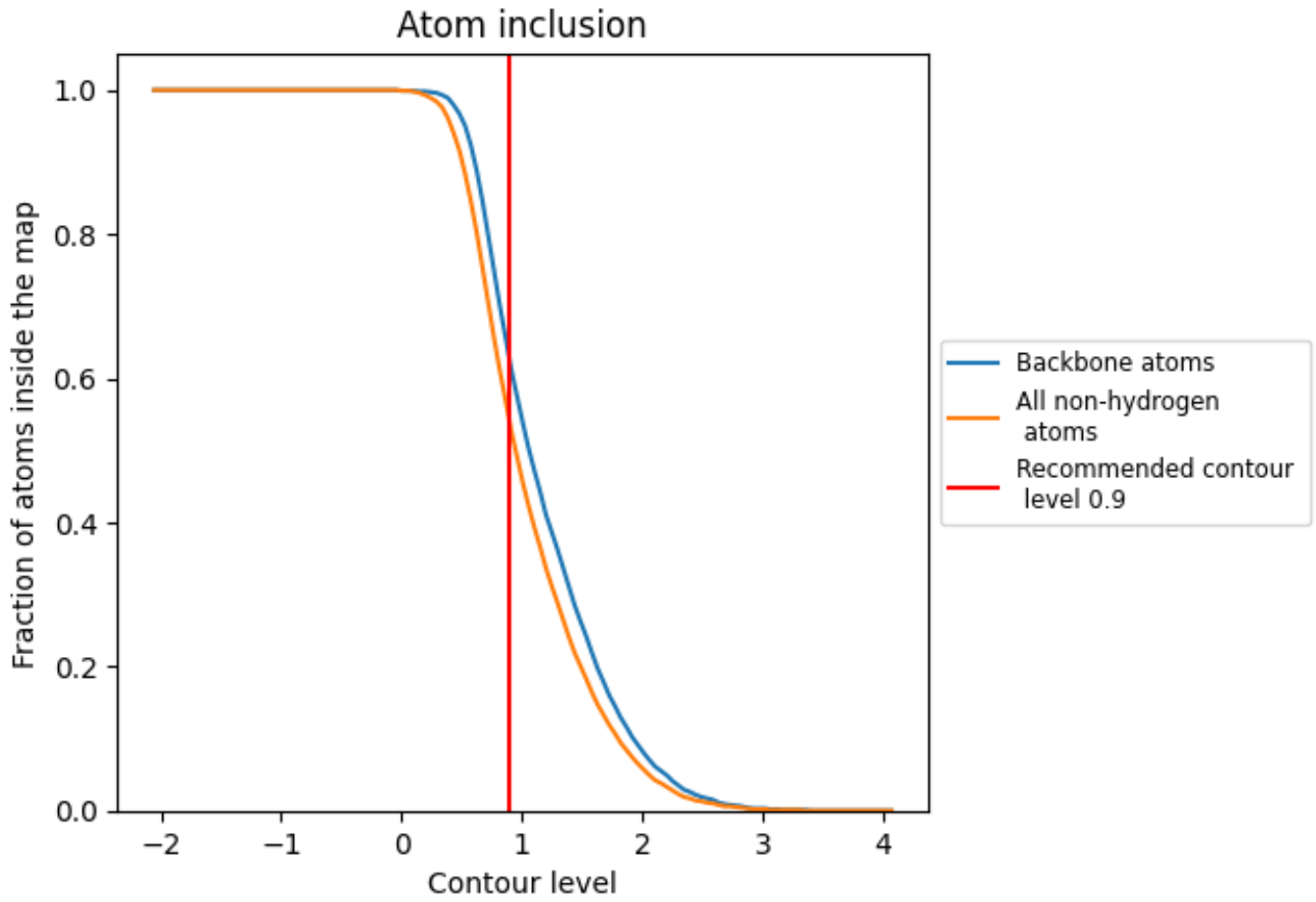
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 54% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5360	0.3950
B	0.5350	0.3950
C	0.5360	0.3950