Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:50 PM UTC

PDB ID	:	8U8B / pdb_00008u8b
EMDB ID	:	EMD-42020
Title	:	Cryo-EM structure of LRRK2 bound to type II inhibitor rebastinib
Authors	:	Zhu, H.; Sun, J.
Deposited on	:	2023-09-16
Resolution	:	3.70 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:

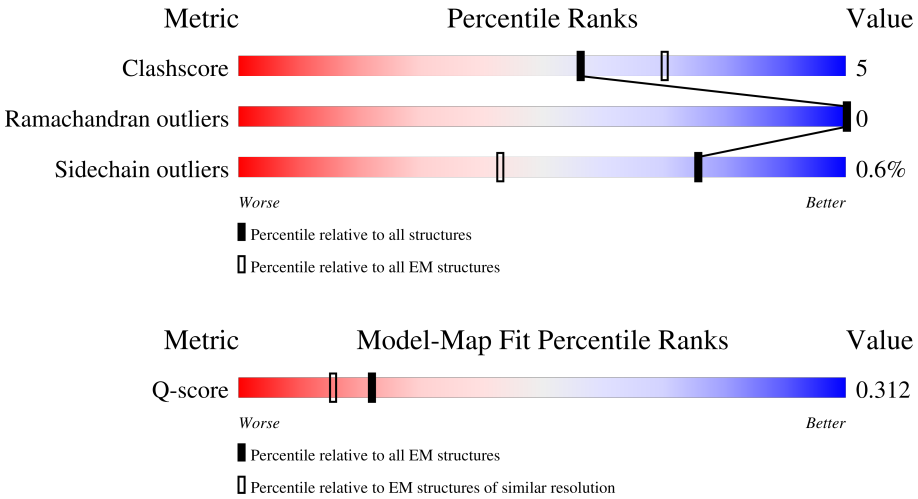
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	24% 60% 8% 32%
1	B	2527	23% 60% 8% 32%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24694 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.

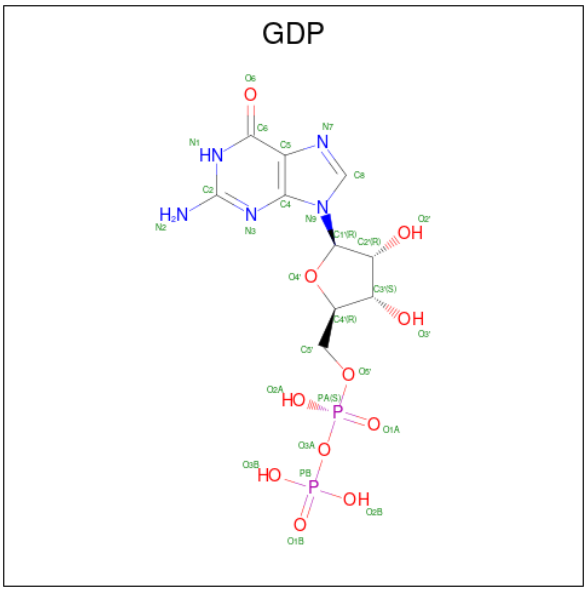
- Molecule 1 is a protein called Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1712	Total	C	N	O	S	0	0
			12278	7922	2090	2194	72		
1	B	1712	Total	C	N	O	S	0	0
			12278	7922	2090	2194	72		

There are 6 discrepancies between the modelled and reference sequences:

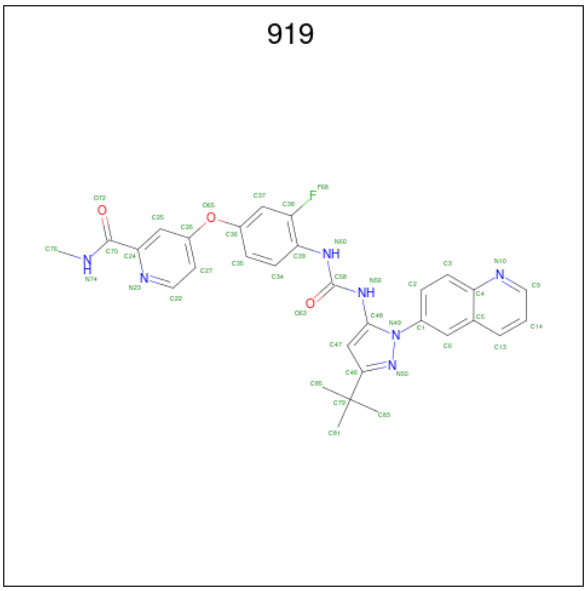
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	HIS	ARG	conflict	UNP Q5S007
A	1647	THR	SER	conflict	UNP Q5S007
A	2397	THR	MET	conflict	UNP Q5S007
B	50	HIS	ARG	conflict	UNP Q5S007
B	1647	THR	SER	conflict	UNP Q5S007
B	2397	THR	MET	conflict	UNP Q5S007

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 3 is 4-[4-({[3-tert-butyl-1-(quinolin-6-yl)-1H-pyrazol-5-yl]carbamoyl}amino)-3-fluorophenoxy]-N-methylpyridine-2-carboxamide (CCD ID: 919) (formula: $C_{30}H_{28}FN_7O_3$) (labeled as "Ligand of Interest" by depositor).



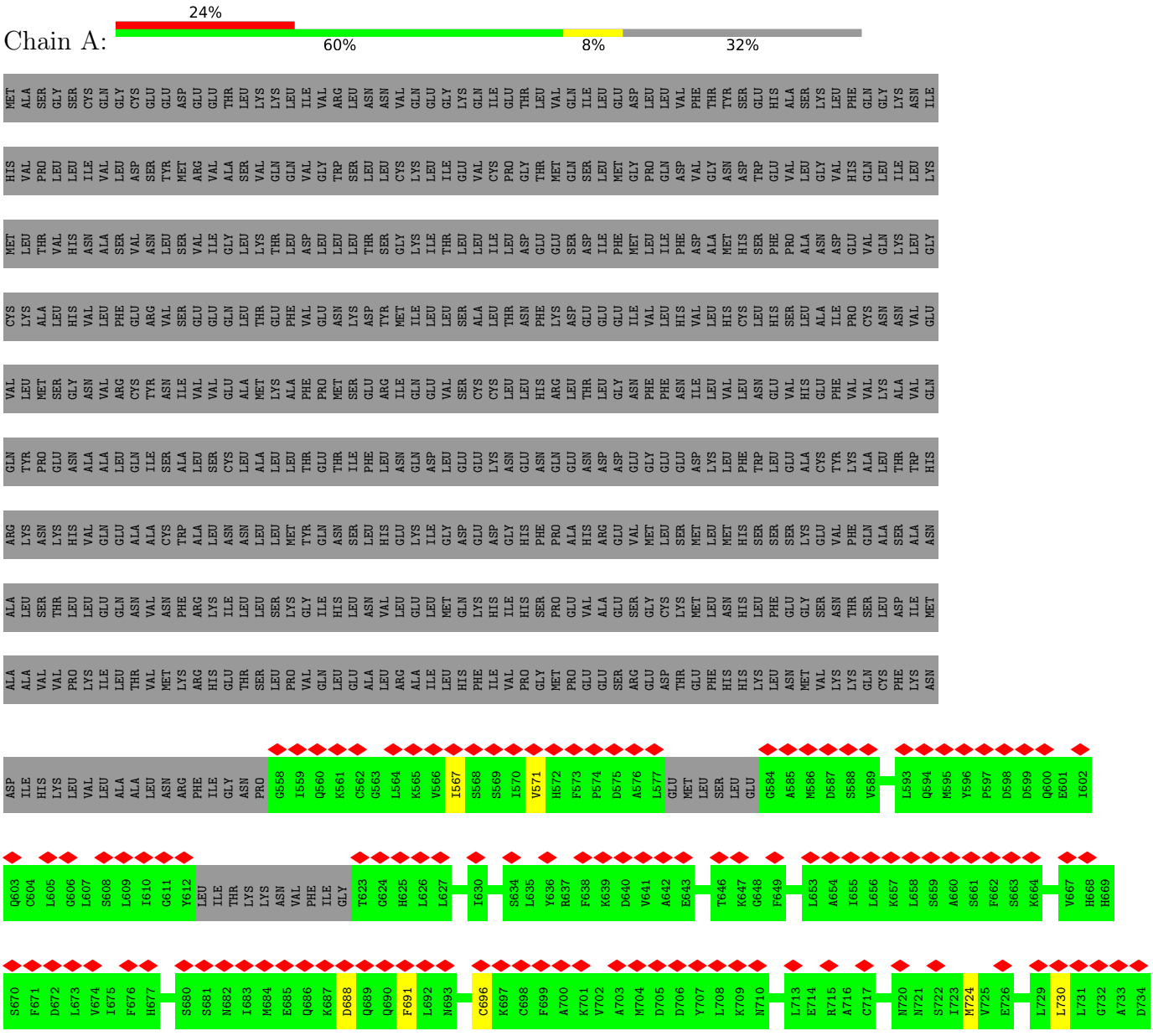
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	F	N	O	0
			41	30	1	7	3	
3	B	1	Total	C	F	N	O	0
			41	30	1	7	3	

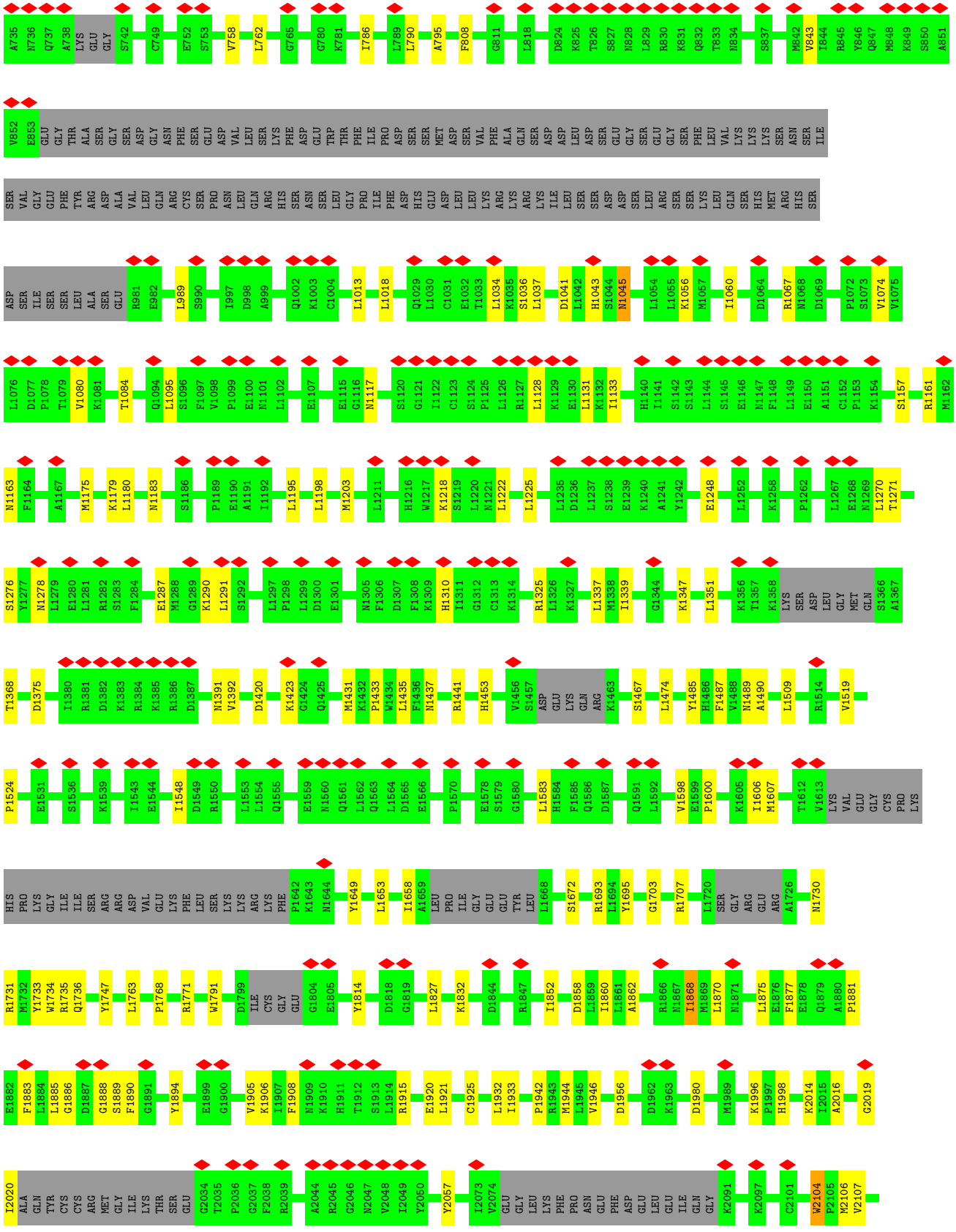
3 Residue-property plots (i)

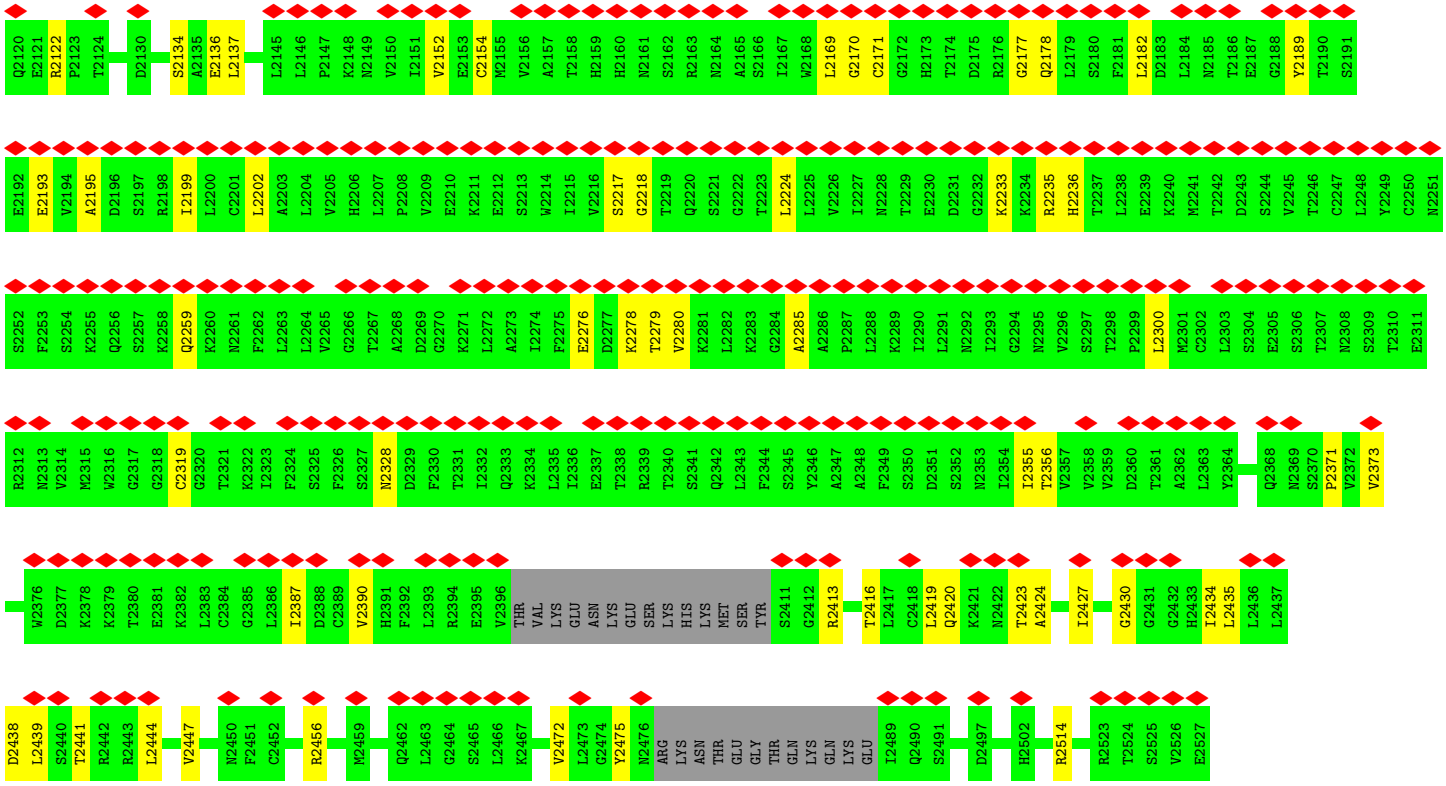
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



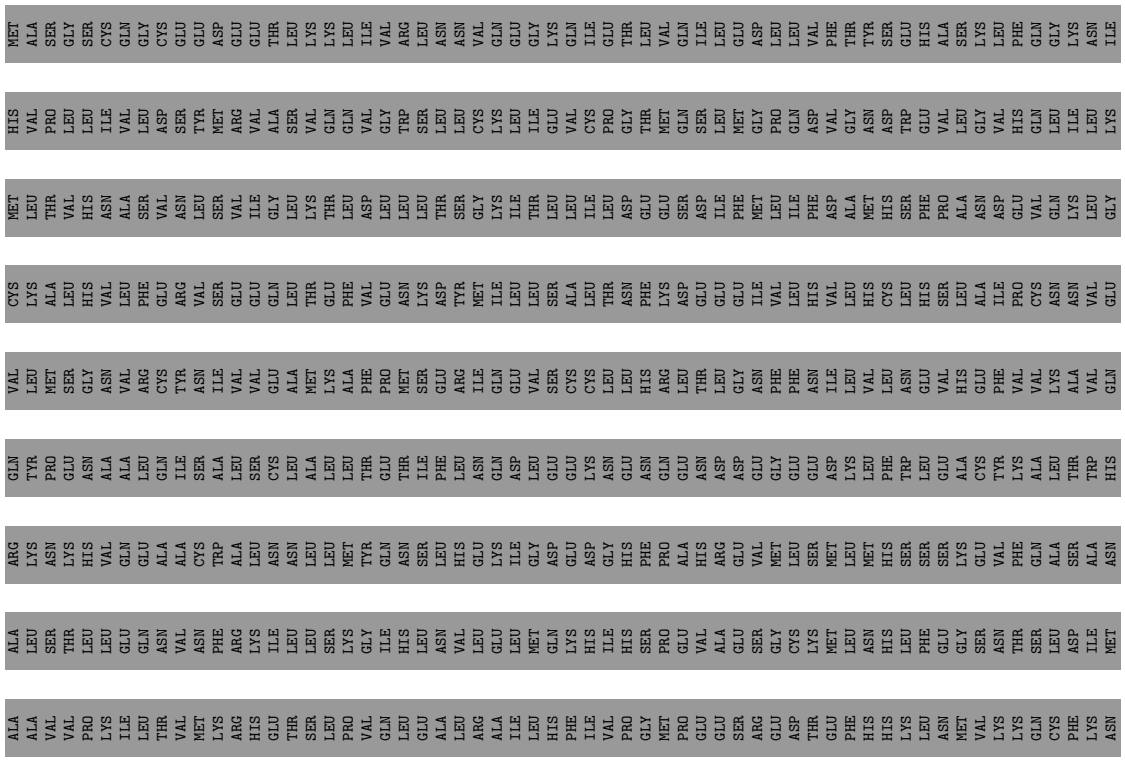

A735 N736 Q737 A738 LYS GLU GLY S742 C749 E752 S753 V758 L762 G765 G780 K781 I786 L789 L790 A795 F808 G811 L818 D824 K825 T826 S827 N828 L829 R830 K831 Q832 T833 N834 S837 M842 V843 I844 R845 Y846 Q847 M848 K849 S850 A851
V852 E853 GLU GLY THR ALA SER GLY SER ASP GLY ASN PHE SER GLU ASP VAL LEU SER LYS 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 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 LEU SER SER ASP ASP SER LEU ARG SER SER LYS LEU HIS MET ARG HIS SER
ASP SER ILE SER LEU ALA SER GLU R981 E982 L989 S990 I997 D998 A999 Q1002 K1003 C1004 L1013 L1018 Q1029 L1030 C1031 E1032 T1033 L1034 K1035 S1036 L1037 D1041 L1042 H1043 S1044 N1045 L1054 L1055 K1056 M1057 I1060 D1064 R1067 N1068 D1069 P1072 S1073 V1074 V1075
L1076 D1077 P1078 T1079 V1080 K1081 T1084 Q1094 L1095 S1096 F1097 V1098 P1099 E1100 N1101 L1102 E1107 E1115 G1116 N1117 S1120 G1121 I1122 C1123 S1124 P1125 L1126 R1127 L1128 K1129 E1130 L1131 K1132 I1133 H1140 I1141 S1142 S1143 L1144 S1145 E1146 N1147 F1148 L1149 E1150 A1151 C1152 P1153 K1154 S1157 R1161 M1162
N1163 F1164 A1167 M1175 K1179 L1180 N1183 S1186 P1189 E1190 A1191 I1192 L1195 L1198 M1203 L1211 H1216 W1217 K1218 S1219 L1220 N1221 L1222 L1225 L1235 D1236 L1237 S1238 E1239 K1240 A1241 Y1242 E1248 L1252 K1258 P1262 L1267 E1268 N1269 L1270 T1271
S1276 Y1277 N1278 L1279 E1280 L1281 R1282 S1283 F1284 E1287 M1288 G1289 K1290 L1291 S1292 L1297 P1298 L1299 D1300 E1301 N1305 F1306 D1307 F1308 K1309 H1310 I1311 G1312 C1313 K1314 R1325 L1326 K1327 L1337 M1338 I1339 G1344 K1347 L1351 K1356 T1357 K1358 LYS SER ASP LEU GLY MET GLN S1366 A1367
T1368 D1375 T1380 R1381 D1382 K1383 R1384 K1385 R1386 D1387 N1391 V1392 D1420 K1423 G1424 Q1425 M1431 K1432 P1433 W1434 L1435 F1436 N1437 R1441 H1453 V1456 S1457 ASP GLU LYS GLN ARG K1463 S1467 L1474 Y1485 H1486 F1487 Y1488 N1489 A1490 L1509 R1514 V1519
P1524 E1531 S1536 K1539 I1543 E1544 I1548 D1549 R1550 L1553 L1554 Q1555 E1559 N1560 Q1561 L1562 Q1563 L1564 D1565 E1566 P1570 E1578 S1579 G1580 L1583 H1584 F1585 Q1586 D1587 Q1591 L1592 V1598 E1599 P1600 K1605 I1606 M1607 T1612 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 Y1649 L1653 I1658 A1659 LEU PRO ILE GLY GLU GLU TYR LEU L1668 S1672 R1693 L1694 Y1695 G1703 R1707 L1720 SER GLY ARG GLU ARG A1726 N1730
R1731 M1732 Y1733 W1734 R1735 Q1736 Y1747 L1763 P1768 R1771 W1791 D1799 ILE CYS GLY GLU G1804 E1805 Y1814 D1818 G1819 L1827 K1832 D1844 R1847 I1852 D1858 L1859 I1860 L1861 A1862 R1866 N1867 I1868 M1869 L1870 N1871 L1875 E1876 F1877 E1878 Q1879 A1880 P1881
E1882 F1883 L1884 L1885 G1886 D1887 G1888 S1889 F1890 G1891 Y1894 E1899 G1900 V1905 K1906 I1907 F1908 N1909 K1910 H1911 T1912 S1913 L1914 R1915 E1920 L1921 C1925 L1932 I1933 P1942 R1943 M1944 L1945 V1946 D1956 D1962 K1963 D1980 M1989 K1996 P1997 H1998 K2014 I2015 A2016 G2019
I2020 ALA GLN TYR CYS CYS ARG MET GLY ILE LYS THR SER GLU G2034 T2035 P2036 G2037 P2038 R2039 A2044 R2045 G2046 N2047 V2048 I2049 Y2050 Y2057 I2073 V2074 GLU GLY LEU LYS PHE PRO ASN GLU PHE ASP GLU LEU GLU ILE GLN GLY K2091 K2097 C2101 W2104 P2105 M2106 V2107

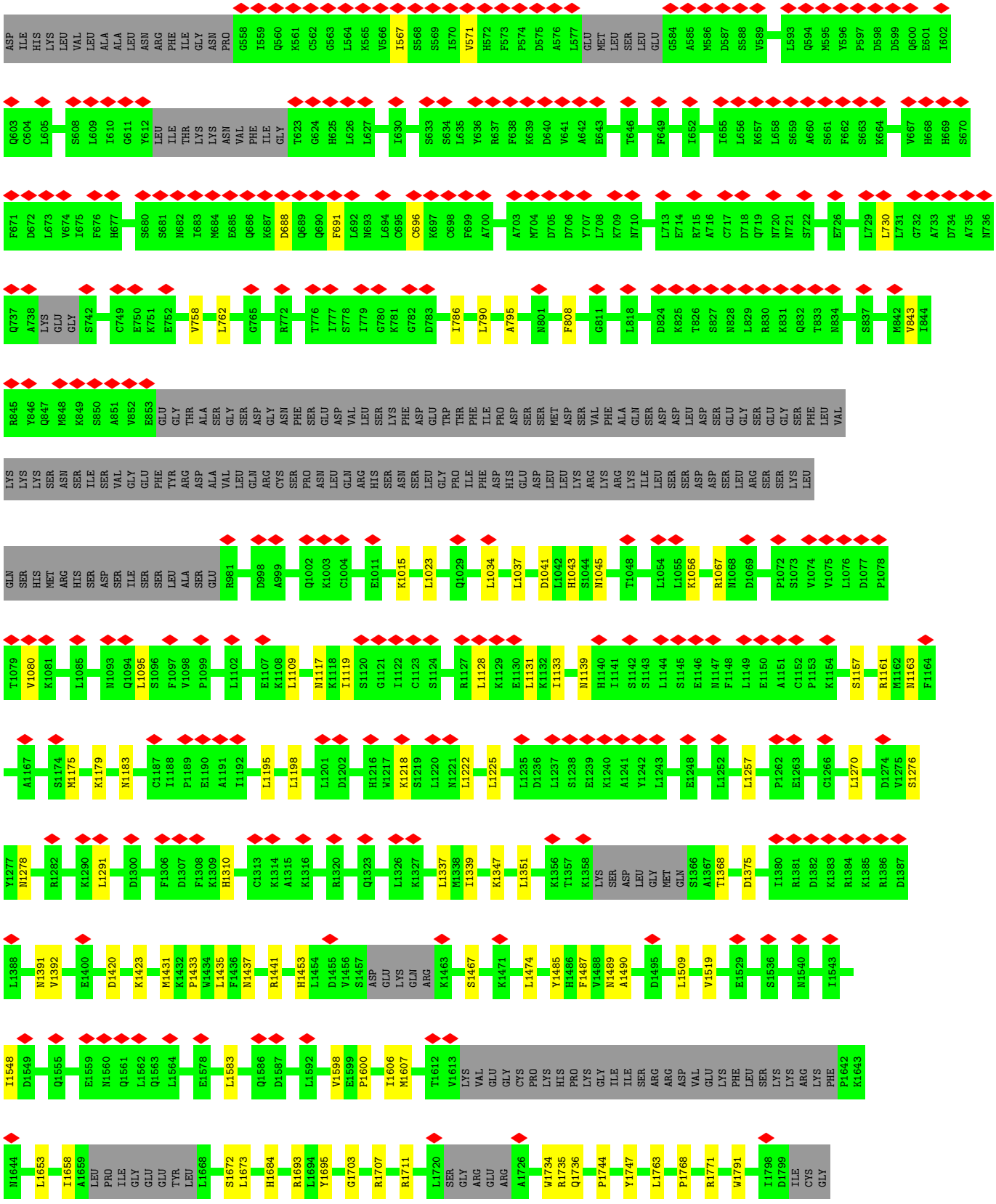


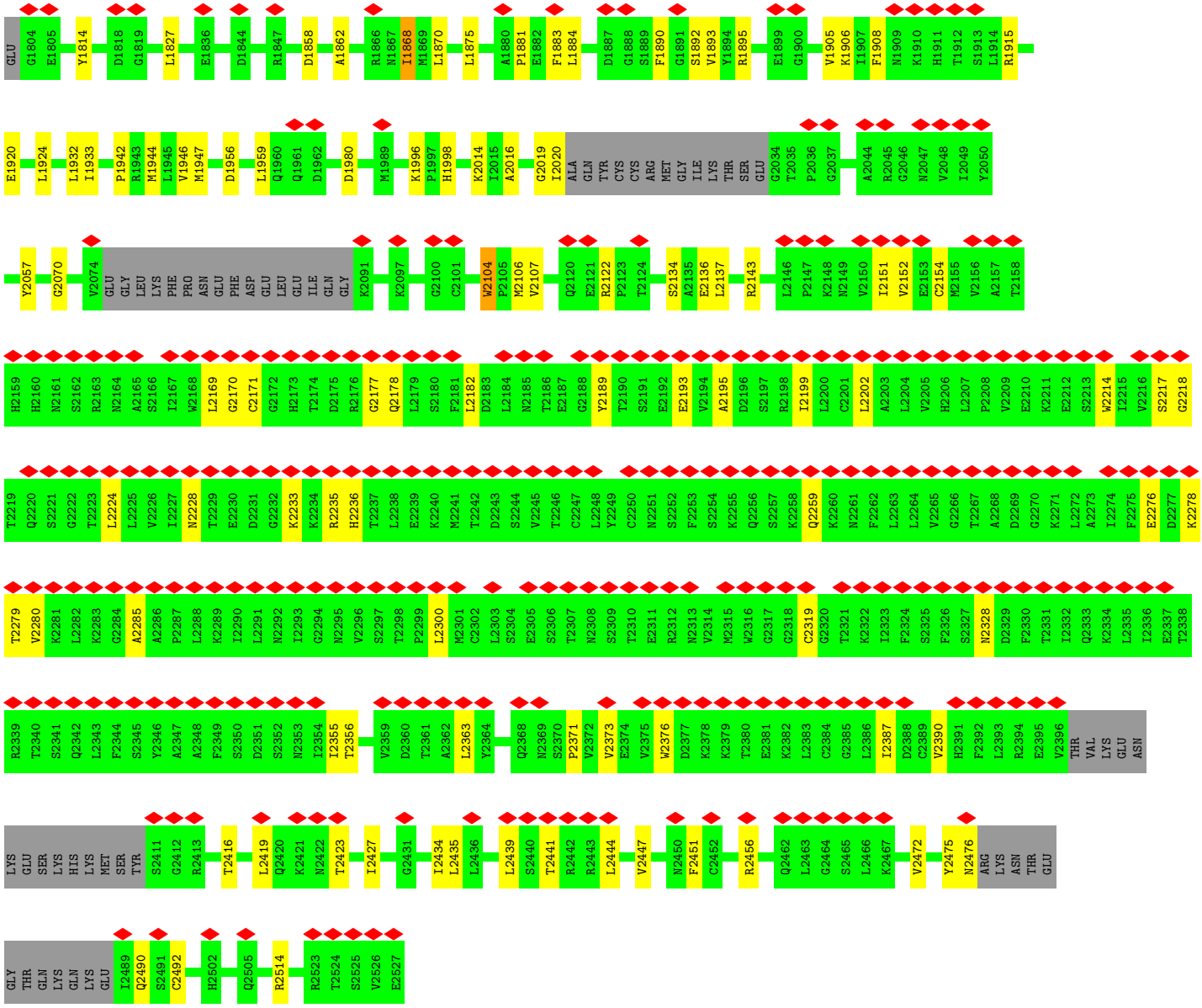
• Molecule 1: Leucine-rich repeat serine/threonine-protein kinase 2

Chain B:






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 L593 Q594 M595 Y596 P597 D598 D599 Q600 E601 I602
Q603 C604 L605 S608 L609 I610 G611 Y612 LEU ILE THR LYS LYS ASN VAL PHE ILE GLY T623 G624 H625 L626 L627 I630 S633 S634 L635 Y636 R637 F638 K639 D640 V641 A642 E643 T646 F649 I652 I655 L656 K657 L658 S659 A660 S661 F662 S663 K664 V667 H668 H669 S670
F671 D672 L673 V674 I675 F676 H677 S680 S681 N682 I683 M684 E685 Q686 K687 D688 Q689 Q690 F691 L692 N693 L694 C695 C696 K697 C698 F699 A700 A703 M704 D705 D706 Y707 L708 K709 N710 L713 E714 R715 A716 C717 D718 Q719 N720 N721 S722 E726 L729 L730 L731 G732 A733 D734 A735 N736
Q737 A738 LYS GLU GLY S742 C749 E750 K751 E752 V758 L762 G765 R772 T776 I777 S778 I779 G780 K781 G782 D783 I786 L790 A795 N801 F808 G811 L818 D824 K825 T826 S827 N828 L829 R830 K831 Q832 T833 N834 S837 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 D998 A999 Q1002 K1003 C1004 E1011 K1015 L1023 Q1029 L1034 L1037 D1041 L1042 H1043 S1044 N1045 T1048 L1054 L1055 K1056 R1067 N1068 D1069 P1072 S1073 V1074 V1075 L1076 D1077 P1078
T1079 V1080 K1081 L1085 N1093 Q1094 L1095 S1096 F1097 V1098 P1099 L1102 E1107 K1108 L1109 N1117 K1118 I1119 S1120 G1121 I1122 C1123 S1124 R1127 L1128 K1129 E1130 L1131 K1132 I1133 N1139 H1140 I1141 S1142 S1143 L1144 S1145 E1146 N1147 F1148 L1149 E1150 A1151 C1152 P1153 K1154 S1157 R1161 M1162 N1163 F1164
A1167 S1174 M1175 K1179 N1183 C1187 I1188 P1189 E1190 A1191 I1192 L1195 L1198 L1201 D1202 H1216 W1217 K1218 S1219 L1220 N1221 L1222 L1225 L1235 D1236 L1237 S1238 E1239 K1240 A1241 Y1242 L1243 E1248 L1262 L1257 P1262 E1263 C1266 L1270 D1274 V1275 S1276
Y1277 N1278 R1282 K1290 L1291 D1300 F1306 D1307 F1308 K1309 H1310 C1313 K1314 A1315 K1316 R1320 Q1323 L1326 K1327 L1337 M1338 I1339 K1347 L1351 K1356 T1357 K1358 LYS SER ASP LEU GLY MET GLN S1366 A1367 T1368 D1375 I1380 R1381 D1382 K1383 R1384 K1385 R1386 D1387
L1388 N1391 V1392 E1400 D1420 K1423 M1431 K1432 P1433 W1434 L1435 F1436 N1437 R1441 H1453 L1454 D1455 V1456 S1457 ASP GLU LYS GLN ARG K1463 S1467 K1471 L1474 Y1485 H1486 F1487 V1488 N1489 A1490 D1495 L1509 V1519 E1529 S1536 N1540 I1543
I1548 D1549 Q1555 E1559 N1560 Q1561 L1562 Q1563 L1564 E1578 L1583 Q1586 D1587 L1592 V1598 E1599 P1600 I1606 M1607 T1612 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 L1653 I1658 A1659 LEU PRO ILE GLY GLU GLU TYR LEU L1668 S1672 L1673 H1684 R1693 L1694 Y1695 G1703 R1707 R1711 L1720 SER GLY ARG GLU ARG A1726 W1734 R1735 Q1736 P1744 Y1747 L1763 P1768 R1771 W1791 I1798 D1799 ILE CYS GLY


GLU G1804 E1805 Y1814 D1818 G1819 L1827 E1836 D1844 R1847 D1858 A1862 R1866 N1867 I1868 M1869 L1870 L1875 A1880 P1881 E1882 F1883 L1884 D1887 G1888 S1889 F1890 G1891 S1892 V1893 Y1894 R1895 E1899 G1900 V1905 K1906 I1907 F1908 N1909 K1910 H1911 T1912 S1913 L1914 R1915
E1920 L1924 L1932 I1933 P1942 R1943 M1944 L1945 V1946 M1947 D1956 L1959 Q1960 Q1961 D1962 D1980 M1989 K1996 P1997 H1998 K2014 I2015 A2016 G2019 I2020 ALA GLN TYR CYS CYS ARG MET GLY ILE LYS THR SER GLU G2034 T2035 P2036 G2037 A2044 R2045 G2046 N2047 V2048 I2049 Y2050
Y2057 G2070 V2074 GLU GLY LEU LYS PHE PRO ASN GLU PHE ASP GLU LEU GLU ILE GLN GLY K2091 K2097 G2100 C2101 W2104 P2105 M2106 V2107 Q2120 E2121 R2122 P2123 T2124 S2134 A2135 E2136 L2137 R2143 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 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 G2317 G2318 C2319 G2320 T2321 K2322 I2323 P2324 S2325 F2326 S2327 N2328 D2329 P2330 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 V2359 D2360 T2361 A2362 L2363 Y2364 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 T2416 L2419 Q2420 K2421 N2422 T2423 I2427 G2431 I2434 L2435 L2436 L2439 S2440 T2441 R2442 R2443 L2444 V2447 N2450 F2451 C2452 R2456 Q2462 L2463 G2464 S2465 L2466 K2467 V2472 Y2475 N2476 ARG LYS ASN THR GLU
GLY THR GLN LYS GLN LYS GLU T2489 Q2490 S2491 C2492 H2502 Q2505 R2514 R2523 T2524 S2525 V2526 E2527

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75005	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 ($e^-/Å^2$)	67.53	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	3.862	Depositor
Minimum map value	-2.223	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.8	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, 919

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	0.14	0/12507	0.41	0/17088
1	B	0.15	0/12507	0.42	0/17088
All	All	0.15	0/25014	0.42	0/34176

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2104	TRP	Peptide
1	B	2104	TRP	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	12278	0	11696	122	0
1	B	12278	0	11696	115	0
2	A	28	0	12	1	0
2	B	28	0	12	1	0
3	A	41	0	28	3	0
3	B	41	0	28	3	0
All	All	24694	0	23472	237	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 5.

All (237) 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:1933:ILE:HD13	1:B:2014:LYS:HD2	1.77	0.67
1:B:1161:ARG:O	1:B:1163:ASN:ND2	2.28	0.67
1:A:1933:ILE:HD13	1:A:2014:LYS:HD2	1.77	0.66
1:B:2427:ILE:HB	1:B:2435:LEU:HB2	1.78	0.66
1:A:1161:ARG:O	1:A:1163:ASN:ND2	2.29	0.65
1:B:1351:LEU:HD21	1:B:1392:VAL:HG21	1.78	0.65
1:A:1653:LEU:HG	1:A:1658:ILE:HB	1.79	0.64
1:B:1653:LEU:HG	1:B:1658:ILE:HB	1.80	0.64
1:A:2427:ILE:HB	1:A:2435:LEU:HB2	1.78	0.64
1:A:1351:LEU:HD21	1:A:1392:VAL:HG21	1.79	0.63
1:B:2373:VAL:HB	1:B:2387:ILE:HB	1.81	0.62
1:A:1906:LYS:HE3	1:A:1908:PHE:HE1	1.64	0.62
1:A:1921:LEU:O	1:A:1925:CYS:HB2	2.01	0.61
1:B:1906:LYS:HE3	1:B:1908:PHE:HE1	1.64	0.61
1:A:1034:LEU:HD13	1:A:1037:LEU:HD11	1.82	0.61
1:A:2300:LEU:HA	1:A:2319:CYS:HA	1.83	0.60
1:B:2259:GLN:OE1	1:B:2328:ASN:ND2	2.34	0.60
1:B:2300:LEU:HA	1:B:2319:CYS:HA	1.83	0.60
1:B:1034:LEU:HD13	1:B:1037:LEU:HD11	1.83	0.59
1:A:2279:THR:HG22	1:A:2285:ALA:HB1	1.86	0.58
1:A:2373:VAL:HB	1:A:2387:ILE:HB	1.84	0.58
1:A:2259:GLN:OE1	1:A:2328:ASN:ND2	2.34	0.58
1:B:2236:HIS:NE2	1:B:2280:VAL:O	2.36	0.58
1:A:1041:ASP:OD1	1:A:1043:HIS:ND1	2.36	0.58
1:B:1905:VAL:HG12	1:B:1946:VAL:HG22	1.86	0.57
1:B:2279:THR:HG22	1:B:2285:ALA:HB1	1.85	0.57
1:A:1827:LEU:HD23	1:A:1832:LYS:HZ3	1.68	0.57
1:B:688:ASP:HB3	1:B:691:PHE:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1041:ASP:OD1	1:B:1043:HIS:ND1	2.38	0.57
1:B:1932:LEU:HD22	3:B:2602:919:H85	1.87	0.56
1:B:1881:PRO:HB2	1:B:1883:PHE:HB3	1.86	0.56
1:A:688:ASP:HB3	1:A:691:PHE:HB3	1.87	0.56
1:B:1583:LEU:HG	1:B:1600:PRO:HB3	1.86	0.56
1:B:1222:LEU:HD22	1:B:1225:LEU:HD11	1.86	0.56
1:A:1128:LEU:HD12	1:A:1131:LEU:HD13	1.88	0.56
1:B:762:LEU:HD11	1:B:790:LEU:HD23	1.88	0.56
1:B:1420:ASP:OD1	1:B:1453:HIS:ND1	2.39	0.55
1:A:1932:LEU:HD22	3:A:2602:919:H85	1.87	0.55
1:B:1509:LEU:HA	1:B:1519:VAL:HG21	1.89	0.55
1:A:1583:LEU:HG	1:A:1600:PRO:HB3	1.87	0.55
1:A:2134:SER:OG	1:A:2136:GLU:OE1	2.24	0.55
1:A:1441:ARG:NH1	1:A:1791:TRP:O	2.34	0.55
1:A:2420:GLN:HE21	1:A:2424:ALA:HB3	1.72	0.55
1:B:2434:ILE:HD11	1:B:2472:VAL:HG11	1.90	0.54
1:A:1420:ASP:OD1	1:A:1453:HIS:ND1	2.41	0.54
1:A:1509:LEU:HA	1:A:1519:VAL:HG21	1.91	0.53
1:B:2419:LEU:HD11	1:B:2439:LEU:HD11	1.90	0.53
1:B:1095:LEU:HB2	1:B:1117:ASN:HD22	1.73	0.53
1:B:2152:VAL:HG21	1:B:2169:LEU:HD12	1.91	0.53
1:B:1128:LEU:HD12	1:B:1131:LEU:HD13	1.89	0.53
1:A:1222:LEU:HD22	1:A:1225:LEU:HD11	1.90	0.53
1:A:1881:PRO:HB2	1:A:1883:PHE:HB3	1.91	0.53
1:A:1905:VAL:HG12	1:A:1946:VAL:HG22	1.90	0.53
1:A:2419:LEU:HD11	1:A:2439:LEU:HD11	1.91	0.53
1:A:762:LEU:HD11	1:A:790:LEU:HD23	1.90	0.52
1:A:2152:VAL:HG21	1:A:2169:LEU:HD12	1.92	0.52
1:A:1996:LYS:HE2	1:A:1998:HIS:HB3	1.90	0.52
1:A:2236:HIS:NE2	1:A:2280:VAL:O	2.41	0.52
1:B:1375:ASP:N	1:B:1375:ASP:OD1	2.43	0.51
1:B:1996:LYS:HE2	1:B:1998:HIS:HB3	1.91	0.51
1:A:1375:ASP:OD1	1:A:1375:ASP:N	2.43	0.51
1:A:2434:ILE:HD11	1:A:2472:VAL:HG11	1.93	0.51
1:A:1870:LEU:HD21	1:A:1875:LEU:HD22	1.93	0.51
1:A:2356:THR:HG21	1:A:2416:THR:HA	1.92	0.51
1:B:2057:TYR:HD1	1:B:2122:ARG:HH12	1.58	0.51
1:B:1195:LEU:HD12	1:B:1198:LEU:HD13	1.93	0.50
1:B:1870:LEU:HD21	1:B:1875:LEU:HD22	1.93	0.50
1:B:2134:SER:OG	1:B:2136:GLU:OE1	2.25	0.50
1:A:1095:LEU:HB2	1:A:1117:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1906:LYS:HE3	1:A:1908:PHE:CE1	2.46	0.49
1:A:2456:ARG:NH1	1:A:2475:TYR:OH	2.46	0.49
1:B:1337:LEU:HD23	1:B:1392:VAL:HG12	1.94	0.49
1:B:1351:LEU:HD11	1:B:1392:VAL:HG11	1.95	0.49
1:A:1270:LEU:HD12	1:A:1291:LEU:HD13	1.95	0.49
1:B:1056:LYS:HE3	1:B:1080:VAL:HG22	1.95	0.49
1:B:1368:THR:OG1	2:B:2601:GDP:O1B	2.28	0.49
1:B:2355:ILE:HG22	1:B:2356:THR:HG23	1.95	0.48
1:A:2057:TYR:HD1	1:A:2122:ARG:HH12	1.61	0.48
1:B:1906:LYS:HE3	1:B:1908:PHE:CE1	2.45	0.48
1:A:1548:ILE:HD12	1:A:1598:VAL:HG21	1.95	0.48
1:B:1270:LEU:HD12	1:B:1291:LEU:HD13	1.94	0.48
1:B:1441:ARG:NH1	1:B:1791:TRP:O	2.38	0.48
1:B:1734:TRP:CD1	1:B:1736:GLN:H	2.31	0.48
1:B:2356:THR:HG21	1:B:2416:THR:HA	1.96	0.48
1:A:1036:SER:O	1:A:1036:SER:OG	2.30	0.48
1:A:1693:ARG:NH2	1:A:1858:ASP:OD1	2.47	0.48
1:B:1133:ILE:HG12	1:B:1157:SER:HB3	1.95	0.48
1:A:1695:TYR:HB2	1:A:1763:LEU:HB3	1.96	0.48
1:B:1431:MET:HE2	1:B:1435:LEU:HD11	1.96	0.48
1:A:2355:ILE:HG22	1:A:2356:THR:HG23	1.95	0.48
1:B:1884:LEU:O	1:B:1895:ARG:N	2.47	0.47
1:A:1734:TRP:CD1	1:A:1736:GLN:H	2.31	0.47
1:A:2019:GLY:HA2	3:A:2602:919:H13	1.96	0.47
1:B:1023:LEU:HB2	1:B:1045:ASN:HD22	1.79	0.47
1:B:2177:GLY:N	1:B:2195:ALA:O	2.47	0.47
1:B:1606:ILE:HG22	1:B:1607:MET:HE2	1.97	0.47
1:A:1056:LYS:HE3	1:A:1080:VAL:HG22	1.96	0.47
1:A:2170:GLY:HA3	1:A:2199:ILE:HD11	1.97	0.46
1:B:1548:ILE:HD12	1:B:1598:VAL:HG21	1.96	0.46
1:A:1339:ILE:HG22	1:A:1347:LYS:HG2	1.97	0.46
1:A:1375:ASP:HA	1:A:1391:ASN:HA	1.97	0.46
1:A:1351:LEU:HD11	1:A:1392:VAL:HG11	1.97	0.46
1:A:2423:THR:HB	1:A:2439:LEU:HB2	1.97	0.46
1:B:1067:ARG:HG2	1:B:1883:PHE:HE1	1.80	0.46
1:B:2276:GLU:HG3	1:B:2279:THR:H	1.81	0.46
1:B:2456:ARG:NH1	1:B:2475:TYR:OH	2.49	0.46
1:B:2143:ARG:NH2	1:B:2451:PHE:O	2.49	0.46
1:A:795:ALA:HB2	1:A:808:PHE:HE2	1.81	0.46
1:A:1276:SER:O	1:A:1278:ASN:ND2	2.49	0.46
1:B:1339:ILE:HG22	1:B:1347:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1375:ASP:HA	1:B:1391:ASN:HA	1.97	0.46
1:B:2019:GLY:HA2	3:B:2602:919:H13	1.97	0.46
1:A:1467:SER:HB2	1:A:1487:PHE:HZ	1.81	0.46
1:B:1956:ASP:HB2	1:B:1998:HIS:HA	1.98	0.46
1:B:2170:GLY:HA3	1:B:2199:ILE:HD11	1.97	0.46
1:A:1161:ARG:HH21	1:A:1179:LYS:HB3	1.81	0.45
1:A:2177:GLY:N	1:A:2195:ALA:O	2.50	0.45
1:B:1489:ASN:OD1	1:B:1490:ALA:N	2.49	0.45
1:B:1920:GLU:HA	3:B:2602:919:H3	1.99	0.45
1:A:2104:TRP:CH2	1:A:2107:VAL:HG21	2.51	0.45
1:B:1747:TYR:CE2	1:B:1768:PRO:HG3	2.52	0.45
1:A:1431:MET:HE2	1:A:1435:LEU:HD11	1.99	0.45
1:A:1489:ASN:OD1	1:A:1490:ALA:N	2.48	0.45
1:A:1730:ASN:H	1:A:1730:ASN:HD22	1.64	0.45
1:A:1980:ASP:OD2	1:A:2514:ARG:NH1	2.44	0.45
1:B:1433:PRO:O	1:B:1437:ASN:ND2	2.49	0.45
1:B:1933:ILE:HG13	1:B:2016:ALA:HB2	1.98	0.45
1:A:2152:VAL:HG21	1:A:2169:LEU:HB2	1.99	0.45
1:B:1161:ARG:HH21	1:B:1179:LYS:HB3	1.82	0.45
1:B:1276:SER:O	1:B:1278:ASN:ND2	2.49	0.45
1:B:1703:GLY:O	1:B:1707:ARG:HD2	2.16	0.45
1:A:1133:ILE:HG12	1:A:1157:SER:HB3	1.99	0.45
1:B:795:ALA:HB2	1:B:808:PHE:HE2	1.82	0.45
1:A:1218:LYS:HE2	1:A:1218:LYS:HB3	1.78	0.45
1:B:2104:TRP:CH2	1:B:2107:VAL:HG21	2.52	0.45
1:B:1868:ILE:HD12	1:B:1868:ILE:HA	1.81	0.44
1:A:1606:ILE:HG22	1:A:1607:MET:HE2	1.99	0.44
1:A:1287:GLU:O	1:A:1290:LYS:NZ	2.48	0.44
1:A:1433:PRO:O	1:A:1437:ASN:ND2	2.50	0.44
1:A:2276:GLU:HG3	1:A:2279:THR:H	1.82	0.44
1:B:2423:THR:HB	1:B:2439:LEU:HB2	2.00	0.44
1:A:1368:THR:OG1	2:A:2601:GDP:O1B	2.32	0.44
1:A:1956:ASP:HB2	1:A:1998:HIS:HA	1.99	0.44
1:B:1695:TYR:HB2	1:B:1763:LEU:HB3	1.98	0.44
1:B:1771:ARG:NH1	1:B:1862:ALA:O	2.51	0.44
1:A:1933:ILE:HG13	1:A:2016:ALA:HB2	1.99	0.44
1:A:1672:SER:H	1:A:1735:ARG:HH12	1.65	0.44
1:B:1942:PRO:HD2	1:B:1944:MET:HE3	1.99	0.44
1:A:2182:LEU:HD13	1:A:2189:TYR:HB3	2.00	0.44
1:A:2178:GLN:HA	1:A:2193:GLU:HA	2.00	0.43
1:A:1034:LEU:HB3	1:A:1037:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1175:MET:HE3	1:A:1175:MET:HB2	1.82	0.43
1:B:696:CYS:HB3	1:B:843:VAL:HG12	2.01	0.43
1:B:730:LEU:HD21	1:B:2441:THR:HG22	1.99	0.43
1:A:730:LEU:HD21	1:A:2441:THR:HG22	1.99	0.43
1:A:1747:TYR:CE2	1:A:1768:PRO:HG3	2.53	0.43
1:A:1885:LEU:HD12	1:A:1886:GLY:H	1.84	0.43
1:B:1467:SER:HB2	1:B:1487:PHE:HZ	1.82	0.43
1:B:2106:MET:HE3	1:B:2137:LEU:HA	2.00	0.43
1:A:696:CYS:HB3	1:A:843:VAL:HG12	2.00	0.43
1:A:1771:ARG:NH1	1:A:1862:ALA:O	2.52	0.43
1:B:1183:ASN:OD1	1:B:1183:ASN:N	2.52	0.43
1:B:1673:LEU:HD23	1:B:1673:LEU:HA	1.86	0.43
1:A:989:LEU:HB2	1:A:1018:LEU:HD23	2.01	0.43
1:B:1672:SER:H	1:B:1735:ARG:HH12	1.66	0.43
1:A:1074:VAL:HG23	1:A:1095:LEU:HD21	2.01	0.43
1:A:1703:GLY:O	1:A:1707:ARG:HD2	2.18	0.43
1:A:1868:ILE:HD12	1:A:1868:ILE:HA	1.81	0.43
1:A:1013:LEU:HD12	1:A:1013:LEU:HA	1.89	0.43
1:A:1195:LEU:HD12	1:A:1198:LEU:HD13	2.00	0.43
1:A:1325:ARG:HG3	1:A:1524:PRO:HG3	2.00	0.43
1:B:2152:VAL:HG21	1:B:2169:LEU:HB2	2.00	0.43
1:B:2182:LEU:HD13	1:B:2189:TYR:HB3	2.00	0.43
1:A:1942:PRO:HD2	1:A:1944:MET:HE3	2.01	0.42
1:B:1423:LYS:H	1:B:1423:LYS:HG2	1.67	0.42
1:A:1180:LEU:O	1:A:1203:MET:HA	2.19	0.42
1:A:567:ILE:O	1:A:571:VAL:HG13	2.19	0.42
1:A:2202:LEU:HG	1:A:2217:SER:HB2	2.02	0.42
1:B:1218:LYS:HE2	1:B:1218:LYS:HB3	1.79	0.42
1:B:567:ILE:O	1:B:571:VAL:HG13	2.18	0.42
1:B:2154:CYS:HB3	1:B:2202:LEU:HD13	2.02	0.42
1:A:1877:PHE:HE1	1:A:1894:TYR:HB2	1.84	0.42
1:B:1980:ASP:OD2	1:B:2514:ARG:NH1	2.41	0.42
1:B:2152:VAL:HG12	1:B:2171:CYS:HB3	2.02	0.42
1:A:1920:GLU:HA	3:A:2602:919:H3	2.02	0.42
1:A:2276:GLU:HG3	1:A:2278:LYS:H	1.85	0.42
1:B:758:VAL:HG11	1:B:786:ILE:HD12	2.02	0.42
1:B:2218:GLY:HA2	1:B:2224:LEU:HG	2.01	0.42
1:B:2276:GLU:HG3	1:B:2278:LYS:H	1.84	0.42
1:A:2152:VAL:HG12	1:A:2171:CYS:HB3	2.01	0.42
1:B:1109:LEU:HB3	1:B:1128:LEU:HD13	2.02	0.42
1:B:1684:HIS:NE2	1:B:1744:PRO:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2202:LEU:HG	1:B:2217:SER:HB2	2.02	0.42
1:A:1183:ASN:OD1	1:A:1183:ASN:N	2.52	0.42
1:A:1474:LEU:HD23	1:A:1474:LEU:HA	1.84	0.42
1:B:2444:LEU:HD21	1:B:2447:VAL:HG23	2.01	0.42
1:B:2476:ASN:N	1:B:2490:GLN:O	2.52	0.42
1:A:2444:LEU:HD21	1:A:2447:VAL:HG23	2.02	0.41
1:B:1175:MET:HE3	1:B:1175:MET:HB2	1.81	0.41
1:A:1888:GLY:HA3	1:A:1890:PHE:CZ	2.55	0.41
1:A:2154:CYS:HB3	1:A:2202:LEU:HD13	2.02	0.41
1:B:1474:LEU:HD23	1:B:1474:LEU:HA	1.82	0.41
1:B:2178:GLN:HA	1:B:2193:GLU:HA	2.02	0.41
1:B:1924:LEU:HD21	1:B:1947:MET:HE1	2.02	0.41
1:A:1060:ILE:O	1:A:1084:THR:OG1	2.36	0.41
1:A:1067:ARG:HG2	1:A:1883:PHE:HE1	1.86	0.41
1:A:1423:LYS:H	1:A:1423:LYS:HG2	1.68	0.41
1:A:2218:GLY:HA2	1:A:2224:LEU:HG	2.02	0.41
1:A:2413:ARG:O	1:A:2430:GLY:N	2.42	0.41
1:A:2371:PRO:HB2	1:A:2390:VAL:HG23	2.03	0.41
1:B:1711:ARG:HE	1:B:1711:ARG:HB2	1.55	0.41
1:A:2106:MET:HE3	1:A:2137:LEU:HA	2.02	0.41
1:B:1257:LEU:HD23	1:B:1257:LEU:HA	1.87	0.41
1:A:1731:ARG:HD2	1:A:1733:TYR:OH	2.21	0.41
1:B:1015:LYS:HB2	1:B:1015:LYS:HE3	1.74	0.41
1:B:1693:ARG:NH2	1:B:1858:ASP:OD1	2.53	0.41
1:A:758:VAL:HG11	1:A:786:ILE:HD12	2.03	0.41
1:A:1248:GLU:O	1:A:1271:THR:OG1	2.37	0.41
1:A:1814:TYR:HE2	1:A:1827:LEU:HB2	1.84	0.41
1:A:2438:ASP:OD1	1:A:2438:ASP:N	2.54	0.41
1:B:1814:TYR:HE2	1:B:1827:LEU:HB2	1.85	0.41
1:B:2371:PRO:HB2	1:B:2390:VAL:HG23	2.03	0.41
1:A:724:MET:HE2	1:A:724:MET:HB3	1.97	0.41
1:A:1852:ILE:HB	1:A:1860:ILE:HD12	2.03	0.41
1:B:2151:ILE:HD12	1:B:2151:ILE:H	1.86	0.41
1:B:2214:TRP:CZ3	1:B:2228:ASN:HB2	2.56	0.41
1:A:1860:ILE:O	1:A:1862:ALA:N	2.53	0.40
1:B:1034:LEU:HB3	1:B:1037:LEU:HG	2.02	0.40
1:B:1119:ILE:HB	1:B:1139:ASN:HD22	1.86	0.40
1:A:1045:ASN:HD22	1:A:1045:ASN:N	2.19	0.40
1:A:1337:LEU:HD23	1:A:1392:VAL:HG12	2.03	0.40
1:A:2233:LYS:NZ	1:A:2235:ARG:HH21	2.20	0.40
1:B:2233:LYS:NZ	1:B:2235:ARG:HH21	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2363:LEU:HB2	1:B:2376:TRP:HB2	2.03	0.40
1:A:1607:MET:HE1	1:A:1649:TYR:CE2	2.57	0.40
1:B:1959:LEU:HD13	1:B:2070:GLY:HA3	2.02	0.40
1:B:2143:ARG:NE	1:B:2492:CYS:SG	2.95	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	1066/2527 (42%)	984 (92%)	82 (8%)	0	100	100
1	B	1682/2527 (67%)	1559 (93%)	123 (7%)	0	100	100
All	All	2748/5054 (54%)	2543 (92%)	205 (8%)	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	1202/2281 (53%)	1195 (99%)	7 (1%)	78	79
1	B	1202/2281 (53%)	1194 (99%)	8 (1%)	76	77
All	All	2404/4562 (53%)	2389 (99%)	15 (1%)	76	79

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1045	ASN
1	A	1310	HIS
1	A	1485	TYR
1	A	1868	ILE
1	A	1889	SER
1	A	1915	ARG
1	A	2020	ILE
1	B	1310	HIS
1	B	1485	TYR
1	B	1868	ILE
1	B	1890	PHE
1	B	1892	SER
1	B	1893	VAL
1	B	1915	ARG
1	B	2020	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	560	GLN
1	A	721	ASN
1	A	1087	GLN
1	A	1093	ASN
1	A	1229	HIS
1	A	1405	HIS
1	A	1425	GLN
1	A	1710	ASN
1	A	1730	ASN
1	A	2369	ASN
1	A	2420	GLN
1	A	2502	HIS
1	B	560	GLN
1	B	721	ASN
1	B	1045	ASN
1	B	1087	GLN
1	B	1093	ASN
1	B	1229	HIS
1	B	1710	ASN
1	B	1783	HIS
1	B	2369	ASN
1	B	2502	HIS

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)

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	GDP	B	2601	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
2	GDP	A	2601	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	6 (13%)
3	919	A	2602	-	45,45,45	2.15	7 (15%)	64,65,65	2.10	18 (28%)
3	919	B	2602	-	45,45,45	2.15	8 (17%)	64,65,65	2.08	18 (28%)

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	B	2601	-	-	2/16/32/32	0/3/3/3
2	GDP	A	2601	-	-	2/16/32/32	0/3/3/3
3	919	A	2602	-	-	4/28/28/28	0/5/5/5
3	919	B	2602	-	-	4/28/28/28	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2602	919	C70-N74	8.92	1.45	1.33
3	B	2602	919	C70-N74	8.85	1.45	1.33
3	A	2602	919	C48-N56	5.37	1.47	1.39
3	B	2602	919	C48-N56	5.35	1.47	1.39
3	A	2602	919	C58-N60	4.44	1.47	1.37
3	B	2602	919	C58-N60	4.34	1.47	1.37
3	B	2602	919	C48-N49	-4.34	1.32	1.36
3	A	2602	919	C48-N49	-4.26	1.32	1.36
3	A	2602	919	C5-C4	-3.66	1.36	1.42
3	B	2602	919	C5-C4	-3.63	1.36	1.42
3	B	2602	919	C58-N56	3.52	1.47	1.39
3	A	2602	919	C58-N56	3.45	1.47	1.39
2	A	2601	GDP	C5-C4	3.12	1.47	1.38
2	B	2601	GDP	C5-C4	3.09	1.47	1.38
3	A	2602	919	C39-N60	2.83	1.47	1.41
3	B	2602	919	C39-N60	2.83	1.47	1.41
2	A	2601	GDP	C6-N1	-2.47	1.34	1.38
2	B	2601	GDP	C6-N1	-2.45	1.34	1.38
2	B	2601	GDP	C5-N7	-2.19	1.34	1.39
2	A	2601	GDP	C5-N7	-2.14	1.34	1.39
3	B	2602	919	O63-C58	-2.01	1.19	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2602	919	C24-C70-N74	8.09	121.10	115.56
3	A	2602	919	C24-C70-N74	8.03	121.06	115.56
2	A	2601	GDP	C5-C4-N3	-6.28	118.40	128.39
2	B	2601	GDP	C5-C4-N3	-6.27	118.41	128.39
2	A	2601	GDP	C2-N3-C4	5.09	121.06	112.30
2	B	2601	GDP	C2-N3-C4	5.07	121.04	112.30
2	A	2601	GDP	N9-C4-N3	4.67	135.30	125.95
2	B	2601	GDP	N9-C4-N3	4.67	135.30	125.95
3	A	2602	919	C79-C46-N50	4.48	126.33	120.42
3	B	2602	919	C79-C46-N50	4.33	126.13	120.42
3	A	2602	919	N56-C48-N49	4.23	127.25	120.11
3	A	2602	919	C47-C48-N56	-4.18	125.76	132.60
3	B	2602	919	N56-C48-N49	4.03	126.92	120.11
3	B	2602	919	C47-C48-N56	-3.99	126.07	132.60
3	A	2602	919	C48-C47-C46	3.93	107.66	105.27
3	B	2602	919	C48-C47-C46	3.78	107.58	105.27
3	B	2602	919	C1-N49-C48	-3.73	126.12	129.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2602	919	C46-N50-N49	3.64	107.32	104.27
3	A	2602	919	C47-C46-N50	-3.57	107.64	111.86
3	A	2602	919	C1-N49-C48	-3.53	126.32	129.78
3	A	2602	919	C22-N23-C24	3.51	121.45	116.93
3	B	2602	919	C46-N50-N49	3.51	107.21	104.27
3	B	2602	919	C47-C46-N50	-3.49	107.73	111.86
3	B	2602	919	C22-N23-C24	3.44	121.36	116.93
3	B	2602	919	C1-N49-N50	3.27	123.41	118.67
3	A	2602	919	C1-N49-N50	3.19	123.29	118.67
3	B	2602	919	C70-C24-N23	3.07	121.01	117.42
2	A	2601	GDP	C6-C5-N7	3.06	135.86	130.29
2	B	2601	GDP	C6-C5-N7	3.05	135.84	130.29
3	A	2602	919	C70-C24-N23	3.04	120.97	117.42
3	B	2602	919	C14-C9-N10	-2.74	119.94	123.97
3	A	2602	919	C14-C9-N10	-2.74	119.95	123.97
3	A	2602	919	C27-C22-N23	-2.70	120.67	123.97
3	B	2602	919	C27-C22-N23	-2.68	120.69	123.97
2	A	2601	GDP	C4-C5-N7	-2.51	106.70	110.67
2	B	2601	GDP	C4-C5-N7	-2.49	106.72	110.67
3	A	2602	919	C37-C38-C39	-2.38	121.00	123.43
3	B	2602	919	C27-C26-C25	-2.37	117.32	120.50
3	A	2602	919	C27-C26-C25	-2.31	117.40	120.50
3	B	2602	919	O72-C70-N74	-2.22	119.38	122.67
3	A	2602	919	O72-C70-N74	-2.21	119.40	122.67
3	B	2602	919	C37-C38-C39	-2.18	121.20	123.43
3	A	2602	919	C25-C24-N23	-2.16	120.67	123.27
2	B	2601	GDP	O6-C6-C5	-2.16	120.83	126.53
2	A	2601	GDP	O6-C6-C5	-2.13	120.91	126.53
3	B	2602	919	C9-N10-C4	2.11	120.12	116.93
3	A	2602	919	C9-N10-C4	2.11	120.12	116.93
3	B	2602	919	C25-C24-N23	-2.10	120.75	123.27

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	GDP	C3'-C4'-C5'-O5'
2	B	2601	GDP	C3'-C4'-C5'-O5'
3	B	2602	919	C2-C1-N49-N50
3	A	2602	919	C2-C1-N49-N50
3	B	2602	919	C6-C1-N49-N50
3	A	2602	919	C6-C1-N49-N50

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Mol	Chain	Res	Type	Atoms
3	A	2602	919	C2-C1-N49-C48
3	A	2602	919	C6-C1-N49-C48
3	B	2602	919	C2-C1-N49-C48
3	B	2602	919	C6-C1-N49-C48
2	A	2601	GDP	O4'-C4'-C5'-O5'
2	B	2601	GDP	O4'-C4'-C5'-O5'

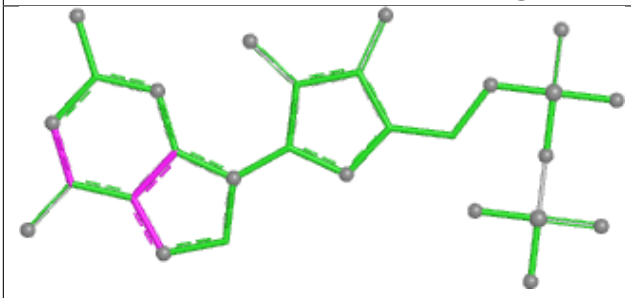
There are no ring outliers.

4 monomers are involved in 8 short contacts:

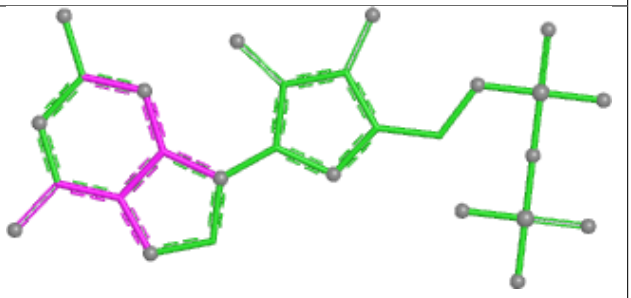
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2601	GDP	1	0
2	A	2601	GDP	1	0
3	A	2602	919	3	0
3	B	2602	919	3	0

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.

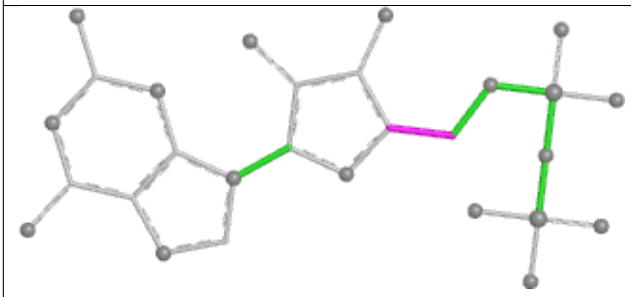
Ligand GDP B 2601



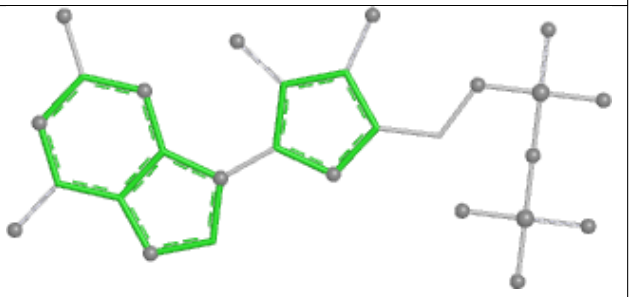
Bond lengths



Bond angles

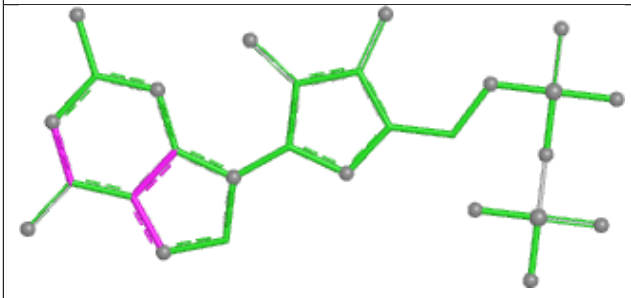


Torsions

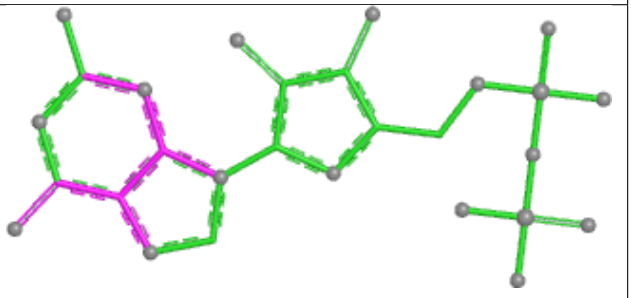


Rings

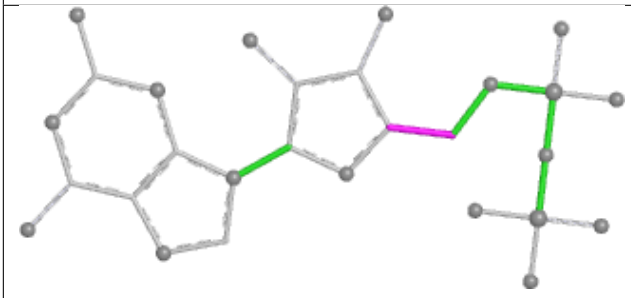
Ligand GDP A 2601



Bond lengths



Bond angles



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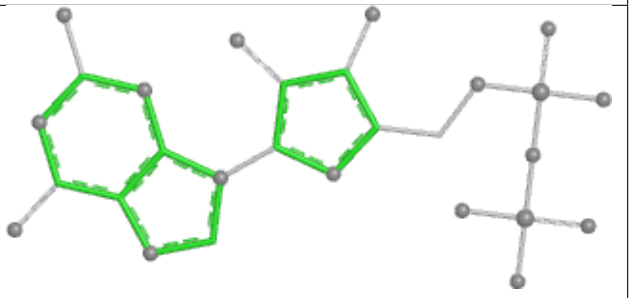
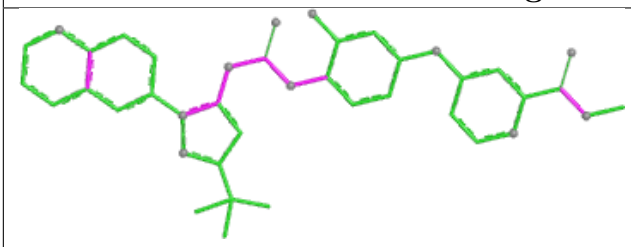
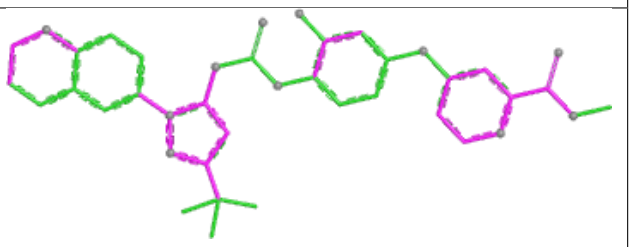
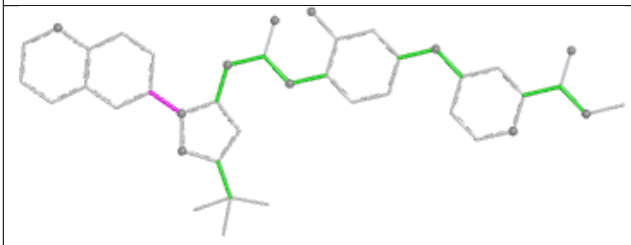
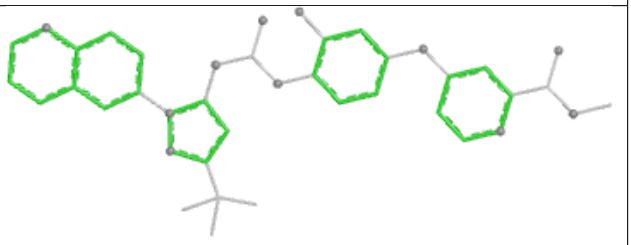


Rings

Ligand 919 A 2602	
	
Bond lengths	Bond angles
	
Torsions	Rings

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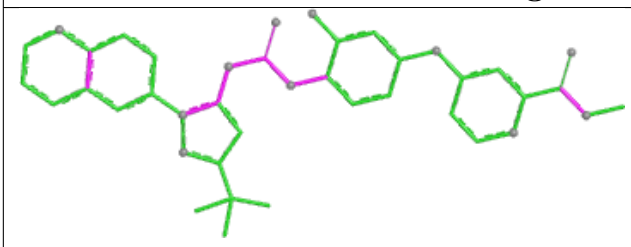
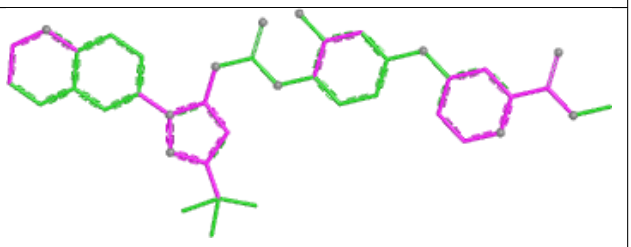
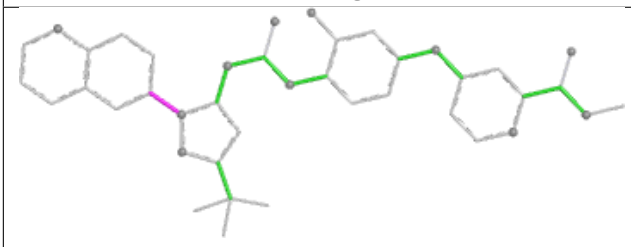
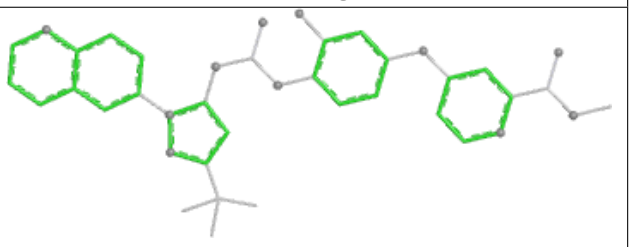
	
Bond lengths	Bond angles
	
Torsions	Rings

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.

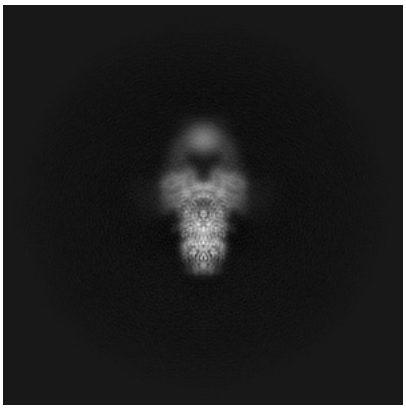
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42020. These allow visual inspection of the internal detail of the map and identification of artifacts.

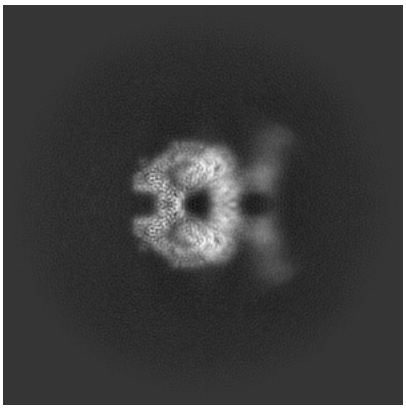
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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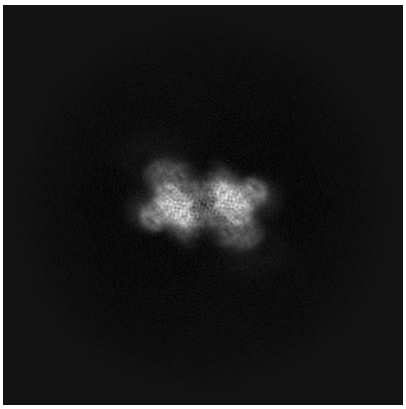
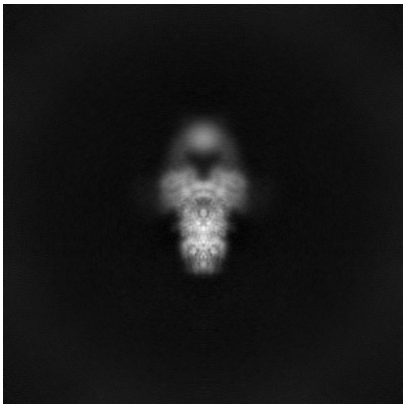


Z

6.1.2 Raw map



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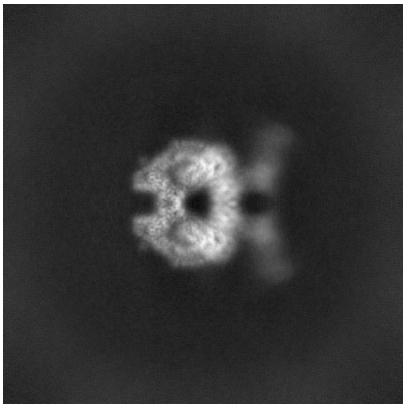
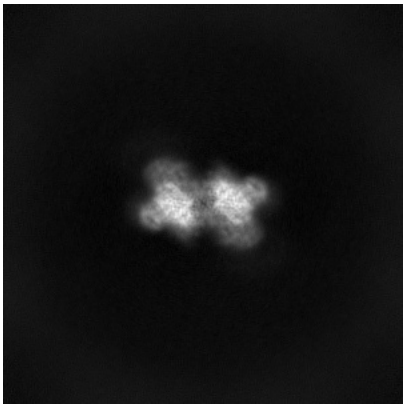


Y



Z

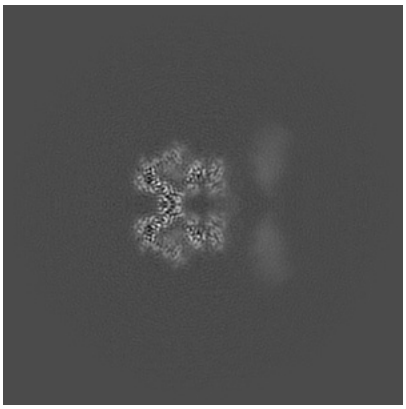
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 192



Y Index: 192

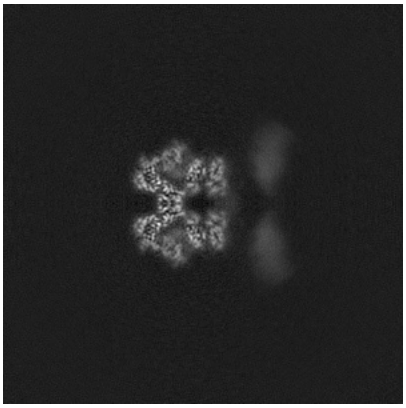


Z Index: 192

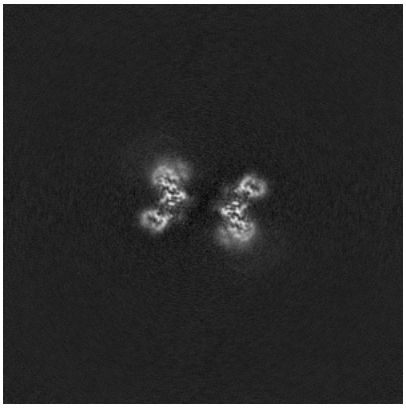
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

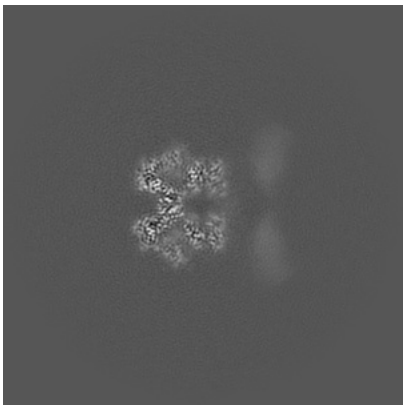
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

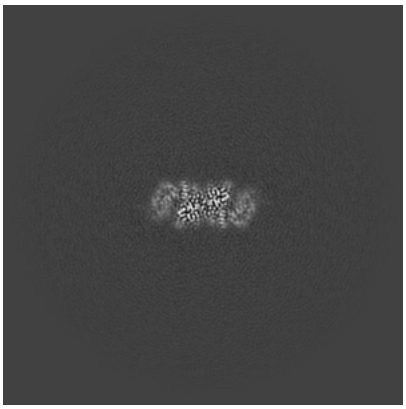
6.3.1 Primary map



X Index: 170



Y Index: 191

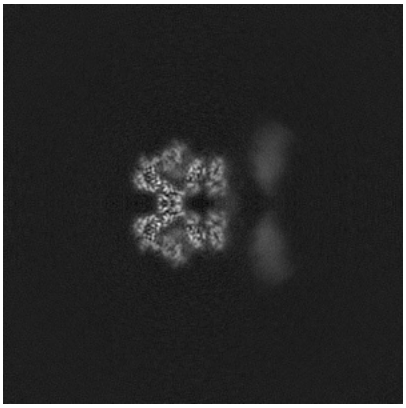


Z Index: 154

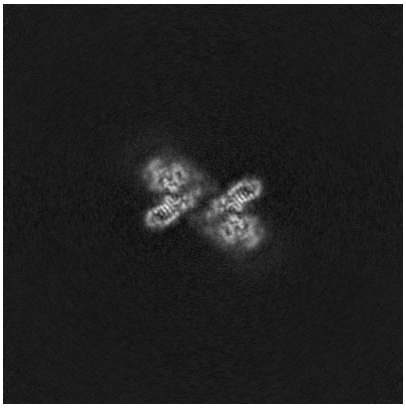
6.3.2 Raw map



X Index: 170



Y Index: 192

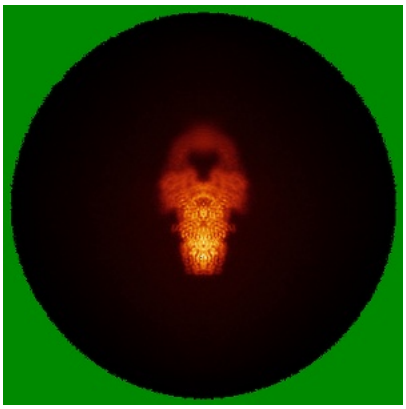


Z Index: 200

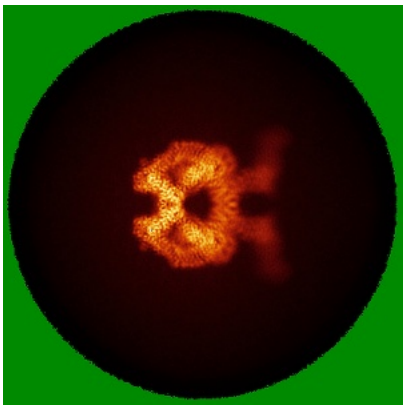
The images above show the largest variance slices of the map in three orthogonal directions.

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

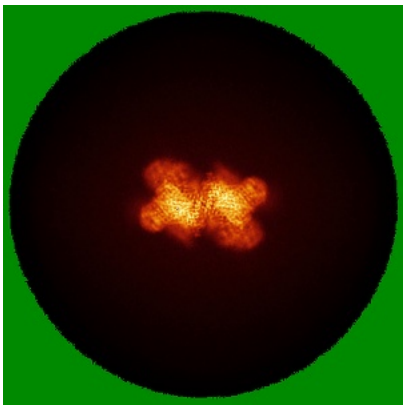
6.4.1 Primary map



X

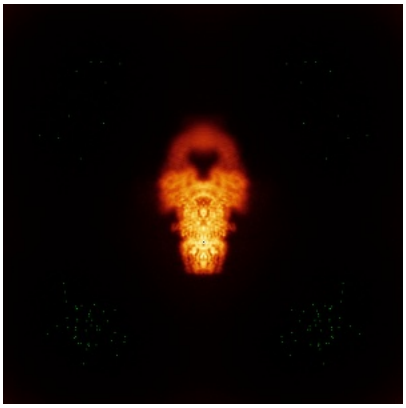


Y

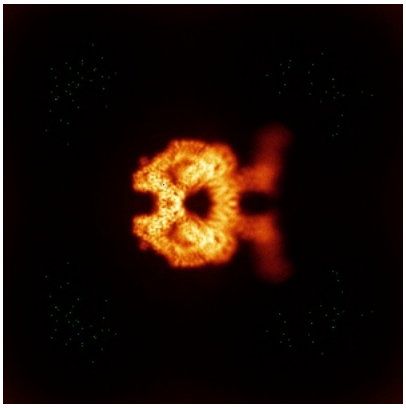


Z

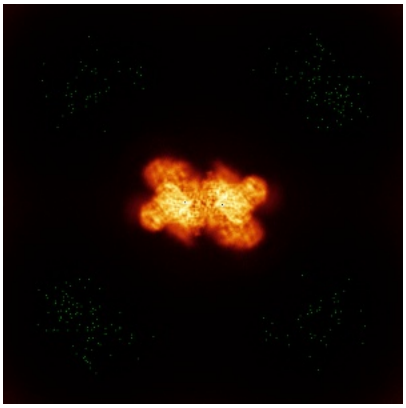
6.4.2 Raw map



X



Y

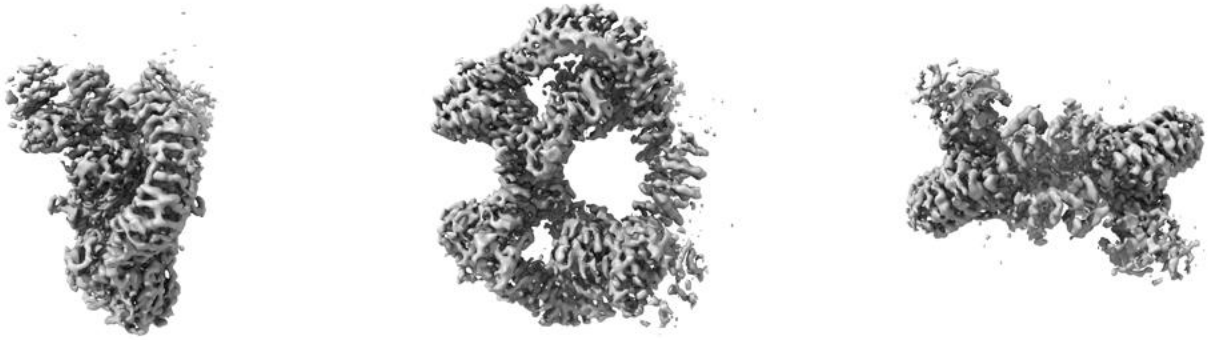


Z

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)

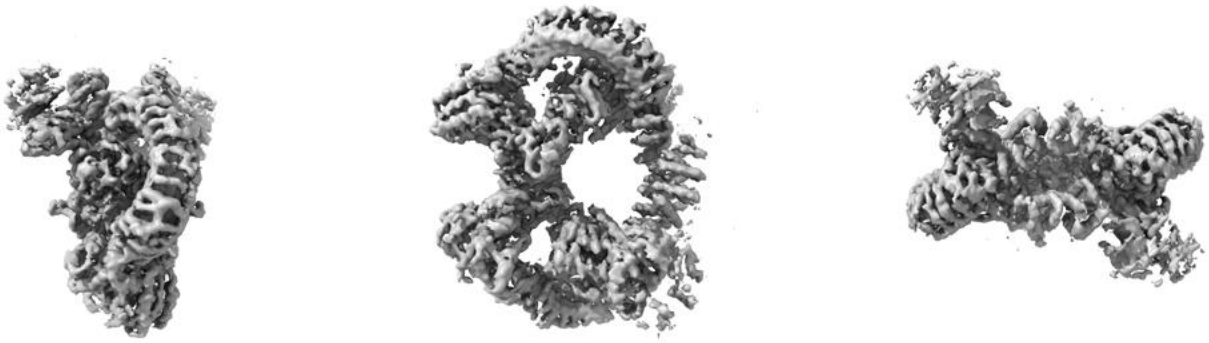
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

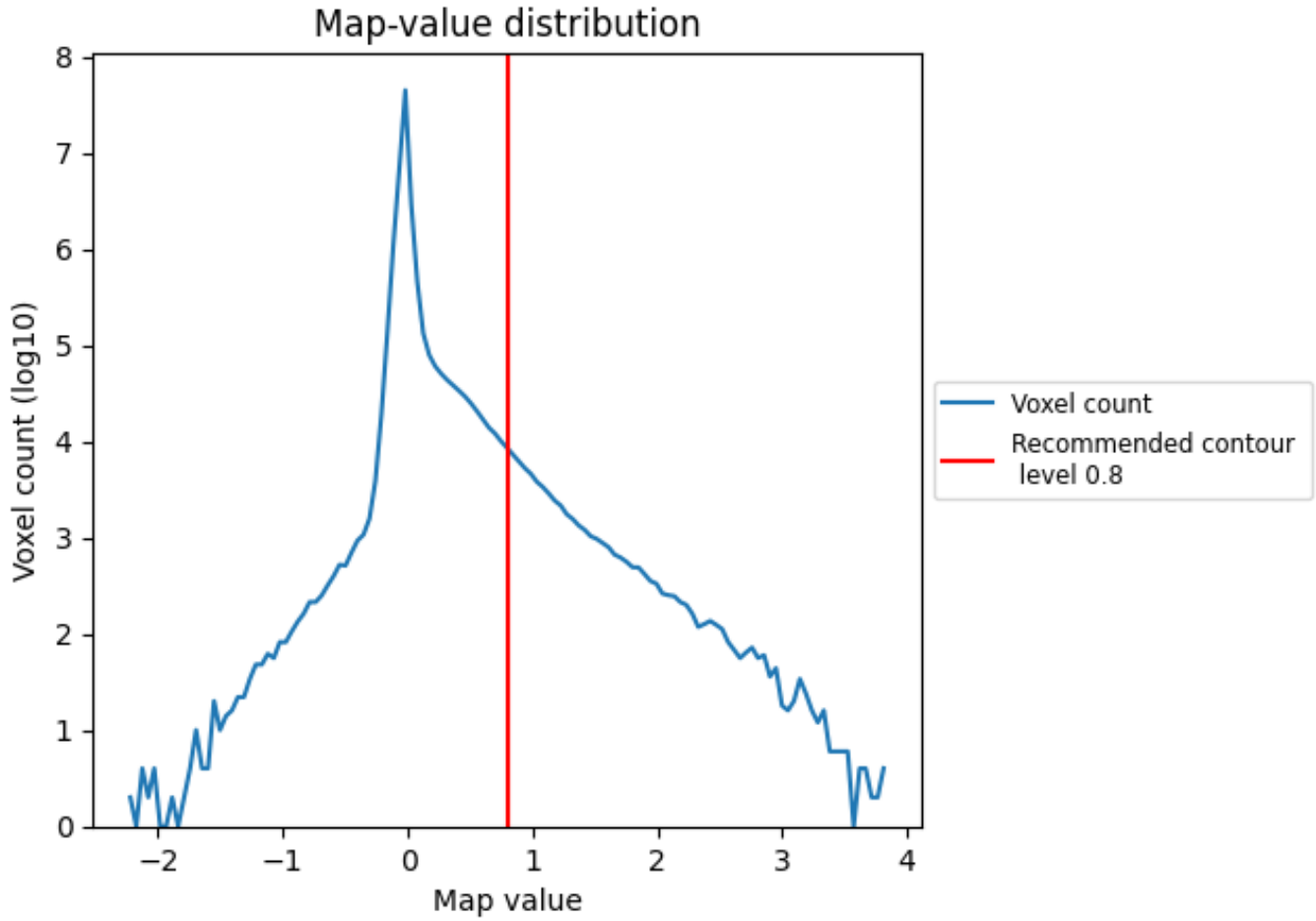
6.6 Mask visualisation (i)

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

7 Map analysis

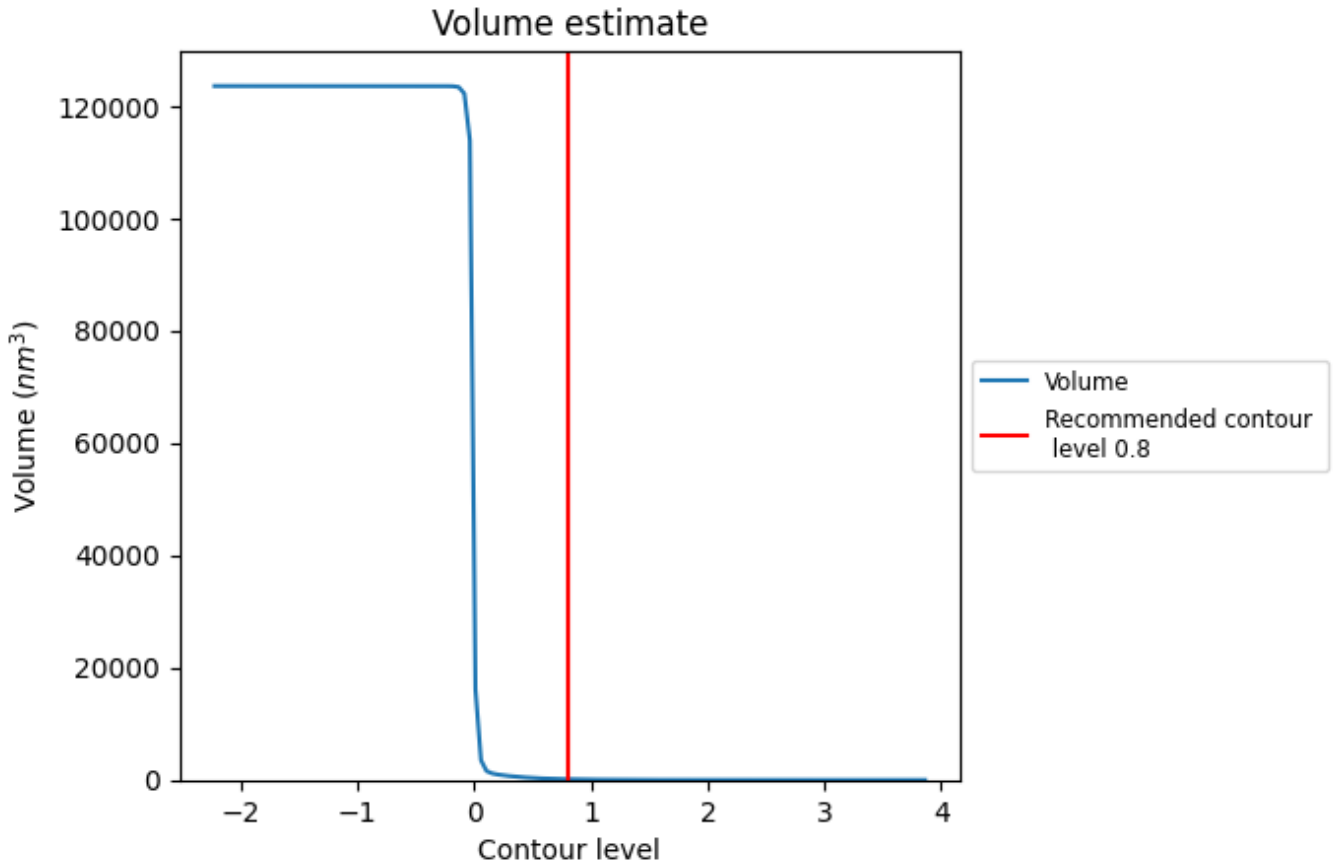
This section contains the results of statistical analysis of the map.

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.

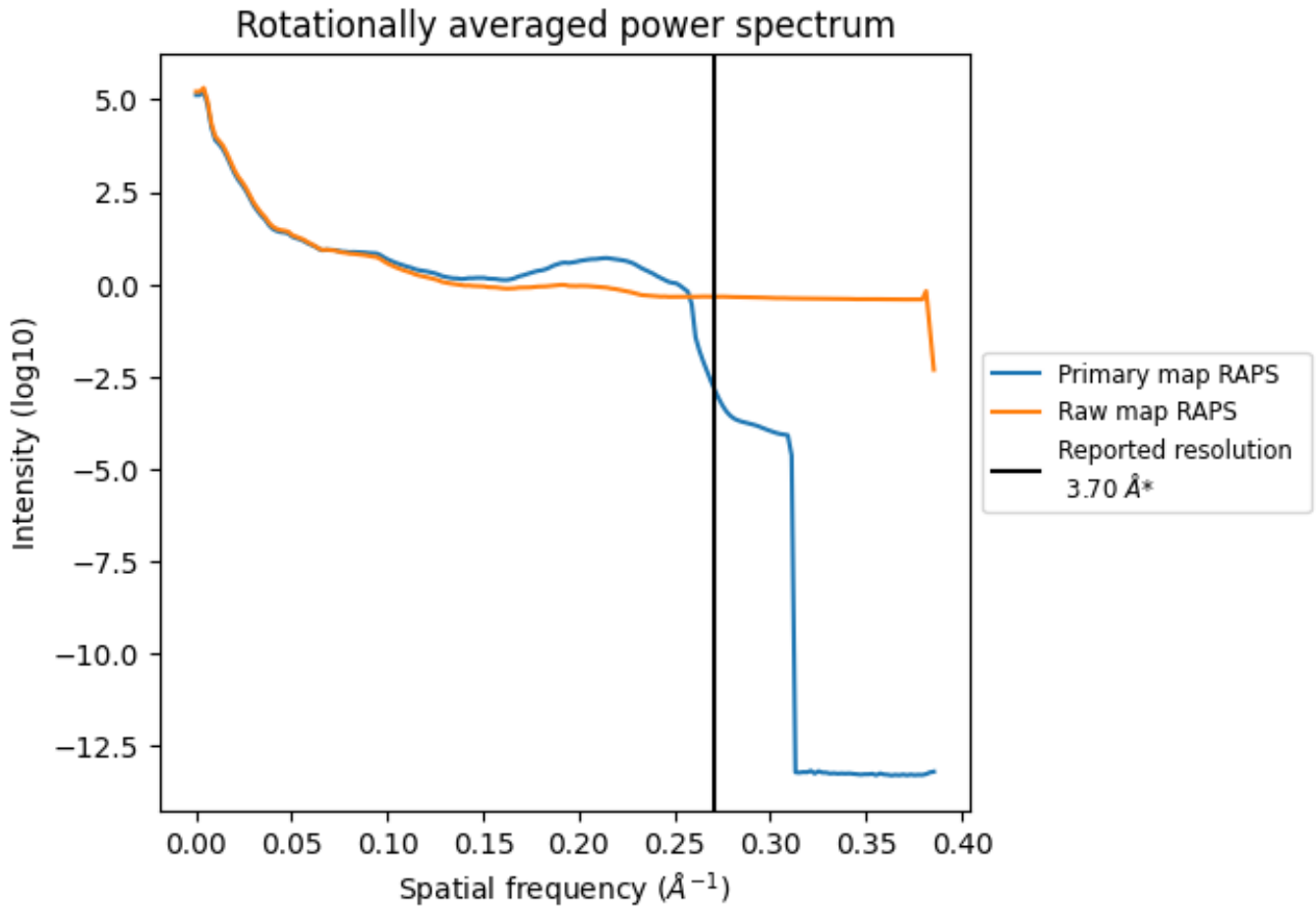
7.2 Volume estimate



The volume at the recommended contour level is 135 nm^3; this corresponds to an approximate mass of 122 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)

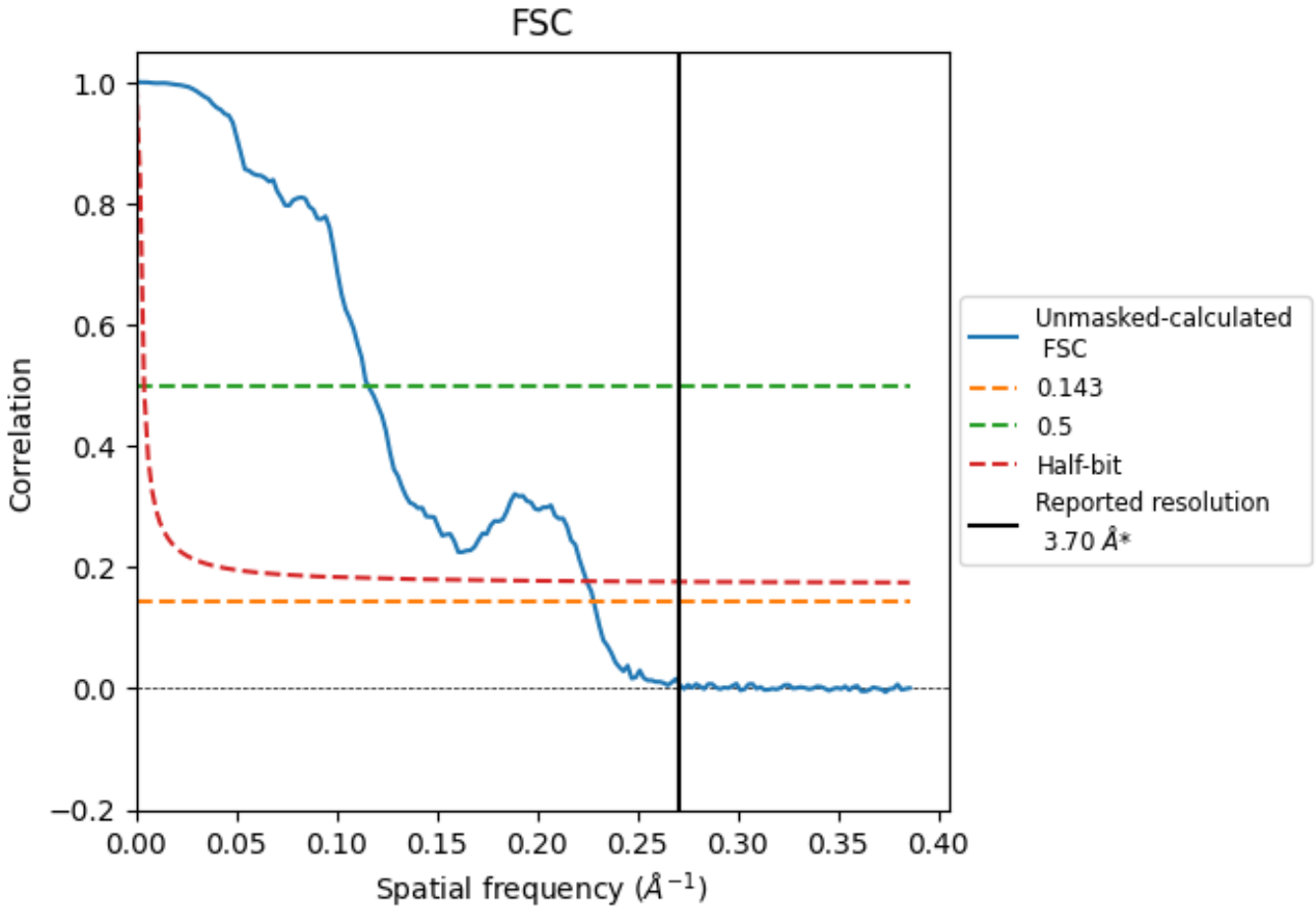


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

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 0.270 Å^{-1}

8.2 Resolution estimates (i)

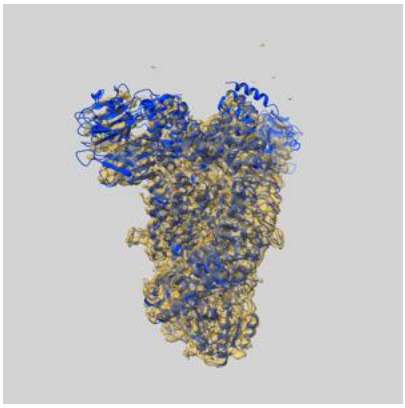
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.38	8.66	4.45

*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 4.38 differs from the reported value 3.7 by more than 10 %

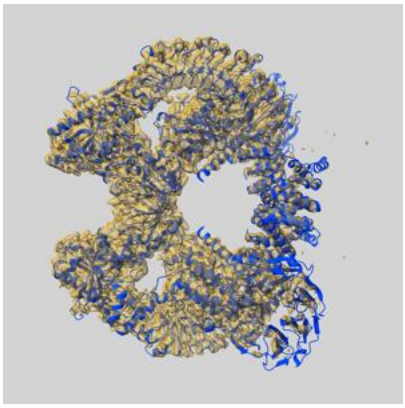
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42020 and PDB model 8U8B. Per-residue inclusion information can be found in section 3 on page 5.

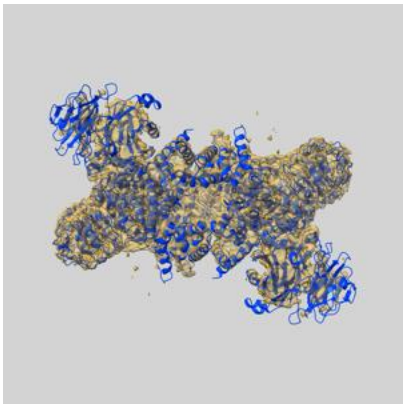
9.1 Map-model overlay



X



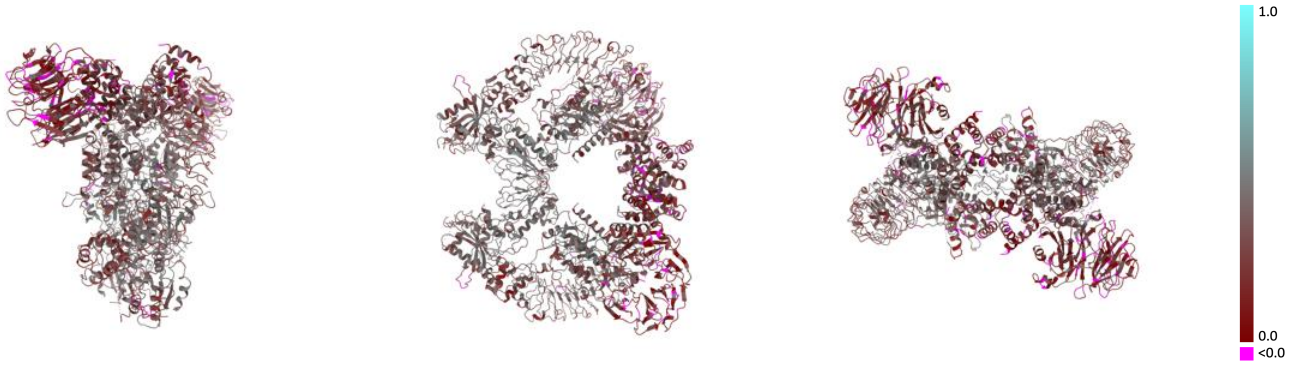
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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)



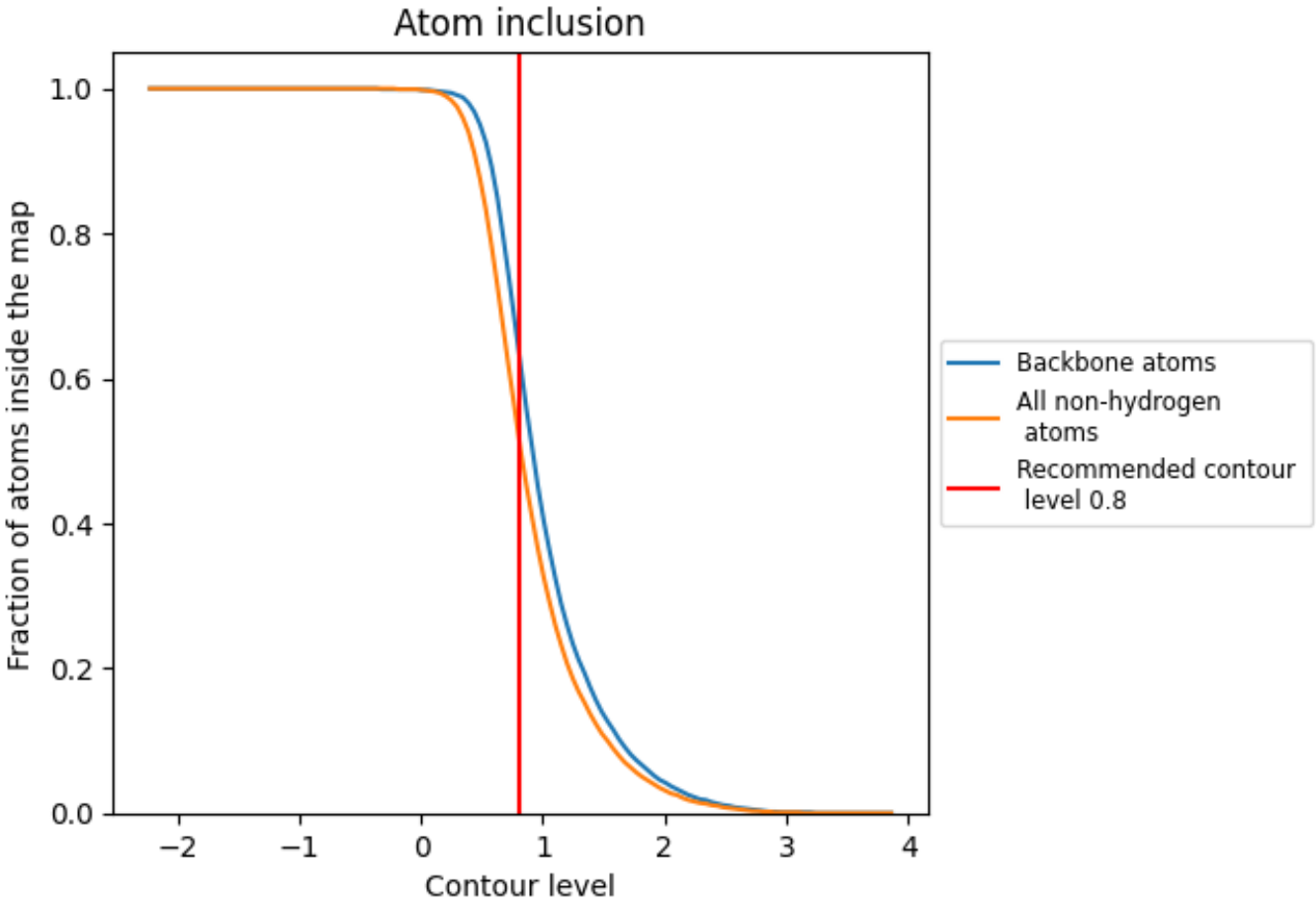
X Y Z

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)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 52% 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 (0.8) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.5230	0.3120
A	0.5210	0.3060
B	0.5250	0.3170