wwPDB EM Validation Summary Report (i)

Nov 13, 2021 – 05:15 am GMT

PDB ID	:	7PGT
EMDB ID	:	EMD-13395
Title	:	The structure of human neurofibromin isoform 2 in opened conformation.
Authors	:	Naschberger, A.; Baradaran, R.; Carroni, M.; Rupp, B.
Deposited on	:	2021-08-15
Resolution	:	4.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

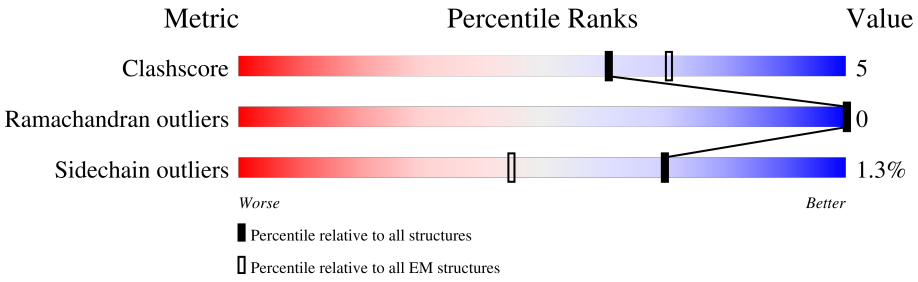
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	F	2839	19% 75% 10% 15%
1	N	2839	13% 74% 11% 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 77424 atoms, of which 38907 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 Neurofibromin.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	2423	Total	C	H	N	O	S	0	0
			38715	12314	19457	3266	3555	123		
1	F	2423	Total	C	H	N	O	S	0	0
			38708	12314	19450	3266	3555	123		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

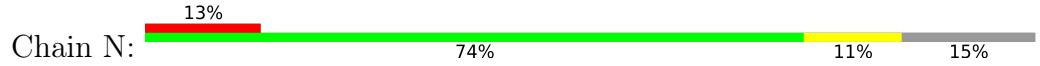
Mol	Chain	Residues	Atoms		AltConf
2	F	1	Total	Zn	0
			1	1	

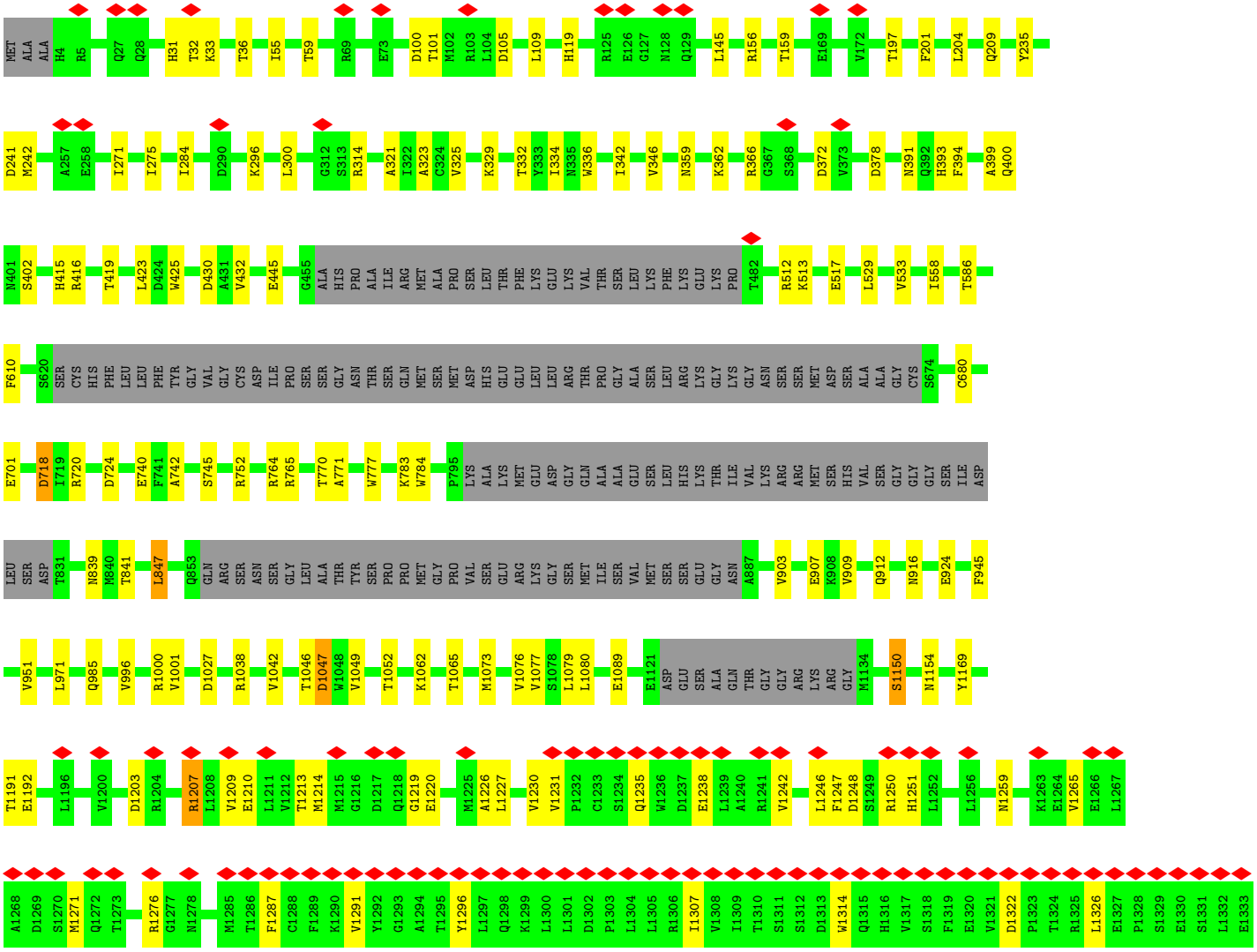
3 Residue-property plots (i)

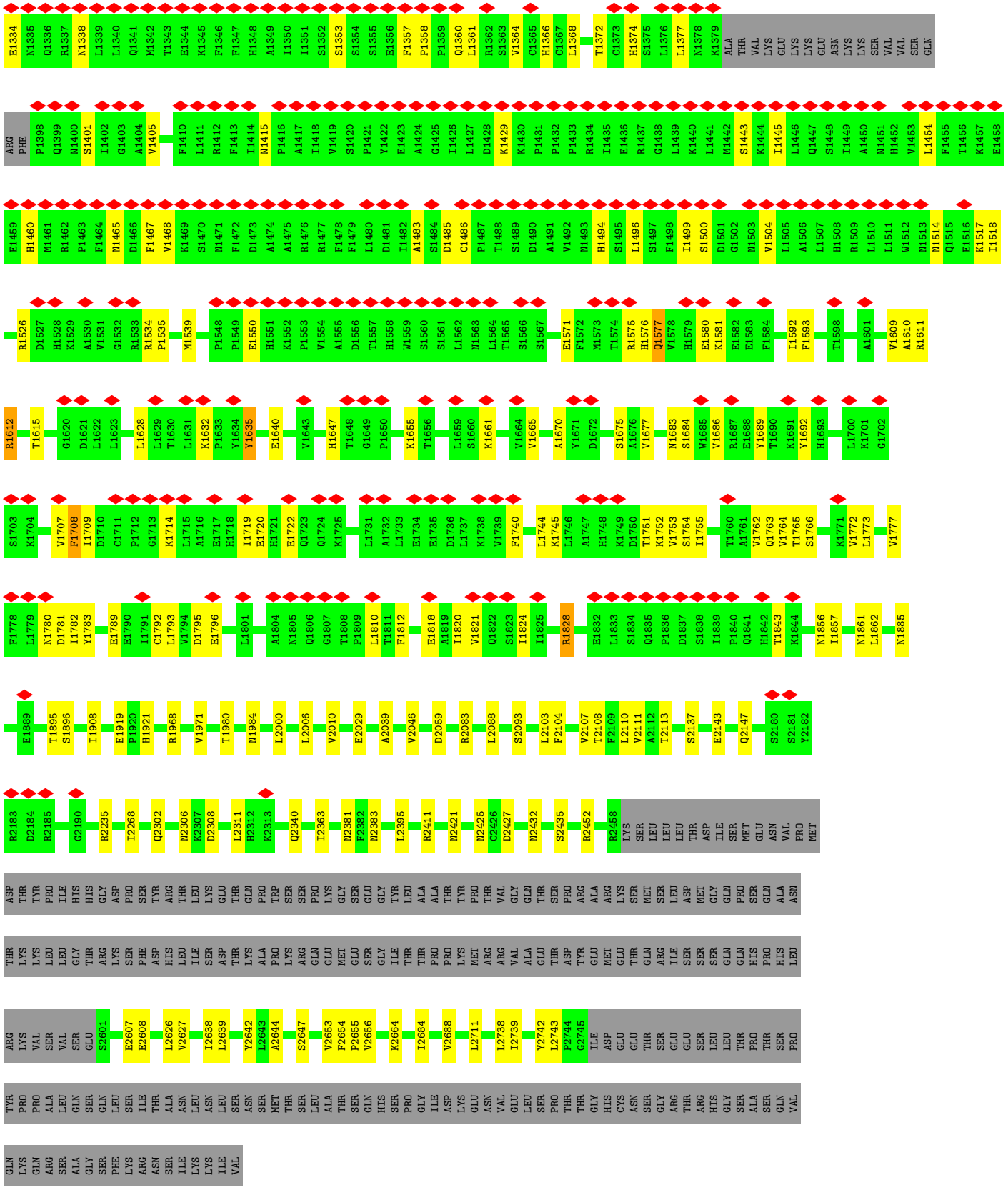
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain N:



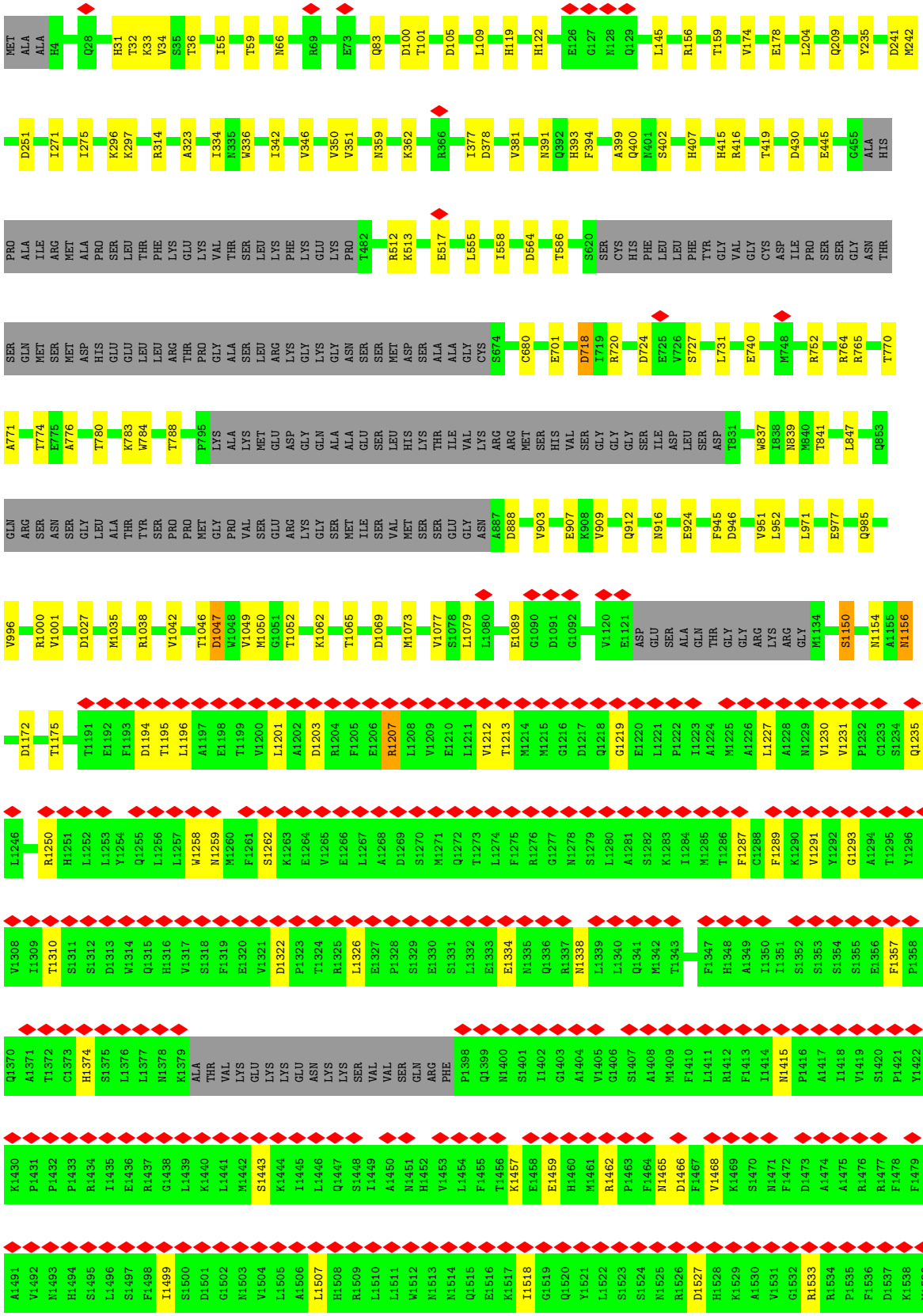


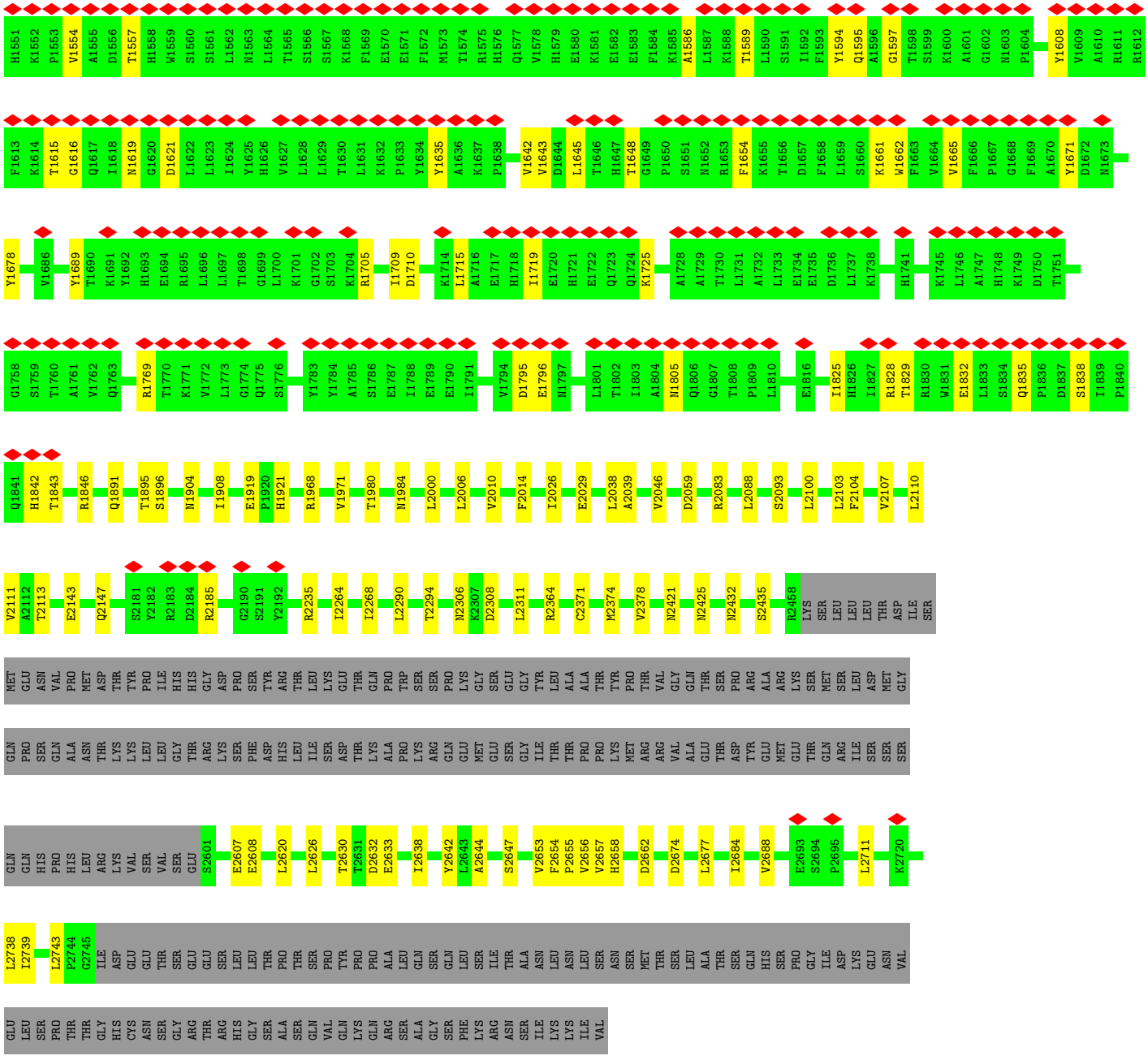


- Molecule 1: Neurofibromin

Chain F:


19%
75%
10%
15%


MET ALA ALA H4 Q28 H31 T32 K33 V34 S35 T36 I55 T59 N66 R69 E73 Q83 D100 T101 D105 L109 H119 H122 E126 G127 N128 Q129 L145 R156 T159 V174 E178 L204 Q209 Y235 D241 M242
D251 I271 I275 K296 K297 R314 A323 I334 N335 W336 I342 V346 V350 V351 N359 K362 R366 I377 D378 V381 N391 Q392 H393 F394 A399 Q400 N401 S402 H407 H415 R416 T419 D430 E445 G455 ALA HIS
PRO ALA ILE ARG MET ALA PRO SER LEU THR PHE LYS GLU LYS VAL THR SER LEU LYS PHE LYS GLU LYS PRO T482 R512 K513 E517 L555 I558 D564 T586 S620 SER CYS HIS PHE LEU LEU PHE TYR GLY VAL GLY CYS ASP ILE PRO SER SER GLY ASN THR
SER GLN MET SER MET ASP HIS GLU GLU LEU LEU ARG THR PRO GLY ALA SER LEU ARG LYS GLY LYS GLY ASN SER SER MET ASP SER ALA ALA GLY CYS S674 C680 E701 D718 I719 R720 D724 E725 V726 S727 L731 E740 M748 R752 R764 R765 T770
A771 T774 E775 A776 T780 K783 W784 T788 P795 LYS ALA LYS MET GLU ASP GLY GLN ALA ALA ALA GLU SER LEU HIS LYS THR ILE VAL LYS ARG ARG MET SER HIS VAL SER GLY GLY GLY GLY SER ILE ASP LEU SER ASP T831 W837 I838 N839 M840 T841 L847 Q853
GLN ARG SER ASN SER GLY LEU ALA THR TYR SER PRO PRO MET GLY PRO VAL SER GLU ARG LYS GLY SER MET ILE SER VAL MET SER SER GLU GLY ASN A887 D888 V903 E907 K908 V909 Q912 N916 E924 F945 D946 V951 L962 L971 E977 Q985
V996 R1000 V1001 D1027 M1035 R1038 V1042 T1046 D1047 W1048 V1049 M1050 G1051 T1052 K1062 T1065 D1069 M1073 V1077 S1078 L1079 L1080 E1089 G1090 D1091 G1092 V1120 E1121 ASP GLU SER ALA GLN THR GLY GLY ARG LYS ARG GLY M1134 S1150 N1154 A1155 N1156
D1172 T1175 T1191 E1192 F1193 D1194 T1195 L1196 A1197 E1198 T1199 V1200 L1201 A1202 D1203 R1204 F1205 E1206 R1207 L1208 V1209 E1210 L1211 V1212 T1213 M1214 M1215 G1216 D1217 Q1218 G1219 E1220 L1221 P1222 I1223 A1224 M1225 A1226 L1227 A1228 N1229 V1230 V1231 P1232 C1233 S1234 Q1235 W1236 D1237 E1238 L1239 A1240 R1241 V1242 L1243 V1244 T1245
L1246 R1250 H1251 L1252 L1253 Y1254 Q1255 L1256 L1257 W1258 N1259 M1260 F1261 S1262 K1263 E1264 V1265 E1266 L1267 A1268 D1269 S1270 M1271 Q1272 T1273 L1274 F1275 R1276 G1277 N1278 S1279 L1280 A1281 S1282 K1283 I1284 M1285 T1286 F1287 G1288 F1289 K1290 V1291 Y1292 G1293 A1294 T1295 Y1296 L1297 Q1298 K1299 L1300 L1301 D1302 P1303 L1304 L1305 R1306 I1307
V1308 I1309 T1310 S1311 S1312 D1313 W1314 Q1315 H1316 V1317 S1318 F1319 E1320 V1321 D1322 P1323 T1324 R1325 L1326 E1327 P1328 S1329 E1330 S1331 L1332 E1333 E1334 N1335 Q1336 R1337 N1338 L1339 L1340 Q1341 M1342 T1343 F1347 H1348 A1349 I1350 I1351 S1352 S1353 S1354 S1355 E1356 F1357 P1358 P1359 Q1360 L1361 R1362 S1363 V1364 C1365 H1366 C1367 L1368 Y1369
Q1370 A1371 T1372 C1373 H1374 S1375 L1376 L1377 N1378 K1379 ALA THR VAL LYS GLU LYS LYS GLU ASN LYS LYS SER VAL VAL SER GLN ARG PHE P1398 Q1399 N1400 S1401 I1402 G1403 A1404 V1405 G1406 S1407 A1408 M1409 F1410 L1411 R1412 F1413 I1414 N1415 P1416 A1417 I1418 V1419 S1420 P1421 Y1422 E1423 A1424 G1425 I1426 L1427 D1428 K1429
K1430 P1431 P1432 P1433 R1434 I1435 E1436 R1437 G1438 L1439 K1440 L1441 M1442 S1443 K1444 I1445 L1446 Q1447 S1448 I1449 A1450 N1451 H1452 V1453 L1454 F1455 T1456 K1457 E1458 E1459 H1460 M1461 R1462 P1463 F1464 N1465 D1466 F1467 V1468 K1469 S1470 N1471 F1472 D1473 A1474 A1475 R1476 R1477 F1478 F1479 I1482 A1483 S1484 D1485 C1486 P1487 T1488 S1489 D1490
A1491 V1492 N1493 H1494 S1495 L1496 S1497 F1498 I1499 S1500 D1501 G1502 N1503 V1504 L1505 A1506 L1507 H1508 R1509 L1510 L1511 W1512 N1513 N1514 Q1515 E1516 K1517 I1518 G1519 Q1520 Y1521 L1522 S1523 S1524 N1525 R1526 D1527 H1528 K1529 A1530 V1531 G1532 R1533 R1534 P1535 F1536 D1537 K1538 M1539 A1540 T1541 L1542 L1543 A1544 Y1545 L1546 G1547 P1548 P1549 E1550


H1551 K1552 P1553 V1554 A1555 D1556 T1557 H1558 W1559 S1560 S1561 L1562 N1563 L1564 T1565 S1566 S1567 K1568 F1569 E1570 E1571 F1572 M1573 T1574 R1575 H1576 Q1577 V1578 H1579 E1580 K1581 E1582 E1583 F1584 K1585 A1586 L1587 K1588 T1589 L1590 S1591 I1592 F1593 Y1594 Q1595 A1596 G1597 T1598 S1599 K1600 A1601 G1602 N1603 P1604 Y1608 V1609 A1610 R1611 R1612
F1613 K1614 T1615 G1616 Q1617 I1618 N1619 G1620 D1621 L1622 L1623 I1624 Y1625 H1626 V1627 L1628 L1629 T1630 L1631 K1632 P1633 Y1634 Y1635 A1636 K1637 P1638 V1642 V1643 D1644 L1645 T1646 H1647 T1648 G1649 P1650 S1651 N1652 R1653 F1654 K1655 T1656 D1657 F1658 L1659 S1660 K1661 W1662 F1663 V1664 V1665 F1666 P1667 G1668 F1669 A1670 Y1671 D1672 N1673
Y1678 V1686 Y1689 T1690 K1691 Y1692 H1693 E1694 R1695 L1696 L1697 T1698 G1699 L1700 K1701 G1702 S1703 K1704 R1705 I1709 D1710 K1714 L1715 A1716 E1717 H1718 I1719 E1720 H1721 E1722 Q1723 Q1724 K1725 A1728 A1729 T1730 L1731 A1732 L1733 E1734 E1735 D1736 L1737 K1738 H1741 K1745 L1746 A1747 H1748 K1749 D1750 T1751
G1758 S1759 T1760 A1761 V1762 Q1763 R1769 T1770 K1771 V1772 L1773 G1774 Q1775 S1776 Y1783 Y1784 A1785 S1786 E1787 I1788 E1789 E1790 I1791 V1794 D1795 E1796 N1797 L1801 T1802 I1803 A1804 N1805 Q1806 G1807 T1808 P1809 L1810 E1816 I1825 H1826 I1827 R1828 T1829 R1830 W1831 E1832 L1833 S1834 Q1835 P1836 D1837 S1838 I1839 P1840
Q1841 H1842 T1843 R1846 Q1891 T1895 S1896 N1904 I1908 E1919 P1920 H1921 R1968 V1971 T1980 N1984 L2000 L2006 V2010 F2014 I2026 E2029 L2038 A2039 V2046 D2059 R2083 L2088 S2093 L2100 L2103 F2104 V2107 L2110
V2111 A2112 T2113 E2143 Q2147 S2181 Y2182 R2183 D2184 R2185 G2190 S2191 Y2192 R2235 I2264 I2268 L2290 T2294 N2306 K2307 D2308 L2311 R2364 C2371 M2374 V2378 N2421 N2425 N2432 S2435 R2458 LYS SER LEU LEU LEU THR ASP ILE SER
MET GLU ASN VAL PRO MET ASP THR TYR PRO ILE HIS HIS GLY GLY ASP PRO SER TYR ARG THR LEU LYS GLU THR GLN PRO TRP SER SER PRO LYS GLY SER GLU GLY TYR LEU ALA ALA THR TYR PRO THR VAL GLY GLN THR SER PRO ARG ALA ARG LYS SER MET SER LEU ASP MET GLY
GLN PRO SER GLN ALA ASN THR LYS LYS LEU LEU GLY THR ARG LYS SER PHE ASP HIS LEU ILE SER ASP THR LYS ALA PRO LYS ARG GLN GLU MET GLU SER GLY ILE THR THR PRO PRO LYS MET ARG ARG VAL ALA GLU THR ASP TYR GLU MET GLU THR GLN ARG ILE SER SER SER
GLN GLN HIS PRO HIS LEU ARG LYS VAL SER VAL SER GLU S2601 E2607 E2608 L2620 L2626 T2630 T2631 D2632 E2633 I2638 Y2642 L2643 A2644 S2647 V2653 F2654 P2655 V2656 V2657 H2658 D2662 D2674 L2677 I2684 V2688 E2693 S2694 P2695 L2711 K2720
L2738 I2739 L2743 P2744 G2745 ILE ASP GLU GLU THR SER GLU GLU SER LEU LEU THR PRO THR SER PRO TYR PRO PRO ALA LEU GLN SER GLN LEU SER SER ILE THR ALA ASN LEU ASN LEU SER ASN SER MET THR SER LEU ALA THR SER GLN HIS SER PRO GLY ILE ASP LYS GLU ASN VAL
GLU LEU SER PRO THR THR GLY HIS CYS ASN SER GLY ARG THR ARG HIS GLY SER ALA SER GLN VAL GLN LYS GLN ARG SER ALA GLY SER PHE LYS ARG ASN SER ILE LYS LYS ILE VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51951	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0123	Depositor
Map size (Å)	687.98596, 687.98596, 687.98596	wwPDB
Map dimensions	470, 470, 470	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4638, 1.4638, 1.4638	Depositor

5 Model quality

5.1 Standard geometry

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

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	F	0.23	0/19654	0.41	0/26645
1	N	0.23	0/19654	0.42	0/26645
All	All	0.23	0/39308	0.41	0/53290

There are no bond length outliers.

There are no bond angle outliers.

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	F	19258	19450	19458	169	0
1	N	19258	19457	19459	190	0
2	F	1	0	0	0	0
All	All	38517	38907	38917	357	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.

The worst 5 of 357 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:N:1762:VAL:HG21	1:N:1824:ILE:HG23	1.48	0.94
1:N:1372:THR:HG1	1:N:1401:SER:HG	0.95	0.91
1:N:1577:GLN:NE2	1:N:1580:GLU:OE1	2.12	0.82
1:F:235:TYR:OH	1:F:275:ILE:O	1.97	0.81
1:N:2088:LEU:O	1:N:2093:SER:OG	1.99	0.80

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	F	2407/2839 (85%)	2390 (99%)	17 (1%)	0	100	100
1	N	2407/2839 (85%)	2393 (99%)	14 (1%)	0	100	100
All	All	4814/5678 (85%)	4783 (99%)	31 (1%)	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	F	2170/2531 (86%)	2147 (99%)	23 (1%)	73	85
1	N	2170/2531 (86%)	2138 (98%)	32 (2%)	65	80
All	All	4340/5062 (86%)	4285 (99%)	55 (1%)	70	82

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	1812	PHE
1	F	297	LYS
1	F	2432	ASN
1	F	1457	LYS
1	N	1828	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	1693	HIS
1	F	1603	ASN
1	N	1856	ASN
1	F	1891	GLN
1	F	554	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

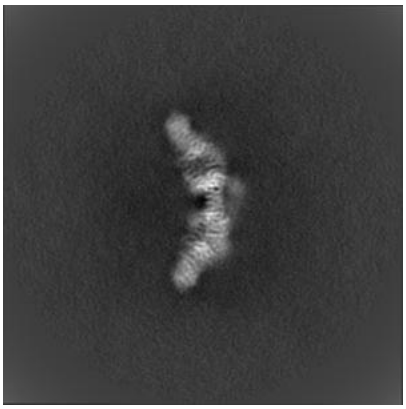
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13395. These allow visual inspection of the internal detail of the map and identification of artifacts.

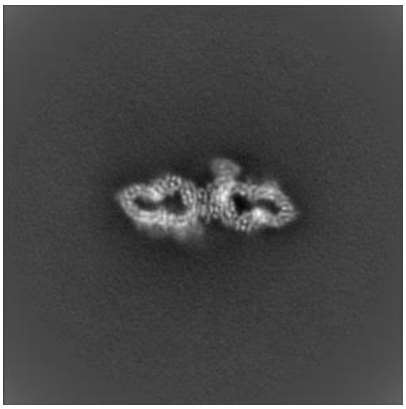
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

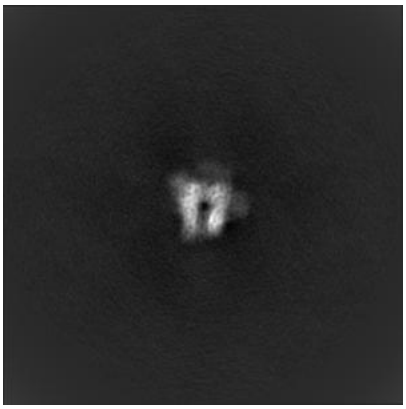
6.1.1 Primary map



X

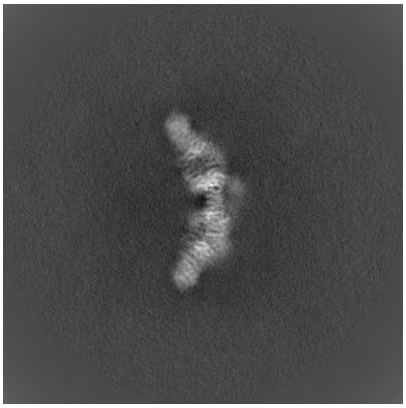


Y

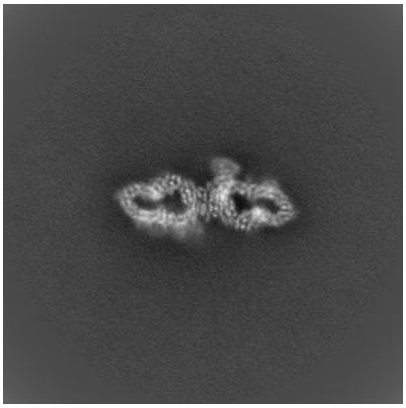


Z

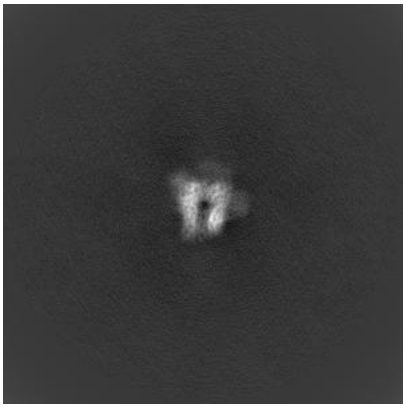
6.1.2 Raw map



X



Y

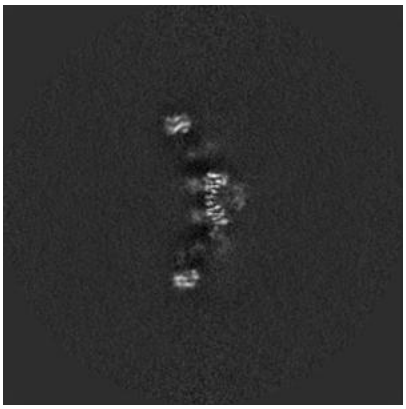


Z

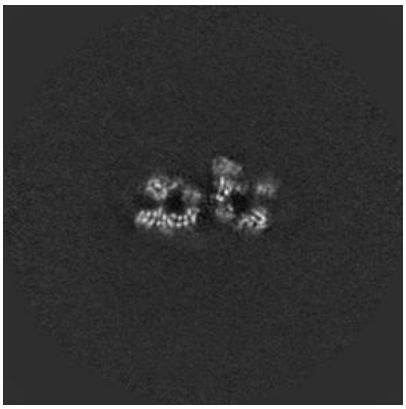
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

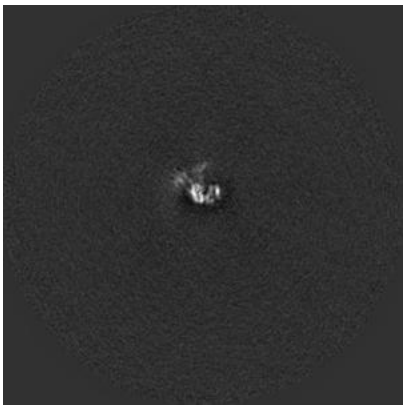
6.2.1 Primary map



X Index: 235



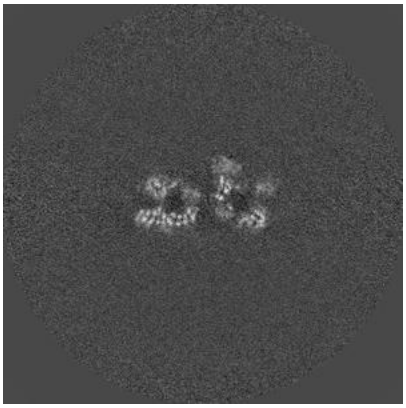
Y Index: 235



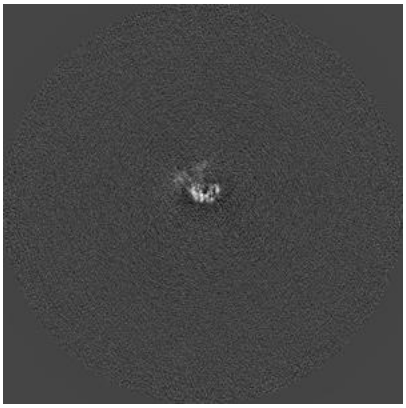
Z Index: 235

6.2.2 Raw map

X Index: 200



Y Index: 200

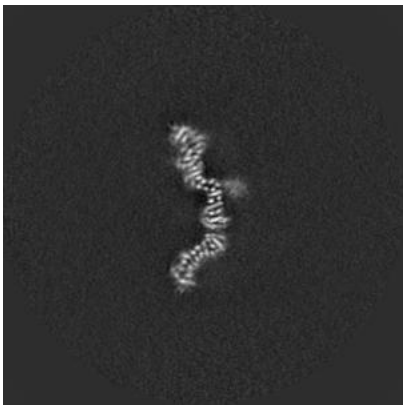


Z Index: 200

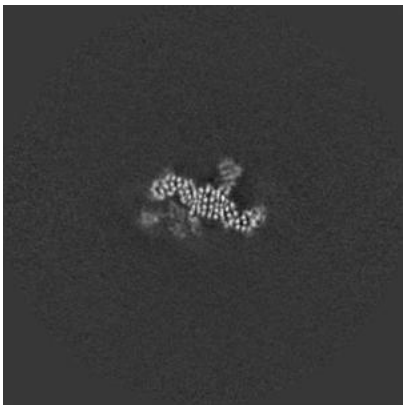
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

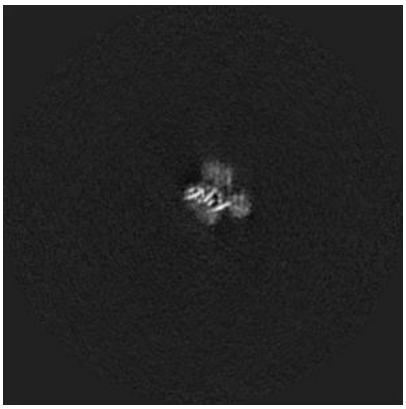
6.3.1 Primary map



X Index: 250

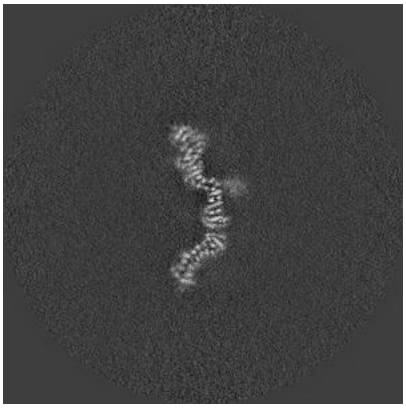


Y Index: 246

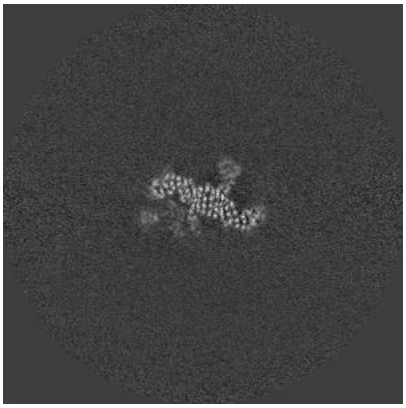


Z Index: 257

6.3.2 Raw map



X Index: 213



Y Index: 209

Z Index: 218

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

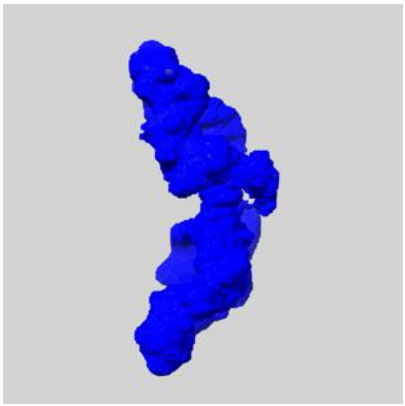
6.5 Mask visualisation (i)

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

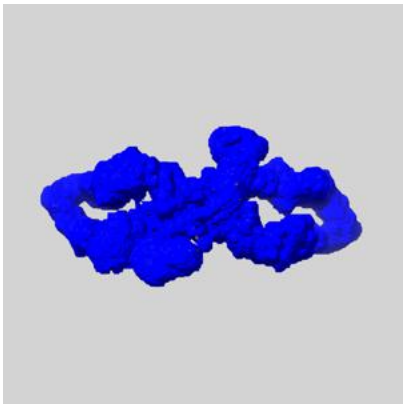
A mask typically either:

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

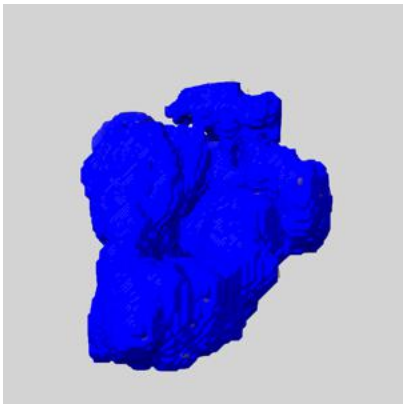
6.5.1 emd_13395_msk_1.map (i)



X



Y

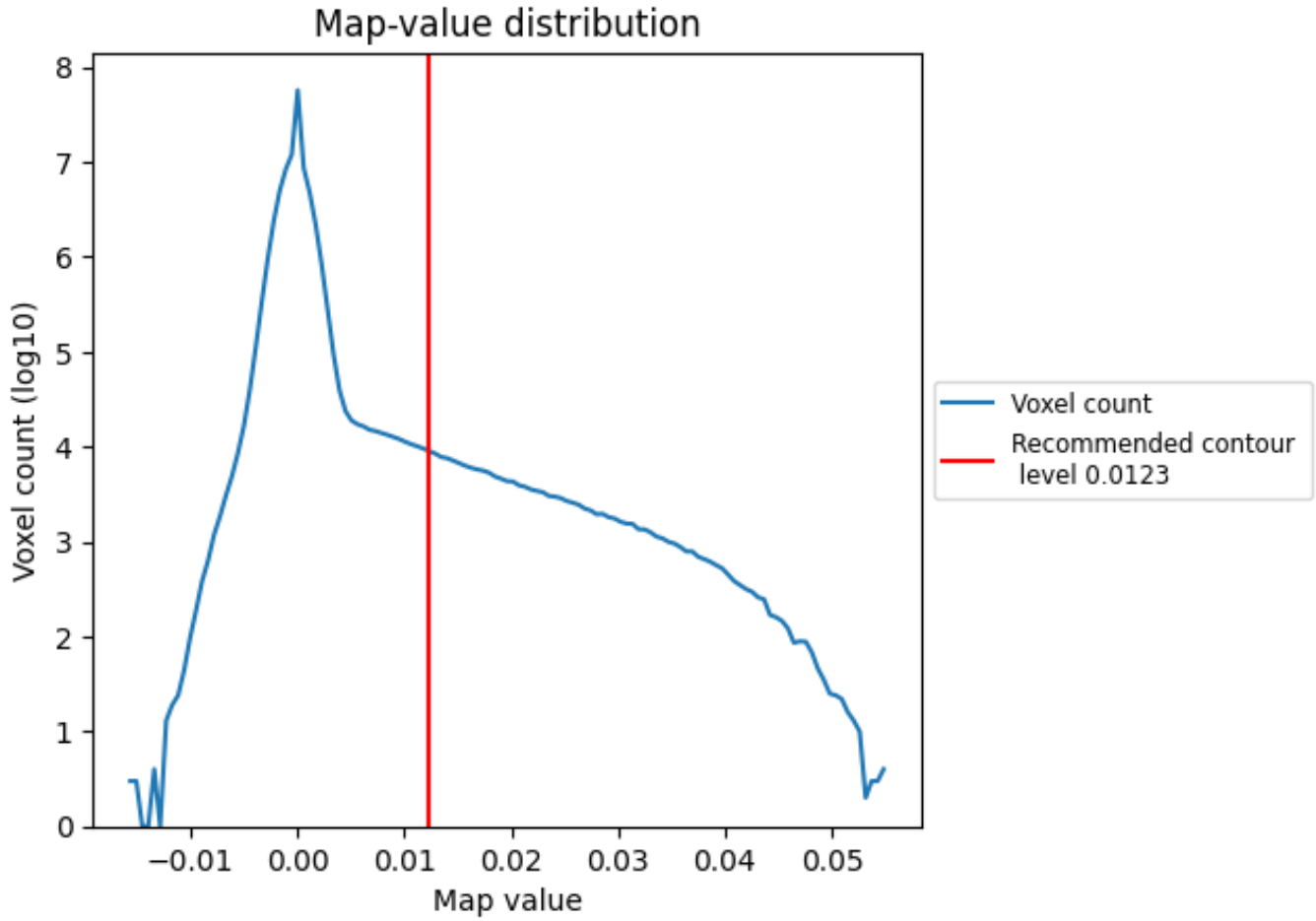


Z

7 Map analysis

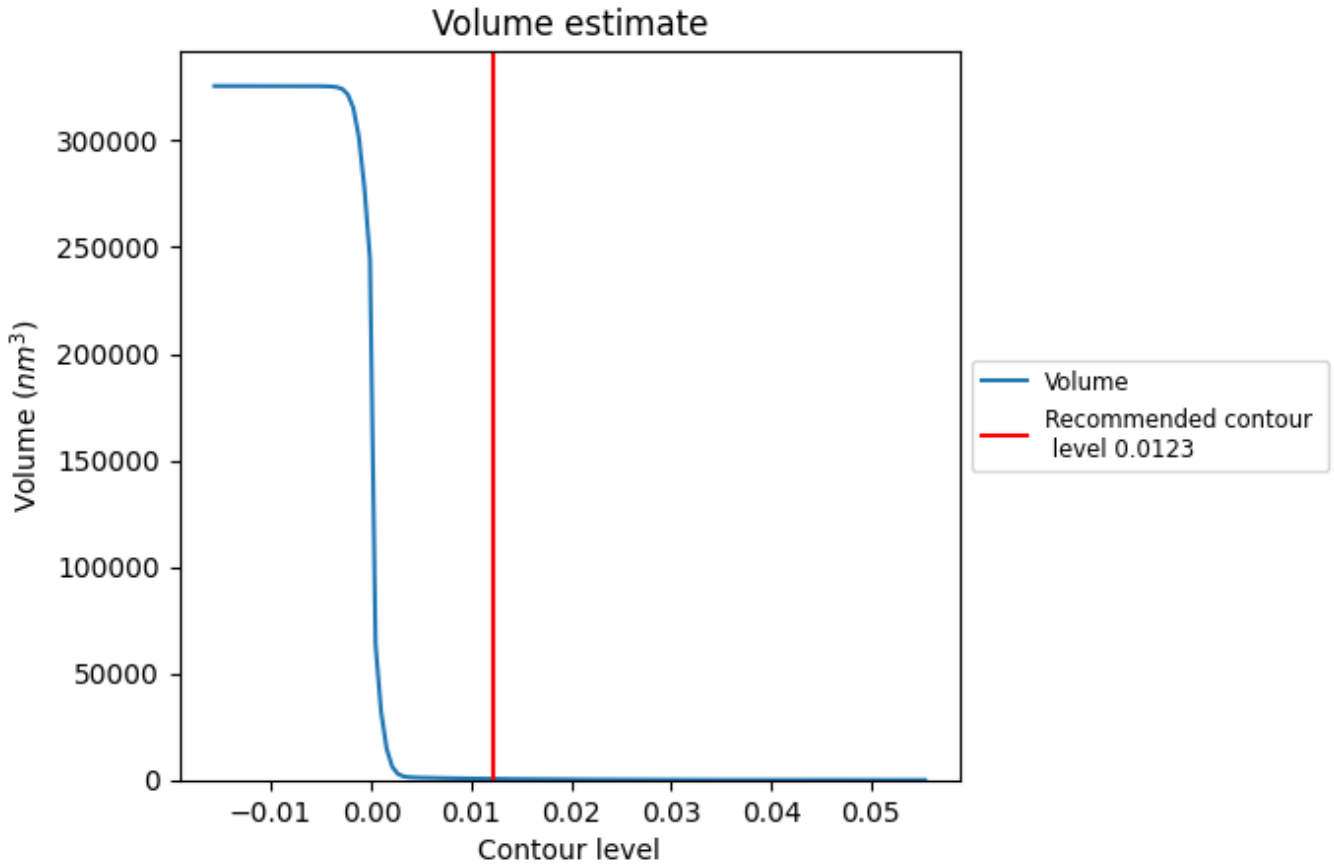
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 510 nm^3; this corresponds to an approximate mass of 460 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.

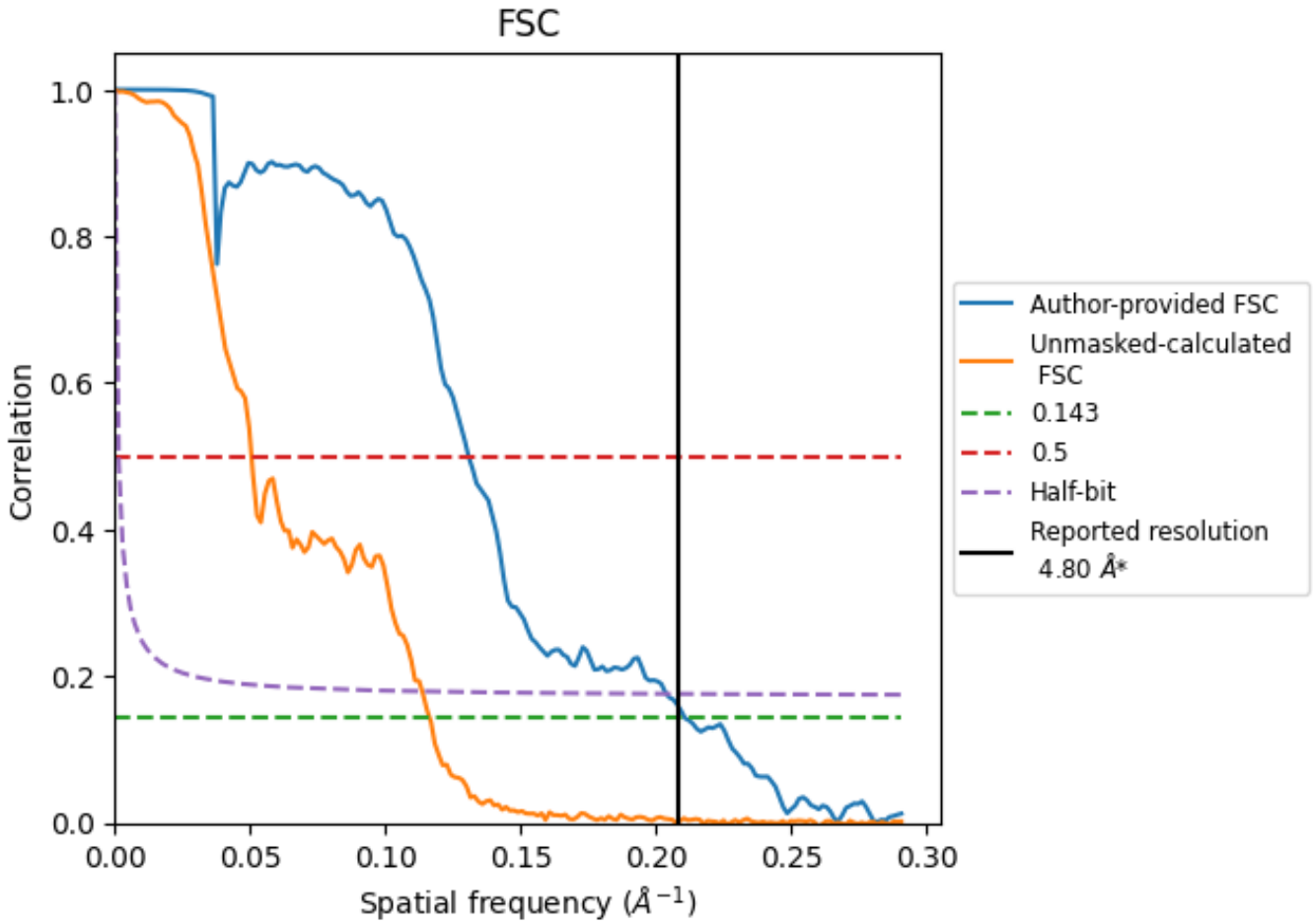
7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

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 0.208 Å^{-1}

8.2 Resolution estimates (i)

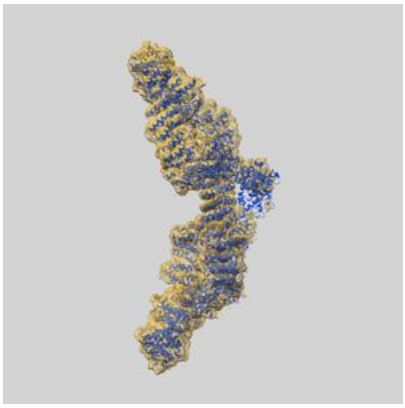
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.75	7.65	4.90
Unmasked-calculated*	8.60	19.80	8.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.60 differs from the reported value 4.8 by more than 10 %

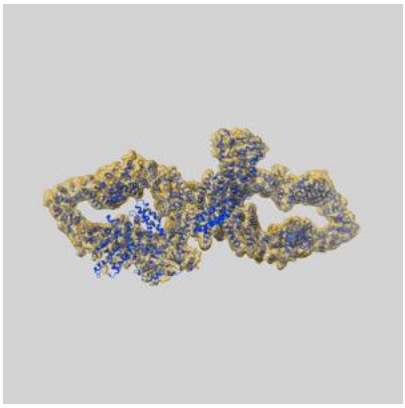
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13395 and PDB model 7PGT. Per-residue inclusion information can be found in section 3 on page 4.

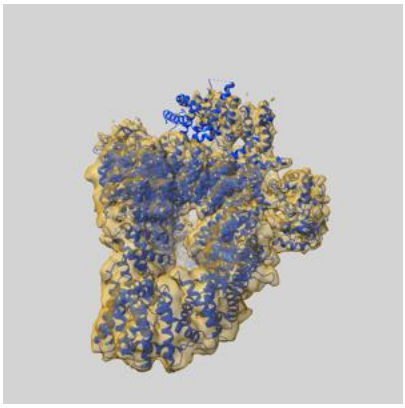
9.1 Map-model overlay



X



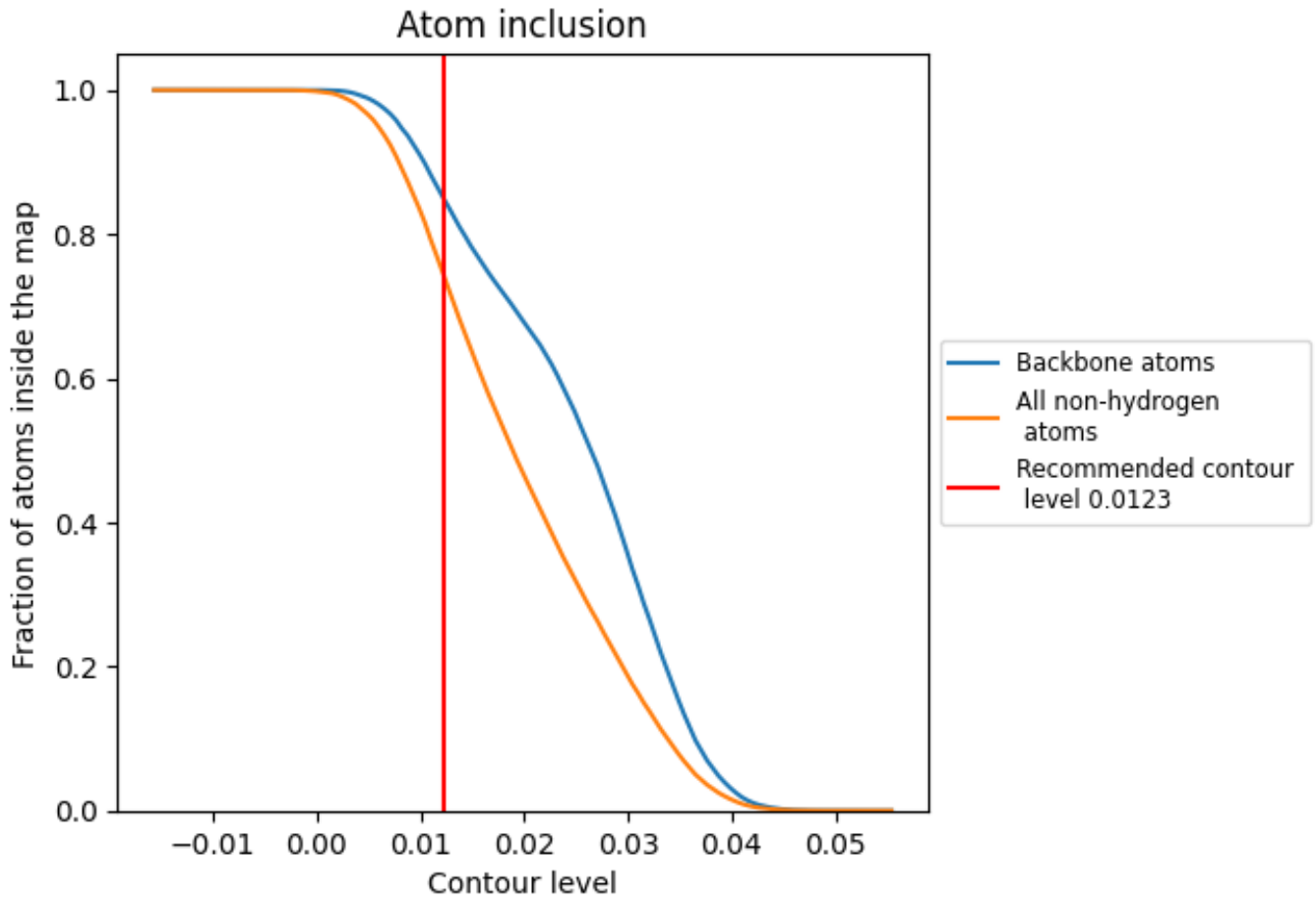
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0123 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 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.