wwPDB EM Validation Summary Report

Jul 7, 2024 – 08:03 am BST

PDB ID	:	7PGU
EMDB ID	:	EMD-13396
Title	:	Autoinhibited structure of human neurofibromin isoform 2 stabilized by Zinc.
Authors	:	Naschberger, A.; Baradaran, R.; Carroni, M.; Rupp, B.
Deposited on	:	2021-08-15
Resolution	:	3.30 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

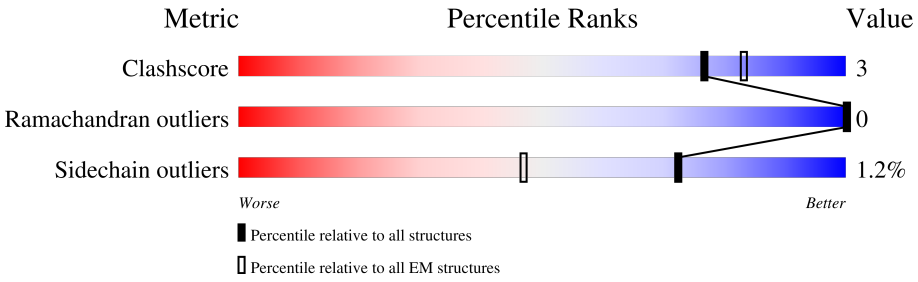
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	18% 78% 7% 15%
1	N	2839	16% 78% 7% 15%

2 Entry composition (i)

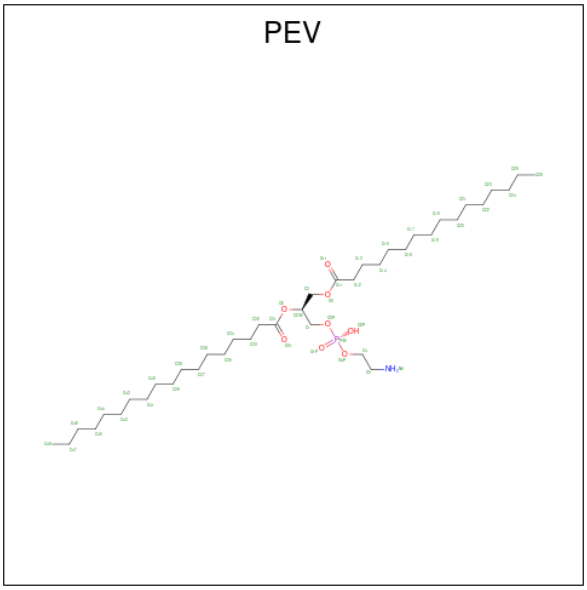
There are 4 unique types of molecules in this entry. The entry contains 77658 atoms, of which 39040 are hydrogens and 0 are deuteriums.

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	F	2423	Total	C	H	N	O	S	0	0
			38701	12314	19443	3266	3555	123		
1	N	2423	Total	C	H	N	O	S	0	0
			38701	12314	19443	3266	3555	123		

- Molecule 2 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula: $C_{39}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
2	F	1	Total	C	H	N	O	P	0
			126	39	77	1	8	1	
2	N	1	Total	C	H	N	O	P	0
			126	39	77	1	8	1	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	F	1	Total Zn 1 1	0
3	N	1	Total Zn 1 1	0

- Molecule 4 is water.

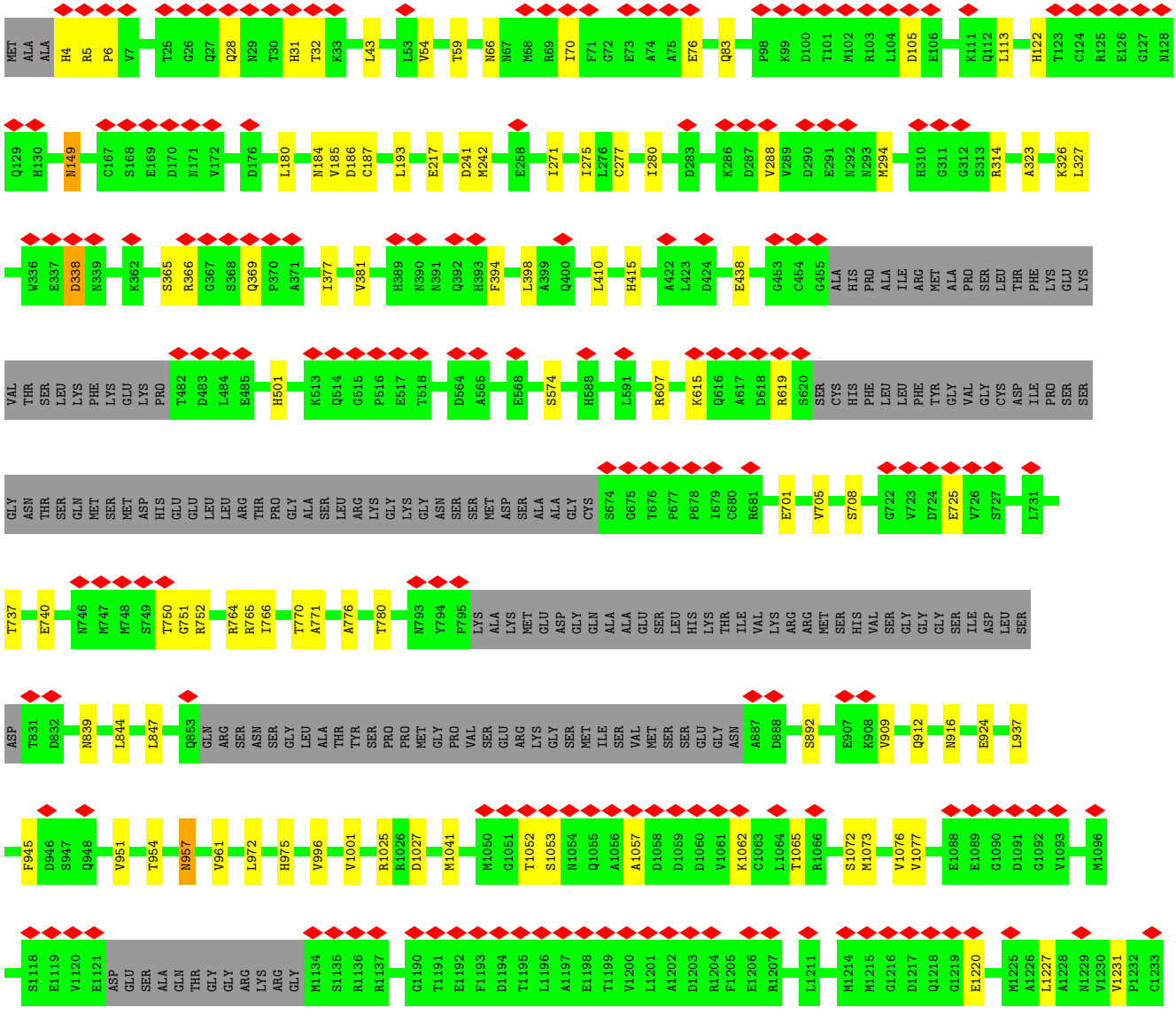
Mol	Chain	Residues	Atoms	AltConf
4	F	1	Total O 1 1	0
4	N	1	Total O 1 1	0

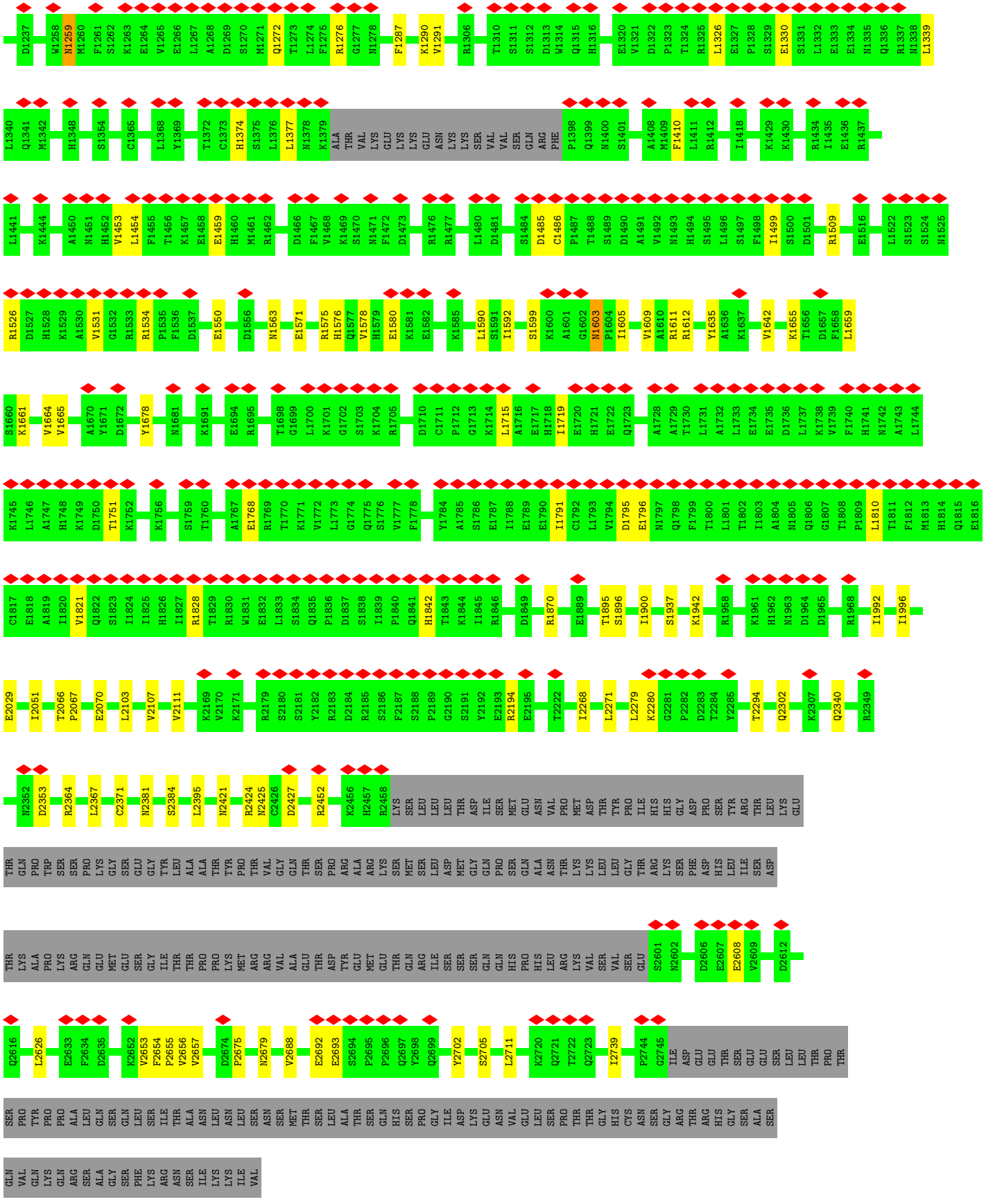
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Neurofibromin

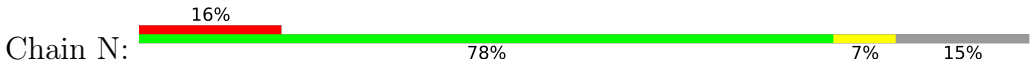
Chain F:

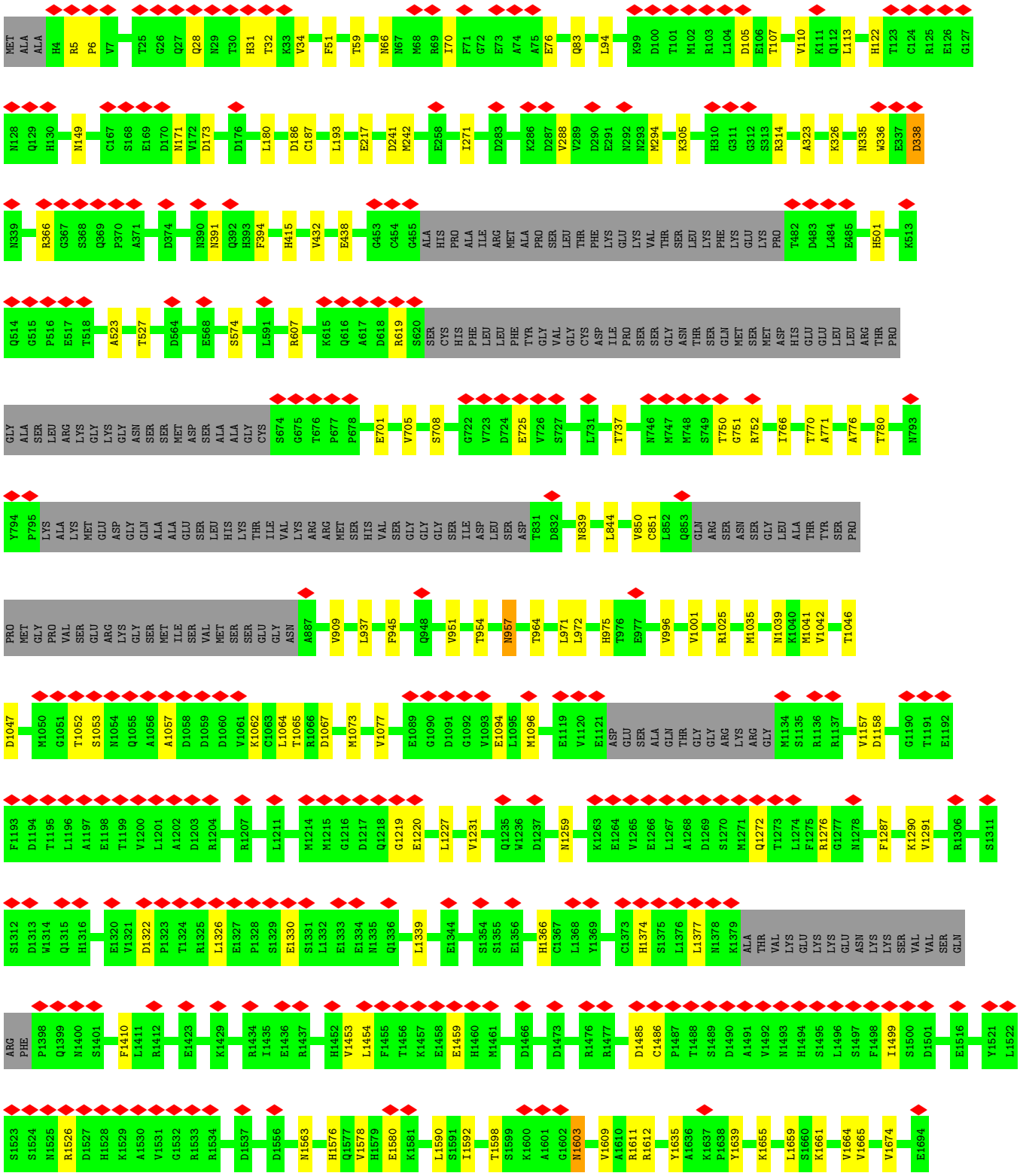


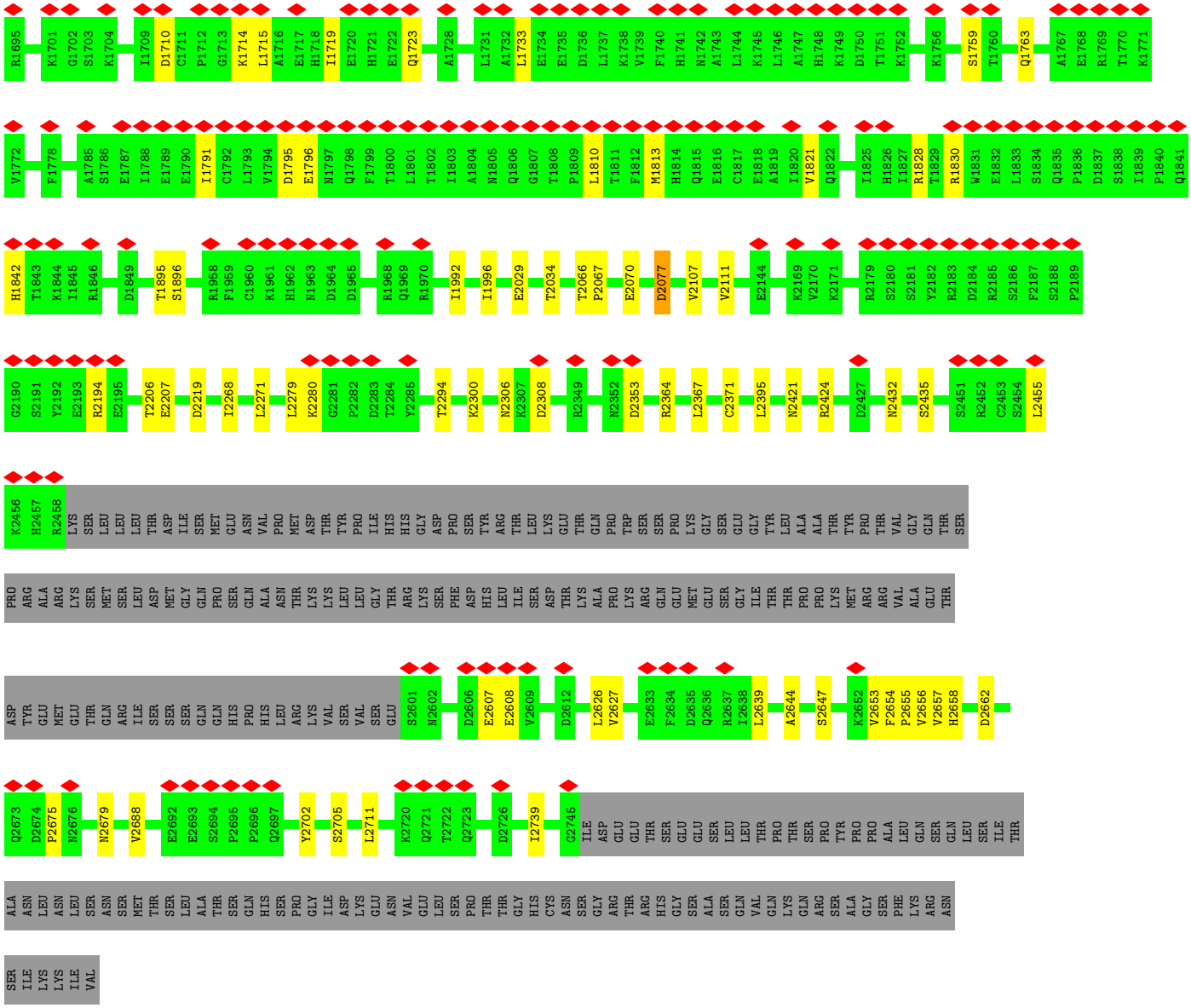

D1237 W1258 N1259 M1260 F1261 S1262 K1263 E1264 V1265 E1266 L1267 A1268 D1269 S1270 M1271 Q1272 T1273 L1274 F1275 R1276 G1277 N1278 F1287 K1290 V1291 R1306 T1310 S1311 S1312 D1313 W1314 Q1315 H1316 E1320 V1321 D1322 P1323 T1324 R1325 L1326 E1327 P1328 S1329 E1330 S1331 L1332 E1333 E1334 N1335 Q1336 R1337 N1338 L1339
L1340 Q1341 M1342 H1348 S1354 G1365 L1368 Y1369 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 A1408 M1409 F1410 L1411 R1412 I1418 K1429 K1430 R1434 I1435 E1436 R1437
L1441 K1444 A1450 N1451 H1452 V1453 L1454 F1455 T1456 K1457 E1458 E1459 H1460 M1461 R1462 D1466 F1467 V1468 K1469 S1470 N1471 F1472 D1473 R1476 R1477 L1480 D1481 S1484 D1485 C1486 P1487 T1488 S1489 D1490 A1491 V1492 N1493 H1494 S1495 L1496 S1497 F1498 I1499 S1500 D1501 R1509 E1516 L1522 S1523 S1524 N1525
R1526 D1527 H1528 K1529 A1530 V1531 G1532 R1533 R1534 P1535 F1536 D1537 E1550 D1556 N1563 E1571 R1575 H1576 Q1577 V1578 H1579 E1580 K1581 E1582 K1585 L1590 S1591 I1592 S1599 K1600 A1601 G1602 N1603 P1604 I1605 V1609 A1610 R1611 R1612 Y1635 A1636 K1637 V1642 K1655 T1656 D1657 F1658 L1659
S1660 K1661 V1664 V1665 A1670 Y1671 D1672 Y1678 N1681 K1691 E1694 R1695 T1698 G1699 L1700 K1701 G1702 S1703 K1704 R1705 D1710 C1711 P1712 G1713 K1714 L1715 A1716 E1717 H1718 I1719 E1720 H1721 E1722 Q1723 A1728 A1729 T1730 L1731 A1732 L1733 E1734 E1735 D1736 L1737 K1738 V1739 F1740 H1741 N1742 A1743 L1744
K1745 L1746 A1747 H1748 K1749 D1750 T1751 K1752 K1756 S1759 T1760 A1767 E1768 R1769 T1770 K1771 V1772 L1773 G1774 Q1775 S1776 V1777 F1778 Y1784 A1785 S1786 E1787 I1788 E1789 E1790 I1791 C1792 L1793 V1794 D1795 E1796 N1797 Q1798 F1799 T1800 L1801 T1802 I1803 A1804 N1805 Q1806 G1807 T1808 P1809 L1810 T1811 F1812 M1813 H1814 Q1815 E1816
C1817 E1818 A1819 I1820 V1821 Q1822 S1823 I1824 I1825 H1826 I1827 R1828 T1829 R1830 W1831 E1832 L1833 S1834 Q1835 P1836 D1837 S1838 I1839 P1840 Q1841 H1842 T1843 K1844 I1845 R1846 D1849 R1870 E1889 T1895 S1896 I1900 S1937 K1942 R1958 K1961 H1962 N1963 D1964 D1965 R1968 I1992 I1996
E2029 I2051 T2066 P2067 E2070 L2103 V2107 V2111 K2169 V2170 K2171 R2179 S2180 S2181 Y2182 R2183 D2184 R2185 S2186 F2187 S2188 P2189 G2190 S2191 Y2192 E2193 R2194 E2195 T2222 I2268 L2271 L2279 K2280 G2281 P2282 D2283 T2284 Y2285 T2294 Q2302 K2307 Q2340 R2349
N2352 D2353 R2364 L2367 C2371 N2381 S2384 L2395 N2421 R2424 N2425 C2426 D2427 R2452 K2456 H2457 R2458 LYS SER LEU LEU LEU THR ASP ILE SER MET GLU ASN VAL PRO MET ASP THR TYR PRO ILE HIS HIS 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 GLY THR ARG LYS SER GLN 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 N2602 D2606 E2607 E2608 V2609 D2612
Q2616 L2626 E2633 F2634 D2635 K2652 V2653 F2654 P2655 V2656 V2657 D2674 P2675 N2679 V2688 E2692 E2693 S2694 P2695 P2696 Q2697 Y2698 Q2699 Y2702 S2705 L2711 K2720 Q2721 T2722 Q2723 I2739 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 ILE THR ALA ASN LEU ASN LEU SER ASN SER MET THR SER LEU ALA THR SER GLN HIS SER 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

• Molecule 1: Neurofibromin

Chain N:






R1695 K1701 G1702 S1703 K1704 I1709 D1710 C1711 P1712 G1713 K1714 L1715 A1716 E1717 H1718 I1719 E1720 H1721 E1722 Q1723 A1728 L1731 A1732 L1733 E1734 E1735 D1736 L1737 K1738 V1739 F1740 H1741 N1742 A1743 L1744 K1745 L1746 A1747 H1748 K1749 D1750 T1751 K1752 K1756 S1759 T1760 Q1763 A1767 E1768 R1769 T1770 K1771
V1772 F1778 A1785 S1786 E1787 I1788 E1789 E1790 I1791 C1792 L1793 V1794 D1795 E1796 N1797 Q1798 F1799 T1800 L1801 T1802 I1803 A1804 N1805 Q1806 G1807 T1808 P1809 L1810 T1811 F1812 M1813 H1814 Q1815 E1816 C1817 E1818 A1819 I1820 V1821 Q1822 I1825 H1826 I1827 R1828 T1829 R1830 W1831 E1832 L1833 S1834 Q1835 P1836 D1837 S1838 I1839 P1840 Q1841
H1842 T1843 K1844 I1845 R1846 D1849 T1895 S1896 R1958 F1959 C1960 K1961 H1962 N1963 D1964 D1965 R1968 Q1969 R1970 I1992 I1996 E2029 T2034 T2066 P2067 E2070 D2077 V2107 V2111 E2144 K2169 V2170 K2171 R2179 S2180 S2181 Y2182 R2183 D2184 R2185 S2186 F2187 S2188 P2189
G2190 S2191 Y2192 E2193 R2194 E2195 T2206 E2207 D2219 I2268 L2271 L2279 K2280 G2281 P2282 D2283 T2284 Y2285 T2294 K2300 N2306 K2307 D2308 R2349 N2352 D2353 R2364 L2367 C2371 L2395 N2421 R2424 D2427 N2432 S2435 S2451 R2452 C2453 S2454 L2455
K2456 H2457 R2458 LYS SER LEU LEU LEU THR ASP ILE SER MET GLU ASN VAL PRO MET ASP THR TYR PRO PRO ILE HIS HIS 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 N2602 D2606 E2607 E2608 V2609 D2612 L2626 V2627 E2633 F2634 D2635 Q2636 R2637 I2638 L2639 A2644 S2647 K2652 V2653 F2654 P2655 V2656 V2657 H2658 D2662
Q2673 D2674 P2675 N2676 N2679 V2688 E2692 E2693 S2694 P2695 P2696 Q2697 Y2702 S2705 L2711 K2720 Q2721 T2722 Q2723 D2726 I2739 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 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	300087	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	163.132	Depositor
Minimum map value	-86.089	Depositor
Average map value	0.013	Depositor
Map value standard deviation	1.447	Depositor
Recommended contour level	30.0	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, PEV

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	0.26	0/19654	0.44	0/26645
1	N	0.26	0/19654	0.44	0/26645
All	All	0.26	0/39308	0.44	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	19443	19458	112	0
1	N	19258	19443	19458	121	0
2	F	49	77	77	0	0
2	N	49	77	77	0	0
3	F	1	0	0	0	0
3	N	1	0	0	0	0
4	F	1	0	0	0	0
4	N	1	0	0	0	0
All	All	38618	39040	39070	231	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 3.

The worst 5 of 231 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:F:66:ASN:OD1	1:F:83:GLN:NE2	2.04	0.91
1:N:66:ASN:OD1	1:N:83:GLN:NE2	2.04	0.90
1:F:1290:LYS:NZ	1:F:1563:ASN:OD1	2.14	0.81
1:N:2675:PRO:O	1:N:2679:ASN:ND2	2.14	0.80
1:N:217:GLU:OE2	1:N:326:LYS:NZ	2.16	0.79

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%)	2370 (98%)	37 (2%)	0	100	100
1	N	2407/2839 (85%)	2367 (98%)	40 (2%)	0	100	100
All	All	4814/5678 (85%)	4737 (98%)	77 (2%)	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%)	2145 (99%)	25 (1%)	71	83

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	2170/2531 (86%)	2143 (99%)	27 (1%)	71 83
All	All	4340/5062 (86%)	4288 (99%)	52 (1%)	72 83

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	149	ASN
1	N	619	ARG
1	N	2367	LEU
1	N	305	LYS
1	N	366	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	1742	ASN
1	N	1856	ASN
1	N	2432	ASN
1	F	2434	GLN
1	F	2432	ASN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	PEV	N	2901	-	48,48,48	0.30	0	51,53,53	0.31	0
2	PEV	F	2901	-	48,48,48	0.29	0	51,53,53	0.28	0

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	PEV	N	2901	-	-	18/52/52/52	-
2	PEV	F	2901	-	-	11/52/52/52	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2901	PEV	C1-O3P-P-O2P
2	N	2901	PEV	O2-C2-C3-O3
2	N	2901	PEV	C1-O3P-P-O2P
2	F	2901	PEV	C17-C18-C19-C20
2	N	2901	PEV	C18-C19-C20-C21

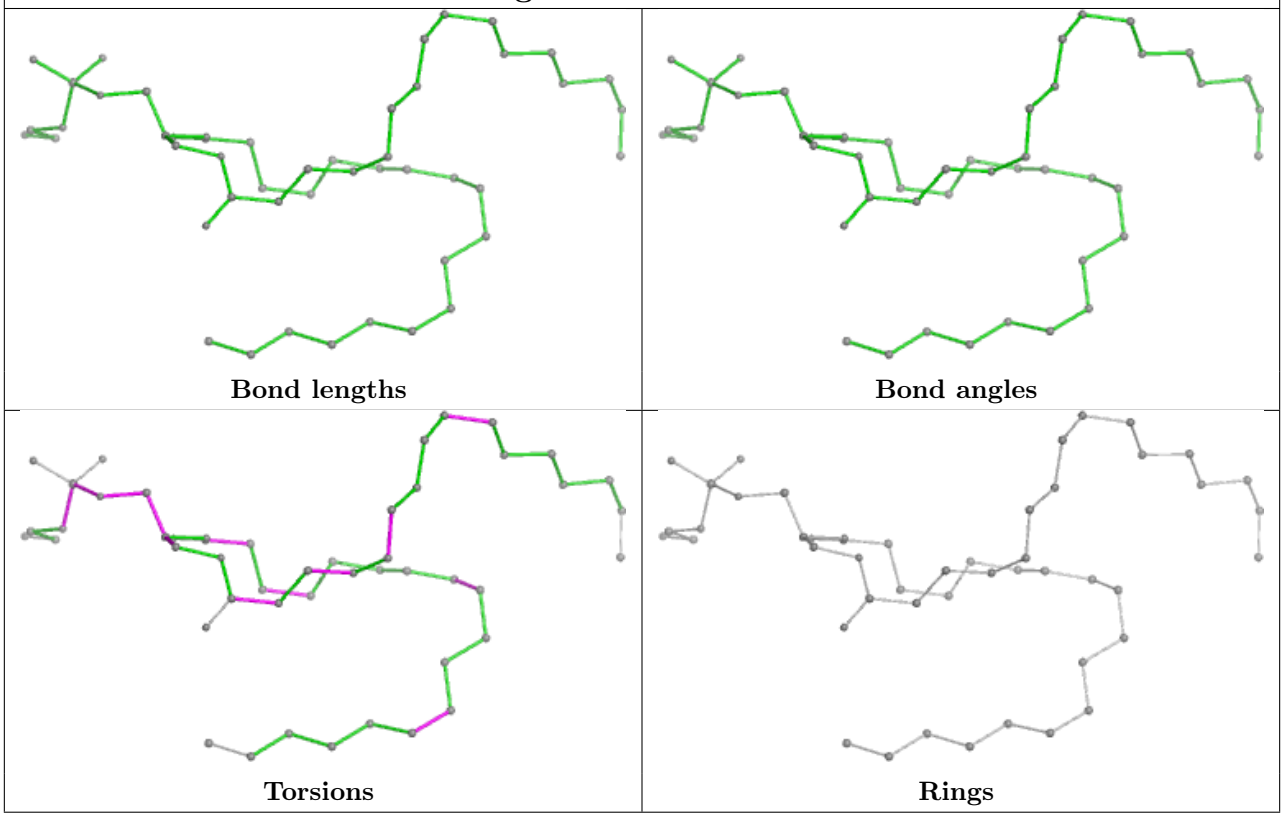
There are no ring outliers.

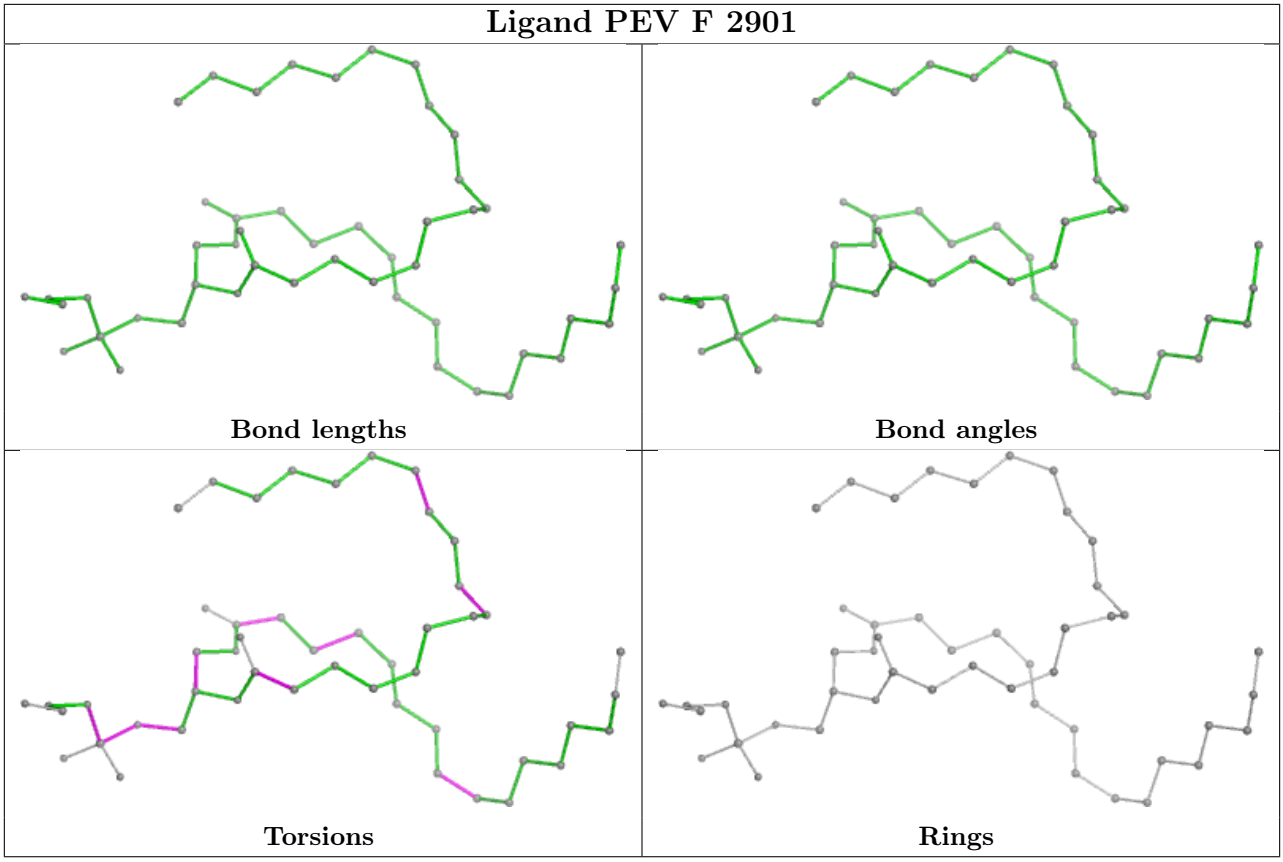
No monomer is involved in short contacts.

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 PEV N 2901





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.

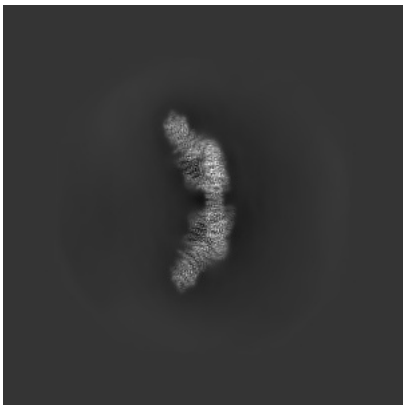
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13396. These allow visual inspection of the internal detail of the map and identification of artifacts.

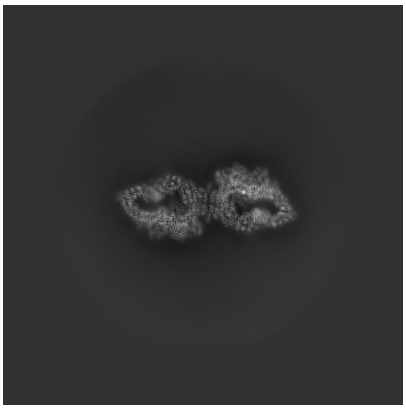
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



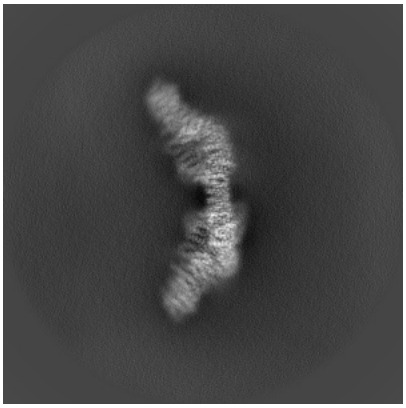
X



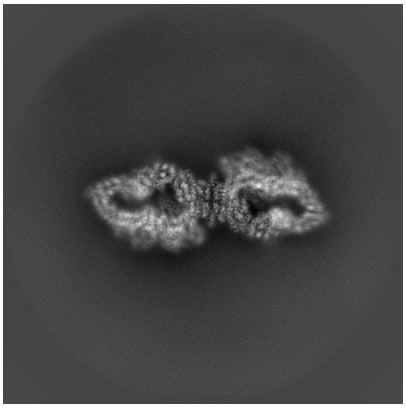
Y

Z

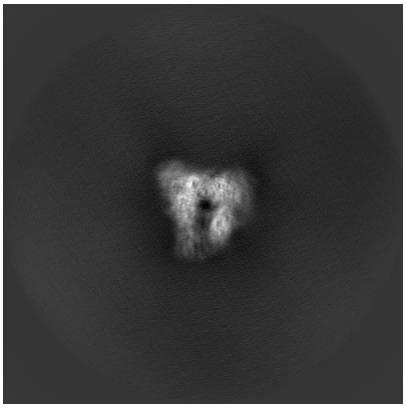
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

6.2.1 Primary map

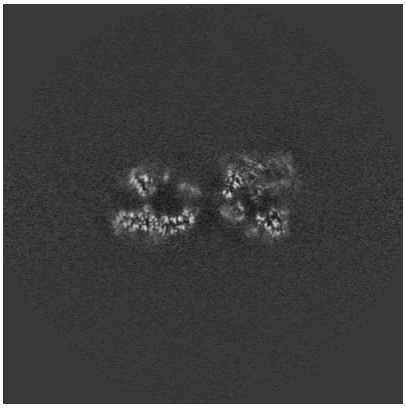
X Index: 235

Y Index: 235

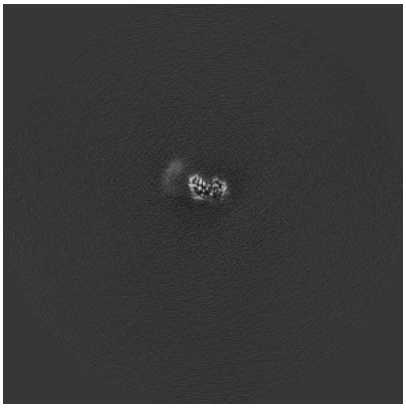
Z Index: 235

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)

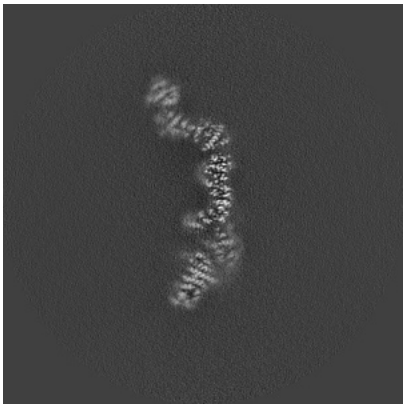
6.3.1 Primary map

X Index: 251

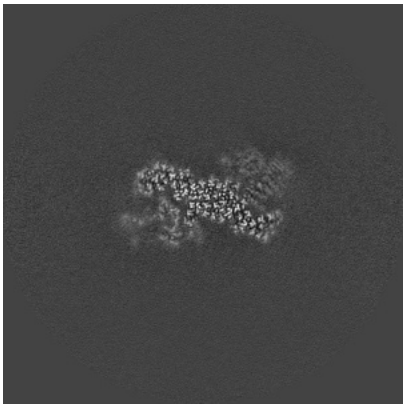
Y Index: 246

Z Index: 270

6.3.2 Raw map



X Index: 188



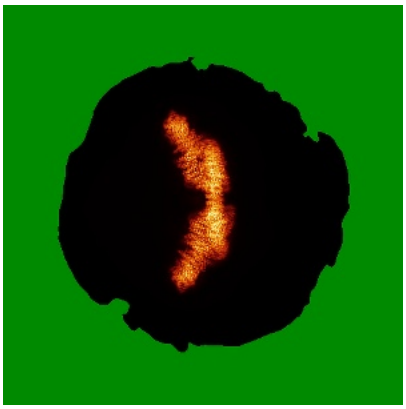
Y Index: 213

Z Index: 178

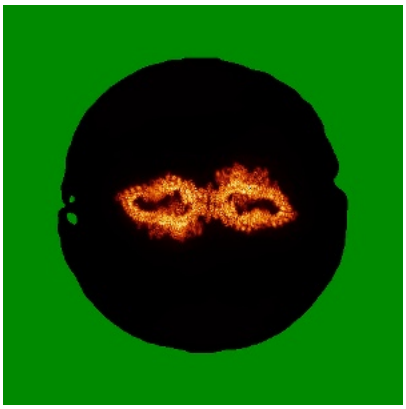
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



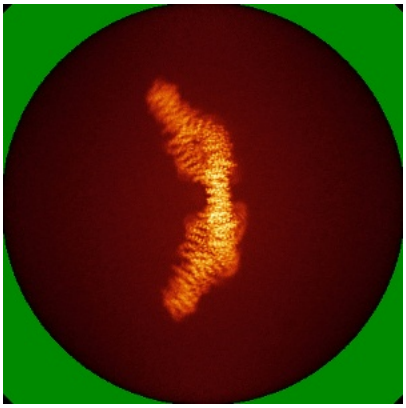
X



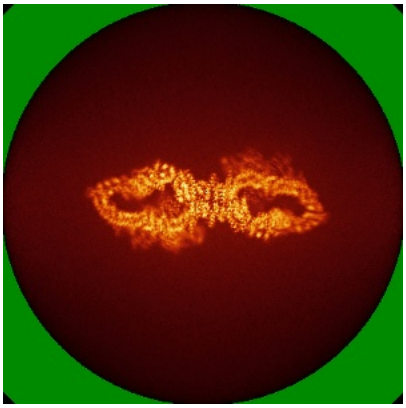
Y

Z

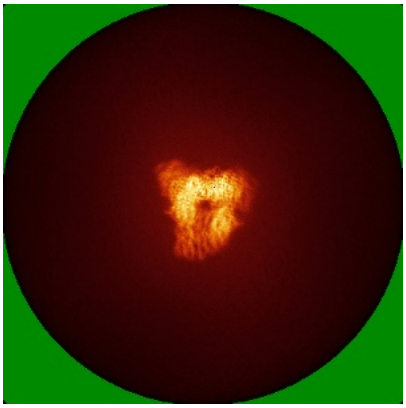
6.4.2 Raw map



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 30.0. 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.

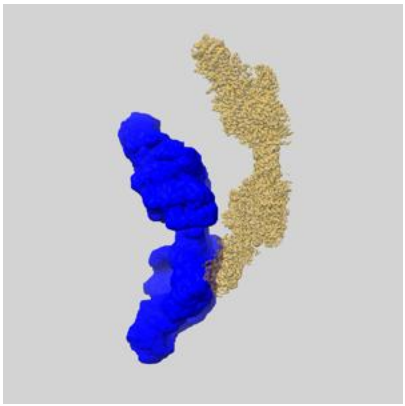
6.6 Mask visualisation (i)

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

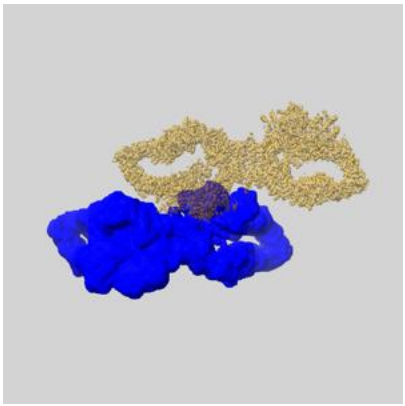
A mask typically either:

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

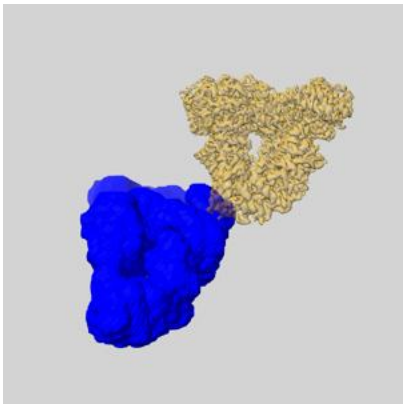
6.6.1 emd_13396_msk_1.map (i)



X



Y

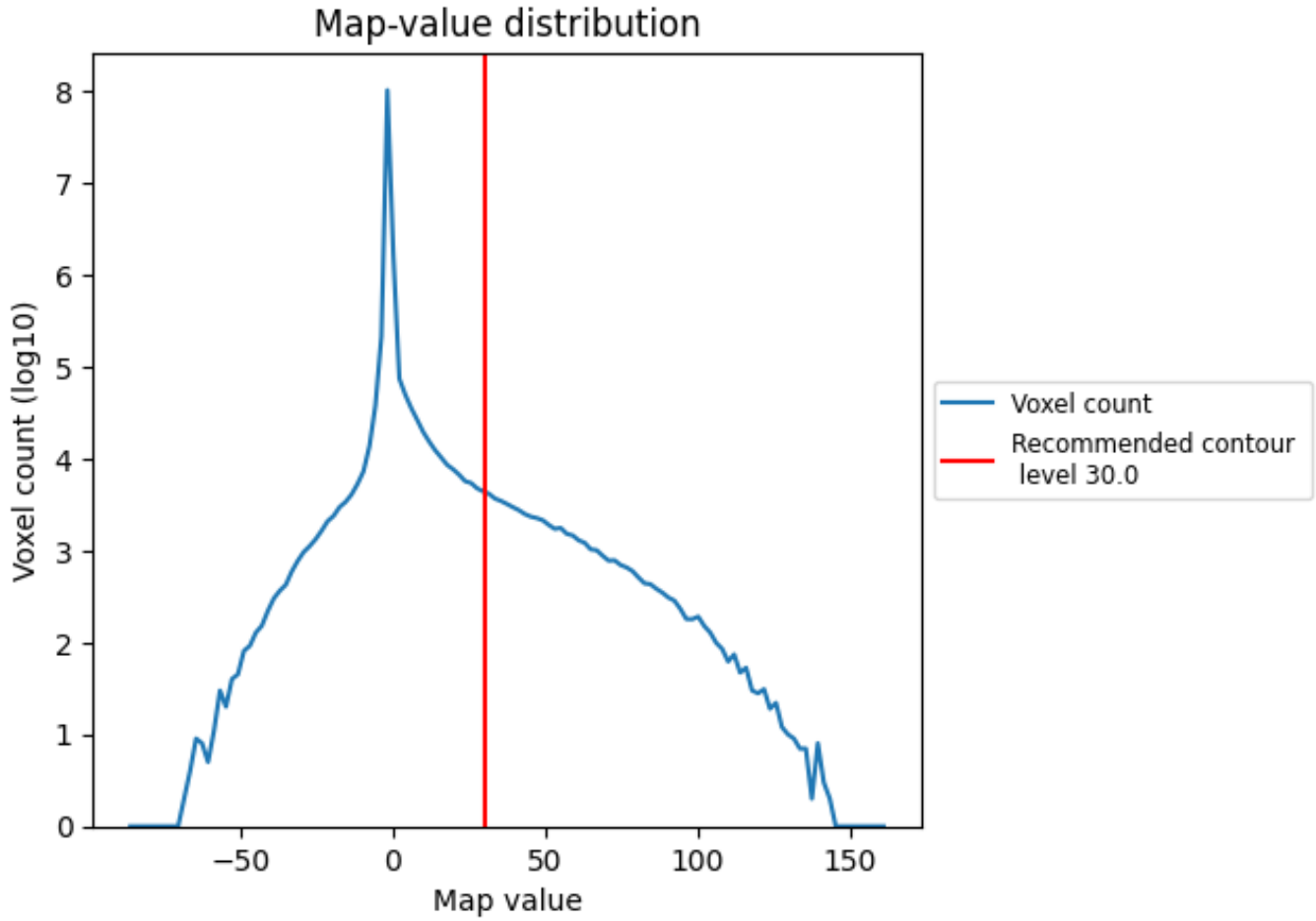


Z

7 Map analysis

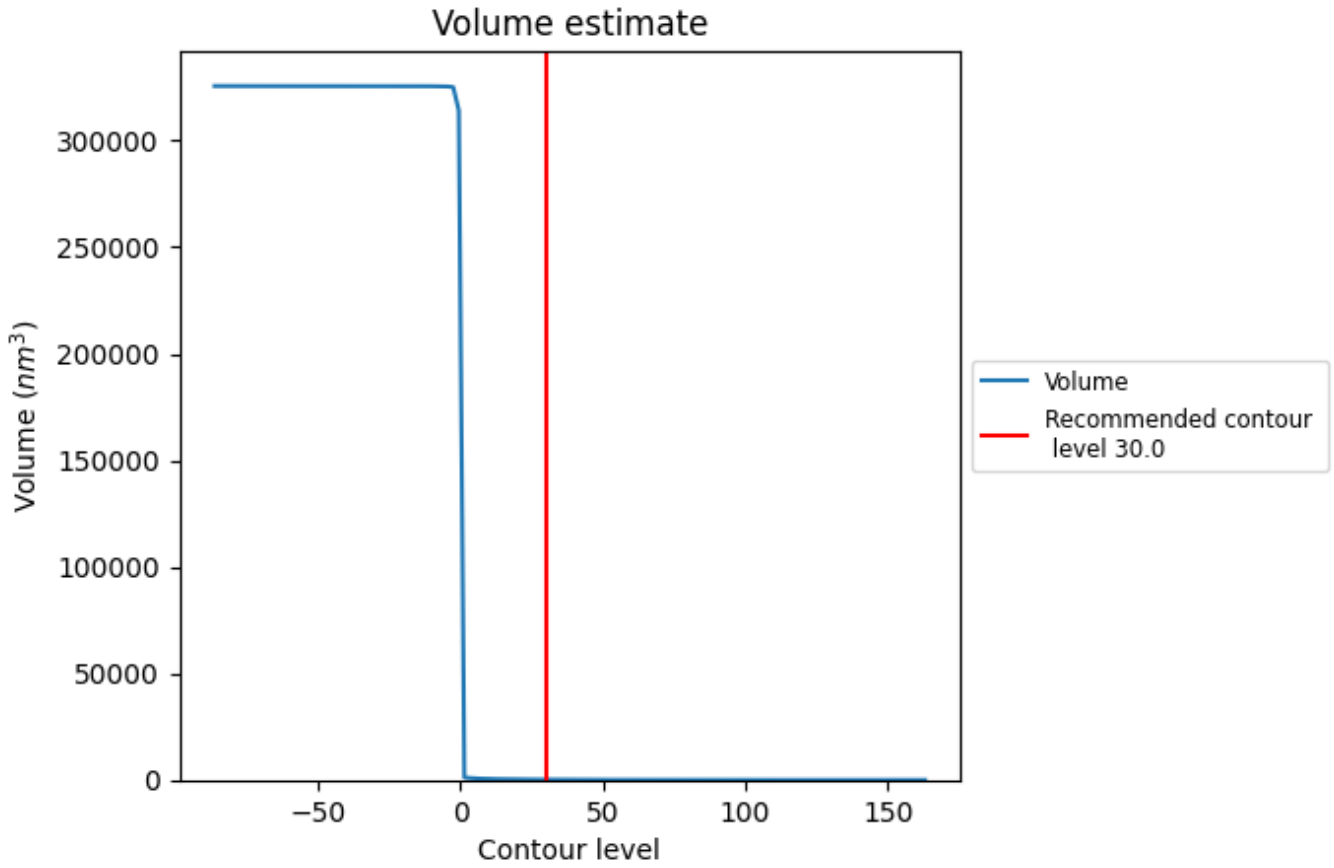
This section contains the results of statistical analysis of the map.

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.

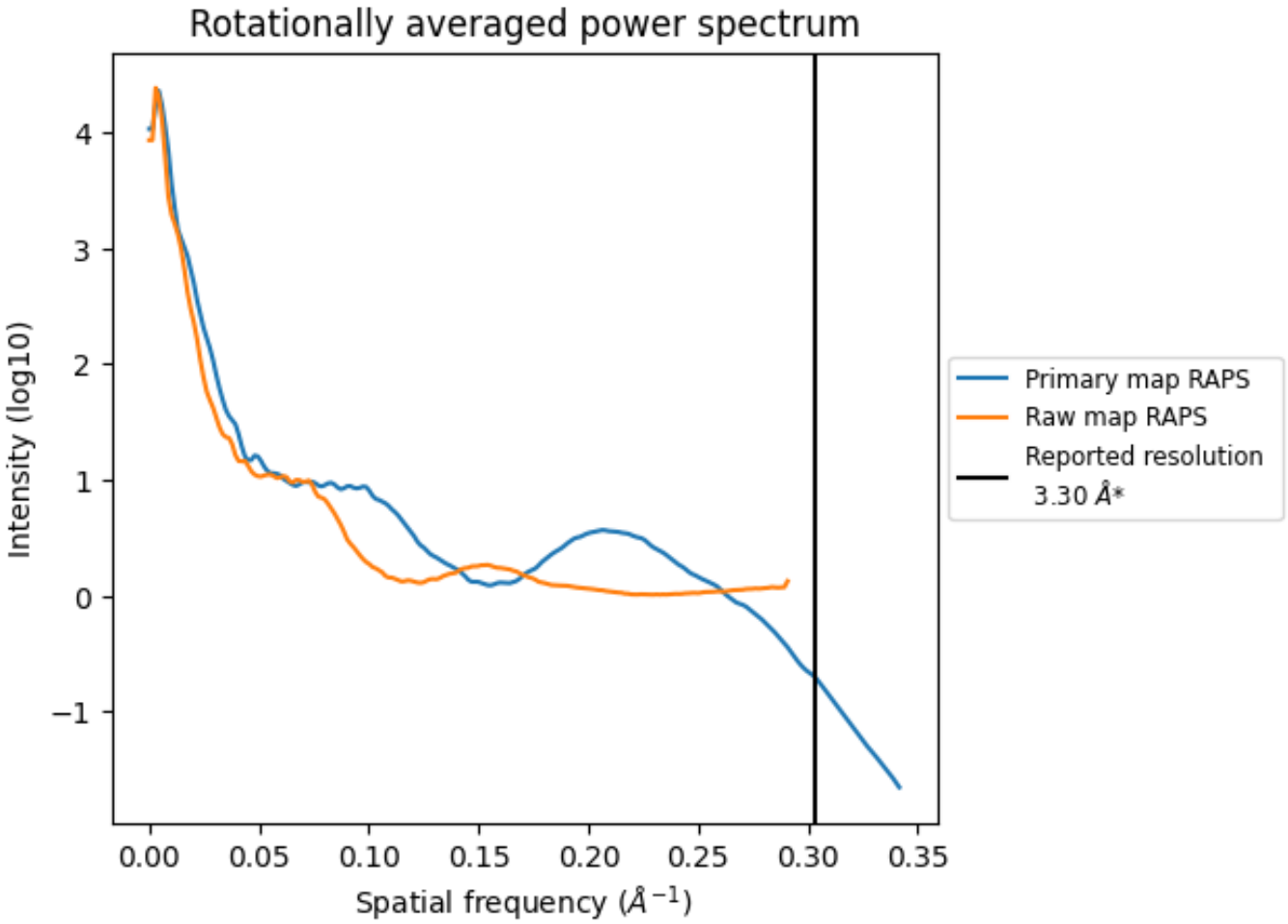
7.2 Volume estimate (i)



The volume at the recommended contour level is 172 nm^3; this corresponds to an approximate mass of 155 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)

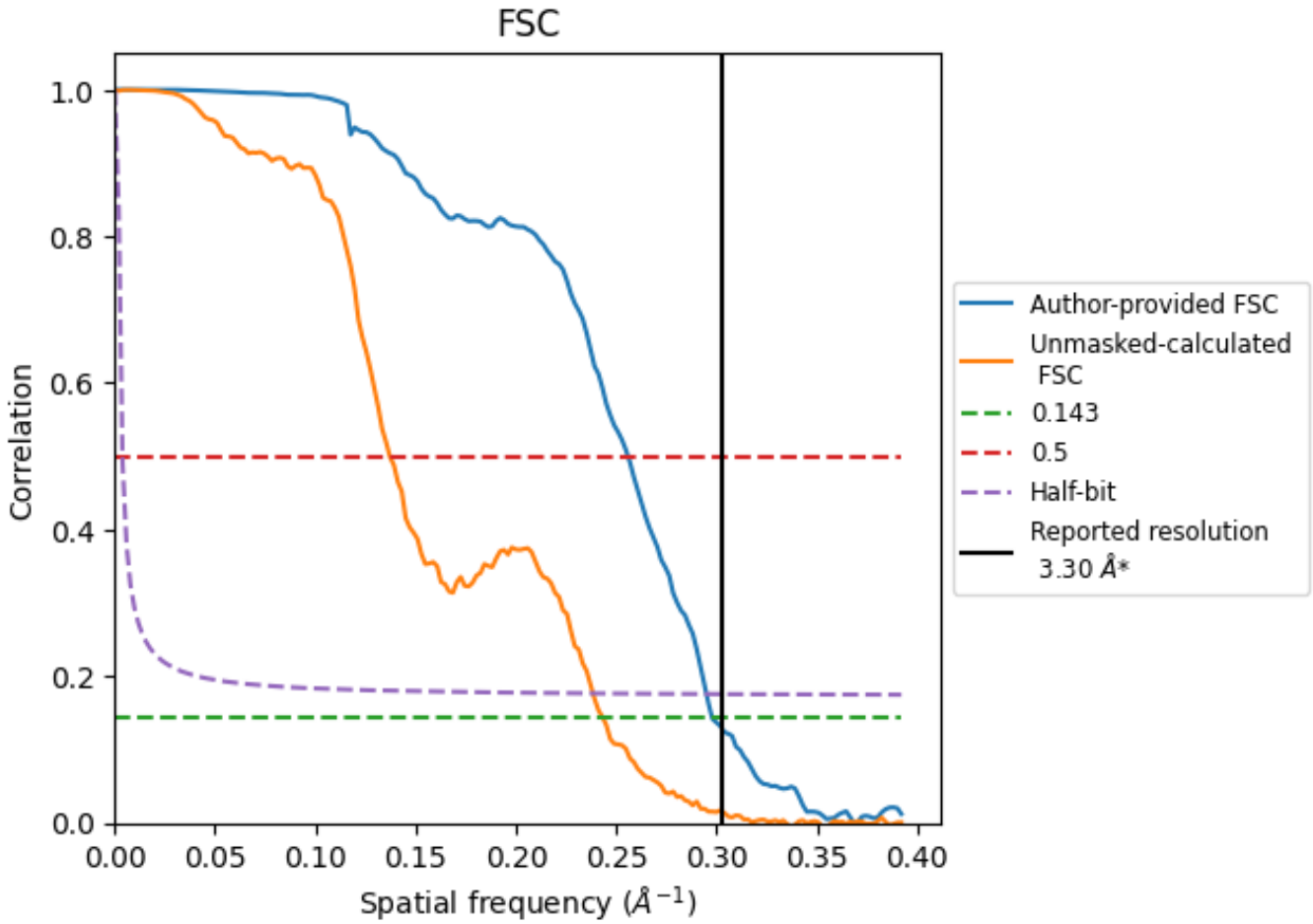


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

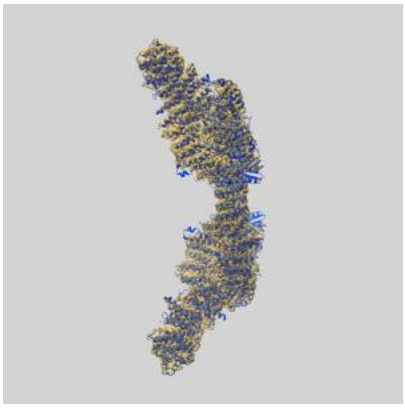
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.36	3.91	3.39
Unmasked-calculated*	4.11	7.29	4.19

*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 4.11 differs from the reported value 3.3 by more than 10 %

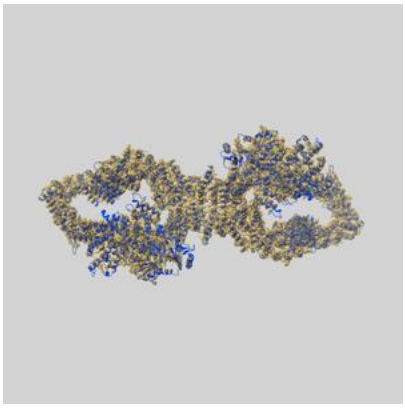
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13396 and PDB model 7PGU. Per-residue inclusion information can be found in section 3 on page 5.

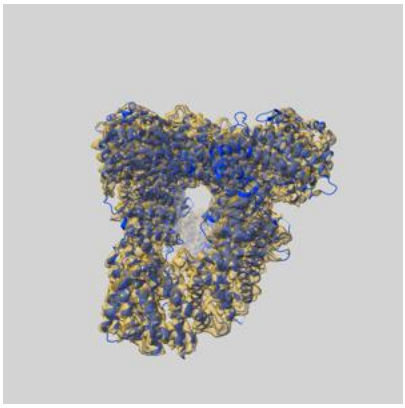
9.1 Map-model overlay



X



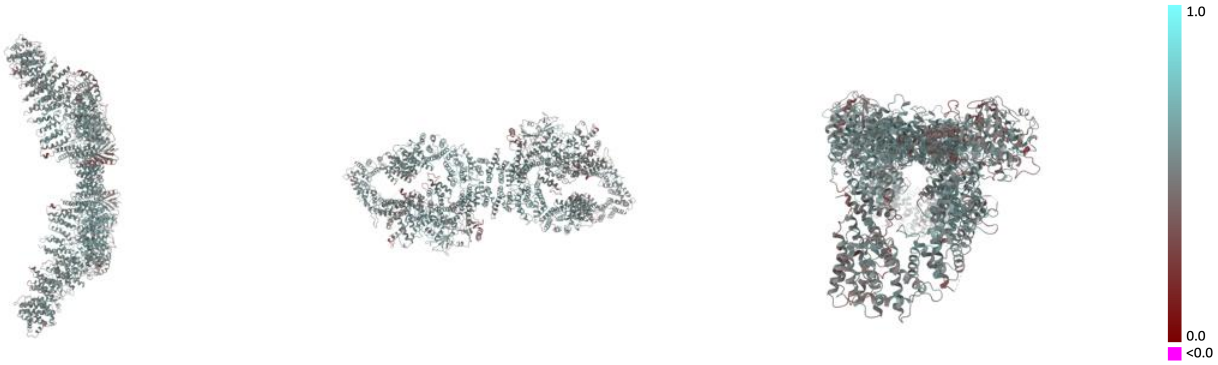
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 30.0 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.

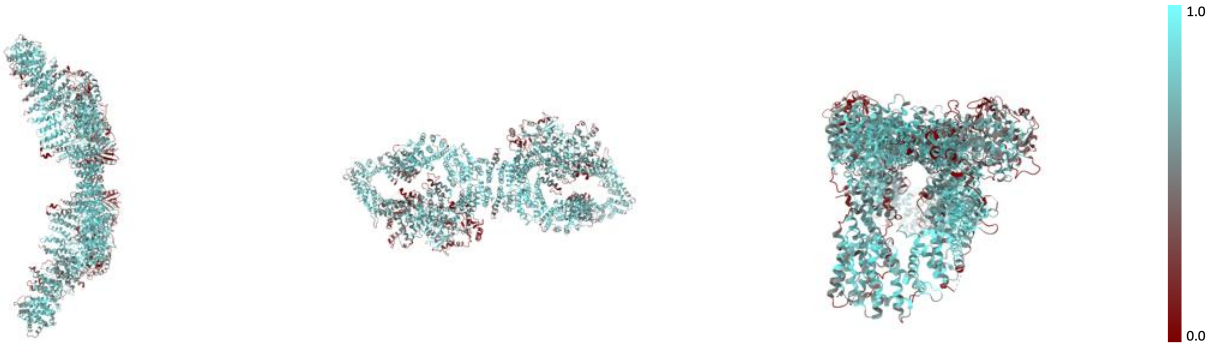
9.2 Q-score mapped to coordinate model (i)



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.

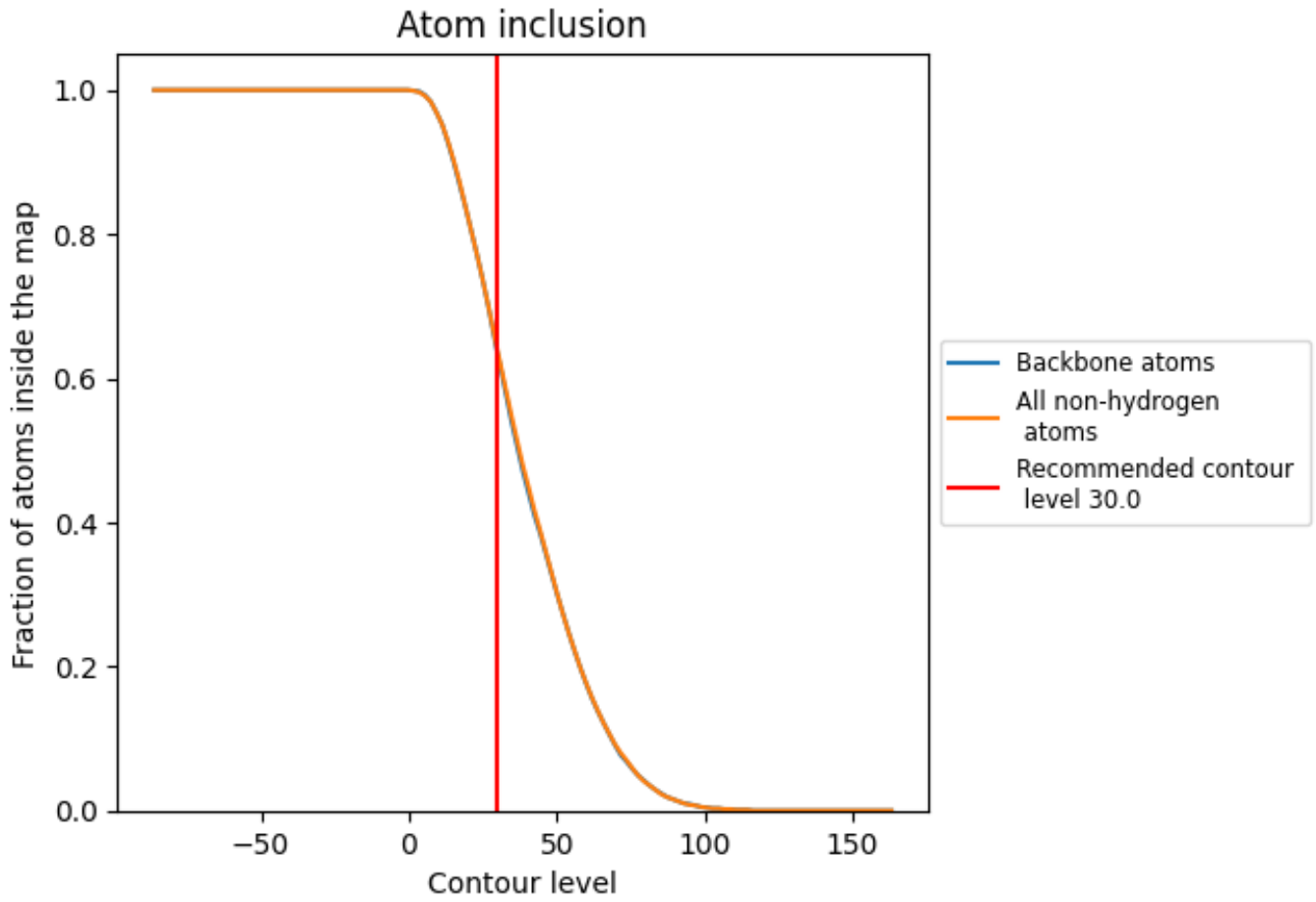
9.3 Atom inclusion mapped to coordinate model (i)



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 (30.0).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 64% 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 (30.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6370	0.5240
F	0.6290	0.5280
N	0.6560	0.5200