wwPDB EM Validation Summary Report

Oct 16, 2022 – 01:22 pm BST

PDB ID	:	7PGQ
EMDB ID	:	EMD-13392
Title	:	GAP-SecPH region of human neurofibromin isoform 2 in closed conformation.
Authors	:	Naschberger, A.; Baradaran, R.; Carroni, M.; Rupp, B.
Deposited on	:	2021-08-15
Resolution	:	3.50 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:

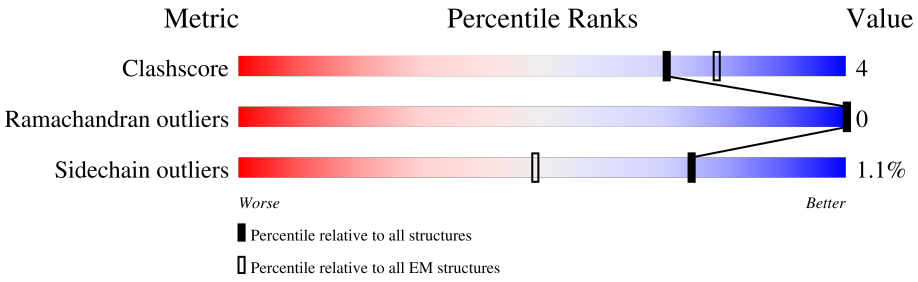
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.50 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	8% 42% 5% 54%
1	N	2839	6% 21% · 77%

2 Entry composition (i)

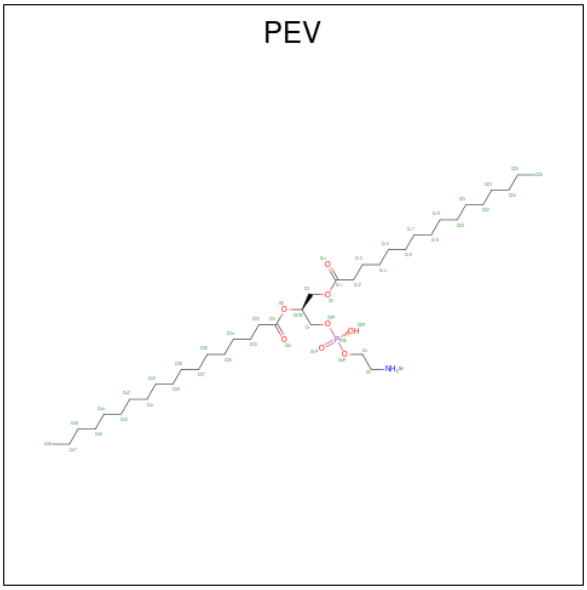
There are 3 unique types of molecules in this entry. The entry contains 31585 atoms, of which 15884 are hydrogens and 0 are deuteriums.

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	1320	Total	C	H	N	O	S	0	0
			21053	6700	10550	1778	1950	75		
1	N	650	Total	C	H	N	O	S	0	0
			10405	3317	5257	868	939	24		

- 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	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

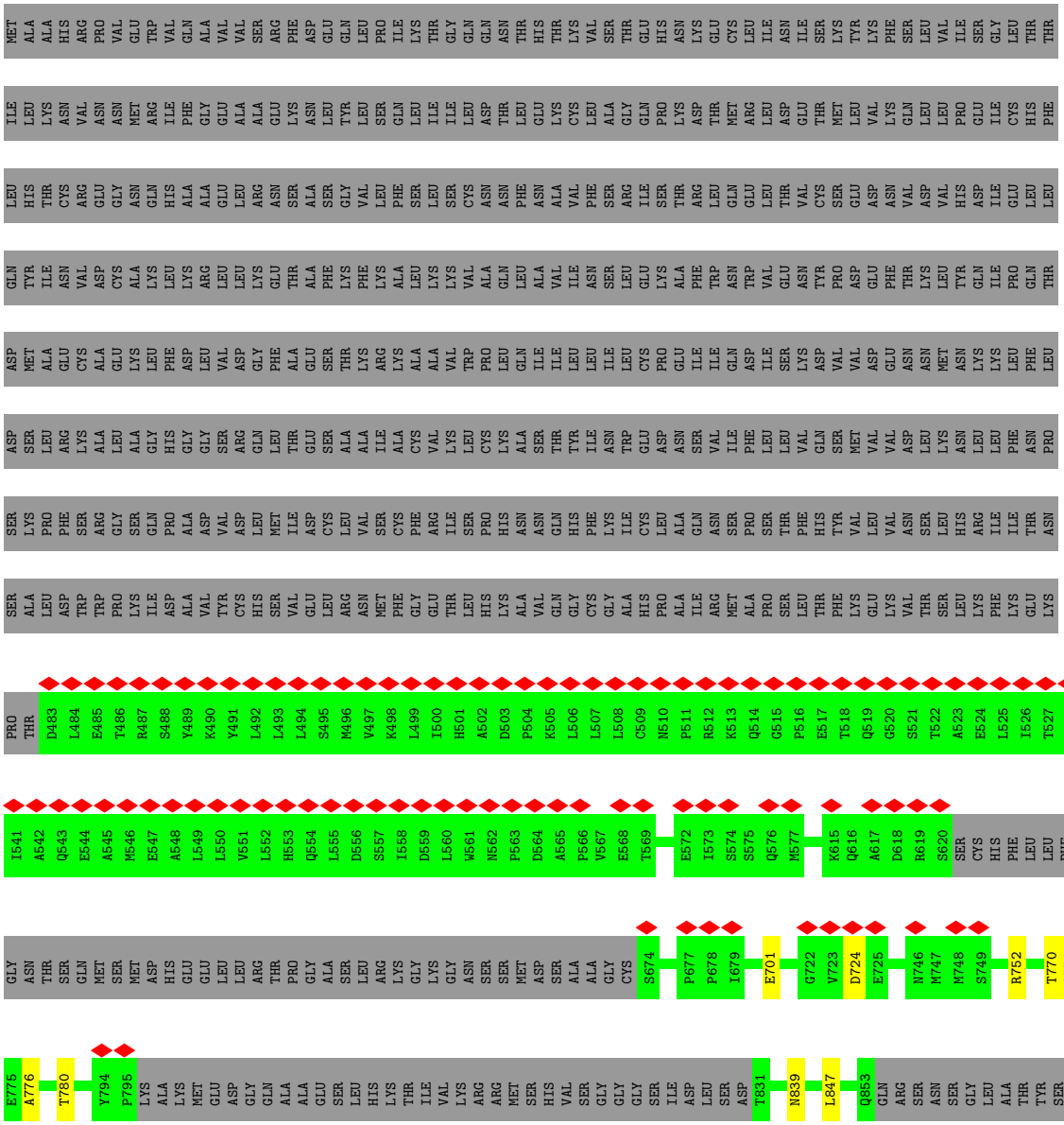
Mol	Chain	Residues	Atoms		AltConf
3	F	1	Total	Zn	0
			1	1	

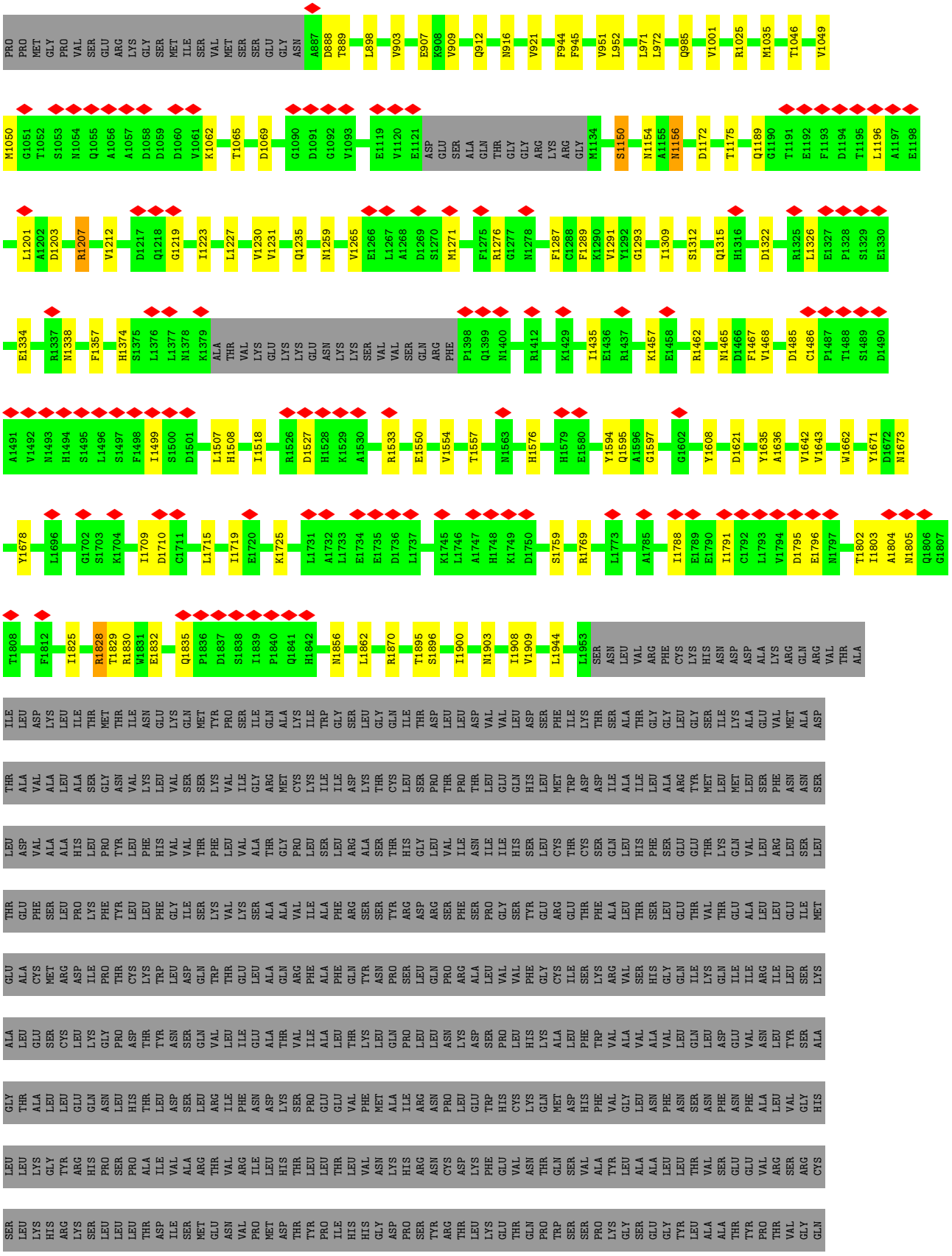
3 Residue-property plots (i)

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 F:




PRO PRO MET GLY PRO VAL SER GLU ARG LYS GLY SER MET ILE SER VAL MET SER SER GLU GLY ASN
A887 D888 T889 L898 V903 E907 K908 V909 Q912 N916 V921 F944 F945 V951 L952 L971 L972 Q985 V1001 R1025 M1035 T1046 V1049
M1050 G1051 T1052 S1053 N1054 Q1055 A1056 A1057 D1058 D1059 D1060 V1061 K1062 T1065 D1069 G1090 D1091 G1092 V1093 E1119 V1120 E1121 ASP GLU SER ALA GLN THR GLY GLY ARG LYS ARG GLY M1134 S1150 N1154 A1155 N1156 D1172 T1175 Q1189 G1190 T1191 E1192 F1193 D1194 T1195 L1196 A1197 E1198
L1201 A1202 D1203 R1207 V1212 D1217 Q1218 G1219 I1223 L1227 V1230 V1231 Q1235 N1259 V1265 E1266 L1267 A1268 D1269 S1270 M1271 F1275 R1276 G1277 N1278 F1287 C1288 F1289 K1290 V1291 Y1292 G1293 I1309 S1312 Q1315 H1316 D1322 R1325 L1326 E1327 P1328 S1329 E1330
E1334 R1337 N1338 F1357 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 R1412 K1429 I1435 E1436 R1437 K1457 E1458 R1462 N1465 D1466 F1467 V1468 D1485 C1486 P1487 T1488 S1489 D1490
A1491 V1492 N1493 H1494 S1495 L1496 S1497 F1498 I1499 S1500 D1501 L1507 H1508 I1518 R1526 D1527 H1528 K1529 A1530 R1533 E1550 V1554 T1557 N1563 H1576 H1579 E1580 Y1594 Q1595 A1596 G1597 G1602 Y1608 D1621 Y1635 A1636 V1642 V1643 W1662 Y1671 D1672 N1673
Y1678 L1696 G1702 S1703 K1704 I1709 D1710 C1711 L1715 I1719 E1720 K1725 L1731 A1732 L1733 E1734 E1735 D1736 L1737 K1745 L1746 A1747 H1748 K1749 D1750 S1759 R1769 L1773 A1785 I1788 E1789 E1790 I1791 C1792 L1793 V1794 D1795 E1796 N1797 T1802 I1803 A1804 N1805 Q1806 G1807
T1808 F1812 I1825 R1828 T1829 R1830 W1831 E1832 Q1835 P1836 D1837 S1838 I1839 P1840 Q1841 H1842 N1856 L1862 R1870 T1895 S1896 I1900 N1903 I1908 V1909 L1944 L1953 SER ASN LEU VAL ARG PHE CYS LYS HIS ASN ASP ASP ALA LYS ARG GLN ARG VAL THR ALA
ILE LEU ASP LYS LEU ILE THR MET THR ILE ASN GLU LYS GLN MET TYR PRO SER ILE GLN ALA LYS ILE TRP GLY SER LEU GLY GLN ILE THR ASP LEU LEU ASP VAL VAL LEU ASP SER PHE ILE LYS THR SER ALA THR GLY GLY LEU GLY SER ILE LYS ALA GLU VAL MET ALA ASP
THR ALA VAL ALA LEU ALA SER GLY ASN VAL LYS LEU VAL SER SER LYS VAL ILE GLY ARG MET CYS LYS ILE ILE ASP LYS THR CYS LEU SER PRO THR PRO THR LEU GLU LEU VAL ASP ASP ILE ALA ILE LEU LEU ALA ARG TYR MET LEU ILE LYS MET LEU SER PHE ASN ASN SER
LEU ASP VAL ALA ALA HIS LEU PRO TYR LEU PHE HIS VAL VAL THR PHE LEU VAL ALA THR GLY PRO LEU SER LEU ARG ALA SER THR HIS GLY LEU ILE ASN ILE ILE HIS SER LEU CYS THR CYS SER GLN LEU HIS PHE SER LEU GLU GLU THR LYS GLN VAL LEU ARG LEU SER SER
THR GLU PHE SER LEU PRO LYS PHE TYR LEU LEU PHE GLY ILE SER LYS VAL LYS SER ALA ALA VAL ILE ALA PHE ARG SER SER TYR ARG ASP ARG SER PHE SER PRO GLY SER TYR GLU ARG GLU THR PHE ALA LEU THR SER LEU GLU GLU THR VAL THR GLU ALA LEU LEU GLU GLU MET
GLU ALA CYS MET ARG ASP ILE PRO THR CYS LYS TRP LEU ASP GLN TRP THR GLU LEU ALA GLN ARG PHE ALA PHE GLN TYR ASN PRO SER LEU GLN PRO ARG ALA LEU VAL VAL PHE GLY CYS ILE SER LYS ARG VAL SER HIS GLY GLN ILE LYS GLN ILE ILE ARG ILE LEU LEU SER LYS
ALA LEU GLU SER CYS LEU LYS GLY PRO ASP THR TYR ASN SER GLN VAL LEU ILE GLU ALA THR VAL ILE ALA LEU THR LYS LEU GLN PRO LEU GLN LEU ASN LYS ASP SER PRO LEU HIS LYS ALA LEU PHE TRP VAL ALA VAL ALA VAL LEU GLN LEU LEU ASP GLU VAL ASN LEU TYR SER ALA
GLY THR ALA LEU LEU GLU GLN ASN LEU HIS THR LEU ASP SER LEU ARG ILE PHE ASN ASP LYS SER PRO GLU GLU VAL PHE MET ALA ILE ARG ASN PRO LEU GLU TRP HIS CYS LYS GLN MET ASP HIS PHE VAL GLY LEU ASN PHE ASN SER ASN PHE ASN PHE ALA LEU VAL GLY HIS
LEU LEU LYS GLY TYR ARG HIS PRO SER LEU THR LEU VAL ASN LYS HIS ARG ASN CYS ASP LYS PHE GLU VAL ASN THR GLN SER VAL ALA TYR LEU ALA ALA LEU LEU LEU THR VAL ALA SER GLU GLU VAL ARG SER CYS
SER LEU LYS HIS ARG ASP LYS SER HIS HIS GLY ASP PRO SER TYR ARG THR LEU LYS GLU THR GLN PRO TRP SER SER PRO GLY LYS GLY SER GLU GLY TYR LEU ALA THR TYR PRO SER VAL THR GLY

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 SER ASN VAL LEU LEU ASP GLU VAL LEU THR ASP PRO LYS ILE GLN ALA LEU LEU LEU THR VAL LEU ALA THR LEU VAL LYS TYR THR THR ASP GLU

PHE ASP GLN ARG ILE LEU TYR GLU TYR LEU ALA GLU ALA SER VAL VAL PHE PRO LYS VAL PHE PRO VAL VAL HIS ASN LEU LEU ASP SER LYS ILE ASN THR LEU LEU SER LEU CYS GLN ASP PRO ASN LEU LEU ASN PRO ILE HIS GLY ILE VAL GLN SER VAL VAL TYR HIS GLU GLU

SER PRO PRO GLN TYR GLN THR SER TYR LEU GLN SER PHE GLY PHE ASN GLY LEU TRP ARG PHE ALA GLY PRO PHE SER LYS GLN THR GLN ILE PRO ASP TYR ALA GLU LEU ILE VAL LYS PHE LEU ASP ALA LEU ILE ASP THR TYR LEU PRO GLY 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

• Molecule 1: Neurofibromin

Chain N:

MET ALA ALA HIS ARG PRO VAL GLU TRP VAL GLN ALA VAL VAL SER ARG PHE ASP GLU GLN LEU PRO ILE LYS THR GLY GLN GLN ASN THR HIS THR LYS VAL SER THR GLU HIS ASN LYS GLU CYS LEU ILE ASN ILE SER LYS TYR LYS PHE SER LEU VAL ILE SER GLY LEU THR THR

ILE LEU LYS ASN VAL ASN ASN MET ARG ILE PHE GLY GLU ALA ALA GLU LYS ASN LEU TYR LEU SER GLN LEU ILE ILE LEU ASP THR LEU GLU LYS CYS LEU ALA GLY GLN PRO LYS ASP THR MET ARG LEU ASP GLU THR MET LEU VAL LYS GLN LEU LEU PRO GLU ILE CYS HIS PHE

LEU HIS THR CYS ARG GLU GLY ASN GLN HIS ALA ALA GLU LEU ARG ASN SER ALA SER GLY VAL LEU PHE SER LEU SER CYS ASN ASN PHE ASN ALA VAL PHE SER ARG ILE SER THR ARG LEU GLN GLU LEU THR VAL CYS SER GLU ASP ASN VAL ASP VAL HIS ASP ILE GLU LEU LEU

GLN TYR ILE ASN VAL ASP CYS ALA LYS LEU LYS ARG LEU LEU LYS GLU THR ALA PHE LYS PHE LYS ALA LEU LYS LYS VAL ALA GLN LEU ALA VAL ILE ASN SER LEU GLU LYS ALA PHE TRP ASN TRP VAL GLU ASN TYR PRO ASP GLU PHE THR LYS LEU TYR GLN ILE PRO GLN THR

ASP MET ALA GLU CYS ALA GLU LYS LEU PHE ASP LEU VAL ASP GLY PHE ALA GLU SER THR LYS ARG LYS ALA ALA VAL TRP PRO LEU GLN ILE ILE LEU LEU ILE LEU CYS PRO GLU ILE ILE GLN ASP ILE SER LYS ASP VAL VAL ASP GLU ASN ASN MET ASN LYS LYS LEU PHE LEU

ASP SER LEU ARG LYS ALA LEU ALA GLY HIS GLY GLY SER ARG GLN LEU THR GLU SER ALA ALA ILE ALA CYS VAL LYS LEU CYS LYS ALA SER THR TYR ILE ASN TRP GLU ASP ASN SER VAL ILE PHE LEU LEU VAL GLN SER MET VAL VAL ASP LEU LYS ASN LEU LEU PHE ASN PRO

SER LYS PRO PHE SER ARG GLY SER GLN PRO ALA ASP VAL ASP LEU MET ILE ASP CYS LEU VAL SER CYS PHE ARG ILE SER PRO HIS ASN ASN GLN HIS PHE LYS ILE CYS LEU ALA GLN ASN SER PRO SER THR PHE HIS TYR VAL LEU VAL ASN SER LEU HIS ARG ILE ILE THR ASN

SER ALA LEU ASP TRP TRP PRO LYS ILE ASP ALA VAL TYR CYS HIS SER VAL GLU LEU ARG ASN MET PHE GLY GLU THR LEU HIS LYS ALA VAL GLN GLY CYS GLY 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

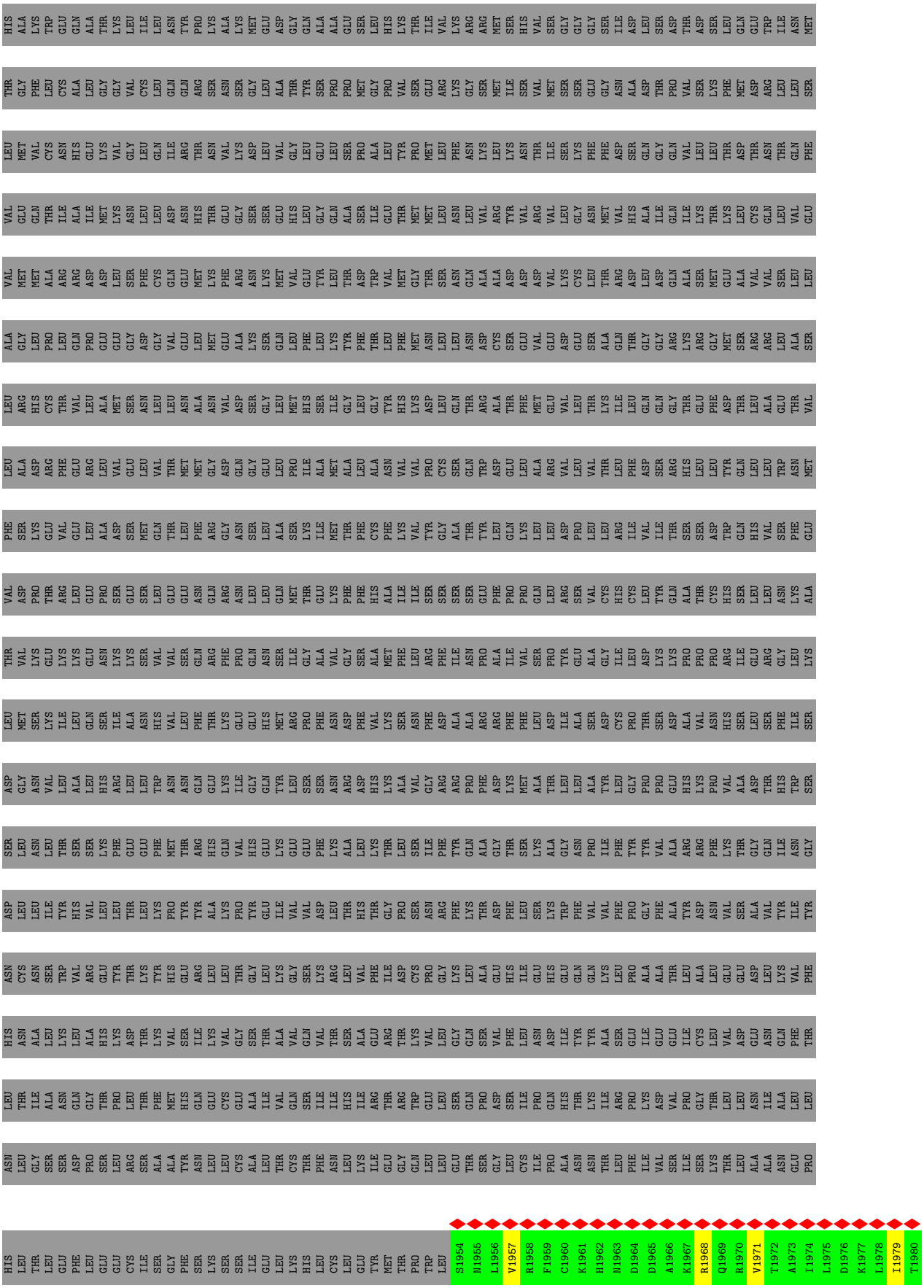
PRO THR ASP LEU GLU THR ARG SER TYR LYS TYR LEU LEU LEU SER MET VAL LYS LEU ILE HIS ALA ASP PRO LYS LEU LEU LEU CYS ASN PRO ARG LYS GLN GLY PRO GLU THR GLN GLY SER THR ALA GLU LEU ILE THR GLY LEU VAL GLN LEU VAL PRO GLN SER HIS MET PRO GLU

ILE ALA GLN GLU ALA MET GLU ALA LEU LEU VAL LEU HIS GLN LEU ASP SER ILE ASP LEU TRP ASN PRO ASP ALA PRO VAL GLU THR PHE TRP GLU ILE SER SER GLN MET LEU PHE TYR ILE CYS LYS LYS LEU THR SER HIS GLN MET LEU SER SER THR GLU ILE LEU LYS TRP LEU

ARG GLU ILE LEU ILE CYS ARG ASN LYS PHE LEU LEU LYS ASN LYS GLN ALA ASP ARG SER 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 SER GLY THR PRO PRO ILE CYS ARG GLN ALA GLN THR LYS LEU GLU VAL ALA LEU TYR MET PHE LEU TRP ASN PRO ASP THR GLU ALA VAL LEU VAL ALA MET SER CYS PHE ARG HIS LEU CYS GLU GLU ALA ASP ILE ARG

CYS GLY VAL ASP GLU VAL SER VAL HIS ASN LEU LEU PRO ASN TYR ASN THR PHE MET GLU PHE ALA SER VAL SER ASN MET MET SER THR GLY ARG ALA ALA LEU GLN LYS ARG VAL MET ALA LEU LEU ARG ARG ILE GLU HIS PRO THR ALA GLY ASN THR GLU ALA TRP GLU ASP THR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N1955
L1956
V1957
R1958
F1959
C1960
K1961
H1962
N1963
D1964
D1965
A1966
K1967
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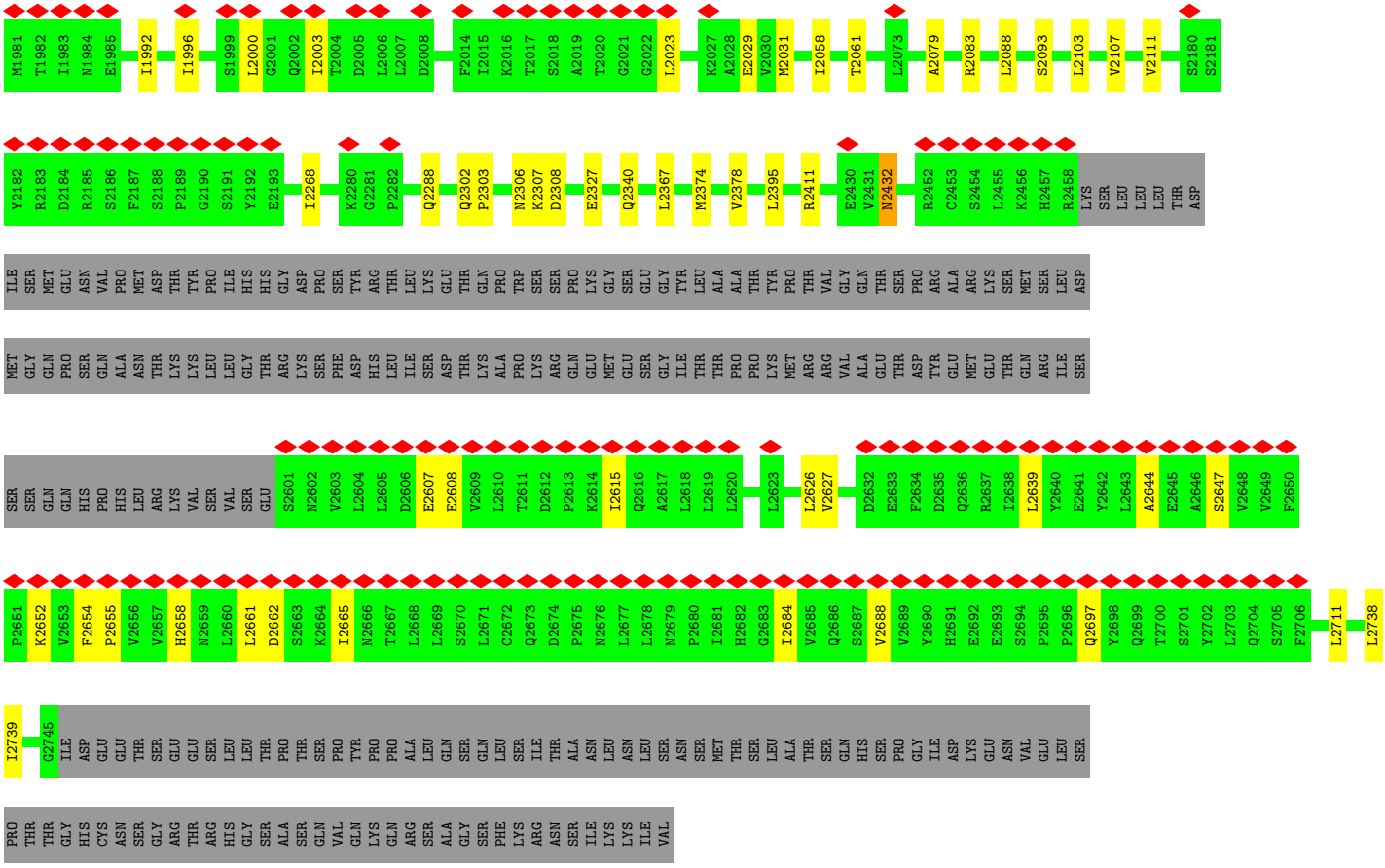

M1981 T1982 I1983 N1984 E1985 I1992 I1996 S1999 L2000 G2001 Q2002 I2003 T2004 D2005 L2006 L2007 D2008 F2014 I2015 K2016 T2017 S2018 A2019 T2020 G2021 G2022 L2023 K2027 A2028 E2029 V2030 M2031 I2058 T2061 L2073 A2079 R2083 L2088 S2093 L2103 V2107 V2111 S2180 S2181
Y2182 R2183 D2184 R2185 S2186 F2187 S2188 P2189 G2190 S2191 Y2192 E2193 I2268 K2280 G2281 P2282 Q2288 Q2302 P2303 N2306 K2307 D2308 E2327 Q2340 L2367 M2374 V2378 L2395 R2411 E2430 V2431 N2432 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 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 V2603 L2604 L2605 D2606 E2607 E2608 V2609 L2610 T2611 D2612 P2613 K2614 I2615 Q2616 A2617 L2618 L2619 L2620 L2623 L2626 V2627 D2632 E2633 F2634 D2635 Q2636 R2637 I2638 L2639 Y2640 E2641 Y2642 L2643 A2644 E2645 A2646 S2647 V2648 V2649 F2650
P2651 K2652 V2653 F2654 P2655 V2656 V2657 H2658 N2659 L2660 L2661 D2662 S2663 K2664 I2665 N2666 T2667 L2668 L2669 S2670 L2671 C2672 Q2673 D2674 P2675 N2676 L2677 L2678 N2679 P2680 I2681 H2682 G2683 I2684 V2685 Q2686 S2687 V2688 V2689 Y2690 H2691 E2692 E2693 S2694 P2695 P2696 Q2697 Y2698 Q2699 T2700 S2701 Y2702 L2703 Q2704 S2705 F2706 L2711 L2738
I2739 G2745 ILE ASP GLU 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	100684	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)	0.5	Depositor
Maximum defocus (nm)	2.1	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.151	Depositor
Minimum map value	-0.062	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.72, 1.72, 1.72	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEV, 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	0.25	0/10719	0.43	0/14518
1	N	0.26	0/5257	0.45	0/7144
All	All	0.25	0/15976	0.44	0/21662

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	10503	10550	10556	83	0
1	N	5148	5257	5257	33	0
2	F	49	77	77	0	0
3	F	1	0	0	0	0
All	All	15701	15884	15890	115	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 4.

The worst 5 of 115 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:1230:VAL:HG21	1:F:1518:ILE:HG22	1.47	0.94
1:N:2088:LEU:O	1:N:2093:SER:OG	1.91	0.87
1:F:907:GLU:N	1:F:907:GLU:OE1	2.12	0.82
1:F:1219:GLY:O	1:F:1259:ASN:ND2	2.15	0.80
1:F:985:GLN:N	1:F:985:GLN:OE1	2.15	0.78

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	1308/2839 (46%)	1291 (99%)	17 (1%)	0	100	100
1	N	646/2839 (23%)	640 (99%)	6 (1%)	0	100	100
All	All	1954/5678 (34%)	1931 (99%)	23 (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	1180/2531 (47%)	1163 (99%)	17 (1%)	67	85
1	N	581/2531 (23%)	579 (100%)	2 (0%)	92	97
All	All	1761/5062 (35%)	1742 (99%)	19 (1%)	74	88

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1635	TYR
1	N	2367	LEU
1	N	2432	ASN
1	F	1828	ARG
1	F	1374	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1856	ASN
1	F	1943	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	F	2901	-	48,48,48	0.31	0	51,53,53	0.25	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	F	2901	-	-	9/52/52/52	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

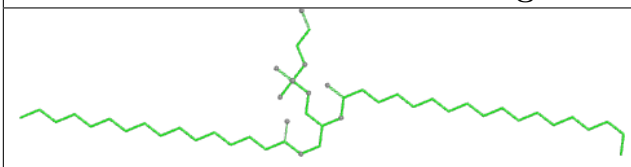
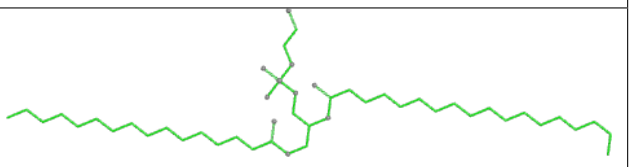
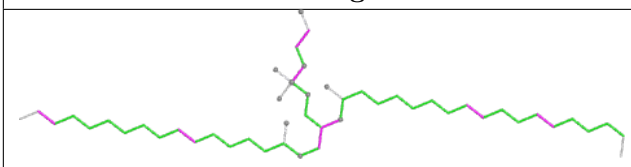
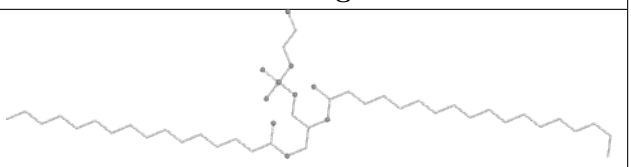
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2901	PEV	O4P-C4-C5-N6
2	F	2901	PEV	C4-O4P-P-O3P
2	F	2901	PEV	C37-C38-C39-C40
2	F	2901	PEV	C41-C42-C43-C44
2	F	2901	PEV	C15-C16-C17-C18

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 F 2901	
 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.

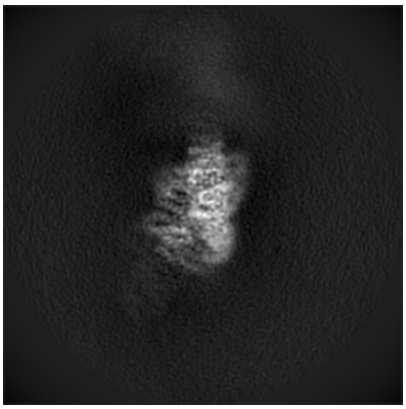
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13392. These allow visual inspection of the internal detail of the map and identification of artifacts.

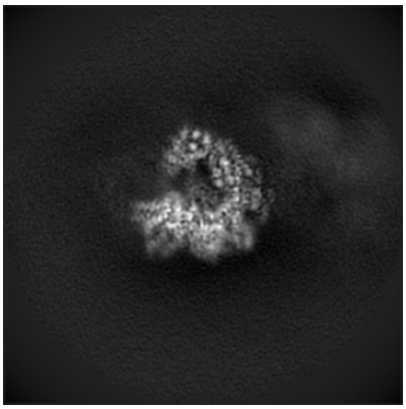
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

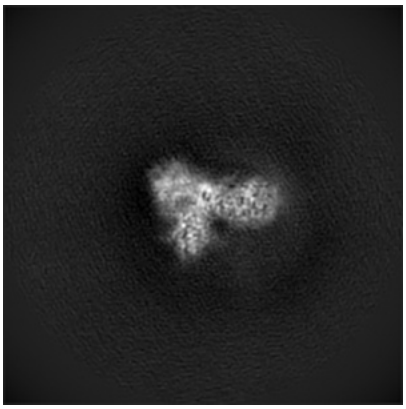
6.1.1 Primary map



X

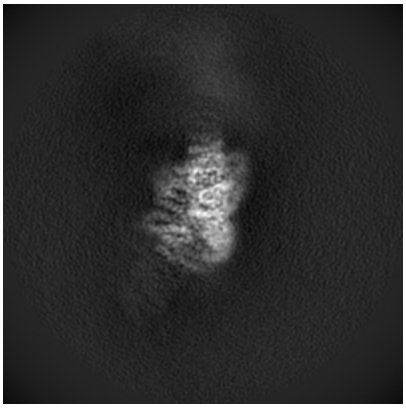


Y

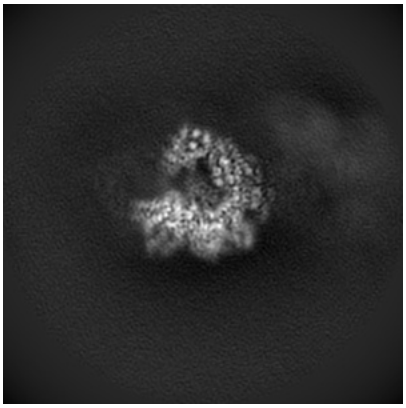


Z

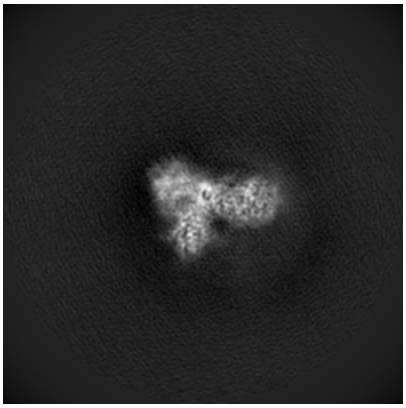
6.1.2 Raw map



X



Y

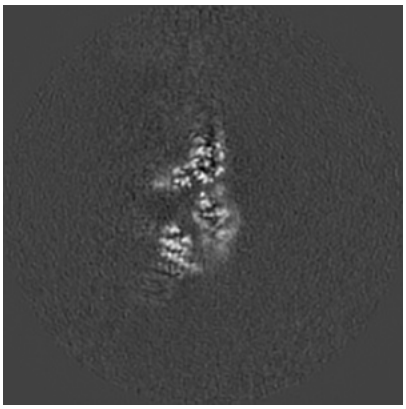


Z

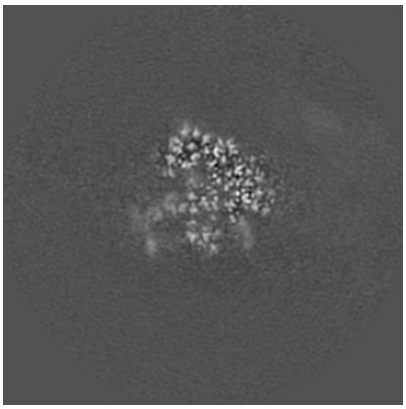
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

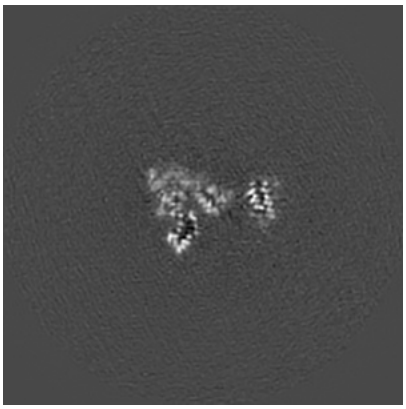
6.2.1 Primary map



X Index: 100

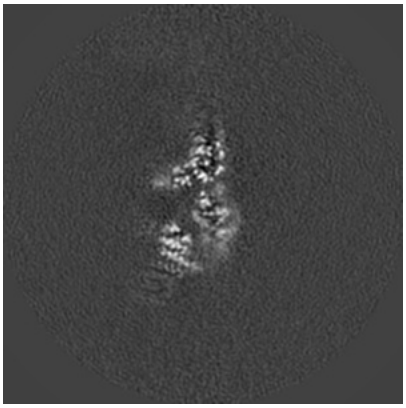


Y Index: 100

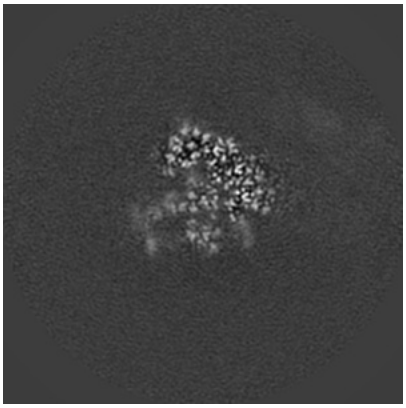


Z Index: 100

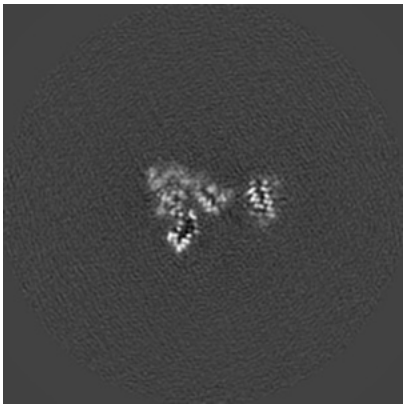
6.2.2 Raw map



X Index: 100



Y Index: 100

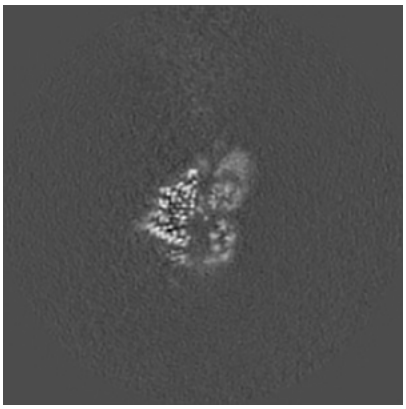


Z Index: 100

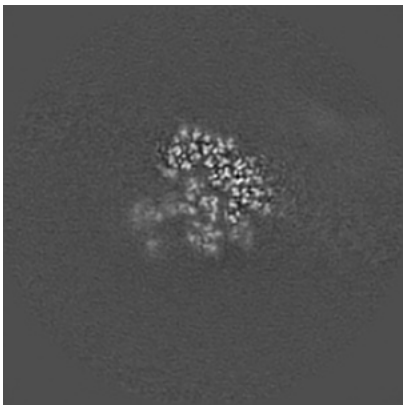
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

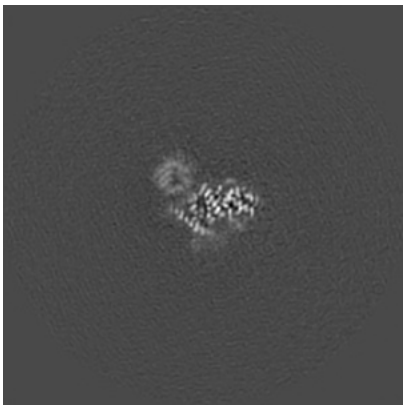
6.3.1 Primary map



X Index: 89

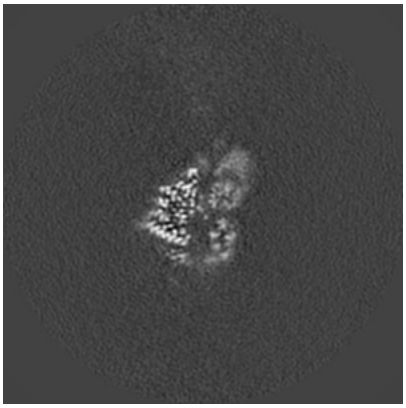


Y Index: 99

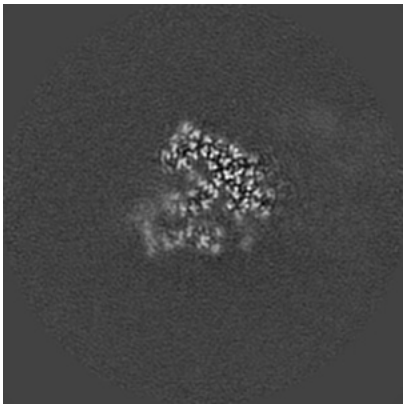


Z Index: 117

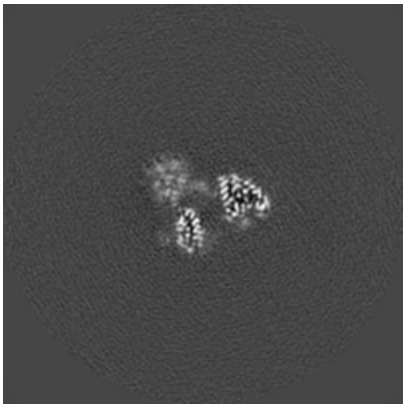
6.3.2 Raw map



X Index: 89



Y Index: 102

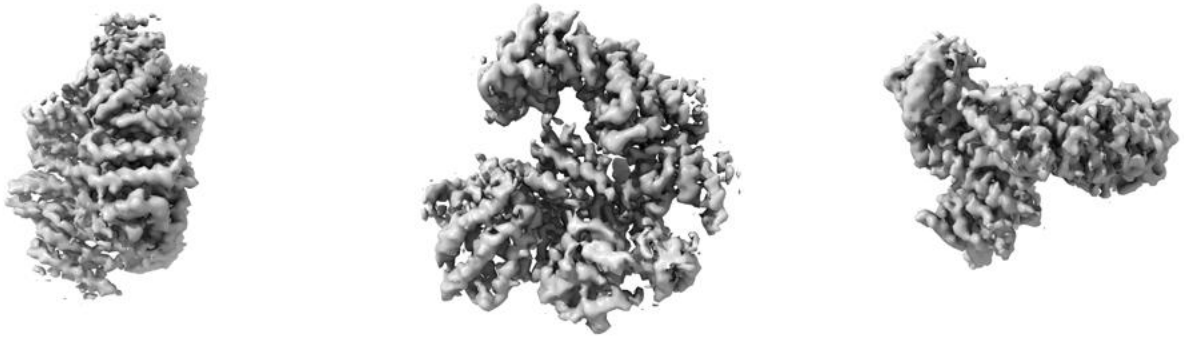


Z Index: 108

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

6.4 Orthogonal surface views (i)

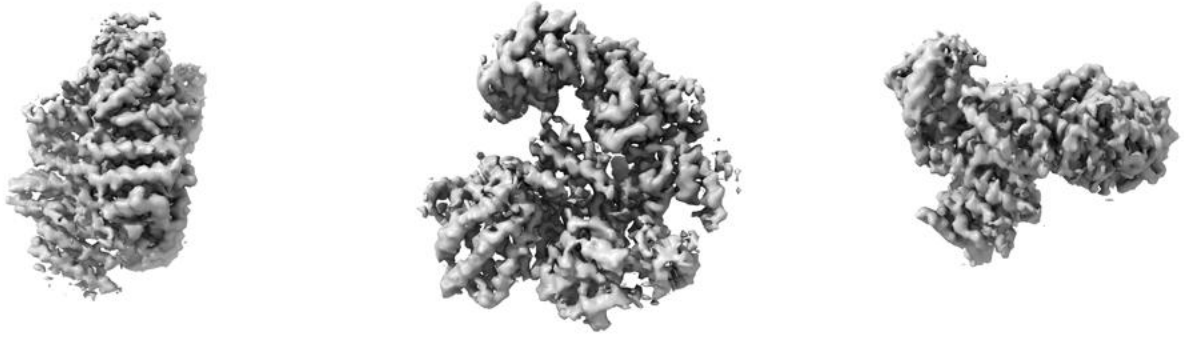
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

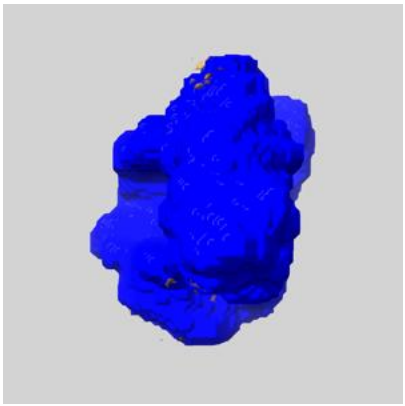
6.5 Mask visualisation (i)

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

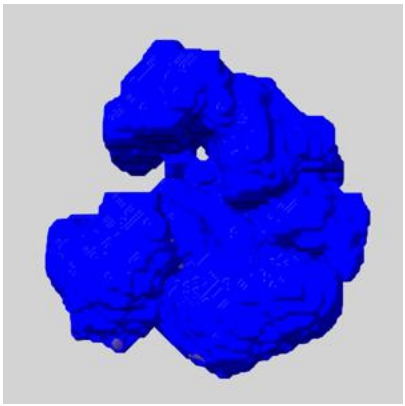
A mask typically either:

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

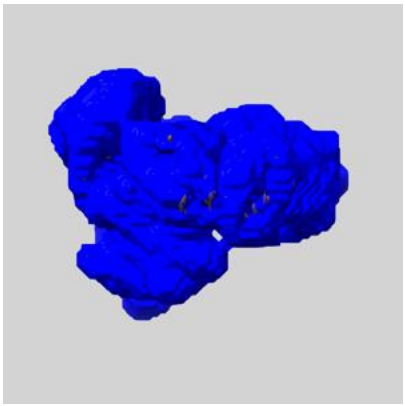
6.5.1 emd_13392_msk_1.map (i)



X



Y

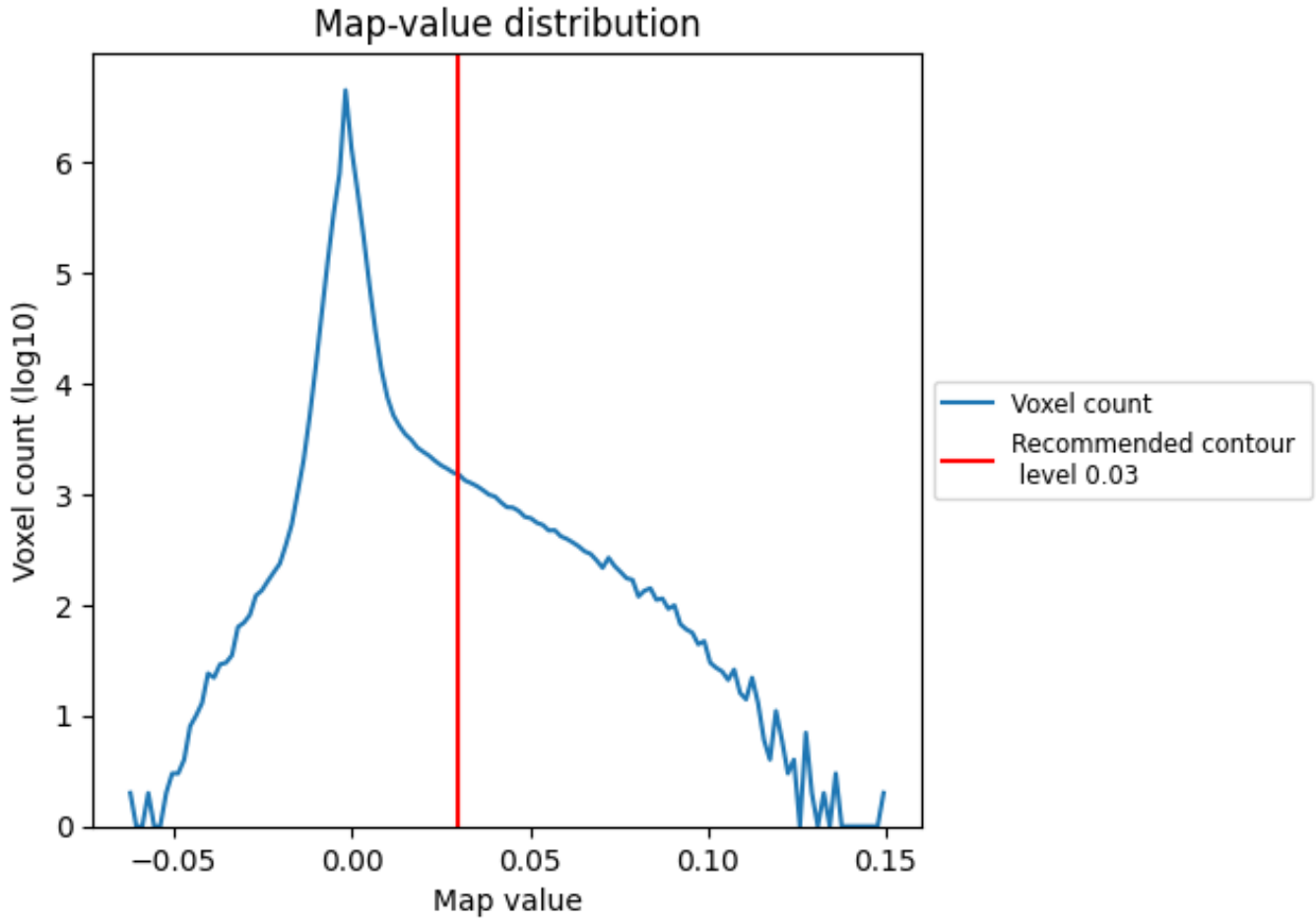


Z

7 Map analysis

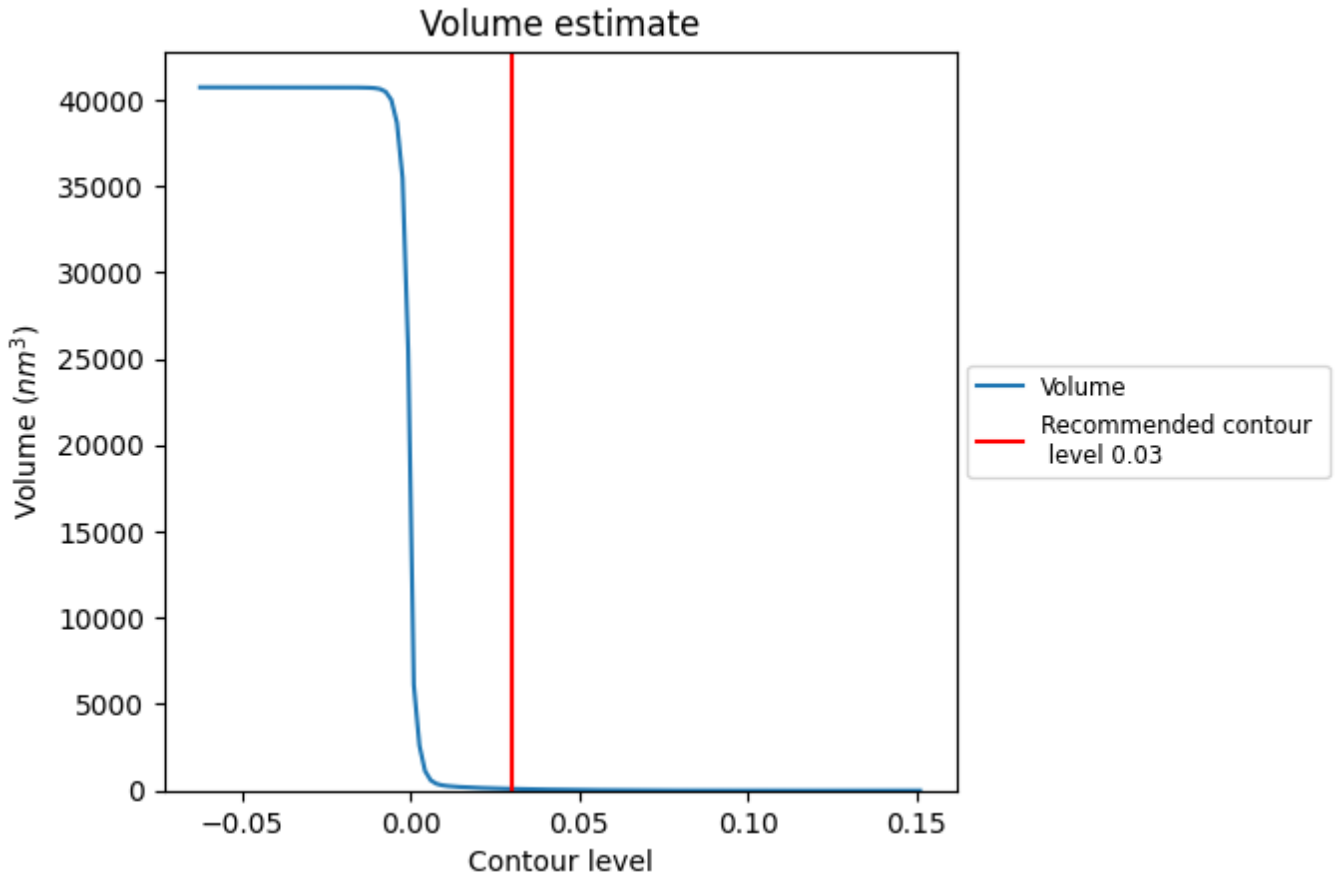
This section contains the results of statistical analysis of the map.

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.

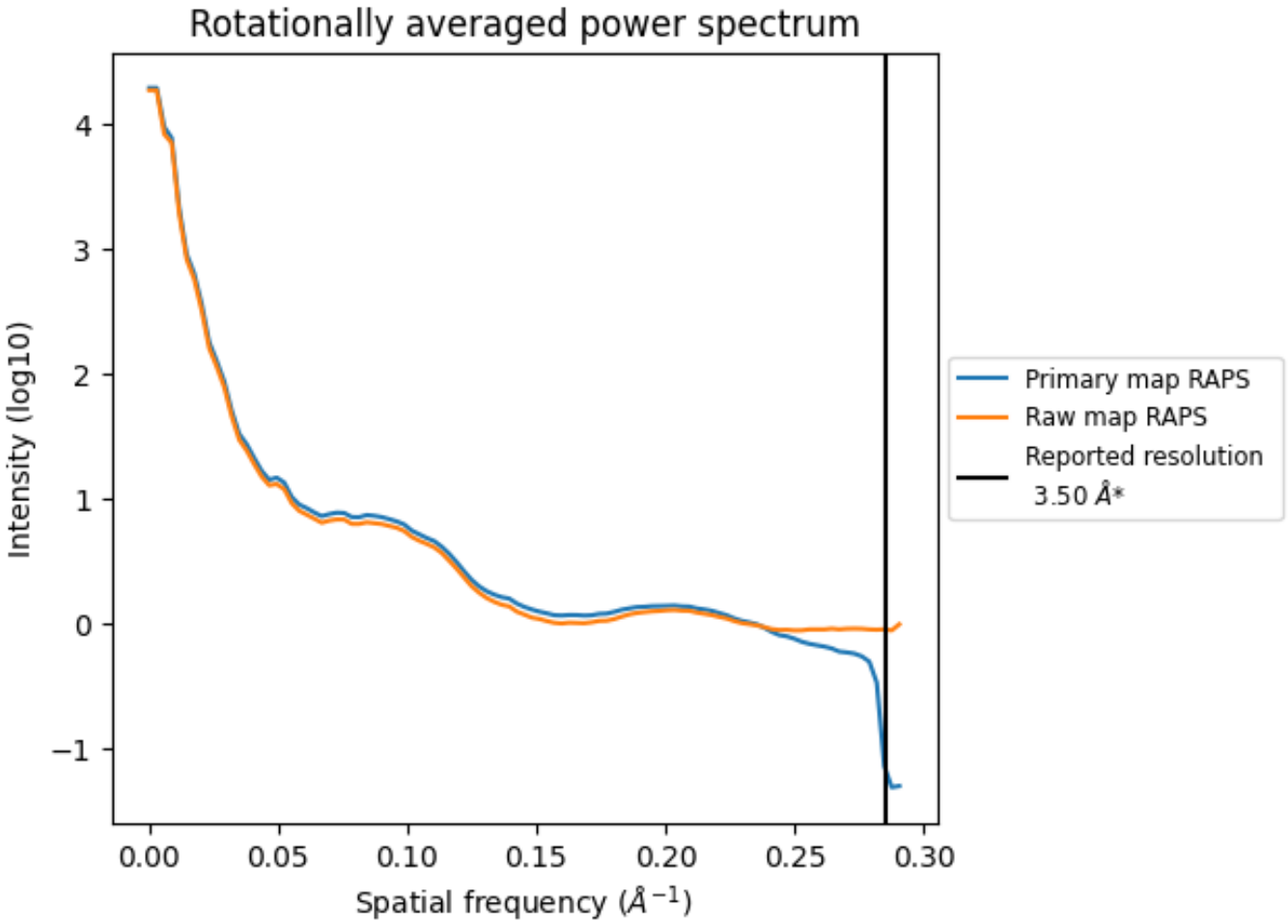
7.2 Volume estimate (i)



The volume at the recommended contour level is 100 nm^3; this corresponds to an approximate mass of 90 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)

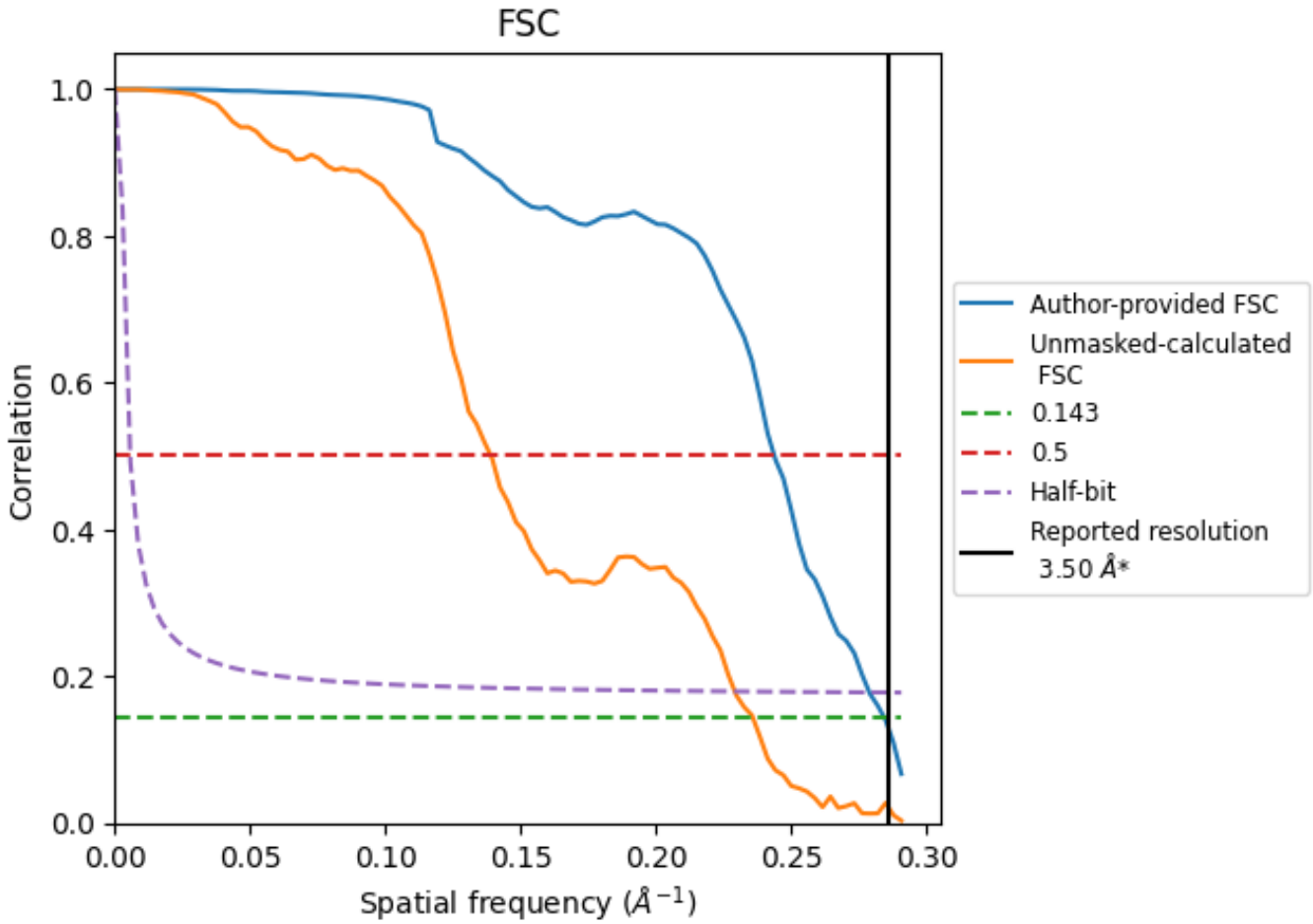


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

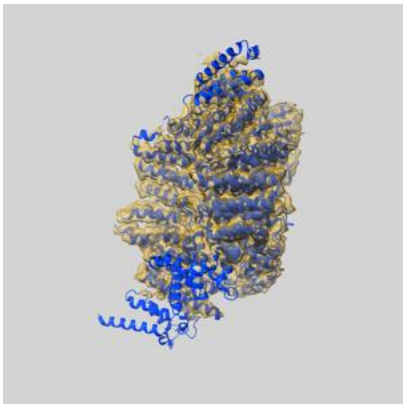
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	4.10	3.59
Unmasked-calculated*	4.24	7.19	4.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.5 by more than 10 %

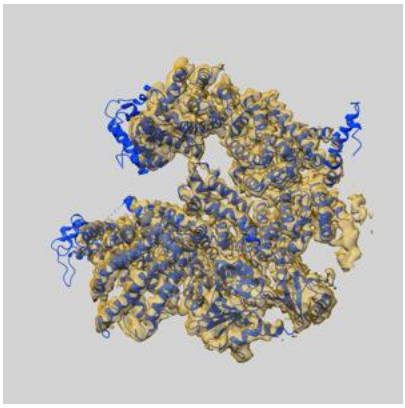
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13392 and PDB model 7PGQ. Per-residue inclusion information can be found in section 3 on page 4.

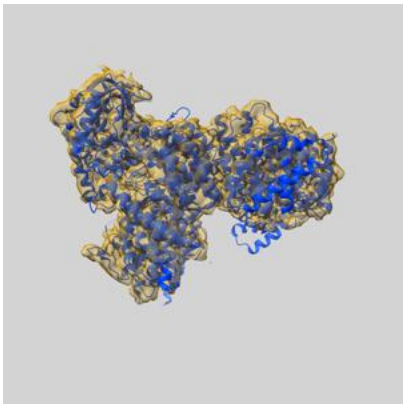
9.1 Map-model overlay



X



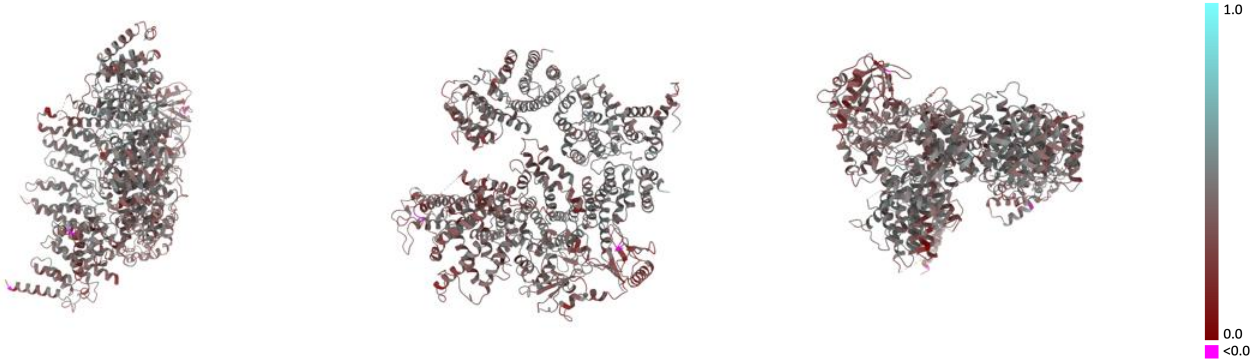
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

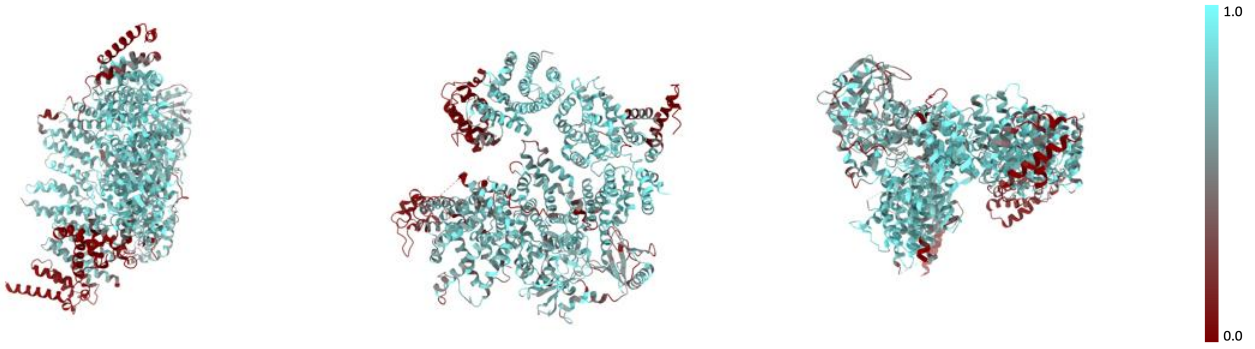
9.2 Q-score mapped to coordinate model



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.

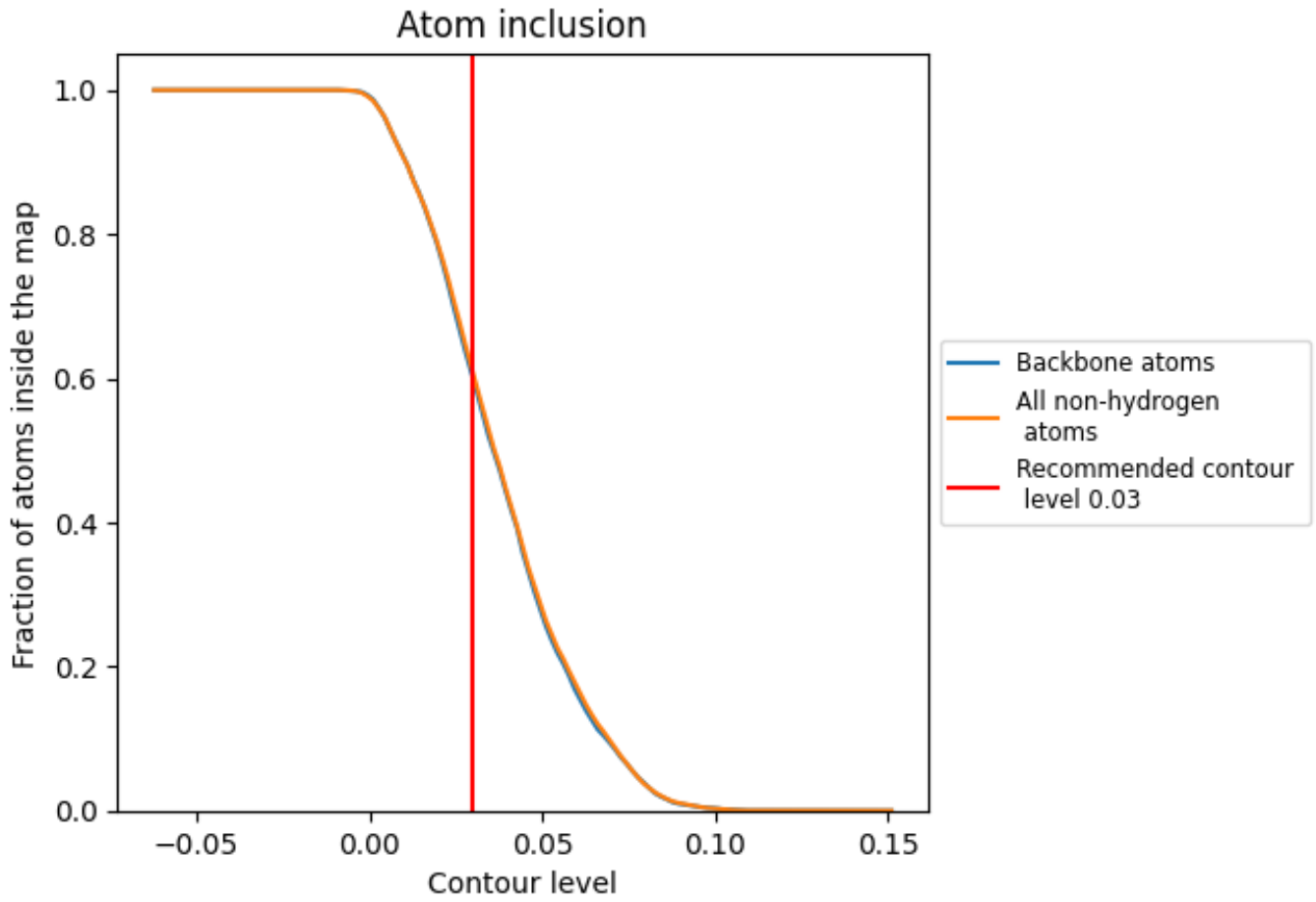
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 61% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6067	0.3950
F	0.6333	0.3830
N	0.5902	0.4190