



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2021 – 05:16 am GMT

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](mailto: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.

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

EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.4 (270009), CSD as541be (2020)  
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

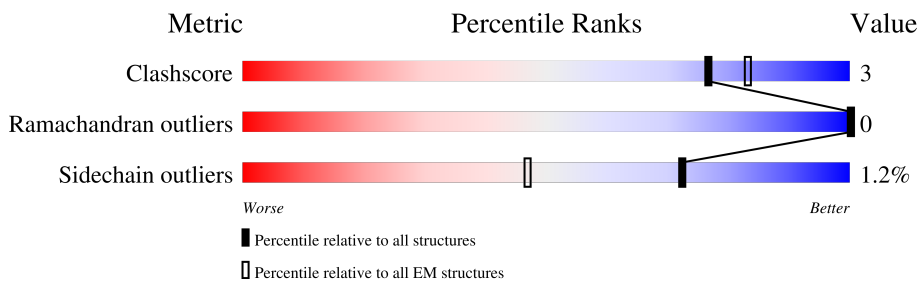
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	N	2839	

## 2 Entry composition i

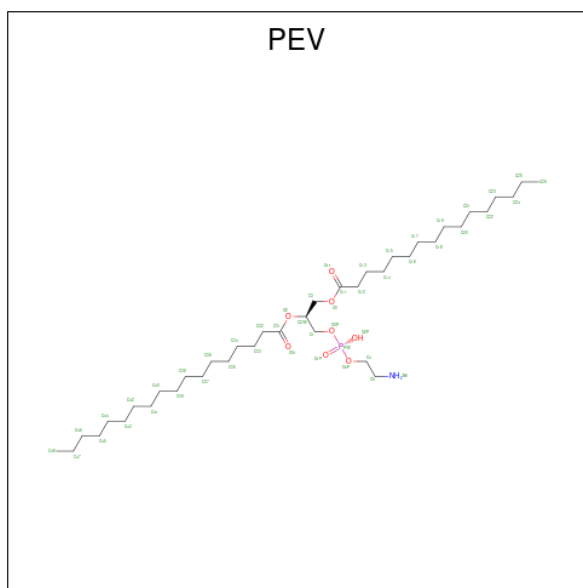
There are 4 unique types of molecules in this entry. The entry contains 77658 atoms, of which 39040 are hydrogens and 0 are deuteriums.

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
			Total	C	H	N	O	S		
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<sub>39</sub>H<sub>78</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
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).

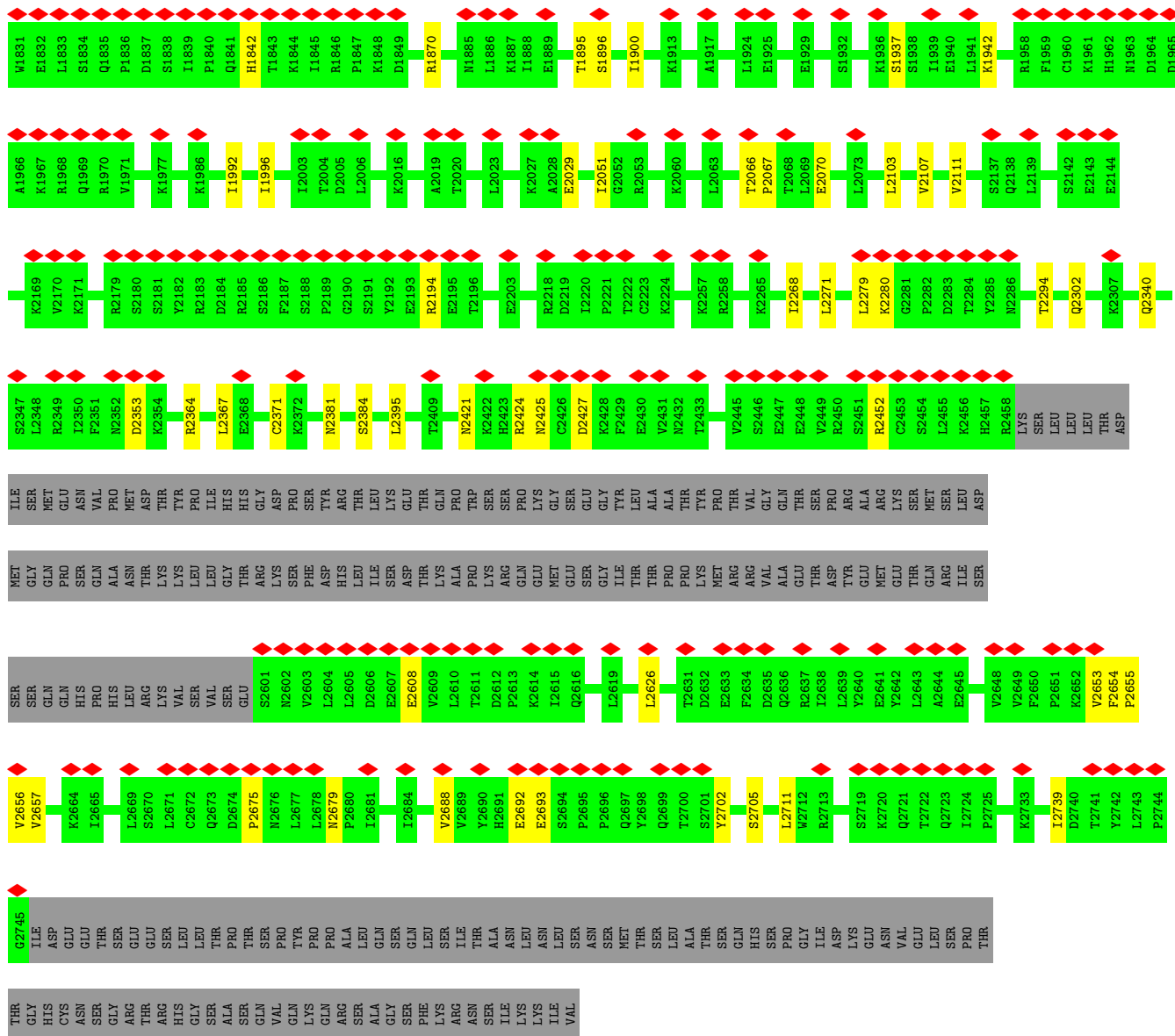
Mol	Chain	Residues	Atoms		AltConf
3	F	1	Total 1	Zn 1	0
3	N	1	Total 1	Zn 1	0

- Molecule 4 is water.

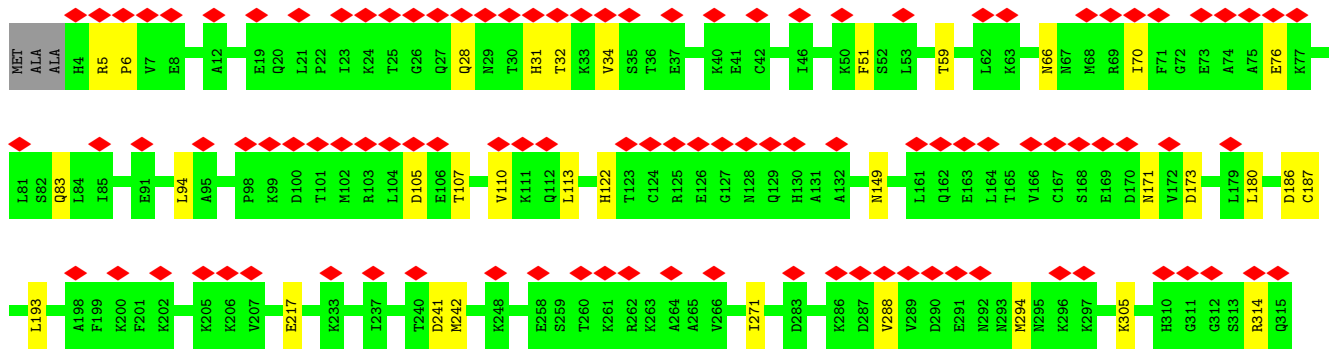
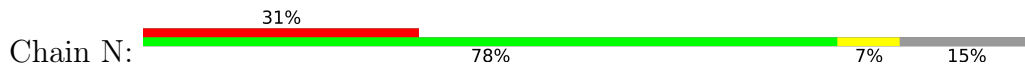
Mol	Chain	Residues	Atoms		AltConf
4	F	1	Total 1	O 1	0
4	N	1	Total 1	O 1	0



K1771	V1772	L1773	G1774	Q1775	S1776	V1777	F1778	L1779	M1780	D1781	I1782	Y1783	Y1784	A1785	S1786	E1787	I1788	E1789	E1790	I1791	C1792	L1793	V1794	D1795	E1796	M1797	Q1798	F1799	T1800	L1801	T1802	I1803	A1804	M1805	Q1806	G1807	T1808	P1809	L1810	T1811	F1812	M1813	H1814	Q1815	E1816	C1817	E1818	A1819	I1820	Y1821	Q1822	I1823	I1824	I1825	H1826	I1827	R1828	T1829	R1830
D1644	L1645	T1646	H1647	T1648	G1649	P1650	K1655	T1656	D1657	F1658	L1659	K1661	V1664	V1665	A1670	Y1671	D1672	M1673	L1674	S1675	A1676	V1677	Y1678	E1679	Y1680	M1681	C1682	M1683	V1684	V1685	F1686	R1687	E1688	Y1689	T1690	K1691	H1692	E1693	R1694	R1695	L1696	L1697	T1698	G1699	K1701	G1702	S1703	K1704	R1705	L1706	F1707	F1708	I1709	D1710					
K1568	F1569	E1570	E1571	R1575	H1576	Q1577	V1578	H1579	E1580	K1581	E1582	F1584	K1585	A1586	L1587	K1588	T1589	L1590	S1591	T1592	A1596	G1597	T1598	S1599	K1600	A1601	G1602	M1603	F1604	V1609	A1610	R1611	R1612	F1613	K1614	Q1617	I1618	L1623	L1629	K1632	Y1635	A1636	K1637	E1640	I1641	V1642	V1643												
V1492	M1493	H1494	S1495	L1496	S1497	F1498	I1499	S1500	D1501	G1502	M1503	V1504	A1506	R1509	L1510	Q1515	E1516	K1517	I1518	G1519	Q1520	Y1521	L1522	S1523	S1524	M1525	R1526	D1527	H1528	K1529	V1531	G1532	R1533	R1534	P1535	F1536	D1537	K1538	M1539	L1542	L1543	A1544	P1548	P1549	E1550	H1551	K1552	P1553	V1554	S1561	L1562	M1563							
P1432	P1433	R1434	I1435	E1436	G1438	L1439	K1440	L1441	M1442	S1443	K1444	I1445	L1446	Q1447	S1448	I1449	A1450	M1451	H1452	V1453	L1454	F1455	T1456	K1457	E1458	E1459	H1460	M1461	R1462	P1463	F1464	M1465	D1466	F1467	V1468	K1469	S1470	M1471	F1472	D1473	A1474	A1475	R1476	R1477	F1478	F1479	L1480	I1482	S1484	D1485	C1486	P1487	T1488	D1489	A1491				
Y1369	Q1370	A1371	L1372	C1373	H1374	S1375	L1377	M1378	K1379	ALA	THR	VAL	GLY	LYS	LYS	GLU	ASN	LYS	LYS	SER	VAL	VAL	GLN	ARG	PHE	F1398	Q1399	M1400	S1401	I1402	G1403	A1404	G1406	S1407	A1408	M1409	F1410	L1411	R1412	M1415	P1416	A1417	I1418	V1419	S1420	E1423	A1424	L1427	D1428	K1429	K1430	F1431							
I1307	V1308	I1309	T1310	S1311	S1312	D1313	W1314	Q1315	H1316	V1317	S1318	F1319	E1320	V1321	D1322	T1324	R1325	L1326	P1328	S1329	E1330	S1331	L1332	E1333	E1334	M1335	Q1336	R1337	M1338	L1339	L1340	Q1341	M1342	T1343	E1344	K1345	F1347	A1349	I1350	I1351	S1352	S1353	S1354	S1355	E1356	F1357	P1358	L1361	R1362	S1363	V1364	C1365	L1366						
W1286	D1287	E1288	L1246	F1247	D1248	S1249	R1250	H1251	L1252	L1253	Y1254	Q1255	L1256	L1257	W1258	M1259	M1260	F1261	S1262	K1263	E1264	V1265	E1266	L1267	A1268	D1269	S1270	M1271	Q1272	T1273	L1274	F1275	R1276	G1277	M1278	S1279	L1280	I1284	F1287	K1290	V1291	A1294	T1295	Y1296	L1297	Q1298	K1299	L1300	L1301	D1302	F1303	L1304	L1305	R1306					
L1153	V1157	M1162	I1165	K1171	L1183	T1184	K1185	G1190	T1191	E1192	F1193	D1194	T1195	L1196	A1197	E1198	T1199	V1200	L1201	E1099	L1203	M1096	E1097	L1113	C1117	S1118	E1119	S980	V996	V1001	M1004	M1005	V1006	R1025	R1026	D1027	M1041	V1049	M1050	G1051	T1052	S1053																	
Q1054	Q1055	A1056	A1057	D1058	D1060	V1061	K1062	C1063	L1064	T1065	R1066	S1072	M1073	V1076	V1077	E1088	E1089	G1090	D1091	L953	T954	R957	V961	L972	H975	T976	E977	G978	S979	S980	V996	V1001	M1004	M1005	V1006	R1025	R1026	D1027	M1041	V1049	M1050	G1051	T1052	S1053															
GLY	SER	ILE	ASP	LEU	SER	ASP	T831	D832	S833	M839	L844	L847	L852	Q853	GLN	ARG	ASN	SER	GLY	LEU	ALA	THR	TYR	SER	PRO	PRO	MET	GLY	VAL	SER	GLU	ARG	LYS	GLY	SER	ILE	VAL	VAL	SER	SER	GLU	GLY	ASN	A887	D888	T889	S892	K893	V903										



• Molecule 1: Neurofibromin









## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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

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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.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

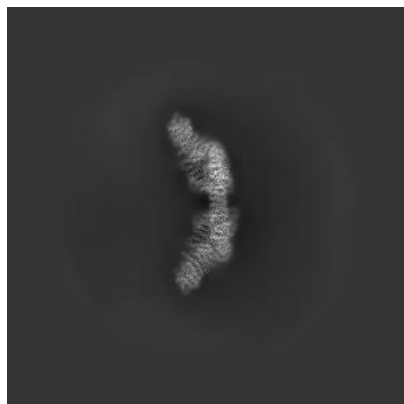
## 6 Map visualisation [i](#)

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.

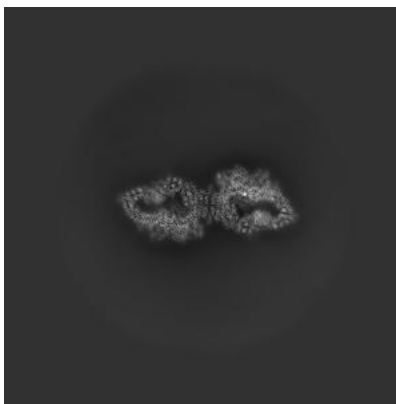
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

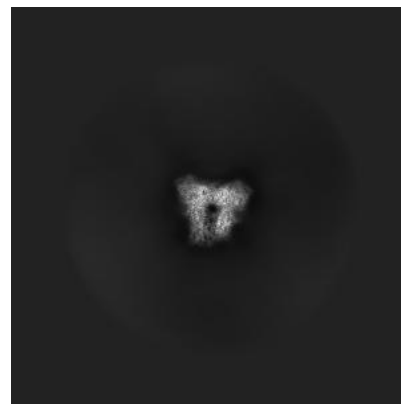
#### 6.1.1 Primary map



X

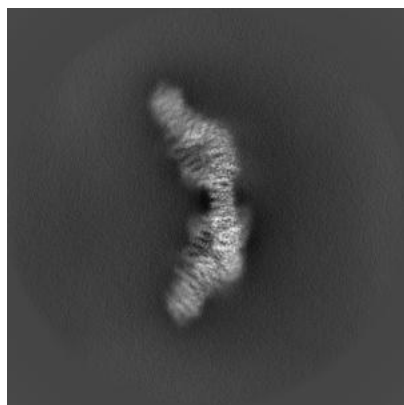


Y

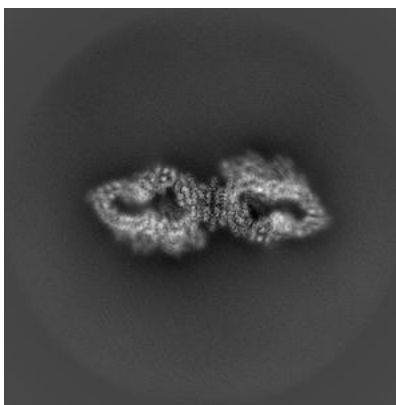


Z

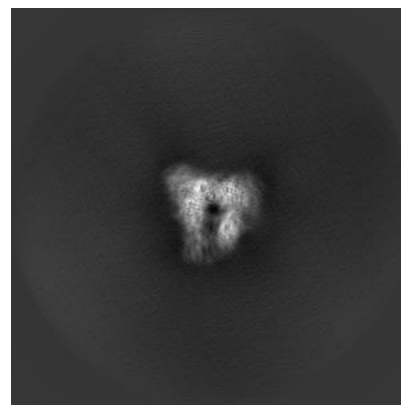
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

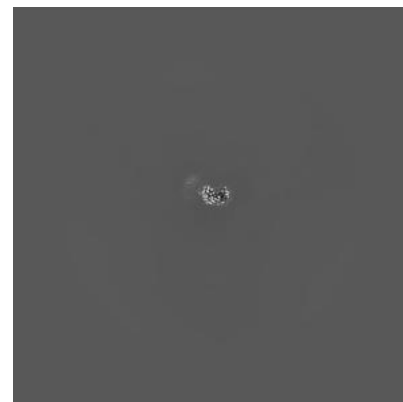
### 6.2.1 Primary map



X Index: 235



Y Index: 235

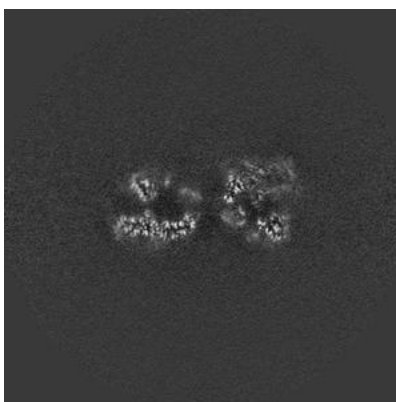


Z Index: 235

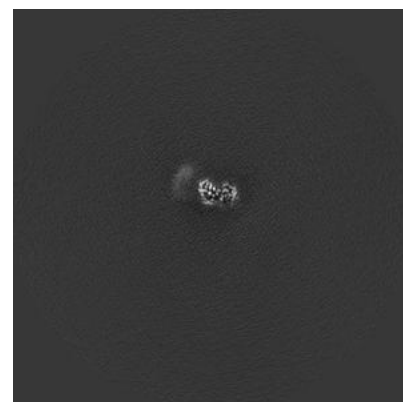
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

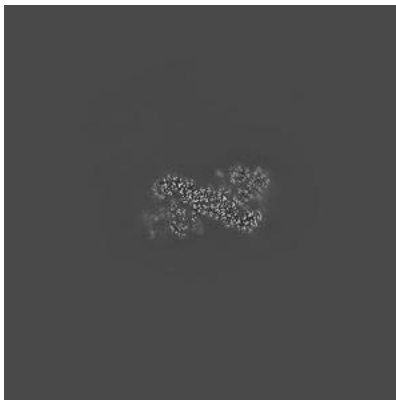


## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 251

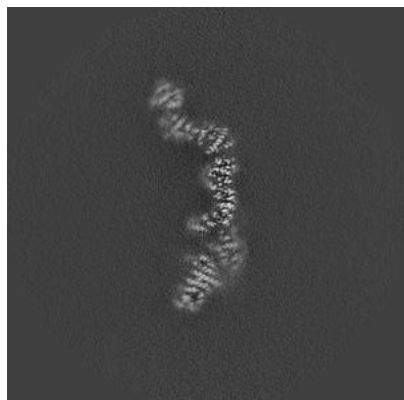


Y Index: 246

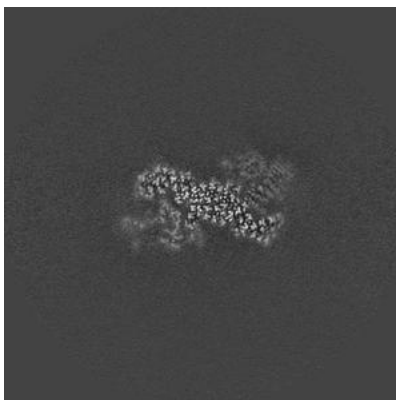


Z Index: 270

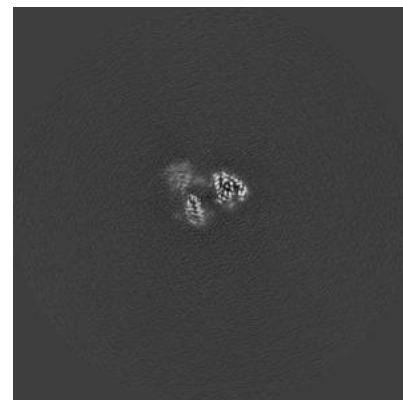
### 6.3.2 Raw map



X Index: 188



Y Index: 213

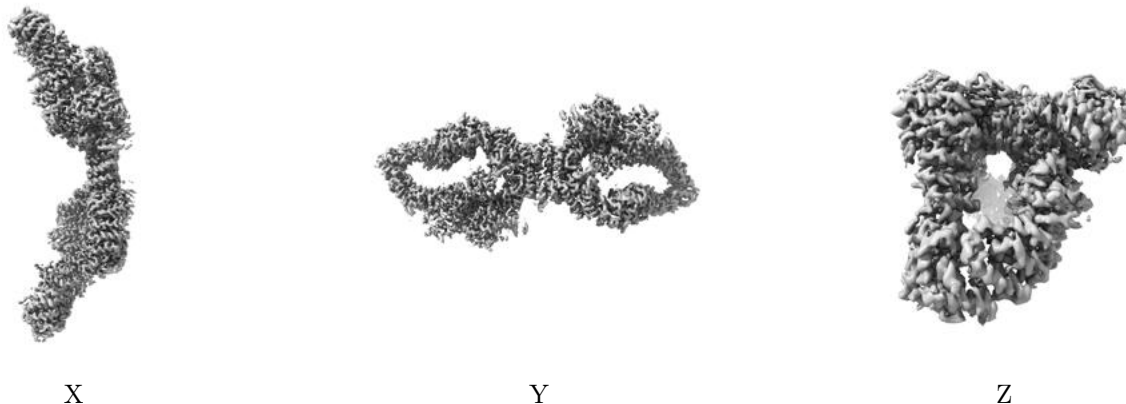


Z Index: 178

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

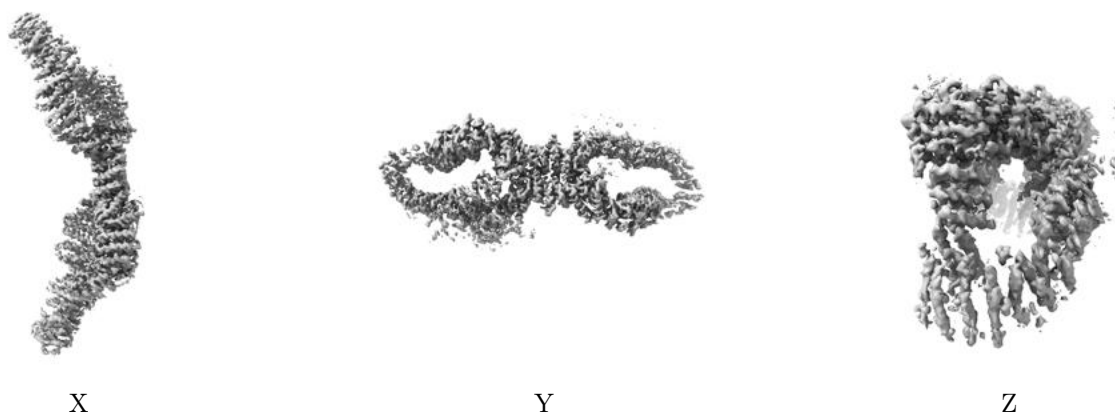
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



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.

### 6.4.2 Raw map



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.

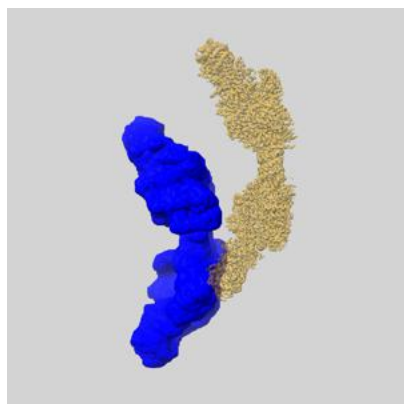
## 6.5 Mask visualisation [i](#)

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

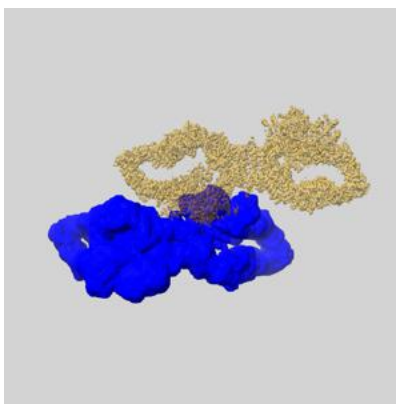
A mask typically either:

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

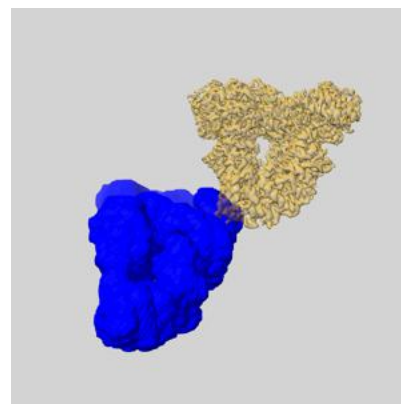
### 6.5.1 emd\_13396\_msk\_1.map [i](#)



X



Y

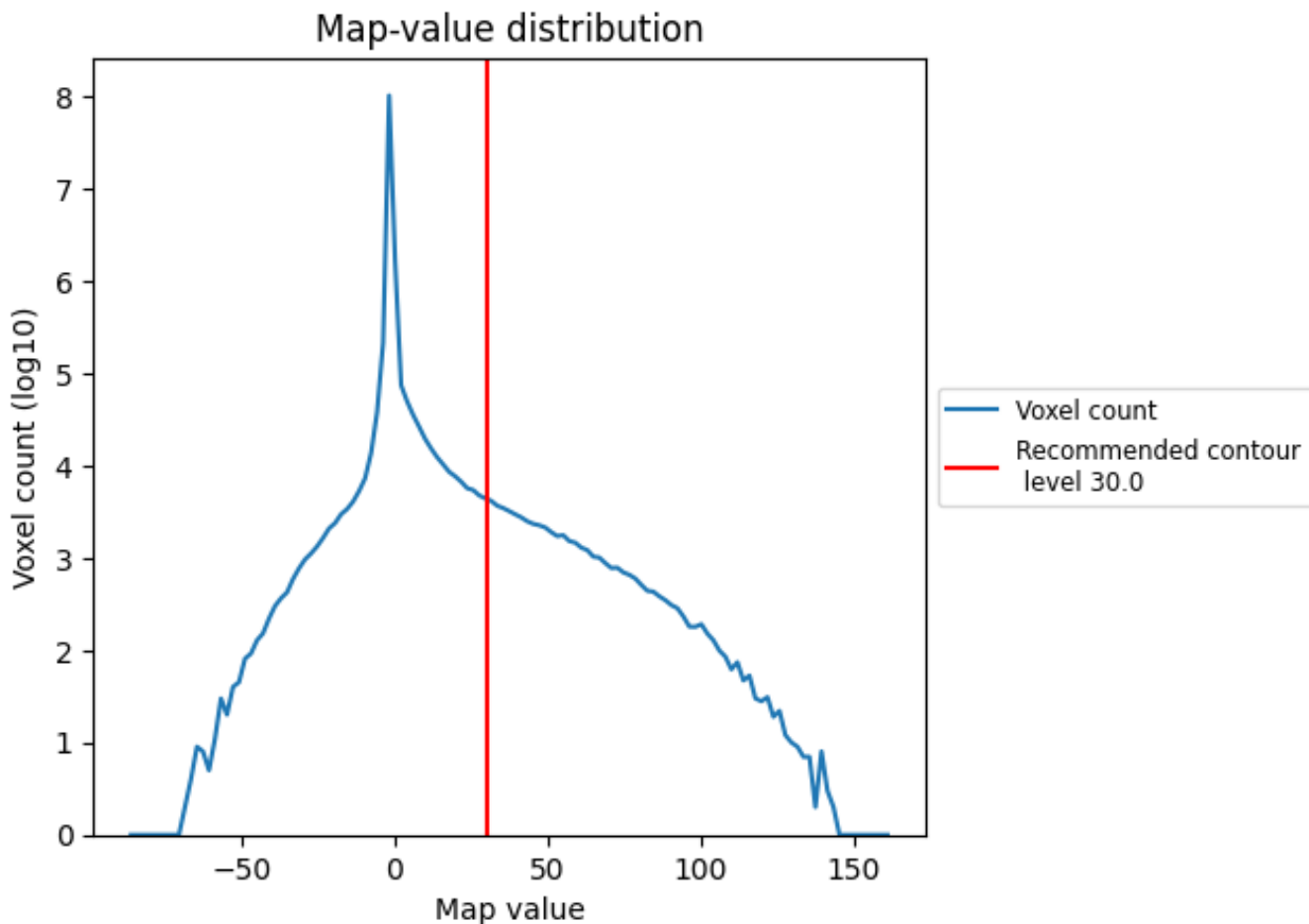


Z

## 7 Map analysis [i](#)

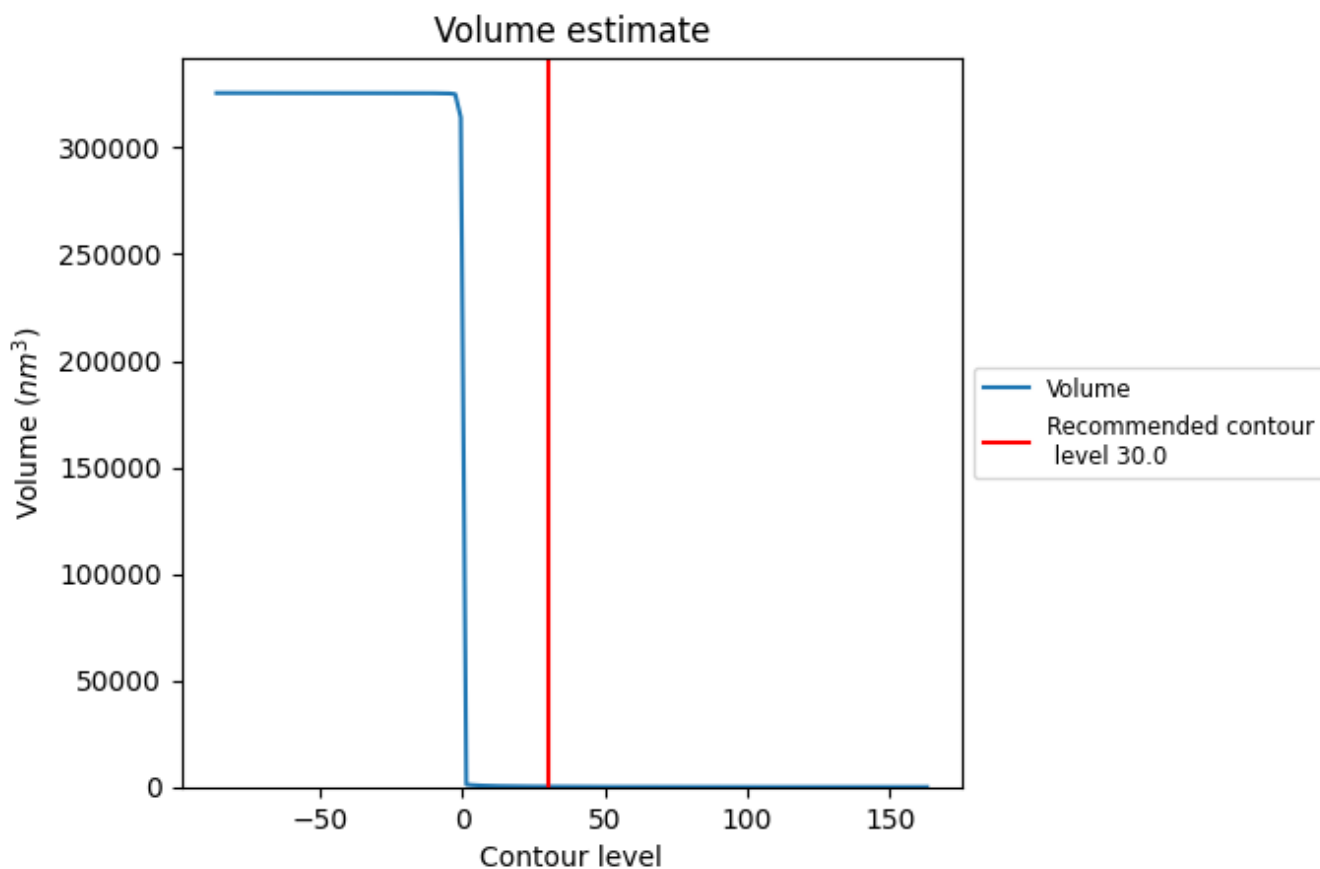
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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<sup>3</sup>; 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.

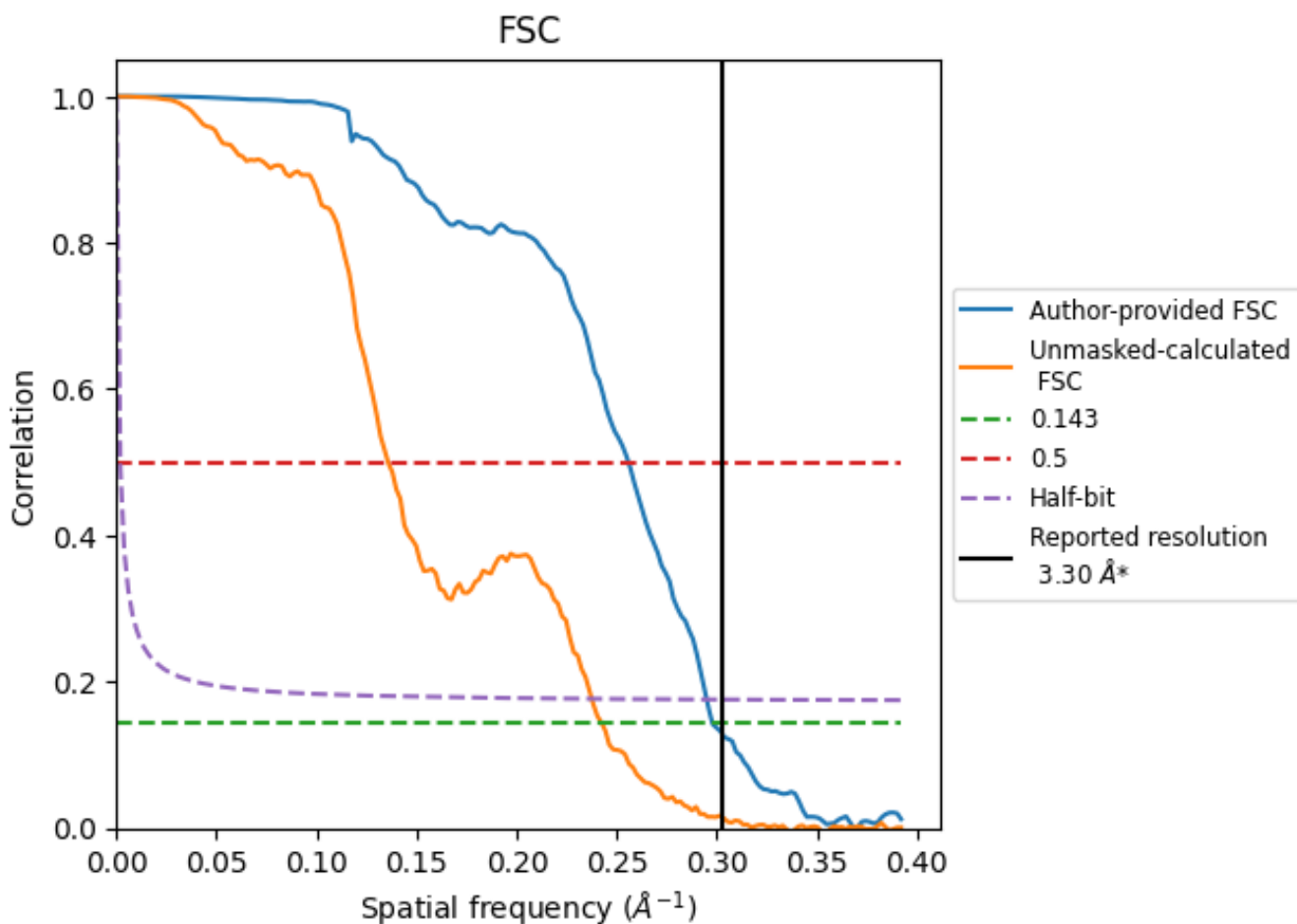
## 7.3 Rotationally averaged power spectrum [i](#)

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

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.303 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

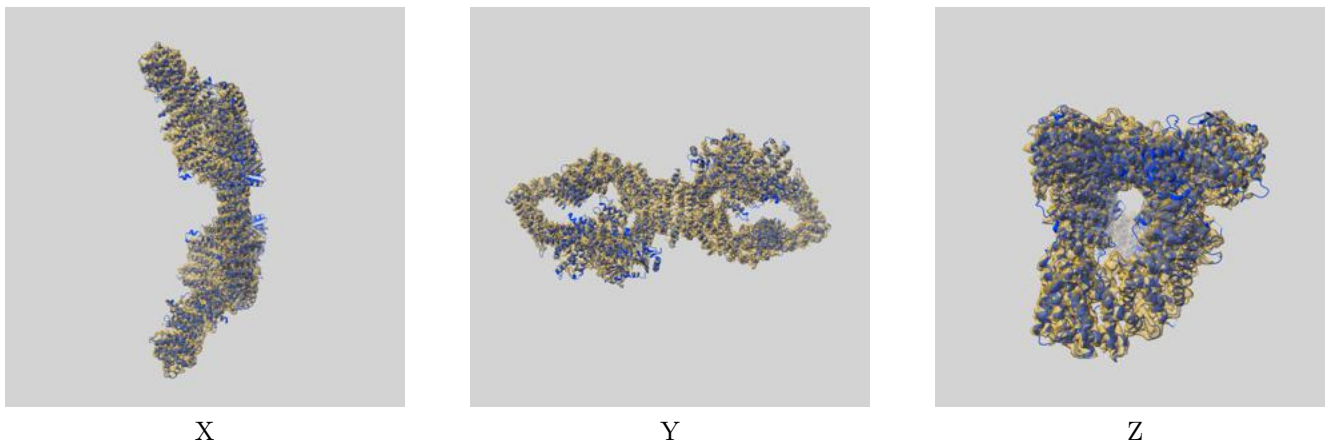
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.36	3.91	3.39
Unmasked-calculated*	4.12	7.36	4.21

\*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 4.12 differs from the reported value 3.3 by more than 10 %

## 9 Map-model fit [i](#)

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.

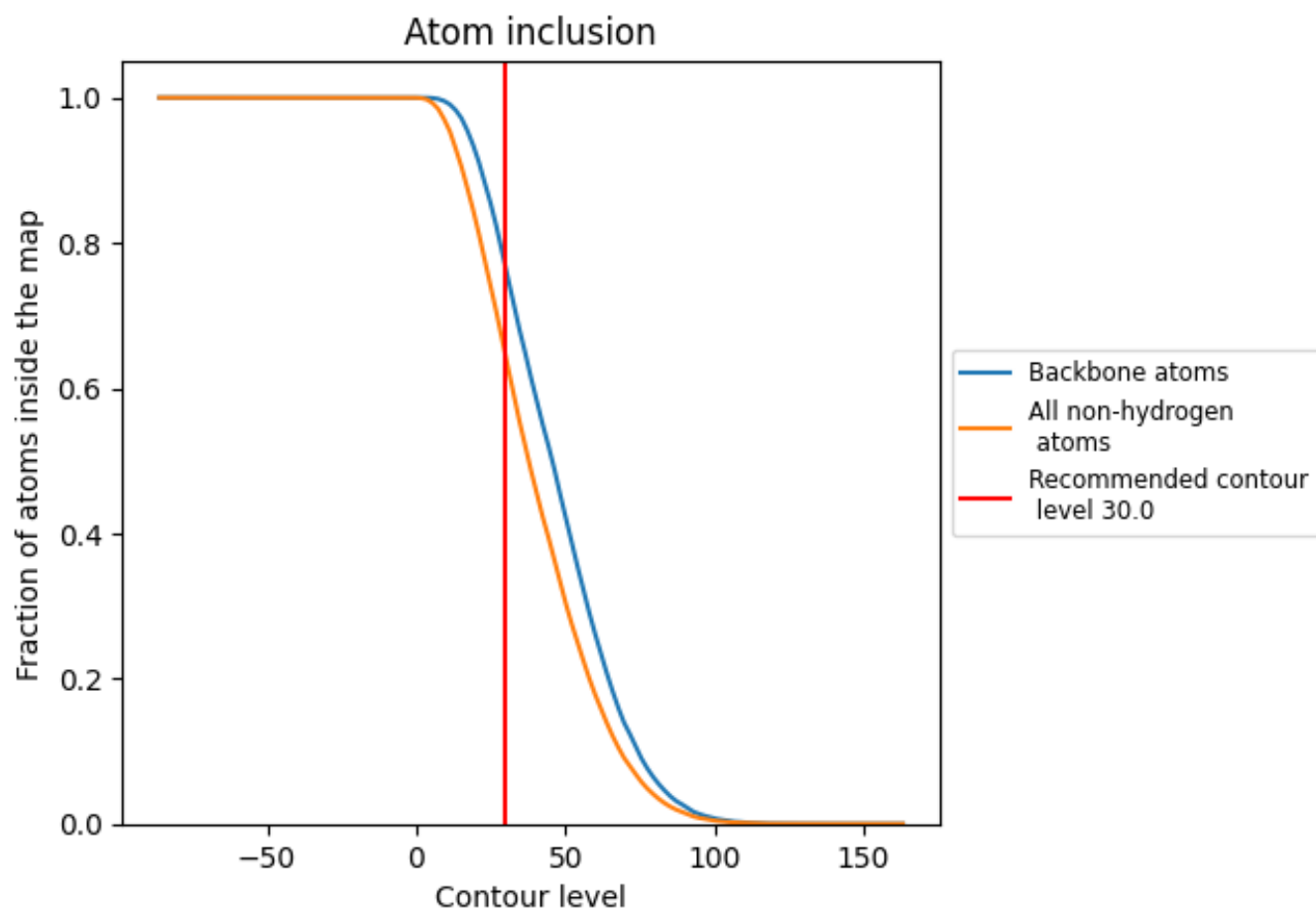
### 9.1 Map-model overlay [i](#)



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 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.