



wwPDB EM Validation Summary Report ⓘ

May 19, 2025 – 07:39 AM EDT

PDB ID : 8E20 / pdb_00008e20
EMDB ID : EMD-27826
Title : Cryo-EM structure of the full-length human NF1 dimer
Authors : Darling, J.E.; Merk, A.; Grishammer, R.; Ognjenovic, J.
Deposited on : 2022-08-12
Resolution : 3.60 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

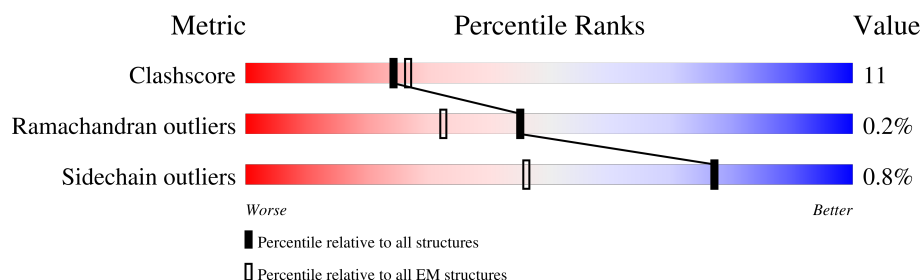
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



The reported resolution of this entry is 3.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	A	2818	
1	B	2818	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29341 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

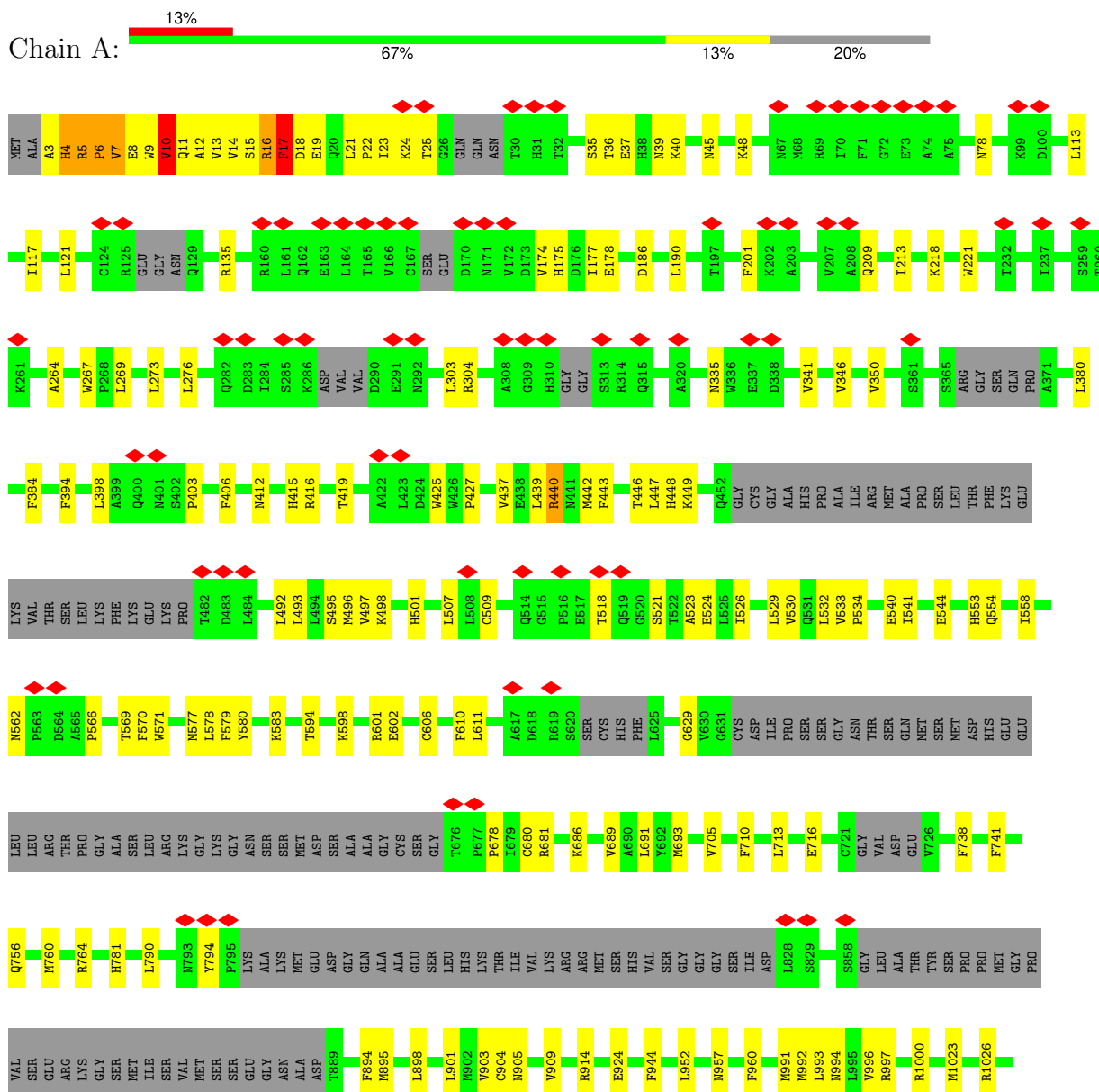
- Molecule 1 is a protein called Isoform I of Neurofibromin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2260	Total	C	N	O	S	0	0
			14633	9327	2661	2593	52		
1	B	2255	Total	C	N	O	S	0	0
			14708	9372	2661	2621	54		

3 Residue-property plots [i](#)

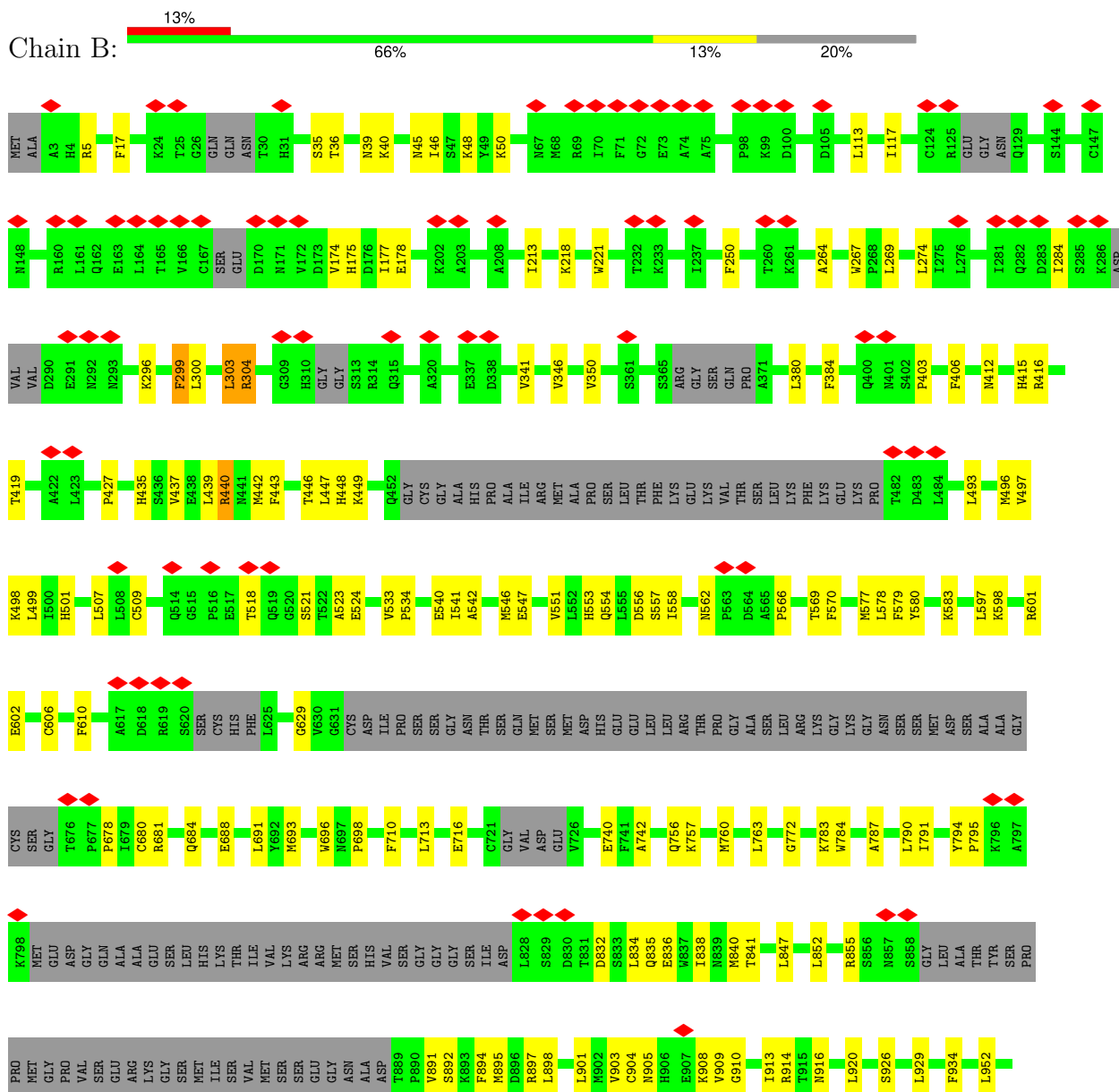
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





- Molecule 1: Isoform I of Neurofibromin



K2203	R1849	E1768	A1707	S1570	E1495	PHE	C1367	D1302	SER	N957
W2204	L1856	E1769	A1708	T1571	K1496	THR	G1367	P1303	ALA	M968
Q2207	L1856	I1770	T1709	F1572	L1501	GLN	V1371	L1304	THR	L972
A2253	L1867	C1771	T1710	Y1573	S1502	GLU	V1372	ARG	GLY	H975
L2269	E1868	L1772	L1710	Q1574	S1503	HIS	S1373	ILE	ARG	S987
H2291	I1879	V1773	L1712	A1575	ASN	MET	Q1374	VAL	LYS	E989
Q2303	L1901	D1774	E1713	G1576	ARG	ARG	F1442	THR	GLY	M1134
L2324	L1902	E1775	E1714	T1577	ASP	F1443	F1443	SER	M1149	M992
M2353	L1903	Q1776	D1715	S1578	HIS	M1444	M1444	ASP	L1246	L993
K2375	E1904	Q1777	L1716	K1579	ALA	D1445	D1445	TRP	L1152	M994
C2432	F1905	F1778	L1717	A1580	VAL	F1446	F1446	GLN	D1248	R997
SER	S1917	T1779	K1717	G1581	GLY	Y1447	Y1447	HIS	M1162	M1023
LEU	K1921	L1780	F1719	N1582	R1513	K1448	K1448	VAL	Y1253	L1023
LYS	C1924	T1781	H1720	P1583	P1514	S1449	S1449	SER	Y1254	A1024
HIS	Y1927	I1787	A1722	I1584	F1515	M1450	M1450	PHE	Q1256	R1025
ARG	W1931	P1788	L1723	F1585	D1516	F1451	G1386	GLU	H1170	E1034
LYS	M2033	L1789	L1723	Y1586	K1517	D1452	A1387	VAL	D1172	F1037
SER	I2057	T1790	H1727	Y1587	L1521	A1453	F1389	PRO	L1173	R1038
LEU	L2062	H1792	K1730	K1593	L1522	A1454	L1390	THR	Q1174	M1041
THR	R2062	H1793	T1730	T1594	L1525	R1455	R1391	ARG	A1177	T1175
ASP	Y2063	Q1794	K1731	G1595	E1529	F1457	R1456	LEU	F1261	R1176
ILE	M2064	E1795	V1732	I1596	HIS	F1458	M1394	GLU	K1263	F1178
SER	L2066	C1796	S1733	I1597	PRO	L1459	I1397	SER	E1264	F1179
MET	L2066	E1797	V1736	D1600	LYS	D1460	L1397	GLU	E1266	M1180
GLU	L2073	A1798	G1737	Y1604	VAL	I1461	Y1401	S1331	L1267	T1052
ASN	D2074	I1799	S1738	L1607	ALA	A1462	E1402	V1132	L1332	S1053
PRO	L2082	L1803	T1739	L1610	THR	S1463	A1403	E1333	L1269	N1054
ASP	S2159	H1805	A1740	L1611	ASP	THR	GLY	E1334	S1270	Q1055
THR	SER	I1806	W1741	K1612	THR	CYS	ILE	M1335	M1271	A1056
PRO	TYR	R1807	V1743	P1612	TRP	PRO	LEU	Q1336	Q1272	A1057
ILE	ARG	R1808	T1744	Y1613	SER	THR	ASP	R1337	Q1273	D1058
HIS	ASP	R1809	S1745	Y1614	LEU	SER	LYS	Q1188	Q1189	D1059
HIS	ARG	W1810	A1746	F1686	ASN	ASP	LYS	M1338	G1190	D1060
GLY	SER	E1747	E1748	V1687	THR	ALA	PRO	E1339	T1191	S1072
ASP	PHE	L1811	R1748	I1688	LEU	VAL	PRO	L1340	G1277	V1076
PRO	PRO	S1812	T1749	D1689	SER	ASN	P1412	Q1341	L1278	L1079
TYR	GLY	S1813	K1750	C1690	THR	HIS	R1413	M1342	S1279	L1080
ARG	TYR	Q1814	V1751	P1691	ARG	SER	I1414	T1343	L1280	THR
THR	GLY	P1815	L1752	Y1618	GLU	LEU	I1415	E1344	A1281	VAL
LEU	LEU	D1816	G1753	I1619	GLU	ILE	R1416	K1283	S1282	LEU
LYS	ARG	SER	Q1754	K1693	VAL	SER	G1417	ALA	K1284	ALA
GLU	E2174	ILE	S1755	V1621	GLU	ASP	L1418	ASP	I1284	ASP
GLN	M2192	PRO	V1756	L1624	K1660	GLY	K1419	ARG	M1285	ARG
PRO		HIS	F1757	E1696	L1569	ASN	M1421	PHE	T1286	F1107
		THR	L1758	H1697		VAL	I1420	GLU	C1288	F1110
		LYS	M1759	I1698		LEU	M1421	GLN	F1289	M1111
		I1824	D1760	E1699		ALA	S1422	S1352	L1208	
		R1825	S1765	H1700		LEU	K1423	S1353	ARG	
		L1838	Y1761	E1701			I1424	S1354	GLU	
		L1841	Y1762	Q1702			L1425	S1355	Q1218	
			Y1763	R1632			Q1426	E1356	L1293	
			A1764	F1633			S1427	F1357	A1294	
			S1765	K1634			I1428	P1358	T1295	
			E1766	L1705			A1429	Q1359	A1299	
			I1767	D1636			N1430	P1360		
							H1431	L1361		
							VAL	R1362		
							LEU			

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

PRO	V2682
LYS	
ARG	A2625
GLN	
GLU	F2629
MET	
GLU	
SER	
GLY	
ILE	
THR	
THR	
PRO	
LYS	
MET	
PRO	
ARG	
GLN	
TYR	
THR	
ASP	
THR	
VAL	
ALA	
GLU	
GLY	
SER	
LEU	
LEU	
ALA	
GLN	
SER	
GLY	
GLN	
LEU	
SER	
ILE	
ALA	
LEU	
GLN	
SER	
GLY	
GLN	
LEU	
SER	
ILE	
VAL	
ASN	
ASN	
THR	
SER	
LEU	
ALA	
THR	
SER	
GLN	
HIS	
SER	
PRO	
GLY	
ILE	

E2672	
F2675	
Q2676	
F2697	
L2722	
PRO	
GLY	
ILE	
ASP	
GLU	
GLU	
THR	
ARG	
THR	
ARG	
HIS	
GLY	
SER	
ALA	
SER	
GLN	
VAL	
GLN	
LYS	
ARG	
SER	
ALA	
GLY	
SER	
PHE	
LYS	
ARG	
ASN	
SER	
ILE	
LYS	
ILE	
VAL	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	692875	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	9.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0133	Depositor
Map size (\AA)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.27	0/14889	0.54	8/20401 (0.0%)
1	B	0.24	0/14962	0.50	2/20488 (0.0%)
All	All	0.26	0/29851	0.52	10/40889 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
All	All	0	7

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1921	LYS	N-CA-C	-8.30	102.17	111.14
1	A	17	PHE	N-CA-C	-7.17	103.47	111.28
1	A	10	VAL	N-CA-C	-7.05	103.65	110.42
1	A	2392	LEU	N-CA-C	-6.11	104.54	111.14
1	A	6	PRO	N-CA-C	-5.95	100.21	112.47

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1170	HIS	Peptide
1	A	304	ARG	Sidechain
1	B	304	ARG	Sidechain
1	B	440	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	794	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	14633	0	11225	284	0
1	B	14708	0	11423	259	0
All	All	29341	0	22648	542	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 11.

The worst 5 of 542 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1273:THR:HB	1:B:1276:ARG:HE	1.19	1.01
1:A:5:ARG:HA	1:A:8:GLU:HB2	1.53	0.87
1:B:1248:ASP:HA	1:B:1253:LEU:HB2	1.56	0.87
1:A:1248:ASP:HA	1:A:1253:LEU:HB2	1.61	0.81
1:B:698:PRO:HB3	1:B:836:GLU:HG2	1.61	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2212/2818 (78%)	2077 (94%)	130 (6%)	5 (0%)	44	73
1	B	2205/2818 (78%)	2093 (95%)	108 (5%)	4 (0%)	44	73
All	All	4417/5636 (78%)	4170 (94%)	238 (5%)	9 (0%)	45	73

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	909	VAL
1	B	909	VAL
1	A	4	HIS
1	A	341	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	897/2512 (36%)	887 (99%)	10 (1%)	70	83
1	B	935/2512 (37%)	930 (100%)	5 (0%)	86	93
All	All	1832/5024 (36%)	1817 (99%)	15 (1%)	77	88

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1920	LEU
1	B	1269	ASP
1	A	1921	LYS
1	B	1733	SER
1	B	303	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	501	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	614	ASN
1	B	1759	ASN
1	B	553	HIS
1	B	712	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

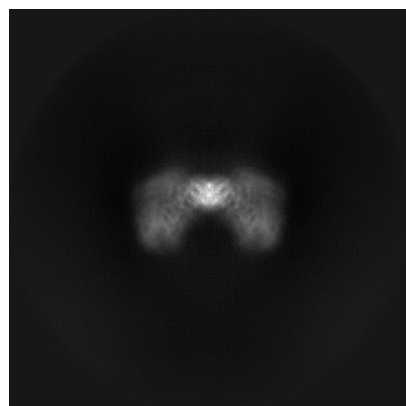
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27826. These allow visual inspection of the internal detail of the map and identification of artifacts.

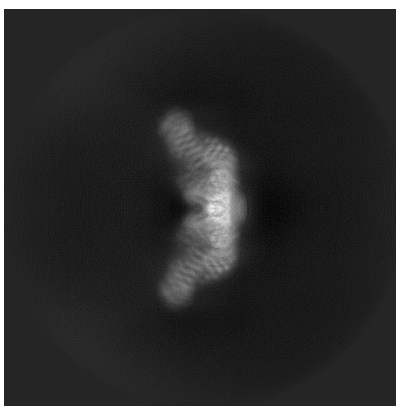
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

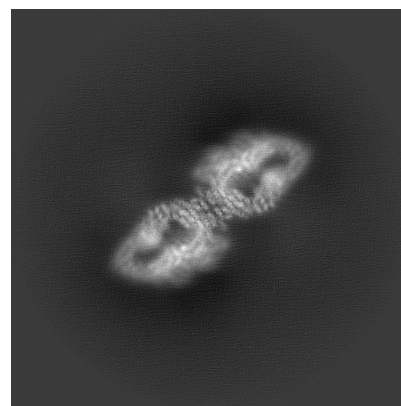
6.1.1 Primary map



X

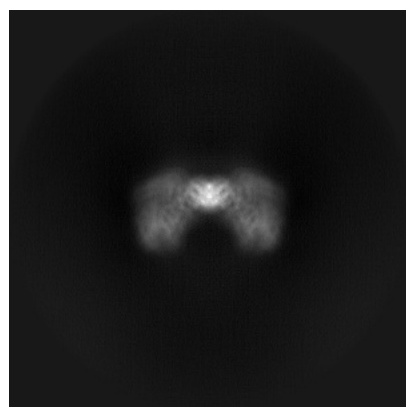


Y

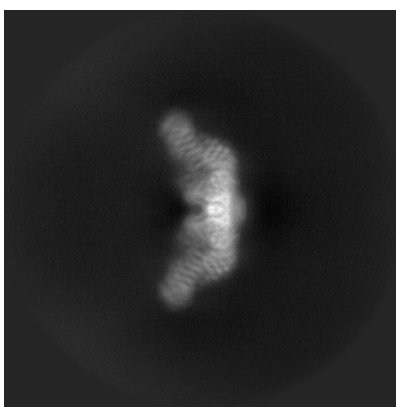


Z

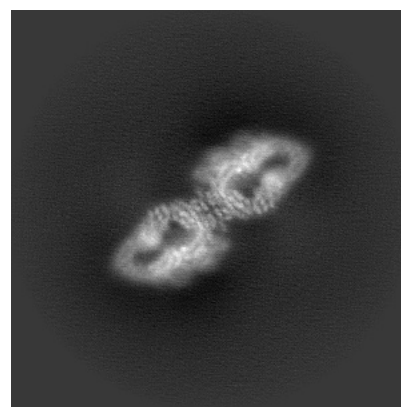
6.1.2 Raw map



X



Y

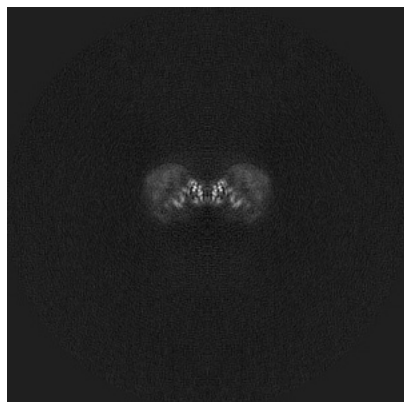


Z

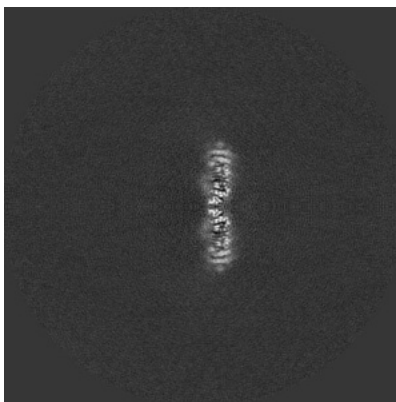
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

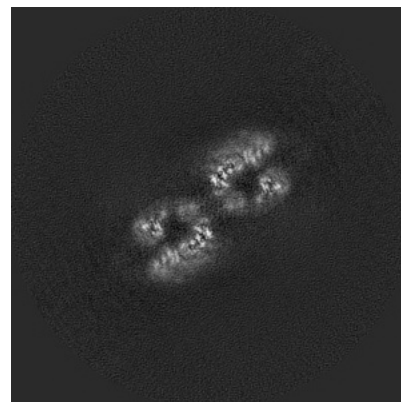
6.2.1 Primary map



X Index: 256

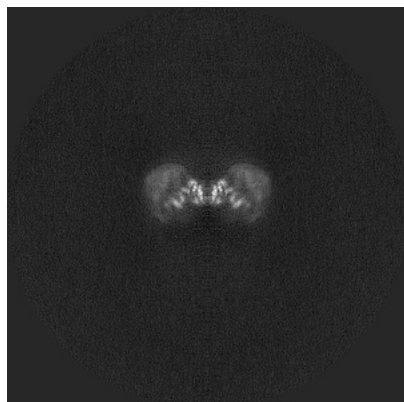


Y Index: 256

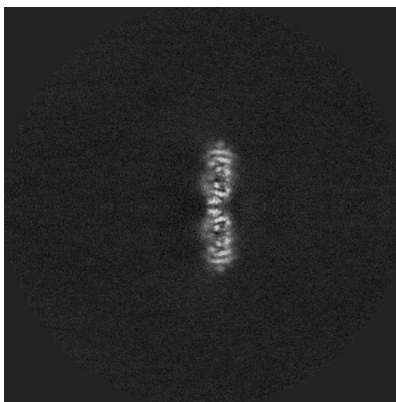


Z Index: 256

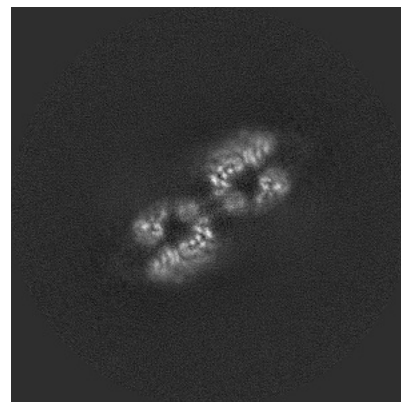
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

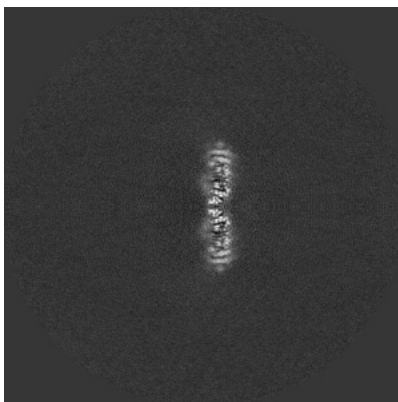
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

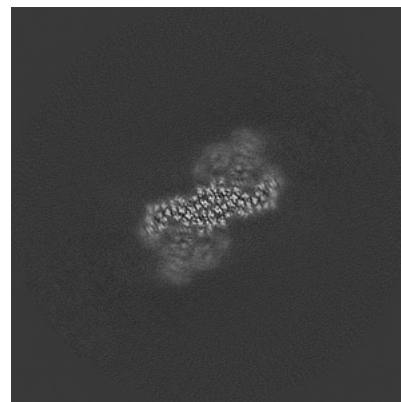
6.3.1 Primary map



X Index: 268

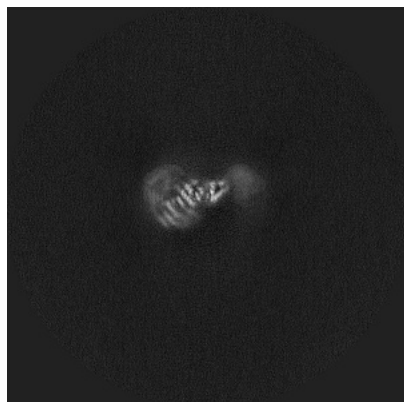


Y Index: 256

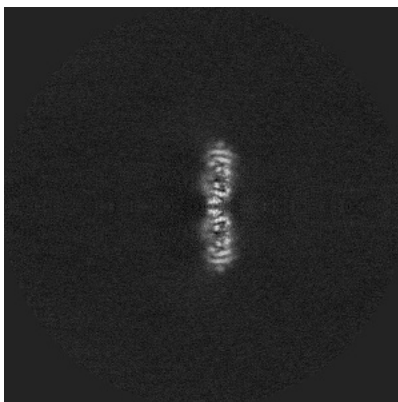


Z Index: 276

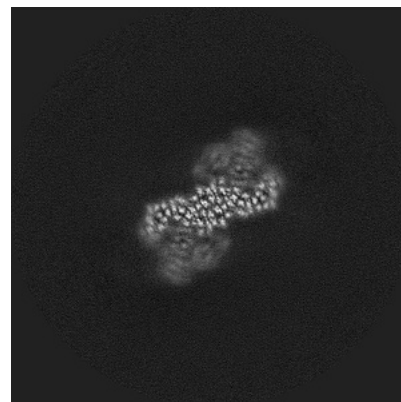
6.3.2 Raw map



X Index: 244



Y Index: 256

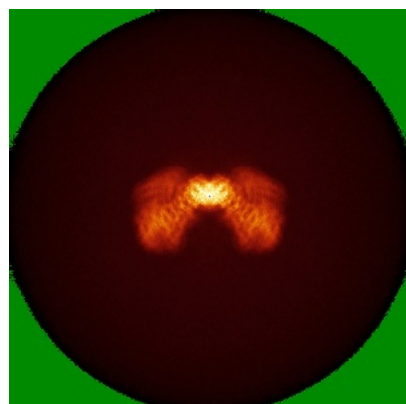


Z Index: 276

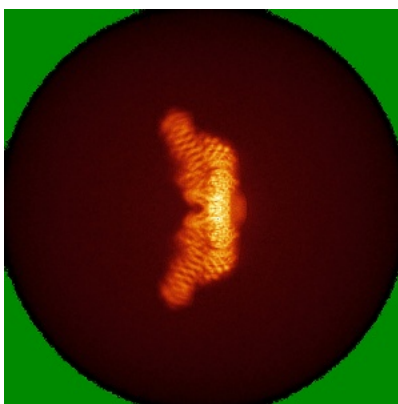
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



X



Y

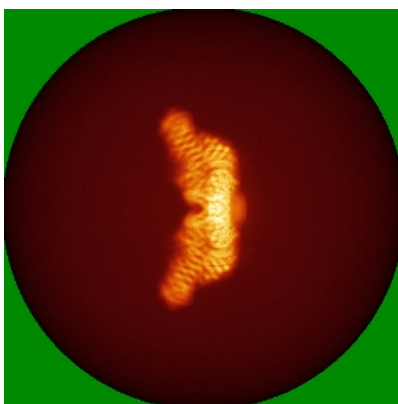


Z

6.4.2 Raw map



X



Y

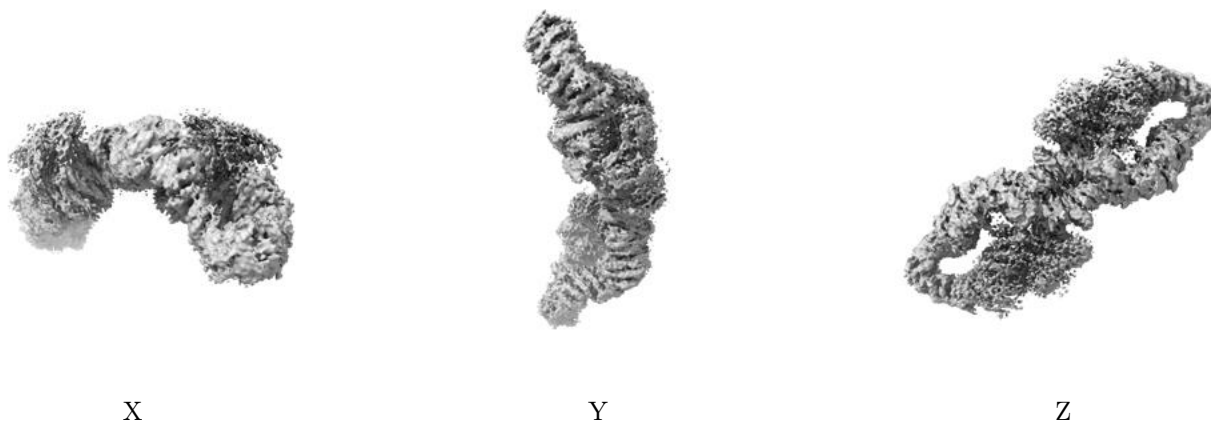


Z

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.

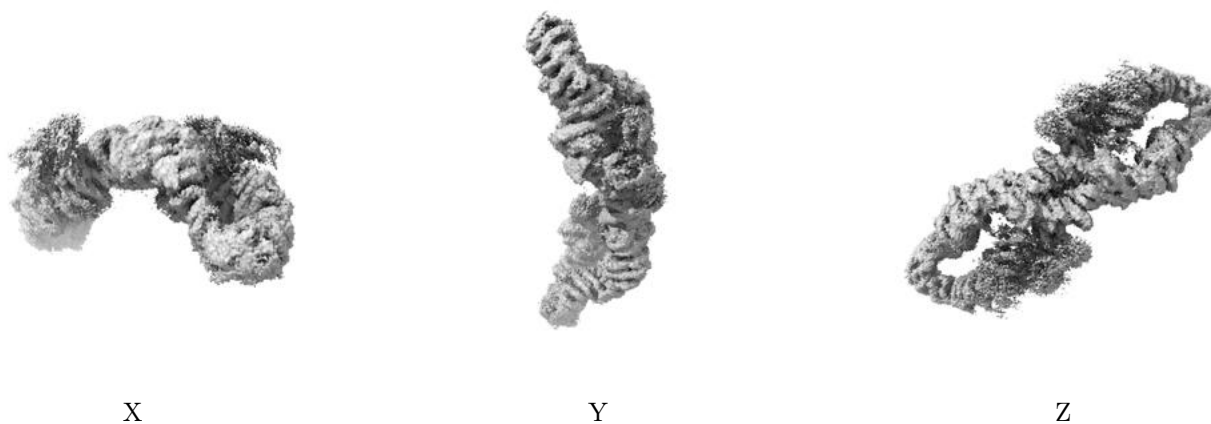
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0133. 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



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

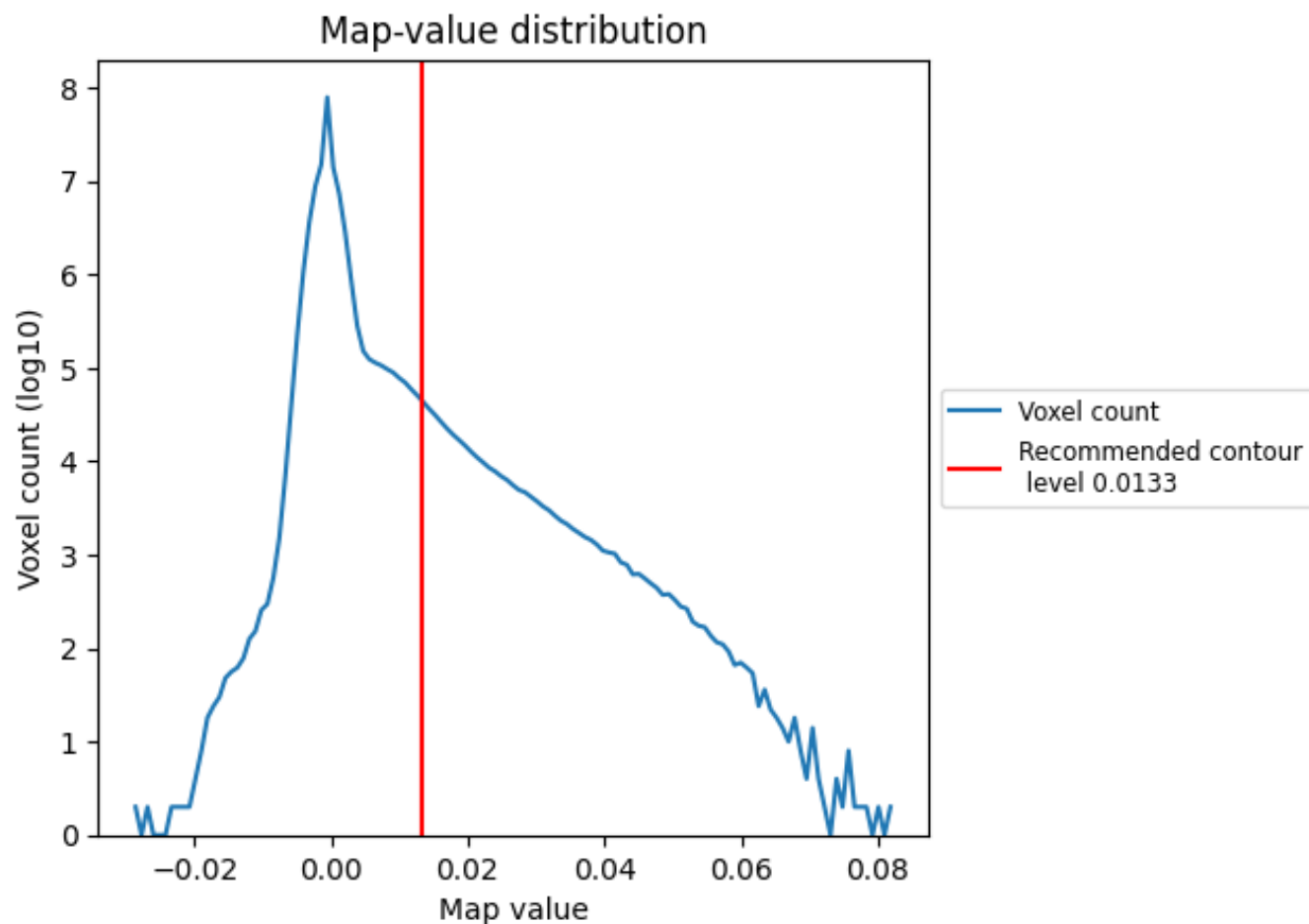
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

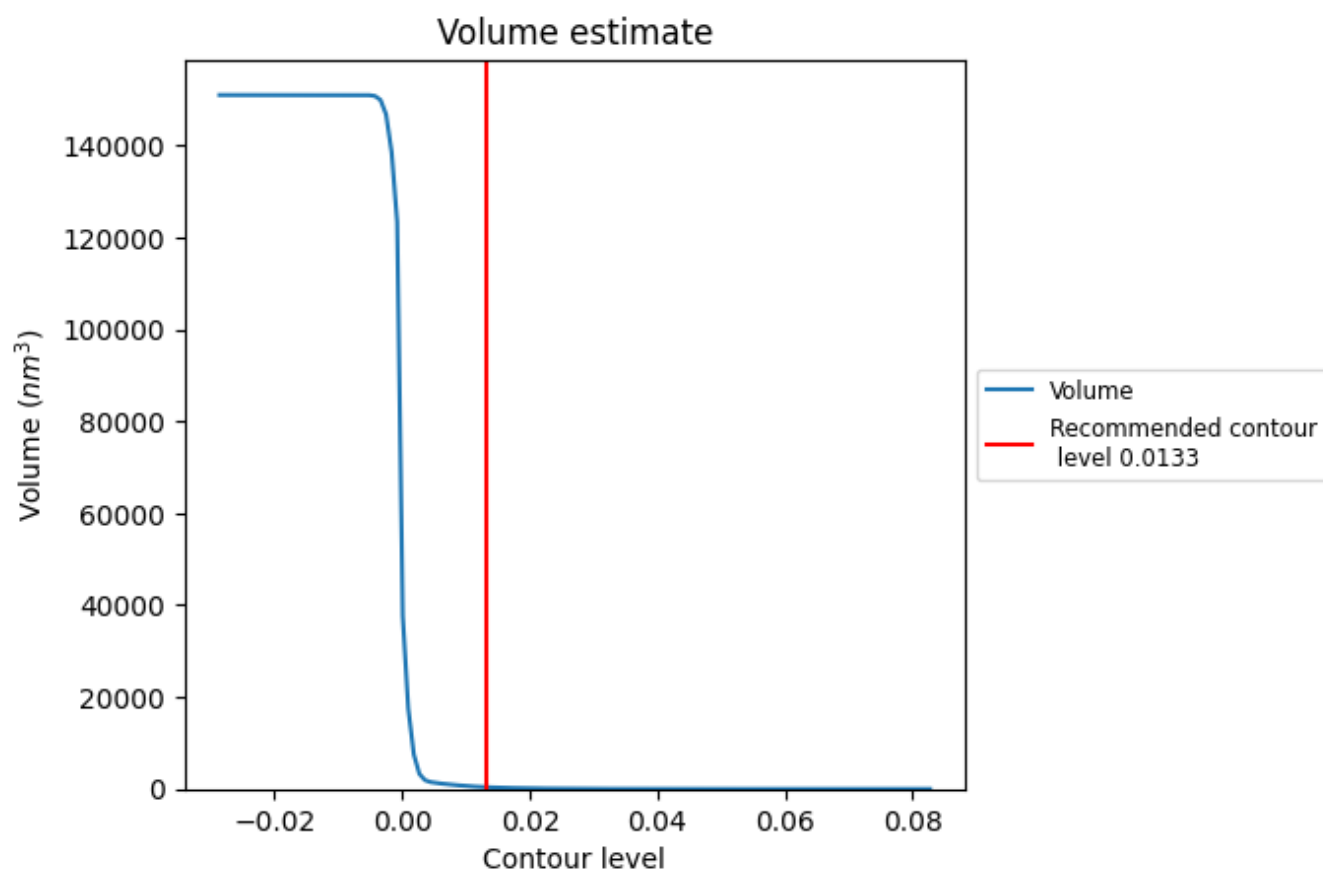
This section contains the results of statistical analysis of the map.

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.

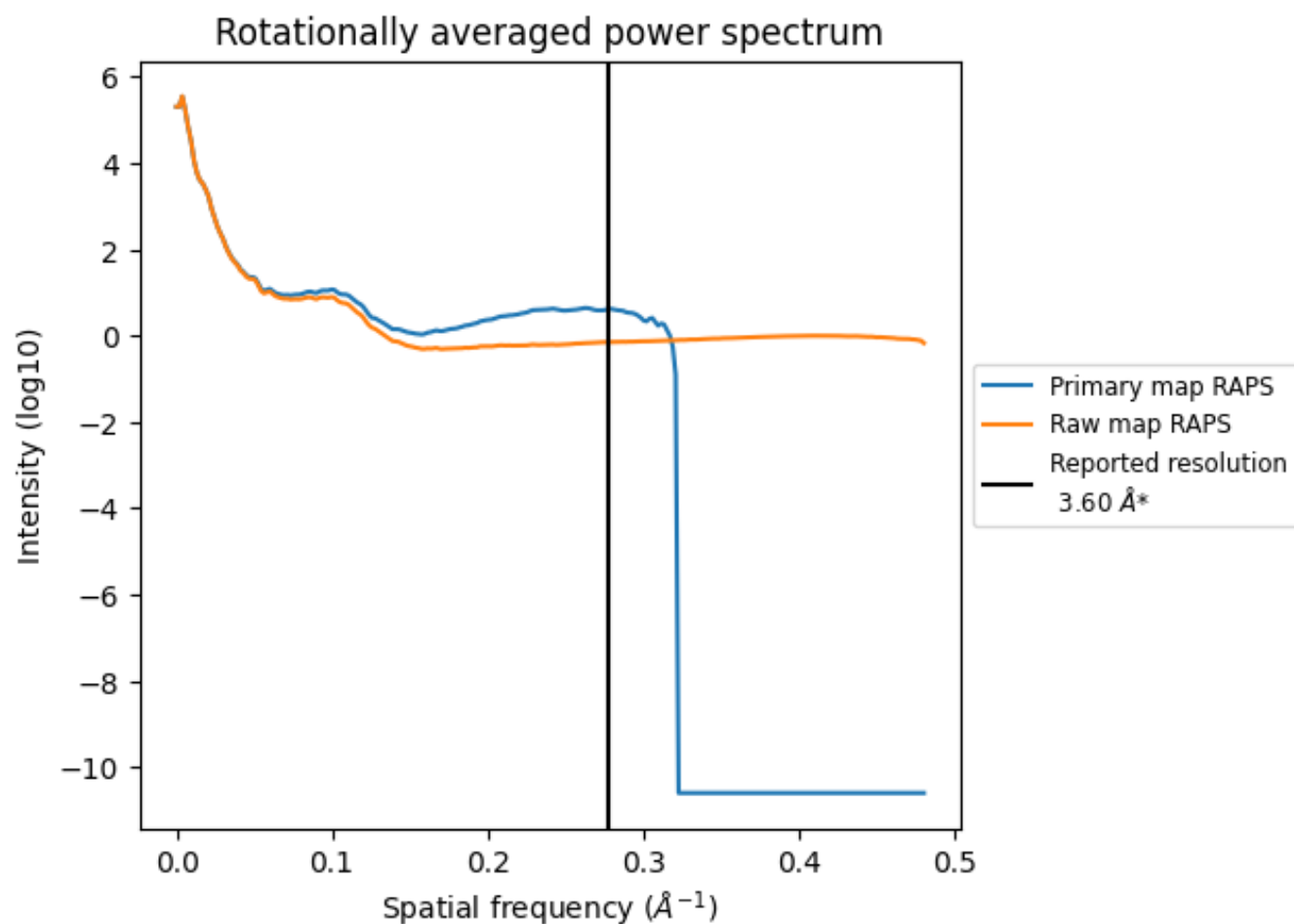
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 381 nm³; this corresponds to an approximate mass of 345 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 ⓘ

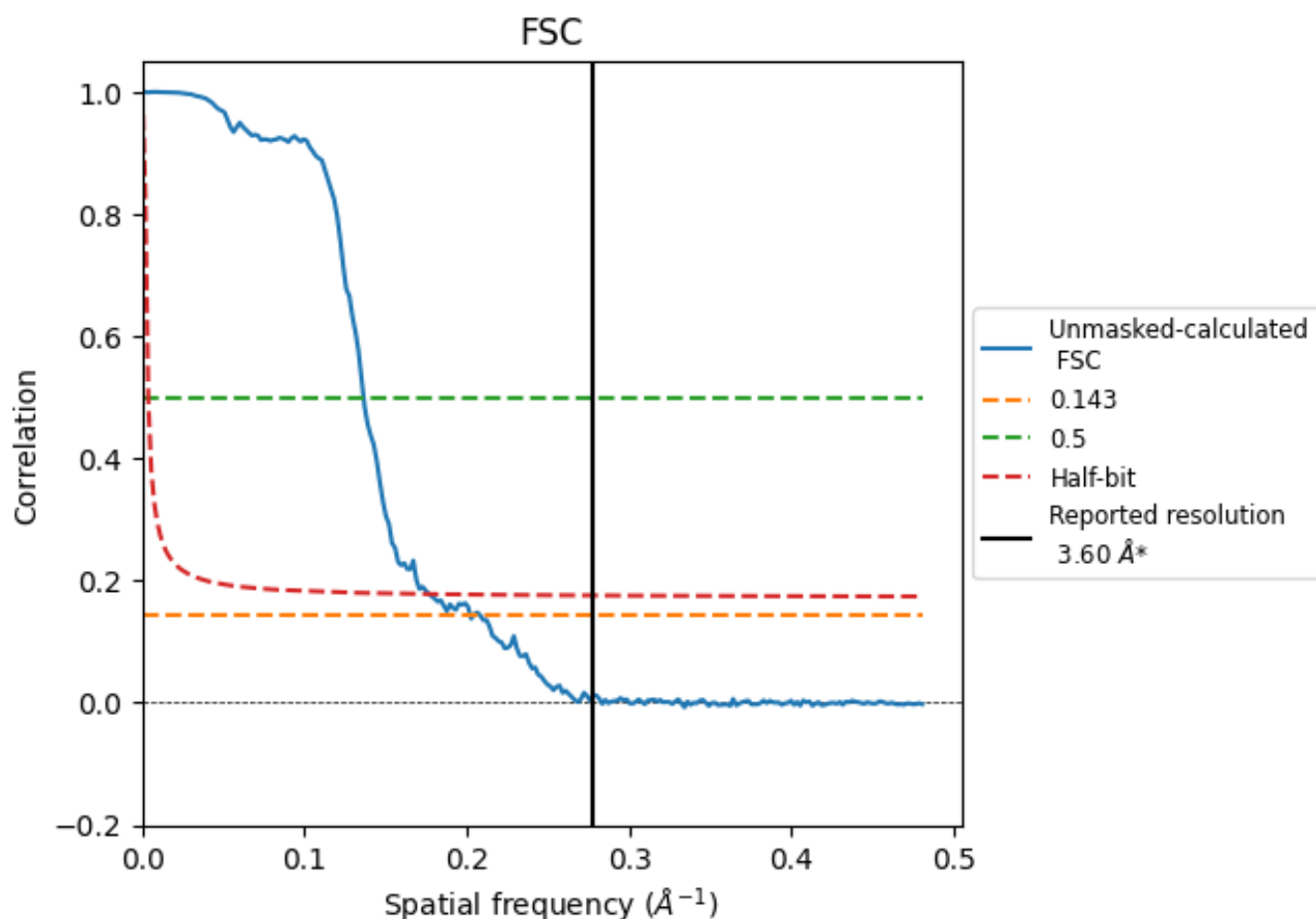


*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

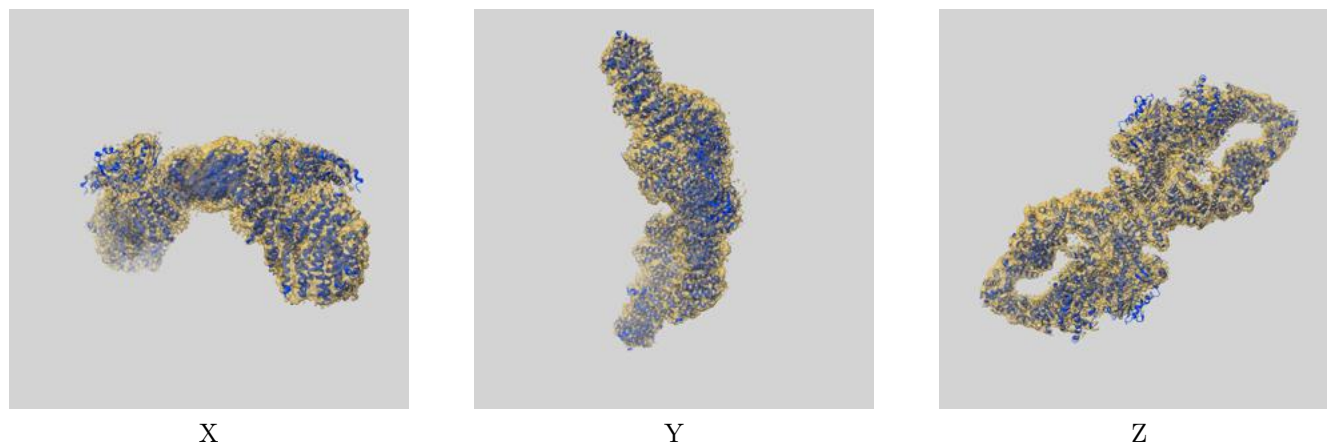
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.94	7.33	5.66

*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 4.94 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

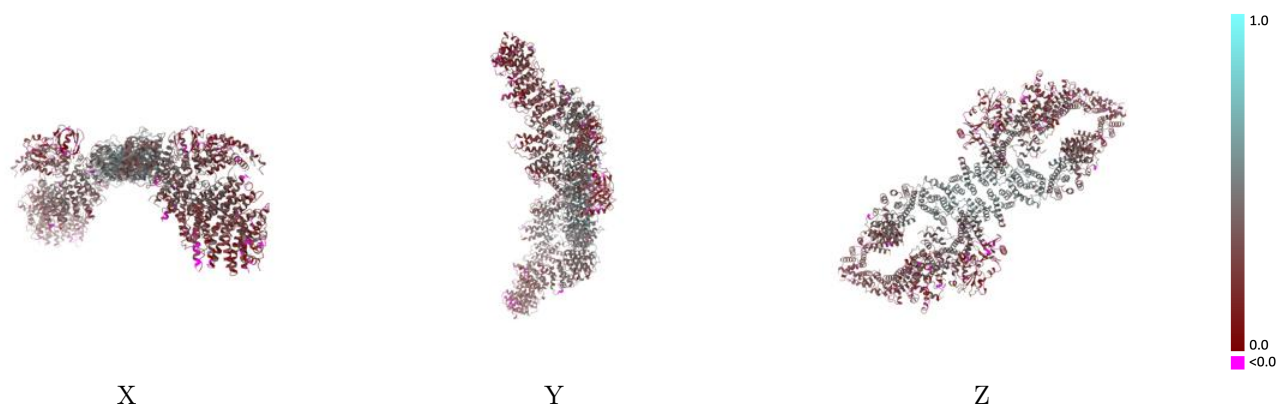
This section contains information regarding the fit between EMDB map EMD-27826 and PDB model 8E20. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



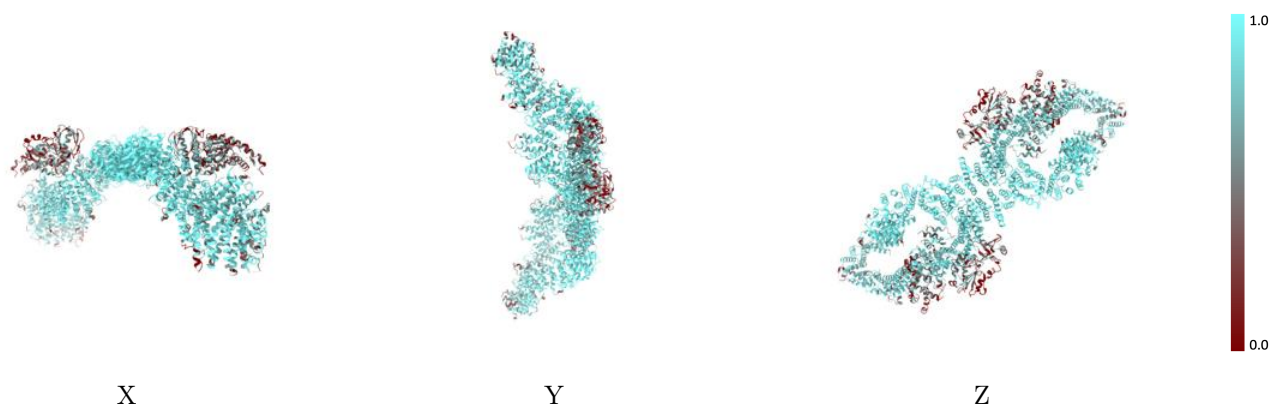
The images above show the 3D surface view of the map at the recommended contour level 0.0133 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



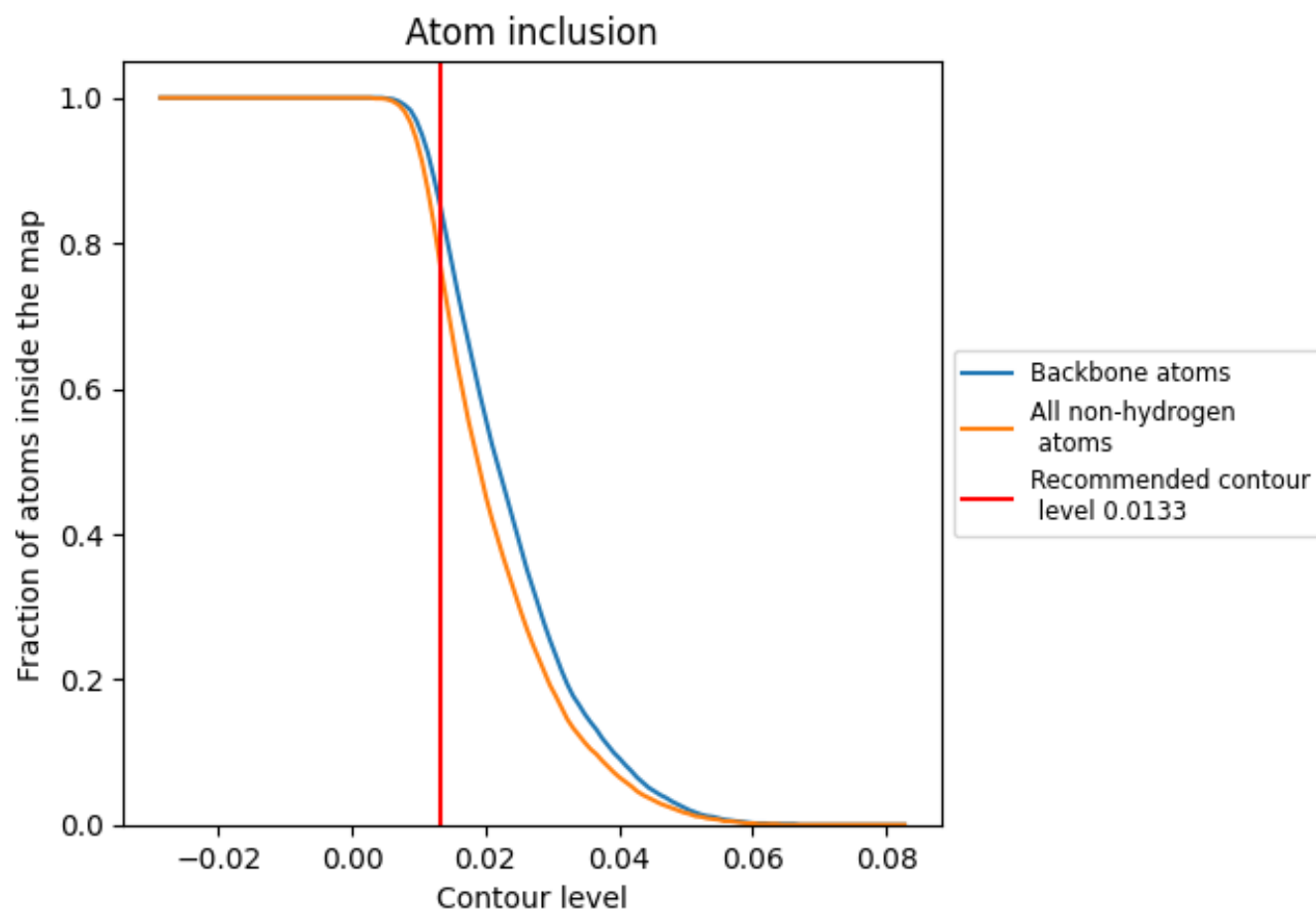
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.0133).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% 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 (0.0133) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7680	<div></div> 0.3230
A	<div></div> 0.7700	<div></div> 0.3250
B	<div></div> 0.7650	<div></div> 0.3200

