



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 10:28 PM UTC

PDB ID : 9MLI / pdb_00009mli
EMDB ID : EMD-48373
Title : Xenorhabdus nematophilus XptA2 RBD C Chimera
Authors : Aller, S.G.; Martin, C.L.
Deposited on : 2024-12-19
Resolution : 3.40 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

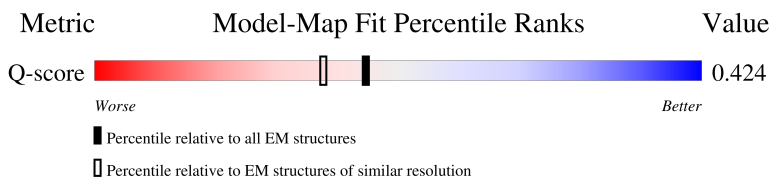
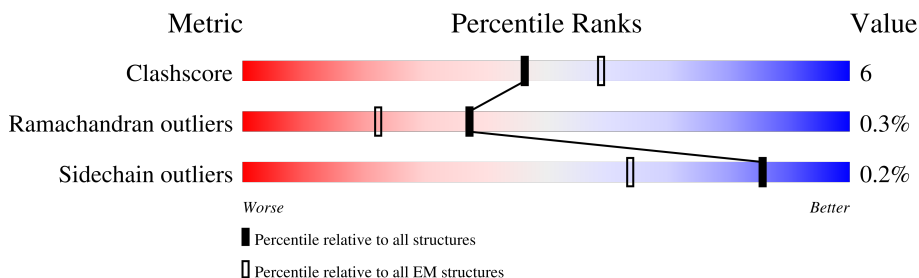
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	2543	
1	B	2543	
1	C	2543	
1	D	2543	

Continued on next page...

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Mol	Chain	Length	Quality of chain
1	E	2543	 85% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 99395 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.

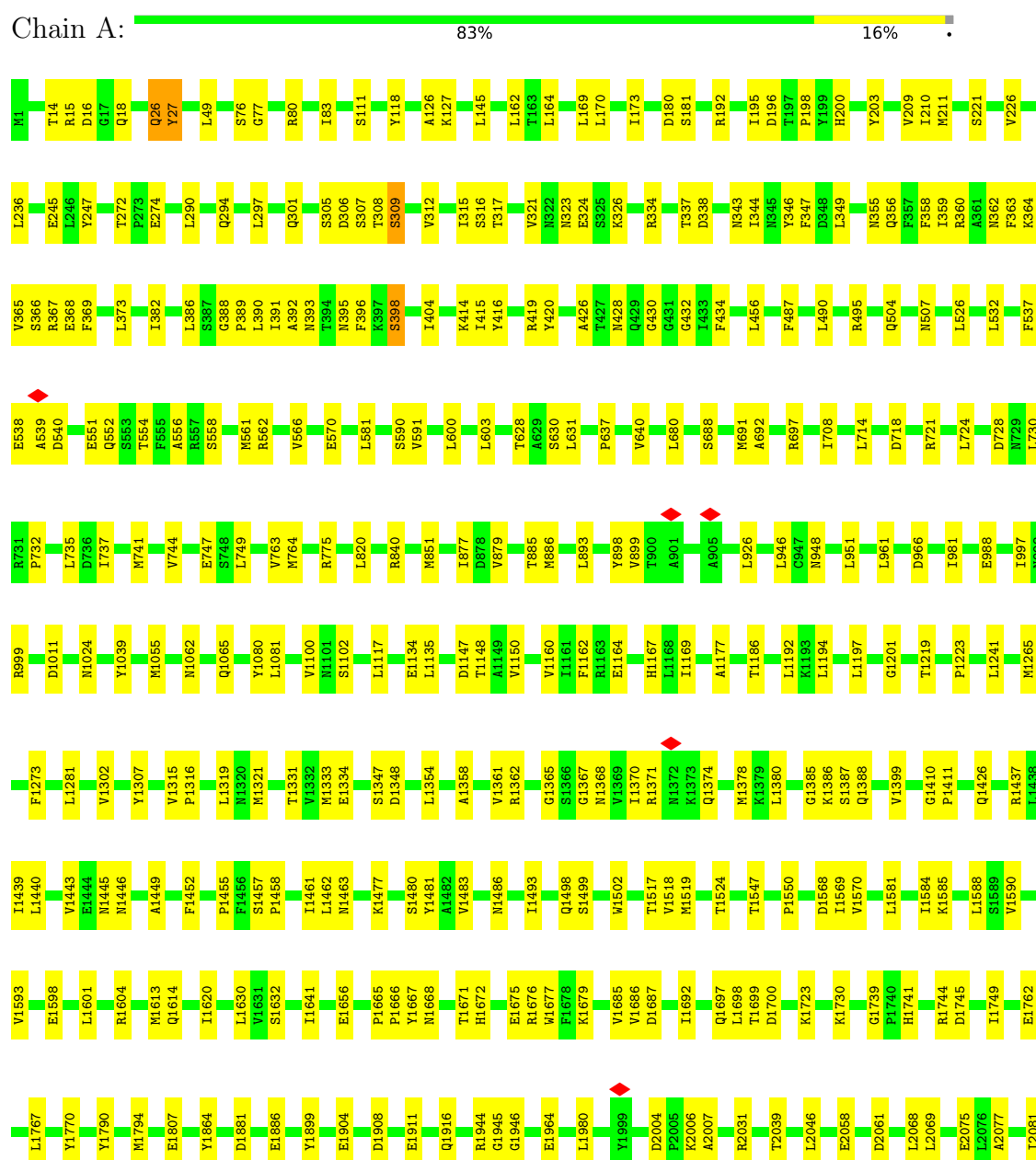
- Molecule 1 is a protein called A component of insecticidal toxin complex (Tc).

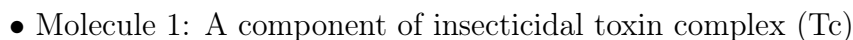
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0
1	B	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0
1	C	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0
1	D	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0
1	E	2519	Total 19879	C 12549	N 3397	O 3863	S 70	0	0

3 Residue-property plots

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: A component of insecticidal toxin complex (Tc)





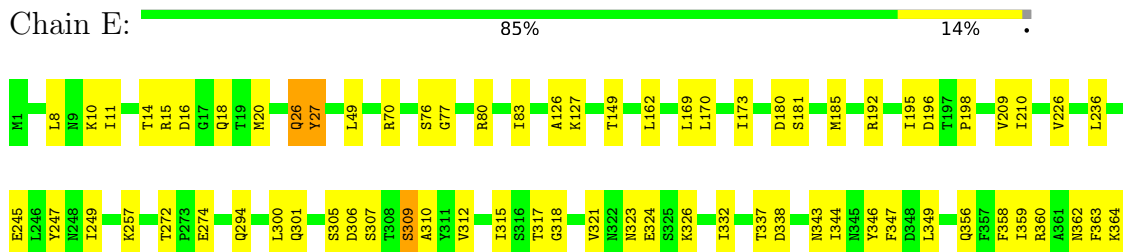
R2519
SER
GLU
ASN
LEU
TYR
PHE
GLN
GLY
ASP
TRP
LYS
ASP
ASP
ASP
LYS
LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 1: A component of insecticidal toxin complex (Tc)

Chain C:  84% 15%

D2434	A2437	V2438	L2439	K2440	G2442	G2443	M2447	P2448	I2454	A2455	L2456	F2466	M2467	L2468	D2469	F2470	E2479	A2496	T2497	D2498	K2501	L2504	E2505	R2519	SER	GLU	ASN	LEU	TYR	PHE	GLN	GLY	ASP	TYR	LYS	ASP	ASP	ASP	LYS	LEU	GLU	HIS	HIS	HIS	HIS	HIS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
W2205	E2231	V2237	H2246	T2247	Q2248	L2253	K2257	Y2264	K2270	L2271	L2281	T2282	F2285	C2286	L2287	R2294	T2303	M2318	L2323	E2329	E2343	V2344	T2345	L2372	K2376	S2382	R2398	Y2408	P2409	L2412	R2416	K2419	V2423																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
Q1916	L1939	T1940	M1941	L1942	G1943	R1944	G1945	G1946	N1955	E1964	L1980	T2003	D2004	P2005	K2006	A2007	R2031	T2039	L2046	E2058	D2061	L2070	M2074	E2075	L2076	A2077	L2081	Q2084	Q2085	R2086	L2130	A2133	Q2137	V2143	A2173	V2177	R2201																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
I1641	E1656	P1665	P1666	M1668	T1671	H1672	E1675	R1676	M1677	F1678	K1679	V1685	V1686	I1692	Q1697	L1698	T1699	D1700	L1711	K1730	R1744	D1745	I1749	E1762	Y1783	Y1784	E1807	D1860	P1861	M1862	R1871	D1881	D1890	Y1899	E1904	E1911	D1912																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
F1456	S1457	P1458	I1461	L1462	V1483	N1486	I1493	Q1498	S1499	I1514	V1518	M1519	T1524	F1527	G1366	G1367	N1368	V1369	I1370	R1371	P1550	L1551	I1569	V1570	T1573	L1581	I1584	K1585	L1588	V1593	E1598	L1601	R1604	Q1614	L1622	N1623	T1624	S1632																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
P1316	L1319	M1320	M1321	T1331	E1334	Q1340	S1347	D1348	L1354	H1355	A1358	R1362	G1365	S1366	G1367	N1368	V1369	I1370	R1371	P1372	K1373	Q1374	I1375	M1378	G1385	K1386	S1387	Q1388	V1399	Q1426	R1437	L1438	I1439	L1440	V1443	E1444	N1445	N1446	A1449	F1452	P1455																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
I997	N998	R999	Y1039	M1055	M1056	R1070	E1074	Y1080	L1081	F1084	V1100	L1117	E1134	T1148	I1157	V1160	F1161	F1162	R1163	E1164	H1167	L1168	I1169	L1192	K1193	L1194	L1197	G1201	L946	C947	N948	P1223	L1241	M1265	N1265	N1446	A1449	F1452	P1455																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
T742	L743	V744	L745	K746	E747	M750	E753	T754	V763	M764	R775	L776	L820	R840	M851	C615	M616	L617	Y618	K626	Y416	Y420	A426	T427	N428	Q429	G430	G431	G432	L456	F487	R495	Q504	N507	L532	F357	F358	I359	R360	A361	N362	F363																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
K364	V365	S366	F367	E368	F369	L373	R374	L386	S387	G388	F389	L391	A392	S398	L401	S402	N403	I404	S405	E408	K414	I415	Y416	Y420	A426	T427	N428	Q429	G430	G431	G432	L456	F487	R495	Q504	N507	L532	F357	F358	I359	R360	A361	N362	F363																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														

- Molecule 1: A component of insecticidal toxin complex (Tc)



ASP	M2318	D2061	I11749	D1568	K1386	D1057	V763	M561	V365
TTR	L2324	L2069	I11757	I1569	S1387	E1061	R775	R562	S366
LYS	L2325	A2077	Y1784	L1581	Q1388	L1081	L776	V566	R367
ASP	E2329	T2081	W1785	T1584	V1399	L1117	R796	E570	E368
ASP	K2332	Q2084	E1786	K1585	G1410	E1134	L820	L581	F369
LEU	L2372	Q2085	Y1790	L1588	P1411	H1167	M830	L589	L373
GLU	S2382	R2086	E1807	S1589	N1416	E1194	R840	S590	R374
HIS	L2115	L2115	D1860	V1590	Y1421	A1177	M851	V591	K375
HIS	R2398	D2132	F1661	E1598	R1437	T1186	M856	L600	I382
HIS	P2409	Q2137	M1862	T1624	L1438	L1194	T877	T601	L386
HIS	L2412	Q2137	D1881	T1624	L1440	A1195	D878	L602	S387
HIS	K2419	V2143	Y1899	S1632	V1443	F1196	V879	L603	G388
HIS	V2423	L2160	E1904	R1633	E1444	T1219	M886	A604	I391
HIS	A2437	A2173	L1905	T1640	N1445	T1219	M886	L614	A392
ASP	Y2441	S2174	D1908	I1664	F1452	P1223	L893	L617	N395
GLU	G2442	V2177	E1911	P1685	P1455	M1285	L893	S630	F396
G2443	R2201	R2201	Q1916	P1666	F1456	F1273	Y898	L631	K397
M2447	M2205	M2205	L1939	N1667	S1457	T900	T900	V640	S398
P2448	E2231	E2231	T1940	N1668	P1458	V1315	A901	N671	L401
L2456	V2237	V2237	M1941	H1672	I1462	L1319	L902	L680	K414
F2466	E2252	E2252	R1944	R1676	N1463	M1321	I903	I687	I415
M2467	L2253	L2253	G1946	K1679	K1477	T1331	A905	R697	Y416
F2470	K2287	K2287	A1954	V1685	V1483	E1334	L926	L714	Y420
D2471	L2263	L2263	N1955	D1686	N1486	S1347	D936	L714	A426
E2479	Y2264	Y2264	S1956	D1687	I1493	D1348	E940	L718	T427
T2497	M2267	M2267	Y1999	I1692	Y1497	L1354	L946	R721	M428
D2498	K2270	K2270	D2004	Q1697	Q1498	H1355	E947	L724	Q429
K2501	L2281	L2281	P2005	L1698	W1502	N1356	N948	D728	G430
L2504	T2282	T2282	K2006	T1699	W1518	R1362	L961	P732	G431
E2505	Q2283	Q2283	A2007	D1700	M1519	G1365	D966	L735	G432
R2519	S2284	S2284	T2010	L1711	T1524	S1386	Y977	D736	L456
SER	F2285	F2285	R2031	M1726	F1527	N1368	I981	I737	F487
GLU	M2288	M2288	T2039	K1730	D1531	R1371	I997	M741	Q804
ASN	R2289	R2289	V2043	G1739	D1531	N1372	R996	V744	N507
LEU	R2294	R2294	L2046	H1741	T1547	L1380	R999	V744	L532
TYR	T2303	T2303	E2058	R1744	P1550	L1380	A1000	V744	E538
PHE	L2317	L2317		D1745	L1551	G1385	L1001	E747	A539
GLN									D540
GLY									E551

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77025	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.962	Depositor
Minimum map value	-0.404	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.0894	Depositor
Map size (Å)	485.46, 485.46, 485.46	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3485, 1.3485, 1.3485	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	0.18	0/20285	0.34	6/27556 (0.0%)
1	B	0.18	0/20285	0.34	7/27556 (0.0%)
1	C	0.18	0/20285	0.34	6/27556 (0.0%)
1	D	0.18	0/20285	0.35	6/27556 (0.0%)
1	E	0.18	0/20285	0.35	6/27556 (0.0%)
All	All	0.18	0/101425	0.34	31/137780 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2497	THR	CA-C-N	13.96	146.83	121.70
1	D	2497	THR	C-N-CA	13.96	146.83	121.70
1	B	2497	THR	CA-C-N	13.93	146.76	121.70
1	B	2497	THR	C-N-CA	13.93	146.76	121.70
1	C	2497	THR	CA-C-N	13.92	146.75	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	B	398	SER	Peptide
1	C	398	SER	Peptide
1	D	398	SER	Peptide
1	E	398	SER	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	19879	0	19498	276	0
1	B	19879	0	19498	251	0
1	C	19879	0	19498	266	0
1	D	19879	0	19498	237	0
1	E	19879	0	19498	253	0
All	All	99395	0	97490	1202	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 6.

The worst 5 of 1202 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:E:2447:MET:HE3	1:E:2448:PRO:HD2	1.58	0.85
1:B:2056:MET:HE2	1:B:2267:MET:HE3	1.59	0.83
1:A:306:ASP:OD1	1:A:307:SER:N	2.14	0.81
1:D:2497:THR:H	1:D:2498:ASP:HB2	1.46	0.81
1:C:2497:THR:H	1:C:2498:ASP:HB2	1.47	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	A	2517/2543 (99%)	2388 (95%)	121 (5%)	8 (0%)	36	65
1	B	2517/2543 (99%)	2392 (95%)	118 (5%)	7 (0%)	36	65
1	C	2517/2543 (99%)	2391 (95%)	119 (5%)	7 (0%)	36	65
1	D	2517/2543 (99%)	2390 (95%)	120 (5%)	7 (0%)	36	65
1	E	2517/2543 (99%)	2384 (95%)	126 (5%)	7 (0%)	36	65
All	All	12585/12715 (99%)	11945 (95%)	604 (5%)	36 (0%)	37	65

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	TYR
1	A	2498	ASP
1	B	27	TYR
1	B	2498	ASP
1	C	27	TYR

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	2167/2192 (99%)	2159 (100%)	8 (0%)	84	83
1	B	2167/2192 (99%)	2161 (100%)	6 (0%)	86	84
1	C	2167/2192 (99%)	2164 (100%)	3 (0%)	88	89
1	D	2167/2192 (99%)	2164 (100%)	3 (0%)	88	89
1	E	2167/2192 (99%)	2165 (100%)	2 (0%)	88	89
All	All	10835/10960 (99%)	10813 (100%)	22 (0%)	85	85

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	317	THR
1	D	1061	GLU
1	C	1315	VAL
1	D	1168	LEU
1	A	2323	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	921	ASN
1	E	921	ASN
1	C	2311	ASN
1	E	863	GLN
1	E	1596	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 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.

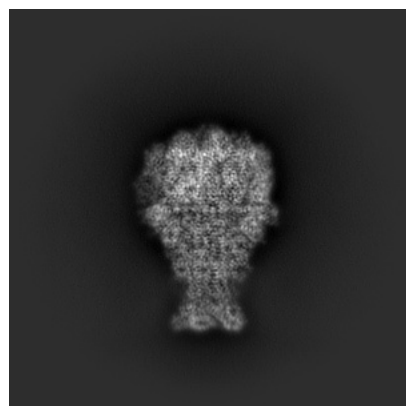
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48373. These allow visual inspection of the internal detail of the map and identification of artifacts.

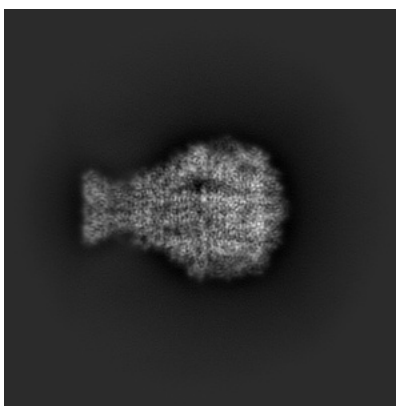
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

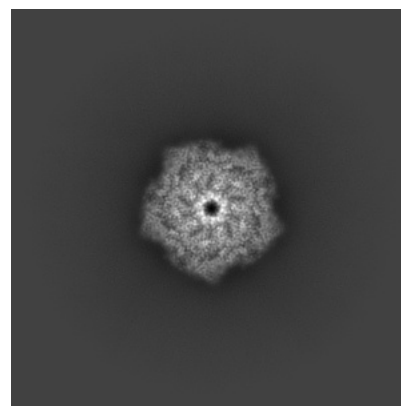
6.1.1 Primary map



X

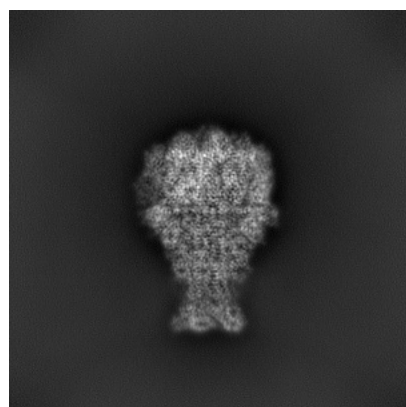


Y

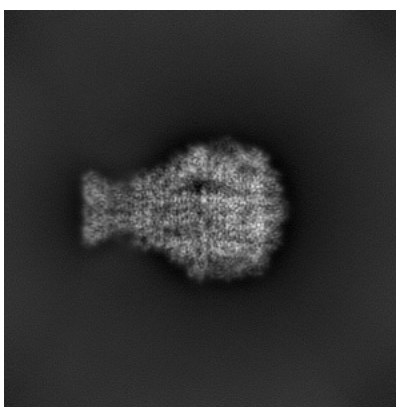


Z

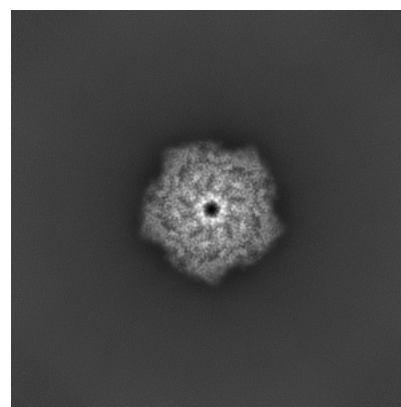
6.1.2 Raw map



X



Y

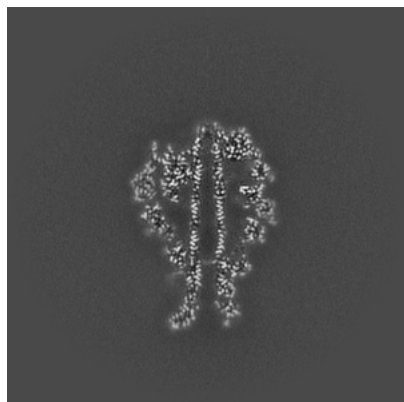


Z

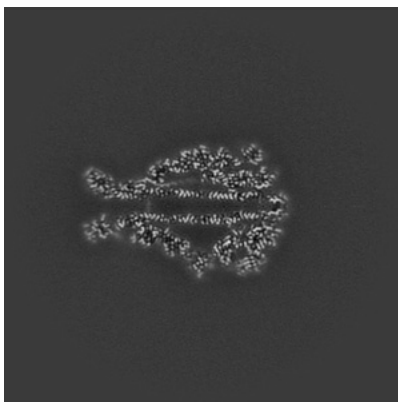
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

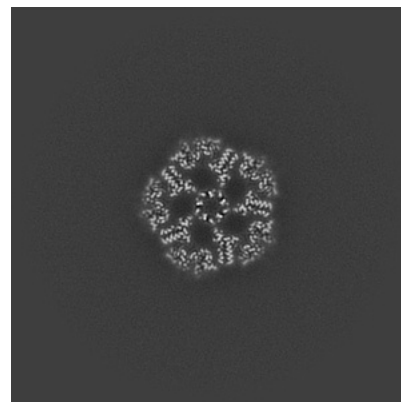
6.2.1 Primary map



X Index: 180

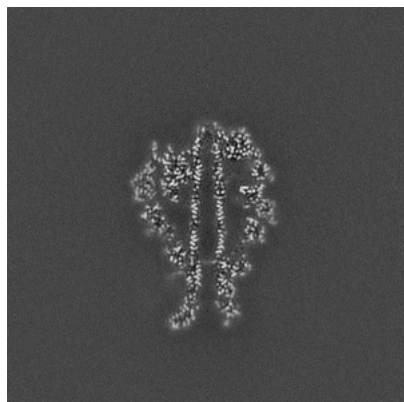


Y Index: 180

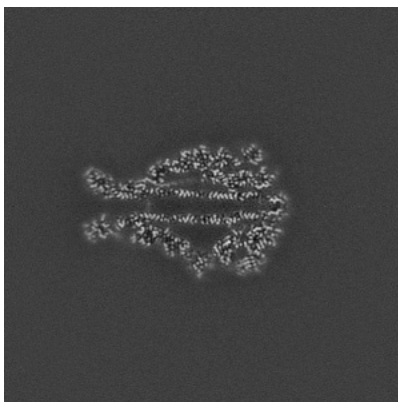


Z Index: 180

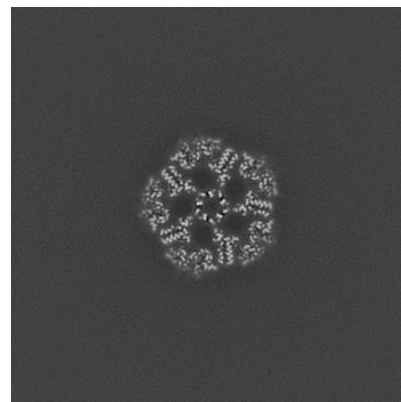
6.2.2 Raw map



X Index: 180



Y Index: 180

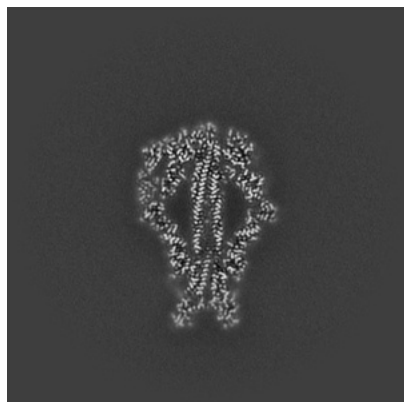


Z Index: 180

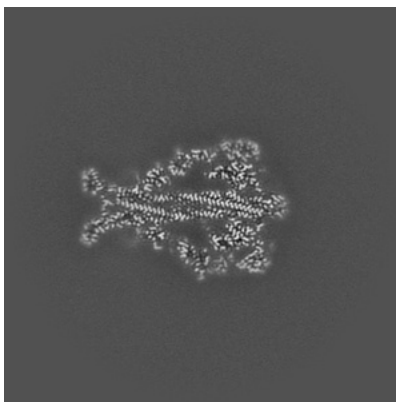
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

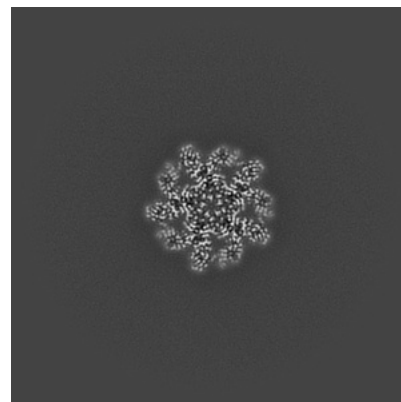
6.3.1 Primary map



X Index: 173

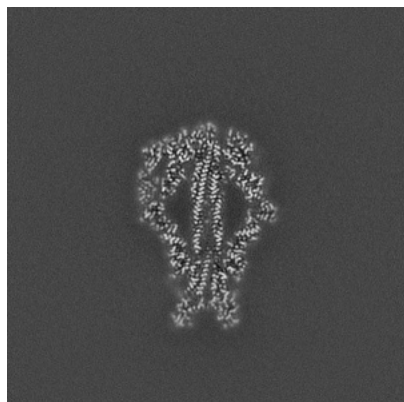


Y Index: 172

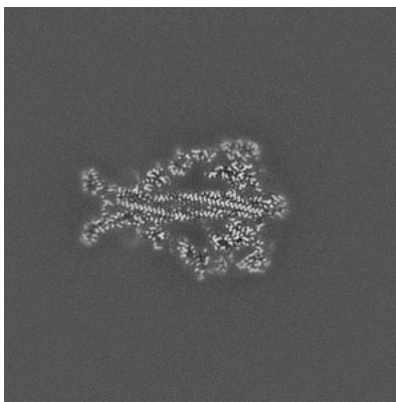


Z Index: 228

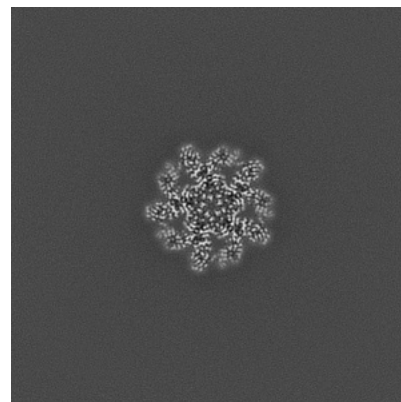
6.3.2 Raw map



X Index: 173



Y Index: 172

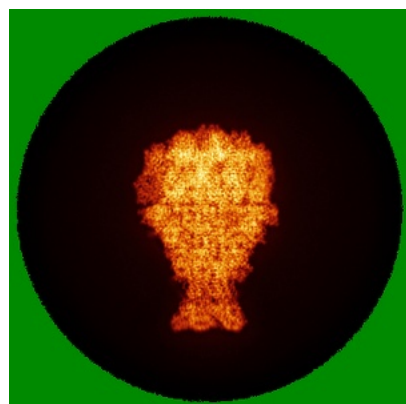


Z Index: 228

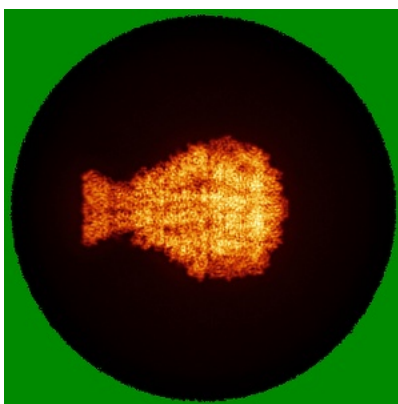
The images above show the largest variance slices of the map in three orthogonal directions.

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

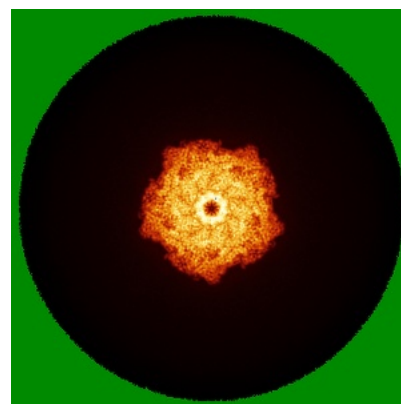
6.4.1 Primary map



X

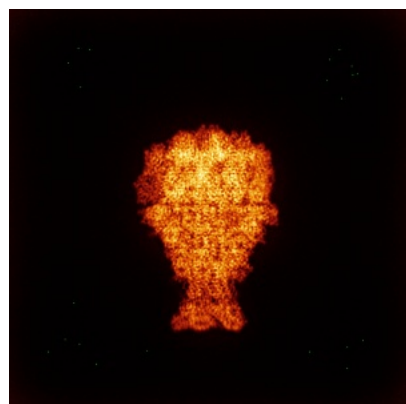


Y

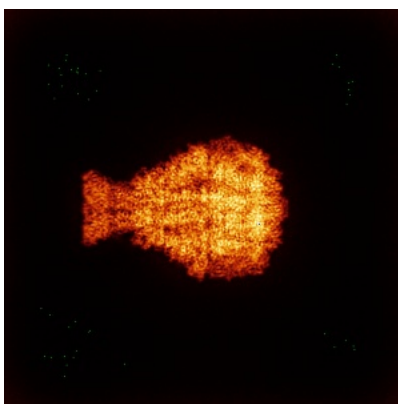


Z

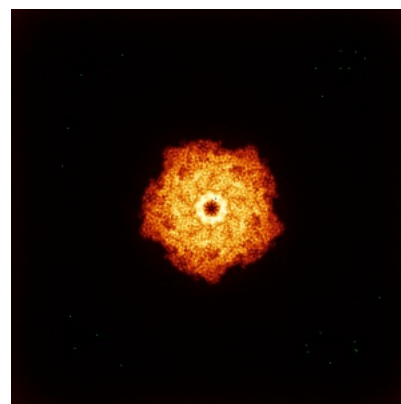
6.4.2 Raw map



X



Y

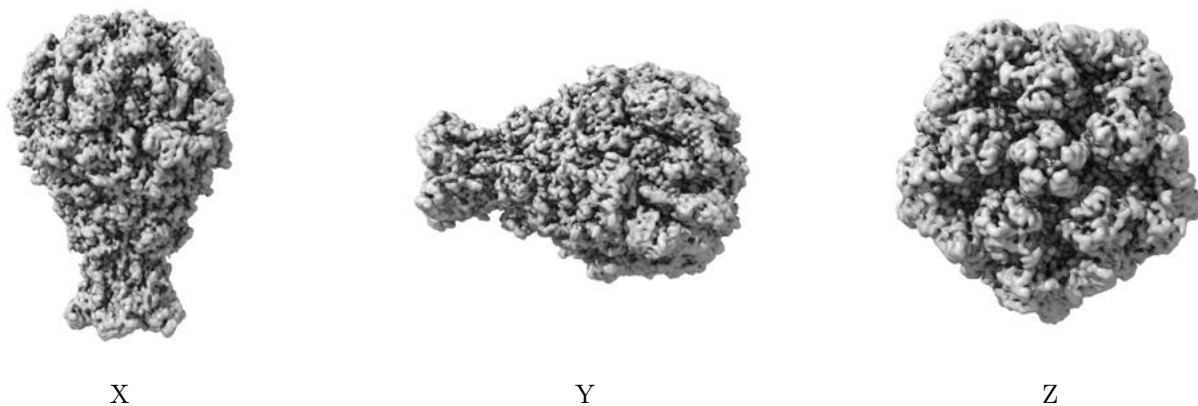


Z

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.

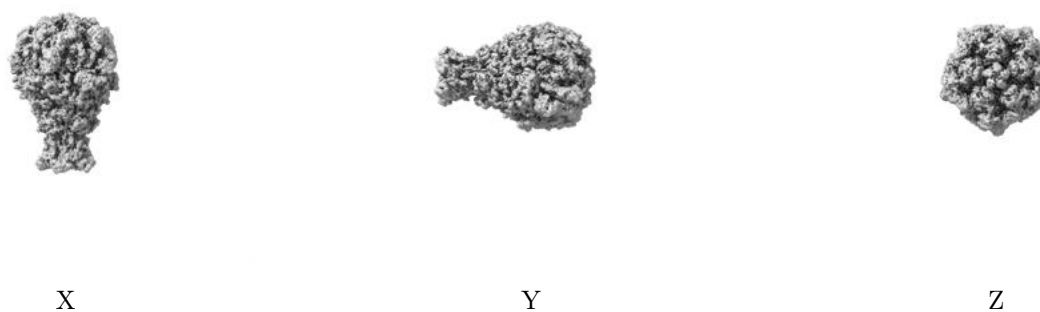
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0894. 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.

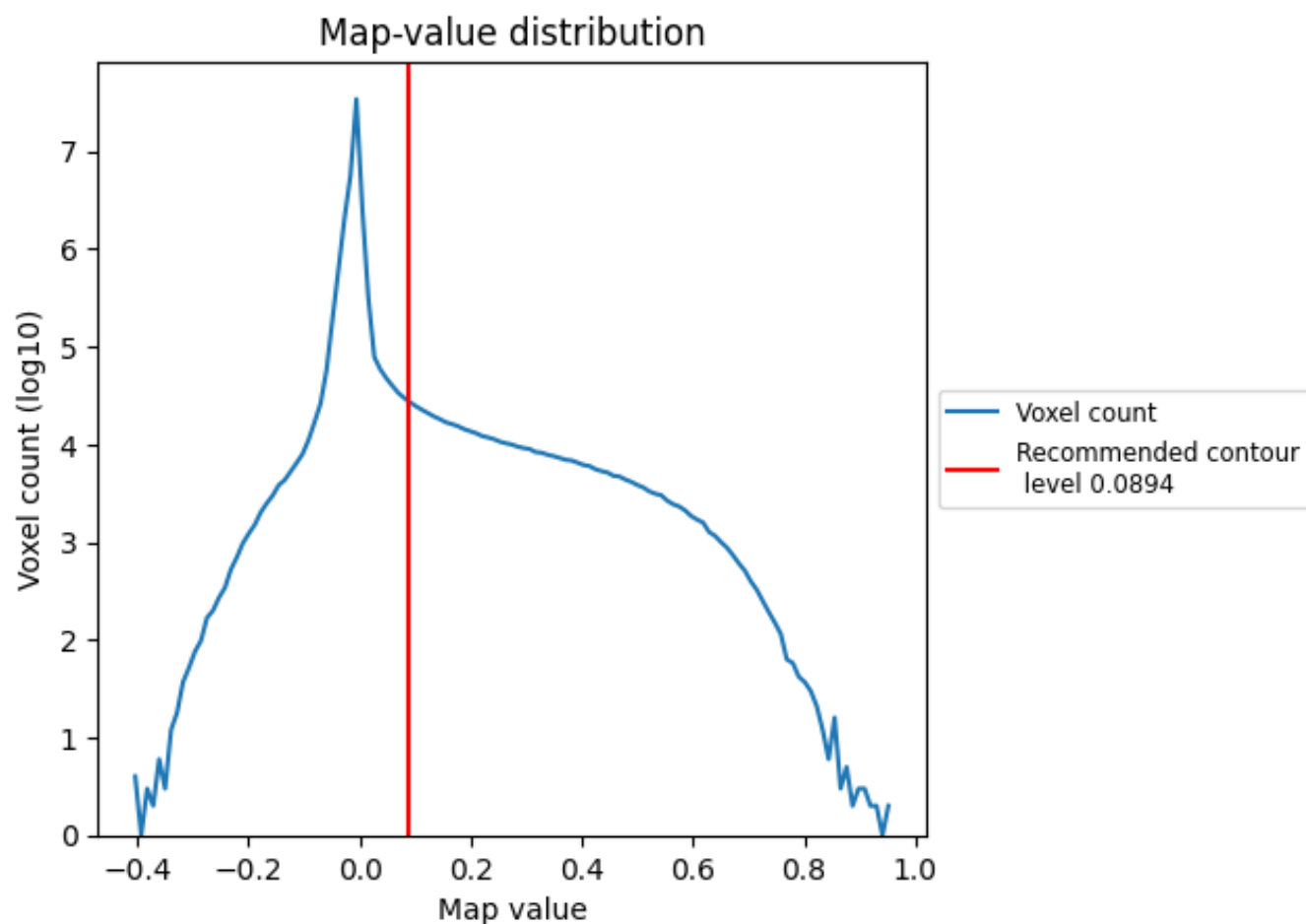
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

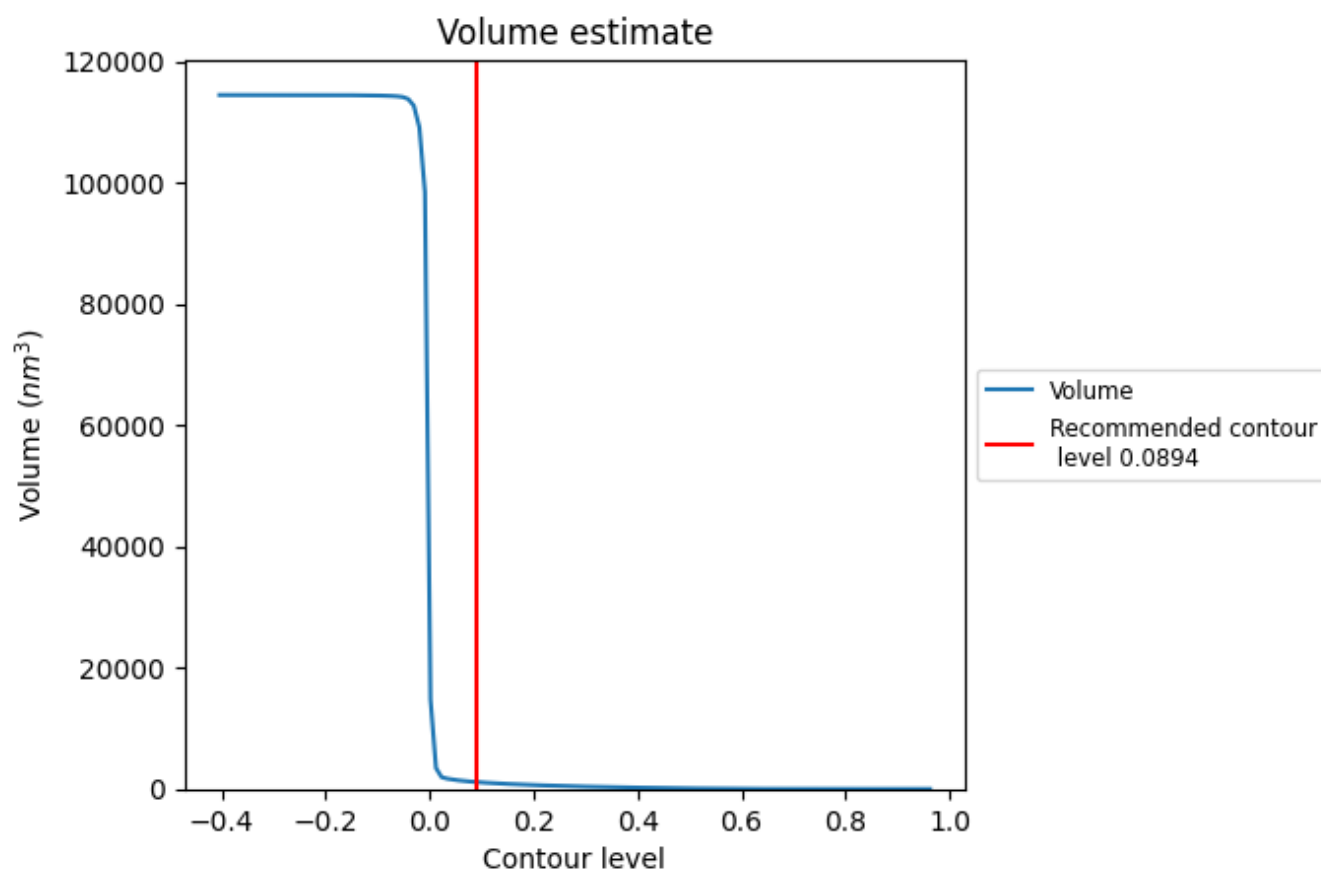
This section contains the results of statistical analysis of the map.

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.

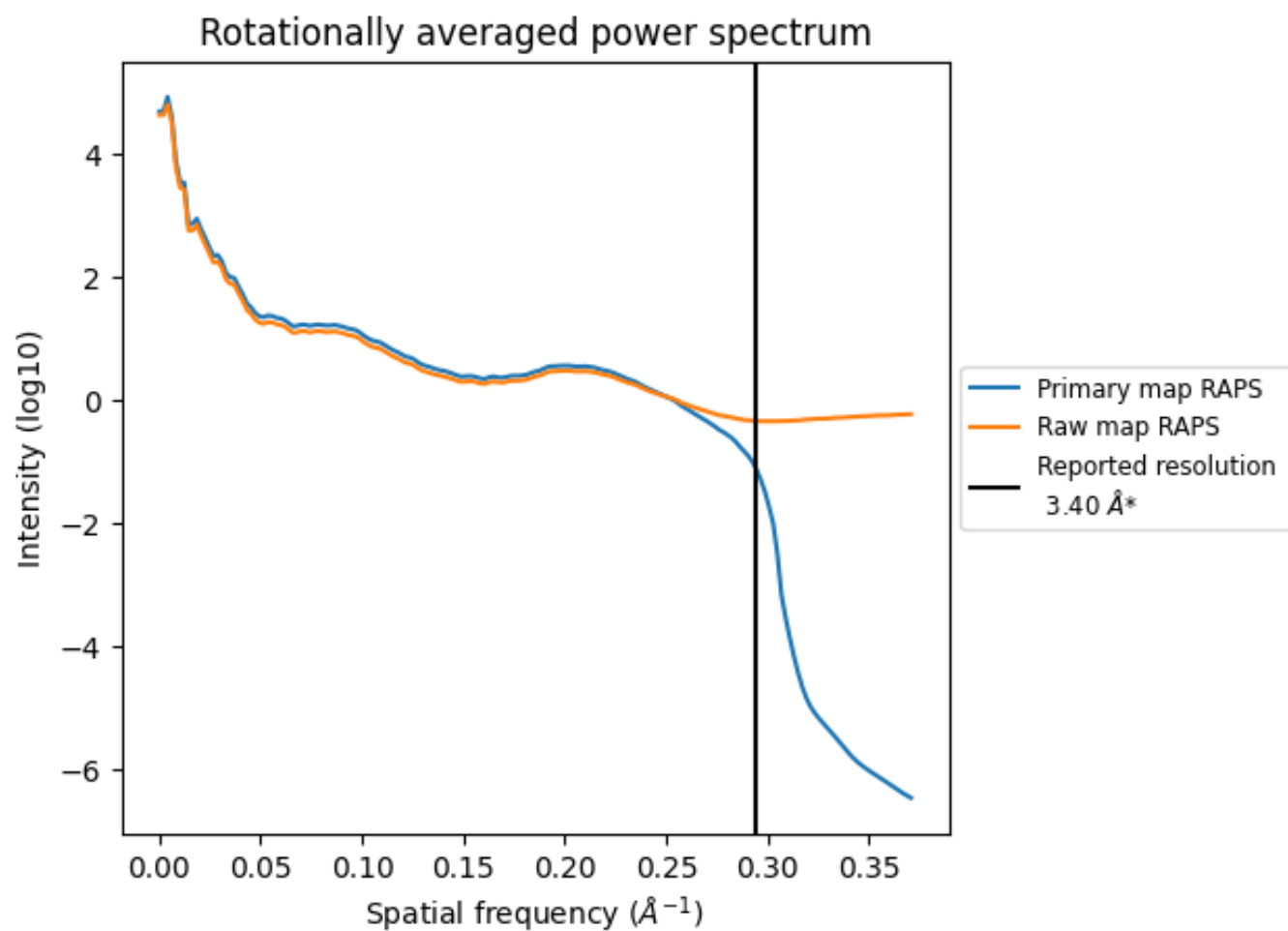
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1142 nm³; this corresponds to an approximate mass of 1031 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 ⓘ

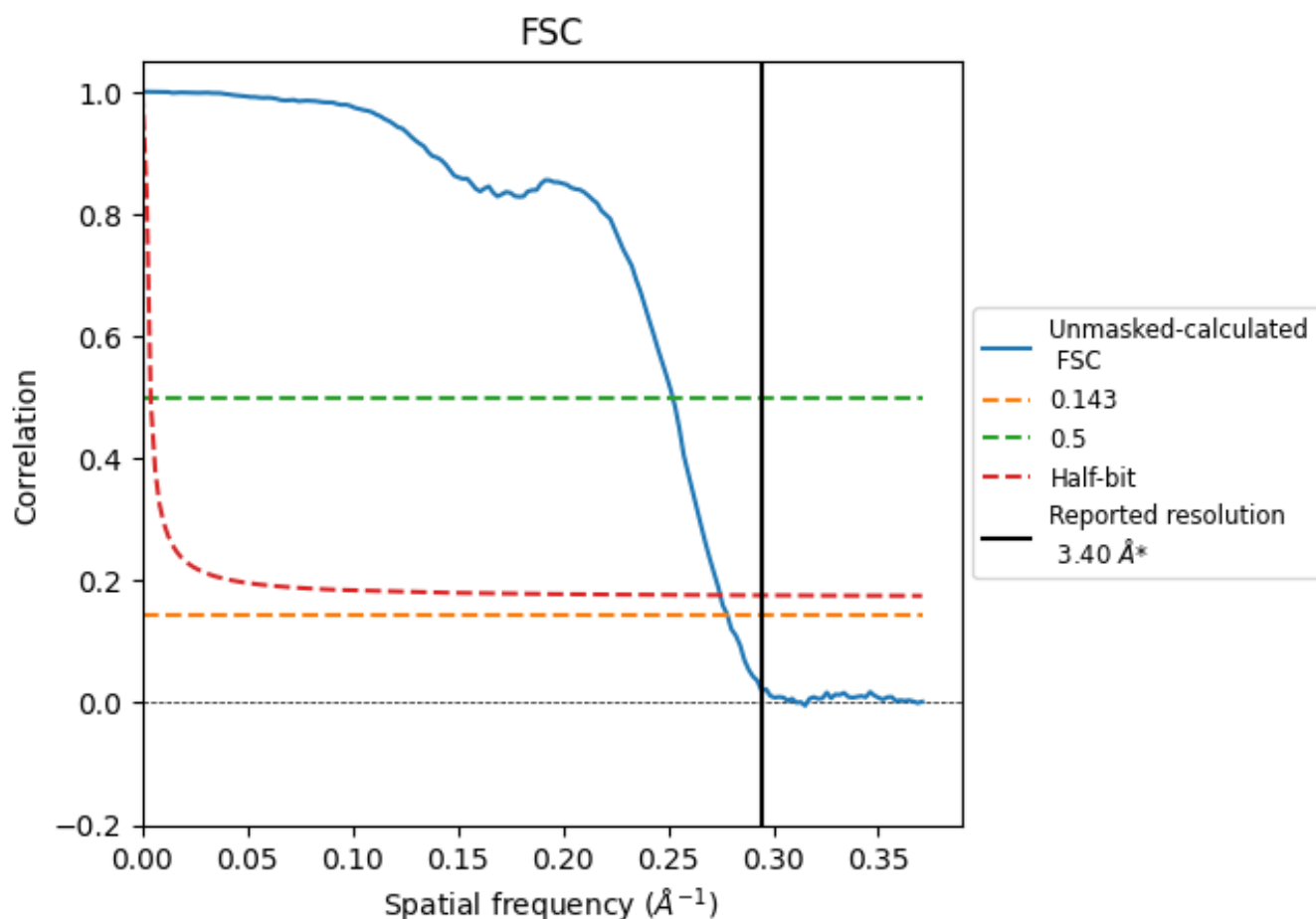


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

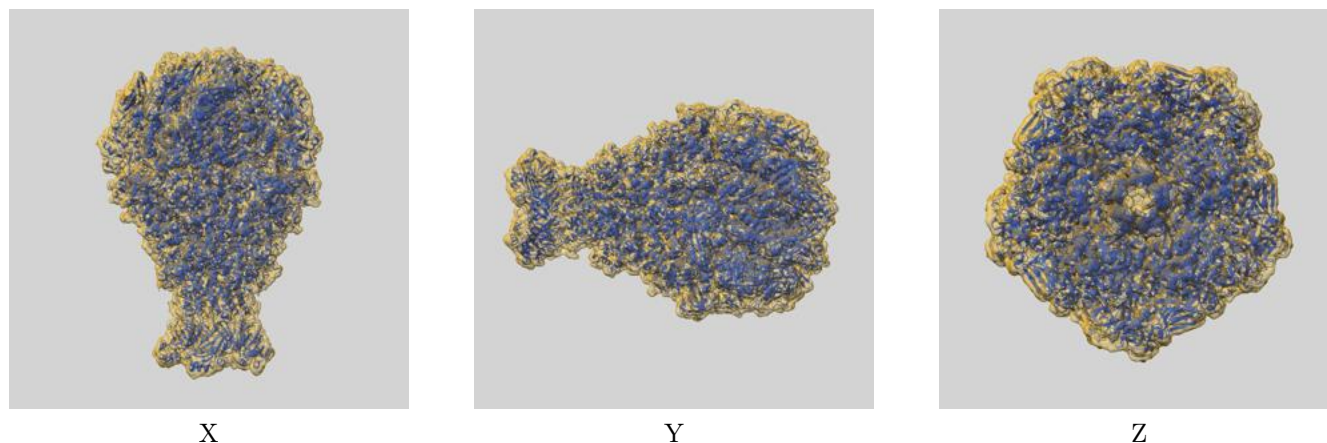
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	3.97	3.64

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

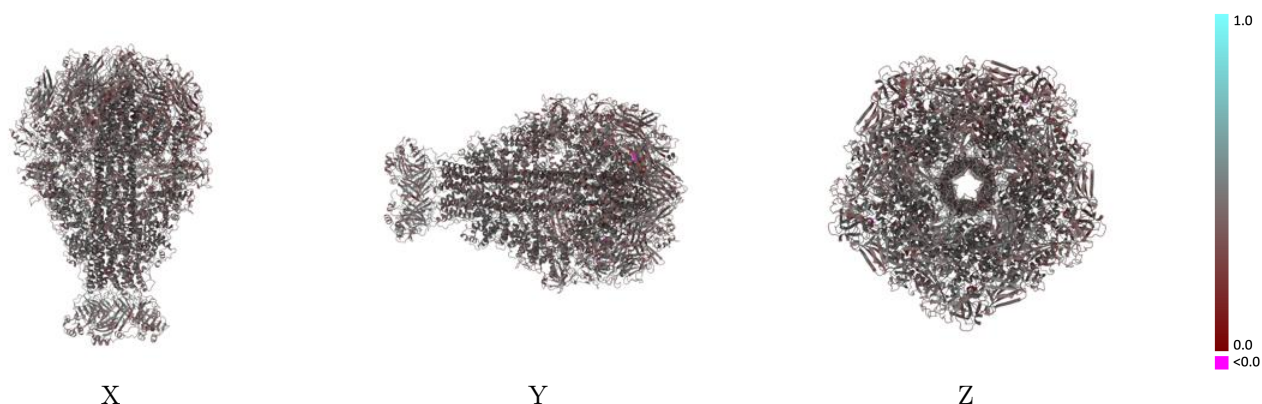
This section contains information regarding the fit between EMDB map EMD-48373 and PDB model 9MLI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



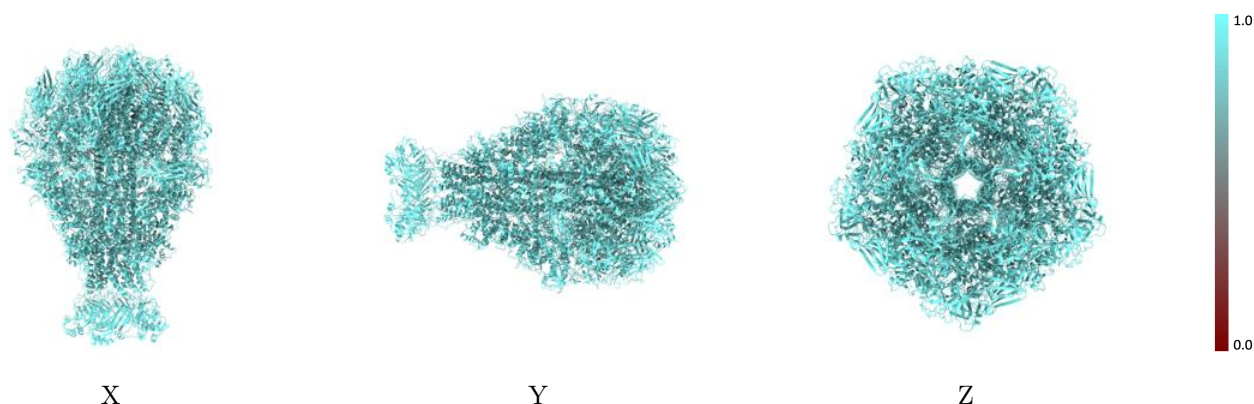
The images above show the 3D surface view of the map at the recommended contour level 0.0894 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



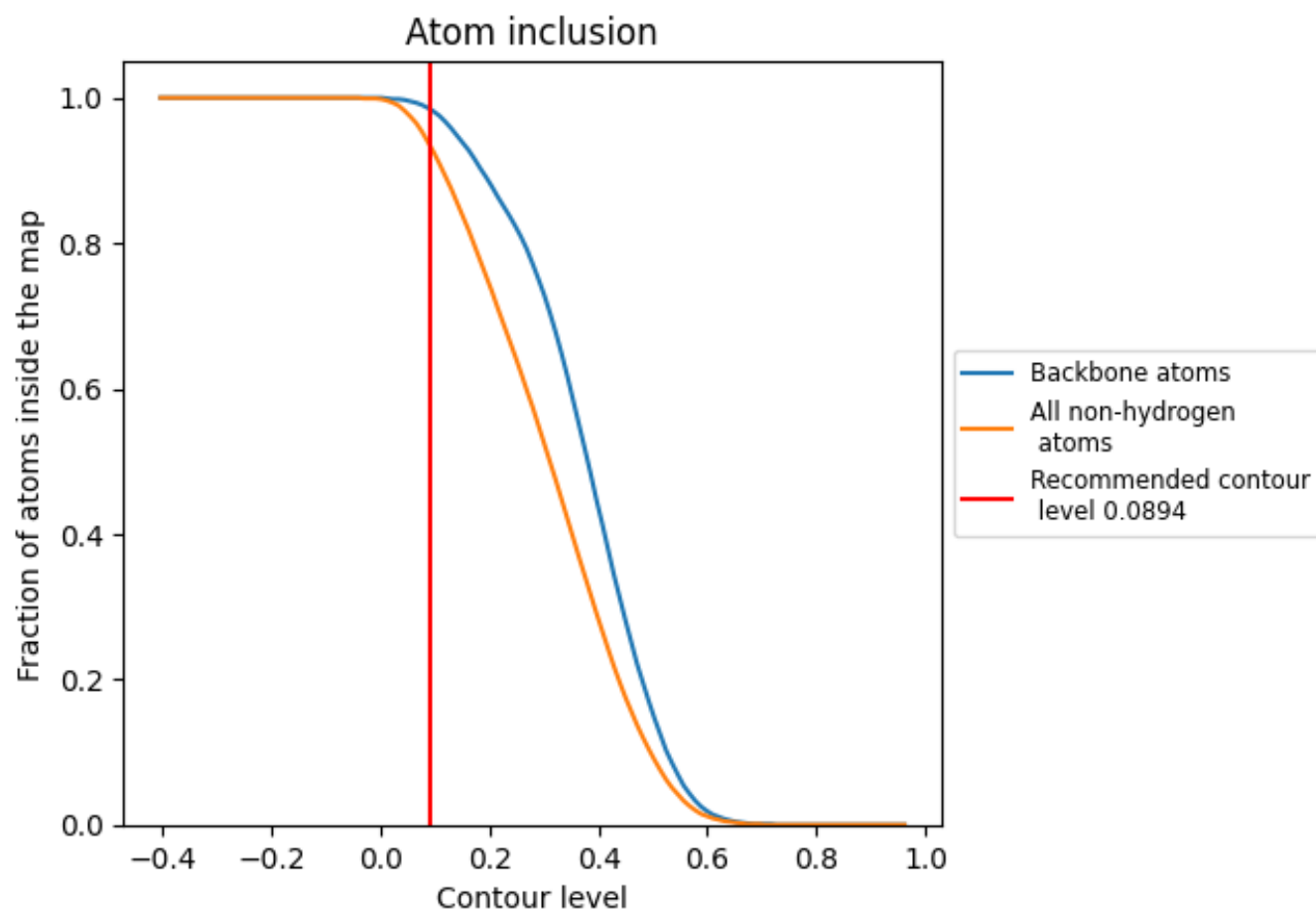
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0894).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.0894) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9360	0.4240
A	0.9350	0.4230
B	0.9410	0.4400
C	0.9400	0.4310
D	0.9330	0.4160
E	0.9330	0.4110

