



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 07:46 PM UTC

PDB ID : 6YEH / pdb_00006yeh
EMDB ID : EMD-10797
Title : Xenorhabdus nematophila XptA1 in complex with porcine mucosa heparin
Authors : Roderer, D.; Broecker, F.; Sitsel, O.; Kaplonek, P.; Leidreiter, F.; Seeberger, P.H.; Raunser, S.
Deposited on : 2020-03-25
Resolution : 3.70 Å(reported)
Based on initial model : 6RW8

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:

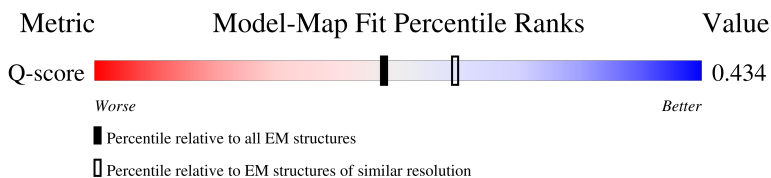
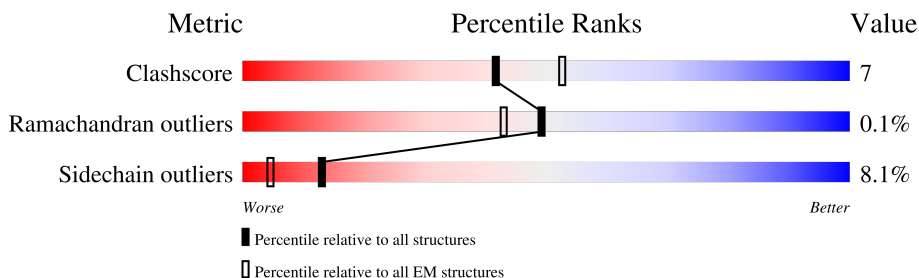
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.70 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	11569 (3.20 - 4.20)

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	2523	
1	B	2523	
1	C	2523	
1	D	2523	

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Mol	Chain	Length	Quality of chain
1	E	2523	 A horizontal bar chart showing the quality of chain E. The bar is divided into three segments: green (71%), yellow (20%), and grey (7%). A small red square is at the start of the green segment, and a small black dot is at the end of the grey segment. 71%20%7%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 93500 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.

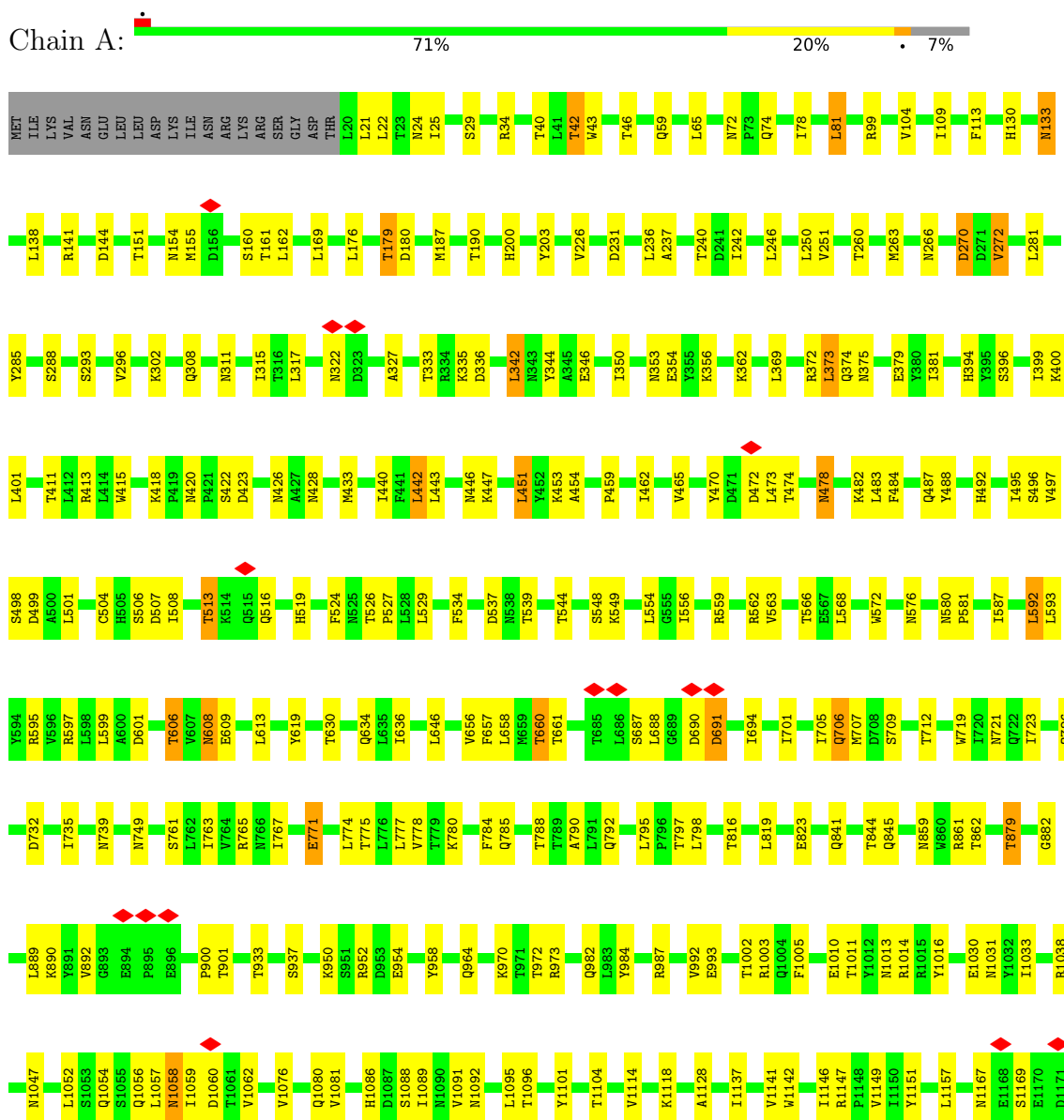
- Molecule 1 is a protein called A component of insecticidal toxin complex (Tc).

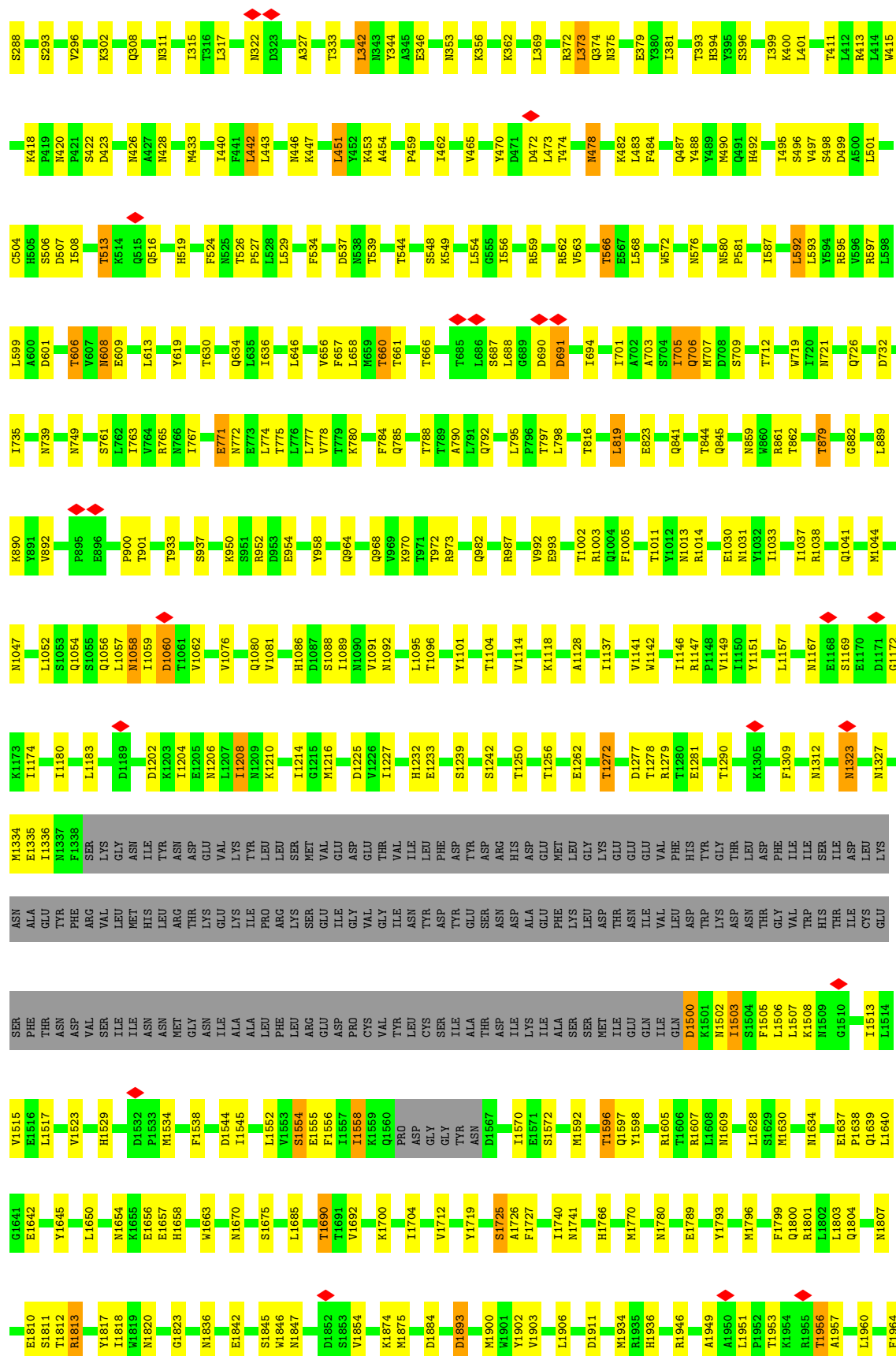
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	B	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	C	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	D	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		
1	E	2337	Total	C	N	O	S	0	0
			18700	11894	3132	3607	67		

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.

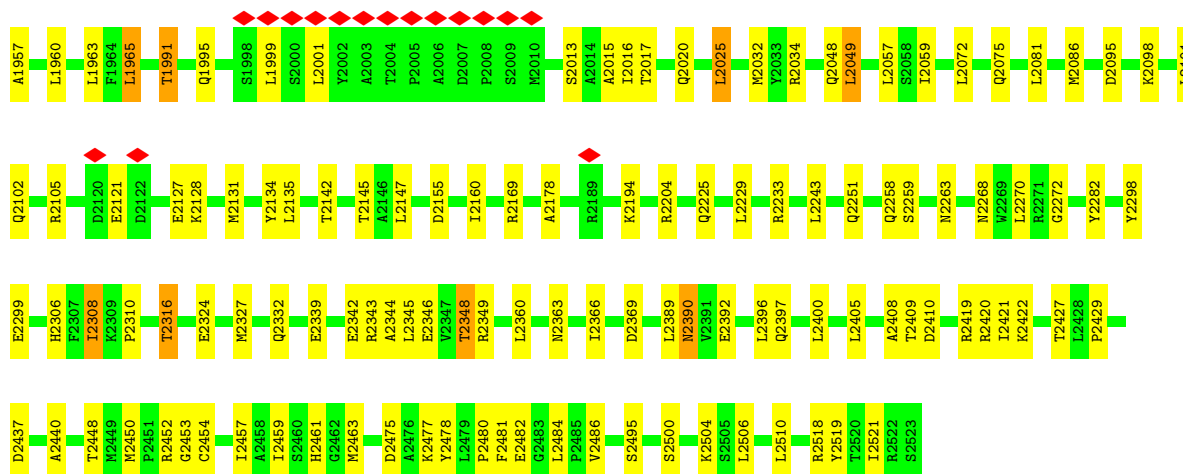
- Molecule 1: A component of insecticidal toxin complex (Tc)





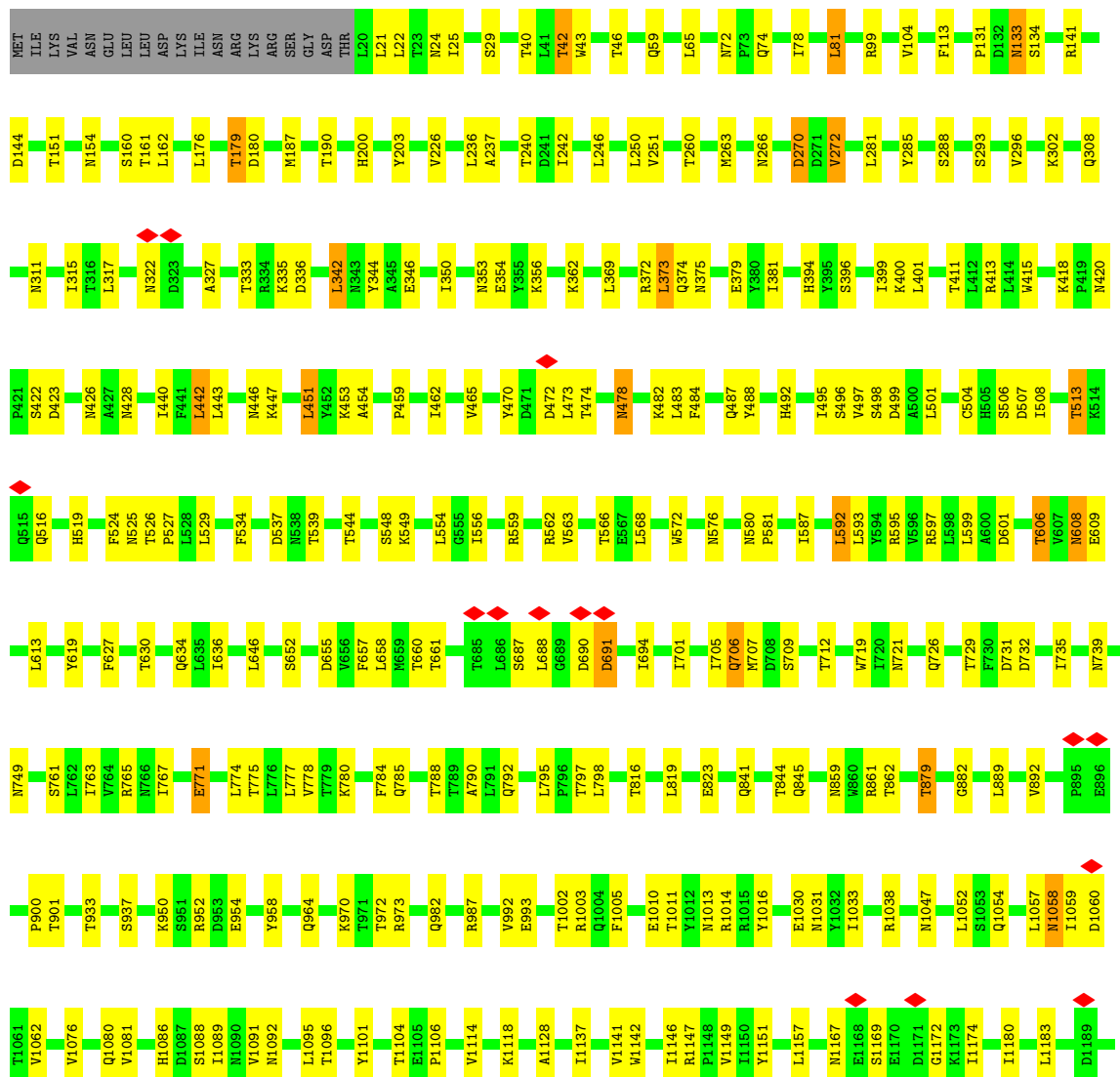






- Molecule 1: A component of insecticidal toxin complex (Tc)

Chain E: 71% 20% 7%



T2448	Y2282	M2086	F1952	L1803	L1640	V1523	PHE	E1335	S1193
M2449	Y2298	D2095	T1953	Q1804	G1641	V1523	THR	I1336	S1194
M2450	E2299	R1954	K1954	E1805	E1642	H1529	ASP	N1337	D1202
R2451	H2306	K2098	R1955	Q1806	Y1645	E1530	VAL	SER	K1203
G2453	F2307	L2101	T1956	N1807	L1650	S1531	SER	LYS	I1204
T2457	T2308	Q2102	A1957	E1810	L1650	D1532	ILE	GLY	E1205
D2475	K2309	R2105	L1960	S1811	N1654	P1533	ILE	ASN	N1206
A2476	P2310	D2120	F1964	R1813	K1655	M1534	ASN	TYR	I1207
K2477	T2316	E2121	L1965	Y1817	E1656	F1538	MET	ASN	N1208
Y2478	M2327	D2122	L1979	Y1818	H1658	I1545	GLY	ASN	N1209
F2481	L2330	E2127	T1991	Y1819	W1663	D1544	THR	ASP	K1210
E2482	E2339	K2128	G1994	N1820	N1670	I1545	GLY	VAL	I1214
L2484	R2343	M2131	Q1995	G1823	N1670	V1553	LYS	LYS	G1215
F2485	A2344	Y2134	S1998	M1836	S1675	S1554	PRO	TYR	M1216
V2486	T2348	L2135	L1999	E1842	L1685	E1555	ARG	LEU	D1225
S2495	R2349	T2142	S2000	S1845	T1690	F1556	LEU	SER	V1226
S2500	T2350	T2145	L2001	W1946	T1691	I1557	ARG	MET	I1227
K2504	L2360	T2145	Y2002	M1847	V1692	Q1560	GLY	VAL	H1232
S2505	N2363	A2146	A2003	D1852	Y1702	ASP	ILE	GLY	E1233
L2506	L2366	L2147	T2004	V1854	Y1703	GLY	GLY	ASP	H1234
L2510	D2369	D2155	P2005	D1863	I1704	TYR	ASP	PHE	S1242
R2518	L2389	T2160	A2006	P1864	R1709	ASN	GLY	TYR	T1250
T2519	T2390	R2169	D2007	K1874	V1712	D1667	SER	ASP	T1256
T2521	V2391	A2178	S2009	M1875	Y1719	I1570	ASP	ARG	E1262
R2522	E2392	R2189	M2010	D1882	D1720	S1572	ALA	ASP	K1270
S2523	L2396	K2194	S2013	G1883	S1725	M1592	ILE	GLY	S1271
	Q2397	R2189	A2014	D1884	A1726	T1596	ALA	LEU	T1272
	L2400	R2204	A2015	D1893	F1727	Q1597	LEU	LYS	D1277
	L2405	Q2225	T2016	D1893	I1740	Y1598	THR	ASP	T1278
	A2408	L2229	T2017	M1900	N1741	R1605	GLU	GLY	R1279
	T2409	R2233	Q2020	Y1901	K1769	T1606	ASN	GLY	T1280
	D2410	R2233	L2025	V1902	M1770	R1607	VAL	VAL	E1281
	R2419	L2243	M2032	V1903	M1770	R1607	ASP	PHE	T1290
	R2420	L2243	Y2033	D1911	N1780	D1625	TRP	LYS	L1293
	I2421	Q2251	R2034	E1923	E1789	D1625	ASP	ASP	L1293
	K2422	Q2258	Q2048	M1934	Y1793	L1628	ASN	THR	K1305
	T2427	S2259	L2049	A1935	M1796	S1829	THR	GLY	F1309
	L2428	Q2268	L2057	H1936	M1796	M1630	VAL	ILE	I1312
	P2429	N2268	S2058	R1946	F1799	M1634	THR	THR	N1323
	L2442	W2269	I2059	A1949	Q1800	L1635	ILE	ASP	N1327
		L2270	L2072	A1950	R1801	P1637	CYS	LEU	L1334
			Q2075	L1951	L1802	Q1639	SER	ASN	
			L2081						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	172596	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	484.0, 484.0, 484.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	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	0.28	0/19100	0.51	2/25936 (0.0%)
1	B	0.28	0/19100	0.51	2/25936 (0.0%)
1	C	0.28	0/19100	0.51	2/25936 (0.0%)
1	D	0.28	0/19100	0.51	2/25936 (0.0%)
1	E	0.28	0/19100	0.51	2/25936 (0.0%)
All	All	0.28	0/95500	0.51	10/129680 (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	2
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	10

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	D	161	THR	CA-C-N	5.58	132.20	121.54
1	D	161	THR	C-N-CA	5.58	132.20	121.54
1	A	161	THR	CA-C-N	5.58	132.19	121.54
1	A	161	THR	C-N-CA	5.58	132.19	121.54
1	E	161	THR	CA-C-N	5.56	132.16	121.54

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1558	ILE	Peptide
1	A	2344	ALA	Peptide
1	B	1558	ILE	Peptide
1	B	2344	ALA	Peptide
1	C	1558	ILE	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	18700	0	18400	262	0
1	B	18700	0	18400	264	0
1	C	18700	0	18400	277	0
1	D	18700	0	18400	262	0
1	E	18700	0	18400	260	0
All	All	93500	0	92000	1258	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 7.

The worst 5 of 1258 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:236:LEU:HB2	1:B:484:PHE:HB2	1.74	0.70
1:A:236:LEU:HB2	1:A:484:PHE:HB2	1.74	0.70
1:C:236:LEU:HB2	1:C:484:PHE:HB2	1.74	0.70
1:D:236:LEU:HB2	1:D:484:PHE:HB2	1.74	0.69
1:E:236:LEU:HB2	1:E:484:PHE:HB2	1.74	0.69

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	2331/2523 (92%)	2158 (93%)	170 (7%)	3 (0%)	48	78
1	B	2331/2523 (92%)	2158 (93%)	170 (7%)	3 (0%)	48	78
1	C	2331/2523 (92%)	2160 (93%)	168 (7%)	3 (0%)	48	78
1	D	2331/2523 (92%)	2159 (93%)	169 (7%)	3 (0%)	48	78
1	E	2331/2523 (92%)	2160 (93%)	168 (7%)	3 (0%)	48	78
All	All	11655/12615 (92%)	10795 (93%)	845 (7%)	15 (0%)	49	78

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1949	ALA
1	C	1949	ALA
1	D	1949	ALA
1	A	2453	GLY
1	B	1949	ALA

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	2049/2222 (92%)	1883 (92%)	166 (8%)	11	36
1	B	2049/2222 (92%)	1883 (92%)	166 (8%)	11	36
1	C	2049/2222 (92%)	1882 (92%)	167 (8%)	10	36
1	D	2049/2222 (92%)	1883 (92%)	166 (8%)	11	36
1	E	2049/2222 (92%)	1883 (92%)	166 (8%)	11	36
All	All	10245/11110 (92%)	9414 (92%)	831 (8%)	13	36

5 of 831 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1965	LEU
1	D	1033	ILE
1	E	2001	LEU
1	C	2142	THR
1	C	1956	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 269 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	519	HIS
1	E	793	HIS
1	E	2102	GLN
1	B	2073	GLN
1	B	1741	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.

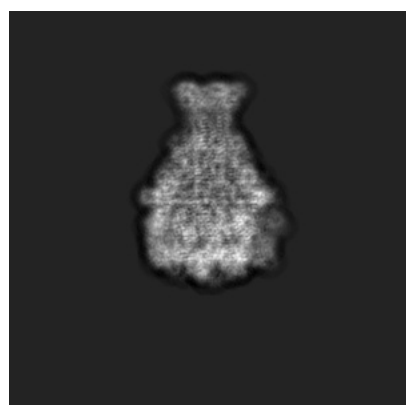
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10797. These allow visual inspection of the internal detail of the map and identification of artifacts.

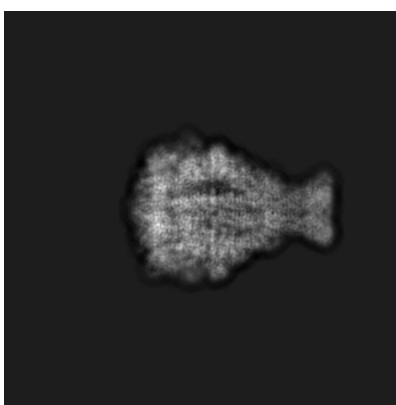
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

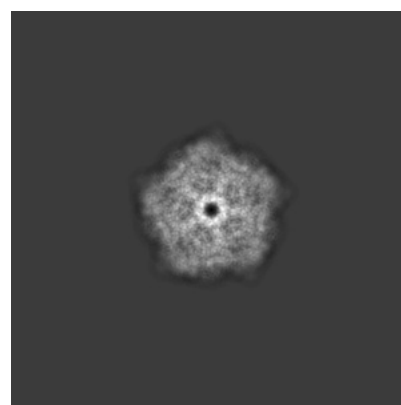
6.1.1 Primary map



X



Y

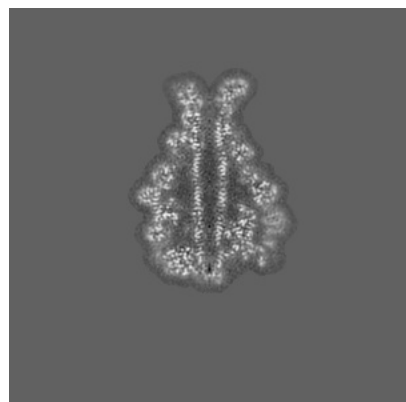


Z

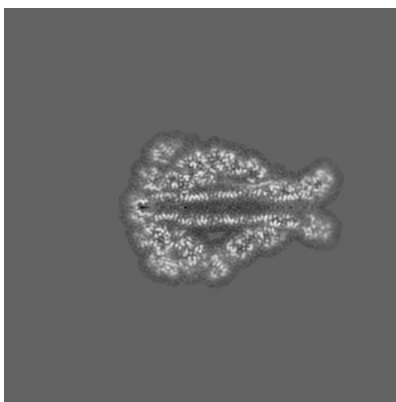
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

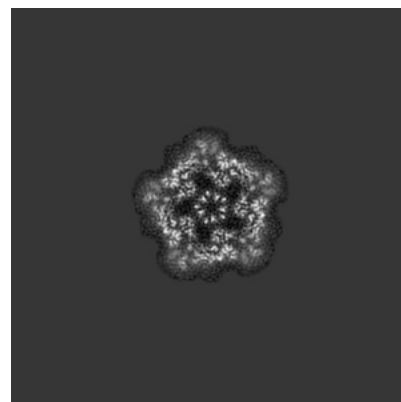
6.2.1 Primary map



X Index: 200



Y Index: 200

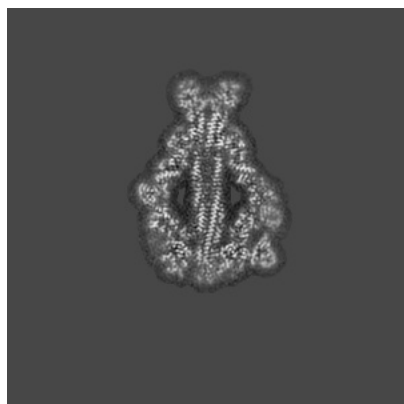


Z Index: 200

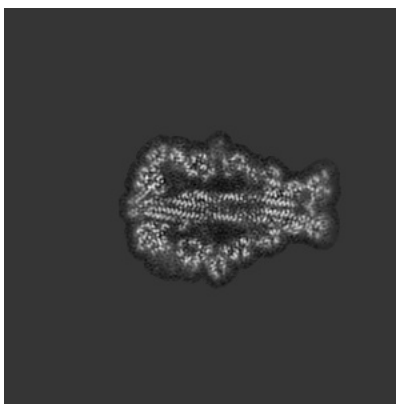
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

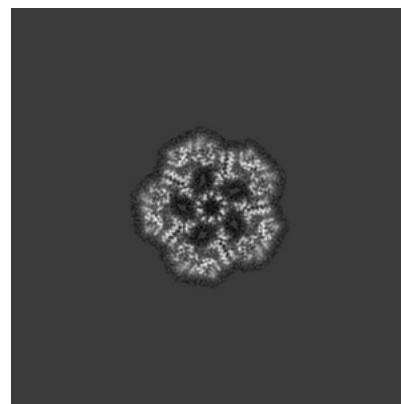
6.3.1 Primary map



X Index: 192



Y Index: 192

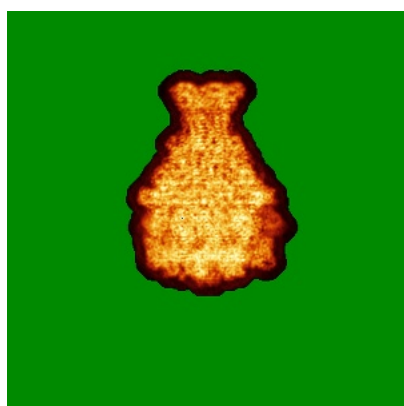


Z Index: 208

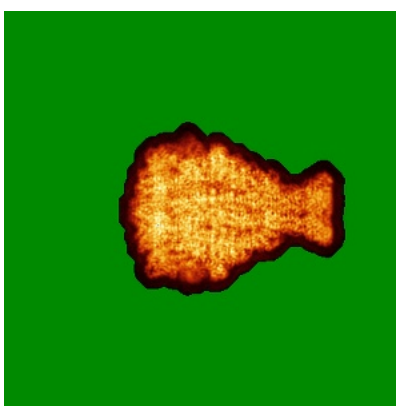
The images above show the largest variance slices of the map in three orthogonal directions.

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

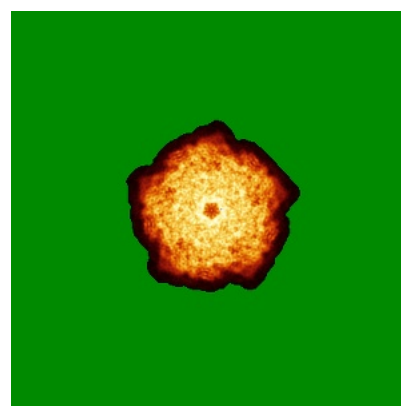
6.4.1 Primary map



X



Y

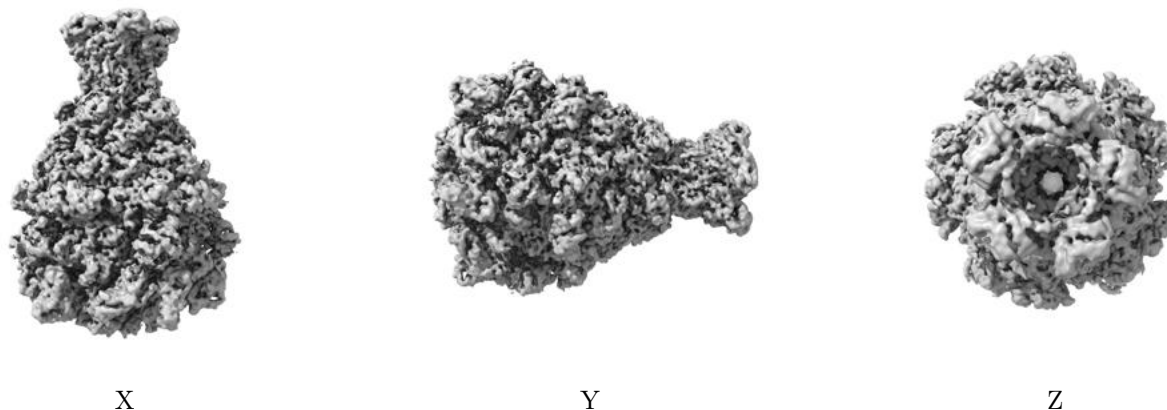


Z

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 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

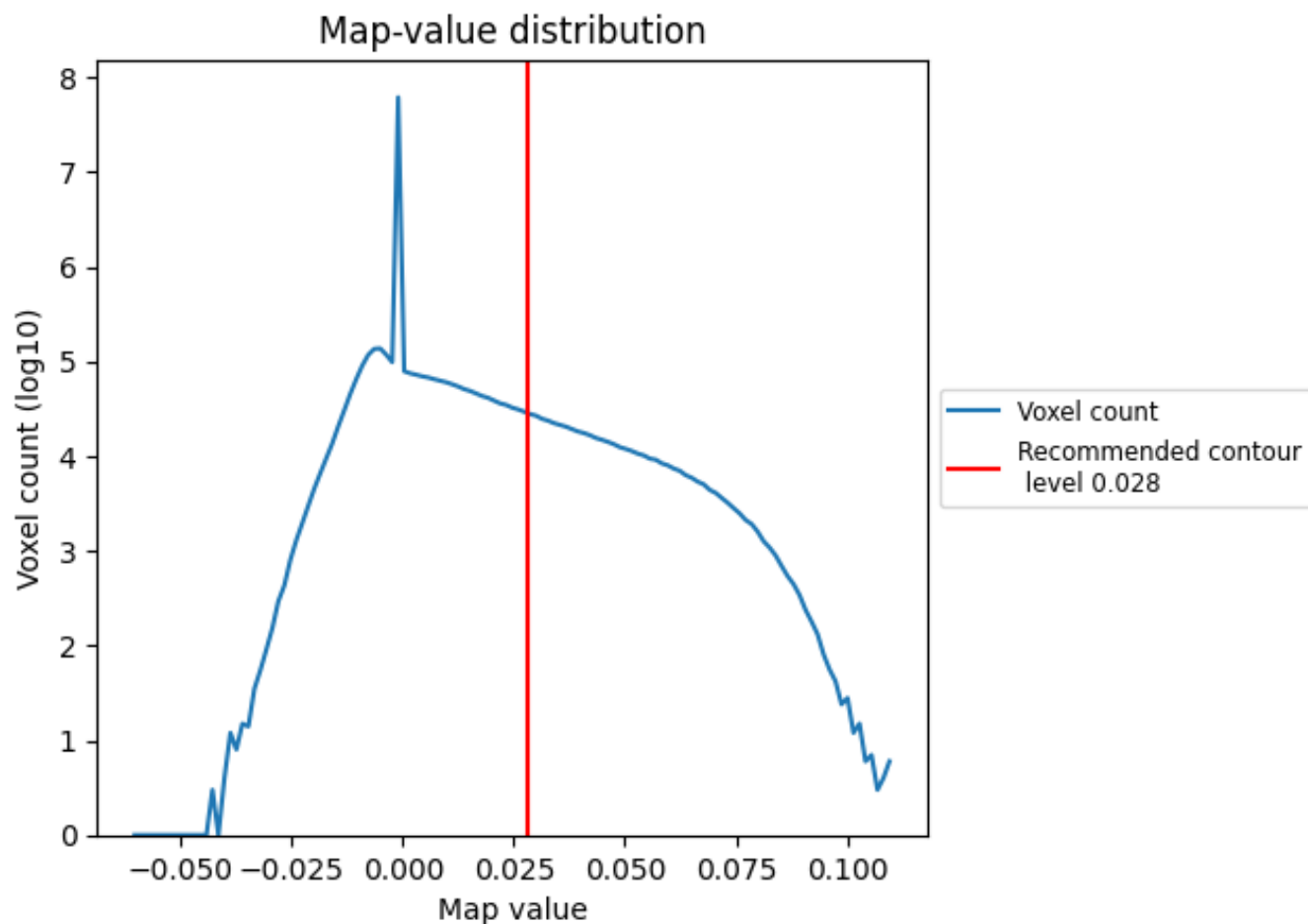
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

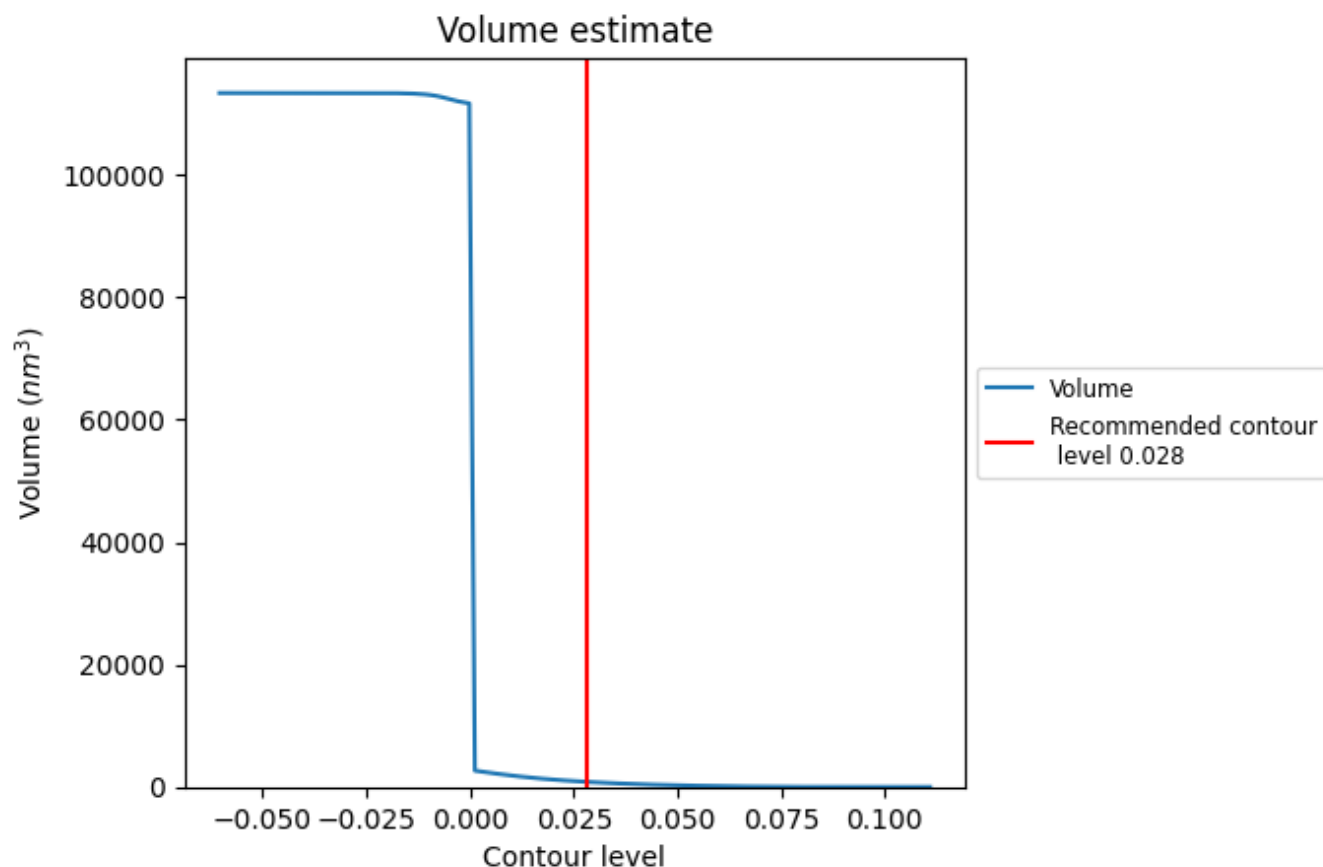
This section contains the results of statistical analysis of the map.

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.

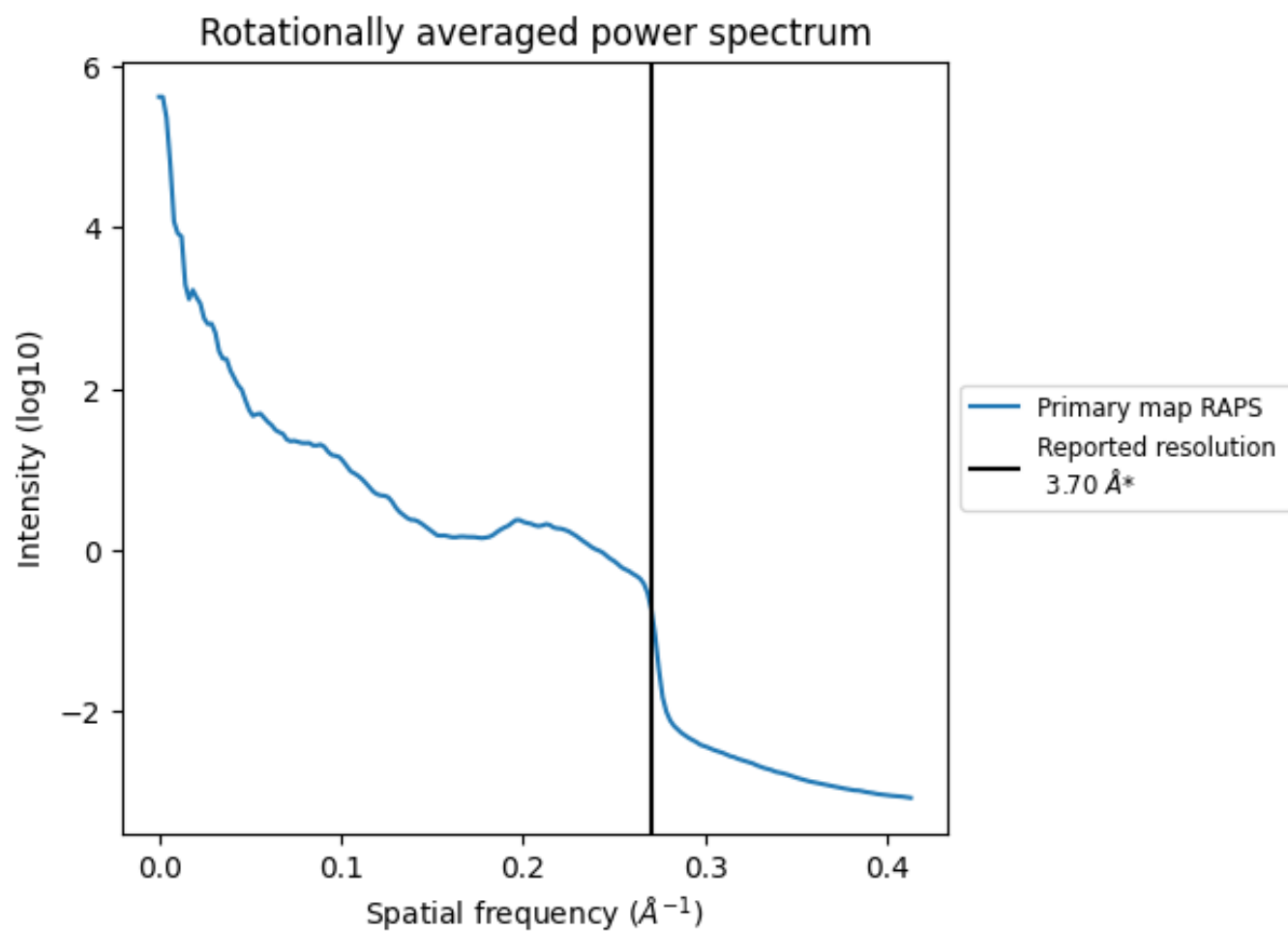
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm³; this corresponds to an approximate mass of 755 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 0.270 Å⁻¹

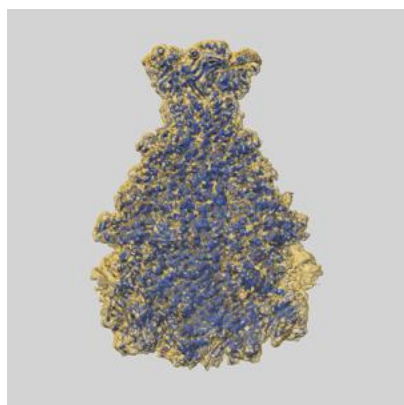
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

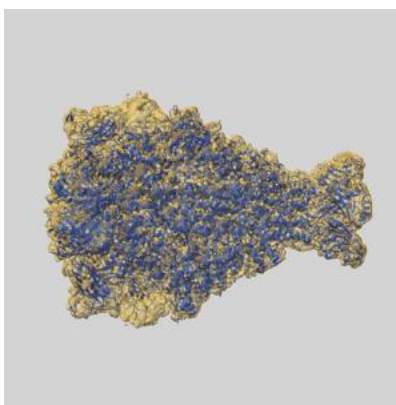
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10797 and PDB model 6YFY. Per-residue inclusion information can be found in section [3](#) on page [5](#).

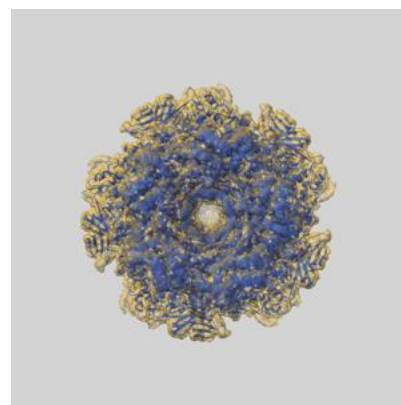
9.1 Map-model overlay [i](#)



X



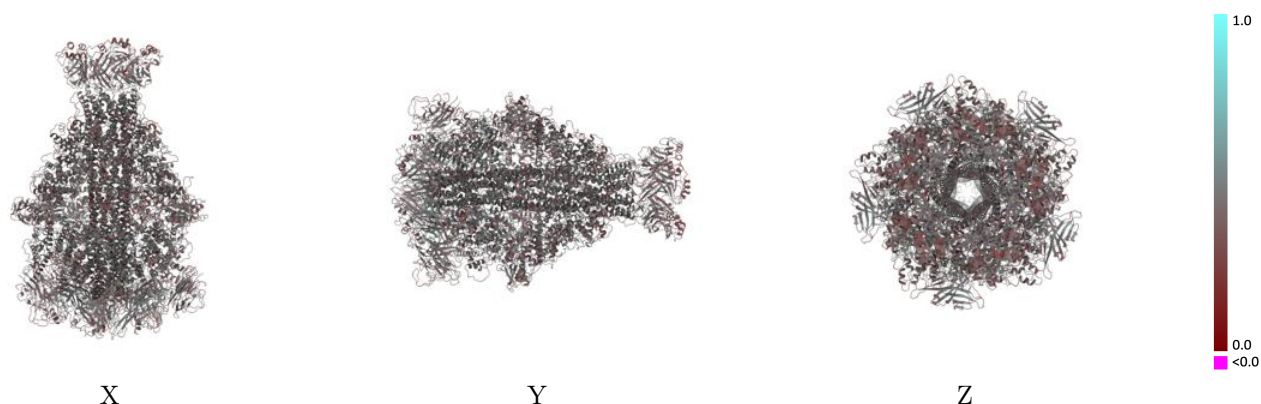
Y



Z

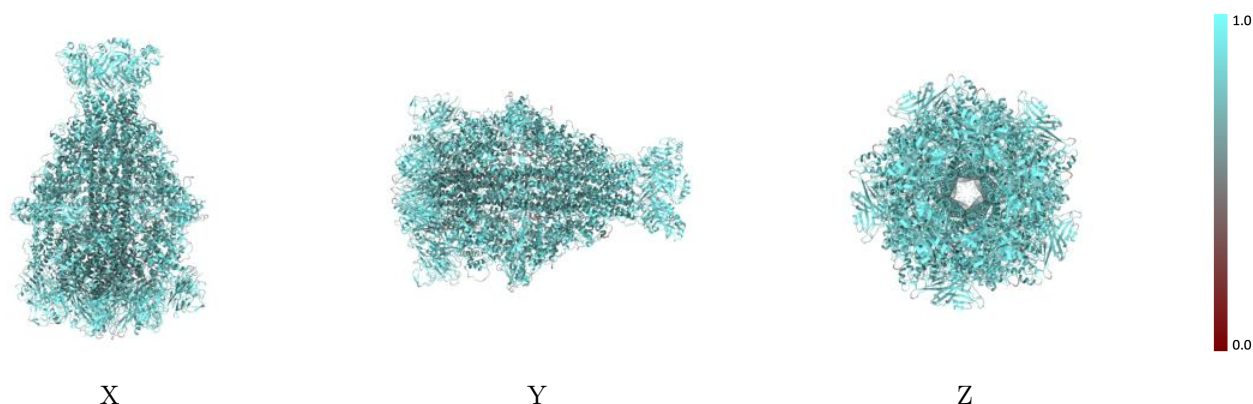
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



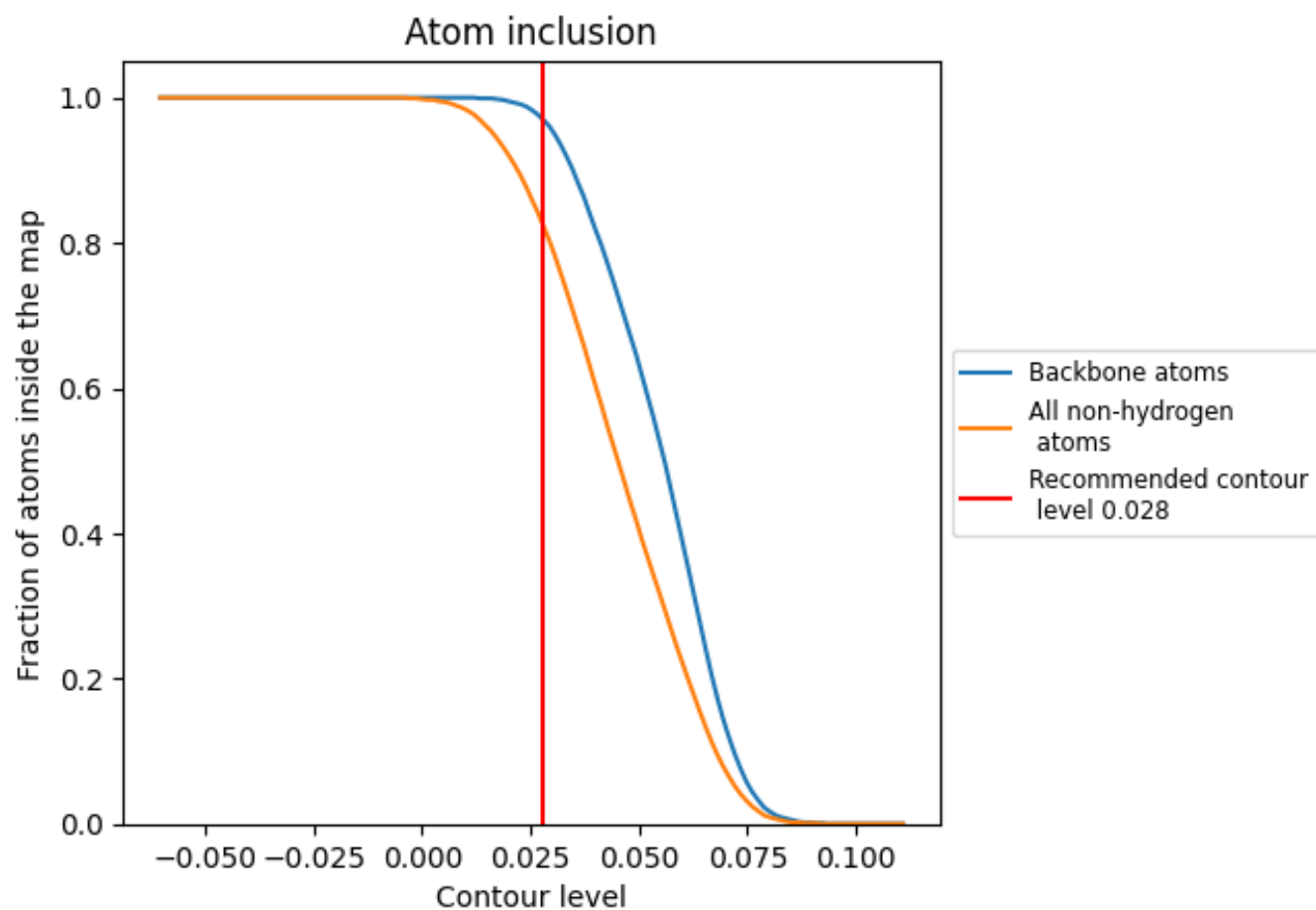
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 82% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8230	0.4340
A	0.8250	0.4360
B	0.8240	0.4360
C	0.8150	0.4230
D	0.8240	0.4370
E	0.8260	0.4360

