



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 05:57 am GMT

PDB ID : 8C8R
EMDB ID : EMD-16492
Title : In situ structure of the Nitrosopumilus maritimus S-layer - Composite map between C2 and C6
Authors : von Kuegelgen, A.; Bharat, T.
Deposited on : 2023-01-20
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
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) : 2.39

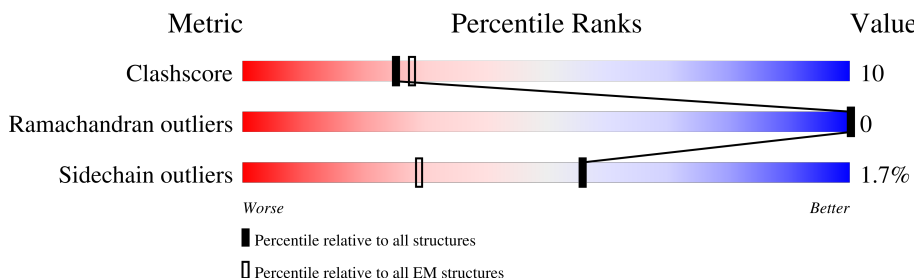
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	1734	<div> <div>7%</div> <div>66%</div> <div>18%</div> <div>•</div> <div>16%</div> </div>
1	B	1734	<div> <div>7%</div> <div>67%</div> <div>17%</div> <div></div> <div>16%</div> </div>
1	C	1734	<div> <div>7%</div> <div>66%</div> <div>18%</div> <div></div> <div>16%</div> </div>
1	D	1734	<div> <div>7%</div> <div>67%</div> <div>17%</div> <div></div> <div>16%</div> </div>
1	E	1734	<div> <div>7%</div> <div>67%</div> <div>17%</div> <div>•</div> <div>16%</div> </div>
1	F	1734	<div> <div>7%</div> <div>66%</div> <div>18%</div> <div>•</div> <div>16%</div> </div>

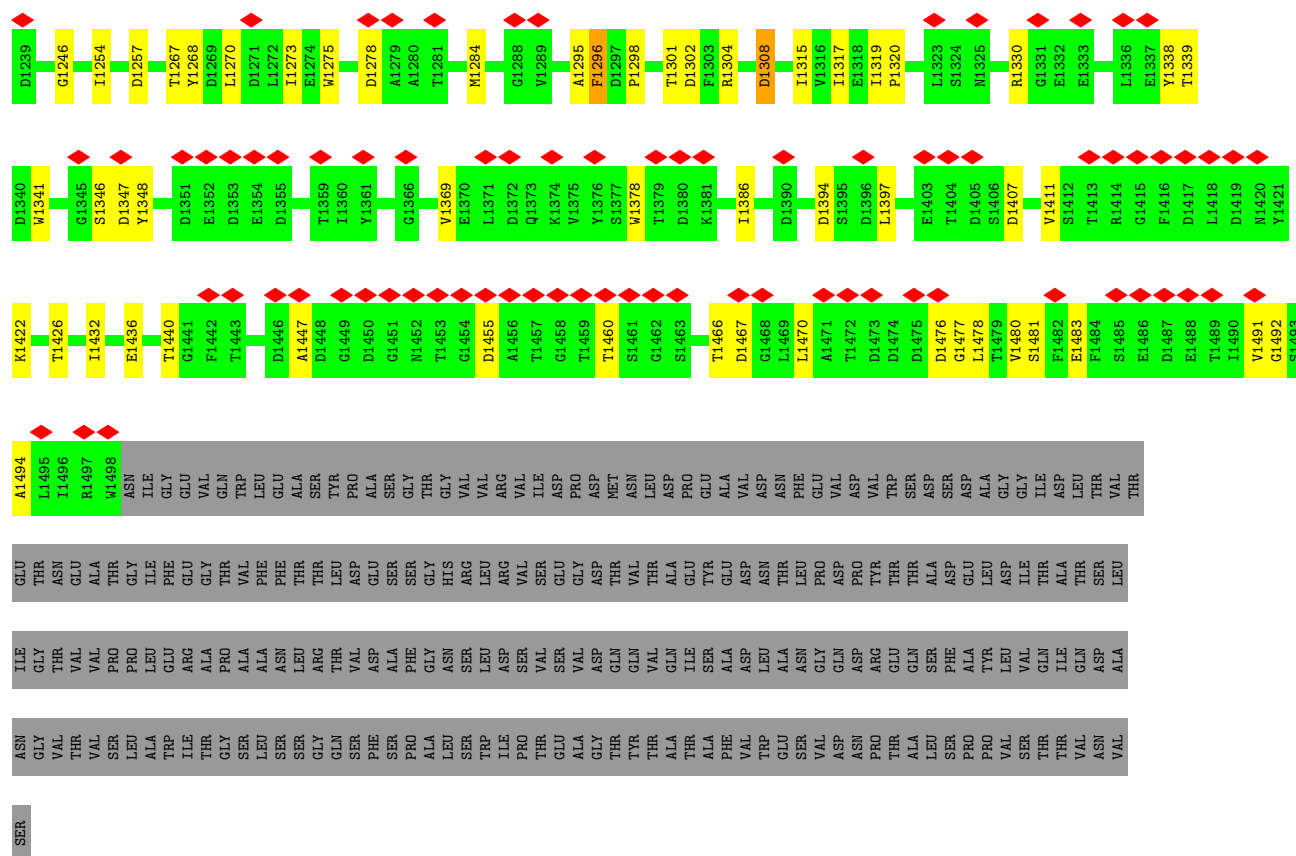
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 65154 atoms, of which 0 are hydrogens and 0 are deuteriums.

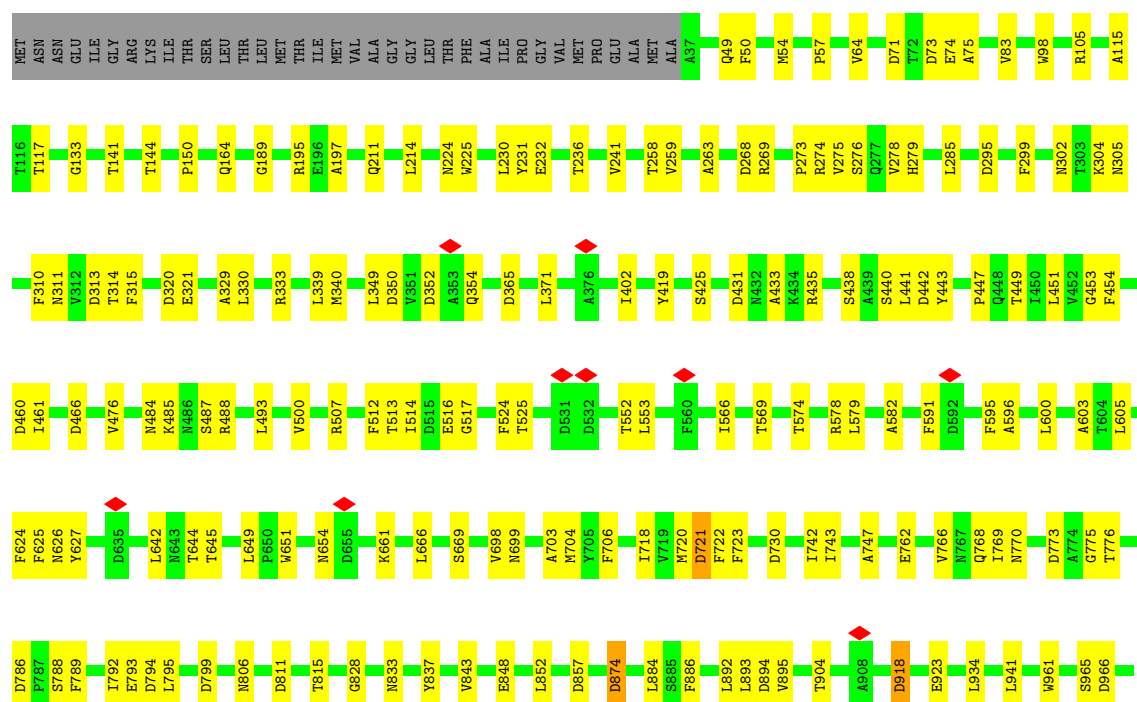
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

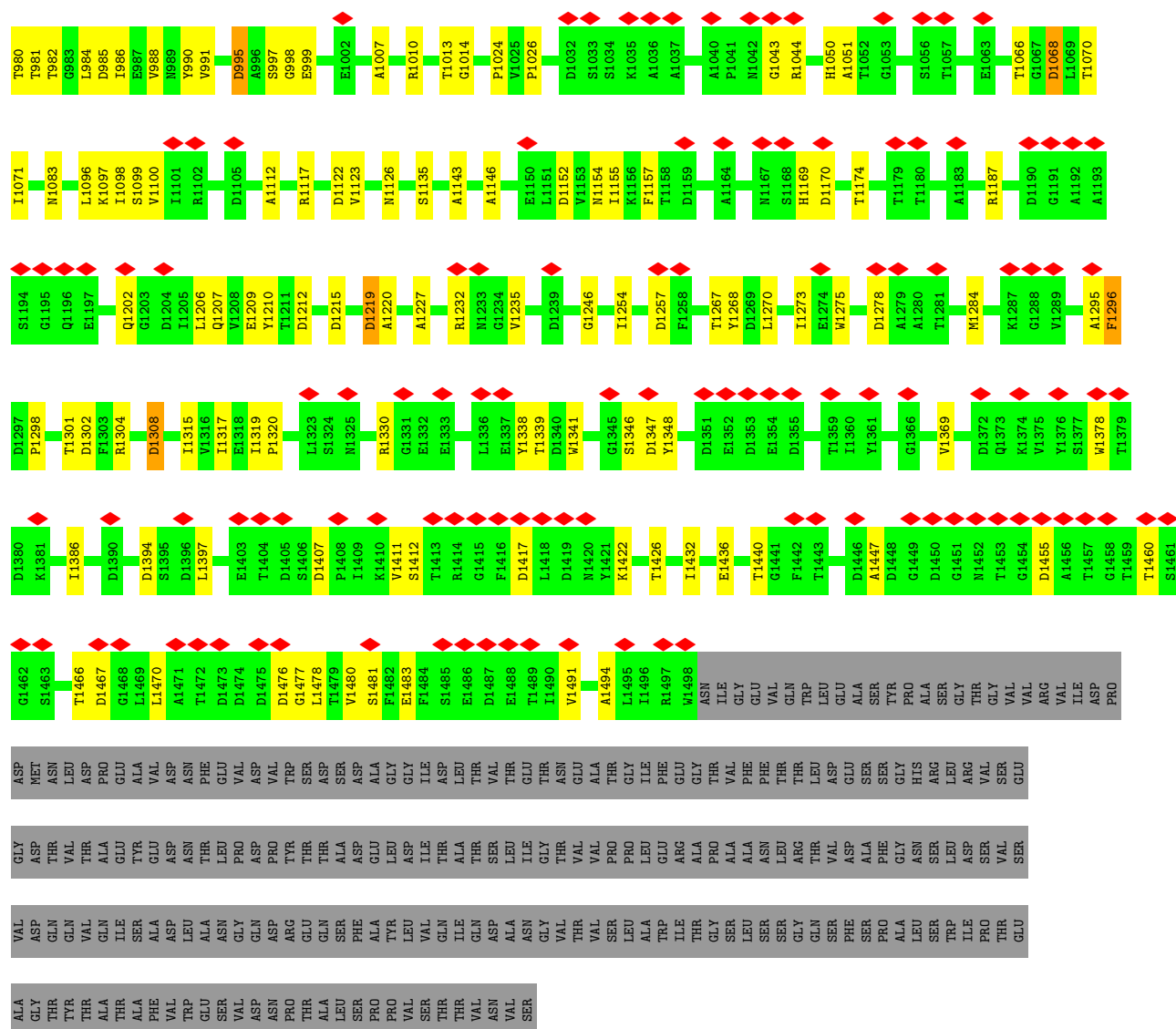
- Molecule 1 is a protein called Cell surface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	B	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	C	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	D	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	E	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		
1	F	1462	Total	C	N	O	S	0	0
			10859	6683	1751	2407	18		

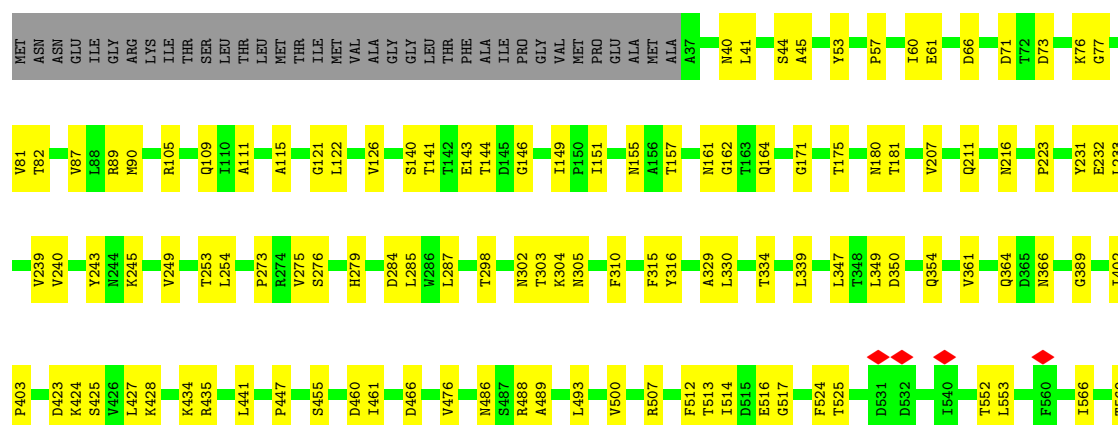


• Molecule 1: Cell surface protein





• Molecule 1: Cell surface protein

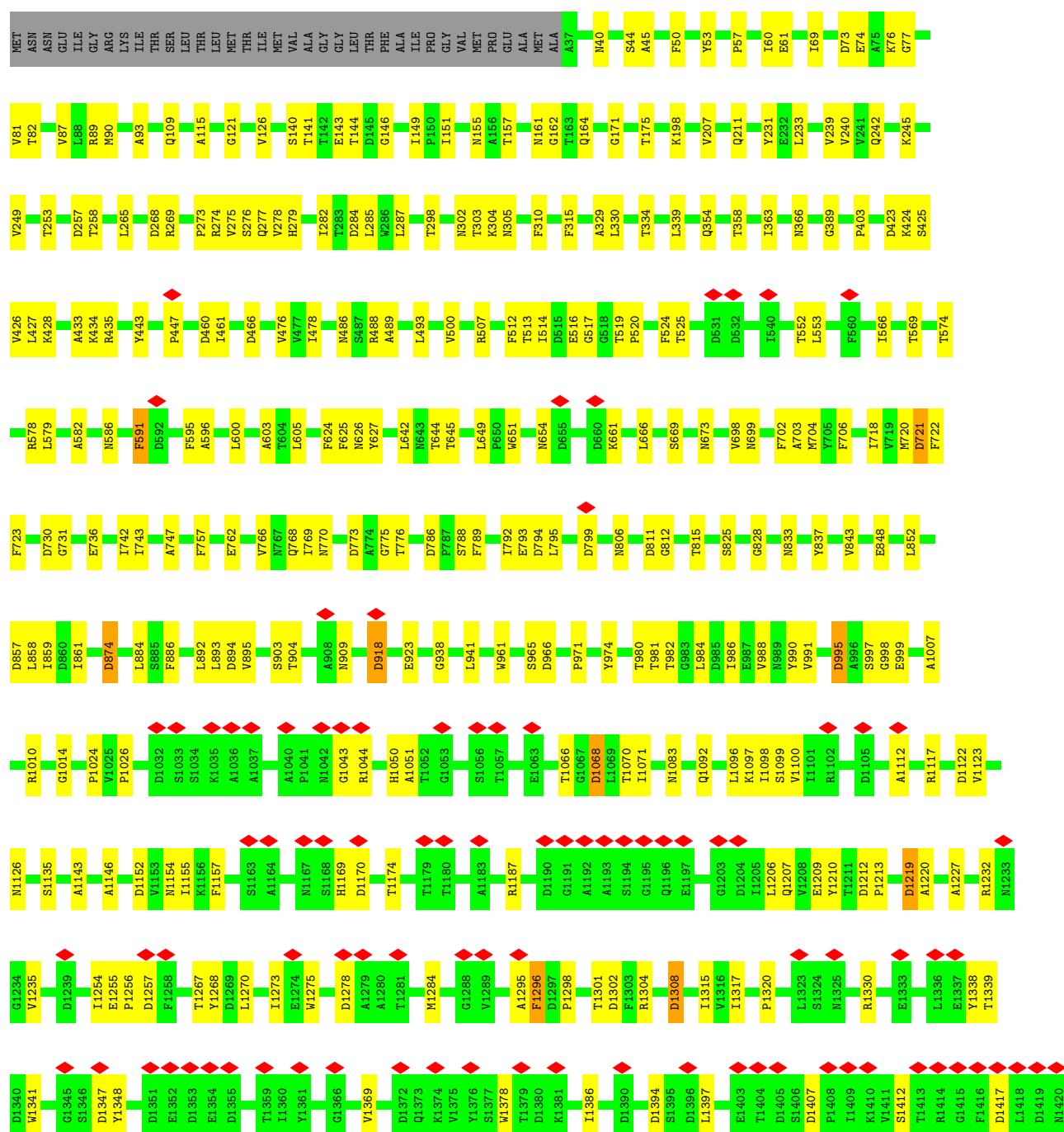






THR	THR	SER	D1448	D1355	L1270	S1169	H1050	D918	D773	L605	D466	L285	D106	MET
LEU	LEU	PRO	G1449	H1169	L1273	D1170	A1051	E923	A774	F624	V476	D295	A115	ASN
ASP	ASP	ALA	D1450	T1359	E1274	D1170	T1052	L934	G775	F625	V477	D296	T116	ASN
GLU	GLU	SER	H1360	I1360	W1275	T1174	G1063	L941	T776	N826	I478	F299	T117	ILE
SER	SER	GLY	H1451	Y1361										GLY
THR	THR	GLY	T1453	G1366	D1278	T1179	S1056	G953	D786	M484	M484	N302	S120	ARG
GLY	GLY	VAL	T1454		A1279	T1180	E1063	G961	F787	K485	K485	G121	G121	LYS
VAL	VAL	VAL	D1455	V1369	T1281	A1183	T1066	S965	S788	M486	M486	N311		ILE
ARG	ARG	VAL	A1456		M1284	R1187	G1067	D966	F789	M443	M443	V312	G133	THR
VAL	VAL	VAL	T1457				D1068			T644	T644	D313	T141	LEU
ASP	ASP	ASP	G1458		G1288	D1190	L1069	Y974	L792	T845	T845	T314	T141	THR
PRO	PRO	GLY	T1459	V1289	V1289	G1191	T1070		D794			F315		LEU
ASP	ASP	ASP	T1460			G1191	I1071		L795	L649	L649	A329	I149	LEU
MET	MET	MET	S1461			A1192	N1083	T980	D799	P650	P650	L330	P150	MET
ASN	ASN	ASN	G1462			A1193	Q1082	T981		M651	M651	R333	I151	ILE
LEU	LEU	ASP	S1463			S1194	Q1092	T982	N806	N654	N654	L339	Q164	VAL
VAL	VAL	ASP				T1379		T983	D811	D655	D655	M340	G189	ALA
THR	THR	GLU				S1194	L1096	L984	T815	V659	V659	L349	R195	GLY
ALA	ALA	GLU	T1301			Q1196	K1097	L985	T815	D660	D660	A197	E196	LEU
GLU	GLU	VAL	D1302			G1196	I1098	L986	S825	K661	K661		A197	THR
ASP	ASP	ASN	F1303			F1303	S1099	F987	S825			A353		PHE
ASN	ASN	ASN	R1304			R1304	V1100	V988	G828	L666	L666	Q354	A203	ALA
THR	THR	PHE	D1380			D1380	T1101	V989	N833					ILE
LEU	LEU	VAL	D1394			D1394	R1101	Y990	N833					PRO
VAL	VAL	ASP	S1395			I1206	R1102	V991	Y837	S669	S669	Q364	V209	GLY
VAL	VAL	VAL	D1396			I1316	D1105	D996	V843			D365	Q210	VAL
TRP	TRP	TRP	L1397			T1317	A1112	S997	V944				Q211	VAL
SER	SER	SER	D1475			I1318	R1117	G998	R845			L371	L214	MET
ASP	ASP	ALA	D1476			T1319	T1117	E999	I845			A376	N224	PRO
ASP	ASP	ASP	T1404			P1320	D1212					I402	W225	ALA
GLY	GLY	ALA	D1405			L1323	D1213	E1002	E848			S425	L230	ALA
LEU	LEU	GLY	S1406			G1324	D1213	A1007	L852			K428	Y231	GLU
ASP	ASP	ILE	D1407			N1325	D1219	R1010	D857			R435	E232	ILE
THR	THR	ASP	P1408			A1227	N1126	G1014	D874			S438	V241	THR
ALA	ALA	LEU	T1409				S1135	P1024	L884			A439	K245	THR
THR	THR	VAL	K1410			R1232	A1143	V1025	S885			S440	K245	THR
VAL	VAL	THR	E1485			N1233	A1146	P1026	F886			L441	T258	ILE
LEU	LEU	THR	S1412			G1234						D442	V259	GLY
GLY	GLY	THR	T1413			V1235						P447	D268	THR
THR	THR	ASN	R1414				E1150	D1032	L892			Q448	R269	THR
ASN	ASN	GLU	R1415			S1238	L1151	S1033	L893			T449	R269	THR
VAL	VAL	ALA	F1416			D1239	D1152	S1034	D894			I450	R274	VAL
THR	THR	THR	D1417			Y1243	V1153	K1035	V895			L451	P273	GLY
PRO	PRO	GLY	L1418			G1246	N1154	A1036	D898			V452	R274	GLY
LEU	LEU	ILE	D1419			I1254	K1155	A1037	F757			G453	V275	GLY
GLU	GLU	PHE	D1419			E1255	K1156					F454	S276	THR
ARG	ARG	GLU	N1420			P1256	F1157						Q277	ALA
ALA	ALA	GLY	I1421			D1257	T1158						V278	ALA
PRO	PRO	THR	K1422			F1257	D1159						H279	ASN
VAL	VAL	VAL	Y1346			D1257	A1164							ILE
ALA	ALA	PHE	D1351			F1258	N1167							ALA
ASN	ASN	GLY	E1352			T1267								GLY
		GLY	F1442			Y1266								GLY
		GLU	T1443			D1269								GLU
		VAL												VAL
		GLN												GLN
		TRP												TRP
		LEU												LEU
		GLU												GLU
		ALA												ALA

- Molecule 1: Cell surface protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, Not provided	
Number of subtomograms used	108621	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; PseudoSubtomograms as described in Zivanov 2022 (https://elifesciences.org/articles/83724)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	121	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.055	Depositor
Minimum map value	-6.789	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.582	Depositor
Recommended contour level	1.45621	Depositor
Map size (\AA)	265.4, 265.4, 265.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.327, 1.327, 1.327	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	0.25	0/11032	0.49	0/15089
1	B	0.25	0/11032	0.49	0/15089
1	C	0.25	0/11032	0.49	0/15089
1	D	0.25	0/11032	0.49	0/15089
1	E	0.25	0/11032	0.49	0/15089
1	F	0.25	0/11032	0.49	0/15089
All	All	0.25	0/66192	0.49	0/90534

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 [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	10859	0	10131	260	0
1	B	10859	0	10136	203	0
1	C	10859	0	10136	234	0
1	D	10859	0	10130	247	0
1	E	10859	0	10135	217	0
1	F	10859	0	10136	236	0
All	All	65154	0	60804	1279	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 10.

The worst 5 of 1279 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:A:269:ARG:HH12	1:A:485:LYS:C	0.98	1.48
1:C:435:ARG:NH1	1:C:812:GLY:HA3	1.24	1.44
1:A:269:ARG:HH12	1:A:486:ASN:N	1.17	1.38
1:A:269:ARG:NH1	1:A:485:LYS:C	1.76	1.37
1:B:354:GLN:NE2	1:C:861:ILE:HD11	1.37	1.36

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	1460/1734 (84%)	1418 (97%)	42 (3%)	0	100	100
1	B	1460/1734 (84%)	1415 (97%)	45 (3%)	0	100	100
1	C	1460/1734 (84%)	1414 (97%)	46 (3%)	0	100	100
1	D	1460/1734 (84%)	1421 (97%)	39 (3%)	0	100	100
1	E	1460/1734 (84%)	1414 (97%)	46 (3%)	0	100	100
1	F	1460/1734 (84%)	1412 (97%)	48 (3%)	0	100	100
All	All	8760/10404 (84%)	8494 (97%)	266 (3%)	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	A	1212/1438 (84%)	1191 (98%)	21 (2%)	56	75
1	B	1212/1438 (84%)	1191 (98%)	21 (2%)	56	75
1	C	1212/1438 (84%)	1190 (98%)	22 (2%)	54	74
1	D	1212/1438 (84%)	1191 (98%)	21 (2%)	56	75
1	E	1212/1438 (84%)	1191 (98%)	21 (2%)	56	75
1	F	1212/1438 (84%)	1191 (98%)	21 (2%)	56	75
All	All	7272/8628 (84%)	7145 (98%)	127 (2%)	56	75

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1278	ASP
1	F	721	ASP
1	D	918	ASP
1	F	661	LYS
1	F	1219	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	242	GLN
1	F	1050	HIS
1	F	806	ASN
1	C	1050	HIS
1	E	1050	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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.

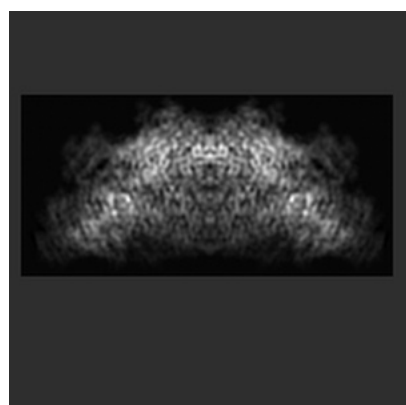
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16492. These allow visual inspection of the internal detail of the map and identification of artifacts.

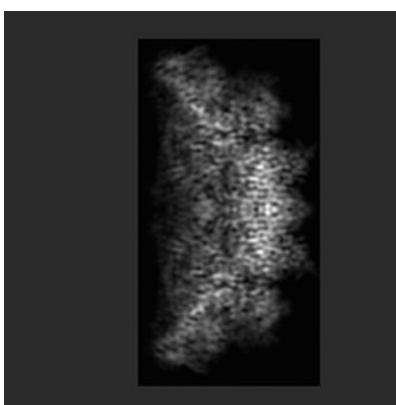
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

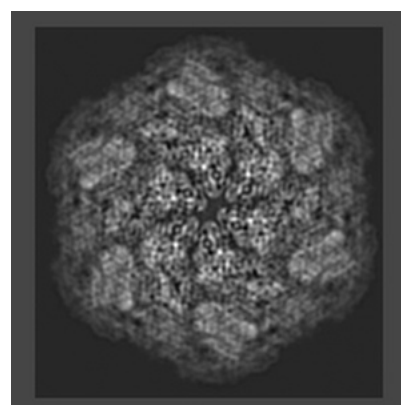
6.1.1 Primary map



X



Y



Z

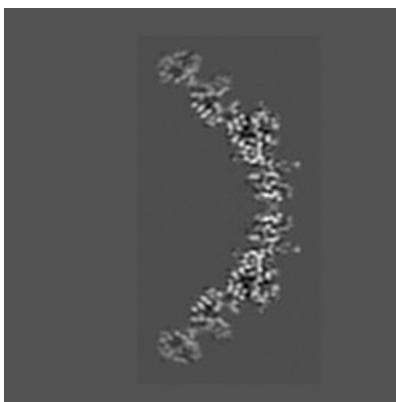
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

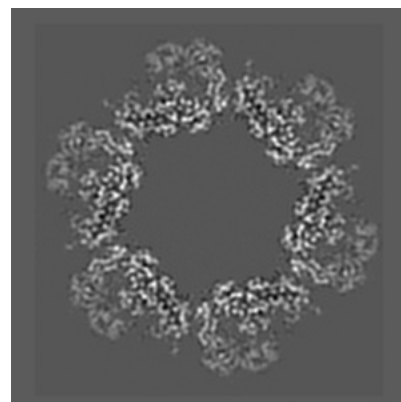
6.2.1 Primary map



X Index: 100



Y Index: 100

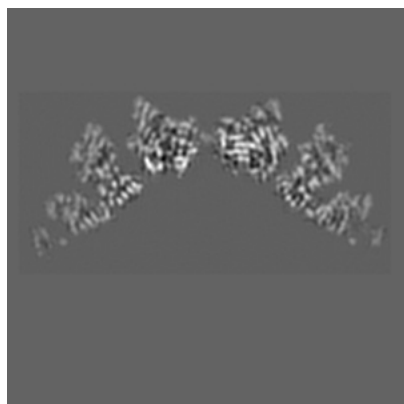


Z Index: 100

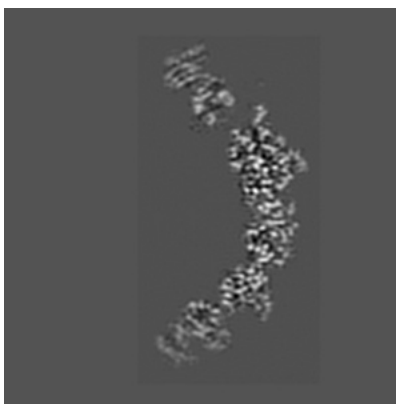
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

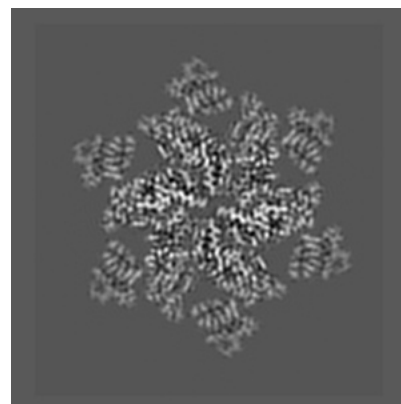
6.3.1 Primary map



X Index: 99



Y Index: 92

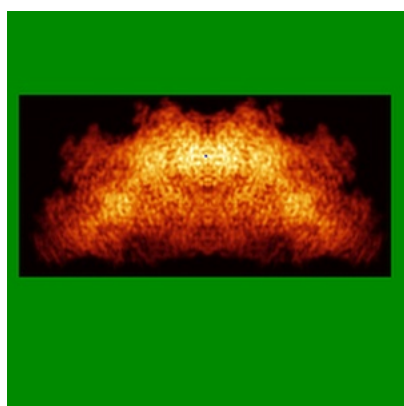


Z Index: 127

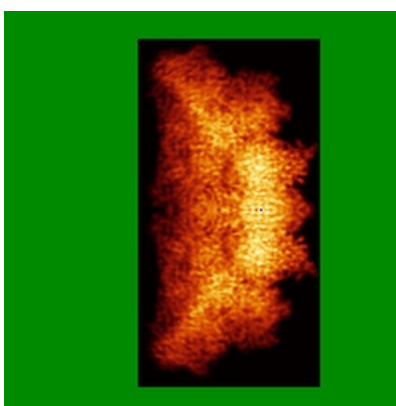
The images above show the largest variance slices of the map in three orthogonal directions.

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

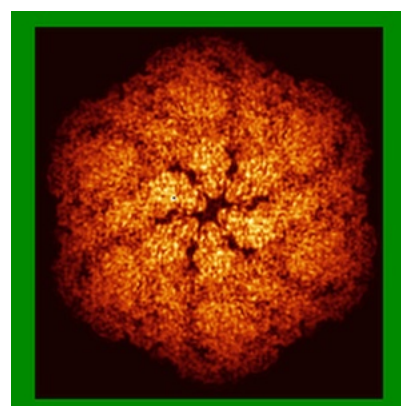
6.4.1 Primary map



X



Y

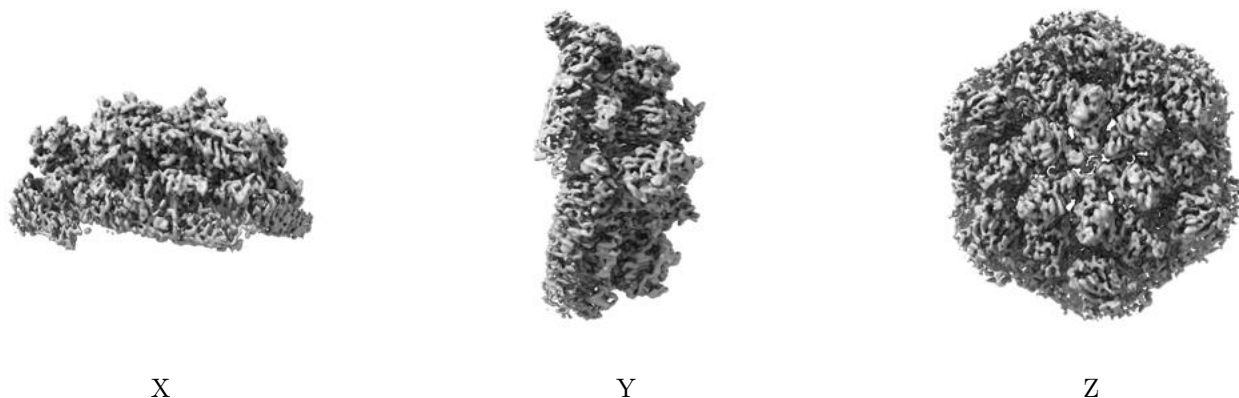


Z

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 1.45621. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

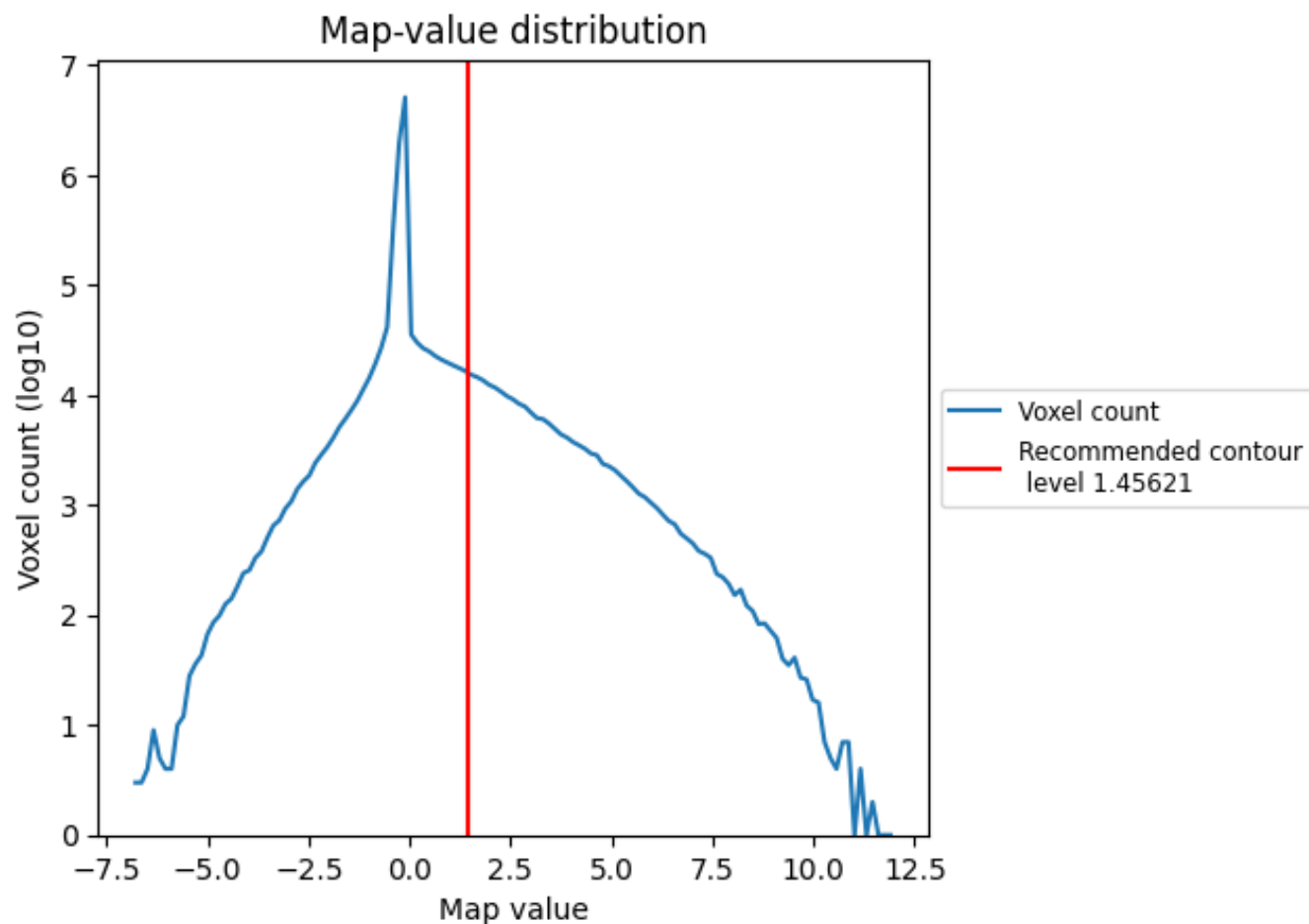
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

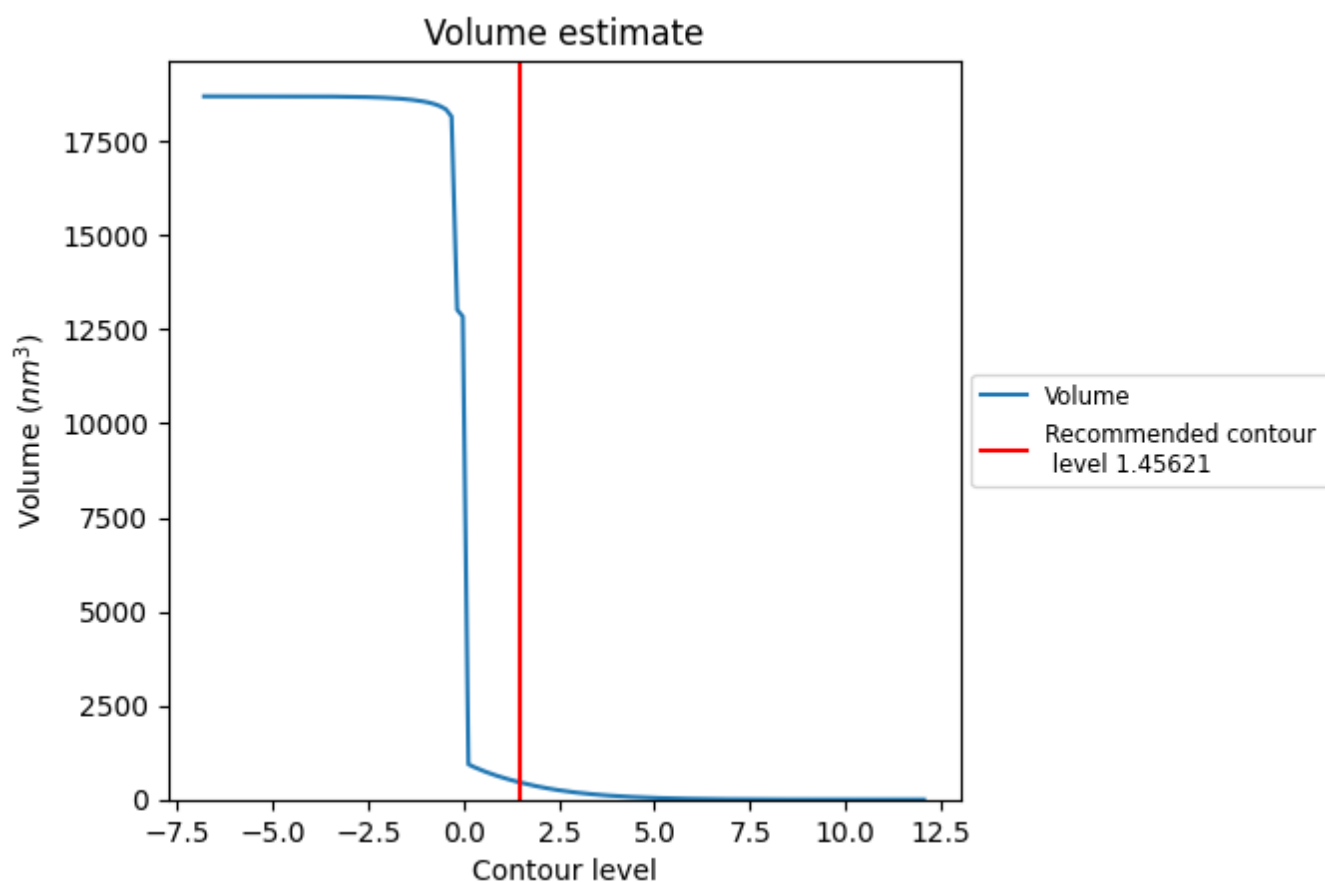
This section contains the results of statistical analysis of the map.

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.

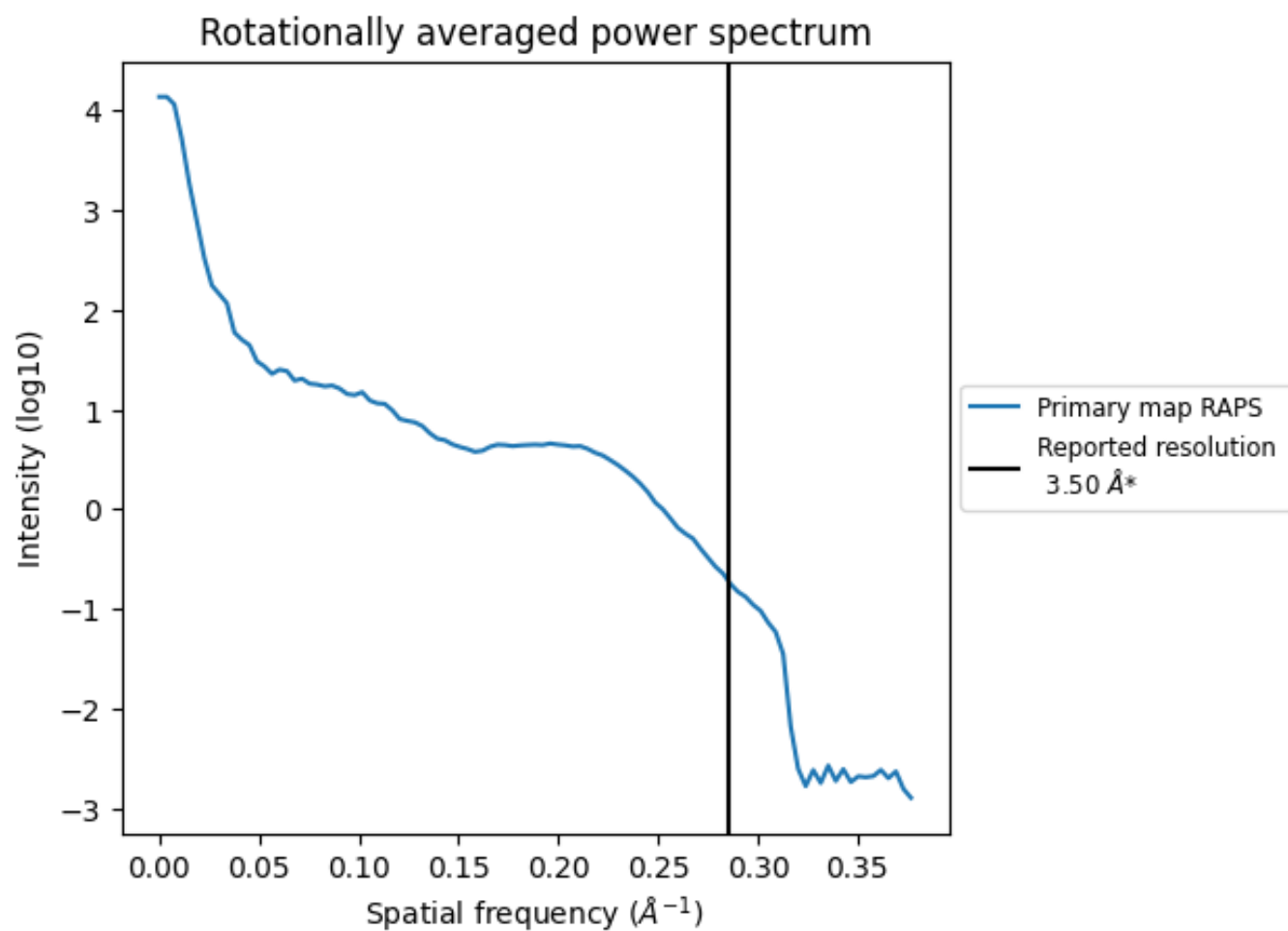
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 462 nm³; this corresponds to an approximate mass of 417 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 0.286 Å⁻¹

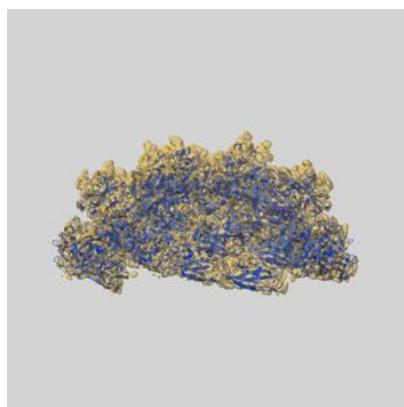
8 Fourier-Shell correlation ⓘ

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

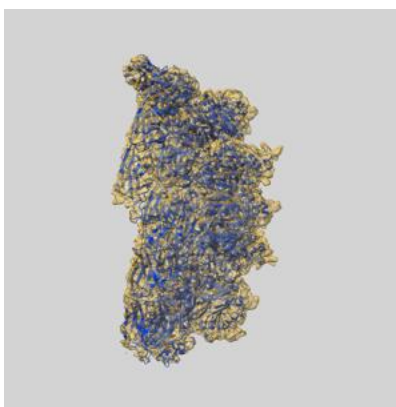
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16492 and PDB model 8C8R. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

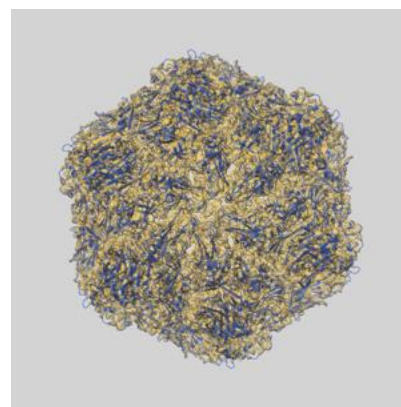
9.1 Map-model overlay [i](#)



X



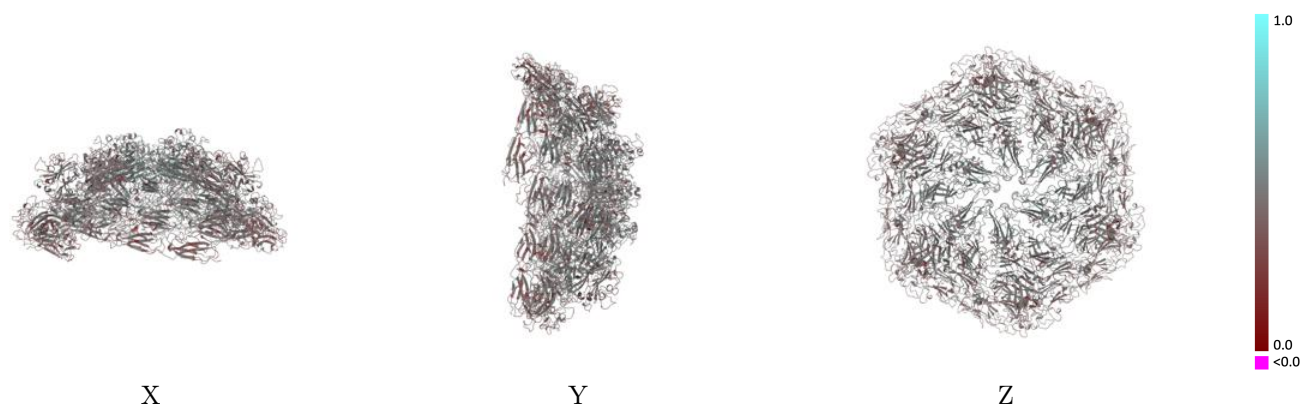
Y



Z

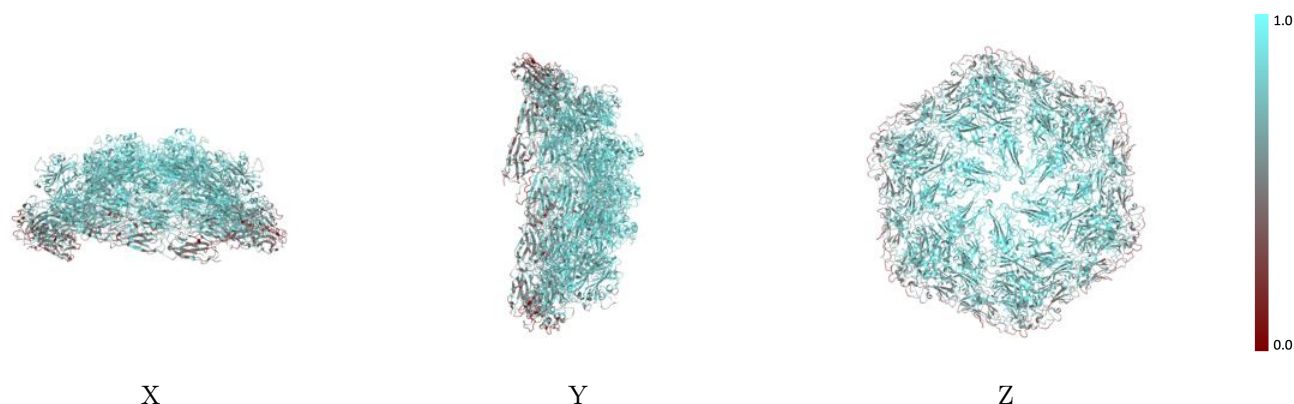
The images above show the 3D surface view of the map at the recommended contour level 1.45621 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



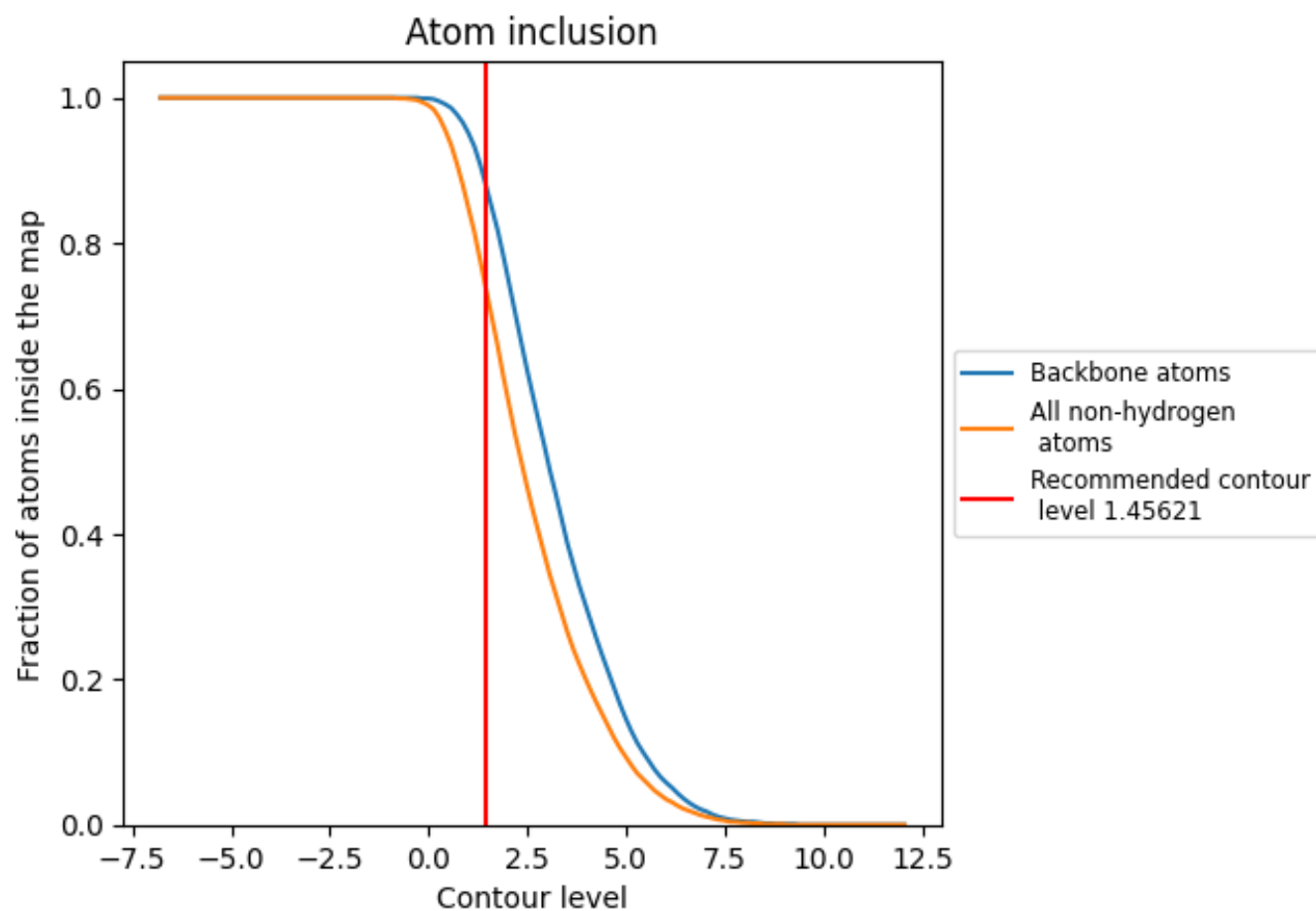
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.45621).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 74% 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 (1.45621) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7360	<div></div> 0.4380
A	<div></div> 0.7430	<div></div> 0.4440
B	<div></div> 0.7370	<div></div> 0.4350
C	<div></div> 0.7300	<div></div> 0.4350
D	<div></div> 0.7430	<div></div> 0.4440
E	<div></div> 0.7340	<div></div> 0.4360
F	<div></div> 0.7290	<div></div> 0.4350

