



## wwPDB EM Validation Summary Report ⓘ

Apr 3, 2024 – 01:54 pm BST

PDB ID : 8C8M  
EMDB ID : EMD-16484  
Title : In vitro structure of the Nitrosopumilus maritimus S-layer - Composite map between two and six-fold symmetrised  
Authors : von Kuegelgen, A.; Bharat, T.  
Deposited on : 2023-01-20  
Resolution : 2.87 Å(reported)

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The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

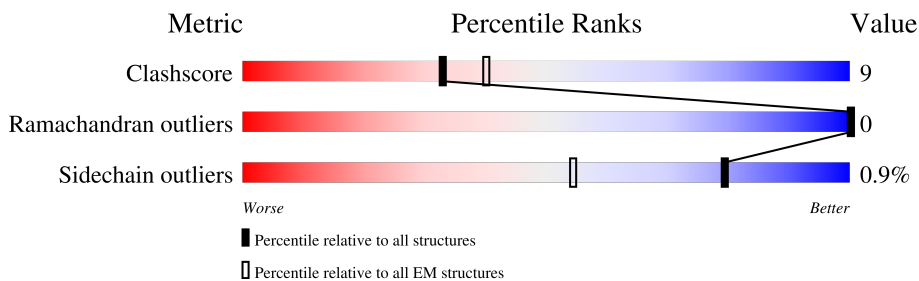
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1734	
1	B	1734	
1	C	1734	
1	D	1734	
1	E	1734	
1	F	1734	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 70506 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.

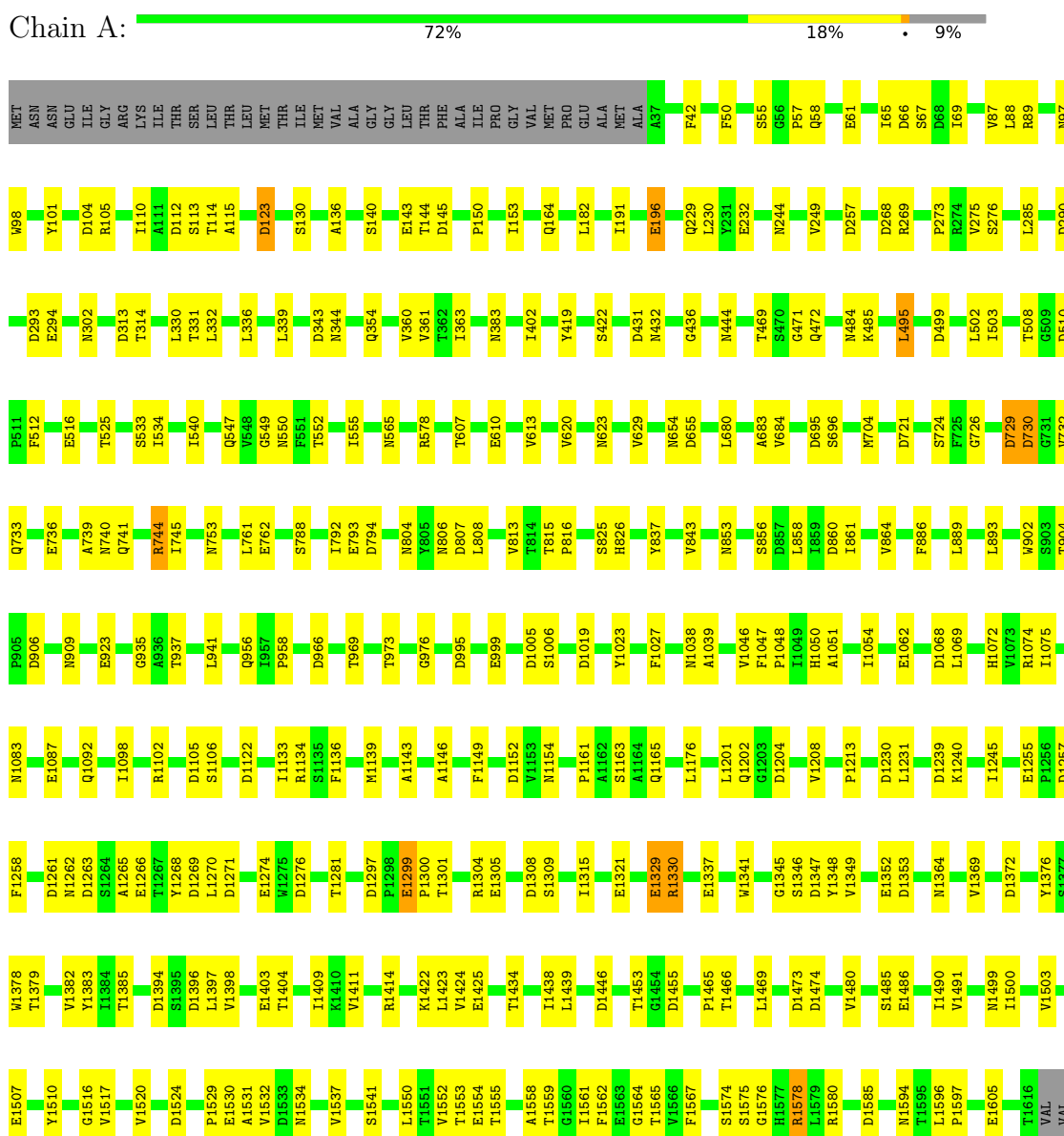
- Molecule 1 is a protein called Cell surface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1580	Total 11751	C 7234	N 1888	O 2610	S 19	0	0
1	B	1580	Total 11751	C 7234	N 1888	O 2610	S 19	0	0
1	C	1580	Total 11751	C 7234	N 1888	O 2610	S 19	0	0
1	D	1580	Total 11751	C 7234	N 1888	O 2610	S 19	0	0
1	E	1580	Total 11751	C 7234	N 1888	O 2610	S 19	0	0
1	F	1580	Total 11751	C 7234	N 1888	O 2610	S 19	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: Cell surface protein









E1098	I1098	E1266	I1267	D1390	S1641	LEU
D1268	R1102	Y1268	L1560	F1393	L1561	ASP
D1269	D1270	D1269	T1561	F1393	V1552	SER
D1271	D1105	D1270	T1553	E1403	T1553	GLU
S1106	S1106	D1271	E1554	T1404	E1554	VAL
D1122	D1122	E1274	T1555	T1404	T1555	ASP
I1133	I1133	W1275	I1409	I1409	I1409	GLN
R1134	R1134	D1276	K1410	K1410	A1558	THR
S1136	S1136	T1281	V1411	V1411	T1559	VAL
F1136	F1136	D1297	R1414	R1414	G1560	ALA
P1298	P1298	P1298	K1422	K1422	F1561	ILE
M1139	M1139	E1299	L1423	L1423	E1562	SER
P1300	P1300	P1300	T1434	T1434	E1563	ASP
T1301	T1301	T1301	T1434	T1434	T1565	LEU
R1304	R1304	R1304	I1438	I1438	V1566	ALA
E1305	E1305	E1305	L1439	L1439	F1567	GLY
D1308	D1308	D1308	S1574	S1574	S1574	GLN
S1309	S1309	S1309	S1576	S1576	G1576	ASP
I1315	I1315	I1315	H1577	H1577	G1576	ARG
P1161	P1161	P1161	L1579	L1579	H1578	GLU
A1162	A1162	A1162	R1580	R1580	H1578	THR
E1329	E1329	E1329	D1585	D1585	L1579	PHE
R1330	R1330	R1330	L1469	L1469	R1580	ALA
Q1165	Q1165	Q1165	S1594	S1594	D1585	PRO
L1176	L1176	L1176	T1595	T1595	M1594	VAL
E1337	E1337	E1337	L1596	L1596	T1595	GLN
D1340	D1340	D1340	P1597	P1597	L1596	ILE
W1341	W1341	W1341	E1605	E1605	L1596	THR
Q1202	Q1202	Q1202	T1616	T1616	P1597	VAL
G1203	G1203	G1203	VAL	VAL	E1605	ALA
D1204	D1204	D1204	THR	THR	T1616	GLY
V1208	V1208	V1208	VAL	VAL	VAL	VAL
P1213	P1213	P1213	VAL	VAL	VAL	THR
D1230	D1230	D1230	VAL	VAL	VAL	THR
L1231	L1231	L1231	VAL	VAL	VAL	THR
D1239	D1239	D1239	VAL	VAL	VAL	THR
K1240	K1240	K1240	VAL	VAL	VAL	THR
I1245	I1245	I1245	VAL	VAL	VAL	THR
D1257	D1257	D1257	VAL	VAL	VAL	THR
F1258	F1258	F1258	VAL	VAL	VAL	THR
T1379	T1379	T1379	VAL	VAL	VAL	THR
D1261	D1261	D1261	VAL	VAL	VAL	THR
N1262	N1262	N1262	VAL	VAL	VAL	THR
S1264	S1264	S1264	VAL	VAL	VAL	THR
A1265	A1265	A1265	VAL	VAL	VAL	THR
I1266	I1266	I1266	VAL	VAL	VAL	THR
T1385	T1385	T1385	VAL	VAL	VAL	THR

● Molecule 1: Cell surface protein



D104	R105	MET	ASN	N302	I534	N740	G935	E1087	L1231
I110	A111	ASN	GLU	F310	I540	R744	A936	Q1092	D1239
D112	S113	GLY	ILE	D313	Q547	I745	T937	I1098	K1240
T114	A115	VAL	ARG	T314	V548	E749	L941	R1102	I1245
THR	THR	LYS	THR	N322	G543	T750	D954	G1103	D1257
ALA	ALA	THR	THR	L330	N850	D751	G956	S1104	F1258
THR	THR	THR	THR	T331	F951	N753	P957	D1105	D1261
THR	THR	THR	THR	L332	T552	L761	D966	S1106	M1262
THR	THR	THR	THR	R333	I555	E762	T969	D1122	M1263
THR	THR	THR	THR	T334	N655	S788	T973	D1264	A1265
THR	THR	THR	THR	L336	R578	I792	T973	A1266	E1266
THR	THR	THR	THR	D343	L579	N804	G976	T1267	Y1268
THR	THR	THR	THR	N344	I580	T805	G983	F1136	D1269
THR	THR	THR	THR	I363	T607	N806	L984	M1139	L1270
THR	THR	THR	THR	S401	E610	D807	D985	A1143	D1271
THR	THR	THR	THR	I402	V613	L808	D985	A1146	E1274
THR	THR	THR	THR	P411	V620	T814	E999	D1152	W1275
THR	THR	THR	THR	Y419	N623	P815	D1005	V1153	T1276
THR	THR	THR	THR	E421	V629	P816	S1006	N1154	T1281
THR	THR	THR	THR	S422	N654	S825	D1019	P1161	D1297
THR	THR	THR	THR	D431	D655	H826	D1019	A1162	P1298
THR	THR	THR	THR	N432	L680	Y837	Y1023	S1163	E1299
THR	THR	THR	THR	R435	A683	V813	F1027	A1164	P1300
THR	THR	THR	THR	G436	V684	T814	N1038	Q1165	T1301
THR	THR	THR	THR	N444	D695	P816	A1039	L1176	D1308
THR	THR	THR	THR	T469	S696	N853	L858	L1201	S1309
THR	THR	THR	THR	Q472	M704	S825	I859	Q1202	I1315
THR	THR	THR	THR	M484	V717	H826	D960	G1203	E1321
THR	THR	THR	THR	R488	D721	N853	D960	D1204	S1322
THR	THR	THR	THR	L495	S724	L833	F725	I1205	K1327
THR	THR	THR	THR	L502	G726	L833	G726	L1206	R1330
THR	THR	THR	THR	I503	D730	L833	I1054	Q1207	E1337
THR	THR	THR	THR	F512	G731	L833	E1062	V1208	D1340
THR	THR	THR	THR	E516	V732	L833	E1062	P1213	W1341
THR	THR	THR	THR	T525	Q733	L833	E1062	S1217	D1340
THR	THR	THR	THR	S533	E736	L833	E1062	G1218	V1341
THR	THR	THR	THR	THR	A739	L833	E1062	D1219	G1345
THR	THR	THR	THR	THR	THR	L833	E1062	A1220	S1346
THR	THR	THR	THR	THR	THR	L833	E1062	N1221	D1347
THR	THR	THR	THR	THR	THR	L833	E1062	T1222	Y1348
THR	THR	THR	THR	THR	THR	L833	E1062	V1223	V1349
THR	THR	THR	THR	THR	THR	L833	E1062	T1224	E1352
THR	THR	THR	THR	THR	THR	L833	E1062	D1285	D1353
THR	THR	THR	THR	THR	THR	L833	E1062	S1226	
THR	THR	THR	THR	THR	THR	L833	E1062	D1230	



ASN	V1369	ASN	V1369
LEU	D1372	LEU	D1372
GLY	Y1376	GLY	Y1376
THR	W1377	THR	W1377
VAL	W1378	VAL	W1378
ASP	T1379	ASP	T1379
ALA	V1382	ALA	V1382
PHE	Y1383	PHE	Y1383
PRO	I1384	PRO	I1384
ALA	T1385	ALA	T1385
LEU	F1393	LEU	F1393
TRP	D1399	TRP	D1399
ILE	E1403	ILE	E1403
PRO	T1404	PRO	T1404
THR	I1409	THR	I1409
ALA	K1410	ALA	K1410
LEU	V1411	LEU	V1411
GLY	R1414	GLY	R1414
ASP	K1422	ASP	K1422
ASN	L1423	ASN	L1423
VAL	T1434	VAL	T1434
ASP	I1438	ASP	I1438
ASN	L1439	ASN	L1439
PRO	D1446	PRO	D1446
THR	T1453	THR	T1453
VAL	P1465	VAL	P1465
THR	L1469	THR	L1469
THR	D1473	THR	D1473
VAL	D1474	VAL	D1474
ASN	V1480	ASN	V1480
VAL	I1490	VAL	I1490
THR	V1491	THR	V1491
VAL	N1499	VAL	N1499
SER	I1500	SER	I1500
LEU	V1503	LEU	V1503
ALA	E1507	ALA	E1507
PRO	Y1510	PRO	Y1510
SER		SER	
LEU		LEU	
GLY	G1516	GLY	G1516
ARG	V1517	ARG	V1517
THR	V1520	THR	V1520
VAL	D1524	VAL	D1524
ALA	P1529	ALA	P1529
PHE	V1532	PHE	V1532
GLY	V1537	GLY	V1537
ASN	S1541	ASN	S1541
SER	L1550	SER	L1550
VAL	T1551	VAL	T1551
THR	V1552	THR	V1552
GLY	T1553	GLY	T1553
ASP	E1554	ASP	E1554
GLN	T1555	GLN	T1555
GLN	A1558	GLN	A1558
VAL	T1559	VAL	T1559
GLN	G1560	GLN	G1560
ILE	L1561	ILE	L1561
SER	F1562	SER	F1562
ALA	E1563	ALA	E1563
ASP	G1564	ASP	G1564
ASP	T1565	ASP	T1565
ASN	V1566	ASN	V1566
THR	F1567	THR	F1567
ARG	S1574	ARG	S1574
GLU	R1578	GLU	R1578
GLN	L1579	GLN	L1579
LEU	R1580	LEU	R1580
SER	D1585	SER	D1585
PHE	M1594	PHE	M1594
ALA	T1595	ALA	T1595
TYR	L1596	TYR	L1596
LEU	P1597	LEU	P1597
VAL	E1605	VAL	E1605
GLY	T1618	GLY	T1618
THR	VAL	THR	VAL
THR	VAL	THR	VAL
SER	PRO	SER	PRO
LEU	PRO	LEU	PRO
ALA	LEU	ALA	LEU
TRP	ALA	TRP	ALA
ILE	TRP	ILE	TRP
THR	ILE	THR	ILE
GLY	THR	GLY	THR
SER	GLY	SER	GLY
LEU	SER	LEU	SER
ALA	ALA	ALA	ALA

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	354860	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; RELION refinement with in-built CTF correction. The function is similar to a Wiener filter, so amplitude correction included.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48.5	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	10.250	Depositor
Minimum map value	-4.662	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.422	Depositor
Recommended contour level	1.05514	Depositor
Map size (Å)	349.44, 349.44, 349.44	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.092, 1.092, 1.092	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	0.75	9/11941 (0.1%)	0.81	18/16339 (0.1%)
1	B	0.69	2/11941 (0.0%)	0.77	8/16339 (0.0%)
1	C	0.69	2/11941 (0.0%)	0.77	6/16339 (0.0%)
1	D	0.68	1/11941 (0.0%)	0.76	7/16339 (0.0%)
1	E	0.69	2/11941 (0.0%)	0.77	7/16339 (0.0%)
1	F	0.70	3/11941 (0.0%)	0.77	5/16339 (0.0%)
All	All	0.70	19/71646 (0.0%)	0.77	51/98034 (0.1%)

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	1
All	All	0	3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	793	GLU	CD-OE2	16.03	1.43	1.25
1	A	1255	GLU	CD-OE1	-15.38	1.08	1.25
1	A	793	GLU	CD-OE1	-13.35	1.10	1.25
1	A	196	GLU	CD-OE1	-10.86	1.13	1.25
1	A	1299	GLU	CD-OE1	-9.95	1.14	1.25

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	ASP	CB-CG-OD1	15.40	132.16	118.30
1	A	123	ASP	CB-CG-OD1	11.60	128.74	118.30
1	A	794	ASP	CB-CG-OD2	10.58	127.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	E	1257	ASP	CB-CG-OD1	-8.15	110.96	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	GLU	Sidechain
1	A	729	ASP	Sidechain
1	B	55	SER	Mainchain

## 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	11751	0	10951	245	0
1	B	11751	0	10951	221	0
1	C	11751	0	10951	248	0
1	D	11751	0	10951	252	0
1	E	11751	0	10949	221	0
1	F	11751	0	10951	248	0
All	All	70506	0	65704	1252	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 9.

The worst 5 of 1252 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:C:1217:SER:CB	1:D:1424:VAL:HG21	1.65	1.25
1:A:1424:VAL:HG21	1:F:1217:SER:CB	1.65	1.24
1:C:816:PRO:HD2	1:D:1083:ASN:HD21	1.01	1.14
1:A:1424:VAL:CG2	1:F:1217:SER:HB2	1.82	1.09
1:C:1217:SER:HB2	1:D:1424:VAL:CG2	1.83	1.08

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	1578/1734 (91%)	1517 (96%)	61 (4%)	0	100	100
1	B	1578/1734 (91%)	1518 (96%)	60 (4%)	0	100	100
1	C	1578/1734 (91%)	1520 (96%)	58 (4%)	0	100	100
1	D	1578/1734 (91%)	1518 (96%)	60 (4%)	0	100	100
1	E	1578/1734 (91%)	1518 (96%)	60 (4%)	0	100	100
1	F	1578/1734 (91%)	1520 (96%)	58 (4%)	0	100	100
All	All	9468/10404 (91%)	9111 (96%)	357 (4%)	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	1312/1438 (91%)	1300 (99%)	12 (1%)	78	92
1	B	1312/1438 (91%)	1301 (99%)	11 (1%)	81	93
1	C	1312/1438 (91%)	1302 (99%)	10 (1%)	81	93
1	D	1312/1438 (91%)	1300 (99%)	12 (1%)	78	92
1	E	1312/1438 (91%)	1300 (99%)	12 (1%)	78	92
1	F	1312/1438 (91%)	1300 (99%)	12 (1%)	78	92
All	All	7872/8628 (91%)	7803 (99%)	69 (1%)	79	92

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	38	ASN
1	F	269	ARG
1	F	1047	PHE
1	C	274	ARG
1	C	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	740	ASN
1	F	956	GLN
1	E	853	ASN
1	F	97	ASN
1	B	1154	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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.

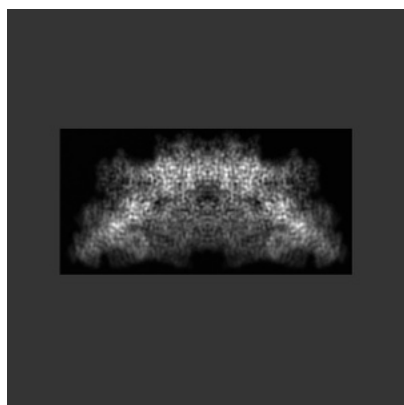
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16484. These allow visual inspection of the internal detail of the map and identification of artifacts.

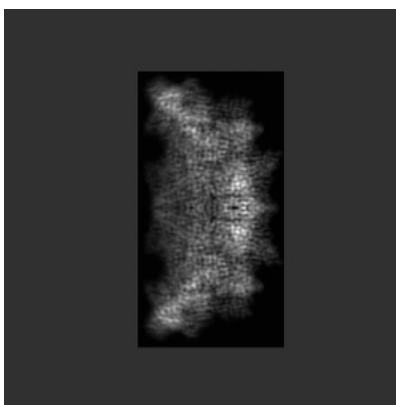
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

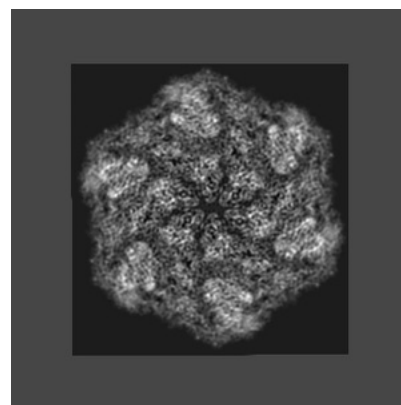
#### 6.1.1 Primary map



X



Y



Z

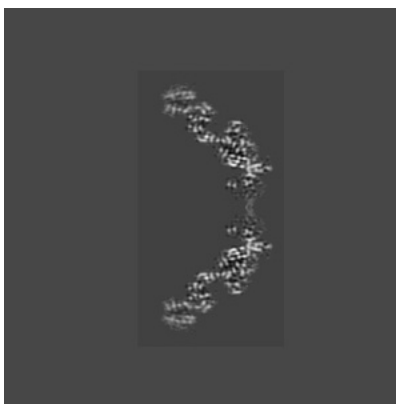
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

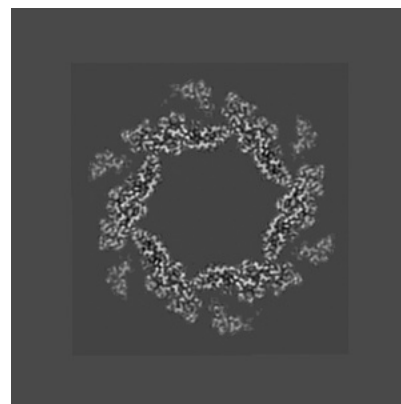
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

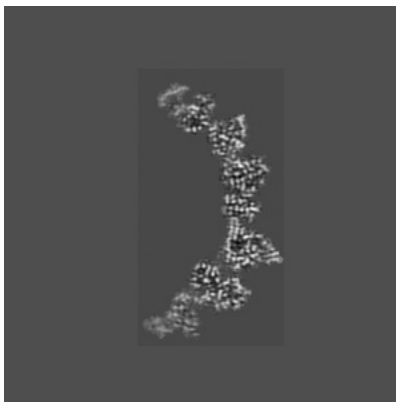
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 156



Y Index: 175

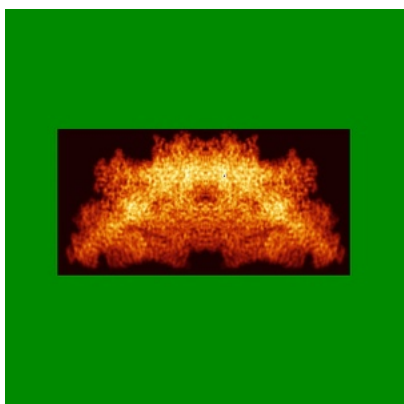


Z Index: 186

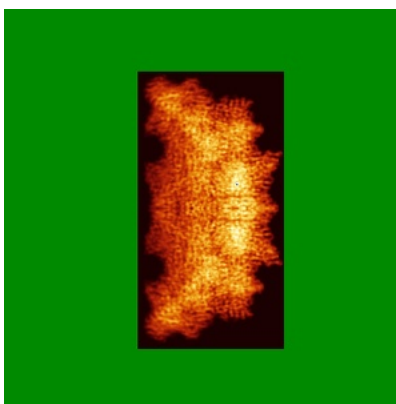
The images above show the largest variance slices of the map in three orthogonal directions.

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

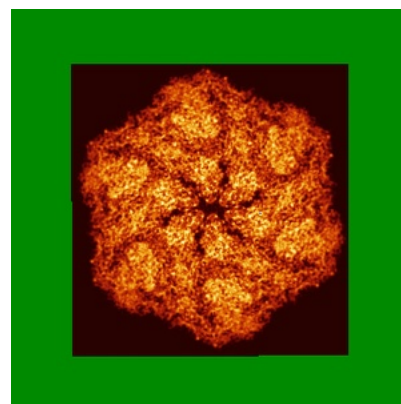
### 6.4.1 Primary map



X



Y



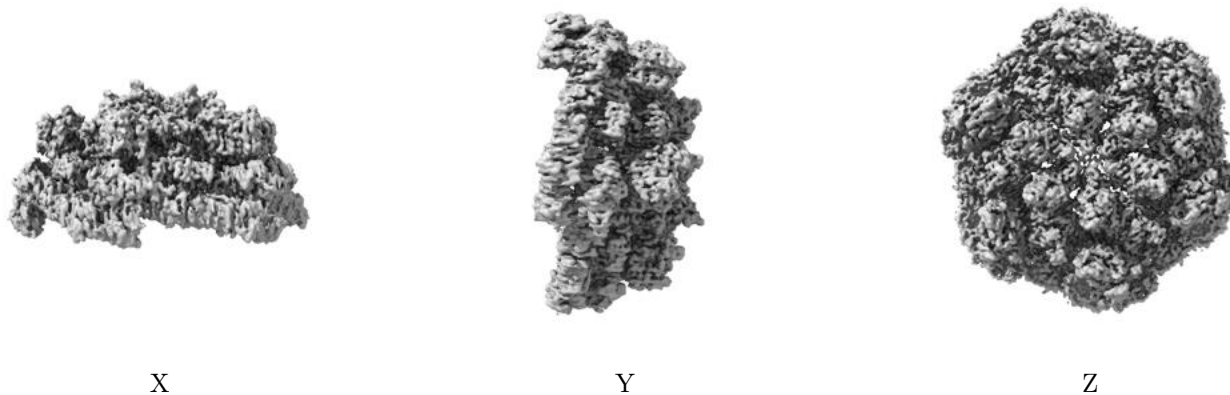
Z

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 1.05514. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

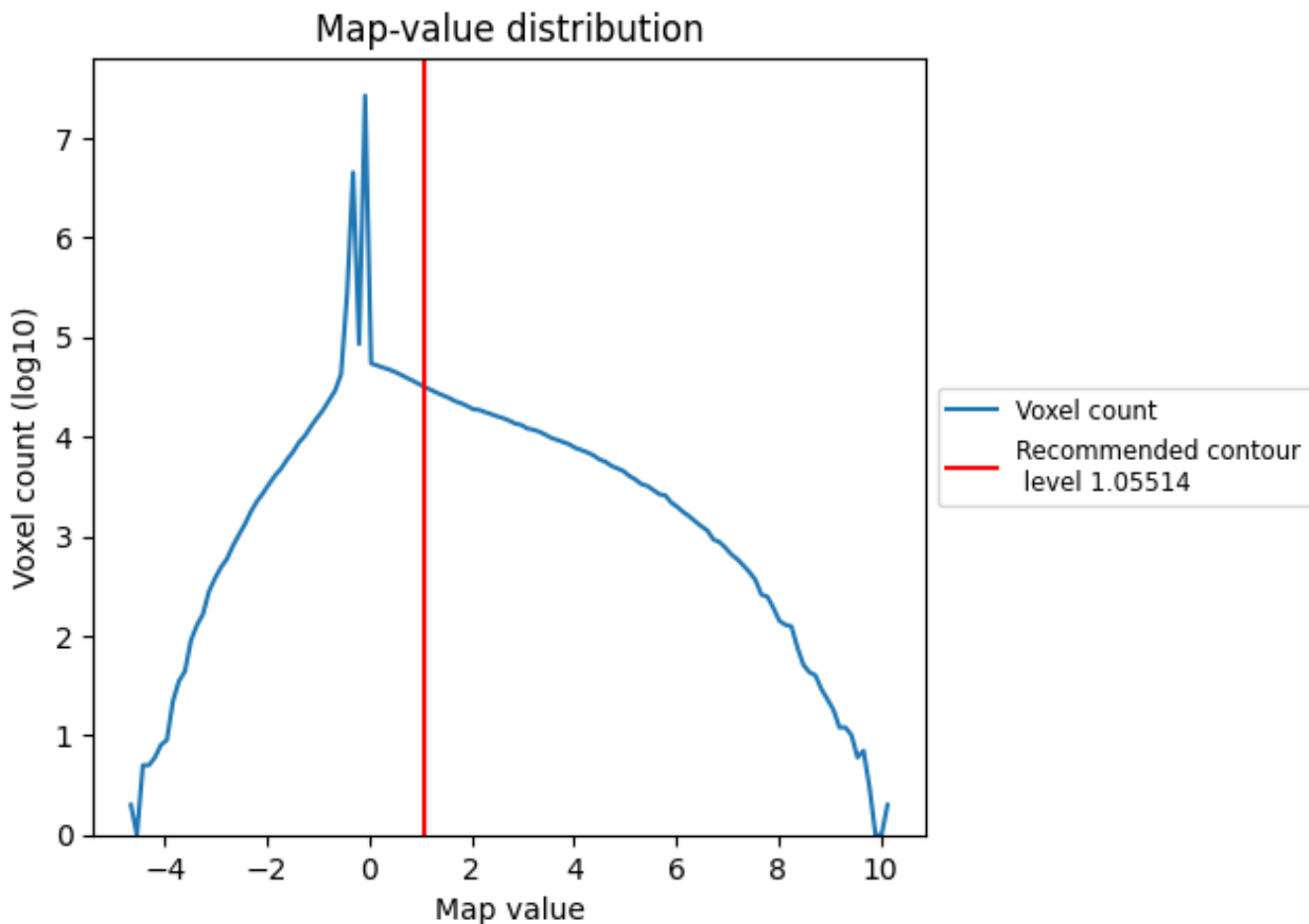
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

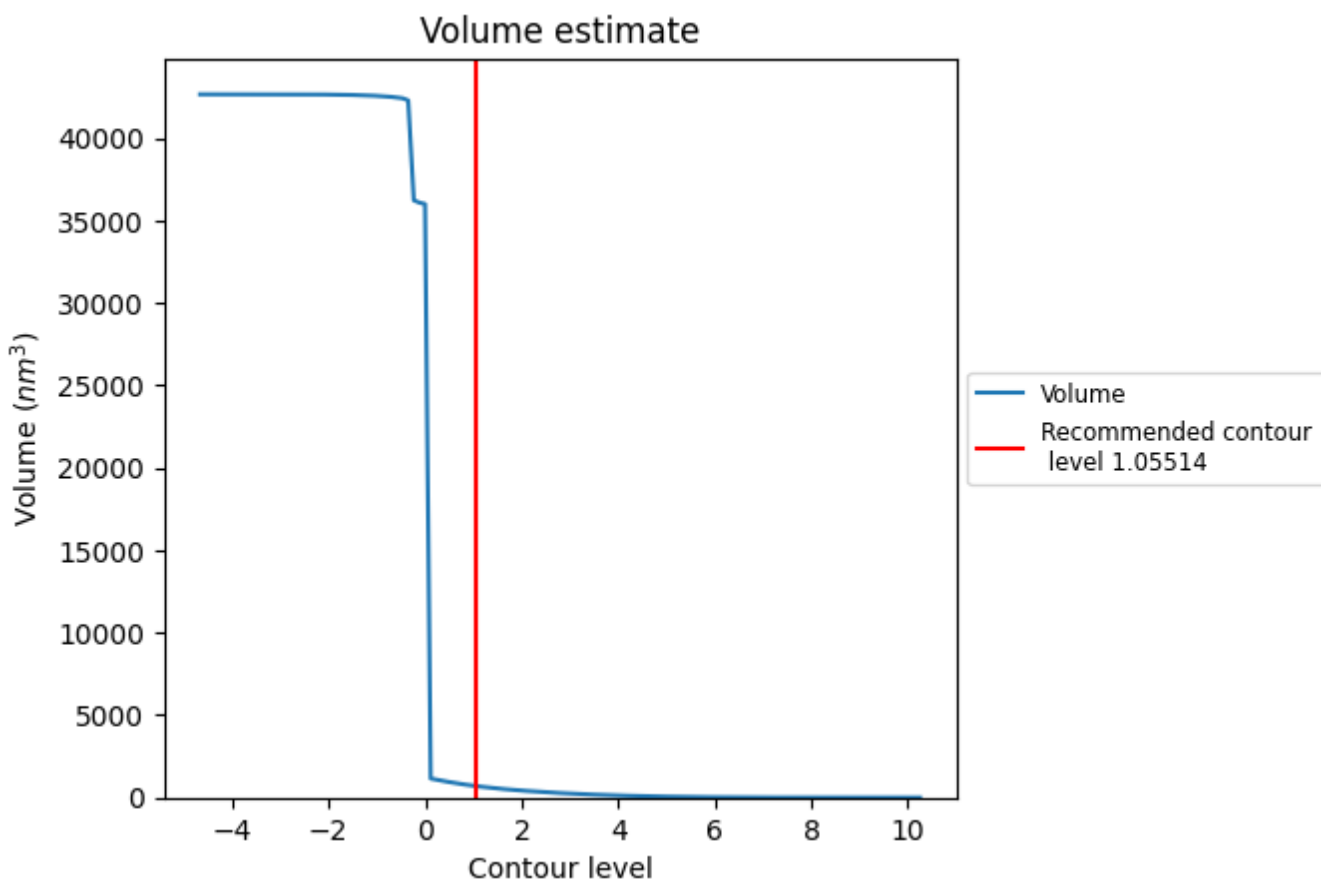
This section contains the results of statistical analysis of the map.

### 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.

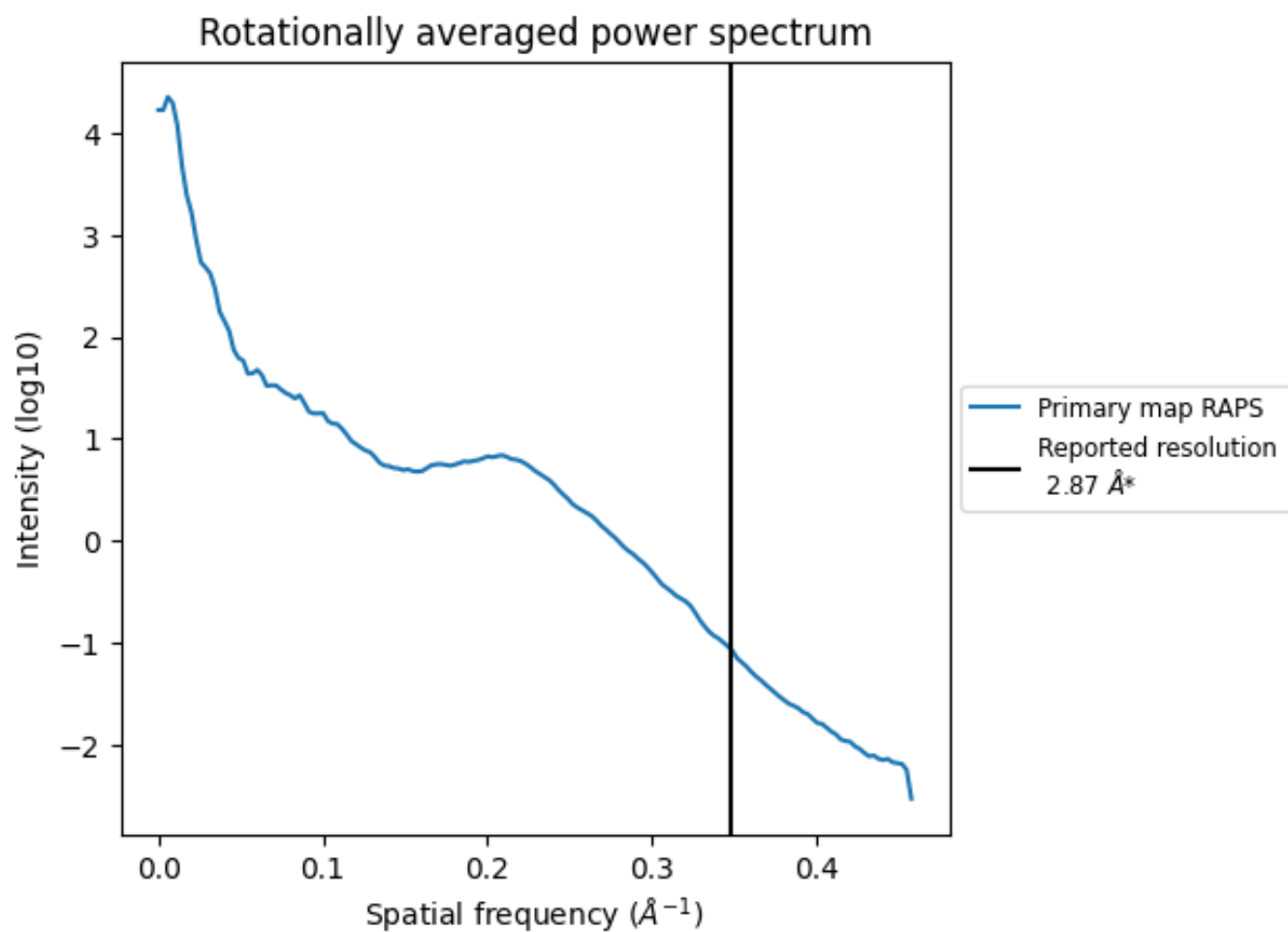
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 697  $\text{nm}^3$ ; this corresponds to an approximate mass of 630 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 0.348 Å<sup>-1</sup>

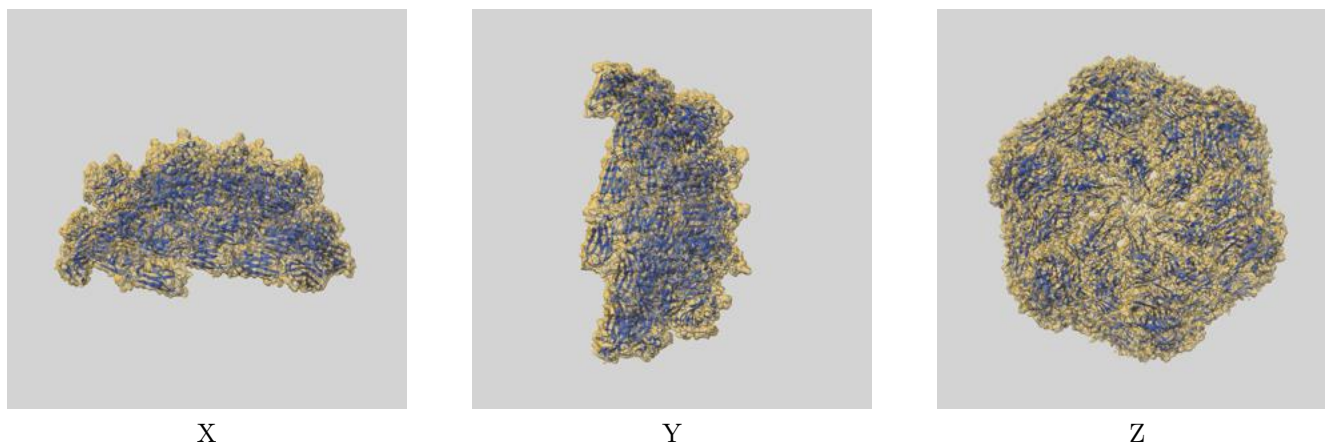
## 8 Fourier-Shell correlation

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

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

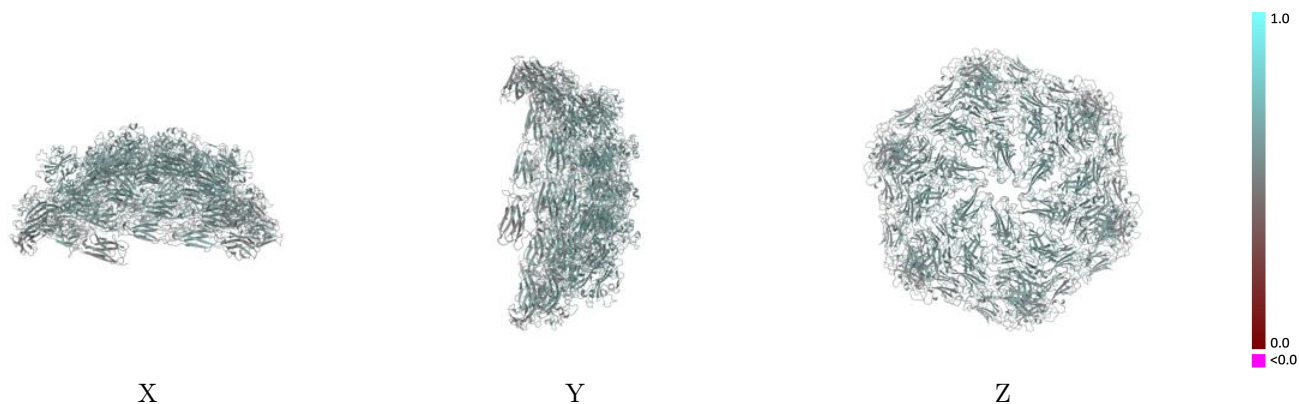
This section contains information regarding the fit between EMDB map EMD-16484 and PDB model 8C8M. Per-residue inclusion information can be found in section 3 on page 4.

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



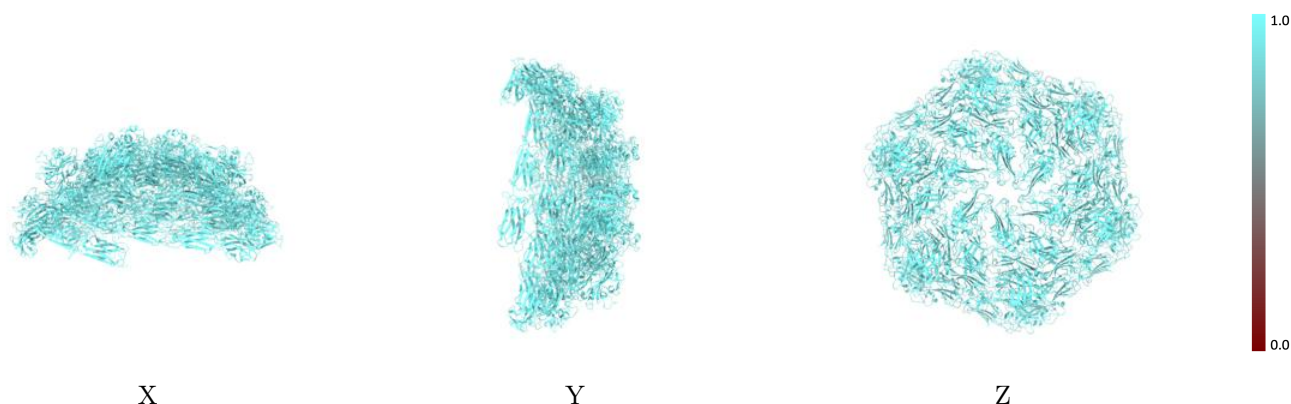
The images above show the 3D surface view of the map at the recommended contour level 1.05514 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



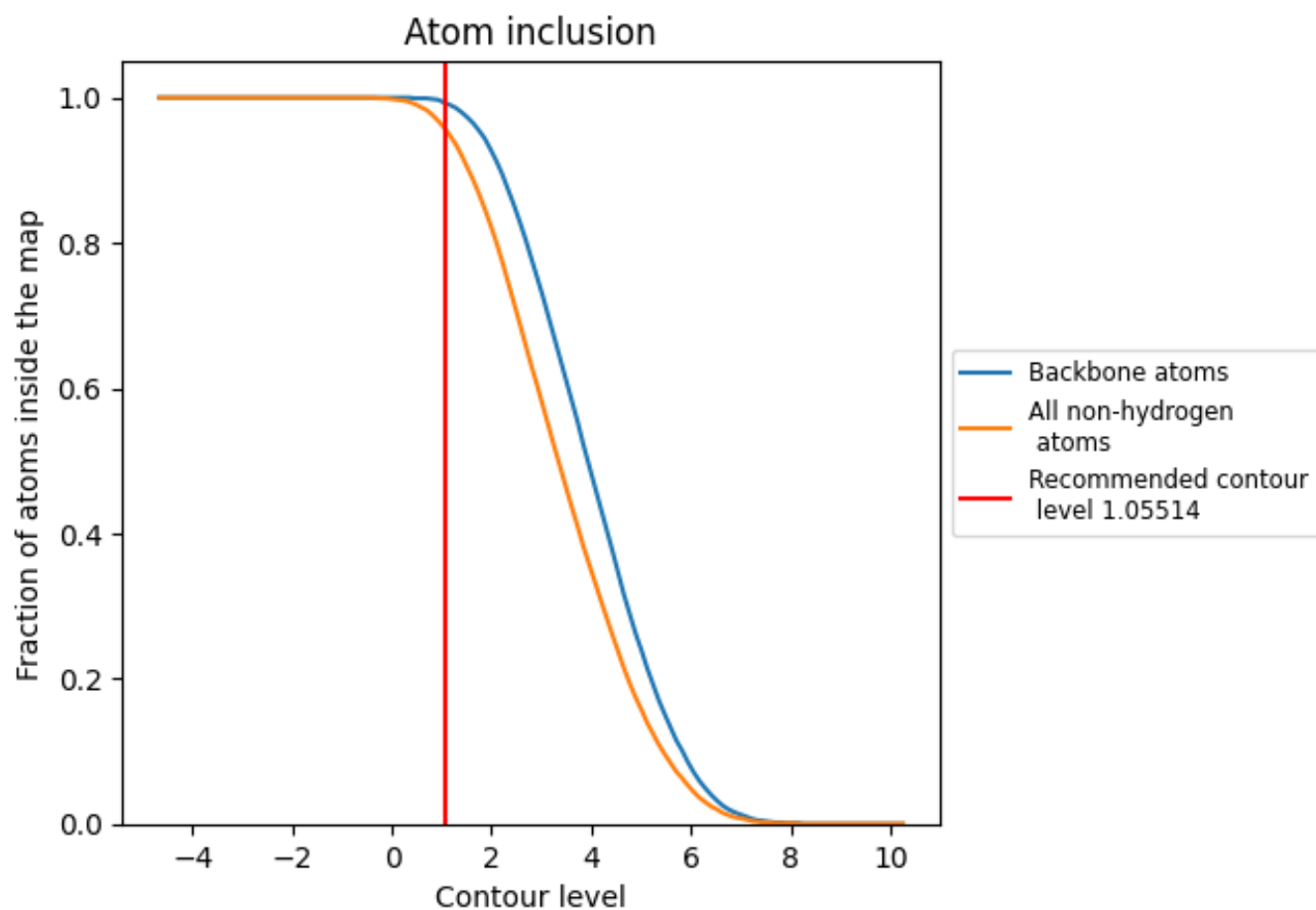
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.05514).

## 9.4 Atom inclusion [i](#)

















At the recommended contour level, 99% of all backbone atoms, 96% 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 (1.05514) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.5560
A	 0.9620	 0.5630
B	 0.9580	 0.5530
C	 0.9530	 0.5520
D	 0.9630	 0.5620
E	 0.9580	 0.5530
F	 0.9540	 0.5520

