



wwPDB EM Validation Summary Report ⓘ

Jun 8, 2024 – 07:49 am 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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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.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) : 2.36.2

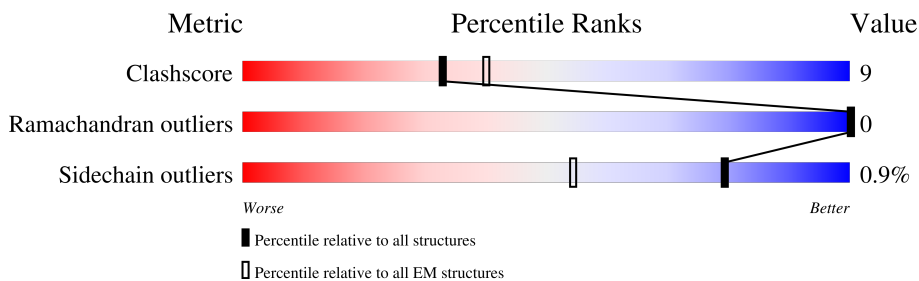
1 Overall quality at a glance

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 ≥ 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.

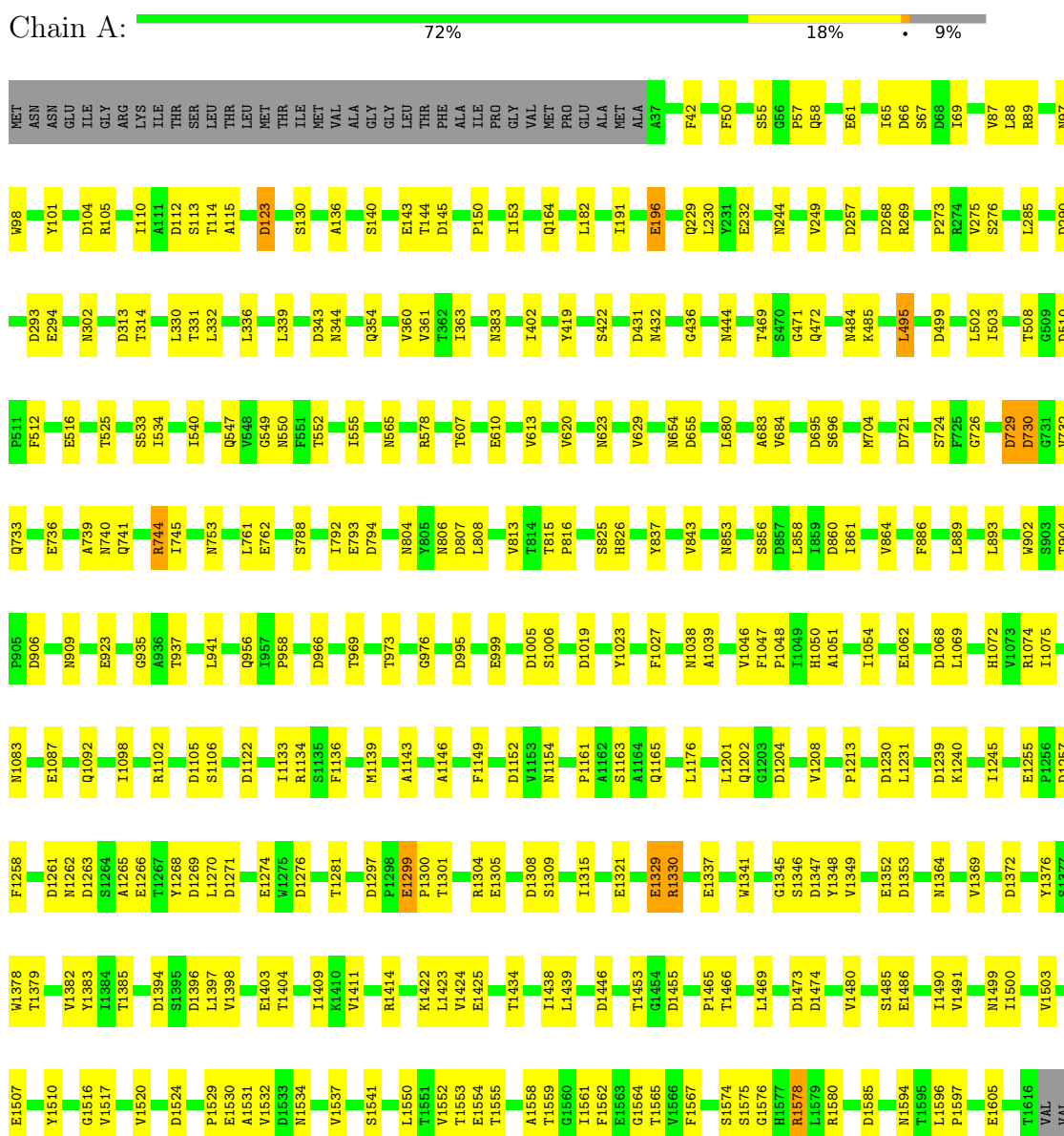
- Molecule 1 is a protein called Cell surface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1580	11751	7234	1888	2610	19	0	0
1	B	1580	11751	7234	1888	2610	19	0	0
1	C	1580	11751	7234	1888	2610	19	0	0
1	D	1580	11751	7234	1888	2610	19	0	0
1	E	1580	11751	7234	1888	2610	19	0	0
1	F	1580	11751	7234	1888	2610	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	THR
D1271	D1271	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	T1281	R1414	R1414	G1560	ALA
M1139	M1139	D1297	F1562	F1562	I1561	THR
M1300	M1300	P1298	E1563	E1563	F1566	ALA
T1301	T1301	E1299	T1565	T1565	V1566	ASP
A1143	A1143	P1300	T1434	T1434	F1567	LEU
A1146	A1146	T1301	I1438	I1438	S1574	GLY
F1149	F1149	R1304	L1439	L1439	S1576	GLN
D1152	D1152	E1305	D1446	D1446	G1576	ASP
W1153	W1153	D1308	D1446	D1446	H1577	ARG
W1154	W1154	S1309	T1453	T1453	H1578	GLU
P1161	P1161	I1315	P1465	P1465	L1579	THR
A1162	A1162	E1321	R1580	R1580	R1580	PHE
A1164	A1164	E1329	D1585	D1585	D1585	ALA
Q1165	Q1165	R1330	M1594	M1594	T1595	THR
L1176	L1176	E1337	L1596	L1596	P1597	LEU
D1340	D1340	D1340	E1605	E1605	E1605	GLN
W1341	W1341	W1341	T1616	T1616	T1616	ALA
G1203	G1203	S1346	VAL	VAL	VAL	GLY
D1204	D1204	D1347	VAL	VAL	VAL	THR
V1208	V1208	Y1348	THR	THR	THR	VAL
P1213	P1213	V1349	VAL	VAL	VAL	VAL
D1230	D1230	E1352	LEU	LEU	LEU	LEU
L1231	L1231	D1353	LEU	LEU	LEU	THR
D1239	D1239	D1353	ALA	ALA	ALA	ALA
K1240	K1240	F1365	ALA	ALA	ALA	ALA
I1245	I1245	V1369	ALA	ALA	ALA	ALA
D1257	D1257	D1372	ASN	ASN	ASN	ASN
F1258	F1258	Y1376	LEU	LEU	LEU	LEU
T1379	T1379	S1377	GLY	GLY	GLY	GLY
D1261	D1261	W1378	THR	THR	THR	THR
N1262	N1262	T1379	VAL	VAL	VAL	VAL
S1263	S1263	V1382	PHE	PHE	PHE	PHE
S1264	S1264	I1383	ALA	ALA	ALA	ALA
A1265	A1265	I1384	PRO	PRO	PRO	PRO
		T1385	LEU	LEU	LEU	LEU
			SER	SER	SER	SER

● Molecule 1: Cell surface protein



MET	ASN	ASN	ASN	D104	N302	I534	N740	G935	E1087	L1231
ASN	GLU	GLU	ILE	R105	F310	I540	R744	A936	Q1092	D1239
THR	VAL	VAL	GLY	I110	D313	Q547	I745	T937	I1098	K1240
GLU	ILE	GLY	ARG	A111	T314	V548	E749	L941	R1102	I1245
VAL	VAL	VAL	LYS	D112	D314	G543	T750	D954	G1103	D1257
ASP	ASP	ASP	LYS	S113	N322	N550	G751	G956	S1104	F1258
GLN	GLN	GLN	THR	T114	L330	F951	N753	P957	D1105	F1258
THR	THR	THR	THR	A115	T331	T552	L761	P958	S1106	D1261
TYR	ALA	ALA	ALA	D123	L332	I555	E762	D966	D1122	M1262
ALA	THR	THR	THR	S130	R333	N655	S788	T969	I1133	M1263
ALA	THR	THR	THR	A136	L336	R578	I792	T973	R1134	S1264
PHE	PHE	PHE	PHE	T144	D343	L579	N804	G976	F1136	A1265
VAL	VAL	VAL	VAL	D145	N344	I580	T805	G983	F1136	Y1267
ASP	ASP	ASP	ASP	P150	I363	E610	N806	L984	M1139	D1269
ASN	ASN	ASN	ASN	I402	S401	V613	D807	D985	A1143	L1270
GLY	GLY	GLY	GLY	I153	I402	V620	L808	D995	A1146	D1271
GLN	GLN	GLN	GLN	Q164	P411	N623	T815	E999	D1152	T1281
THR	THR	THR	THR	L182	Y419	V629	P816	D1005	Y1153	D1297
LEU	LEU	LEU	LEU	I191	E421	S825	S825	S1006	P1161	P1297
ALA	ALA	ALA	ALA	A197	S422	H826	H826	A1162	E1299	P1298
PHE	PHE	PHE	PHE	D431	D431	N654	Y837	D1019	S1163	E1300
ALA	ALA	ALA	ALA	N432	N432	D655	V843	Y1023	A1164	T1301
ALA	ALA	ALA	ALA	P226	R435	L680	V843	F1027	Q1165	D1308
GLY	GLY	GLY	GLY	Q229	G436	A683	N853	N1038	L1176	S1309
VAL	VAL	VAL	VAL	L230	G436	V684	N853	A1039	L1201	I1315
THR	THR	THR	THR	E232	N444	D695	L858	V1046	Q1202	E1321
VAL	VAL	VAL	VAL	F42	T469	S696	I859	F1047	G1203	E1322
SER	SER	SER	SER	F50	Q472	M704	D960	P1048	D1204	S1322
LEU	LEU	LEU	LEU	Q58	M484	V717	V864	T1049	I1205	K1327
LEU	LEU	LEU	LEU	T65	R488	D721	F886	H1050	Q1207	R1330
THR	THR	THR	THR	D66	R488	S724	L889	A1051	V1208	E1337
GLY	GLY	GLY	GLY	D66	L495	F725	L893	I1054	P1213	D1340
THR	THR	THR	THR	D68	L502	G726	N902	E1062	S1217	W1341
SER	SER	SER	SER	T69	I503	D730	T904	D1068	G1218	D1340
SER	SER	SER	SER	V67	F512	G731	P905	L1069	D1219	G1345
ALA	ALA	ALA	ALA	L88	F512	V732	D906	D1222	A1220	S1346
ALA	ALA	ALA	ALA	R89	E516	Q733	N909	H1072	N1221	D1347
ASP	ASP	ASP	ASP	Y94	T525	E736	E923	I1075	V1223	Y1348
ALA	ALA	ALA	ALA	D290	S533	A739		M1083	T1224	V1349
PRO	PRO	PRO	PRO	D293					D1285	E1352
ALA	ALA	ALA	ALA	E294					S1226	D1353
LEU	LEU	LEU	LEU						D1230	
SER	SER	SER	SER							

ASN	V1369
LEU	
GLY	D1372
THR	
VAL	Y1376
ASP	S1377
ALA	W1378
PHE	T1379
PRO	
ALA	V1382
LEU	Y1383
SER	I1384
TRP	T1385
ILE	
ASP	F1393
PRO	
THR	VAL
THR	L1409
GLU	K1410
GLU	V1411
ALA	
ALA	R1414
PHE	
VAL	K1422
TRP	L1423
GLU	
GLU	T1434
TRP	
LEU	I1438
ALA	L1439
THR	
THR	D1446
LEU	
LEU	T1453
THR	
THR	P1465
SER	
THR	L1469
THR	
THR	D1473
VAL	D1474
ASN	
VAL	V1480
SER	
SER	I1490
THR	V1491
THR	
VAL	N1499
VAL	I1500
THR	
THR	V1503
THR	
THR	E1507
GLY	
SER	Y1510
LEU	
ASN	G1516
LEU	V1517
GLY	
GLN	V1520
SER	
THR	D1524
VAL	
ASP	P1529
ALA	
PHE	V1532
PRO	
ALA	V1537
LEU	
LEU	S1541
SER	
TRP	VAL
ILE	L1550
ASP	T1551
ASP	V1552
GLY	T1553
THR	E1554
THR	T1555
TYR	
THR	
ALA	A1558
ALA	T1559
ALA	
PHE	G1560
VAL	L1561
TRP	F1562
GLU	E1563
GLU	G1564
SER	T1565
SER	
LEU	V1566
LEU	F1567
THR	
THR	S1574
ALA	
ALA	R1578
LEU	
LEU	L1579
SER	
SER	PHE
PRO	ALA
PRO	TYR
VAL	D1585
VAL	
SER	M1594
THR	
THR	T1595
THR	
VAL	L1596
VAL	P1597
ASN	
VAL	E1605
SER	
SER	T1618
THR	VAL
THR	VAL
VAL	PRO
VAL	PRO
THR	LEU
THR	ALA
THR	ALA
THR	TRP
THR	ILE
THR	THR
THR	GLY
SER	SER
LEU	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.

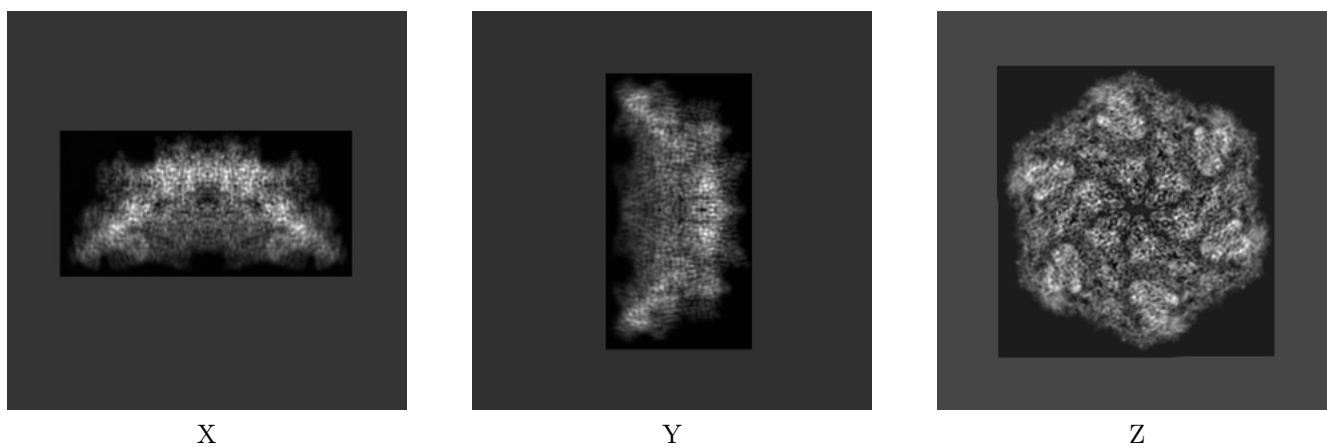
6 Map visualisation [i](#)

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](#)

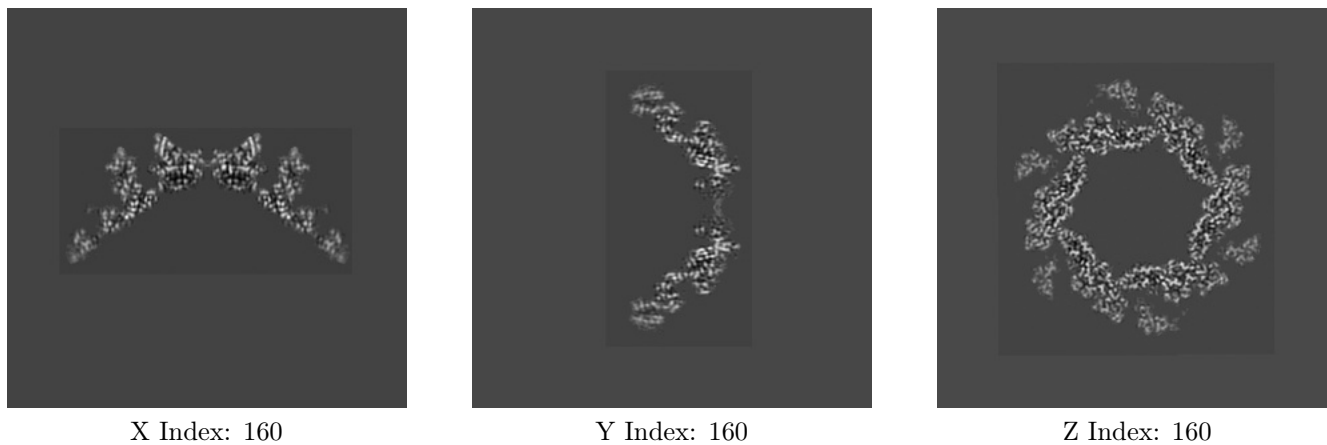
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



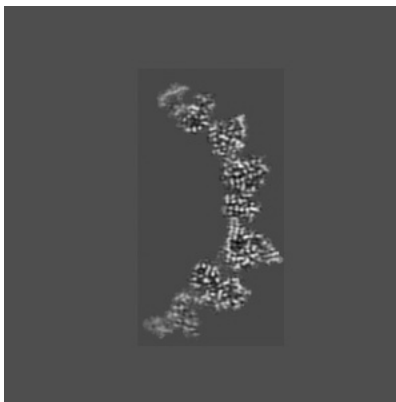
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 156



Y Index: 175

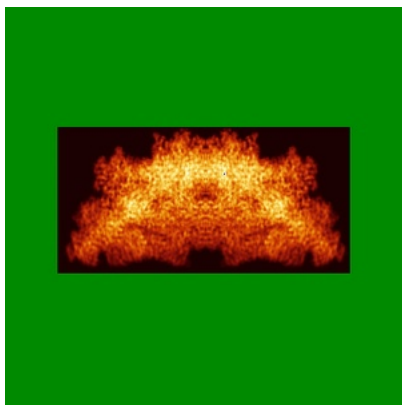


Z Index: 186

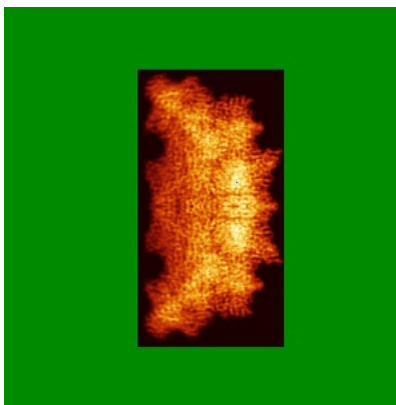
The images above show the largest variance slices of the map in three orthogonal directions.

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

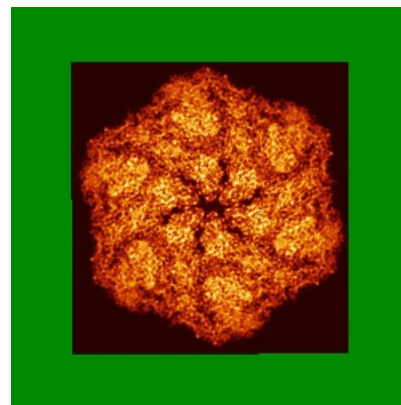
6.4.1 Primary map



X



Y

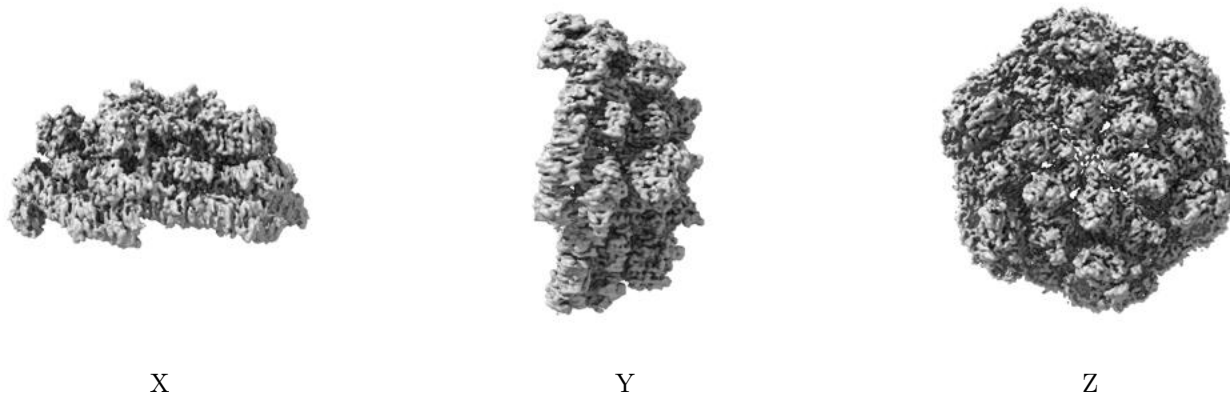


Z

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.

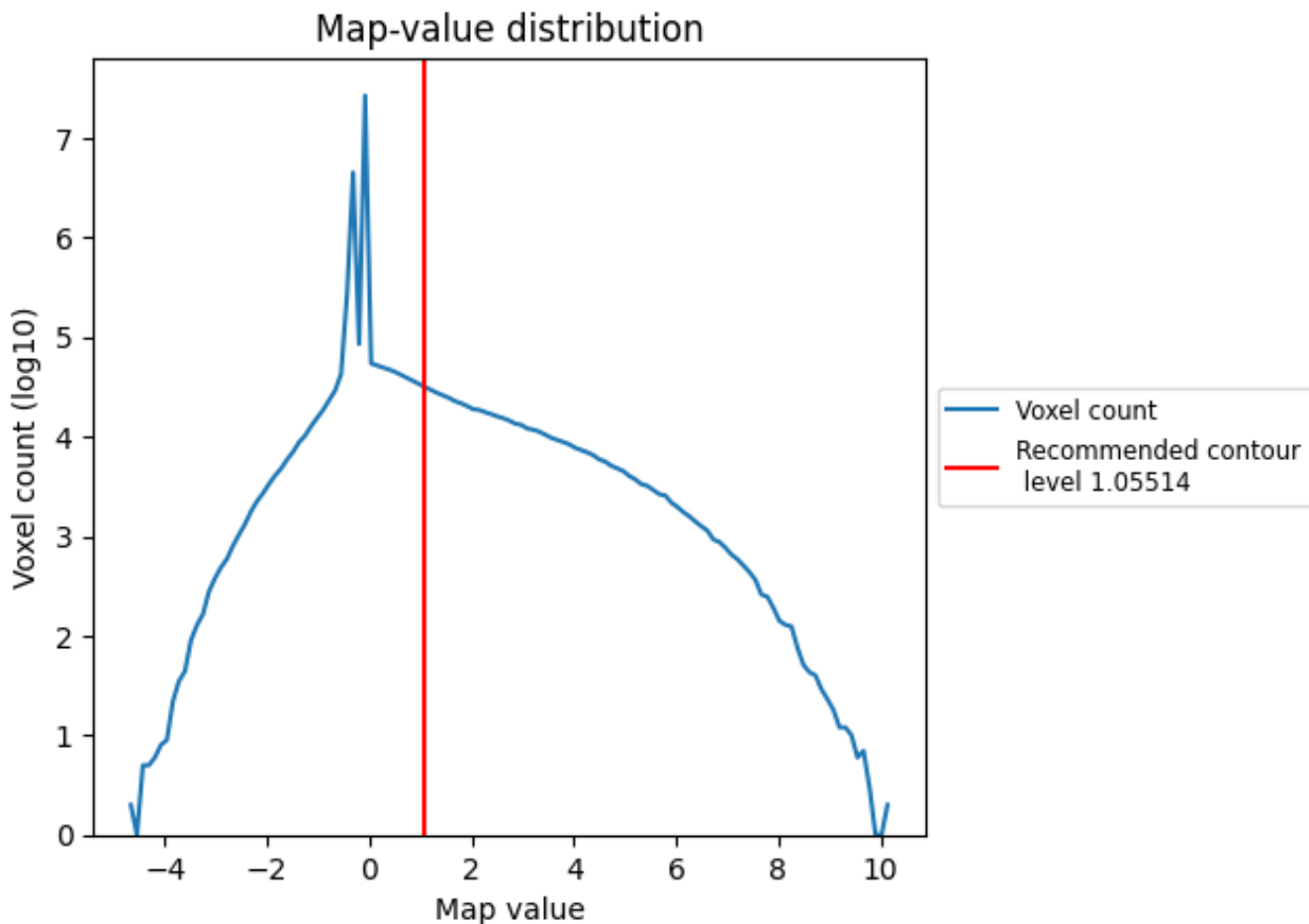
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

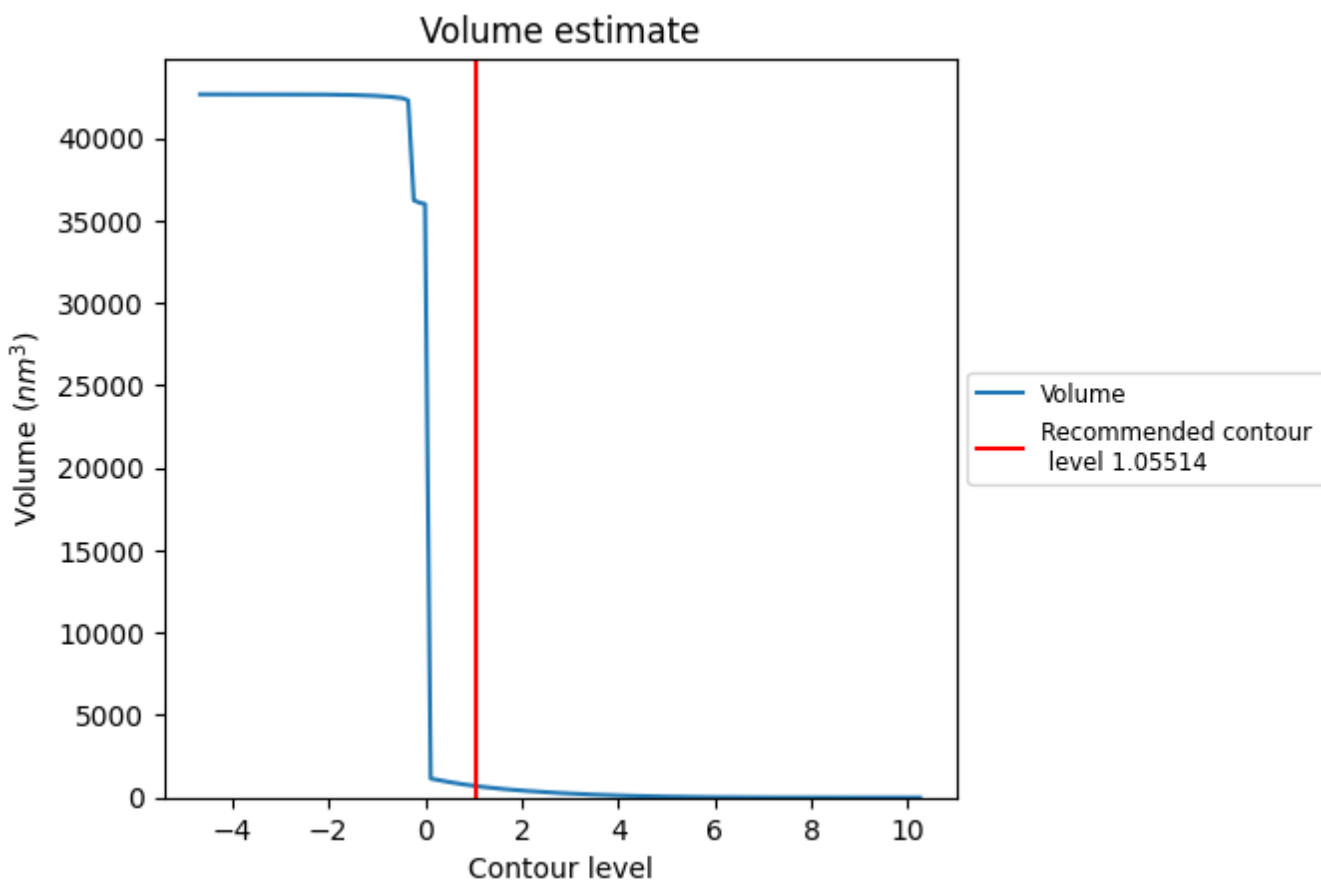
This section contains the results of statistical analysis of the map.

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.

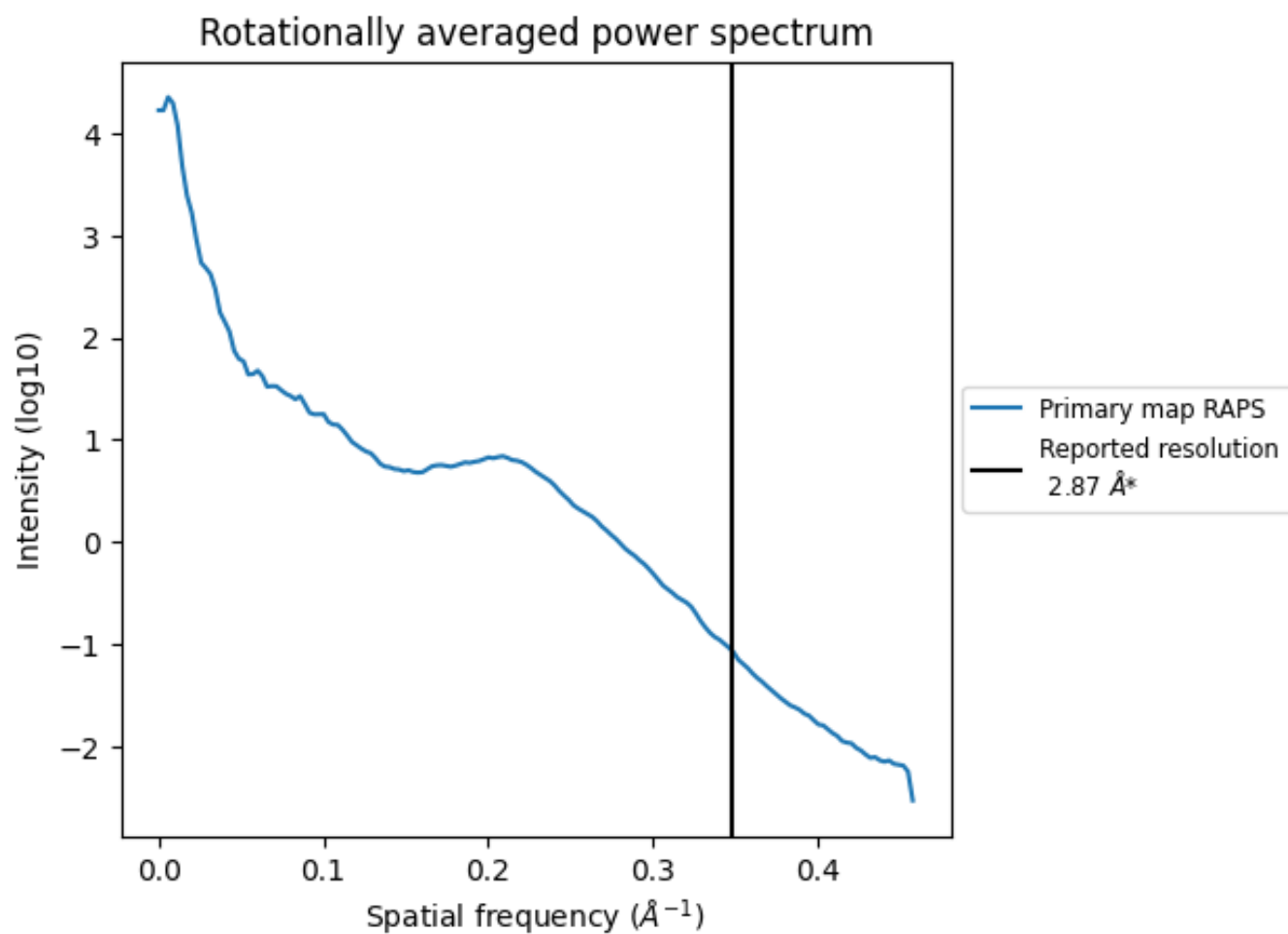
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 697 nm³; 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⁻¹

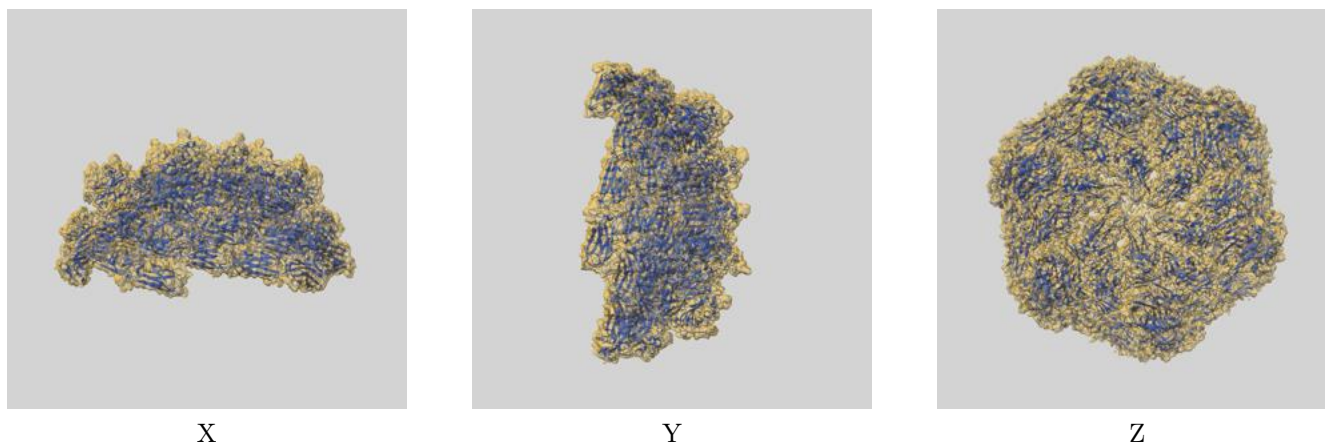
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

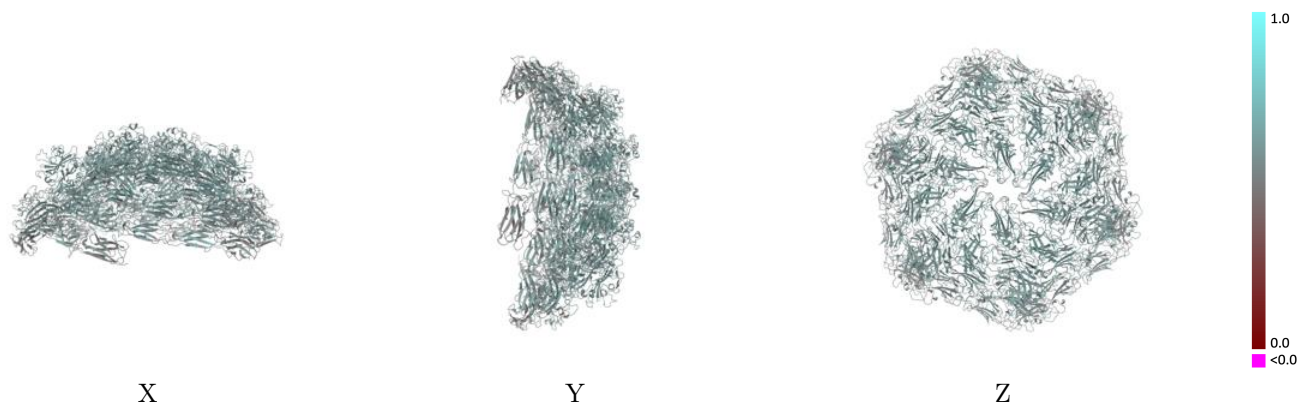
This section contains information regarding the fit between EMDB map EMD-16484 and PDB model 8C8M. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



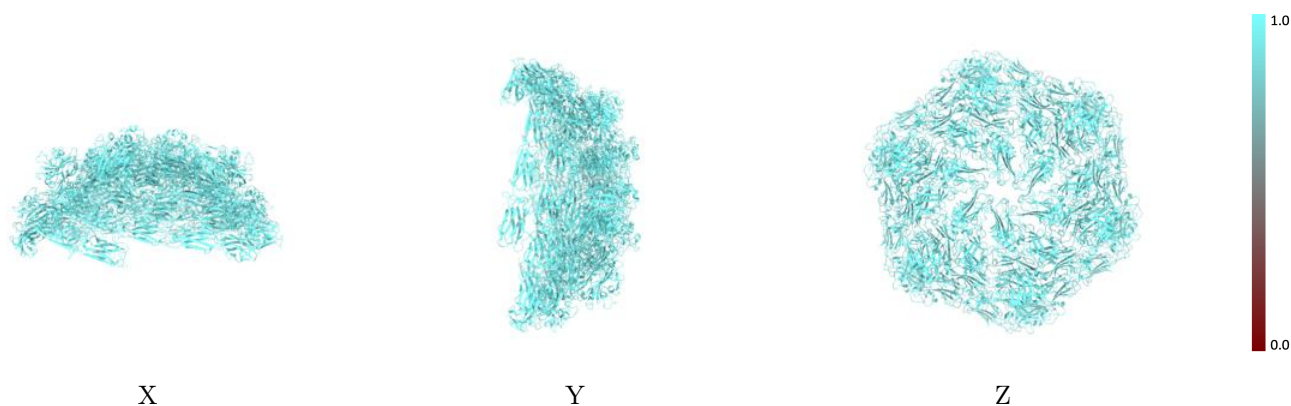
The images above show the 3D surface view of the map at the recommended contour level 1.05514 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



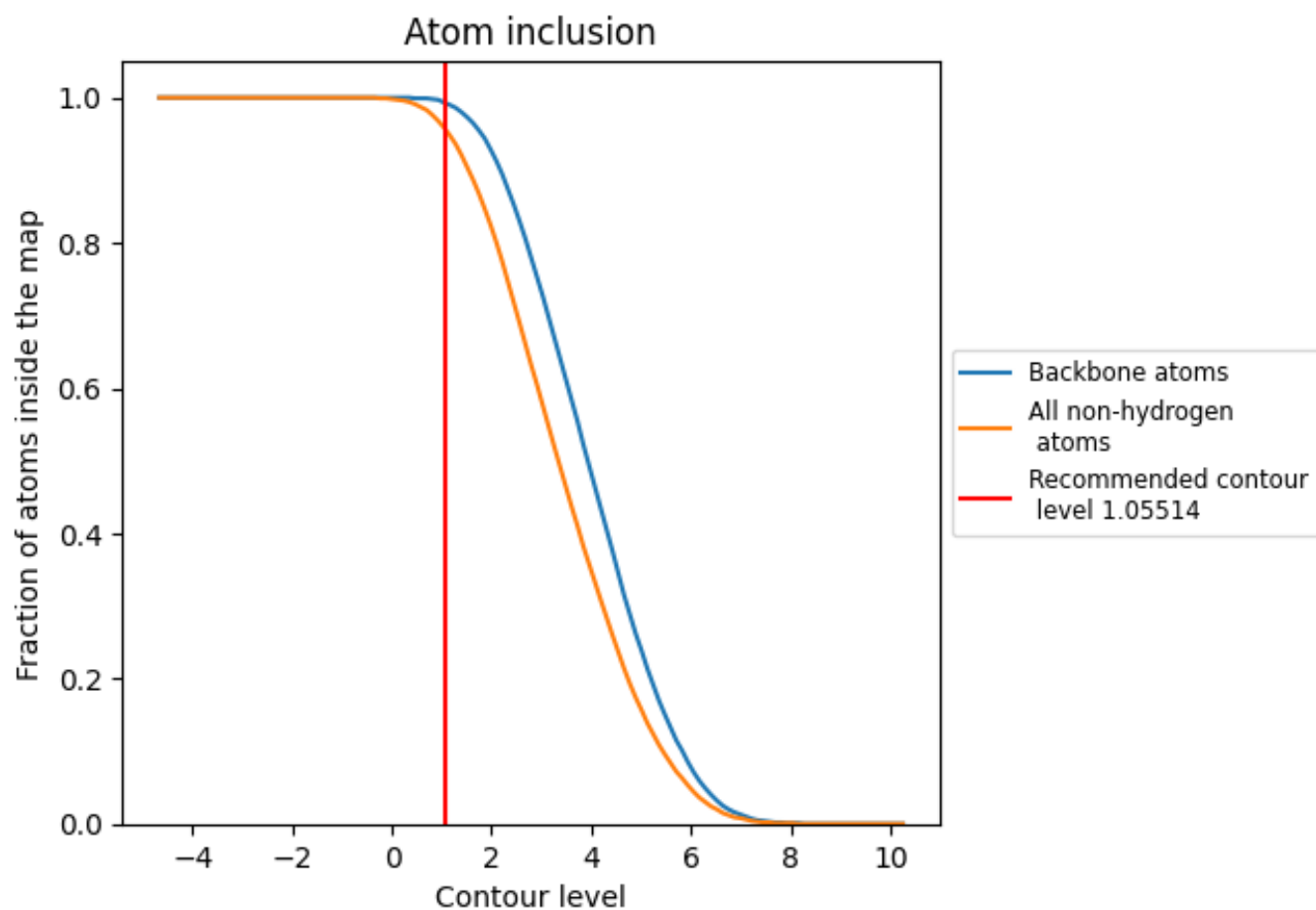
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

