



wwPDB EM Validation Summary Report ⓘ

Jun 1, 2024 – 07:48 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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<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

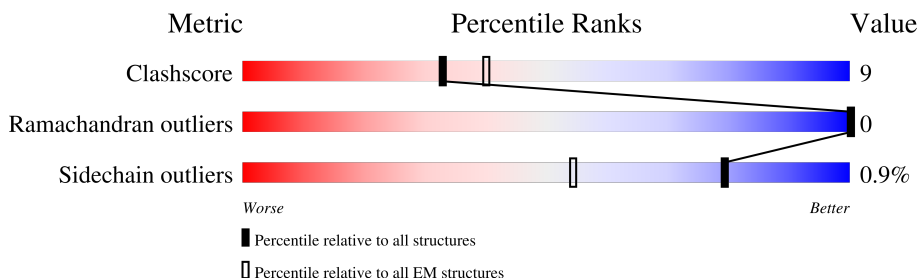
1 Overall quality at a glance

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.

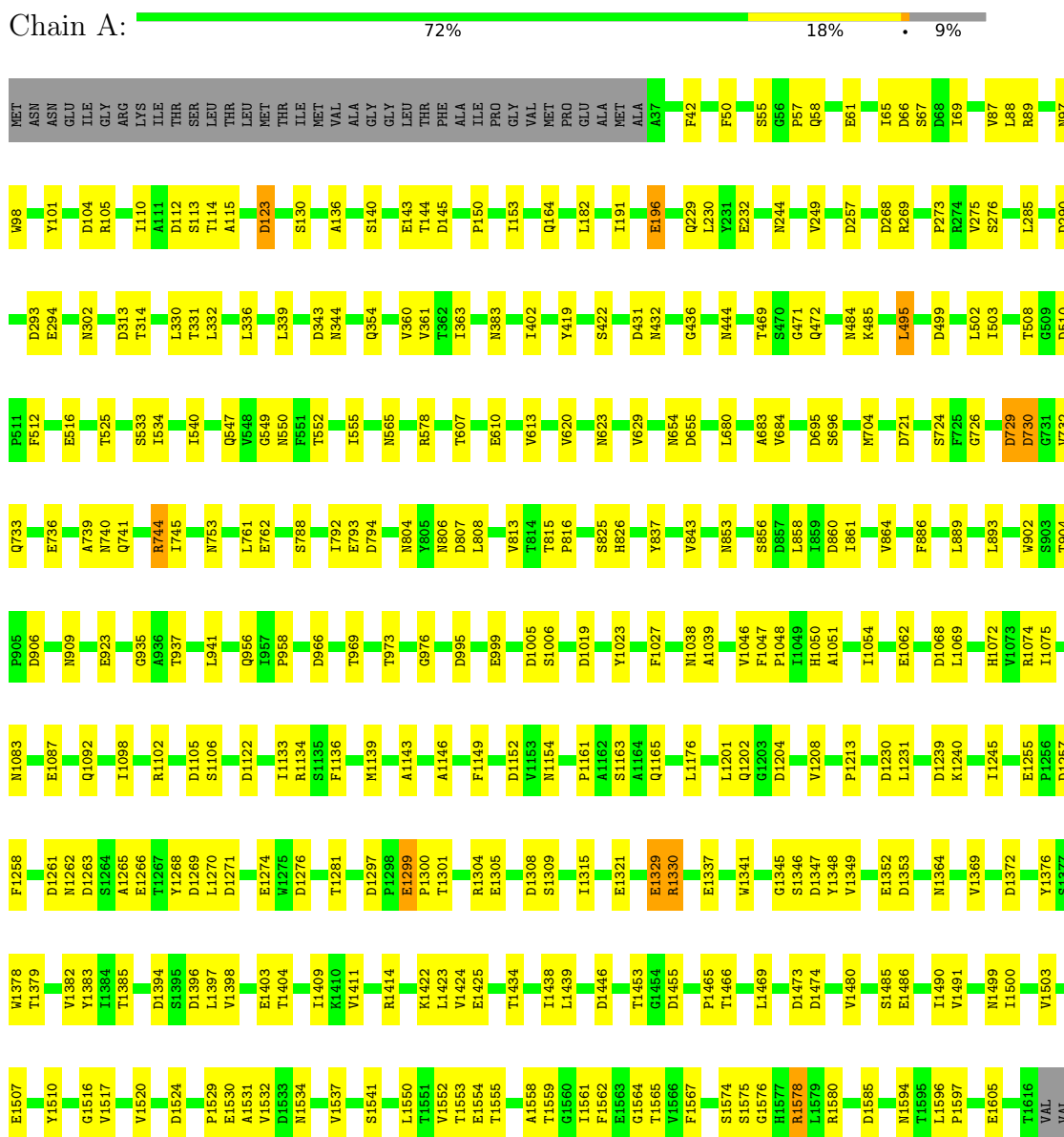
- Molecule 1 is a protein called Cell surface protein.

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

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



SER	LEU	ALA	TRP	THR	GLY	SER	LEU	SER	SER	GLY	GLN	SER	PHE	SER	PRO	PRO	LEU	SER	TRP	ILE	PRO	THR	GLU	ALA	GLY	THR	TYP	THR	ALA	THR	ALA	PHE	VAL	THR	TRP	GLU	SER	VAL	ASP	ASN	PRO	THR	ALA	LEU	SER	PRO	PRO	VAL	SER	THR	THR	VAL	ASN	VAL	SER
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- Molecule 1: Cell surface protein

Chain B: 73% 18% 9%

THR	GLJ	VAL	Y1552	F1393	Y1268	R1102	E923	V732	S276	V87	MET
GLJ	SER	SER	T1553	E1403	D1269	D1105	E923	Q733	Q736	L88	ASN
GLY	ASP	VAL	E1554	E1404	D1270	D1106	G935	E736	L285	R89	GLU
THR	GLN	GLN	T1555	T1404	D1271	S1106	G935	E736	D290	N97	ILE
TYR	GLN	VAL	E1558	I1409	E1274	D1122	L941	A739	D293	W98	GLY
THR	VAL	VAL	T1559	K1410	W1275	I1133	Q956	Q740	D293	Y101	ARG
ALA	GLN	GLN	G1560	V1411	D1276	R1134	Q956	Q741	E294	Y101	LYS
ILE	THR	ILE	I1561	R1414	T1281	S1135	P958	R744	N302	D104	ILE
ALA	SER	ALA	F1562	R1414	T1281	S1135	P958	R744	N302	D104	THR
PHE	ALA	ALA	E1563	K1422	D1297	F1136	D966	I745	F310	R105	SER
VAL	ASP	ASP	K1564	L1423	P1298	M1139	D966	N753	F310	R105	LEU
TRP	LEU	LEU	T1565	L1423	E1299	M1139	T969	N753	D313	I110	THR
GLJ	ALA	ALA	V1566	T1434	P1300	A1143	T969	L761	T314	A111	MET
ASN	ASN	GLY	F1567	T1434	T1301	A1143	T973	L761	T314	A111	THR
VAL	GLY	GLY	E1573	A1146	I792	A1146	T973	I792	L330	T114	ILE
ASP	GLN	GLN	E1574	E1338	R1304	D1152	G976	N804	T331	A115	MET
ASN	ASP	ASP	S1574	L1439	E1305	D1152	G976	N804	L332	A115	VAL
PRO	ARG	ARG	S1575	D1446	G1576	V1153	D995	Y805	L339	D123	ALA
THR	GLU	GLU	E1576	G1576	D1308	N1154	D995	Y805	L339	S130	GLY
GLN	GLN	GLN	H1577	T1453	S1309	N1154	D1005	N806	D807	S130	GLY
LEU	SER	SER	R1578	T1453	D1309	P1161	D1005	N806	D807	S130	GLY
SER	SER	PHE	L1579	T1453	D1309	P1161	D1005	N806	D807	S130	GLY
PRO	ALA	ALA	R1580	P1465	I1315	A1162	S1006	L808	D843	A136	THR
PRO	TYR	TYR	D1585	L1469	E1321	S1163	D1019	V813	N344	A136	THR
VAL	LEU	LEU	E1585	L1469	E1321	S1163	D1019	V813	I363	S140	ALA
SER	VAL	VAL	N1594	D1473	E1329	A1164	Y1023	T815	I363	S140	ALA
THR	THR	GLN	T1595	D1474	R1330	Q1165	Y1023	T815	I363	S140	ALA
VAL	VAL	GLN	L1596	D1474	R1330	Q1165	Y1023	T815	S401	E143	PRO
ASN	ASN	GLN	P1597	V1480	E1337	L1176	F1027	S825	I402	T144	GLY
SER	SER	ASP	E1605	V1480	E1337	L1176	F1027	S825	Y419	D145	VAL
ALA	ALA	GLY	T1616	V1490	D1340	L1201	N1038	H826	S422	P150	MET
VAL	VAL	VAL	T1616	V1491	D1341	Q1202	A1039	H826	I153	I153	GLU
THR	THR	THR	VAL	M1499	S1346	D1204	A1040	H826	D431	I153	GLU
VAL	VAL	SER	VAL	V1503	Y1348	D1204	A1040	H826	N432	Q164	MET
SER	LEU	LEU	PRO	E1507	Y1349	D1204	A1040	H826	R435	L182	ALA
ALA	ALA	ALA	ALA	E1507	Y1349	I1205	V1046	V843	N444	I191	M54
TRP	GLU	TRP	GLU	Y1510	D1353	T1228	F1047	N853	P447	Q229	S55
ILE	ARG	ILE	ARG	Y1510	D1353	T1228	F1047	N853	Q448	L230	G56
THR	ALA	THR	ALA	G1516	F1385	D1230	I1049	S856	Y231	P57	P57
GLY	PRO	GLY	PRO	V1517	F1385	D1231	E1062	A683	E232	Q58	Q58
SER	ALA	SER	ALA	V1517	V1369	L1231	E1062	A683	T469	L233	Q58
LEU	ALA	LEU	ALA	V1520	D1372	D1239	D1068	V684	T469	L233	Q58
SER	ASN	SER	ASN	V1520	D1372	K1240	L1069	D695	S470	N234	E81
LEU	LEU	SER	LEU	D1524	Y1376	I1245	H1072	F886	C471	N234	E81
GLY	ARG	GLY	ARG	D1524	Y1376	I1245	H1072	F886	Q472	N244	T65
GLN	THR	GLN	THR	P1529	S1377	D1257	I1075	L889	N484	V249	D66
SER	ASP	SER	ASP	P1529	S1377	D1257	I1075	L889	K485	V249	S87
PHE	THR	PHE	THR	P1529	S1377	D1257	I1075	L889	K485	V249	S87
SER	ALA	SER	ALA	V1532	V1382	F1258	M1083	L893	D257	I69	I69
PRO	PHE	PRO	PHE	V1532	V1382	F1258	M1083	L893	L495	D257	I69
ALA	GLY	ALA	GLY	V1537	V1383	D1261	E1087	W902	F723	D268	K76
LEU	ASN	LEU	ASN	V1537	V1383	D1261	E1087	W902	T501	R269	K76
SER	SER	SER	SER	S1541	T1385	D1263	Q1092	T904	L502	P273	N84
TRP	TRP	TRP	TRP	S1541	T1385	D1263	Q1092	T904	I503	P273	N84
ILE	LEU	ILE	LEU	L1550	T1550	A1265	I1098	D906	D730	R274	G85
ASP	ASP	ASP	ASP	T1550	T1550	A1265	I1098	D906	T503	R274	G85
SER	SER	SER	SER	T1550	T1550	A1265	I1098	D906	T503	R274	G85

- Molecule 1: Cell surface protein

Chain C:  73% 18% 9%

- Molecule 1: Cell surface protein

Response	Percentage
Doing a good job	73%
Not doing a good job	18%
Unsure	9%



LEU	ASP	TRP	S1641	D1390	E1266	I1098
ILE	SER	ILE	L1550	F1393	I1267	I1098
PRO	SER	PRO	T1551	F1393	Y1268	R1102
GLU	SER	GLU	T1552	E1403	D1269	D1270
ALA	VAL	ALA	T1553	T1404	D1271	D1271
ASP	ASP	GLY	E1554	T1404	S1106	S1106
GLN	GLN	THR	T1555	T1409	D1122	D1122
TYR	VAL	TYR	A1558	T1410	E1274	E1274
ALA	GLN	ALA	T1559	V1411	D1276	D1276
THR	ILE	THR	G1560	R1414	T1281	T1281
ALA	SER	ALA	F1561	R1414	R1133	R1133
PHE	ALA	PHE	F1562	K1422	R1134	R1134
VAL	ASP	VAL	E1563	L1423	F1136	F1136
TRP	LEU	TRP	E1564	L1423	P1298	P1298
GLU	ALA	GLU	T1565	T1434	E1299	E1299
SER	ASN	SER	T1566	T1434	P1300	P1300
VAL	GLY	VAL	F1567	T1438	T1301	T1301
ASP	GLN	ASP	S1574	L1439	R1304	R1304
ASN	ASP	ASN	S1575	L1439	E1305	E1305
PRO	ARG	PRO	G1576	D1446	F1149	F1149
THR	GLN	THR	H1577	D1446	D1308	D1308
ALA	GLN	ALA	R1578	T1453	S1309	S1309
LEU	SER	LEU	L1579	P1465	I1315	I1315
SER	PHE	SER	R1580	P1465	P1161	P1161
PRO	ALA	PRO	D1585	L1469	E1321	E1321
TYR	LEU	TYR	D1585	L1469	A1162	A1162
VAL	VAL	VAL	N1594	D1473	S1163	S1163
SER	GLN	SER	T1595	D1474	A1164	A1164
THR	ILE	THR	L1596	D1474	Q1165	Q1165
VAL	GLN	VAL	P1597	V1480	L1176	L1176
ASN	ASP	ASN	E1605	T1490	D1340	D1340
ALA	ALA	ALA	T1616	T1490	W1341	W1341
GLY	GLY	GLY	VAL	N1499	S1346	S1346
THR	THR	THR	VAL	I1500	D1347	D1347
VAL	VAL	VAL	PRO	I1500	Y1348	Y1348
SER	SER	SER	PRO	V1503	V1349	V1349
LEU	LEU	LEU	LEU	V1503	E1352	E1352
THR	THR	THR	ARG	E1507	D1353	D1353
ALA	ALA	ALA	ALA	Y1510	F1365	F1365
ASN	ASN	ASN	ALA	G1516	V1369	V1369
LEU	LEU	LEU	ALA	V1517	D1239	D1239
SER	SER	SER	ASN	V1520	K1240	K1240
GLY	GLY	GLY	LEU	V1520	T1245	T1245
THR	THR	THR	ARG	D1524	D1257	D1257
VAL	VAL	VAL	THR	D1524	F1257	F1257
PHE	PHE	PHE	ASP	P1529	W1378	W1378
ALA	ALA	ALA	ALA	V1532	T1379	T1379
PRO	PRO	PRO	PHE	V1532	D1261	D1261
ALA	ALA	ALA	GLY	V1537	N1262	N1262
LEU	LEU	LEU	ASN	V1537	I1383	I1383
SER	SER	SER	SER	V1537	S1264	S1264
					A1265	A1265

• Molecule 1: Cell surface protein

Chain F:  72% 18% 9%

MET	ASN	D104	N302	I534	N740	G935	E1087	L1231
ASN	ASN	R105	F310	I540	R744	A936	Q1092	D1239
GLU	GLU	I110	D313	Q547	I745	T937	I1098	K1240
ILE	ILE	A111	T314	G548	E749	L941	R1102	I1245
ARG	ARG	D112	D314	G549	T750	D954	G1103	D1257
LYS	LYS	S113	N322	N550	G751	P955	S1104	F1258
ILE	ILE	A115	L330	F951	D752	Q956	S1105	D1261
THR	THR	D123	T331	T552	N753	P957	S1106	D1263
LEU	LEU	S130	L332	I555	L761	D966	D1122	N1262
THR	THR	A136	R333	N555	E762	T969	T1133	D1263
LEU	LEU	S140	T334	R578	S788	R1134	R1134	A1265
MET	MET	I153	L336	I580	I792	T973	S1135	I1267
ILE	ILE	E143	D343	I580	T804	T976	F1136	Y1268
VAL	VAL	T144	N344	T607	T805	G976	M1139	D1269
GLY	GLY	D145	T363	E610	N806	G983	A1143	L1270
LEU	LEU	P150	S401	E610	L807	L984	A1146	D1271
THR	THR	I153	I402	V613	L808	D985	D1152	E1274
PHE	PHE	Q164	P411	V620	T813	D995	N1153	W1275
ALA	ALA	I182	Y419	N623	T815	E999	N1154	D1276
MET	MET	I191	E421	V629	P816	D1005	P1161	T1281
PRO	PRO	A197	S422	N654	S825	S1006	A1162	D1297
GLU	GLU	A197	D431	D655	H826	D1019	S1163	E1299
ALA	ALA	P226	N432	L680	Y837	Y1023	A1164	P1300
MET	MET	Q229	R435	A683	V843	F1027	Q1165	T1301
ALA	ALA	L230	G436	V684	N853	N1038	L1176	D1308
A37	R38	T231	N444	D695	L858	A1039	L1201	S1309
F42	F50	E232	T469	S696	I859	V1046	Q1202	I1315
Q58	Q68	S251	Q472	M704	D860	F1047	G1203	E1321
T65	D66	D268	N484	V717	V864	P1048	D1204	S1322
D66	S67	R269	R488	D721	F886	H1050	I1205	K1327
D68	D68	S276	L495	S724	L889	A1051	L1206	R1330
I69	I69	H279	L502	F725	L893	I1054	Q1207	E1337
V67	L88	L285	L503	G726	W902	E1062	V1208	D1340
R89	R89	D290	F512	D730	S903	D1068	P1213	D1341
Y94	Y94	D293	E516	G731	T904	L1069	S1217	G1345
N97	N97	E294	T525	V732	P905	H1072	G1218	S1346
Y98	Y98	S533	A739	Q733	D906	I1075	D1219	D1347
				E736	N909	M1083	N1221	Y1348
				A739	E923		T1222	V1349
							H1223	E1352
							T1224	D1353
							D1225	
							S1226	
							D1230	

[illegible]

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 (\AA)	349.44, 349.44, 349.44	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.092, 1.092, 1.092	Depositor

5 Model quality

5.1 Standard geometry

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

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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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.

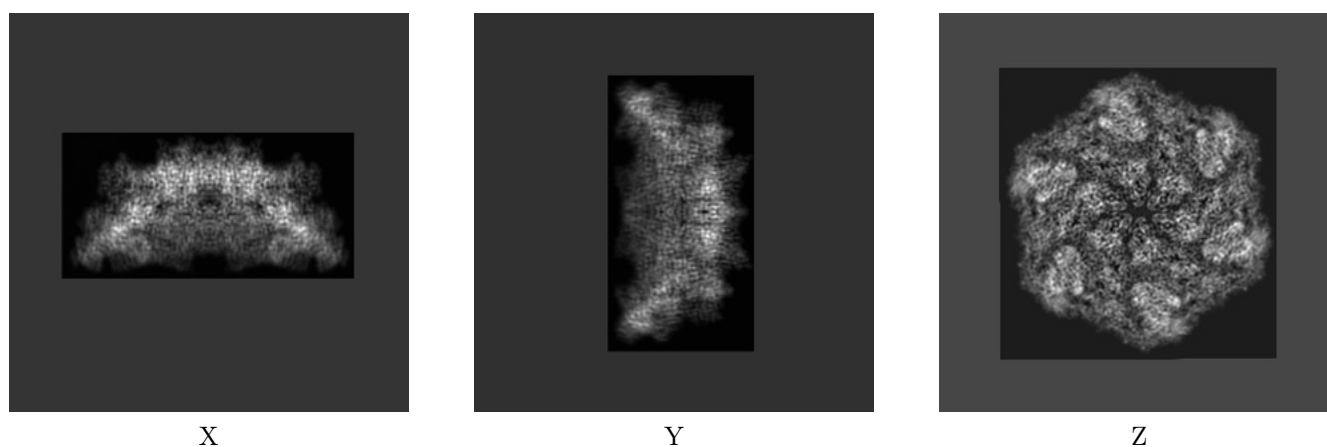
6 Map visualisation [i](#)

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](#)

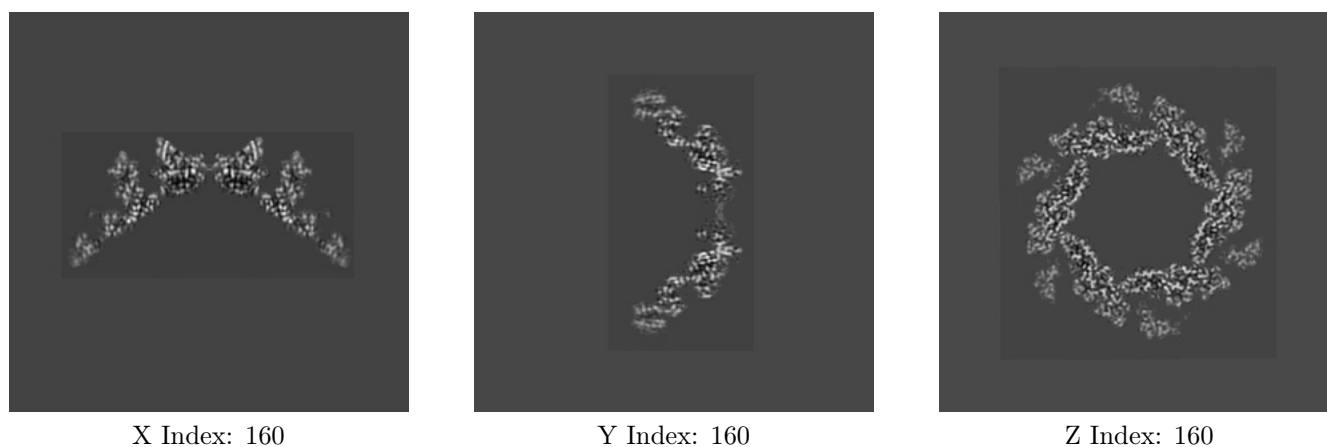
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



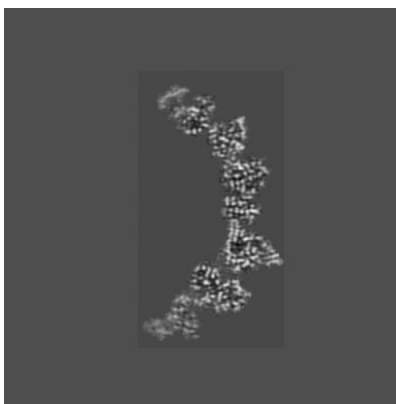
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 156



Y Index: 175

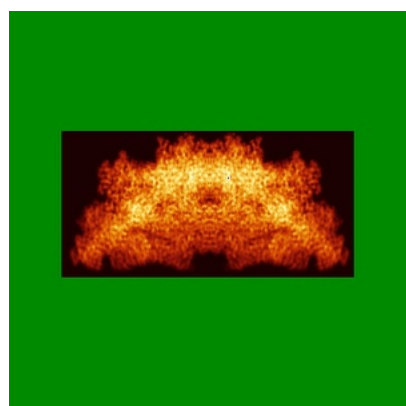


Z Index: 186

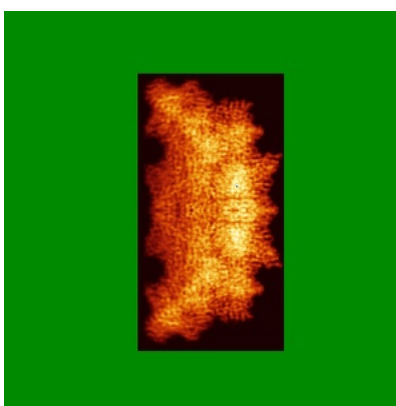
The images above show the largest variance slices of the map in three orthogonal directions.

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

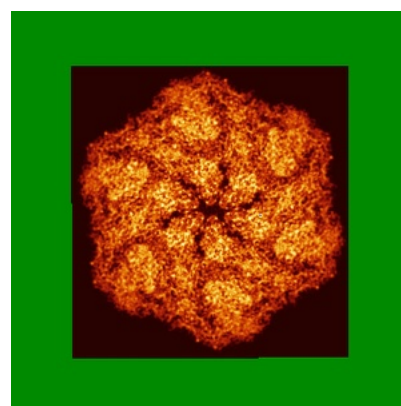
6.4.1 Primary map



X



Y

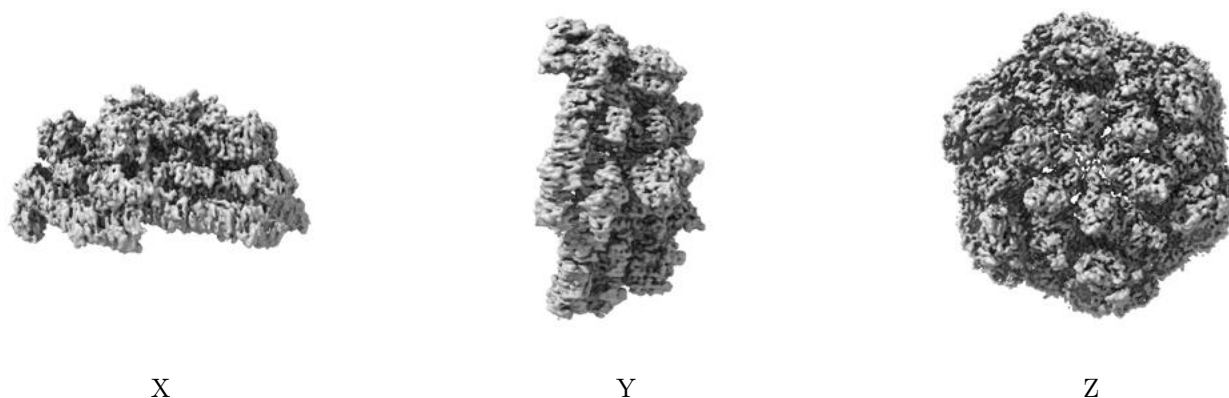


Z

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.

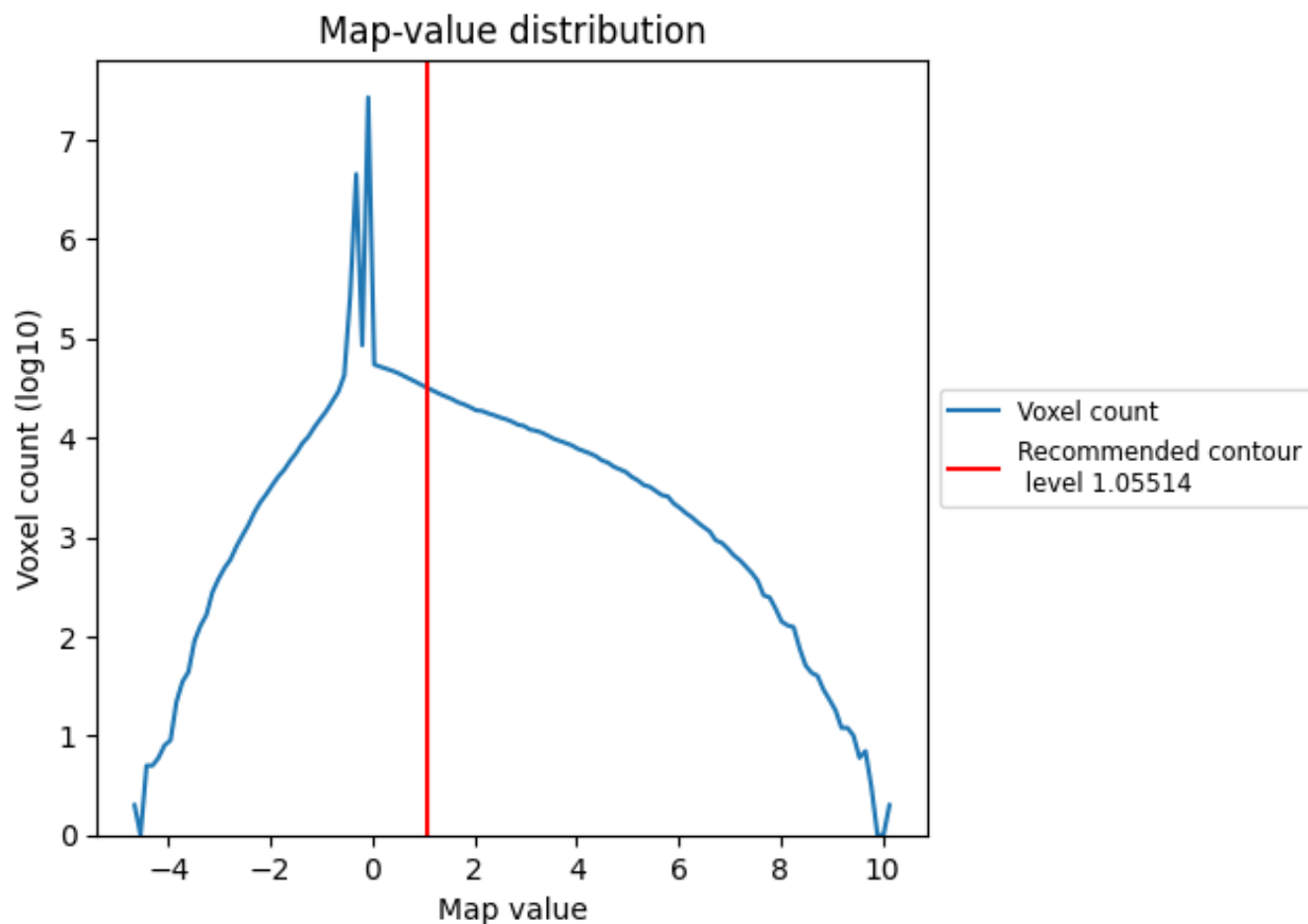
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

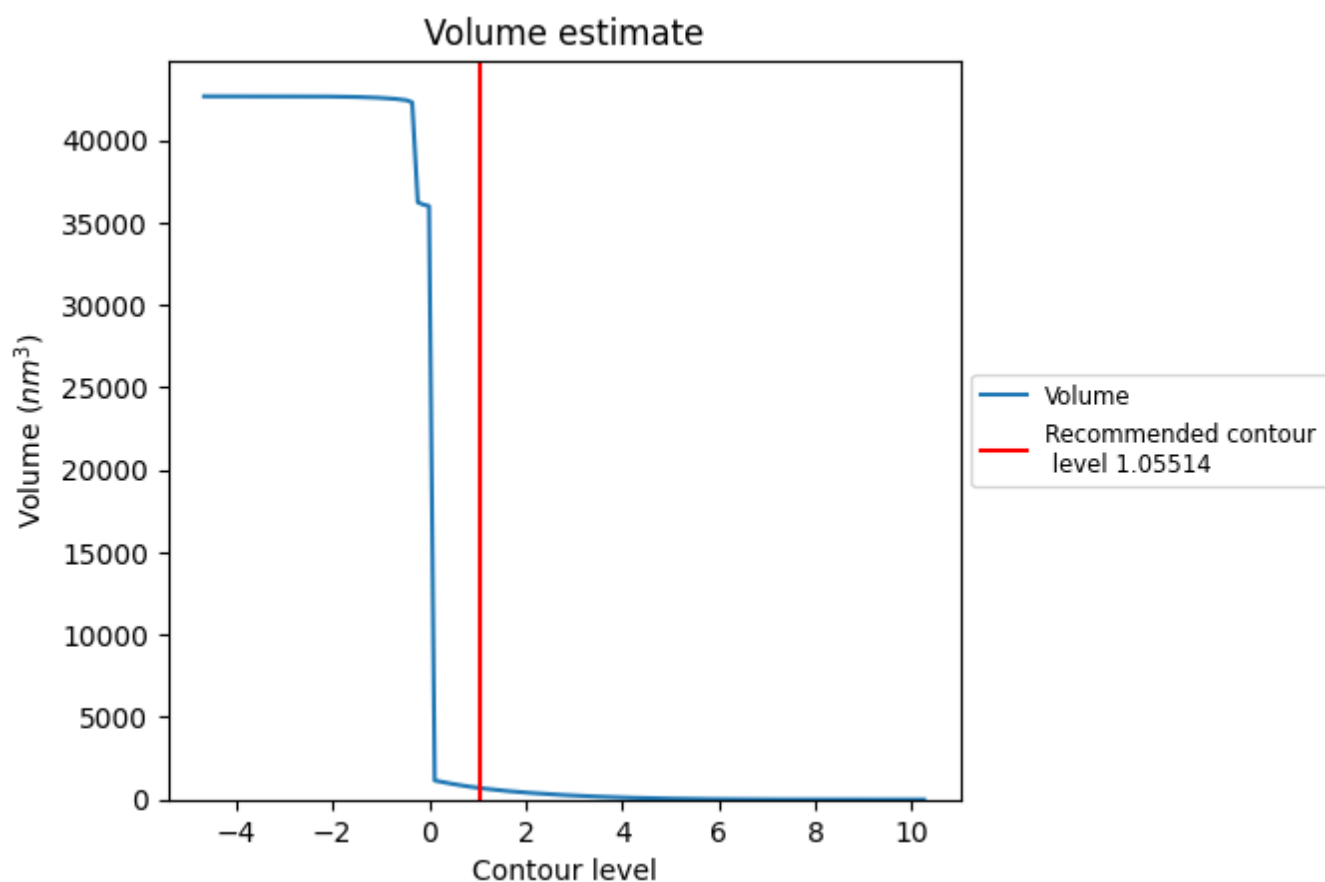
This section contains the results of statistical analysis of the map.

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.

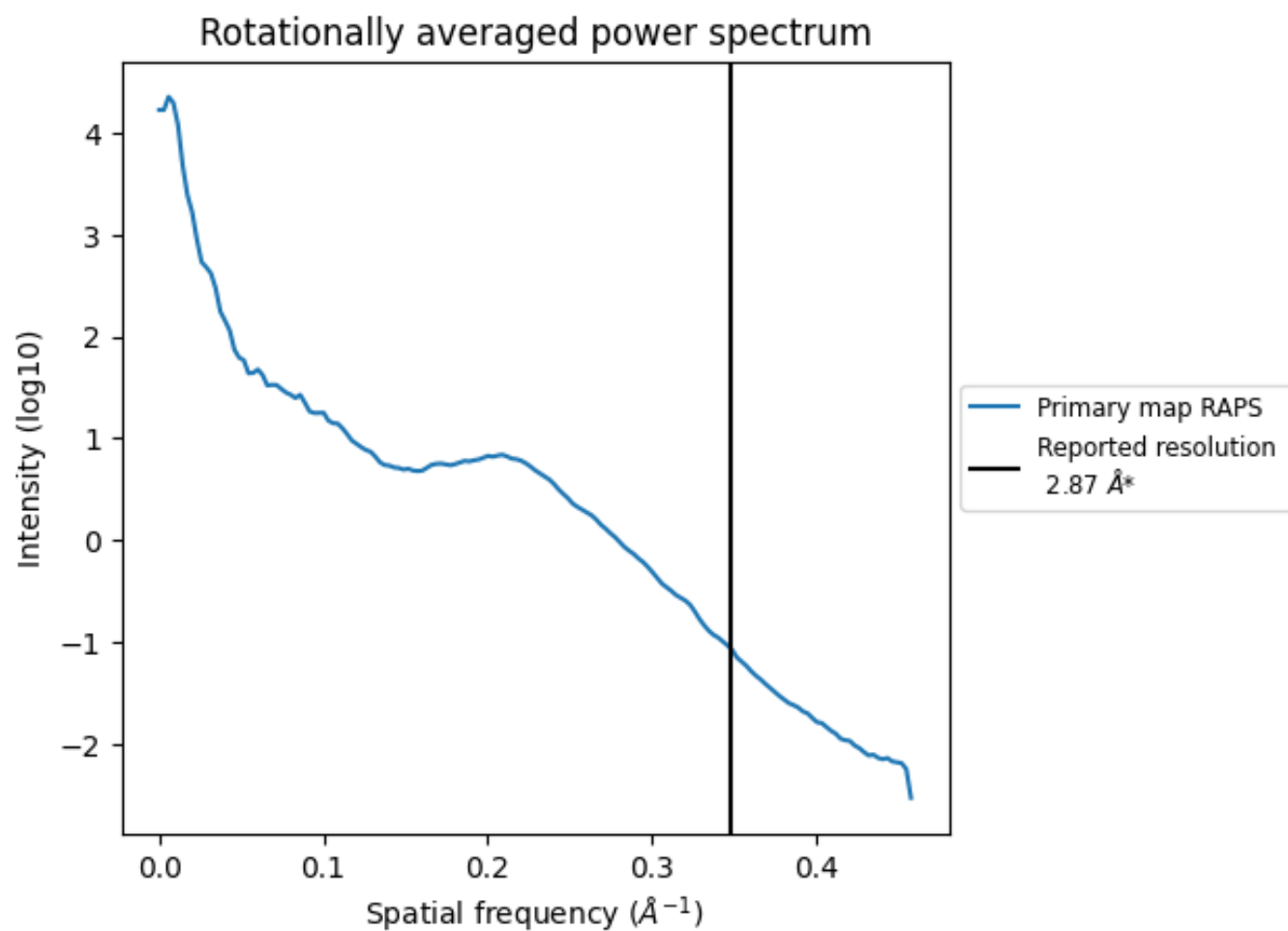
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 697 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

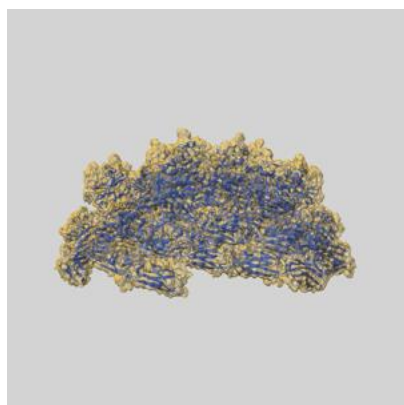
8 Fourier-Shell correlation ⓘ

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

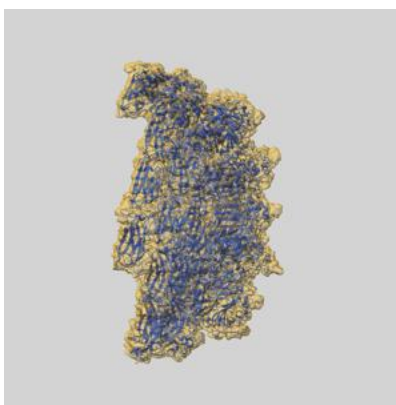
9 Map-model fit [i](#)

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](#).

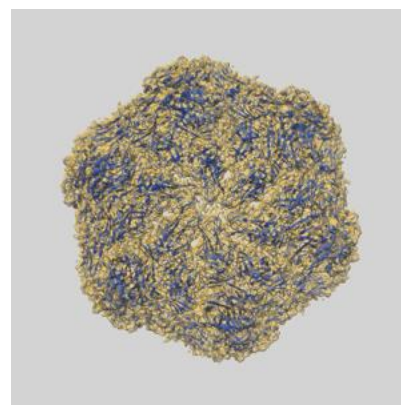
9.1 Map-model overlay [i](#)



X



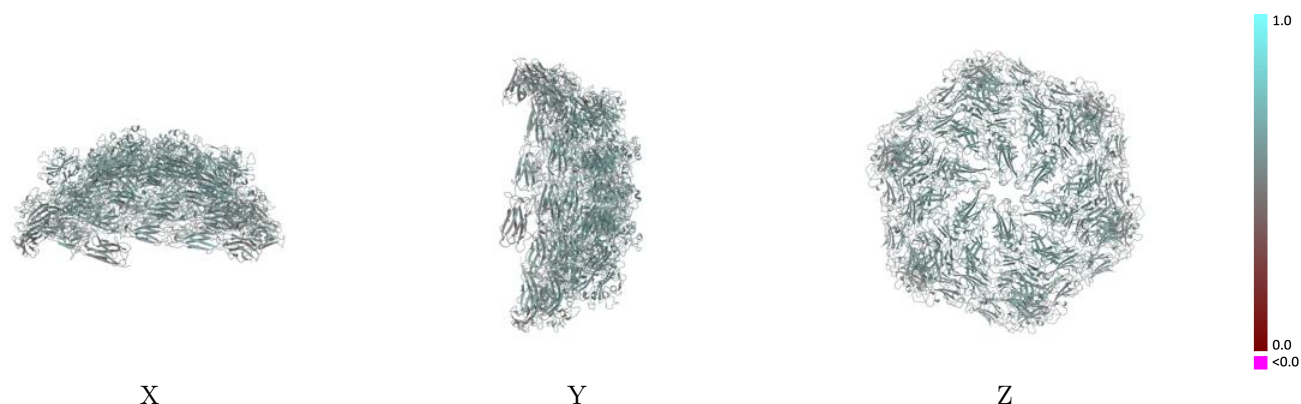
Y



Z

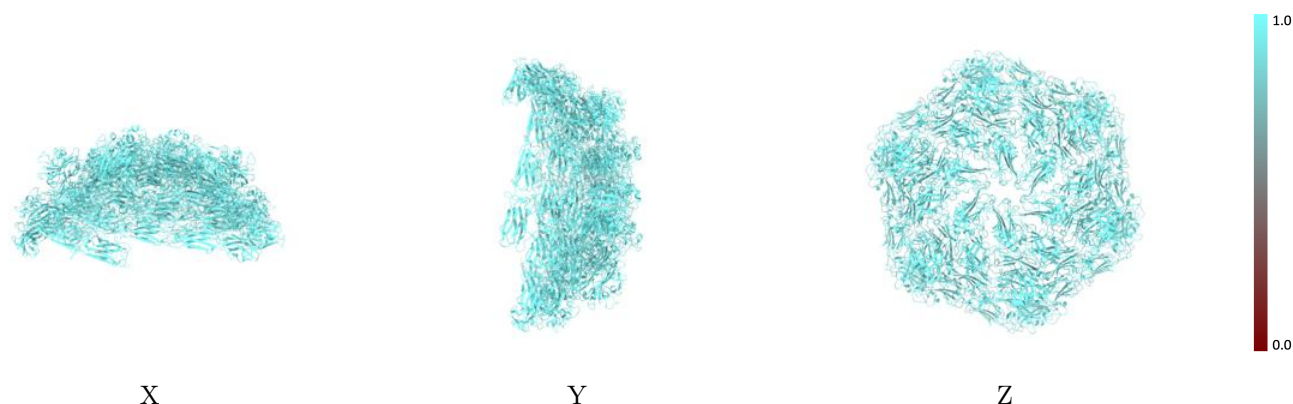
The images above show the 3D surface view of the map at the recommended contour level 1.05514 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



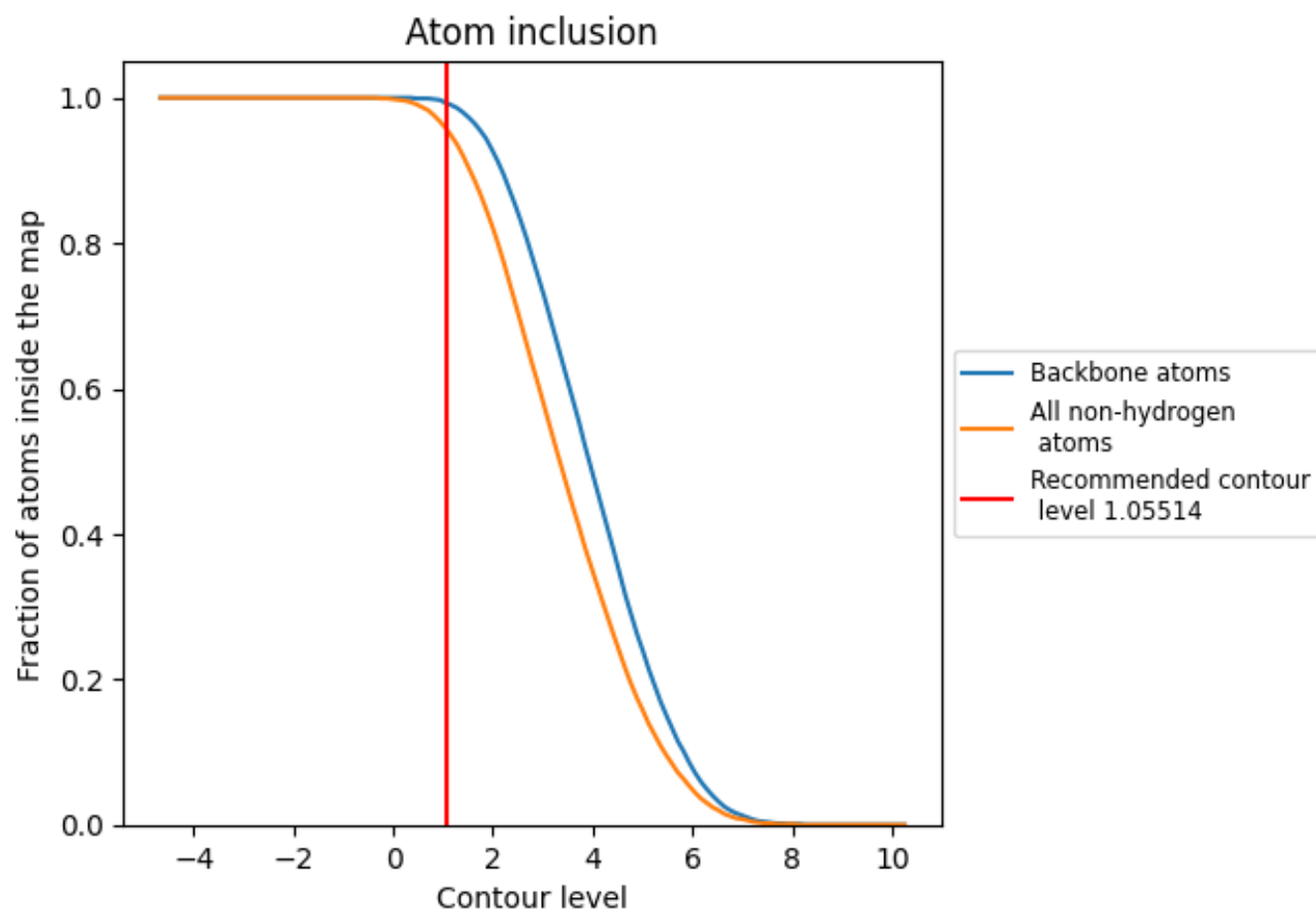
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div></div> 0.9580	<div><div></div></div> 0.5560
A	<div><div></div></div> 0.9620	<div><div></div></div> 0.5630
B	<div><div></div></div> 0.9580	<div><div></div></div> 0.5530
C	<div><div></div></div> 0.9530	<div><div></div></div> 0.5520
D	<div><div></div></div> 0.9630	<div><div></div></div> 0.5620
E	<div><div></div></div> 0.9580	<div><div></div></div> 0.5530
F	<div><div></div></div> 0.9540	<div><div></div></div> 0.5520

1.0

0.0

<0.0