WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Apr 9, 2025 – 01:29 PM JST

PDB ID	:	9LC0 / pdb_00009lc0
EMDB ID	:	EMD-62961
Title	:	tail complex of mature phage N4
Authors	:	Liu, H.; Chen, W.
Deposited on	:	2025-01-03
Resolution	:	3.20 Å(reported)

This is a Full wwPDB EM Validation 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:

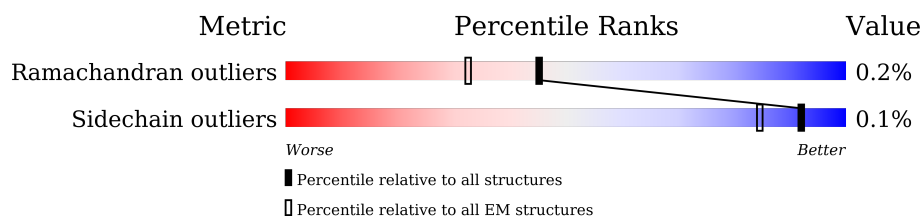|		
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.20 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	Percentile Ranks	Value
Ramachandran outliers		0.2%
Sidechain outliers		0.1%

Worse *Better*

▊ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
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 <=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	556	5% / 13% / 87%
1	B	556	5% / 16% / 84%
1	C	556	5% / 16% / 84%
1	D	556	5% / 12% / 88%
1	E	556	6% / 16% / 84%
1	F	556	6% / 15% / 84%
1	G	556	5% / 13% / 87%
1	L	556	5% / 16% / 84%
1	Q	556	6% / 16% / 84%

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Mol	Chain	Length	Quality of chain
1	V	556	5% / 12% / 88%
1	a	556	6% / 16% / 84%
1	f	556	6% / 16% / 84%
2	M	417	99%
2	R	417	99%
3	I	1382	15% / 100%
3	N	1382	86% / 14%
4	H	236	100%
4	J	236	100%
4	O	236	100%
4	S	236	100%
5	K	299	99%
5	P	299	99%
5	T	299	99%
5	U	299	99%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 51753 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 60 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	73	Total	C	N	O	S	0	0
			589	379	96	110	4		
1	B	91	Total	C	N	O	S	0	0
			729	468	118	138	5		
1	C	88	Total	C	N	O	S	0	0
			703	450	115	133	5		
1	D	69	Total	C	N	O	S	0	0
			559	361	92	103	3		
1	E	91	Total	C	N	O	S	0	0
			729	468	118	138	5		
1	F	88	Total	C	N	O	S	0	0
			703	450	115	133	5		
1	G	73	Total	C	N	O	S	0	0
			589	379	96	110	4		
1	L	91	Total	C	N	O	S	0	0
			729	468	118	138	5		
1	Q	88	Total	C	N	O	S	0	0
			703	450	115	133	5		
1	V	69	Total	C	N	O	S	0	0
			559	361	92	103	3		
1	a	91	Total	C	N	O	S	0	0
			729	468	118	138	5		
1	f	88	Total	C	N	O	S	0	0
			703	450	115	133	5		

- Molecule 2 is a protein called Gp64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	415	Total	C	N	O	S	0	0
			3384	2213	537	616	18		
2	R	415	Total	C	N	O	S	0	0
			3384	2213	537	616	18		

- Molecule 3 is a protein called Non-contractile tail sheath.

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	1381	Total 10866	C 6904	N 1831	O 2082	S 49	0	0
3	N	1190	Total 9403	C 5989	N 1583	O 1789	S 42	0	0

- Molecule 4 is a protein called 30 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	236	Total 1911	C 1201	N 327	O 374	S 9	0	0
4	O	236	Total 1911	C 1201	N 327	O 374	S 9	0	0
4	S	236	Total 1911	C 1201	N 327	O 374	S 9	0	0
4	H	236	Total 1911	C 1201	N 327	O 374	S 9	0	0

- Molecule 5 is a protein called Gp54.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	298	Total 2262	C 1408	N 381	O 463	S 10	0	0
5	P	298	Total 2262	C 1408	N 381	O 463	S 10	0	0
5	T	298	Total 2262	C 1408	N 381	O 463	S 10	0	0
5	U	298	Total 2262	C 1408	N 381	O 463	S 10	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: 60 kDa protein

• Molecule 1: 60 kDa protein

• Molecule 1: 60 kDa protein

Chain C:

5%

16%   84%

• Molecule 1: 60 kDa protein

Chain D:

5%

12%   88%

• Molecule 1: 60 kDa protein

Chain E:

6%

16%   84%

• Molecule 1: 60 kDa protein

6%

Chain F:

15% 84%

• Molecule 1: 60 kDa protein

5%

Chain G:

13% 87%

SER THR VAL THR PHE SER LEU LEU LEU PRO THR ASP ASP THR GLN LEU THR ALA GLN LEU LYS SER HIS THR ASP SER SER PHE VAL VAL LYS ILE ALA LYS PRO ASP GLY SER LEU LEU ASP ALA PRO LEU GLU GLY MET GLY ILE MET SER ARG GLY MET HIS GLY ILE TYR LYS

VAL PRO TYR GLY SER LEU ILE VAL ASP VAL GLY ARG VAL GLN VAL LYS PHE SER GLU PHE ASN THR GLU GLY ILE SER VAL VAL GLY ILE ASN SER ASN ALA

• Molecule 1: 60 kDa protein

Chain L:

5%

16%   84%

MET SER GLY HIS THR PRO PHE ASN **T9** **E18** **D22** **S67** **L73** **D74** **E75** **L76** **Q77** **L78** **I79** **H80** **N81** **N82** **L83** **D84** **K85** **L86** **Q87** **E88** **L89** **Y90** **N91** **Q92** **L93** **S94** **K95** **L96** **T97** **G98** **L99** TYR ASP ASN LEU GLN ALA LEU LEU ARG VAL TYR ASP ASN LEU THR PRO ILE

ASN THR VAL ALA SER ASN ILE ASP ALA VAL ASN THR VAL ALA THR ASP ILE ALA LYS VAL ILE ILE VAL SER ALA GLN ILE ASP LYS VAL ILE THR VAL ALA ASN SER ILE THR ASN VAL ASN THR VAL ALA GLY SER ILE ASP ALA VAL ASN THR VAL SER THR ASN ILE ASN ALA ILE

LYS ASN VAL ASN THR ASN MET ALA ALA LEU ASP ASP LEU ASP ASN HIS MET THR GLU LEU ALA VAL HIS ALA LEU GLY LEU ASP LEU VAL THR ILE ALA GLU GLN LEU LEU ASP THR ILE ILE ALA ASP HIS GLU LYS TYR ALA THR ALA GLU GLY LEU ILE ILE GLY PHE ASN GLN

ALA GLN THR TYR ALA ALA ASN THR VAL GLY ALA MET LEU ARG GLN VAL ILE THR MET GLY ASN ASP LYS GLY TYR ALA VAL ALA GLY LYS THR LEU SER ALA ARG GLY TRP SER LEU ALA THR GLY SER ILE ASN MET ASN ALA PRO THR ALA GLY ALA VAL ALA ASN LEU VAL

LEU ASN TYR LYS ALA GLY LYS VAL SER VAL SER LEU LEU VAL ALA PRO SER GLN MET ALA LEU ASP GLY LEU ILE MET GLY ALA SER THR ALA ASP ASN THR ALA THR VAL THR ALA PRO LEU ARG PHE LYS ALA ASP LEU THR LYS THR ILE SER GLY VAL ASN THR ARG

ILE MET PRO SER ALA VAL THR LEU ASN VAL ASP ALA TYR GLY ILE THR LEU GLY TYR PRO PRO SER LEU GLN THR VAL GLU PRO VAL MET PHE ILE THR PRO THR GLY LYS ALA PRO LEU THR PRO ARG PHE LYS ALA ASP LEU THR LYS THR ILE SER GLY VAL ASN THR ARG VAL MET VAL

GLY GLU ALA GLU ALA GLN LEU LYS TYR SER GLY GLY TRP ALA ALA VAL SER ASP TRP ASP SER GLY THR TYR CYS ALA PHE ASP THR VAL SER GLU LEU VAL TYR HIS SER THR LEU ILE LYS SER SER THR VAL THR PHE SER LEU LEU LEU PRO THR ASP ASP THR GLN

LEU THR ALA GLN LEU LYS HIS THR ASP SER SER PHE VAL VAL LYS ILE ALA LYS PRO ASP GLY SER LEU LEU ASP ALA PRO LEU GLU GLY MET GLY ILE MET SER ARG GLY MET HIS ILE TYR LYS PRO ILE SER VAL PRO TYR GLY SER LEU ILE VAL ASP VAL GLY ARG VAL GLN VAL LYS

LYS PHE SER GLU PHE ASN THR THR GLU GLY ILE SER VAL VAL GLY ILE ASN SER ASN ALA

• Molecule 1: 60 kDa protein

Chain Q:

6%

16%   84%

MET **S2** **N12** **E13** **G14** **Y15** **C16** **C17** **E18** **N61** **K62** **L63** **T64** **S67** **A68** **I69** **Y70** **T71** **K72** **L73** **D74** **E75** **L76** **Q77** **L78** **I79** **H80** **N81** **N82** **L83** **D84** **K85** **L86** **Q87** **E88** **L89** TYR ASN GLN LEU SER GLN LYS SER LEU THR GLY LEU TYR LEU ASP TYR ASP ASN LEU GLN ALA LEU LEU ARG VAL TYR

ASP ASN LEU THR PRO ILE ASN THR VAL ALA SER ASN ILE ASP ALA VAL ASN THR VAL ALA THR ASP ILE ALA LYS VAL ILE ILE VAL SER ALA GLN ILE ASP LYS VAL ILE THR VAL ALA ASN SER ILE THR ASN VAL ASN THR VAL ALA GLY SER ILE ASP ALA VAL ASN THR VAL SER

THR ASN ILE ASN ALA ILE LYS ASN VAL ASN THR ASN MET ALA ALA LEU ASP ASP LEU ASP ASN HIS MET THR GLU LEU ALA VAL HIS ALA LEU GLY LEU ASP LEU VAL THR ILE ALA GLU GLN LEU LEU ASP THR ILE ILE ALA ASP HIS GLU LYS TYR ALA THR ALA GLU GLY LEU ILE ILE GLY PHE ASN GLN ALA GLY

LEU ILE GLY PHE ASN GLN ALA GLN THR TYR ALA ALA ASN THR VAL GLY ALA MET LEU ARG GLN VAL ILE THR MET GLY ASN ASP LYS GLY TYR ALA VAL ALA GLY LYS THR LEU SER ALA ARG GLY TRP SER LEU ALA THR GLY SER ILE ASN MET ASN ALA PRO THR ALA GLY

ALA VAL ALA ASN LEU VAL LEU ASN TYR LYS ALA GLY LYS VAL SER VAL SER LEU LEU VAL ALA PRO SER GLN MET ALA LEU ASP GLY LEU ILE MET GLY ALA SER THR ALA ASP ASN THR ALA THR VAL THR ALA PRO LEU ARG PHE LYS ALA ASP LEU THR LYS THR ILE

• Molecule 1: 60 kDa protein

Chain V:

5%

12% 88%

• Molecule 1: 60 kDa protein

Chain a:

6%

16% 84%

• Molecule 1: 60 kDa protein

Chain f:

6%
16%
84%

• Molecule 2: Gp64

Chain M:

99%

• Molecule 2: Gp64

Chain R:

99%

MET S2 Y167 G214 S215 Y216 T246 P247 A254 E258 D340 E371 C416 GLY

• Molecule 3: Non-contractile tail sheath

Chain I:

15%

100%

MET S2 K10 L13 D21 F34 K35 K36 D37 R47 R48 N49 L242 S510 A513 Q589 S813 N814 K849 R983 A1006 K1122 N1143 E1144 S1184 M1187 N1188 A1191 G1192 L1193 Y1194 A1195 V1196 F1197 T1198 G1199 D1200 P1201 G1202 N1203 S1204 N1205

I1206 K1207 I1208 M1209 W1210 D1211 K1212 P1213 S1214 V1215 G1216 G1217 R1218 D1219 V1220 R1221 I1222 R1223 N1224 M1225 H1226 V1227 T1228 S1229 S1230 A1231 T1232 I1233 S1234 D1235 Q1236 F1237 V1238 S1239 D1240 N1241 N1242 L1243 V1244 F1245 T1246 R1247 E1248 E1249 Q1250 V1251 A1252 A1253 Y1254 G1255 F1256 T1257 A1258 S1259 S1260 V1261 S1262 V1263 R1264 A1265

Q1266 D1269 I1270 E1271 S1272 G1273 A1274 L1275 G1276 L1277 T1278 T1279 E1280 Y1281 V1282 A1283 V1284 P1285 E1286 T1287 A1288 G1289 T1290 V1291 G1292 Q1293 G1294 F1295 A1296 K1297 K1298 D1299 S1300 V1301 G1302 N1303 C1304 T1305 M1306 S1307 W1308 E1309 V1310 G1311 D1312 A1313 V1314 Q1315 W1316 Q1317 V1318 E1319 I1320 L1321 N1322 A1323 E1324 N1325 S1326

T1327 V1328 V1329 K1330 T1331 E1332 I1333 V1334 V1335 A1336 P1337 T1338 I1339 T1340 W1341 M1342 A1343 E1344 E1345 I1346 T1347 A1348 E1349 Y1350 G1351 Y1352 L1353 T1354 D1355 H1356 M1357 V1358 W1359 R1360 V1361 R1362 P1363 Y1364 R1365 A1366 D1367 G1368 A1369 S1370 N1371 V1372 A1373 K1374 Q1375 F1376 D1377 M1378 T1379 V1380 T1381 L1382

• Molecule 3: Non-contractile tail sheath

Chain N:

86%   14%

MET S2 K10 D21 F34 K35 K36 N49 L242 N501 S510 D551 D722 T811 K849 N852 A1006 D1062 D1097 R1105 N1143 E1144 E1149 E1150 S1184 N1185 P1186 M1187 N1188 P1189 V1190 A1191 GLY LEU TYR ALA VAL PHE THR GLY ASP

PRO GLY ASN SER ASN ILE LYS ILE MET TRP ASP LYS SER PRO SER VAL GLY GLY ARG ASP VAL ILE ARG ASN MET HIS VAL THR SER SER ALA THR ILE SER ASP GLN PHE VAL SER ASP ASN ASN LEU VAL PHE THR ARG GLU GLN GLN VAL ALA ALA TYR GLY PHE THR ALA SER SER

VAL SER VAL ARG ALA GLN GLU HIS ASP ILE GLU SER GLY ALA LEU GLY LEU THR THR GLU TYR VAL ALA VAL PRO GLU THR ALA GLY THR GLY THR GLY PHE ALA LYS LYS ASP SER SER VAL GLY ASN CYS THR MET SER TRP GLU VAL GLY VAL ASP ALA VAL GLN TRP GLN VAL GLU ILE

LEU ASN ALA GLU ASN SER THR VAL VAL LYS THR GLU ILE VAL VAL ALA PRO THR ILE THR TRP MET ALA GLU GLU ILE THR ALA GLU TYR GLY TYR LEU THR ASP HIS MET VAL TRP ARG VAL ARG PRO TYR ARG ALA ASP GLY ALA SER ASN VAL ALA LYS GLN PHE ASP MET THR ALA

THR LEU

• Molecule 4: 30 kDa protein

Chain J:

100%

M1 D24 R115 R236

• Molecule 4: 30 kDa protein

Chain O:

100%

• Molecule 4: 30 kDa protein

Chain S:

100%

• Molecule 4: 30 kDa protein

Chain H:

100%

• Molecule 5: Gp54

Chain K:

99%

• Molecule 5: Gp54

Chain P:

99%

• Molecule 5: Gp54

Chain T:

99%

• Molecule 5: Gp54

Chain U:

99%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47179	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	32	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	57.334	Depositor
Minimum map value	-45.213	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.815	Depositor
Recommended contour level	5.2	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.25	0/597	0.48	0/808
1	B	0.26	0/740	0.41	0/1003
1	C	0.27	0/716	0.50	0/972
1	D	0.24	0/567	0.41	0/767
1	E	0.26	0/740	0.40	0/1003
1	F	0.26	0/716	0.46	0/972
1	G	0.25	0/597	0.44	0/808
1	L	0.27	0/740	0.44	0/1003
1	Q	0.27	0/716	0.51	0/972
1	V	0.25	0/567	0.41	0/767
1	a	0.25	0/740	0.40	0/1003
1	f	0.26	0/716	0.44	0/972
2	M	0.28	0/3499	0.48	1/4784 (0.0%)
2	R	0.28	0/3499	0.47	1/4784 (0.0%)
3	I	0.27	0/11163	0.49	1/15218 (0.0%)
3	N	0.27	0/9670	0.49	1/13182 (0.0%)
4	H	0.30	0/1952	0.50	0/2654
4	J	0.30	0/1952	0.50	0/2654
4	O	0.30	0/1952	0.51	0/2654
4	S	0.30	0/1952	0.51	0/2654
5	K	0.30	0/2289	0.50	0/3103
5	P	0.31	0/2289	0.51	0/3103
5	T	0.31	0/2289	0.50	0/3103
5	U	0.31	0/2289	0.50	0/3103
All	All	0.28	0/52947	0.49	4/72046 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	R	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	246	THR	C-N-CD	-8.30	102.33	120.60
2	M	246	THR	C-N-CD	-7.38	104.35	120.60
3	I	242	LEU	CA-CB-CG	5.48	127.90	115.30
3	N	242	LEU	CA-CB-CG	5.47	127.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	246	THR	Peptide
2	R	246	THR	Peptide

5.2   Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	71/556 (13%)	67 (94%)	4 (6%)	0	100	100
1	B	89/556 (16%)	83 (93%)	5 (6%)	1 (1%)	12	44
1	C	86/556 (16%)	74 (86%)	11 (13%)	1 (1%)	11	43
1	D	67/556 (12%)	63 (94%)	3 (4%)	1 (2%)	8	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	89/556 (16%)	85 (96%)	4 (4%)	0	100	100
1	F	86/556 (16%)	76 (88%)	8 (9%)	2 (2%)	5	29
1	G	71/556 (13%)	65 (92%)	6 (8%)	0	100	100
1	L	89/556 (16%)	86 (97%)	3 (3%)	0	100	100
1	Q	86/556 (16%)	74 (86%)	11 (13%)	1 (1%)	11	43
1	V	67/556 (12%)	62 (92%)	4 (6%)	1 (2%)	8	38
1	a	89/556 (16%)	83 (93%)	5 (6%)	1 (1%)	12	44
1	f	86/556 (16%)	77 (90%)	9 (10%)	0	100	100
2	M	413/417 (99%)	385 (93%)	27 (6%)	1 (0%)	44	75
2	R	413/417 (99%)	391 (95%)	21 (5%)	1 (0%)	44	75
3	I	1379/1382 (100%)	1314 (95%)	65 (5%)	0	100	100
3	N	1188/1382 (86%)	1122 (94%)	66 (6%)	0	100	100
4	H	234/236 (99%)	228 (97%)	6 (3%)	0	100	100
4	J	234/236 (99%)	224 (96%)	10 (4%)	0	100	100
4	O	234/236 (99%)	227 (97%)	7 (3%)	0	100	100
4	S	234/236 (99%)	227 (97%)	7 (3%)	0	100	100
5	K	296/299 (99%)	284 (96%)	11 (4%)	1 (0%)	37	69
5	P	296/299 (99%)	288 (97%)	7 (2%)	1 (0%)	37	69
5	T	296/299 (99%)	287 (97%)	8 (3%)	1 (0%)	37	69
5	U	296/299 (99%)	287 (97%)	8 (3%)	1 (0%)	37	69
All	All	6489/12410 (52%)	6159 (95%)	316 (5%)	14 (0%)	45	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Q	61	ASN
2	M	247	PRO
2	R	247	PRO
1	C	61	ASN
1	F	17	CYS
1	F	61	ASN
1	B	69	ILE
5	P	225	THR
5	K	225	THR
5	T	225	THR

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Mol	Chain	Res	Type
5	U	225	THR
1	D	79	ILE
1	V	79	ILE
1	a	69	ILE

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	68/455 (15%)	68 (100%)	0	100	100
1	B	84/455 (18%)	84 (100%)	0	100	100
1	C	81/455 (18%)	81 (100%)	0	100	100
1	D	64/455 (14%)	64 (100%)	0	100	100
1	E	84/455 (18%)	84 (100%)	0	100	100
1	F	81/455 (18%)	79 (98%)	2 (2%)	42	71
1	G	68/455 (15%)	68 (100%)	0	100	100
1	L	84/455 (18%)	84 (100%)	0	100	100
1	Q	81/455 (18%)	81 (100%)	0	100	100
1	V	64/455 (14%)	64 (100%)	0	100	100
1	a	84/455 (18%)	84 (100%)	0	100	100
1	f	81/455 (18%)	81 (100%)	0	100	100
2	M	370/371 (100%)	370 (100%)	0	100	100
2	R	370/371 (100%)	370 (100%)	0	100	100
3	I	1154/1155 (100%)	1152 (100%)	2 (0%)	92	97
3	N	997/1155 (86%)	996 (100%)	1 (0%)	92	98
4	H	209/209 (100%)	208 (100%)	1 (0%)	86	93
4	J	209/209 (100%)	209 (100%)	0	100	100
4	O	209/209 (100%)	209 (100%)	0	100	100
4	S	209/209 (100%)	209 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	K	243/244 (100%)	243 (100%)	0	100	100
5	P	243/244 (100%)	243 (100%)	0	100	100
5	T	243/244 (100%)	242 (100%)	1 (0%)	89	94
5	U	243/244 (100%)	243 (100%)	0	100	100
All	All	5623/10324 (54%)	5616 (100%)	7 (0%)	92	98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	17	CYS
1	F	55	GLN
3	I	814	ASN
3	I	849	LYS
3	N	849	LYS
4	H	9	CYS
5	T	278	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	55	GLN
1	F	52	ASN
1	F	87	GLN
1	f	87	GLN
3	I	904	ASN
3	I	1325	ASN
3	N	89	GLN
3	N	343	GLN
3	N	852	ASN
3	N	904	ASN
4	J	49	HIS
4	J	138	ASN
4	J	148	ASN
4	O	148	ASN
4	S	58	ASN
4	H	138	ASN
4	H	148	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-62961. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
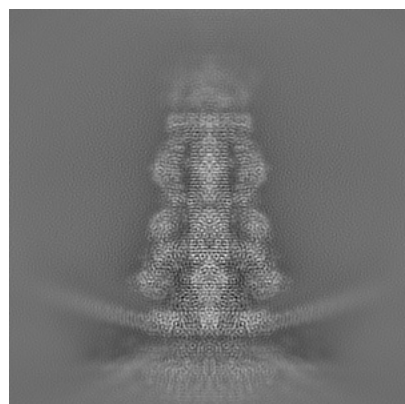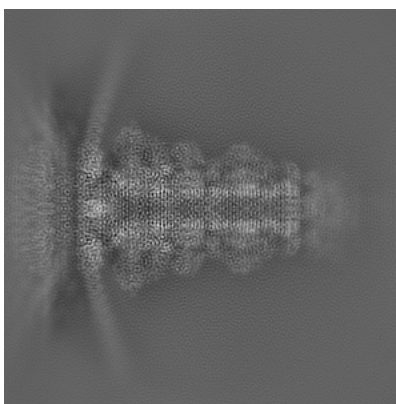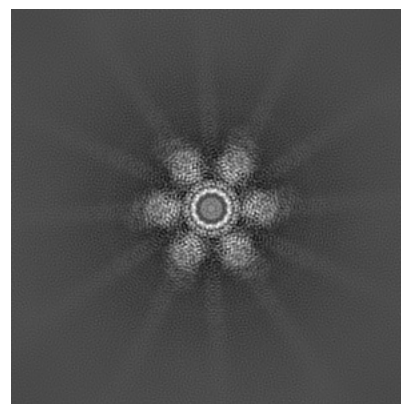
6.1.1 Primary map

X　　　　　　　　　　Y　　　　　　　　　　Z

6.1.2 Raw map

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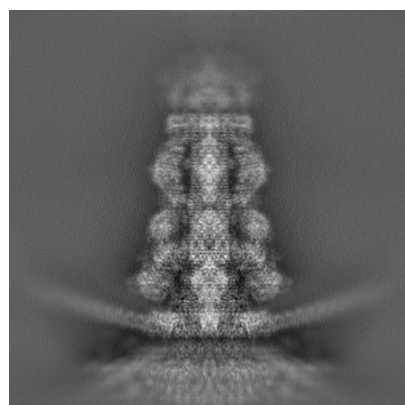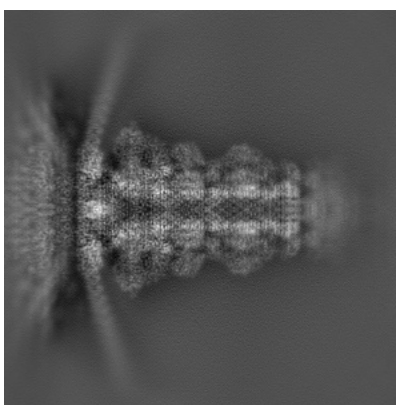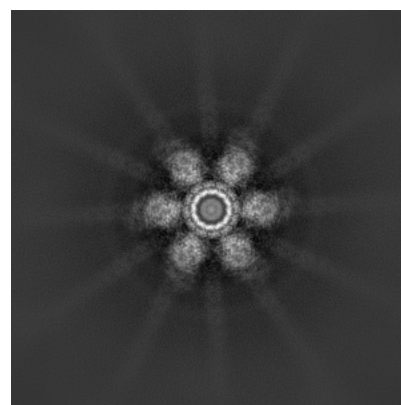
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map
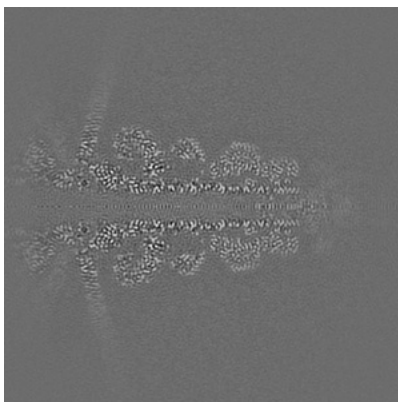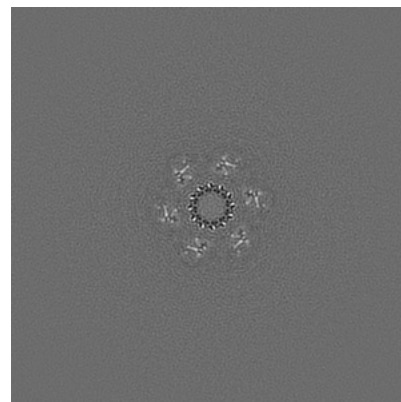
X Index: 240   Y Index: 240   Z Index: 240

6.2.2 Raw map
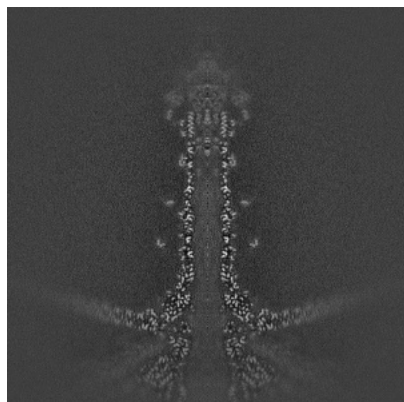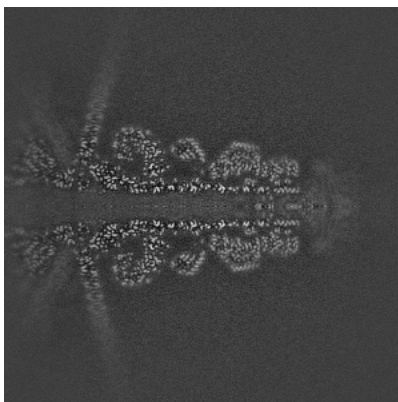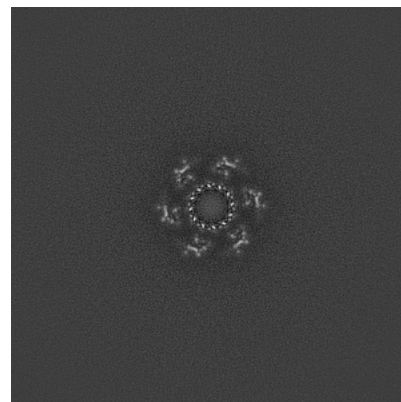
X Index: 240   Y Index: 240   Z Index: 240

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

6.3   Largest variance slices ⓘ

6.3.1   Primary map
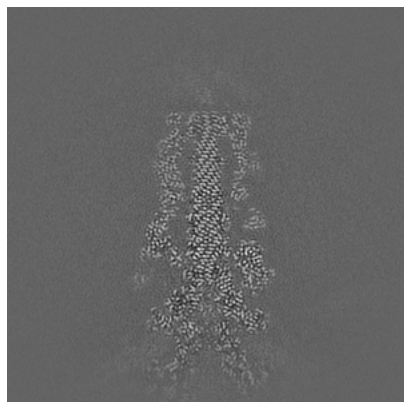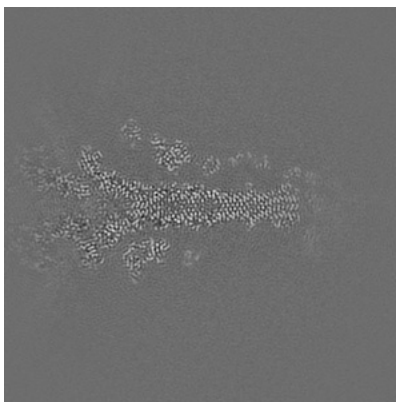
X Index: 220   Y Index: 258   Z Index: 189
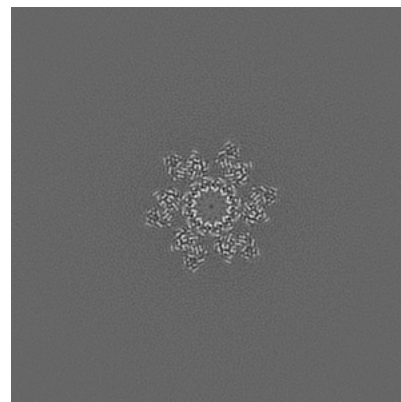
6.3.2   Raw map
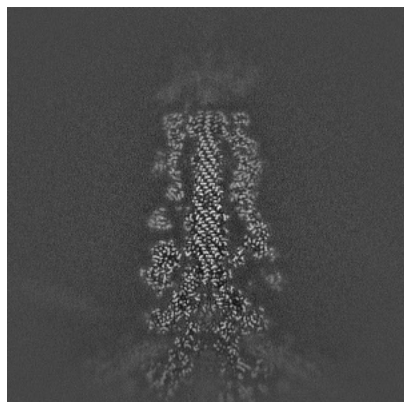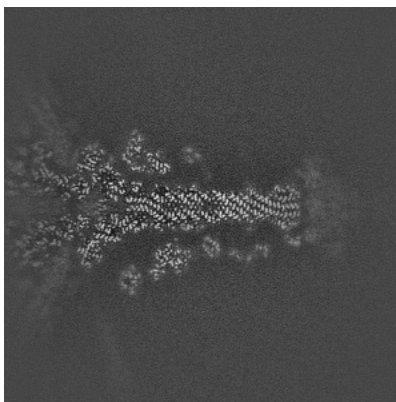
X Index: 260   Y Index: 221   Z Index: 189
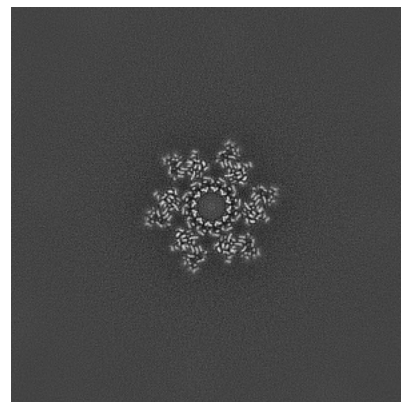
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map
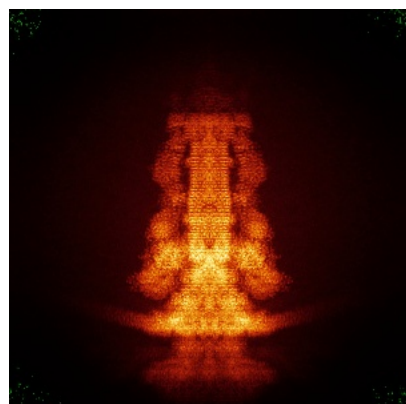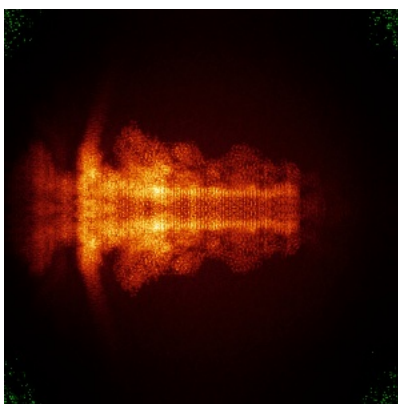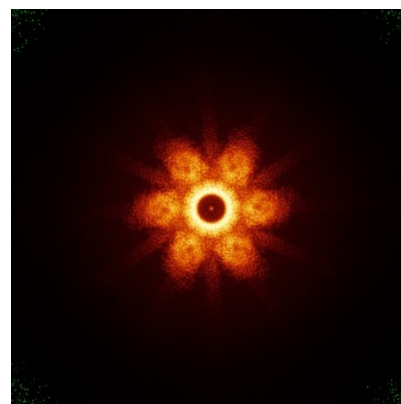
| X | Y | Z |

6.4.2 Raw map

| X | Y | Z |
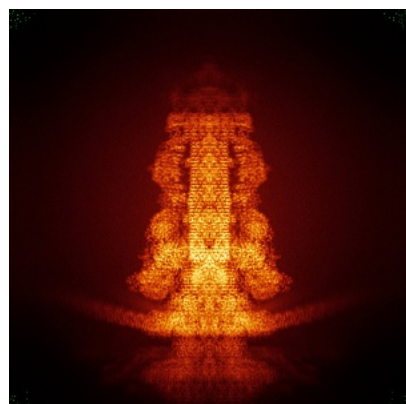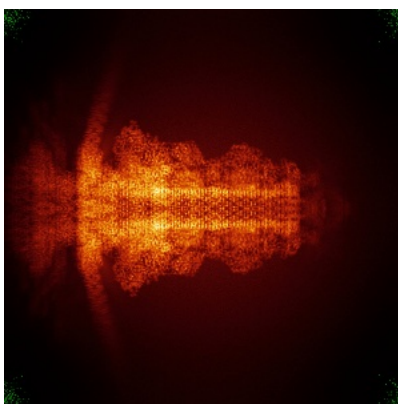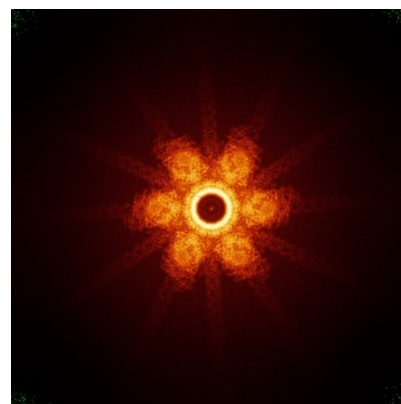
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X   Y   Z
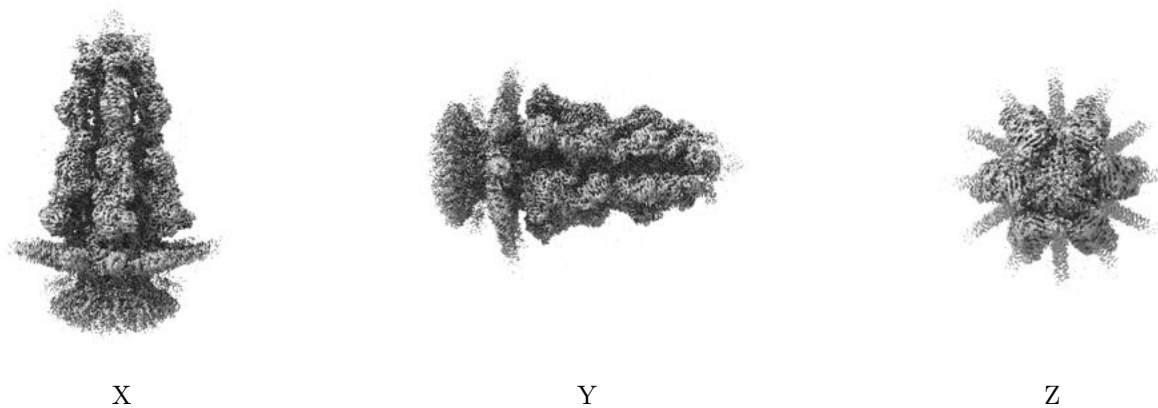
The images above show the 3D surface view of the map at the recommended contour level 5.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X   Y   Z
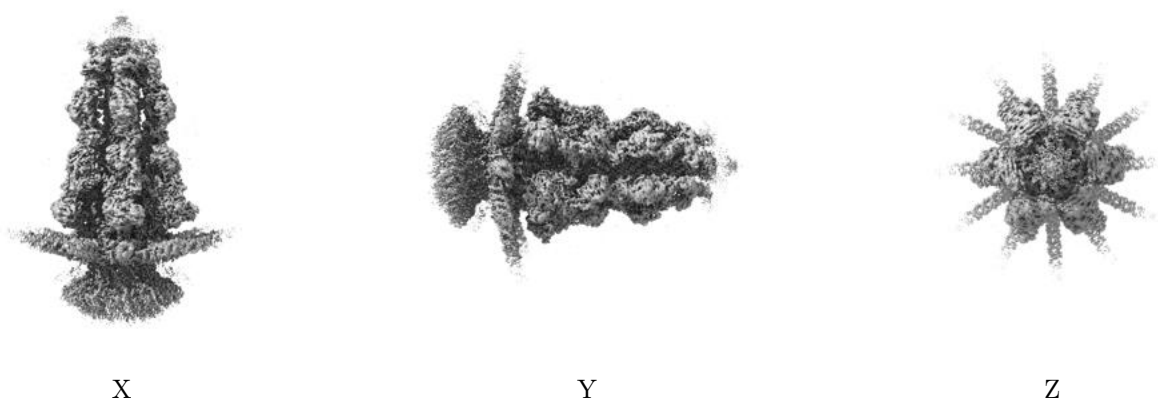
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
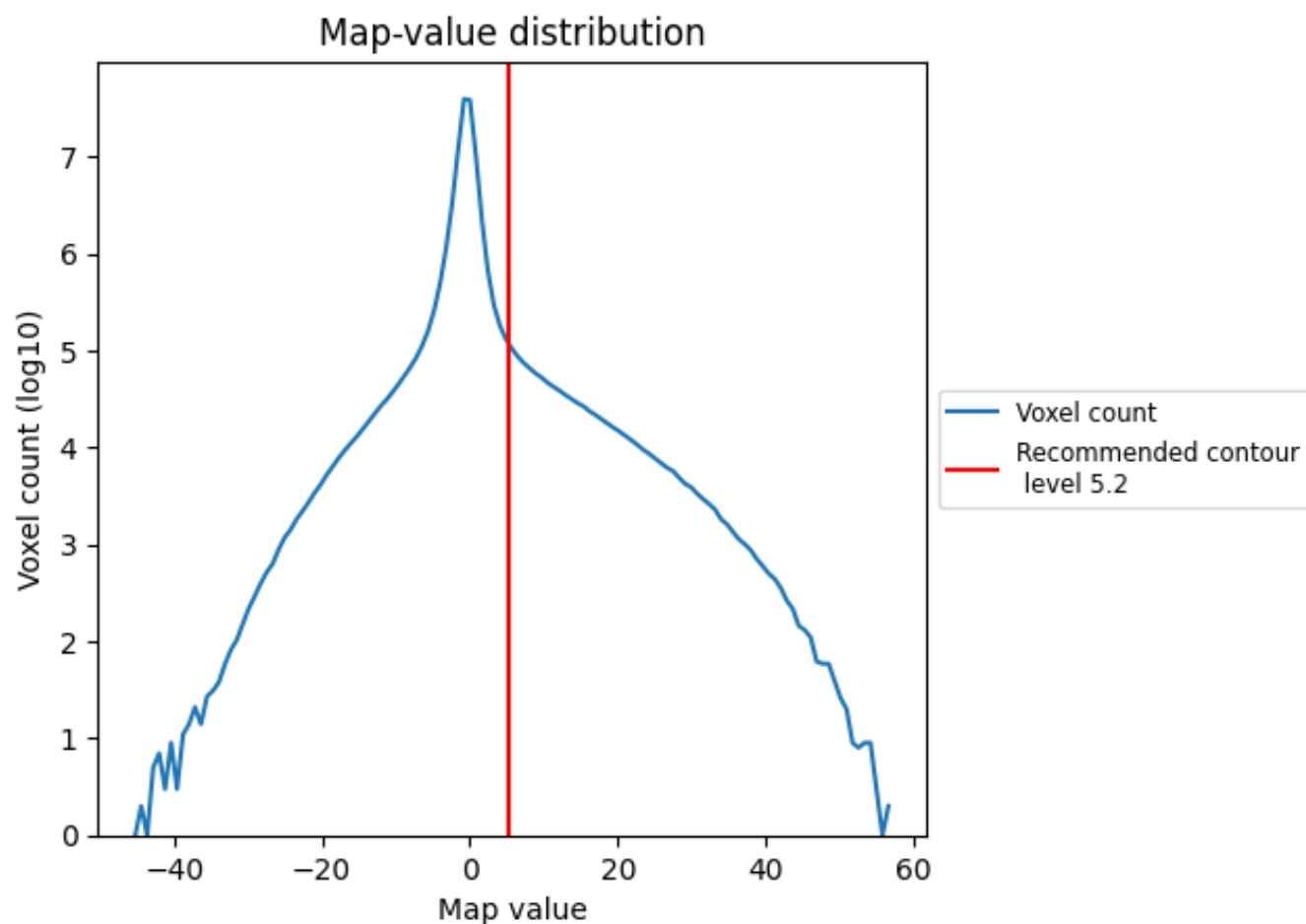
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
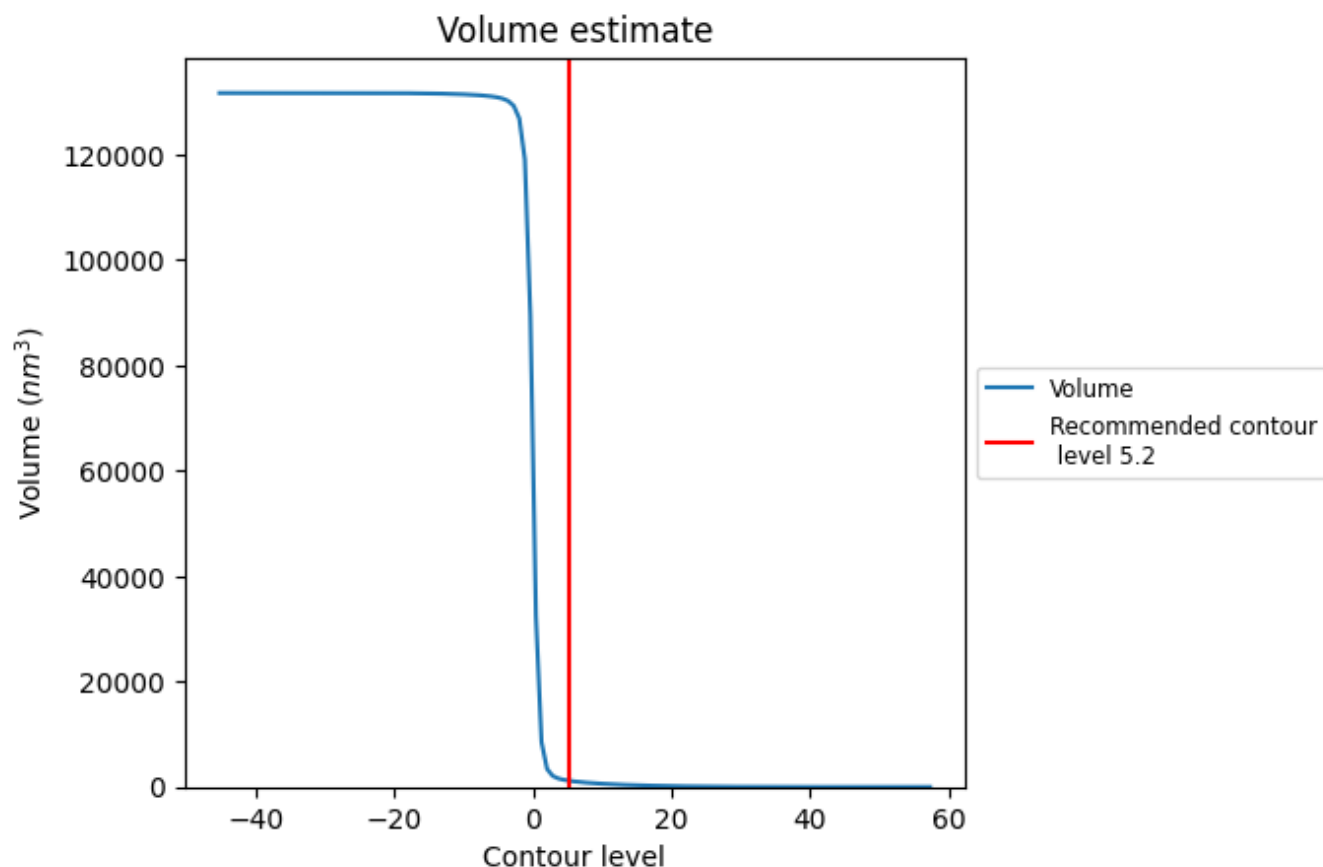
The volume at the recommended contour level is 1187 nm^3; this corresponds to an approximate mass of 1072 kDa.

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 ⓘ
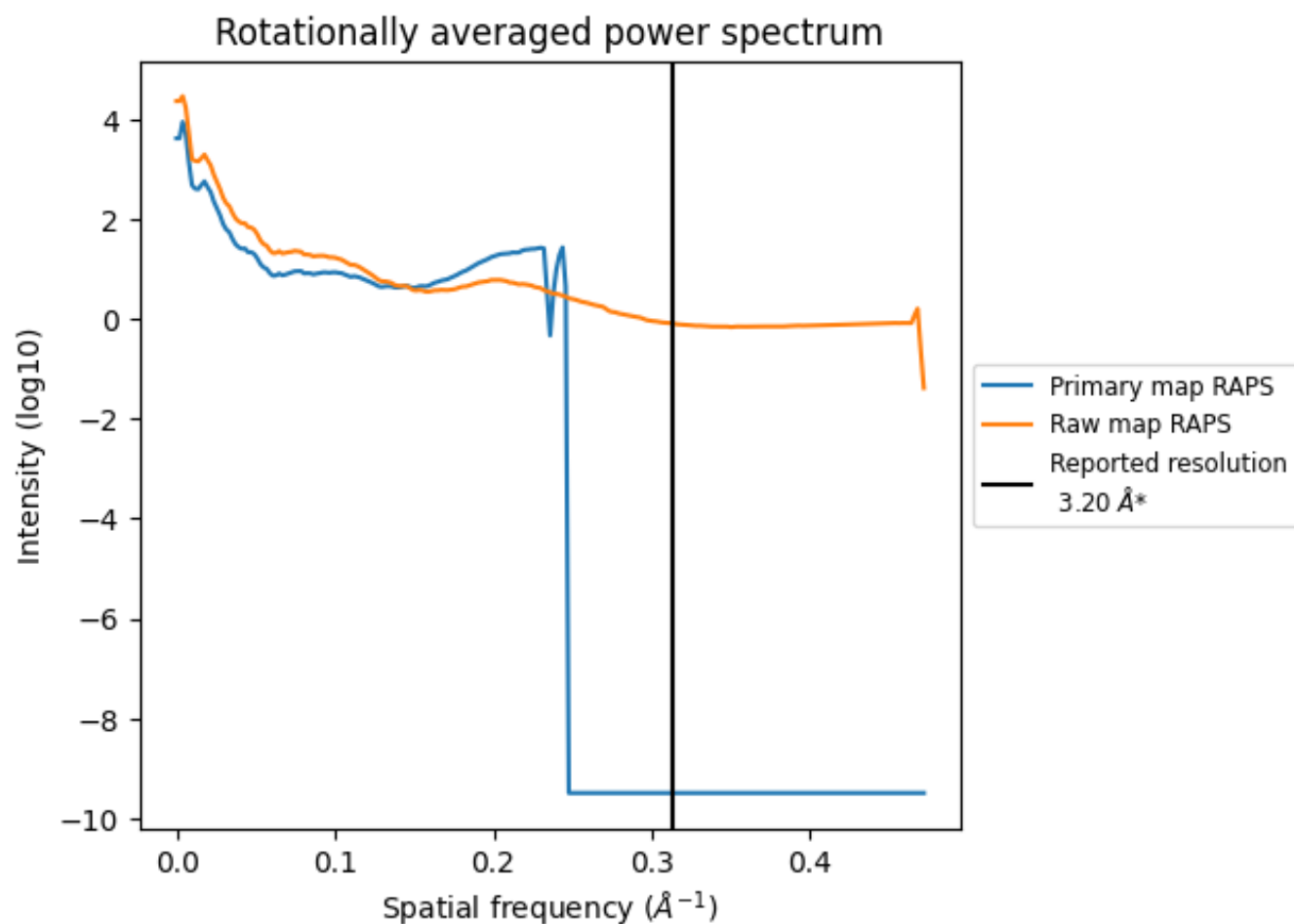
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ
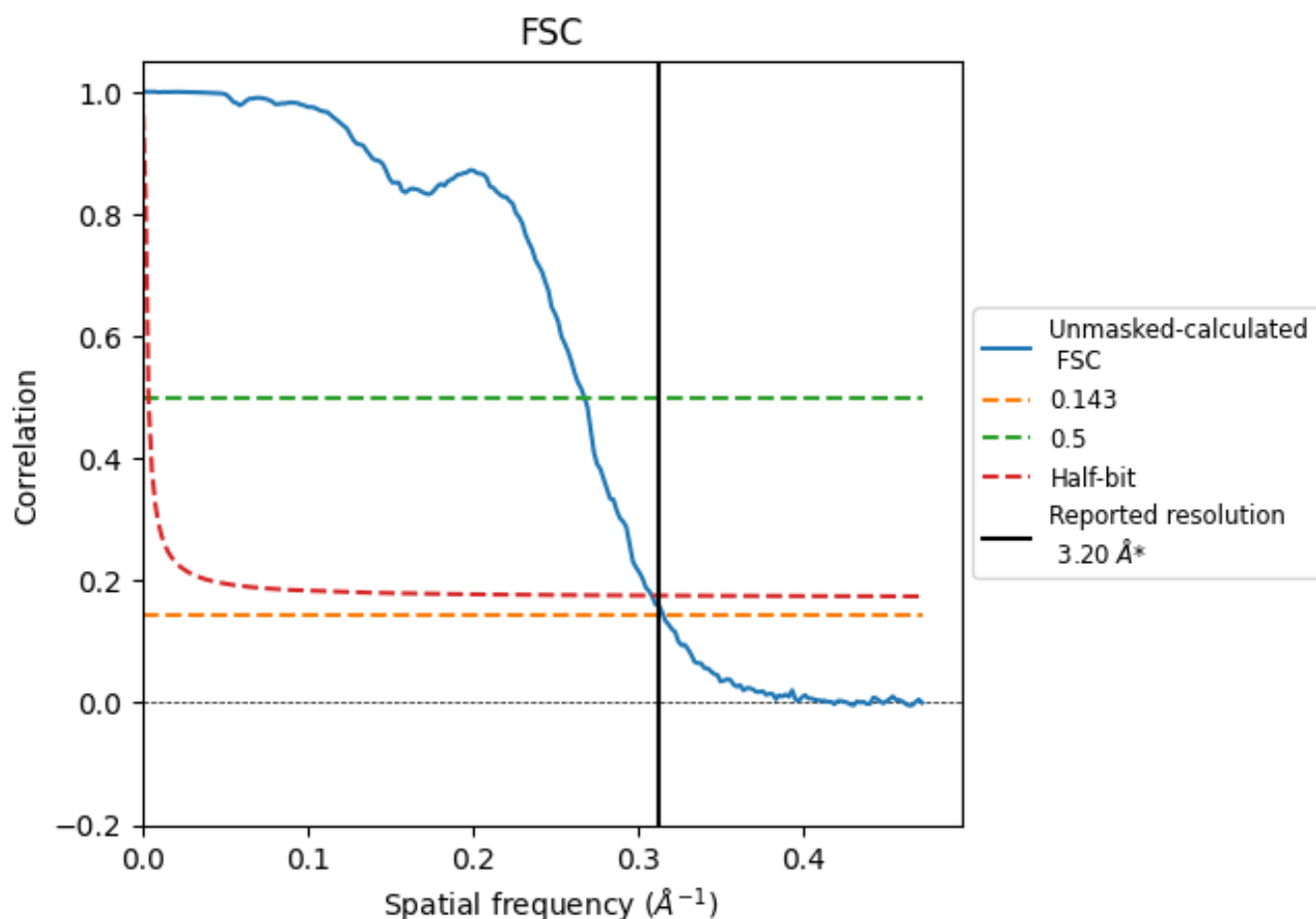
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.74	3.25

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-62961 and PDB model 9LC0. Per-residue inclusion information can be found in section 3 on page 6.

9.1   Map-model overlays

9.1.1   Map-model overlay (i)
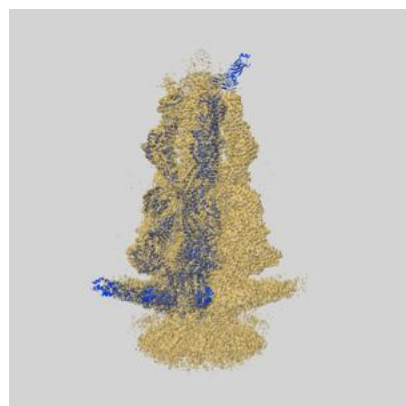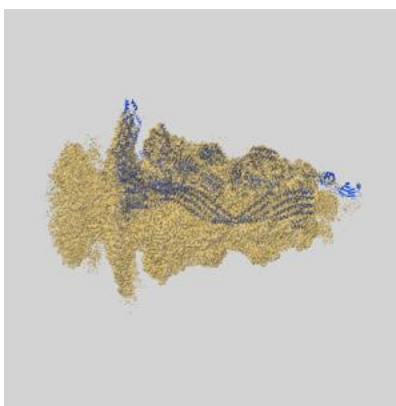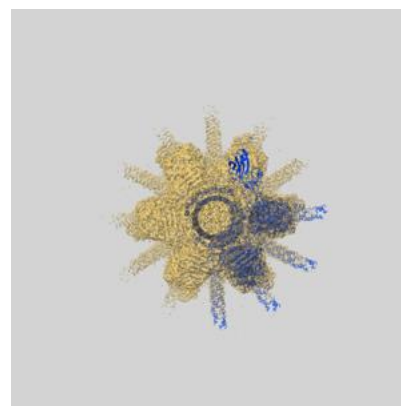
| X | Y | Z |

9.1.2   Map-model assembly overlay (i)
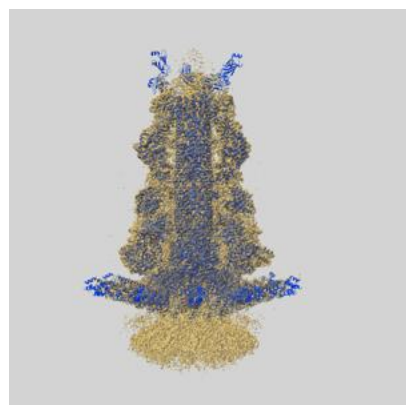
| X | Y | Z |
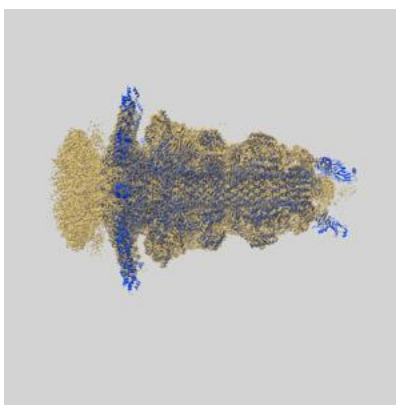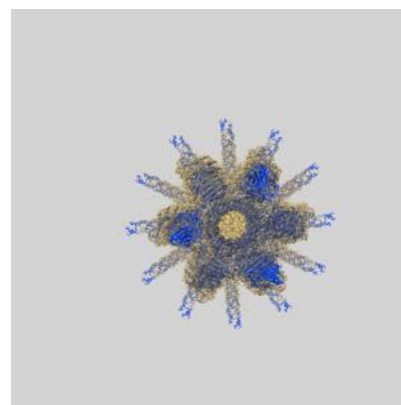
The images above show the 3D surface view of the map at the recommended contour level 5.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

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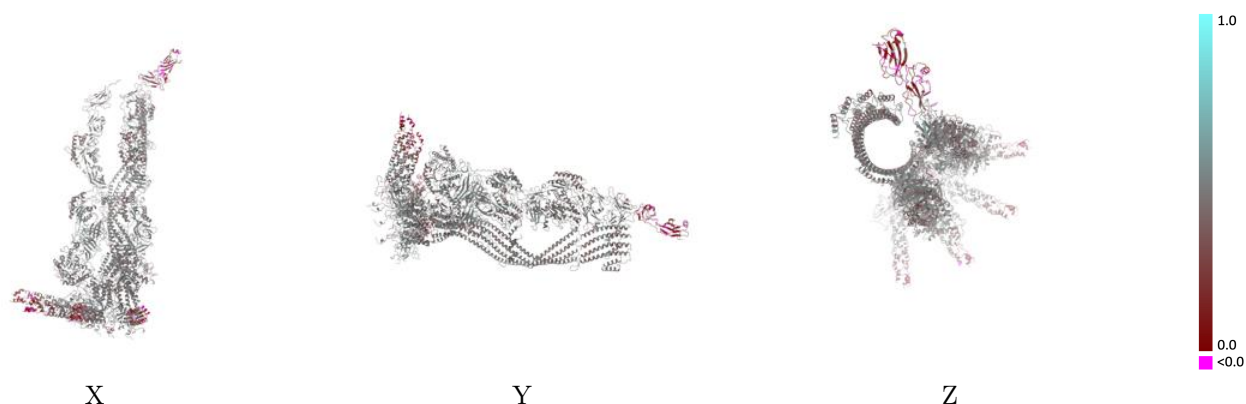
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X　　　　　　　　Y　　　　　　　　Z
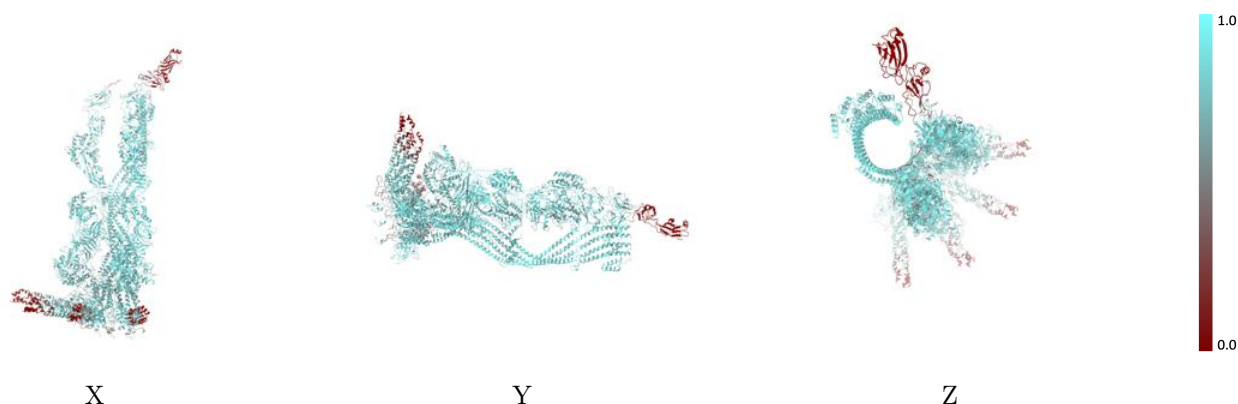
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.2).

9.4   Atom inclusion ⓘ
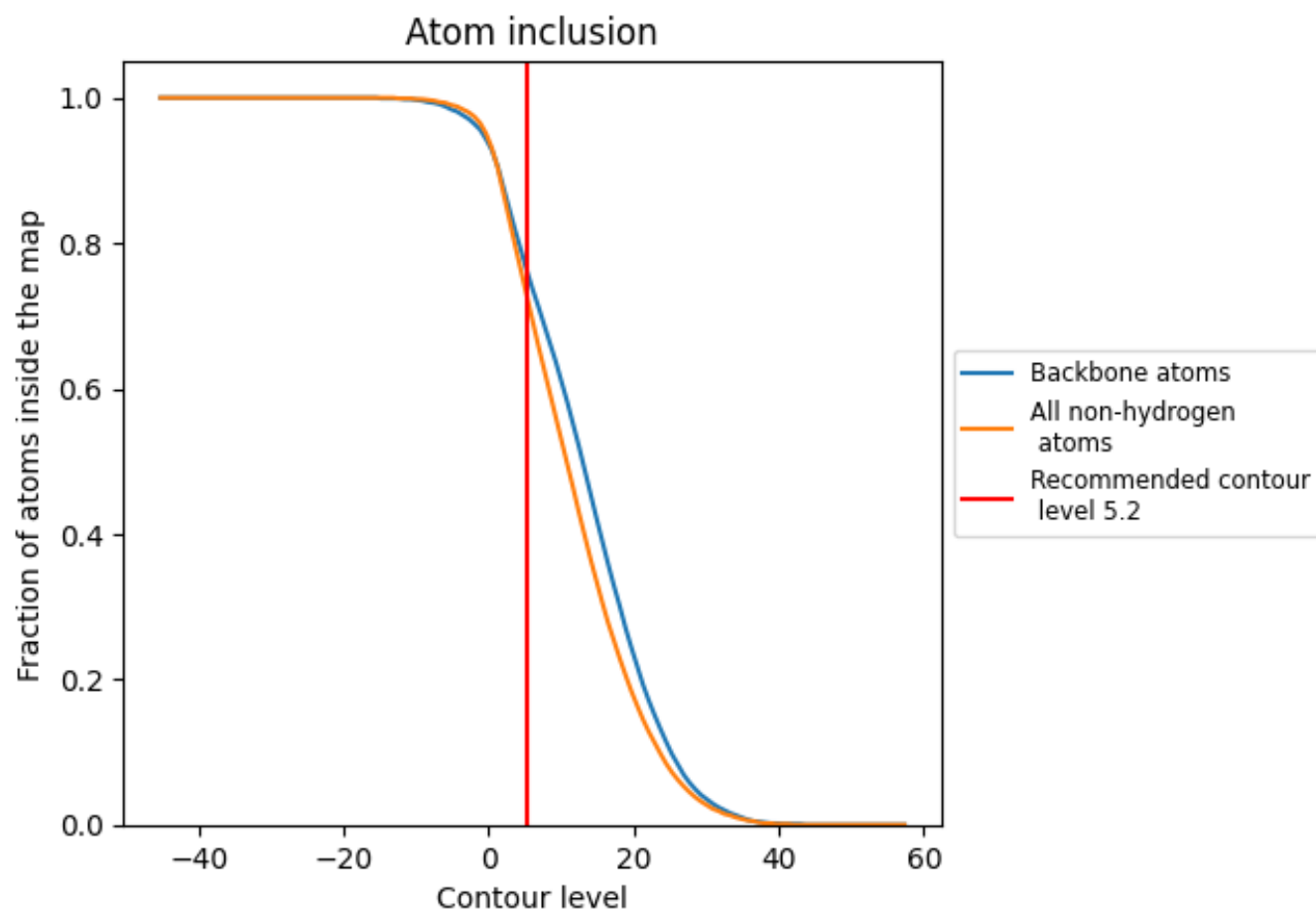
At the recommended contour level, 76% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7300	0.4360
A	0.4710	0.3390
B	0.5290	0.3640
C	0.5310	0.3630
D	0.4640	0.3270
E	0.5170	0.3690
F	0.5010	0.3600
G	0.4950	0.3350
H	0.7820	0.4650
I	0.6980	0.4230
J	0.7900	0.4690
K	0.8190	0.4550
L	0.5320	0.3680
M	0.7940	0.4570
N	0.7920	0.4610
O	0.7730	0.4650
P	0.8090	0.4540
Q	0.5340	0.3580
R	0.7880	0.4590
S	0.7890	0.4720
T	0.8170	0.4540
U	0.8180	0.4550
V	0.4480	0.3340
a	0.5120	0.3590
f	0.4920	0.3610

1.0

0.0
<0.0