W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Apr 18, 2024 – 07:23 pm BST

PDB ID	:	8RJL
EMDB ID	:	EMD-19251
Title	:	Structure of a first order Sierpinski triangle formed by the H369R mutant of
		the citrate synthase from Synechococcus elongatus
Authors	:	Lo, Y.K.; Bohn, S.; Sendker, F.L.; Schuller, J.M.; Hochberg, G.
Deposited on	:	2023-12-21
Resolution	:	3.34 Å(reported)

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

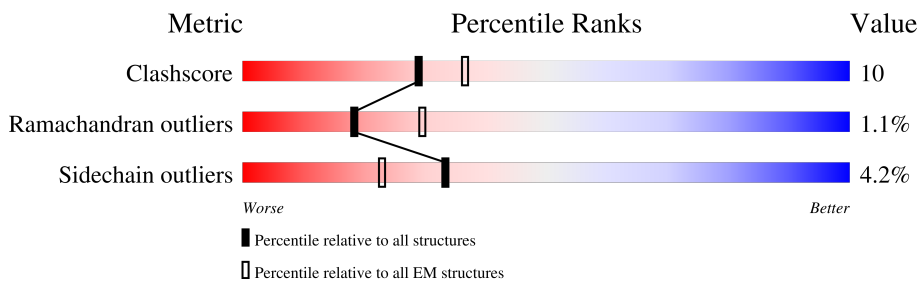|		
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 3.34 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
Clashscore		10
Ramachandran outliers		1.1%
Sidechain outliers		4.2%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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 <=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	394	13% / 44% / 10% · / 45%
1	B	394	11% / 44% / 10% · / 44%
1	C	394	· / 59% / 8% · / 31%
1	D	394	· / 52% / 15% · / 31%
1	E	394	13% / 43% / 10% · / 45%
1	F	394	14% / 44% / 9% · / 45%
1	G	394	· / 55% / 13% / 31%
1	H	394	· / 54% / 13% · / 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	394	11% 45% 10% · 44%
1	J	394	11% 45% 10% · 44%
1	K	394	60% 8% · 31%
1	L	394	58% 9% · 31%
1	M	394	53% 14% · 31%
1	N	394	52% 15% · 31%
1	O	394	54% 14% 31%
1	P	394	56% 12% 31%
1	Q	394	54% 13% · 31%
1	R	394	54% 13% · 31%

2   Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 36300 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 Citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1729	1122	291	308	8		
1	B	219	Total	C	N	O	S	0	0
			1740	1126	294	312	8		
1	C	273	Total	C	N	O	S	0	0
			2167	1393	371	395	8		
1	D	272	Total	C	N	O	S	0	0
			2156	1386	373	389	8		
1	G	270	Total	C	N	O	S	0	0
			2146	1380	370	388	8		
1	H	273	Total	C	N	O	S	0	0
			2162	1389	370	395	8		
1	E	218	Total	C	N	O	S	0	0
			1729	1122	291	308	8		
1	I	219	Total	C	N	O	S	0	0
			1740	1126	294	312	8		
1	K	273	Total	C	N	O	S	0	0
			2167	1393	371	395	8		
1	M	272	Total	C	N	O	S	0	0
			2156	1386	373	389	8		
1	O	270	Total	C	N	O	S	0	0
			2146	1380	370	388	8		
1	Q	273	Total	C	N	O	S	0	0
			2162	1389	370	395	8		
1	F	218	Total	C	N	O	S	0	0
			1729	1122	291	308	8		
1	J	219	Total	C	N	O	S	0	0
			1740	1126	294	312	8		
1	L	273	Total	C	N	O	S	0	0
			2167	1393	371	395	8		
1	N	272	Total	C	N	O	S	0	0
			2156	1386	373	389	8		
1	P	270	Total	C	N	O	S	0	0
			2146	1380	370	388	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	273	2162	1389	370	395	8	0	0

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	ARG	HIS	engineered mutation	UNP Q31QM5
A	387	LEU	-	expression tag	UNP Q31QM5
A	388	GLU	-	expression tag	UNP Q31QM5
A	389	HIS	-	expression tag	UNP Q31QM5
A	390	HIS	-	expression tag	UNP Q31QM5
A	391	HIS	-	expression tag	UNP Q31QM5
A	392	HIS	-	expression tag	UNP Q31QM5
A	393	HIS	-	expression tag	UNP Q31QM5
A	394	HIS	-	expression tag	UNP Q31QM5
B	369	ARG	HIS	engineered mutation	UNP Q31QM5
B	387	LEU	-	expression tag	UNP Q31QM5
B	388	GLU	-	expression tag	UNP Q31QM5
B	389	HIS	-	expression tag	UNP Q31QM5
B	390	HIS	-	expression tag	UNP Q31QM5
B	391	HIS	-	expression tag	UNP Q31QM5
B	392	HIS	-	expression tag	UNP Q31QM5
B	393	HIS	-	expression tag	UNP Q31QM5
B	394	HIS	-	expression tag	UNP Q31QM5
C	369	ARG	HIS	engineered mutation	UNP Q31QM5
C	387	LEU	-	expression tag	UNP Q31QM5
C	388	GLU	-	expression tag	UNP Q31QM5
C	389	HIS	-	expression tag	UNP Q31QM5
C	390	HIS	-	expression tag	UNP Q31QM5
C	391	HIS	-	expression tag	UNP Q31QM5
C	392	HIS	-	expression tag	UNP Q31QM5
C	393	HIS	-	expression tag	UNP Q31QM5
C	394	HIS	-	expression tag	UNP Q31QM5
D	369	ARG	HIS	engineered mutation	UNP Q31QM5
D	387	LEU	-	expression tag	UNP Q31QM5
D	388	GLU	-	expression tag	UNP Q31QM5
D	389	HIS	-	expression tag	UNP Q31QM5
D	390	HIS	-	expression tag	UNP Q31QM5
D	391	HIS	-	expression tag	UNP Q31QM5
D	392	HIS	-	expression tag	UNP Q31QM5
D	393	HIS	-	expression tag	UNP Q31QM5
D	394	HIS	-	expression tag	UNP Q31QM5

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	369	ARG	HIS	engineered mutation	UNP Q31QM5
G	387	LEU	-	expression tag	UNP Q31QM5
G	388	GLU	-	expression tag	UNP Q31QM5
G	389	HIS	-	expression tag	UNP Q31QM5
G	390	HIS	-	expression tag	UNP Q31QM5
G	391	HIS	-	expression tag	UNP Q31QM5
G	392	HIS	-	expression tag	UNP Q31QM5
G	393	HIS	-	expression tag	UNP Q31QM5
G	394	HIS	-	expression tag	UNP Q31QM5
H	369	ARG	HIS	engineered mutation	UNP Q31QM5
H	387	LEU	-	expression tag	UNP Q31QM5
H	388	GLU	-	expression tag	UNP Q31QM5
H	389	HIS	-	expression tag	UNP Q31QM5
H	390	HIS	-	expression tag	UNP Q31QM5
H	391	HIS	-	expression tag	UNP Q31QM5
H	392	HIS	-	expression tag	UNP Q31QM5
H	393	HIS	-	expression tag	UNP Q31QM5
H	394	HIS	-	expression tag	UNP Q31QM5
E	369	ARG	HIS	engineered mutation	UNP Q31QM5
E	387	LEU	-	expression tag	UNP Q31QM5
E	388	GLU	-	expression tag	UNP Q31QM5
E	389	HIS	-	expression tag	UNP Q31QM5
E	390	HIS	-	expression tag	UNP Q31QM5
E	391	HIS	-	expression tag	UNP Q31QM5
E	392	HIS	-	expression tag	UNP Q31QM5
E	393	HIS	-	expression tag	UNP Q31QM5
E	394	HIS	-	expression tag	UNP Q31QM5
I	369	ARG	HIS	engineered mutation	UNP Q31QM5
I	387	LEU	-	expression tag	UNP Q31QM5
I	388	GLU	-	expression tag	UNP Q31QM5
I	389	HIS	-	expression tag	UNP Q31QM5
I	390	HIS	-	expression tag	UNP Q31QM5
I	391	HIS	-	expression tag	UNP Q31QM5
I	392	HIS	-	expression tag	UNP Q31QM5
I	393	HIS	-	expression tag	UNP Q31QM5
I	394	HIS	-	expression tag	UNP Q31QM5
K	369	ARG	HIS	engineered mutation	UNP Q31QM5
K	387	LEU	-	expression tag	UNP Q31QM5
K	388	GLU	-	expression tag	UNP Q31QM5
K	389	HIS	-	expression tag	UNP Q31QM5
K	390	HIS	-	expression tag	UNP Q31QM5
K	391	HIS	-	expression tag	UNP Q31QM5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	392	HIS	-	expression tag	UNP Q31QM5
K	393	HIS	-	expression tag	UNP Q31QM5
K	394	HIS	-	expression tag	UNP Q31QM5
M	369	ARG	HIS	engineered mutation	UNP Q31QM5
M	387	LEU	-	expression tag	UNP Q31QM5
M	388	GLU	-	expression tag	UNP Q31QM5
M	389	HIS	-	expression tag	UNP Q31QM5
M	390	HIS	-	expression tag	UNP Q31QM5
M	391	HIS	-	expression tag	UNP Q31QM5
M	392	HIS	-	expression tag	UNP Q31QM5
M	393	HIS	-	expression tag	UNP Q31QM5
M	394	HIS	-	expression tag	UNP Q31QM5
O	369	ARG	HIS	engineered mutation	UNP Q31QM5
O	387	LEU	-	expression tag	UNP Q31QM5
O	388	GLU	-	expression tag	UNP Q31QM5
O	389	HIS	-	expression tag	UNP Q31QM5
O	390	HIS	-	expression tag	UNP Q31QM5
O	391	HIS	-	expression tag	UNP Q31QM5
O	392	HIS	-	expression tag	UNP Q31QM5
O	393	HIS	-	expression tag	UNP Q31QM5
O	394	HIS	-	expression tag	UNP Q31QM5
Q	369	ARG	HIS	engineered mutation	UNP Q31QM5
Q	387	LEU	-	expression tag	UNP Q31QM5
Q	388	GLU	-	expression tag	UNP Q31QM5
Q	389	HIS	-	expression tag	UNP Q31QM5
Q	390	HIS	-	expression tag	UNP Q31QM5
Q	391	HIS	-	expression tag	UNP Q31QM5
Q	392	HIS	-	expression tag	UNP Q31QM5
Q	393	HIS	-	expression tag	UNP Q31QM5
Q	394	HIS	-	expression tag	UNP Q31QM5
F	369	ARG	HIS	engineered mutation	UNP Q31QM5
F	387	LEU	-	expression tag	UNP Q31QM5
F	388	GLU	-	expression tag	UNP Q31QM5
F	389	HIS	-	expression tag	UNP Q31QM5
F	390	HIS	-	expression tag	UNP Q31QM5
F	391	HIS	-	expression tag	UNP Q31QM5
F	392	HIS	-	expression tag	UNP Q31QM5
F	393	HIS	-	expression tag	UNP Q31QM5
F	394	HIS	-	expression tag	UNP Q31QM5
J	369	ARG	HIS	engineered mutation	UNP Q31QM5
J	387	LEU	-	expression tag	UNP Q31QM5
J	388	GLU	-	expression tag	UNP Q31QM5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	389	HIS	-	expression tag	UNP Q31QM5
J	390	HIS	-	expression tag	UNP Q31QM5
J	391	HIS	-	expression tag	UNP Q31QM5
J	392	HIS	-	expression tag	UNP Q31QM5
J	393	HIS	-	expression tag	UNP Q31QM5
J	394	HIS	-	expression tag	UNP Q31QM5
L	369	ARG	HIS	engineered mutation	UNP Q31QM5
L	387	LEU	-	expression tag	UNP Q31QM5
L	388	GLU	-	expression tag	UNP Q31QM5
L	389	HIS	-	expression tag	UNP Q31QM5
L	390	HIS	-	expression tag	UNP Q31QM5
L	391	HIS	-	expression tag	UNP Q31QM5
L	392	HIS	-	expression tag	UNP Q31QM5
L	393	HIS	-	expression tag	UNP Q31QM5
L	394	HIS	-	expression tag	UNP Q31QM5
N	369	ARG	HIS	engineered mutation	UNP Q31QM5
N	387	LEU	-	expression tag	UNP Q31QM5
N	388	GLU	-	expression tag	UNP Q31QM5
N	389	HIS	-	expression tag	UNP Q31QM5
N	390	HIS	-	expression tag	UNP Q31QM5
N	391	HIS	-	expression tag	UNP Q31QM5
N	392	HIS	-	expression tag	UNP Q31QM5
N	393	HIS	-	expression tag	UNP Q31QM5
N	394	HIS	-	expression tag	UNP Q31QM5
P	369	ARG	HIS	engineered mutation	UNP Q31QM5
P	387	LEU	-	expression tag	UNP Q31QM5
P	388	GLU	-	expression tag	UNP Q31QM5
P	389	HIS	-	expression tag	UNP Q31QM5
P	390	HIS	-	expression tag	UNP Q31QM5
P	391	HIS	-	expression tag	UNP Q31QM5
P	392	HIS	-	expression tag	UNP Q31QM5
P	393	HIS	-	expression tag	UNP Q31QM5
P	394	HIS	-	expression tag	UNP Q31QM5
R	369	ARG	HIS	engineered mutation	UNP Q31QM5
R	387	LEU	-	expression tag	UNP Q31QM5
R	388	GLU	-	expression tag	UNP Q31QM5
R	389	HIS	-	expression tag	UNP Q31QM5
R	390	HIS	-	expression tag	UNP Q31QM5
R	391	HIS	-	expression tag	UNP Q31QM5
R	392	HIS	-	expression tag	UNP Q31QM5
R	393	HIS	-	expression tag	UNP Q31QM5
R	394	HIS	-	expression tag	UNP Q31QM5

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: Citrate synthase

Chain A:

• Molecule 1: Citrate synthase

Chain B:

• Molecule 1: Citrate synthase

Chain C:

59% 8% 31%

• Molecule 1: Citrate synthase

Chain D:

52% 15% 31%

• Molecule 1: Citrate synthase

Chain G:

55% 13% 31%

• Molecule 1: Citrate synthase

Chain H:

54% 13% 31%

• Molecule 1: Citrate synthase

Chain E:

13%

43% 10% 45%

• Molecule 1: Citrate synthase

Chain I:

11%

45%   10%   44%

• Molecule 1: Citrate synthase

Chain K:

60%   8%   31%

• Molecule 1: Citrate synthase

Chain M:

53%   14%   •   31%

• Molecule 1: Citrate synthase

Chain O:

54%   14%   31%

• Molecule 1: Citrate synthase

Chain Q:

54%   13%   •   31%

LYS GLY ILE TYR P313 F317 Y318 V322 L332 V336 G344 A347 Q352 F359 Q363 I364 Y365 T366 G367 S368 R369 N370 L371 D372 Y373 T374 P375 ILE ALA ASP ARG ASP LEU ALA ILE GLU SER ASP LEU GLU HIS HIS HIS HIS HIS

• Molecule 1: Citrate synthase

Chain F:

14%

44% 9% • 45%

MET THR ALA VAL SER GLU PHE ARG PRO GLY LEU GLU GLY VAL PRO ALA THR LEU SER SER ILE SER PHE VAL ASP GLY GLN ARG GLY VAL LEU GLU Y33 R34 S37 I38 E39 Q40 L41 A42 GLN GLN SER SER F47 L53 L54 I55 W56 G57 H58 L59 P60 T61 Q62 Q63 E64 L65

T66 I72 R73 Y74 K79 F80 R81 H94 P95 F109 R112 ARG ALA LEU ASP ASP PRO E119 Y120 A123 V126 K144 G145 Q150 P151 R152 D153 E154 L155 D156 N160 F161 L162 T166 E167 R168 E169 P170 D171 P172 V173 A174 A175 R176 I177 F178 D179 I180 C181

L182 T183 L184 E187 H188 T189 I190 N191 A192 S196 L204 T205 D206 V211 V215 A219 GLY PRO LEU HIS GLY ALA ASN GLU GLU VAL LEU ASP MET LEU GLU ALA ILE GLY SER VAL GLU ASN VAL GLU PRO TYR LEU ASP HIS CYS ILE ALA THR LYS THR ARG ILE

MET GLY PHE GLY HIS ARG VAL TYR LYS VAL LYS ASP PRO ARG ALA VAL ILE LEU GLN ASN LEU ALA GLU GLN LEU PHE ASP ILE PHE GLY HIS ASP PRO TYR TYR GLU ILE ALA VAL ALA VAL GLU LYS ALA ALA GLU ARG LEU SER HIS LYS GLY ILE TYR P313 N314 V315 D316 F317

Y318 S319 G320 L321 V322 Y323 R324 K325 L326 G327 S330 F333 T334 F337 G344 E351 Q352 L353 ASN GLU ASN ARG ILE PHE ARG PRO THR GLN ILE TYR THR GLY SER ARG ASN LEU ASP TYR PRO ILE ALA ASP ARG ASP LEU ALA ILE GLU SER ASP LEU GLU HIS HIS

HIS HIS HIS HIS

• Molecule 1: Citrate synthase

Chain J:

11%

45% 10% • 44%

MET THR ALA VAL SER GLU PHE ARG PRO GLY LEU GLU GLY VAL PRO ALA THR LEU SER SER ILE SER PHE VAL ASP GLY GLN ARG GLY VAL LEU GLU Y33 R34 G35 I36 S37 I38 E39 Q40 L41 A42 Q43 Q44 S45 SER F47 L48 E49 G57 H58 T61 Q62 Q63 E64 L65 T66 E67

F68 E71 I72 R73 Y74 H75 R76 R77 I78 K79 F80 R81 I82 R83 D84 P90 F109 Y110 S111 ARG ALA LEU ASP ASP PRO E119 Y120 I121 R122 A123 A130 K131 Q140 R143 Q150 P151 R152 D153 A159 L162 T166 E167 R168 E169 P170 D171 P172 V173 A174

A175 R176 I180 C181 L182 E187 H188 T189 I190 N191 F195 V199 S202 D206 P207 A219 GLY PRO LEU HIS GLY ALA ASN GLU GLU VAL LEU ASP MET LEU GLU ALA ILE GLY SER VAL GLU ASN VAL GLU PRO TYR LEU ASP HIS CYS ILE ALA THR LYS THR ARG

ILE MET GLY PHE GLY HIS ARG VAL TYR LYS VAL LYS ASP PRO ARG ALA VAL ILE LEU GLN ASN LEU ALA GLU GLN LEU PHE ASP ILE PHE GLY HIS ASP PRO TYR TYR GLU ILE ALA VAL ALA VAL GLU LYS ALA ALA GLU ARG LEU SER HIS LYS GLY ILE TYR P313 N314 V315 D316

F317 Y318 S319 G320 L321 V322 Y323 R324 K325 L326 D331 A340 Q352 LEU ASN GLU ASN ARG ILE LEU ARG PRO THR GLN ILE ILE ALA ASP ARG ASP LEU ALA ILE GLU SER ASP LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Citrate synthase

Chain L:

58% 9% 31%

• Molecule 1: Citrate synthase

Chain N:

52% 15% 31%

• Molecule 1: Citrate synthase

Chain P:

56% 12% 31%

GLY HIS ARG VAL TYR LYS VAL LYS ASP PRO ARG ALA VAL ILE LEU GLN ASN LEU ALA GLU GLN LEU PHE ASP ILE PHE GLY HIS ASP PRO TYR TYR GLU ILE ALA VAL ALA VAL GLU LYS ALA ALA ALA GLU ARG LEU SER HIS LYS GLY ILE TYR **P313** **D316** **F317** **V336** **I339**

V342 **L346** **K350** **E351** **Q352** **L353** **R357** **I358** **T362** **Q363** **I364** **Y365** **T366** **G367** **S368** **R369** **D372** **P375** ILE ALA ASP ARG ASP ASP LEU ALA ILE GLU SER ASP LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Citrate synthase

Chain R:

54%   13%   •   31%

MET THR ALA VAL **S5** **E6** **F7** **R8** **P9** **G10** **L11** **E12** **G13** **V14** **S19** **S20** **I21** **S22** **F23** **V24** **D25** **R28** **G29** **V30** **F47** **Q63** **T66** **R73** **R76** **R83** **K87** **L106** **Y110** **S111** **R112** ARG ALA LEU ASP ASP **P118** **E119** **Y120** **A123** **V126** **L141**

R152 **D156** **Y163** **R176** **L182** **F195** **V199** **L204** **T205** **D206** **P207** **V211** **T217** **L218** **A219** GLY PRO LEU HIS GLY GLY ALA ASN GLU GLU VAL LEU ASP MET LEU GLU ALA ILE GLY SER VAL GLU ASN VAL GLU PRO TYR LEU ASP HIS CYS ILE ALA THR LYS

THR ARG ILE MET GLY PHE GLY HIS ARG VAL TYR LYS VAL LYS ASP PRO ARG ALA VAL ILE LEU GLN ASN LEU ALA GLU GLN LEU PHE ASP ILE PHE GLY HIS ASP PRO TYR TYR GLU ILE ALA VAL ALA VAL GLU LYS ALA ALA ALA GLU ARG LEU SER HIS LYS GLY ILE TYR **P313**

F317 **Y318** **L321** **V322** **L332** **V336** **G344** **A347** **Q352** **F359** **Q363** **T366** **G367** **S368** **R369** **N370** **L371** **D372** **Y373** **T374** **P375** ILE ALA ASP ARG ASP ASP LEU ALA ILE GLU GLU SER ASP LEU GLU HIS HIS HIS HIS HIS HIS

4   Experimental information   ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.855	Depositor
Minimum map value	-0.625	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	395.0, 395.0, 395.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.79, 0.79, 0.79	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	0.41	0/1772	0.57	0/2408
1	B	0.42	0/1783	0.58	0/2422
1	C	0.54	0/2220	0.66	1/3017 (0.0%)
1	D	0.69	3/2209 (0.1%)	0.74	3/3001 (0.1%)
1	E	0.41	0/1772	0.57	0/2408
1	F	0.41	0/1772	0.57	0/2408
1	G	0.58	0/2199	0.74	2/2988 (0.1%)
1	H	0.56	0/2216	0.72	1/3013 (0.0%)
1	I	0.42	0/1783	0.58	0/2422
1	J	0.42	0/1783	0.58	0/2422
1	K	0.54	0/2220	0.67	1/3017 (0.0%)
1	L	0.54	0/2220	0.68	1/3017 (0.0%)
1	M	0.61	1/2209 (0.0%)	0.72	2/3001 (0.1%)
1	N	0.61	1/2209 (0.0%)	0.72	2/3001 (0.1%)
1	O	0.66	2/2199 (0.1%)	0.76	3/2988 (0.1%)
1	P	0.58	0/2199	0.74	2/2988 (0.1%)
1	Q	0.56	0/2216	0.71	0/3013
1	R	0.56	0/2216	0.72	1/3013 (0.0%)
All	All	0.54	7/37197 (0.0%)	0.68	19/50547 (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
1	B	0	1
1	D	0	1
1	G	0	1
1	I	0	1
1	J	0	1
1	M	0	1
1	N	0	1

Continued on next page...

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
1	P	0	1
All	All	0	9

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	15	PRO	N-CA	14.10	1.71	1.47
1	O	15	PRO	N-CA	13.91	1.71	1.47
1	O	14	VAL	C-N	6.08	1.45	1.34
1	D	14	VAL	C-N	6.08	1.45	1.34
1	M	361	PRO	N-CD	-5.09	1.40	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	15	PRO	CA-N-CD	-8.56	99.52	111.50
1	D	15	PRO	CA-N-CD	-8.22	100.00	111.50
1	G	106	LEU	CA-CB-CG	7.78	133.19	115.30
1	P	106	LEU	CA-CB-CG	7.77	133.17	115.30
1	O	106	LEU	CA-CB-CG	7.76	133.15	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	79	LYS	Peptide
1	D	189	THR	Peptide
1	G	367	GLY	Mainchain
1	I	79	LYS	Peptide
1	M	189	THR	Peptide

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	1729	0	1714	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1740	0	1722	29	0
1	C	2167	0	2144	55	0
1	D	2156	0	2147	57	0
1	E	1729	0	1714	38	0
1	F	1729	0	1714	36	0
1	G	2146	0	2127	42	0
1	H	2162	0	2130	54	0
1	I	1740	0	1722	27	0
1	J	1740	0	1722	27	0
1	K	2167	0	2144	39	0
1	L	2167	0	2144	46	0
1	M	2156	0	2147	41	0
1	N	2156	0	2147	49	0
1	O	2146	0	2127	46	0
1	P	2146	0	2127	41	0
1	Q	2162	0	2130	59	0
1	R	2162	0	2130	55	0
All	All	36300	0	35952	721	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 721 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:D:15:PRO:N	1:D:15:PRO:CA	1.71	1.34
1:O:15:PRO:N	1:O:15:PRO:CA	1.70	1.33
1:C:365:TYR:CE1	1:D:20:SER:HA	1.80	1.17
1:C:365:TYR:OH	1:D:20:SER:O	1.63	1.13
1:P:369:ARG:HH21	1:P:369:ARG:HG3	1.13	1.13

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	210/394 (53%)	190 (90%)	15 (7%)	5 (2%)	6	31
1	B	211/394 (54%)	184 (87%)	25 (12%)	2 (1%)	17	51
1	C	267/394 (68%)	228 (85%)	37 (14%)	2 (1%)	22	57
1	D	266/394 (68%)	222 (84%)	39 (15%)	5 (2%)	8	36
1	E	210/394 (53%)	190 (90%)	15 (7%)	5 (2%)	6	31
1	F	210/394 (53%)	190 (90%)	15 (7%)	5 (2%)	6	31
1	G	264/394 (67%)	225 (85%)	39 (15%)	0	100	100
1	H	267/394 (68%)	234 (88%)	31 (12%)	2 (1%)	22	57
1	I	211/394 (54%)	184 (87%)	25 (12%)	2 (1%)	17	51
1	J	211/394 (54%)	184 (87%)	25 (12%)	2 (1%)	17	51
1	K	267/394 (68%)	228 (85%)	37 (14%)	2 (1%)	22	57
1	L	267/394 (68%)	227 (85%)	37 (14%)	3 (1%)	14	47
1	M	266/394 (68%)	223 (84%)	39 (15%)	4 (2%)	10	40
1	N	266/394 (68%)	222 (84%)	40 (15%)	4 (2%)	10	40
1	O	264/394 (67%)	224 (85%)	39 (15%)	1 (0%)	34	68
1	P	264/394 (67%)	225 (85%)	39 (15%)	0	100	100
1	Q	267/394 (68%)	234 (88%)	31 (12%)	2 (1%)	22	57
1	R	267/394 (68%)	234 (88%)	31 (12%)	2 (1%)	22	57
All	All	4455/7092 (63%)	3848 (86%)	559 (12%)	48 (1%)	18	47

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	B	191	ASN
1	C	72	ILE
1	D	27	GLN
1	D	317	PHE

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	179/329 (54%)	169 (94%)	10 (6%)	21	54
1	B	181/329 (55%)	177 (98%)	4 (2%)	52	76
1	C	229/329 (70%)	218 (95%)	11 (5%)	25	59
1	D	227/329 (69%)	216 (95%)	11 (5%)	25	59
1	E	179/329 (54%)	169 (94%)	10 (6%)	21	54
1	F	179/329 (54%)	169 (94%)	10 (6%)	21	54
1	G	226/329 (69%)	223 (99%)	3 (1%)	69	83
1	H	228/329 (69%)	212 (93%)	16 (7%)	15	46
1	I	181/329 (55%)	177 (98%)	4 (2%)	52	76
1	J	181/329 (55%)	177 (98%)	4 (2%)	52	76
1	K	229/329 (70%)	222 (97%)	7 (3%)	40	69
1	L	229/329 (70%)	218 (95%)	11 (5%)	25	59
1	M	227/329 (69%)	217 (96%)	10 (4%)	28	61
1	N	227/329 (69%)	217 (96%)	10 (4%)	28	61
1	O	226/329 (69%)	223 (99%)	3 (1%)	69	83
1	P	226/329 (69%)	223 (99%)	3 (1%)	69	83
1	Q	228/329 (69%)	209 (92%)	19 (8%)	11	38
1	R	228/329 (69%)	213 (93%)	15 (7%)	16	48
All	All	3810/5922 (64%)	3649 (96%)	161 (4%)	33	62

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	324	ARG
1	P	81	ARG
1	J	187	GLU
1	L	106	LEU
1	R	112	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	100	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	94	HIS
1	P	363	GLN
1	O	160	ASN
1	O	363	GLN

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 monosaccharides 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-19251. 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 ⓘ
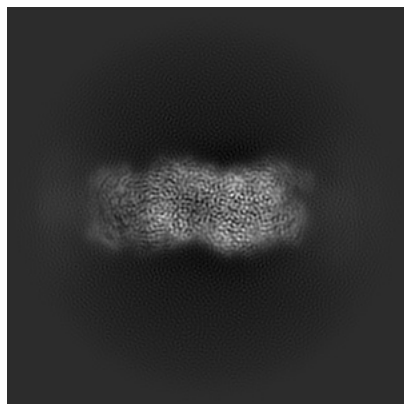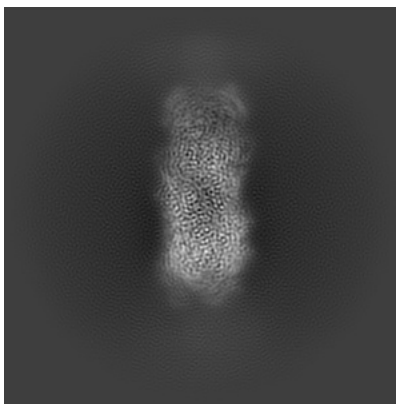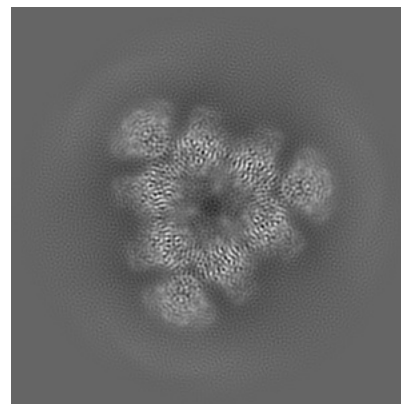
6.1.1 Primary map

X   Y   Z

6.1.2 Raw map

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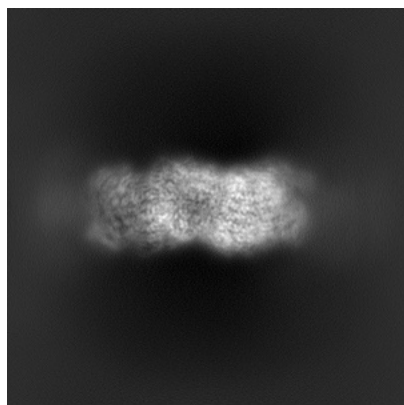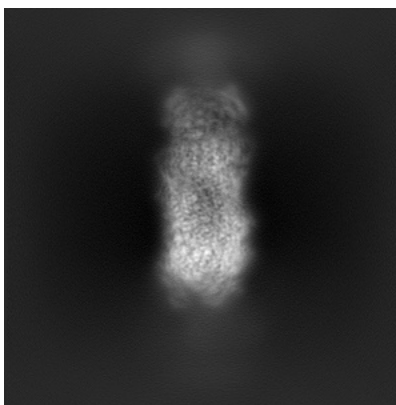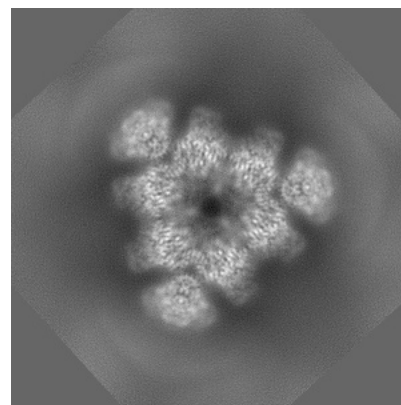
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
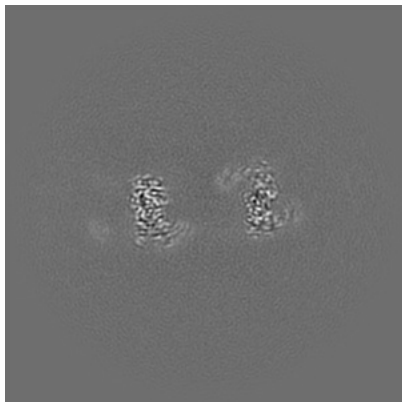
6.2.1 Primary map
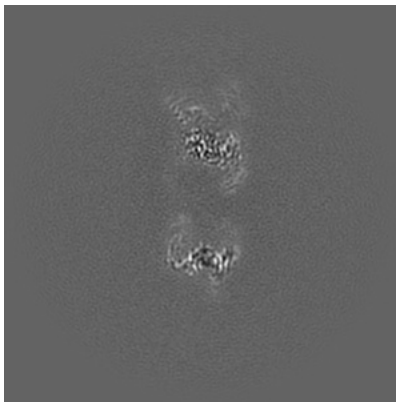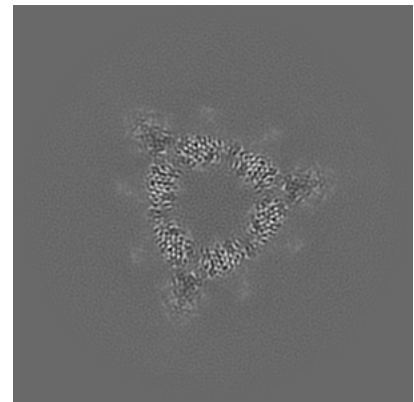
| X Index: 250 | Y Index: 250 | Z Index: 250 |

6.2.2 Raw map
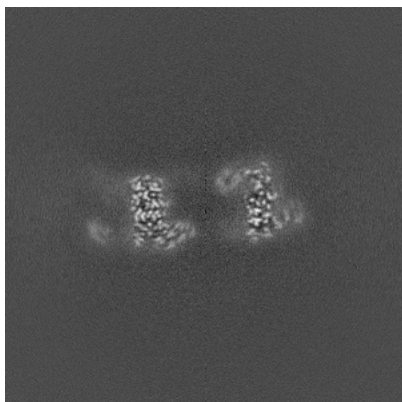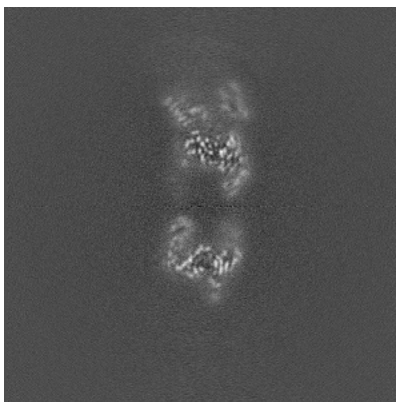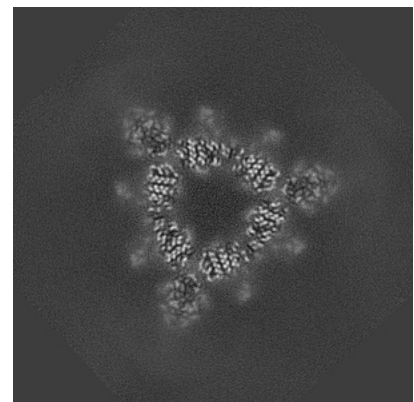
| X Index: 250 | Y Index: 250 | Z Index: 250 |

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
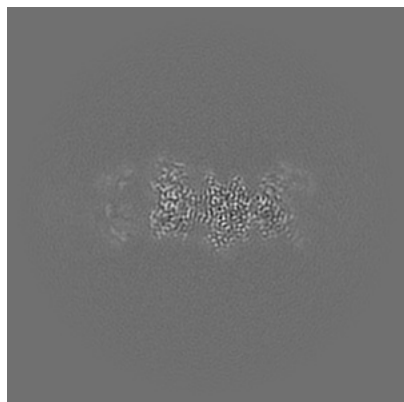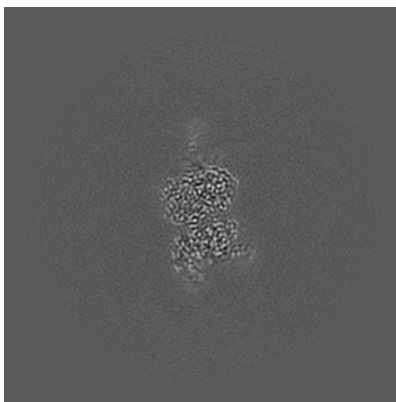
| X Index: 187 | Y Index: 191 | Z Index: 261 |
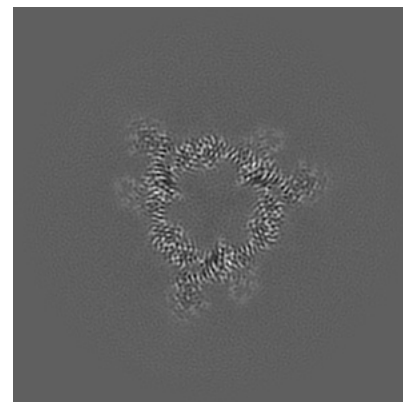
6.3.2 Raw map
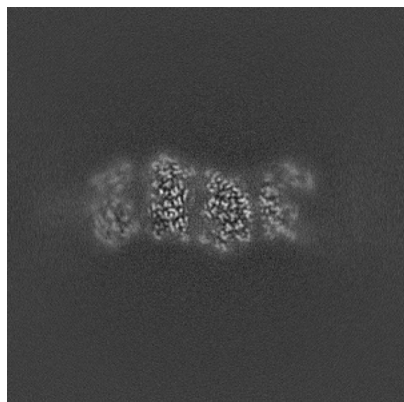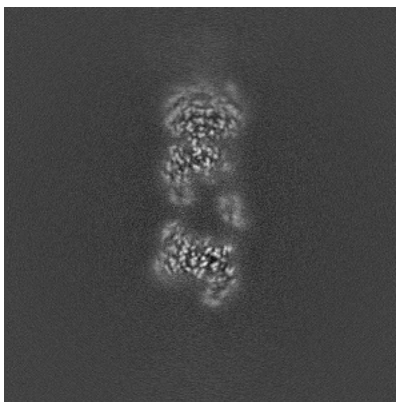
| X Index: 193 | Y Index: 275 | Z Index: 239 |
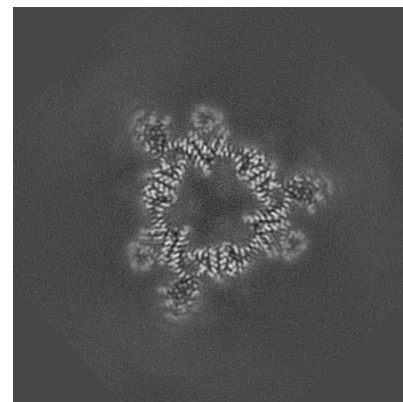
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1　Primary map
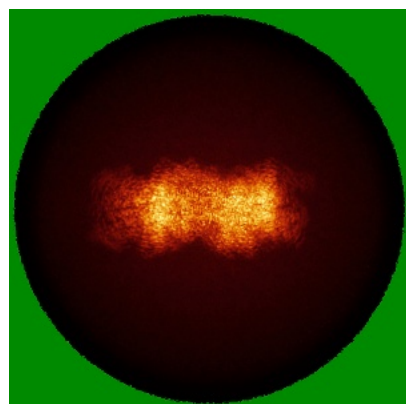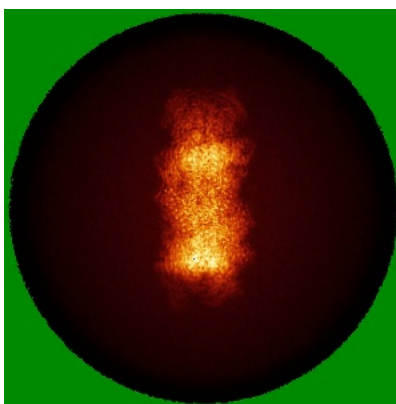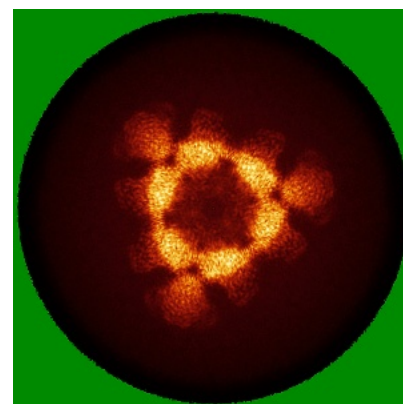
X　　　　　　　　　Y　　　　　　　　　Z

6.4.2　Raw map

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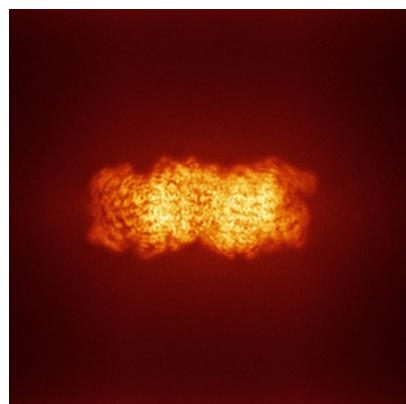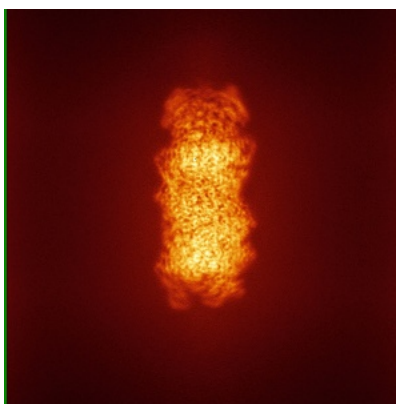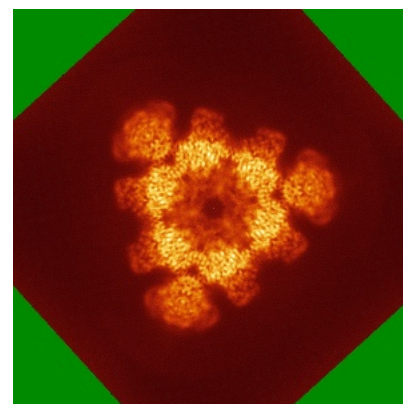
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X	Y	Z
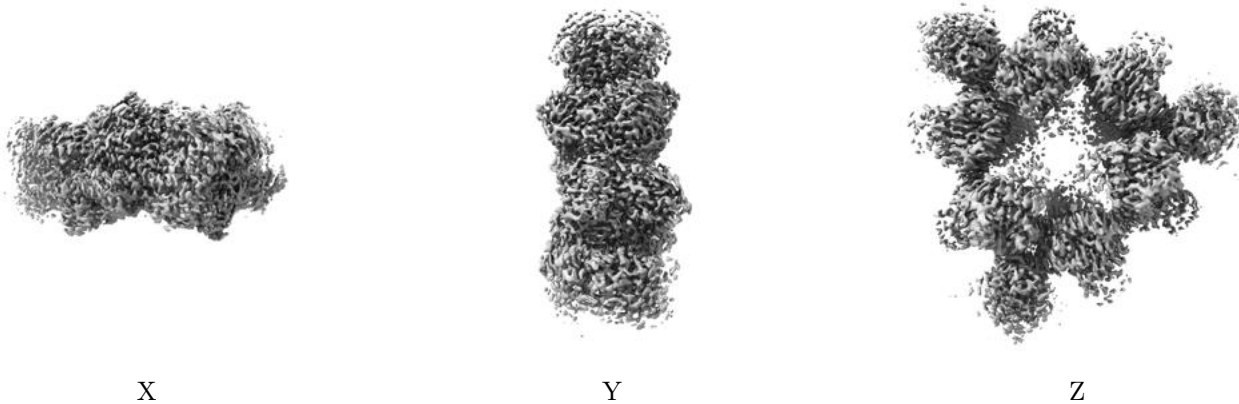
The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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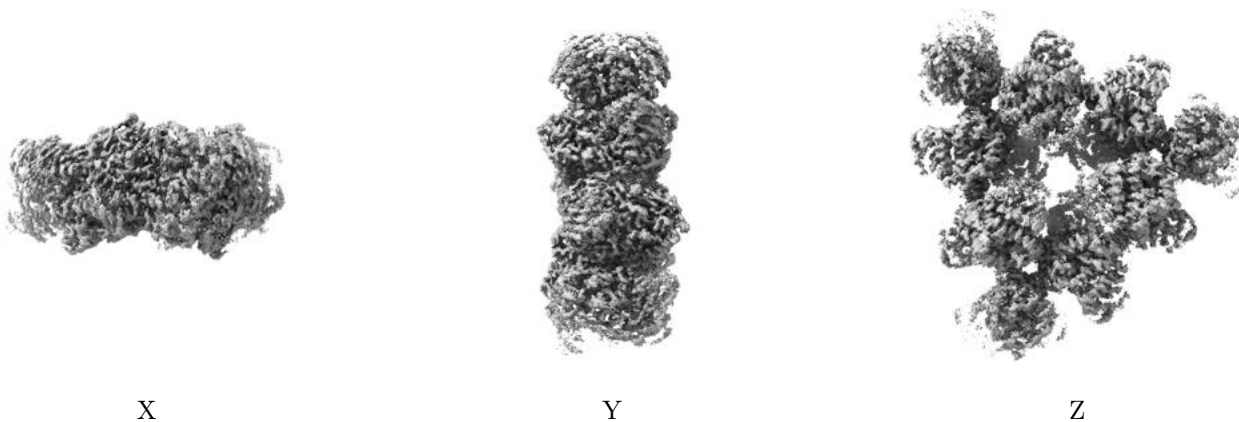
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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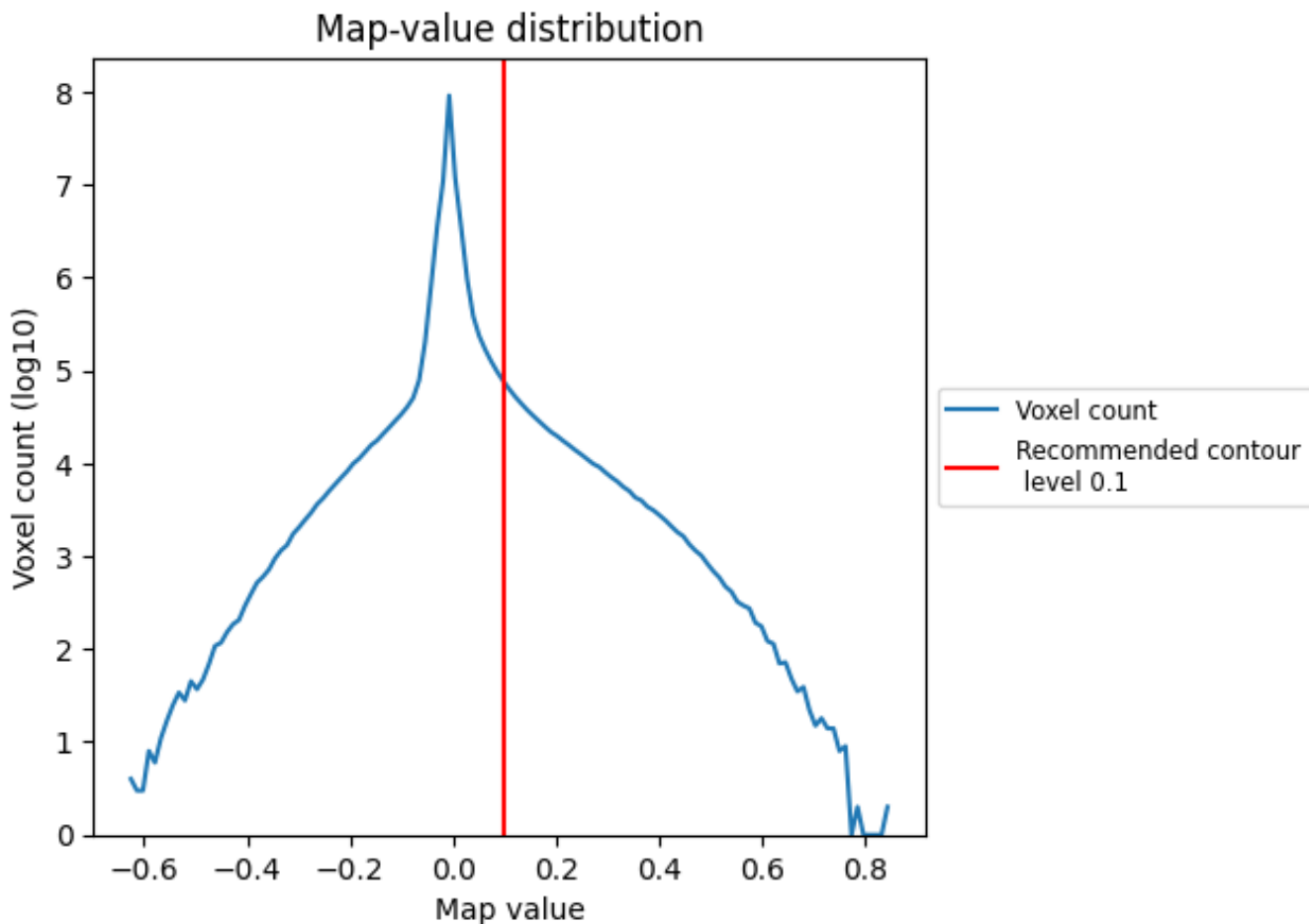
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
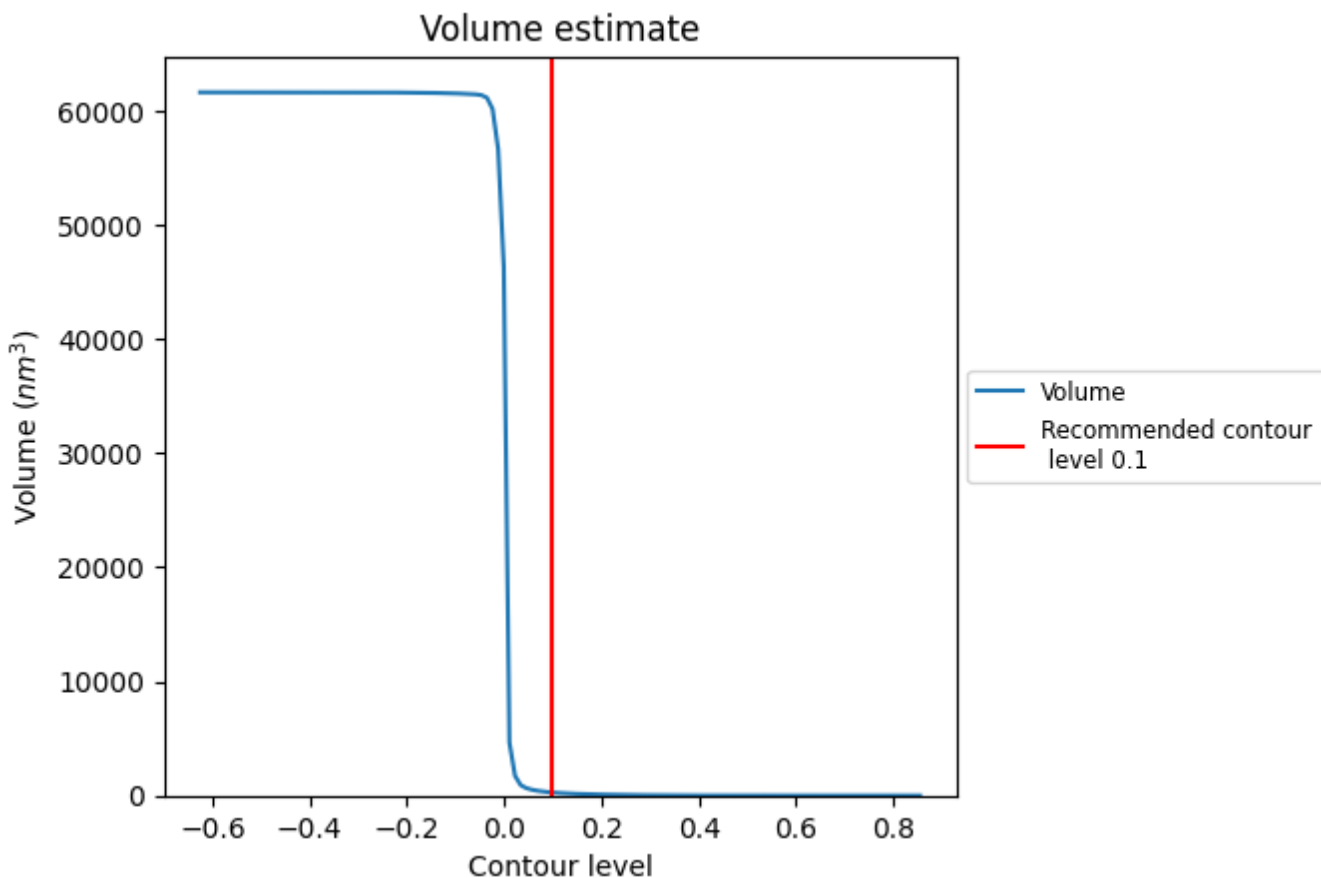
Volume estimate

The volume at the recommended contour level is 266 nm^3; this corresponds to an approximate mass of 241 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 ⓘ
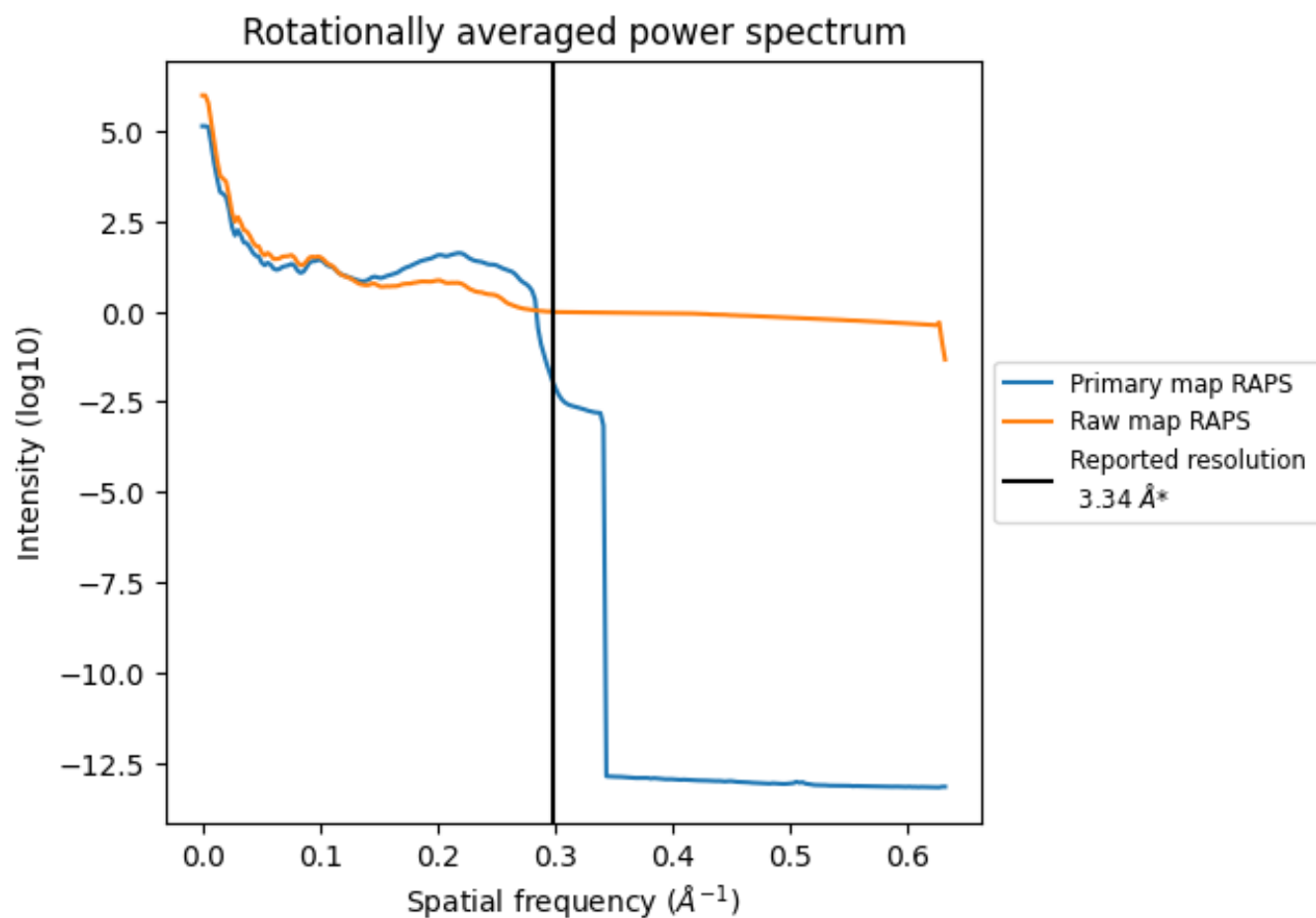
*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

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 ⓘ
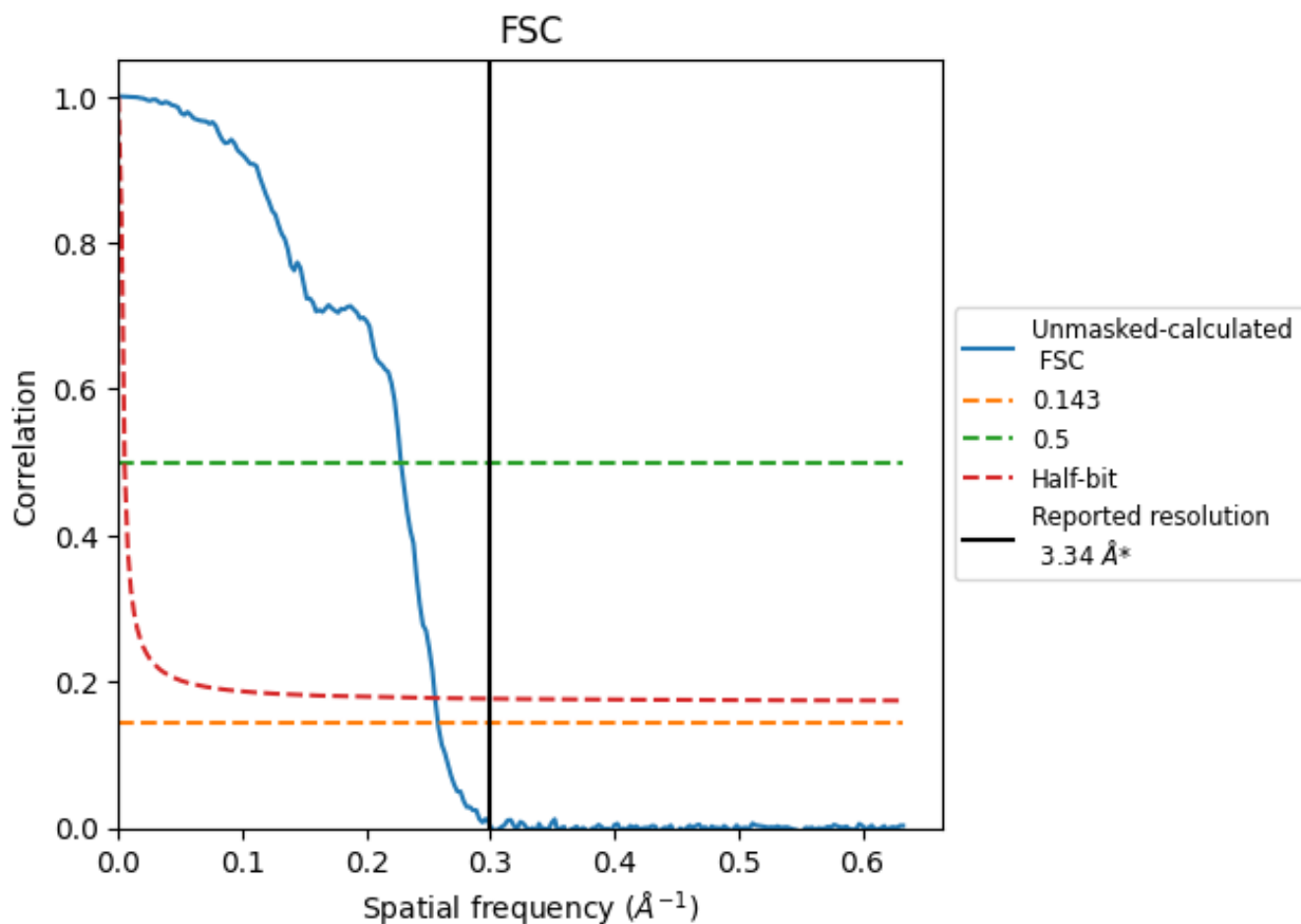
*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	4.39	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.34 by more than 10 %

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-19251 and PDB model 8RJL. Per-residue inclusion information can be found in section 3 on page 9.

9.1　Map-model overlay ⓘ

X　　　　　　　　　　　　　Y　　　　　　　　　　　　　Z
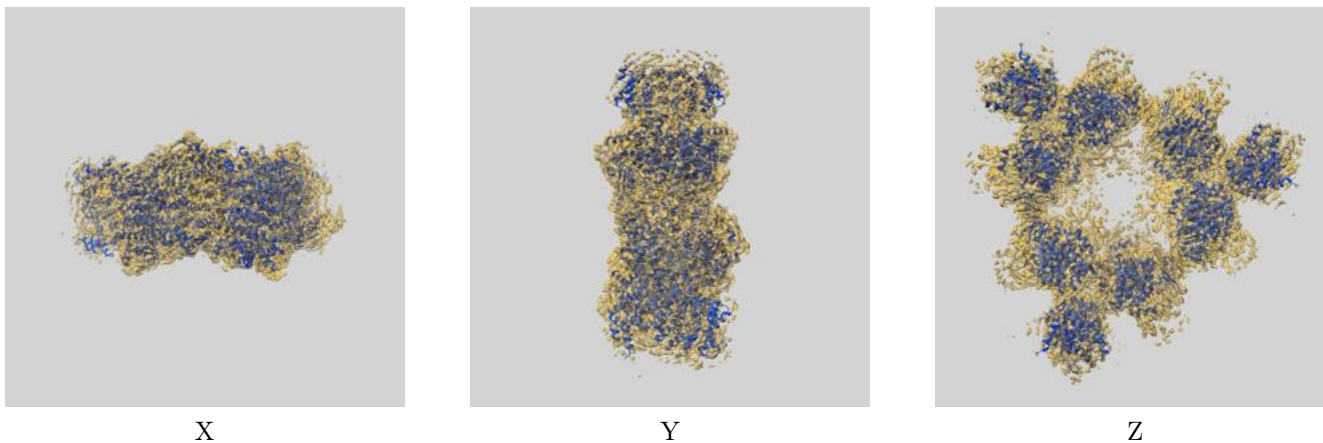
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　　Y　　　　　　　　　　Z
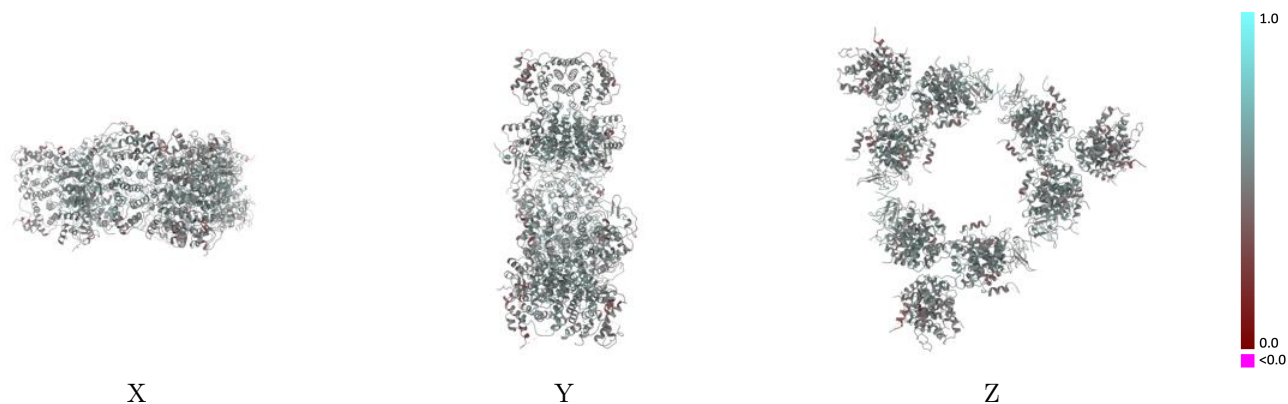
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
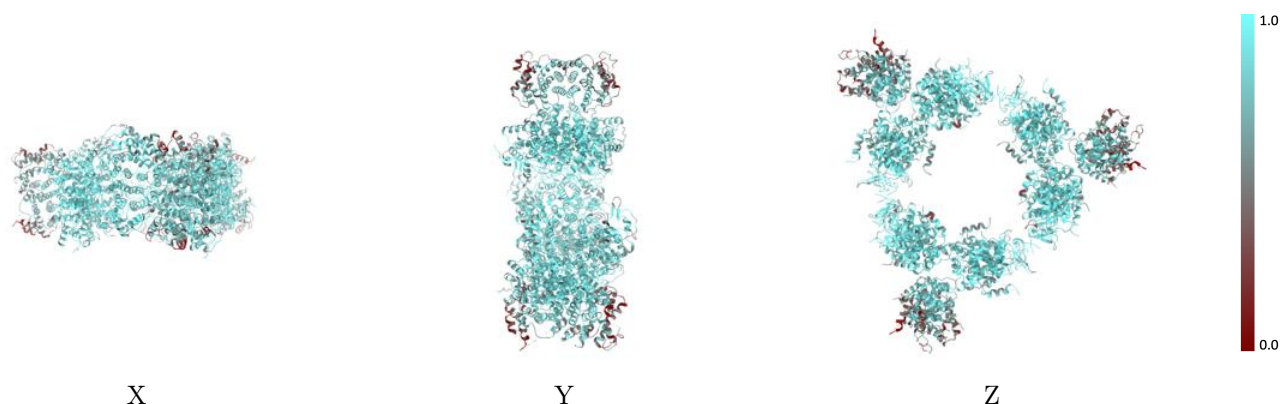
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4   Atom inclusion ⓘ
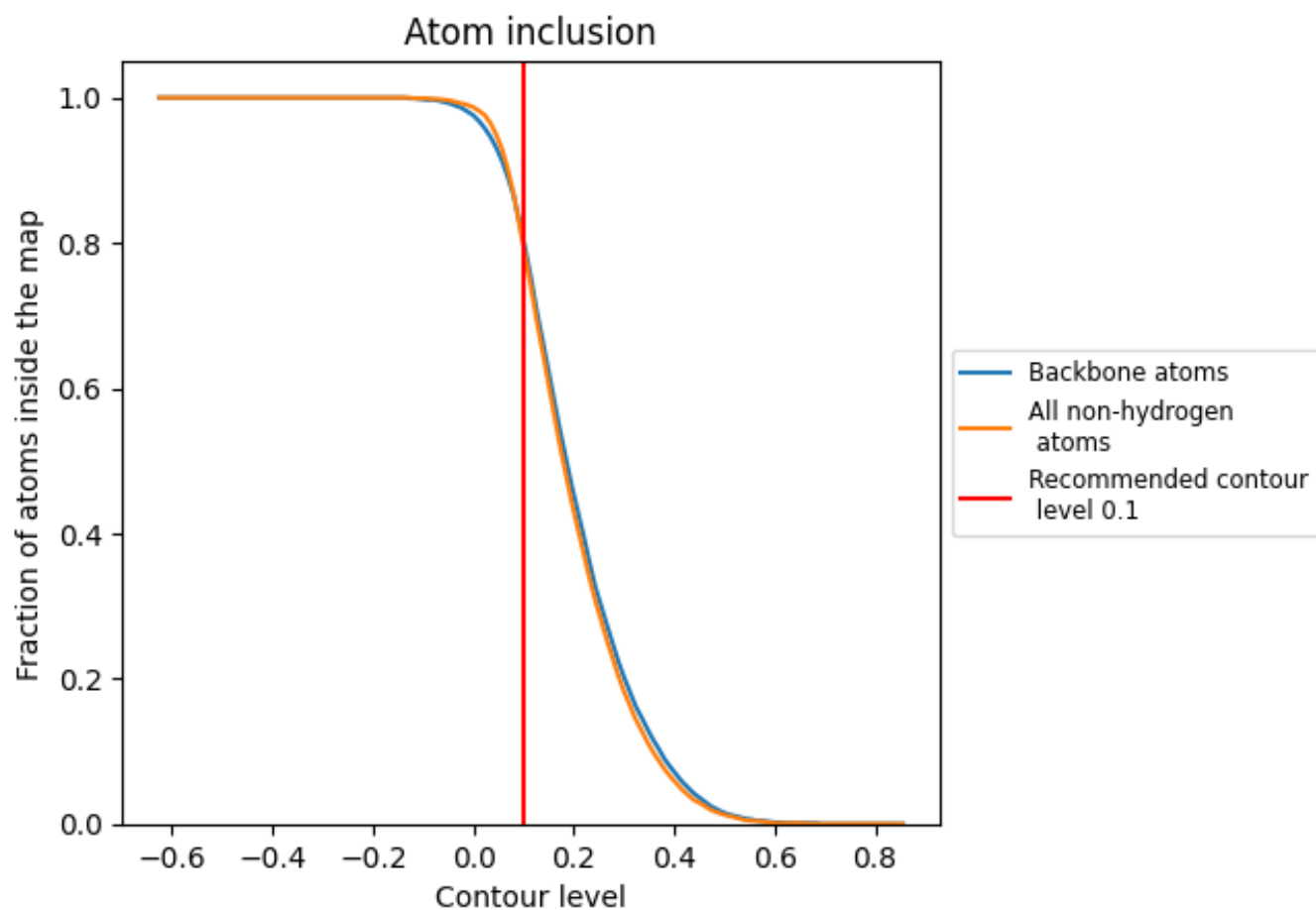
At the recommended contour level, 80% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7940	0.5040
A	0.6240	0.4820
B	0.6560	0.4850
C	0.8430	0.5100
D	0.8660	0.5220
E	0.6210	0.4780
F	0.6170	0.4780
G	0.8650	0.5150
H	0.8570	0.5070
I	0.6570	0.4840
J	0.6530	0.4840
K	0.8450	0.5130
L	0.8460	0.5110
M	0.8640	0.5220
N	0.8640	0.5210
O	0.8630	0.5120
P	0.8670	0.5120
Q	0.8530	0.5030
R	0.8530	0.5060

1.0

0.0
<0.0