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 ⓘ

Mar 12, 2024 – 06:53 PM JST

PDB ID	:	8H33
EMDB ID	:	EMD-34449
Title	:	Cryo-EM Structure of the KBTBD2-Cul3-Rbx1 tetrameric complex
Authors	:	Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on	:	2022-10-07
Resolution	:	7.86 Å(reported)

This is a wwPDB EM Validation Summary 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:

# 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 7.86 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		17
Ramachandran outliers		1.3%
Sidechain outliers		10.4%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
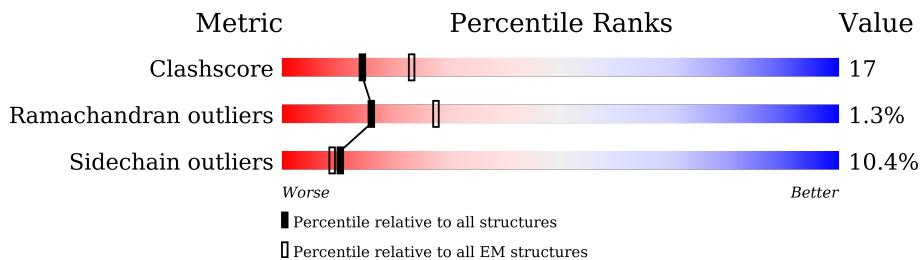
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	623	61% · 27% · 10%
1	B	623	60% · 27% · 11%
1	G	623	60% · 27% · 10%
1	J	623	61% · 26% · 11%
2	D	121	47% · 25% ·· 26%
2	E	121	40% · 28% · 5% · 26%
2	K	121	41% · 27% ·· 26%
2	L	121	38% · 32% ·· 26%
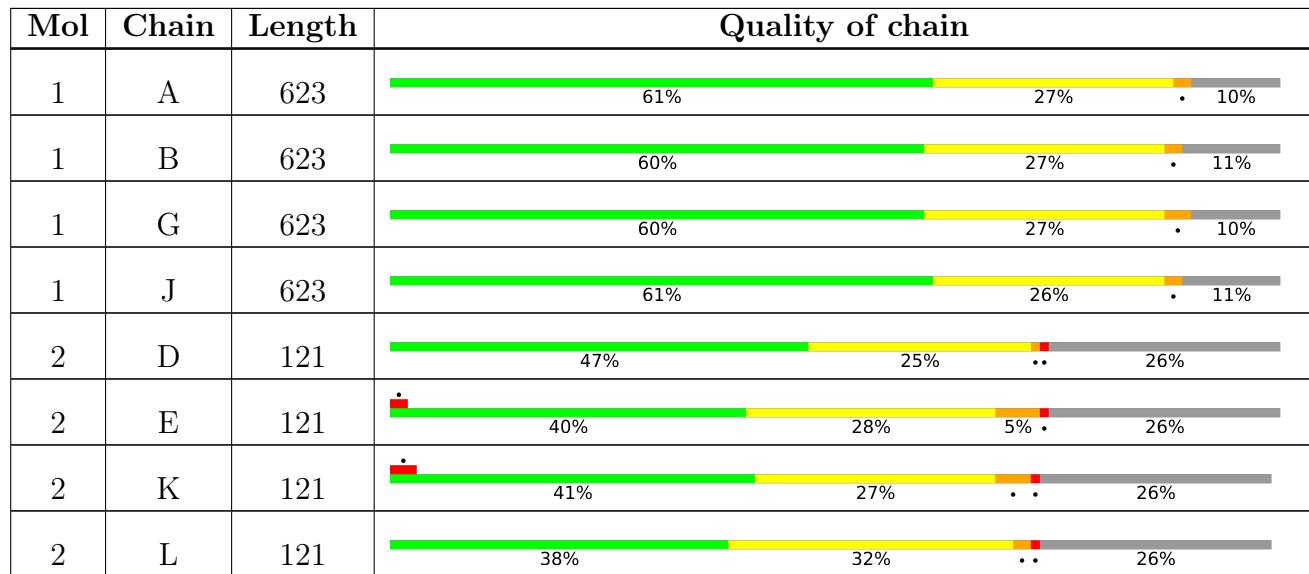
<div align="right">Continued on next page...</div>

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	776	60%　　29%　・7%
3	F	776	59%　　29%　・7%
3	H	776	58%　　31%　・7%
3	I	776	59%　　30%　・7%

2 Entity composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 43620 atoms, of which 72 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 Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	562	Total	C	H	N	O	S	0	0
			4473	2842	18	746	832	35		
1	B	557	Total	C	H	N	O	S	0	0
			4464	2839	18	737	834	36		
1	G	562	Total	C	H	N	O	S	0	0
			4438	2820	18	743	823	34		
1	J	555	Total	C	H	N	O	S	0	0
			4482	2855	18	740	832	37		

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	89	Total	C	N	O	S	0	0
			695	443	121	124	7		
2	K	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
2	L	89	Total	C	N	O	S	0	0
			737	466	135	127	9		
2	E	89	Total	C	N	O	S	0	0
			737	466	135	127	9		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P62877
D	-11	HIS	-	expression tag	UNP P62877
D	-10	HIS	-	expression tag	UNP P62877
D	-9	HIS	-	expression tag	UNP P62877
D	-8	HIS	-	expression tag	UNP P62877
D	-7	HIS	-	expression tag	UNP P62877
D	-6	GLU	-	expression tag	UNP P62877
D	-5	ASN	-	expression tag	UNP P62877
D	-4	LEU	-	expression tag	UNP P62877

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	TYR	-	expression tag	UNP P62877
D	-2	PHE	-	expression tag	UNP P62877
D	-1	GLN	-	expression tag	UNP P62877
D	0	GLY	-	expression tag	UNP P62877
K	-12	HIS	-	expression tag	UNP P62877
K	-11	HIS	-	expression tag	UNP P62877
K	-10	HIS	-	expression tag	UNP P62877
K	-9	HIS	-	expression tag	UNP P62877
K	-8	HIS	-	expression tag	UNP P62877
K	-7	HIS	-	expression tag	UNP P62877
K	-6	GLU	-	expression tag	UNP P62877
K	-5	ASN	-	expression tag	UNP P62877
K	-4	LEU	-	expression tag	UNP P62877
K	-3	TYR	-	expression tag	UNP P62877
K	-2	PHE	-	expression tag	UNP P62877
K	-1	GLN	-	expression tag	UNP P62877
K	0	GLY	-	expression tag	UNP P62877
L	-12	HIS	-	expression tag	UNP P62877
L	-11	HIS	-	expression tag	UNP P62877
L	-10	HIS	-	expression tag	UNP P62877
L	-9	HIS	-	expression tag	UNP P62877
L	-8	HIS	-	expression tag	UNP P62877
L	-7	HIS	-	expression tag	UNP P62877
L	-6	GLU	-	expression tag	UNP P62877
L	-5	ASN	-	expression tag	UNP P62877
L	-4	LEU	-	expression tag	UNP P62877
L	-3	TYR	-	expression tag	UNP P62877
L	-2	PHE	-	expression tag	UNP P62877
L	-1	GLN	-	expression tag	UNP P62877
L	0	GLY	-	expression tag	UNP P62877
E	-12	HIS	-	expression tag	UNP P62877
E	-11	HIS	-	expression tag	UNP P62877
E	-10	HIS	-	expression tag	UNP P62877
E	-9	HIS	-	expression tag	UNP P62877
E	-8	HIS	-	expression tag	UNP P62877
E	-7	HIS	-	expression tag	UNP P62877
E	-6	GLU	-	expression tag	UNP P62877
E	-5	ASN	-	expression tag	UNP P62877
E	-4	LEU	-	expression tag	UNP P62877
E	-3	TYR	-	expression tag	UNP P62877
E	-2	PHE	-	expression tag	UNP P62877
E	-1	GLN	-	expression tag	UNP P62877

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P62877

- Molecule 3 is a protein called Cullin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	720	Total 5651	C 3540	N 1003	O 1071	S 37	0	0
3	H	720	Total 5719	C 3589	N 1019	O 1073	S 38	0	0
3	I	720	Total 5722	C 3585	N 1013	O 1086	S 38	0	0
3	C	720	Total 5753	C 3613	N 1022	O 1081	S 37	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	TRP	-	expression tag	UNP Q13618
F	-6	SER	-	expression tag	UNP Q13618
F	-5	HIS	-	expression tag	UNP Q13618
F	-4	PRO	-	expression tag	UNP Q13618
F	-3	GLN	-	expression tag	UNP Q13618
F	-2	PHE	-	expression tag	UNP Q13618
F	-1	GLU	-	expression tag	UNP Q13618
F	0	LYS	-	expression tag	UNP Q13618
H	-7	TRP	-	expression tag	UNP Q13618
H	-6	SER	-	expression tag	UNP Q13618
H	-5	HIS	-	expression tag	UNP Q13618
H	-4	PRO	-	expression tag	UNP Q13618
H	-3	GLN	-	expression tag	UNP Q13618
H	-2	PHE	-	expression tag	UNP Q13618
H	-1	GLU	-	expression tag	UNP Q13618
H	0	LYS	-	expression tag	UNP Q13618
I	-7	TRP	-	expression tag	UNP Q13618
I	-6	SER	-	expression tag	UNP Q13618
I	-5	HIS	-	expression tag	UNP Q13618
I	-4	PRO	-	expression tag	UNP Q13618
I	-3	GLN	-	expression tag	UNP Q13618
I	-2	PHE	-	expression tag	UNP Q13618
I	-1	GLU	-	expression tag	UNP Q13618
I	0	LYS	-	expression tag	UNP Q13618
C	-7	TRP	-	expression tag	UNP Q13618

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	SER	-	expression tag	UNP Q13618
C	-5	HIS	-	expression tag	UNP Q13618
C	-4	PRO	-	expression tag	UNP Q13618
C	-3	GLN	-	expression tag	UNP Q13618
C	-2	PHE	-	expression tag	UNP Q13618
C	-1	GLU	-	expression tag	UNP Q13618
C	0	LYS	-	expression tag	UNP Q13618

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	D	3	Total 3	Zn 3	0
4	K	3	Total 3	Zn 3	0
4	L	3	Total 3	Zn 3	0
4	E	3	Total 3	Zn 3	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: Kelch repeat and BTB domain-containing protein 2

• Molecule 1: Kelch repeat and BTB domain-containing protein 2

A232 W233 L237 P238 P239 V245 S252 M253 P254 K255 F256 F257 G262 M263 T264 K265 I270 E273 A274 S275 S276 E277 N278 P279 C280 S281 L282 Y283 V286 C287 Y288 S289 K294 K297 P301 P302 A303 D304 L305 I318 A321 G322 G323 Q324 V325 P326 T330

LYS THR ASN HIS SER LYS THR SER LYS LEU GLN THR ALA F344 R345 N348 C349 F350 F353 W360 K363 T364 P365 M366 R370 S374 L375 C378 E379 I382 I385 S389 V390 E393 R396 R397 T398 V399 E400 R401 Y402 W409 P414 L415 W419

S422 V425 V426 I431 M434 T435 L436 N437 M438 M439 Y442 V450 R455 Q456 T457 S458 R459 A466 K470 G476 L477 HIS ILE ALA THR ASN SER GLY ILE ARG LEU PRO SER GLY THR VAL ASP GLY SER S496 E500 D503 P516 ALA LYS ARG TYR

SER D522 V525 I530 C535 M538 R539 K548 Y549 Q553 Y554 D555 L558 W561 R564 Q565 H566 W573 D574 R577 K585 L586 Y587 E593 S594 P595 P598 PRO THR TYR LEU PHE SER THR ASP GLY THR GLU GLU PHE GLU LEU ASP GLY GLU MET

VAL ALA LEU PRO VAL

• Molecule 1: Kelch repeat and BTB domain-containing protein 2

Chain G:

60%   27%   •   10%

MET SER THR GLN ASP E6 R7 Q8 I9 N10 T11 E12 Y13 A14 V15 L18 L21 V34 V37 T40 E41 H45 K46 M47 V48 T51 S54 A58 S62 H71 L74 R75 N76 V77 D78 A79 L82 Q83 I84 Y90 T91 G92 N93 E102

F110 R119 K127 I128 C133 V134 R135 L136 S151 A152 K153 R154 M155 F160 T161 D167 Q171 L172 S173 D179 I180 L181 L186 N187 V188 E189 K190 E191 E192 T193 V194 R195 A198 M199 L200 W201 L202 E203 T206 R209 S210 Q211 Y212 L213 V216 L217 S218

Q219 I220 R221 I222 D223 A224 L225 S226 E227 V228 T229 Q230 R231 A232 W233 L237 V245 S252 M253 P254 K255 F256 F257 G262 M263 T264 K265 M268 M269 I270 E273 S276 E277 C280 S281 L282 Y283 V286 C287 Y288 S289 K294 V295 Y296 K297 P301 P302 A303 D304

L305 H306 I318 A321 G322 G323 Q324 V325 P326 T330 LYS THR ASN HIS SER LYS THR SER LYS LEU GLN THR ALA F344 R345 N348 C349 F350 F353 W360 K363 T364 P365 M366 R370 S374 L375 V376 C377 C378 E379 Y383 A384 I385 S389 V390 E393

R396 R397 T398 V399 E400 R401 Y402 W409 S413 P414 L415 W419 S422 V425 V426 I431 M434 T435 L436 N437 L438 Y442 F443 W449 R455 Q456 T457 S458 R459 A466 G476 L477 HIS ILE ALA THR ASN SER GLY ILE ARG LEU PRO SER GLY THR VAL ASP

GLY SER S496 E500 V525 I530 C535 M538 R539 K548 Y549 Q553 Y554 D555 L558 W561 R564 Q565 H566 W573 R577 K585 L586 Y587 E593 K597 P598 PRO THR TYR LEU PHE SER THR ASP GLY THR GLU GLU PHE GLU LEU ASP GLY

GLU MET VAL ALA LEU PRO VAL

• Molecule 1: Kelch repeat and BTB domain-containing protein 2

Chain J:

61%   26%   •   11%

MET SER THR GLN ASP E6 R7 Q8 I9 N10 T11 L17 L21 I33 V37 M47 V48 T51 C52 S53 R57 A58 M59 V72 R75 L82 T87 Y90 T91 G92 N93 E102 L111 R119 K127 I128 C133 V134 R135 L136 S144 C145

E146 K153 V156 F160 T161 Q166 D167 A168 F169 M170 Q171 L172 S173 D179 I180 L181 S182 V188 E189 K190 E191 E192 T193 V194 R195 E196 A197 A198 W201 L202 E203 Y204 N205 T206 E207 S210 Q211 Y212 L213 S214 L217 S218 Q219 I220 I222 D223 A224 L225 S226 E227

• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain D: 47% 25% 26%

• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain K: 41% 27% 26%

• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain L: 38% 32% 26%
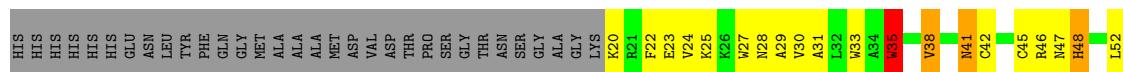
• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain E: 40% 28% 5% 26%

• Molecule 3: Cullin-3

Chain F:

59%　29%　•　7%

• Molecule 3: Cullin-3

Chain H:

58%　31%　•　7%

C462 F466 T467 S468 K469 L470 M473 F474 R475 D476 S480 M484 R488 L491 Q492 A493 V501 D502 L503 T504 V505 R506 V507 L508 T509 T510 G511 Y512 W513 P514 T515 Q516 S517 K521 C522 N523 I524 P525 P526 A527 P528 R529 Y539 K542 R546 Q547 Q551

H552 H553 S556 A557 D558 L559 N560 A561 T562 PHE TYR GLY PRO VAL LYS LYS GLU ASP GLY SER GLU VAL GLY VAL GLY ALA GLN VAL THR GLY SER ASN T587 L592 Q593 V594 S595 T596 F597 Q598 L602 F605 N606 E609 K610 Y611 T612 F613 E614 Q617 T620 D621

I622 R625 E626 L627 V628 R629 Q632 S633 L634 A635 C636 G637 K638 P639 T640 Q641 R642 V643 L644 T645 K646 E647 P648 I653 E654 N655 F659 Q664 F665 L669 H670 R671 V672 K680 Q681 G682 E683 D685 P686 E687 R688 K689 E690 T691 K694 V695 D696 D697 D698 R699 K700

H701 E702 I703 A706 I707 V708 R709 I710 M711 K712 S713 R714 K715 K716 M717 L722 V723 A724 E725 V726 Q729 L735 P736 I741 K742 K743 R744 I749 E750 R751 E752 Y753 L754 A755 R756 T757 P758 V767 A768

• Molecule 3: Cullin-3

Chain I:

TRP SER HIS PRO GLN PHE GLU LYS MET SER ASN LEU SER LYS GLY THR GLY SER ARG LYS ASP THR LYS MET ARG ILE ARG ALA PHE PRO MET THR M25 K47 K72 L73 Y74 L77 I86 R90 L102 Q113 M116 V117 M118 I119 R120 D121 I122 L123 M124 Y125

M126 D127 R128 V129 Y130 V131 Q132 Q133 E137 N138 V139 Y140 N141 L142 G143 L144 R148 D149 Q150 R153 L166 I169 R180 G181 A182 L193 R198 S199 V200 Y201 E202 E203 D204 F205 E206 A207 P208 F209 L210 E211 M212 S213 M219 E220 S221 Q222 K223 F224 L225 A230

E238 N242 R247 V248 M249 H250 K254 S255 T256 E257 E258 P259 V263 V264 E265 R266 E267 L268 I269 S270 K271 H272 I276 S282 V285 H286 M287 G291 C298 M299 Y300 K301 V306 C314 N337 P338 V339 L345 L346 K349 S350 R351 F352 D353 R354

F355 L356 L357 T369 E375 Y376 F377 L378 N379 L380 N381 S382 R383 S384 P385 L390 F391 I392 D393 D394 K395 L396 K397 K398 G399 V400 E407 D413 K414 A415 M416 V417 L418 F419 R420 F421 M422 Q423 E424 K425 D426 V427 F428 K433 L436 A437 R438 R439 T442 V446 S447

I455 L458 L462 C462 F466 T467 S468 K469 L470 F474 R475 D476 S480 E486 F487 R488 L491 V496 S497 L498 G499 G500 L503 R506 V507 L508 T509 T510 G511 Y512 W513 P514 T515 Q516 S517 A518 T519 P520 K521 C522 N523 I524 P525 P526 R529 R546 Q547

H552 H553 S556 A557 D558 L559 N560 A561 T562 PHE TYR GLY PRO VAL LYS LYS GLU ASP GLY SER GLU VAL GLY VAL GLY ALA GLN VAL THR GLY SER ASN T587 L592 Q593 V594 S595 T596 F597 Q598 L602 F605 N606 E609 K610 Y611 T612 F613 E614 Q617 Q618 E619

I622 P623 E624 R625 E626 L627 V628 R629 Q632 S633 L634 A635 C636 G637 K638 P639 T640 Q641 R642 V643 L644 T645 K646 E647 P648 I653 E654 N655 F659 Q664 F665 L669 H670 R671 V672 K673 I674 K680 Q681 G682 E683 E687 R688 K689 E690 T691 R692 Q693 K694 V695 D696 D697

K700 H701 E702 I703 A706 I707 V708 R709 I710 M711 K712 S713 R714 K715 K716 M717 V721 L722 V723 V726 K731 L735 I741 K742 K743 R744 L748 I749 E750 R751 E752 Y753 L754 A755 R756 T757 P758 A768

• Molecule 3: Cullin-3

Chain C:

TRP SER HIS PRO GLN PHE GLU LYS MET SER ASN LEU SER LYS GLY THR GLY SER ARG LYS ASP THR LYS MET ARG ILE ARG ALA PHE PRO MET THR M25 E43 K47 Y58 Y74 L77 I86 R90 L102 Q113 M116 V117 M118 I119 R120 L123 M124

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50236	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 $(e^-/\text{Å}^2)$	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.590	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.0001	Depositor
Map size (Å)	511.488, 511.488, 511.488	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.664, 2.664, 2.664	Depositor

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.39	0/4558	0.49	0/6191
1	B	0.40	0/4548	0.50	0/6172
1	G	0.43	0/4521	0.51	0/6146
1	J	0.40	0/4569	0.48	0/6201
2	D	0.59	0/715	0.62	0/973
2	E	0.57	0/759	0.61	0/1029
2	K	0.55	0/759	0.61	0/1029
2	L	0.55	0/759	0.61	0/1029
3	C	0.43	0/5840	0.52	0/7853
3	F	0.46	0/5728	0.53	0/7706
3	H	0.41	0/5806	0.52	0/7810
3	I	0.46	0/5802	0.54	0/7804
All	All	0.44	0/44364	0.52	0/59943

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4455	18	4288	138	0

Continued on next page...

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

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4446	18	4306	169	0
1	G	4420	18	4240	141	0
1	J	4464	18	4343	139	0
2	D	695	0	608	42	0
2	E	737	0	686	57	0
2	K	737	0	686	54	0
2	L	737	0	686	58	0
3	C	5753	0	5709	193	0
3	F	5651	0	5542	190	0
3	H	5719	0	5634	216	0
3	I	5722	0	5664	182	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	K	3	0	0	0	0
4	L	3	0	0	0	0
All	All	43548	72	42392	1479	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 17.

The worst 5 of 1479 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:G:47:MET:CE	1:J:21:LEU:HD22	1.45	1.44
2:K:24:VAL:C	2:K:25:LYS:HE2	1.43	1.38
2:D:24:VAL:C	2:D:25:LYS:HE2	1.43	1.38
2:L:24:VAL:C	2:L:25:LYS:HE2	1.43	1.35
2:E:24:VAL:C	2:E:25:LYS:HE2	1.43	1.35

There are no symmetry-related clashes.

5.3   Torsion angles (i)

5.3.1   Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	556/623 (89%)	509 (92%)	44 (8%)	3 (0%)	29	69
1	B	549/623 (88%)	506 (92%)	39 (7%)	4 (1%)	22	63
1	G	556/623 (89%)	495 (89%)	53 (10%)	8 (1%)	11	46
1	J	547/623 (88%)	495 (90%)	49 (9%)	3 (0%)	29	69
2	D	87/121 (72%)	61 (70%)	21 (24%)	5 (6%)	1	18
2	E	87/121 (72%)	59 (68%)	23 (26%)	5 (6%)	1	18
2	K	87/121 (72%)	60 (69%)	22 (25%)	5 (6%)	1	18
2	L	87/121 (72%)	62 (71%)	20 (23%)	5 (6%)	1	18
3	C	716/776 (92%)	629 (88%)	82 (12%)	5 (1%)	22	63
3	F	716/776 (92%)	610 (85%)	93 (13%)	13 (2%)	8	40
3	H	716/776 (92%)	615 (86%)	94 (13%)	7 (1%)	15	55
3	I	716/776 (92%)	620 (87%)	87 (12%)	9 (1%)	12	48
All	All	5420/6080 (89%)	4721 (87%)	627 (12%)	72 (1%)	16	48

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	390	VAL
1	B	279	PRO
1	G	221	ARG
2	D	68	CYS
3	F	400	VAL

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	478/560 (85%)	446 (93%)	32 (7%)	16	41
1	B	485/560 (87%)	452 (93%)	33 (7%)	16	41
1	G	470/560 (84%)	427 (91%)	43 (9%)	9	29
1	J	491/560 (88%)	452 (92%)	39 (8%)	12	35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
2	D	66/102 (65%)	58 (88%)	8 (12%)	5	20	
2	E	78/102 (76%)	66 (85%)	12 (15%)	2	14	
2	K	78/102 (76%)	66 (85%)	12 (15%)	2	14	
2	L	78/102 (76%)	67 (86%)	11 (14%)	3	16	
3	C	621/701 (89%)	542 (87%)	79 (13%)	4	18	
3	F	597/701 (85%)	520 (87%)	77 (13%)	4	18	
3	H	610/701 (87%)	556 (91%)	54 (9%)	9	30	
3	I	617/701 (88%)	530 (86%)	87 (14%)	3	16	
All	All	4669/5452 (86%)	4182 (90%)	487 (10%)	10	24	

5 of 487 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	753	TYR
3	C	619	GLU
2	K	35	TRP
3	C	542	LYS
3	C	754	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	657	HIS
3	C	728	GLN
3	F	657	HIS
3	F	618	GLN
2	E	28	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

This section contains visualisations of the EMDB entry EMD-34449. 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 (i)

6.1.1 Primary map
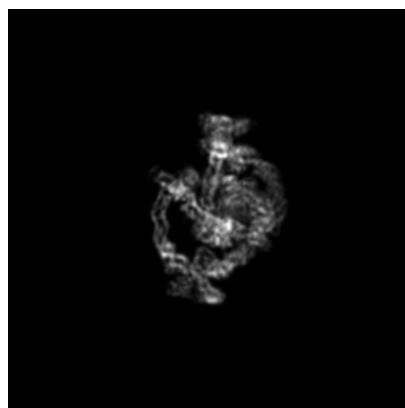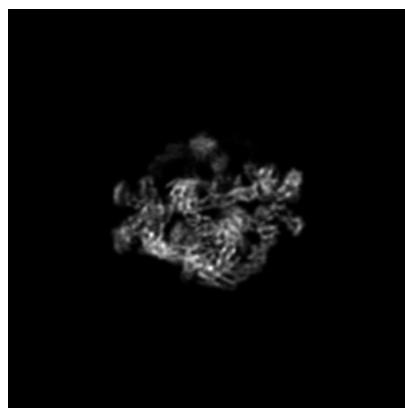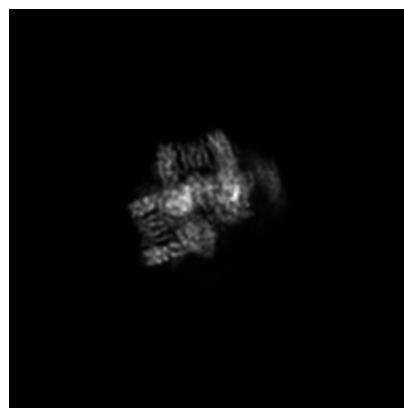
X   Y   Z

6.1.2 Raw map

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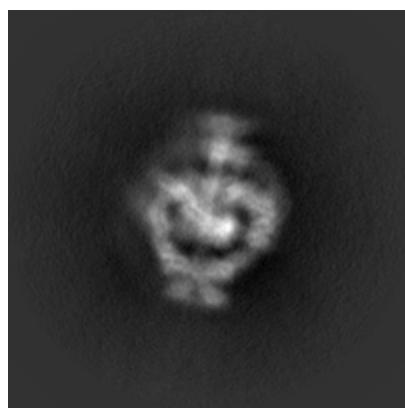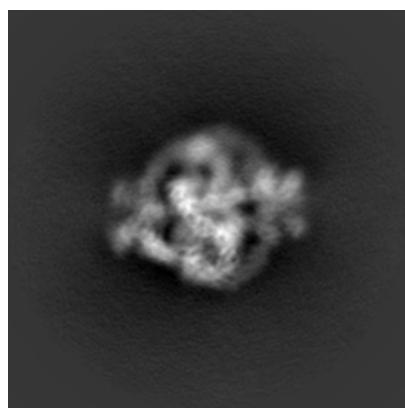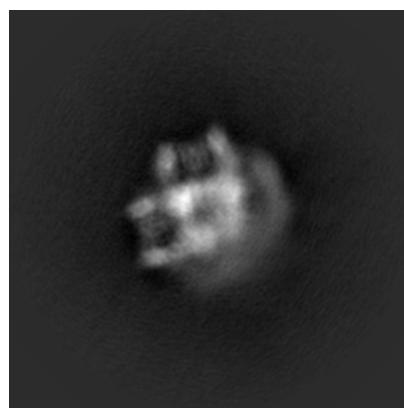
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

| X Index: 96 | Y Index: 96 | Z Index: 96 |

6.2.2 Raw map
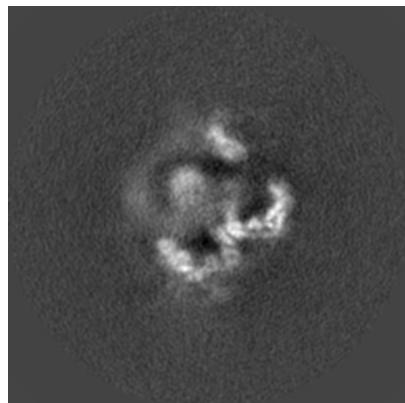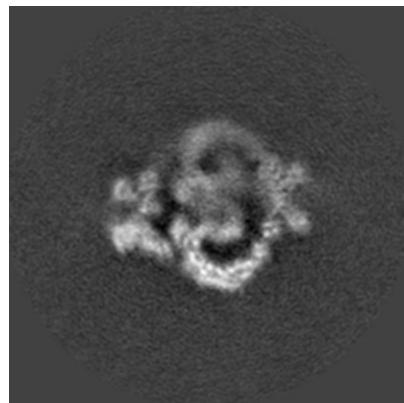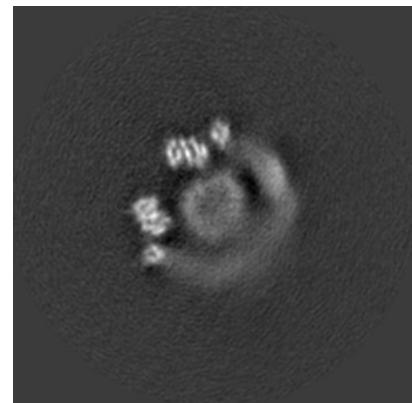
| X Index: 96 | Y Index: 96 | Z Index: 96 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
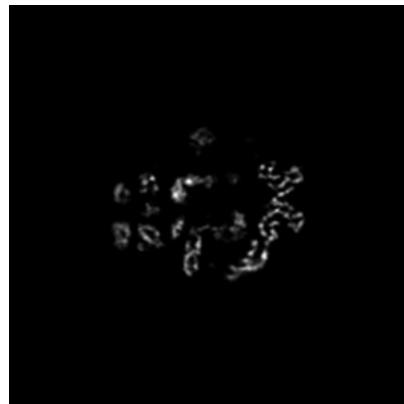
| X Index: 86 | Y Index: 100 | Z Index: 86 |

6.3.2 Raw map
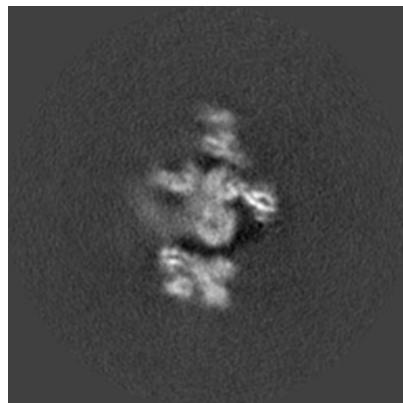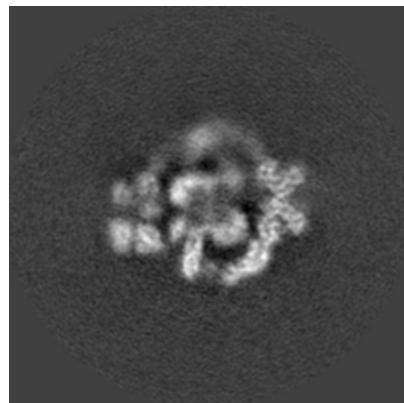
| X Index: 84 | Y Index: 100 | Z Index: 89 |
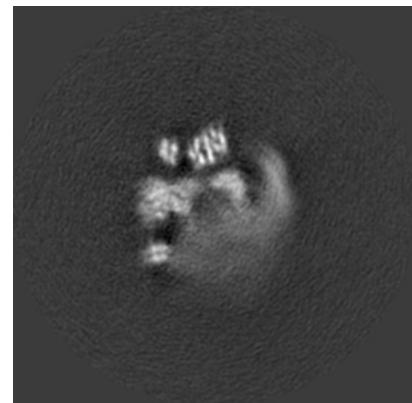
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
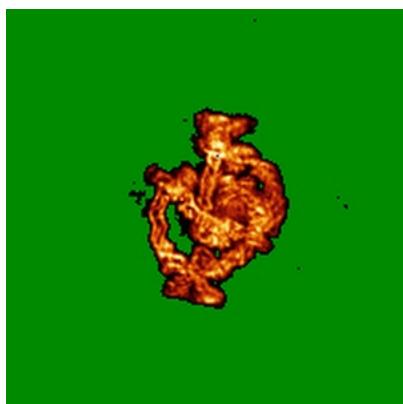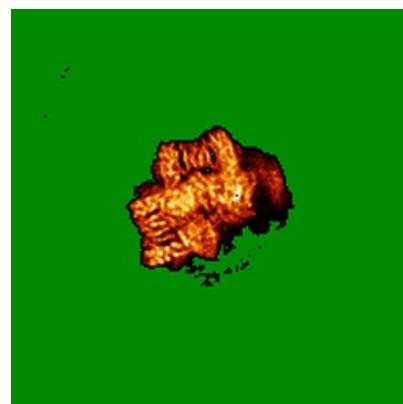
X	Y	Z

6.4.2 Raw map

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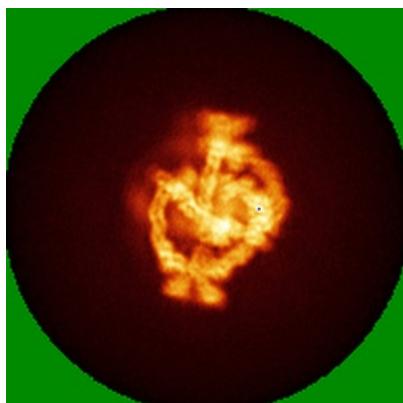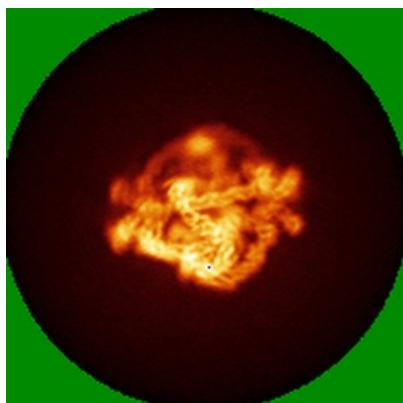
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X   Y   Z
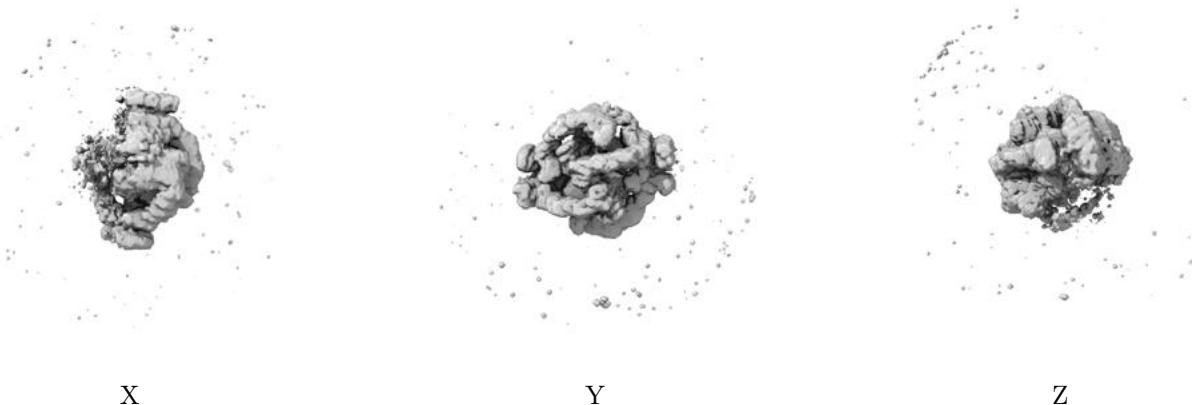
The images above show the 3D surface view of the map at the recommended contour level 0.0001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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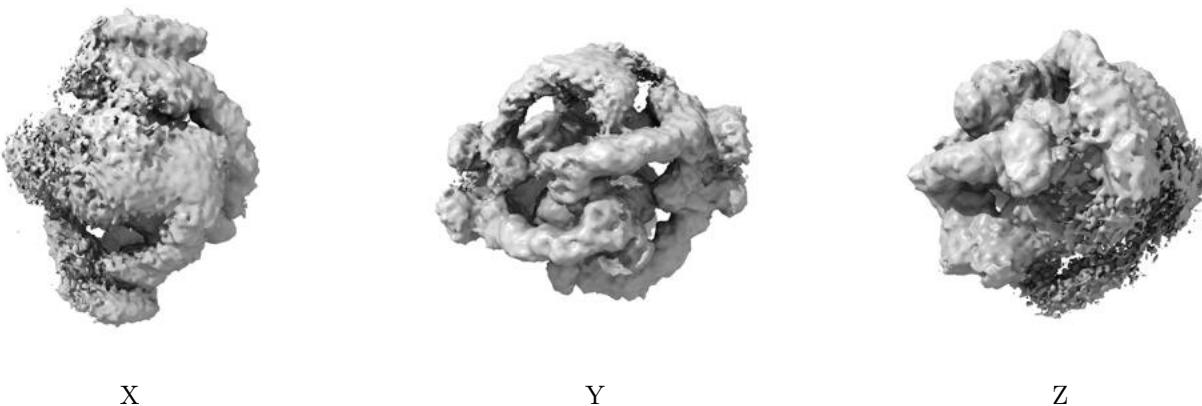
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7　Map analysis ⓘ

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

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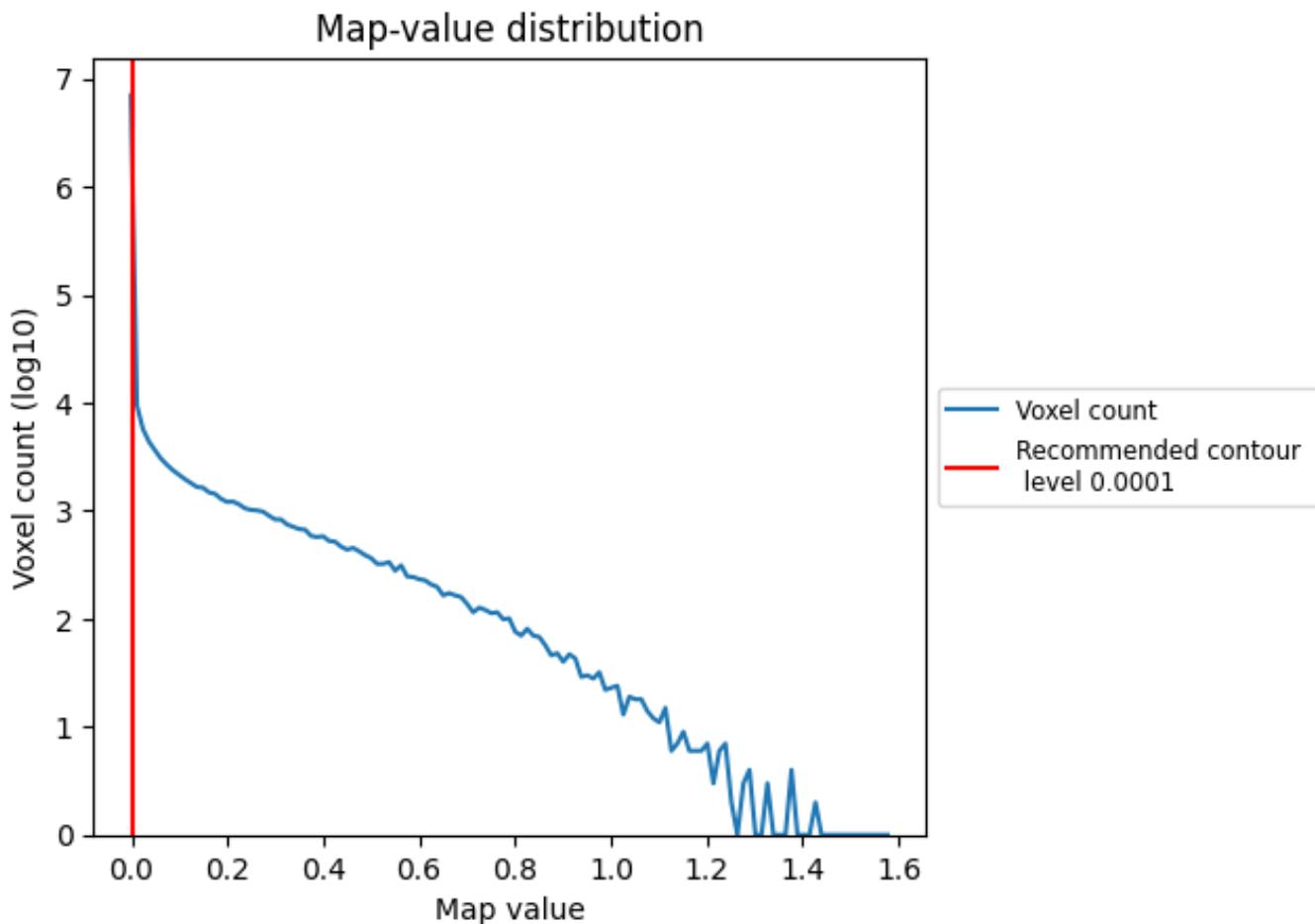
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate (i)
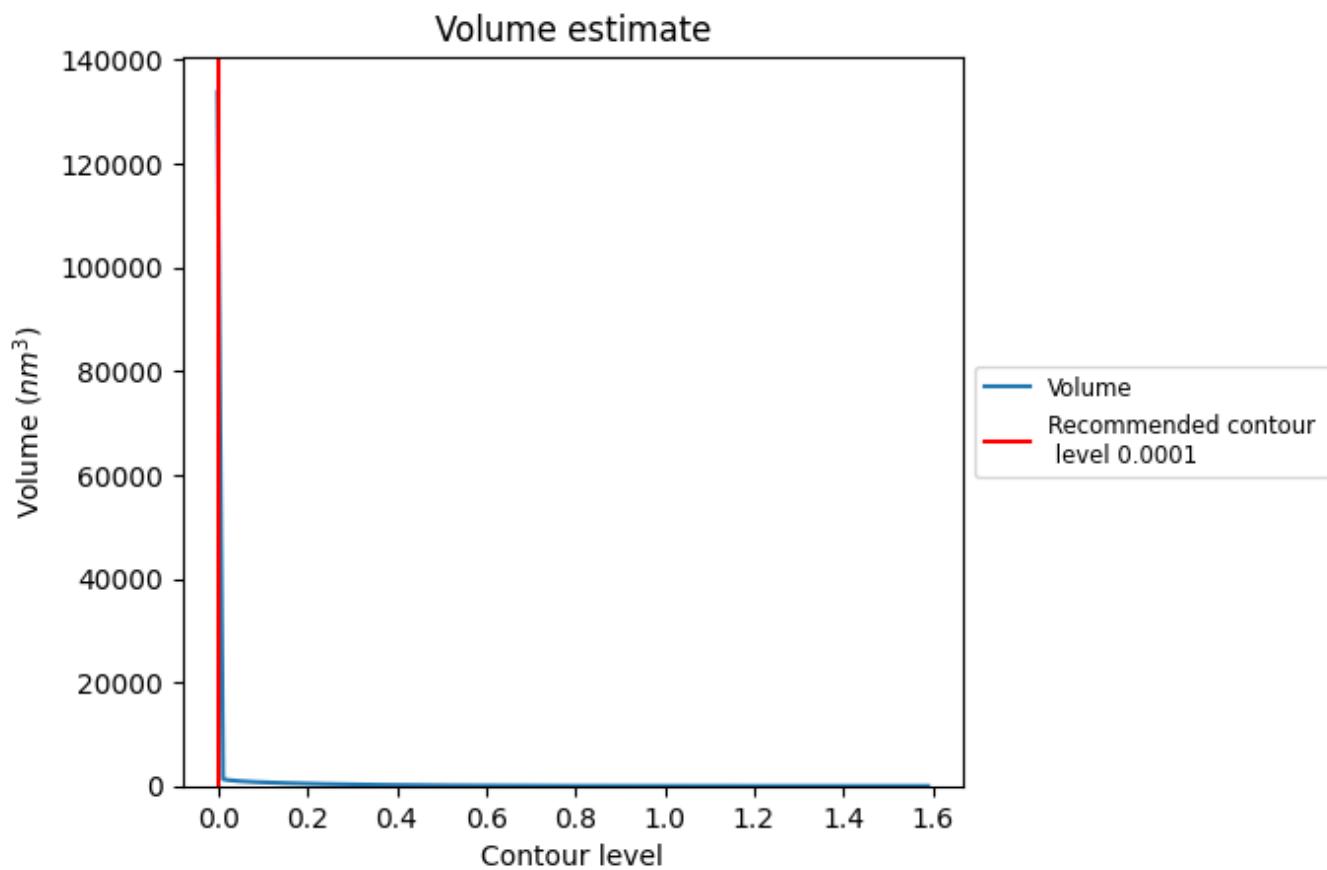
The volume at the recommended contour level is 117945 nm^3; this corresponds to an approximate mass of 106543 kDa.

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 ⓘ
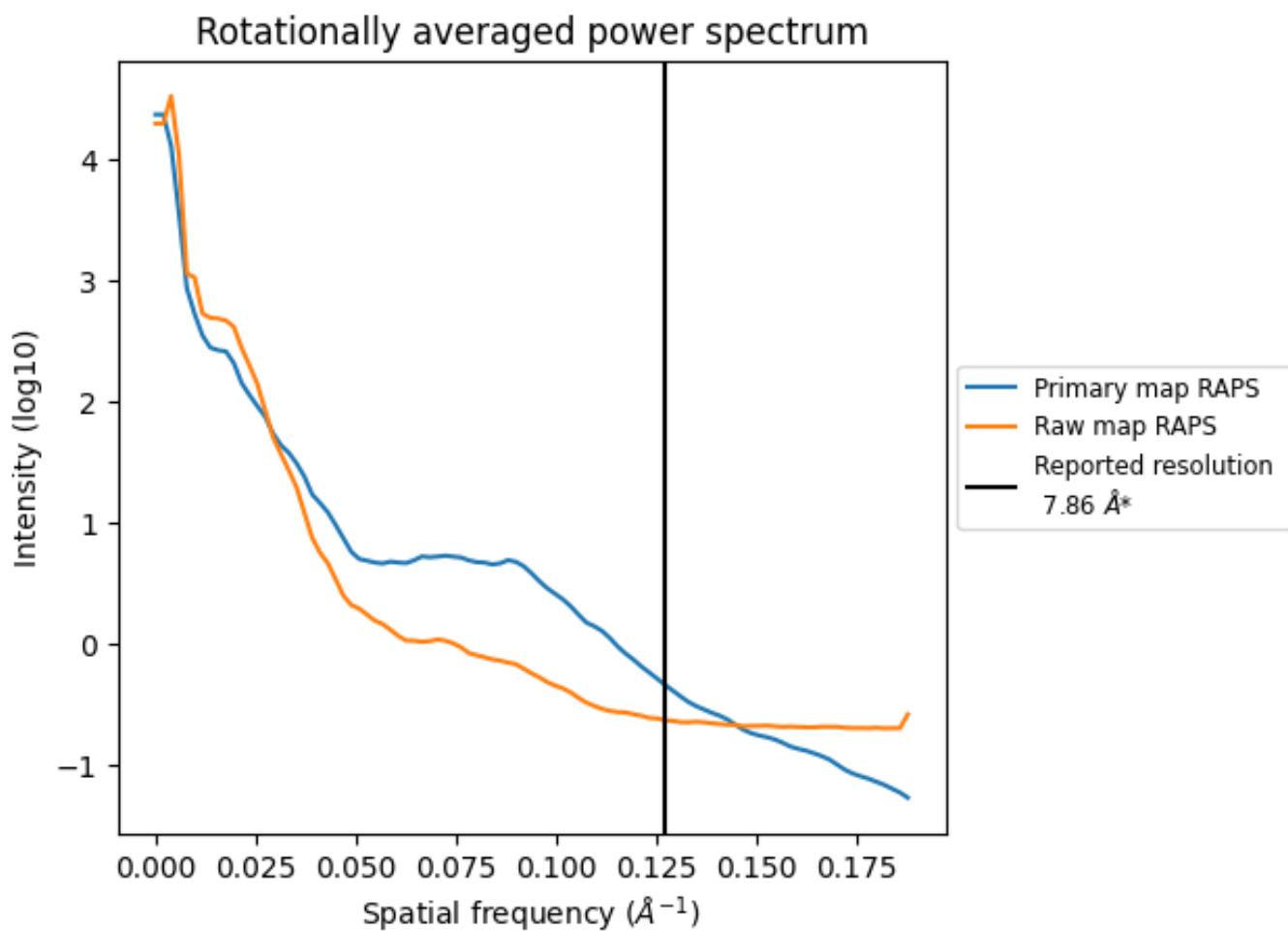
*Reported resolution corresponds to spatial frequency of 0.127 Å^{-1}

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 ⓘ
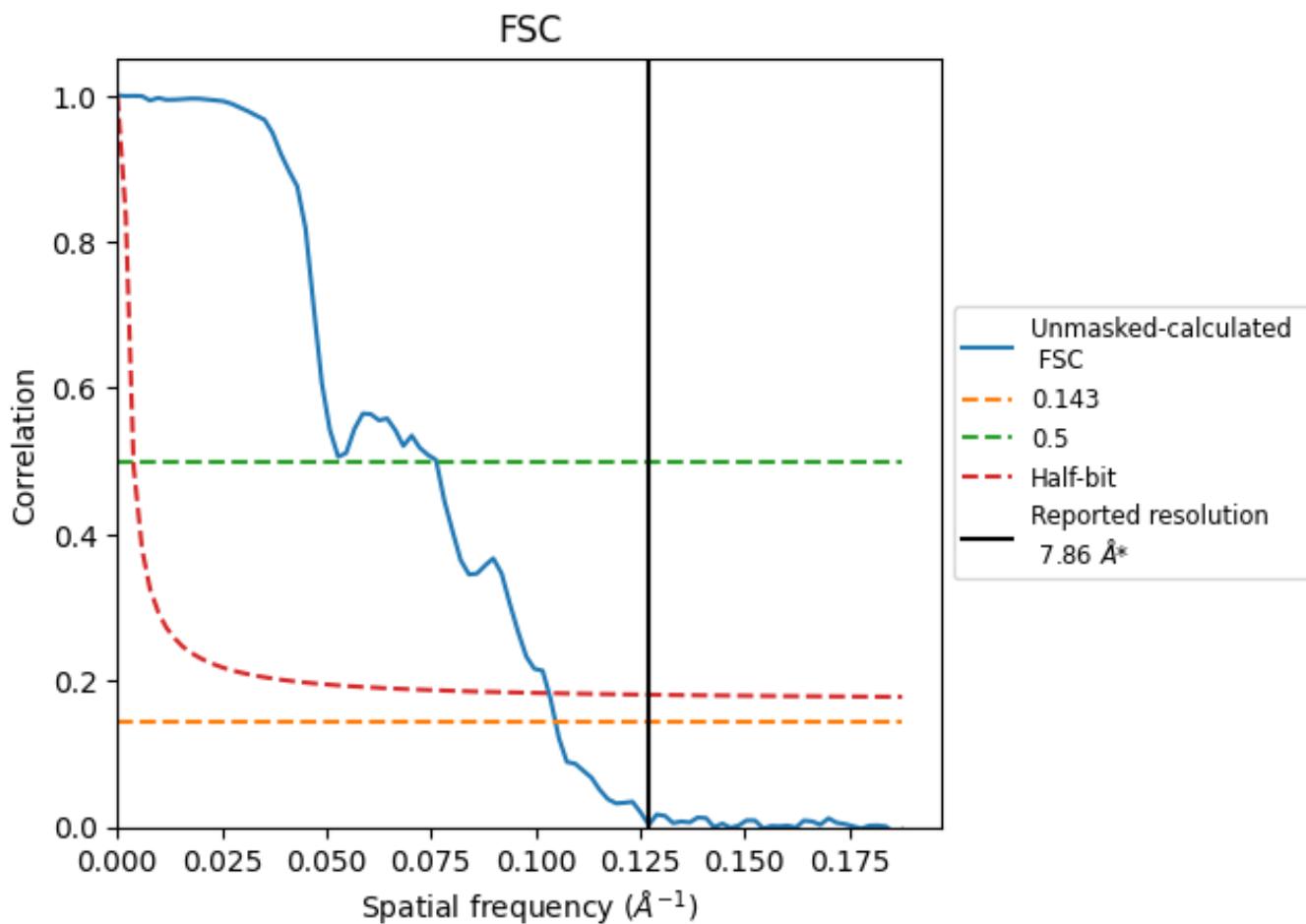
*Reported resolution corresponds to spatial frequency of 0.127 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.86	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.54	13.11	9.69

*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 9.54 differs from the reported value 7.86 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34449 and PDB model 8H33. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)
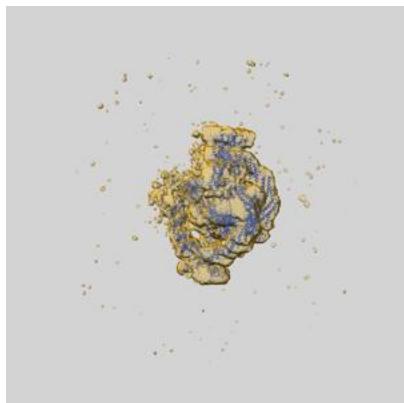
| X | Y | Z |
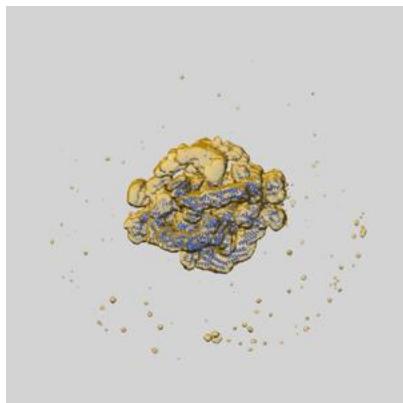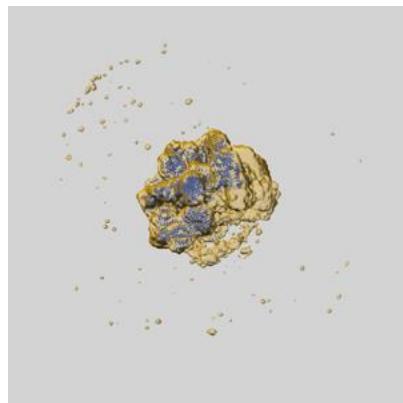
The images above show the 3D surface view of the map at the recommended contour level 0.0001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
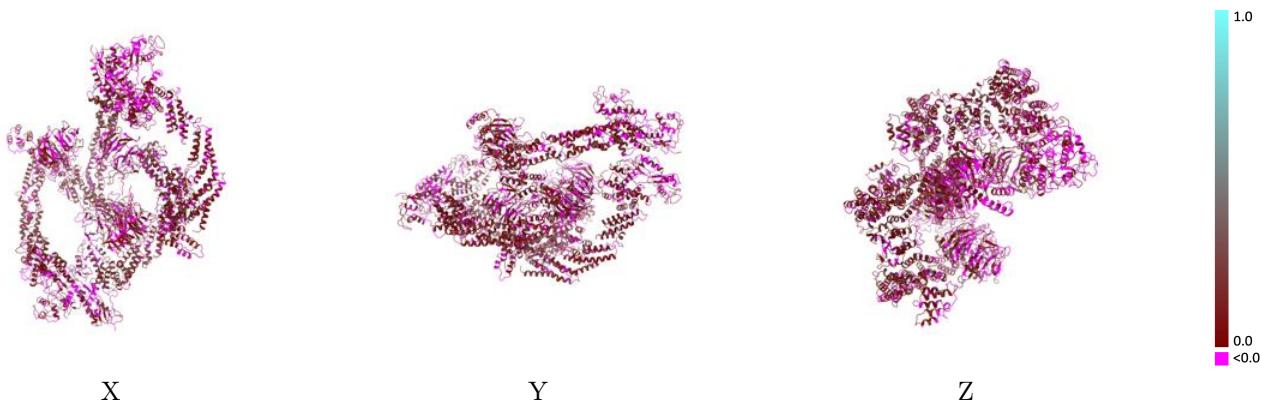
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
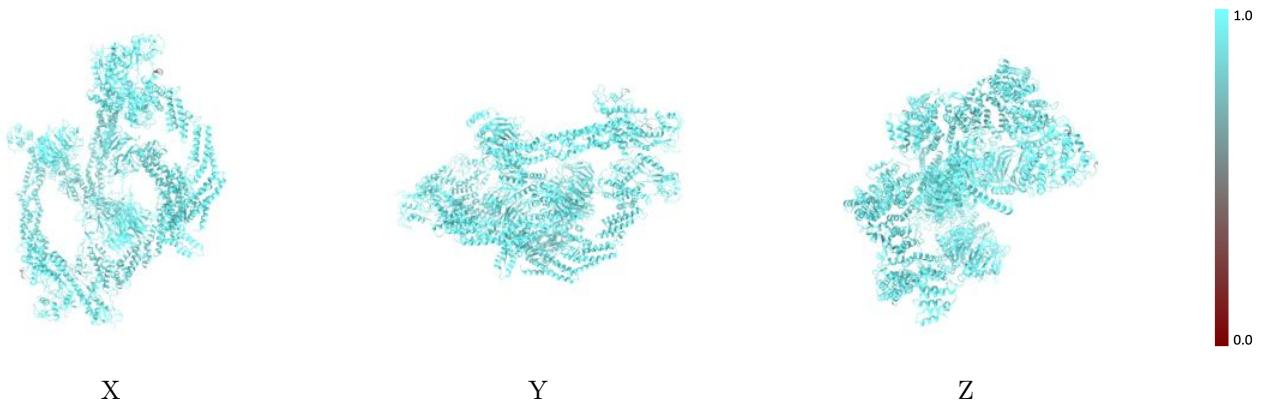
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0001).

9.4   Atom inclusion   ⓘ
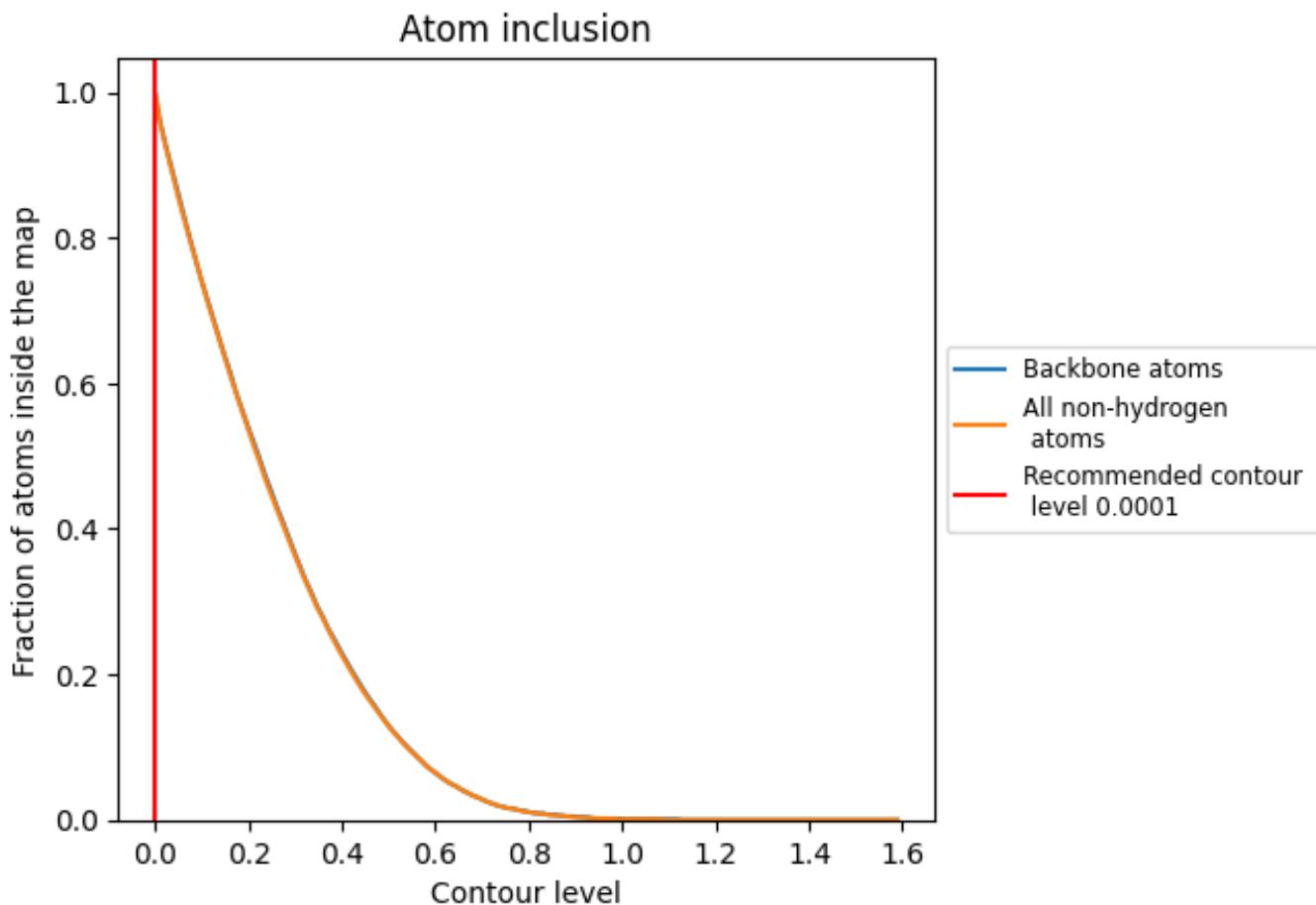
At the recommended contour level, 100% of all backbone atoms, 100% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9970	0.0700
A	0.9980	0.0850
B	0.9980	0.0790
C	0.9930	0.0520
D	0.9990	0.0320
E	0.9750	-0.0190
F	0.9980	0.0840
G	0.9990	0.0850
H	0.9990	0.0780
I	0.9990	0.0810
J	0.9970	0.0570
K	0.9670	0.0000
L	0.9990	0.0280

1.0

0.0
<0.0