WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 04:41 PM EDT

PDB ID	:	7MKA
EMDB ID	:	EMD-23888
Title	:	Structure of EC+EC (leading EC-focused)
Authors	:	Yang, C.; Murakami, K.
Deposited on	:	2021-04-22
Resolution	:	3.54 Å(reported)
Based on initial models	:	5C4J, 6GML, 3PO2

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:
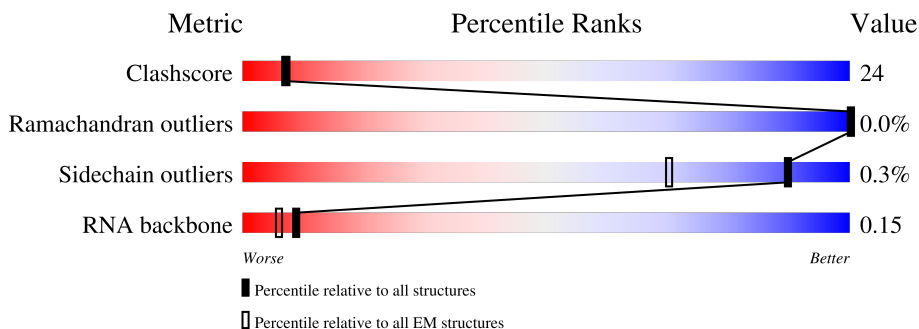
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.54 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.
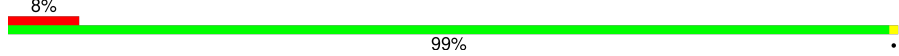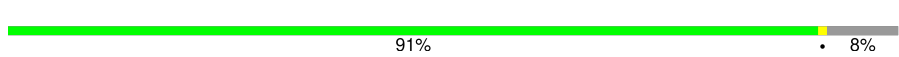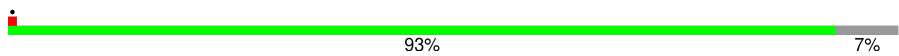
Metric	Percentile Ranks	Value
Clashscore		24
Ramachandran outliers		0.0%
Sidechain outliers		0.3%
RNA backbone		0.15

Worse   *Better*

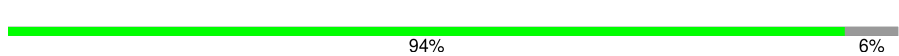▮ Percentile relative to all structures
◫ Percentile relative to all EM structures
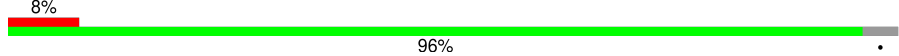
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	N	39	41% 59%
2	O	40	28% 72%
3	a	1733	82% 18%
4	b	1224	94% 5%
5	c	318	83% 17%
6	d	221	8% 75% 24%
7	e	215	99%

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Mol	Chain	Length	Quality of chain
8	f	155	56% 44%
9	g	171	8% 99%
10	h	146	91% 8%
11	i	122	93% 7%
12	j	70	94% 6%
13	k	120	8% 96%
14	l	70	61% 37%
15	r	16	12% 38% 62%

2 Entry composition ⓘ

There are 17 unique types of molecules in this entry. The entry contains 33384 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 DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	N	39	798	382	149	228	39	0	0

- Molecule 2 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	O	40	821	394	140	247	40	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	a	1425	11189	7046	1955	2126	62	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	b	1160	9197	5805	1614	1723	55	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	265	2086	1312	347	414	13	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	d	168	1331	822	237	270	2	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	87	Total	C	N	O	S	0	0
			705	451	119	132	3		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	h	135	Total	C	N	O	S	0	0
			1080	679	182	214	5		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	114	Total	C	N	O	S	0	0
			927	571	168	178	10		

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	j	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	k	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 14 is a protein called DNA-Vdirected RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	l	44	Total 352	C 217	N 70	O 61	S 4	0	0

- Molecule 15 is a RNA chain called RNA (5'-R(P*AP*AP*CP*UP*AP*GP*UP*UP*AP*A P*GP*AP*GP*GP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	16	Total 333	C 150	N 55	O 112	P 16	0	0

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	a	2	Total 2	Zn 2	0
16	b	1	Total 1	Zn 1	0
16	c	1	Total 1	Zn 1	0
16	i	2	Total 2	Zn 2	0
16	j	1	Total 1	Zn 1	0
16	l	1	Total 1	Zn 1	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	a	2	Total 2	Mg 2	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: DNA (40-MER)

Chain N:
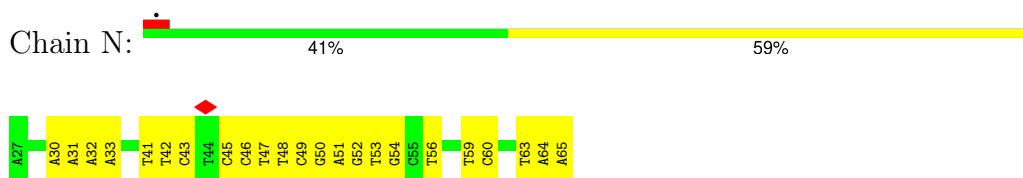
• Molecule 2: DNA (40-MER)

Chain O:
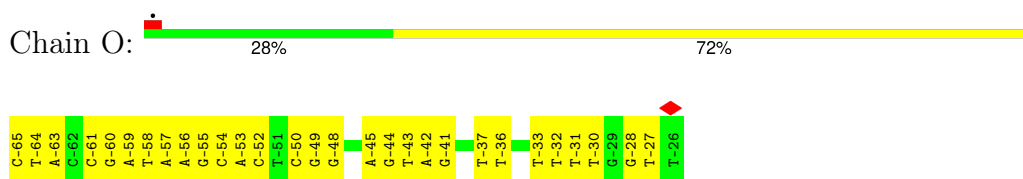
• Molecule 3: DNA-directed RNA polymerase subunit

Chain a:
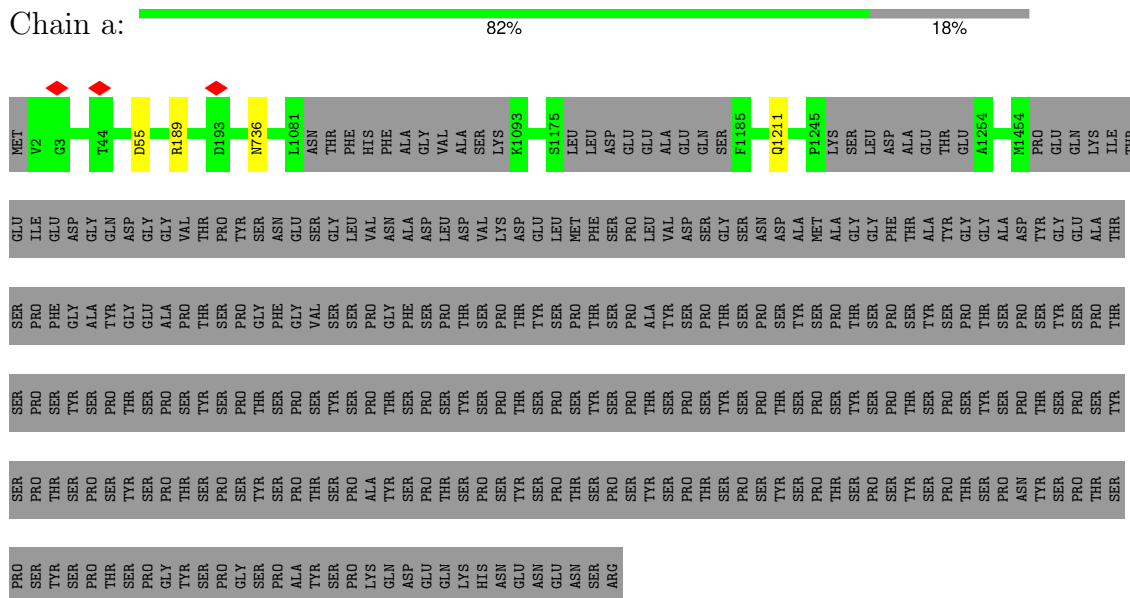
• Molecule 4: DNA-directed RNA polymerase subunit beta

Chain b:
94%   5%

MET SER ASP LEU ALA ASN SER GLU LYS TYR TYR ASP GLU PRO TYR GLY PHE GLU D20 Q76 K133 LYS ARG T136 E146 L147 E150 LEU ILE ALA GLU GLU GLU SER GLU ASP D159 E245 R261 GLU GLY S264 S265 I364 N449 I502 GLY ARG ASP GLY LYS

LEU A509 D668 ILE GLU GLY GLY PHE GLU ASP VAL GLU E678 A713 GLU ALA ASN GLU GLU ASN ASP LEU ASP VAL ASP PRO A726 I729 R730 VAL SER HIS HIS A735 M868 S869 M885 S919 P920 D921 E922 E923 E924 L925 G926 Q927 R928 T929 R995 R1124 K1201

I1212 THR P1214 D1223 PHE

• Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain c:
83%   17%

MET SER GLU E4 D268 LYS VAL ASN PHE ALA SER GLY ASP ASN ASN THR ALA SER ASN MET LEU GLY SER GLU ASN GLU ASP VAL MET MET THR GLY SER GLU GLN ASP PRO TYR SER ASN ALA GLN MET GLY LYS ASN THR GLY SER GLY LEU TYR ASP SER ASN ALA TRP

• Molecule 6: DNA-directed RNA polymerase II subunit RPB4

Chain d:
8%
75%   24%

MET ASN VAL SER SER THR THR PHE GLN THR ARG ARG R14 V18 E19 E20 E21 E22 T26 K75 K76 HIS LYS LYS LYS HIS LEU LYS HIS GLU ASN ALA ASN ASP GLU THR ALA VAL GLU ASP GLU ASP ASP ASP LEU ASP GLU ASP ASP VAL ASN ALA ASP ASP ASP

ASP PHE MET HIS SER E117 T118 R119 E120 K121 E131 Q132 T133 T134 G135 G136 N137 P196 T219 L220 Y221

• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain e:
99%

MET D2 K171 E172 M215

• Molecule 8: DNA-directed RNA polymerases I,II,and III subunit RPABC2

Chain f:
56%   44%

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

HIS GLU GLN ILE ARG ARG LYS THR L69 L155

• Molecule 9: DNA-directed RNA polymerase II subunit RPB7

Chain g:

• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain h:
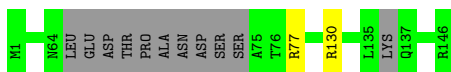
• Molecule 11: DNA-directed RNA polymerase II subunit RPB9

Chain i:
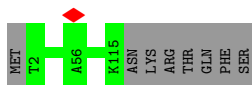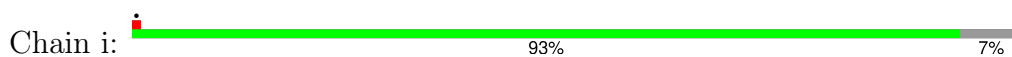
• Molecule 12: DNA-directed RNA polymerases II subunit RPABC5

Chain j:
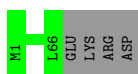
• Molecule 13: DNA-directed RNA polymerase II subunit RPB11

Chain k:
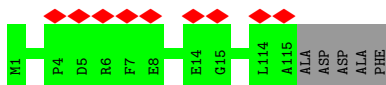
• Molecule 14: DNA-directed RNA polymerases II subunit RPABC4

Chain l:
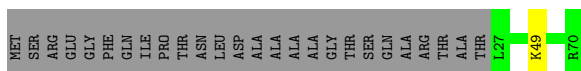
• Molecule 15: RNA (5'-R(P*AP*AP*CP*UP*AP*GP*UP*UP*AP*AP*GP*AP*GP*GP*UP*U)-3')

Chain r:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57690	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1750	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0101	Depositor
Map size (Å)	237.6, 237.6, 237.6	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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 RMSZ	Bond lengths $\#|Z| > 5$	Bond angles RMSZ	Bond angles $\#|Z| > 5$
1	N	0.63	0/896	0.96	0/1379
2	O	0.76	0/918	1.02	1/1416 (0.1%)
3	a	0.34	0/11390	0.50	0/15408
4	b	0.36	0/9371	0.52	1/12636 (0.0%)
5	c	0.34	0/2124	0.47	0/2879
6	d	0.26	0/1339	0.50	0/1793
7	e	0.34	0/1788	0.46	0/2406
8	f	0.37	0/717	0.54	0/967
9	g	0.31	0/1367	0.54	0/1844
10	h	0.35	0/1097	0.50	0/1484
11	i	0.31	0/945	0.48	0/1273
12	j	0.41	0/549	0.47	0/738
13	k	0.33	0/942	0.48	0/1272
14	l	0.31	0/354	0.47	0/468
15	r	0.81	0/370	0.88	1/572 (0.2%)
All	All	0.38	0/34167	0.55	3/46535 (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
3	a	0	1
4	b	0	1
7	e	0	1
9	g	0	2
All	All	0	5

There are no bond length outliers.

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All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	r	40	U	N1-C1'-C2'	-6.58	104.76	112.00
2	O	-48	DG	O4'-C4'-C3'	-5.87	102.15	104.50
4	b	885	MET	CA-CB-CG	5.06	121.90	113.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	a	55	ASP	Peptide
4	b	868	MET	Peptide
7	e	171	LYS	Peptide
9	g	131	GLN	Peptide
9	g	56	ILE	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	N	798	0	440	29	0
2	O	821	0	457	26	0
3	a	11189	0	11225	0	0
4	b	9197	0	9180	0	0
5	c	2086	0	2045	0	0
6	d	1331	0	1345	0	0
7	e	1752	0	1776	0	0
8	f	705	0	731	0	0
9	g	1339	0	1357	0	0
10	h	1080	0	1049	0	0
11	i	927	0	880	0	0
12	j	540	0	553	0	0
13	k	924	0	934	0	0
14	l	352	0	374	0	0
15	r	333	0	172	0	0
16	a	2	0	0	0	0
16	b	1	0	0	0	0
16	c	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	i	2	0	0	0	0
16	j	1	0	0	0	0
16	l	1	0	0	0	0
17	a	2	0	0	0	0
All	All	33384	0	32518	48	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 24.

The worst 5 of 48 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:N:65:DA:H61	2:O:-65:DC:N4	1.48	1.11
1:N:65:DA:N6	2:O:-65:DC:H42	1.48	1.10
1:N:50:DG:H1	2:O:-50:DC:H5	1.19	0.89
1:N:49:DC:O2	2:O:-49:DG:N2	2.06	0.88
1:N:65:DA:N1	2:O:-65:DC:N3	2.29	0.80

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	
3	a	1417/1733 (82%)	1235 (87%)	182 (13%)	0	100	100
4	b	1142/1224 (93%)	983 (86%)	159 (14%)	0	100	100
5	c	263/318 (83%)	225 (86%)	38 (14%)	0	100	100
6	d	164/221 (74%)	156 (95%)	8 (5%)	0	100	100
7	e	212/215 (99%)	193 (91%)	18 (8%)	1 (0%)	25	59
8	f	85/155 (55%)	77 (91%)	8 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	g	169/171 (99%)	152 (90%)	17 (10%)	0	100	100
10	h	129/146 (88%)	111 (86%)	18 (14%)	0	100	100
11	i	112/122 (92%)	104 (93%)	8 (7%)	0	100	100
12	j	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
13	k	113/120 (94%)	106 (94%)	7 (6%)	0	100	100
14	l	42/70 (60%)	30 (71%)	12 (29%)	0	100	100
All	All	3912/4565 (86%)	3426 (88%)	485 (12%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	e	172	GLU

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	
3	a	1240/1520 (82%)	1237 (100%)	3 (0%)	92	97
4	b	999/1061 (94%)	995 (100%)	4 (0%)	89	95
5	c	233/274 (85%)	233 (100%)	0	100	100
6	d	146/200 (73%)	144 (99%)	2 (1%)	62	80
7	e	196/197 (100%)	196 (100%)	0	100	100
8	f	77/137 (56%)	77 (100%)	0	100	100
9	g	152/152 (100%)	152 (100%)	0	100	100
10	h	118/128 (92%)	116 (98%)	2 (2%)	56	76
11	i	108/116 (93%)	108 (100%)	0	100	100
12	j	61/65 (94%)	61 (100%)	0	100	100
13	k	99/102 (97%)	99 (100%)	0	100	100
14	l	39/57 (68%)	38 (97%)	1 (3%)	41	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3468/4009 (86%)	3456 (100%)	12 (0%)	90 96

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	d	75	LYS
6	d	121	LYS
14	l	49	LYS
10	h	77	ARG
4	b	265	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	b	1076	HIS
12	j	53	HIS
4	b	47	GLN
4	b	357	GLN
4	b	395	GLN

5.3.3   RNA   ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	r	15/16 (93%)	9 (60%)	0

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	r	35	C
15	r	36	U
15	r	38	G
15	r	41	C
15	r	42	U

There are no RNA pucker outliers to report.

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 (i)

There are no oligosaccharides in this entry.

5.6   Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 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 (i)

There are no such residues in this entry.

5.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23888. 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
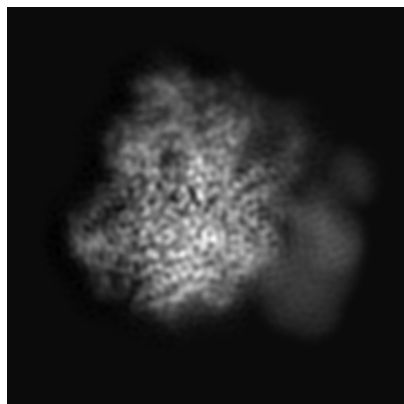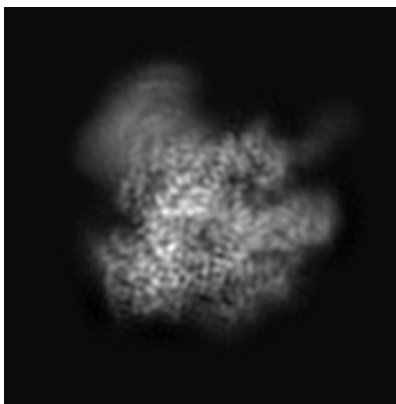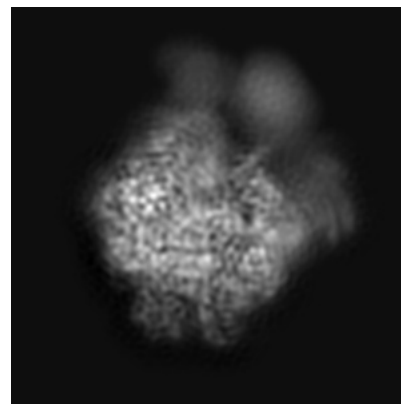
X   Y   Z

6.1.2 Raw map

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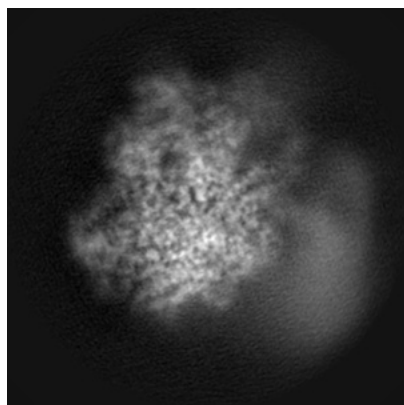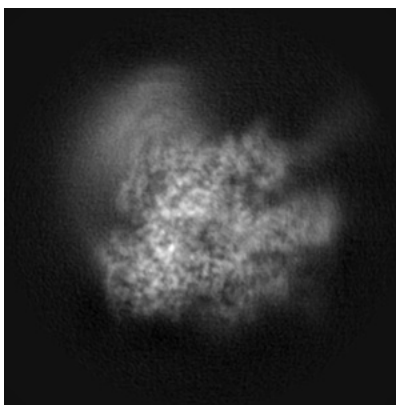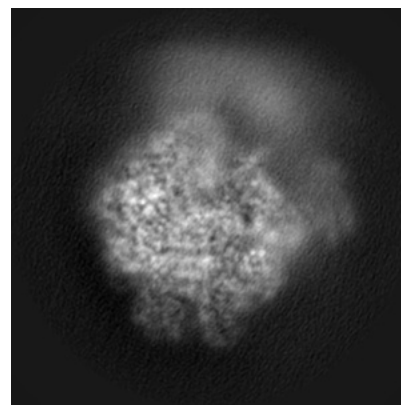
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map
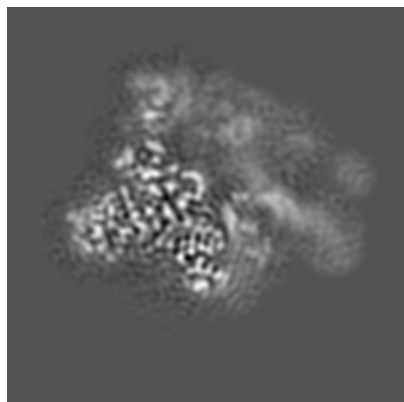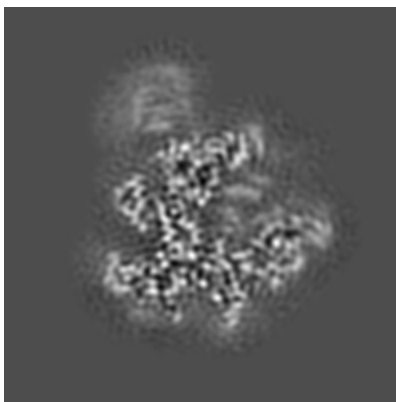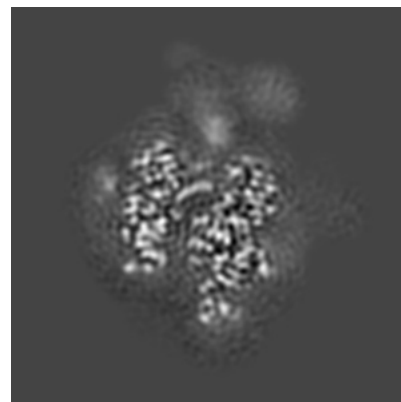
| X Index: 110 | Y Index: 110 | Z Index: 110 |

6.2.2 Raw map
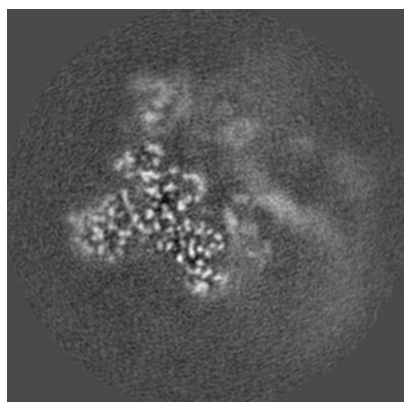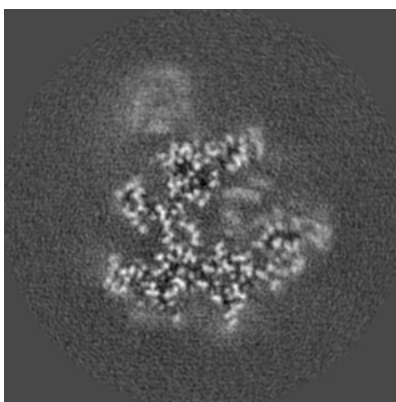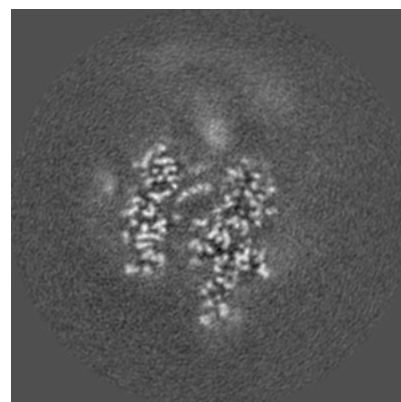
| X Index: 110 | Y Index: 110 | Z Index: 110 |

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

6.3 Largest variance slices ⓘ
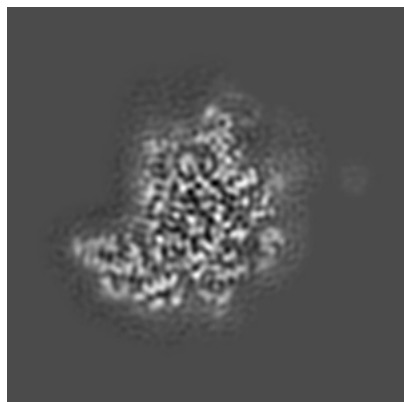
6.3.1 Primary map
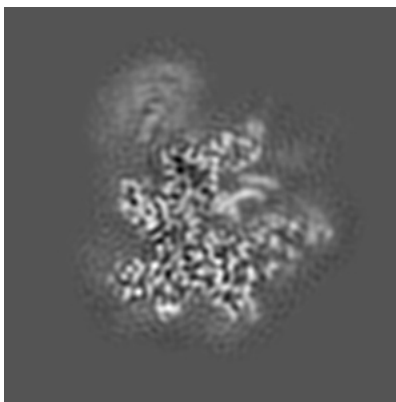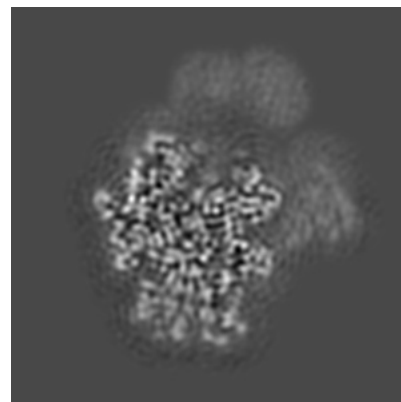
X Index: 78	Y Index: 106	Z Index: 93

6.3.2 Raw map
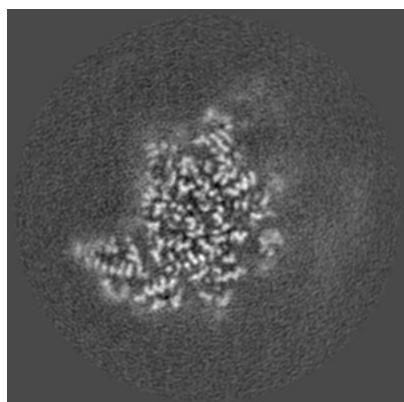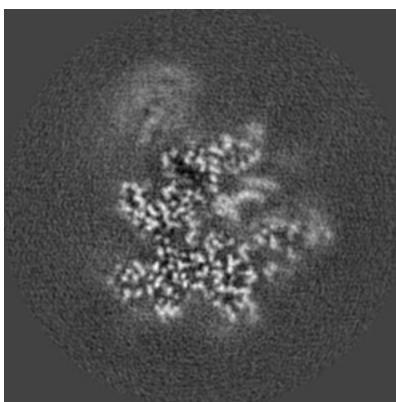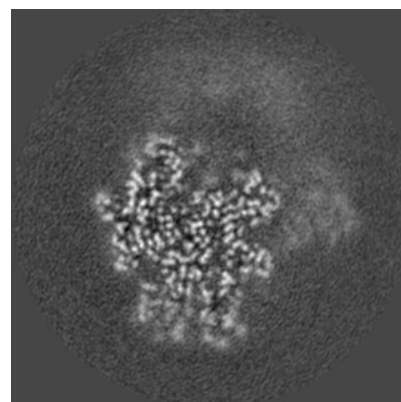
X Index: 78	Y Index: 106	Z Index: 93

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

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

6.4.1 Primary map
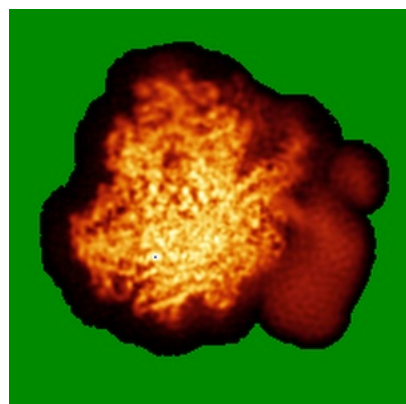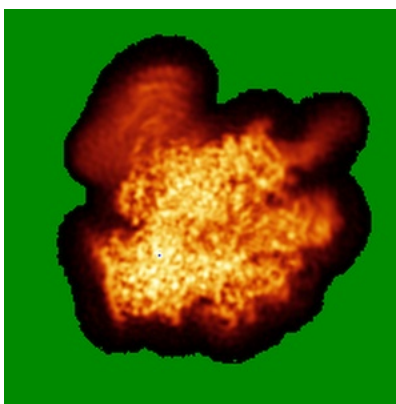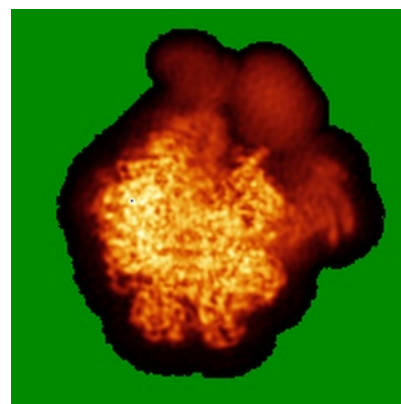
X Y Z

6.4.2 Raw map

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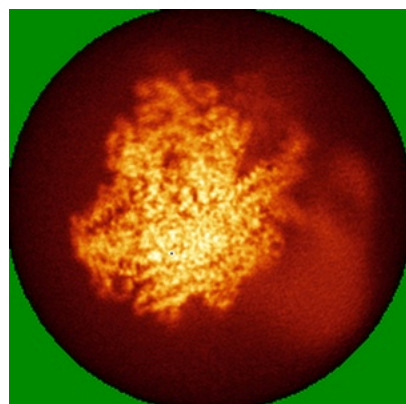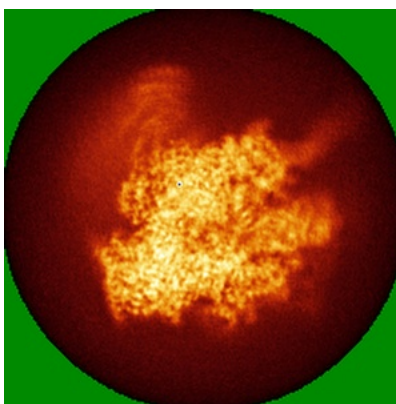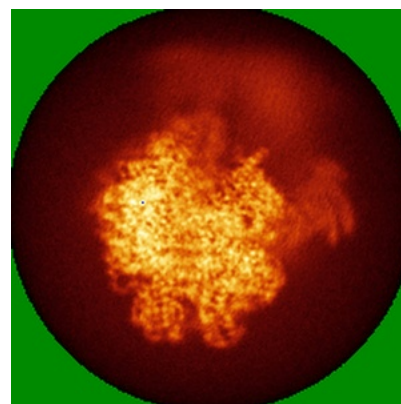
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.0101. 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
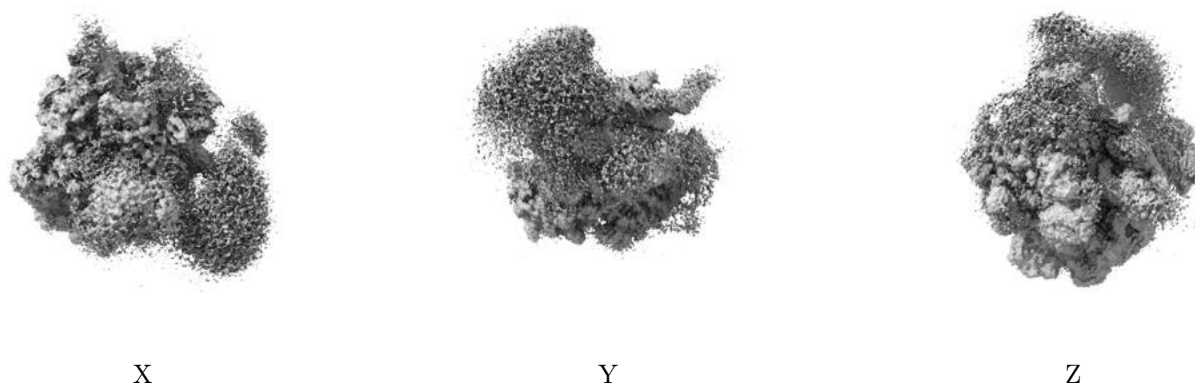
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6   Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure

- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

6.6.1   emd_23888_msk_1.map (i)

X   Y   Z
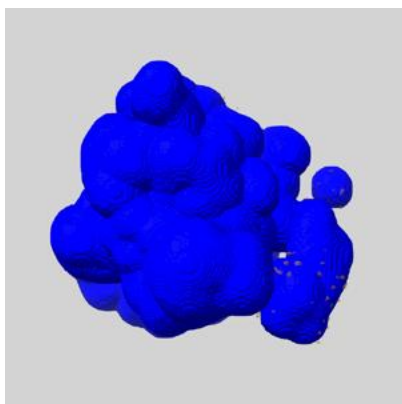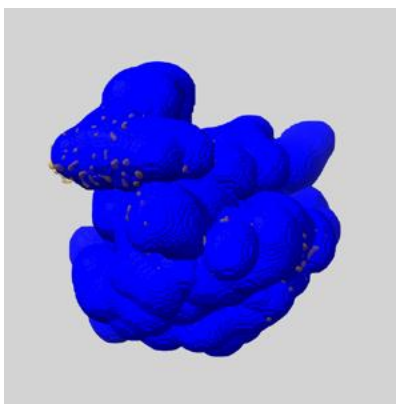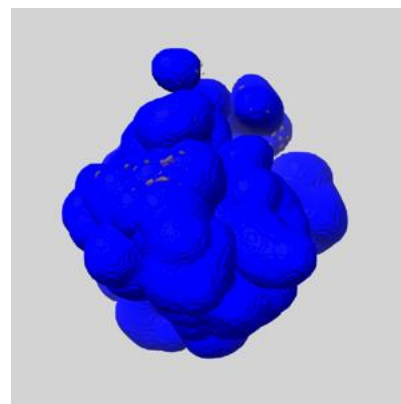
7 Map analysis ⓘ

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

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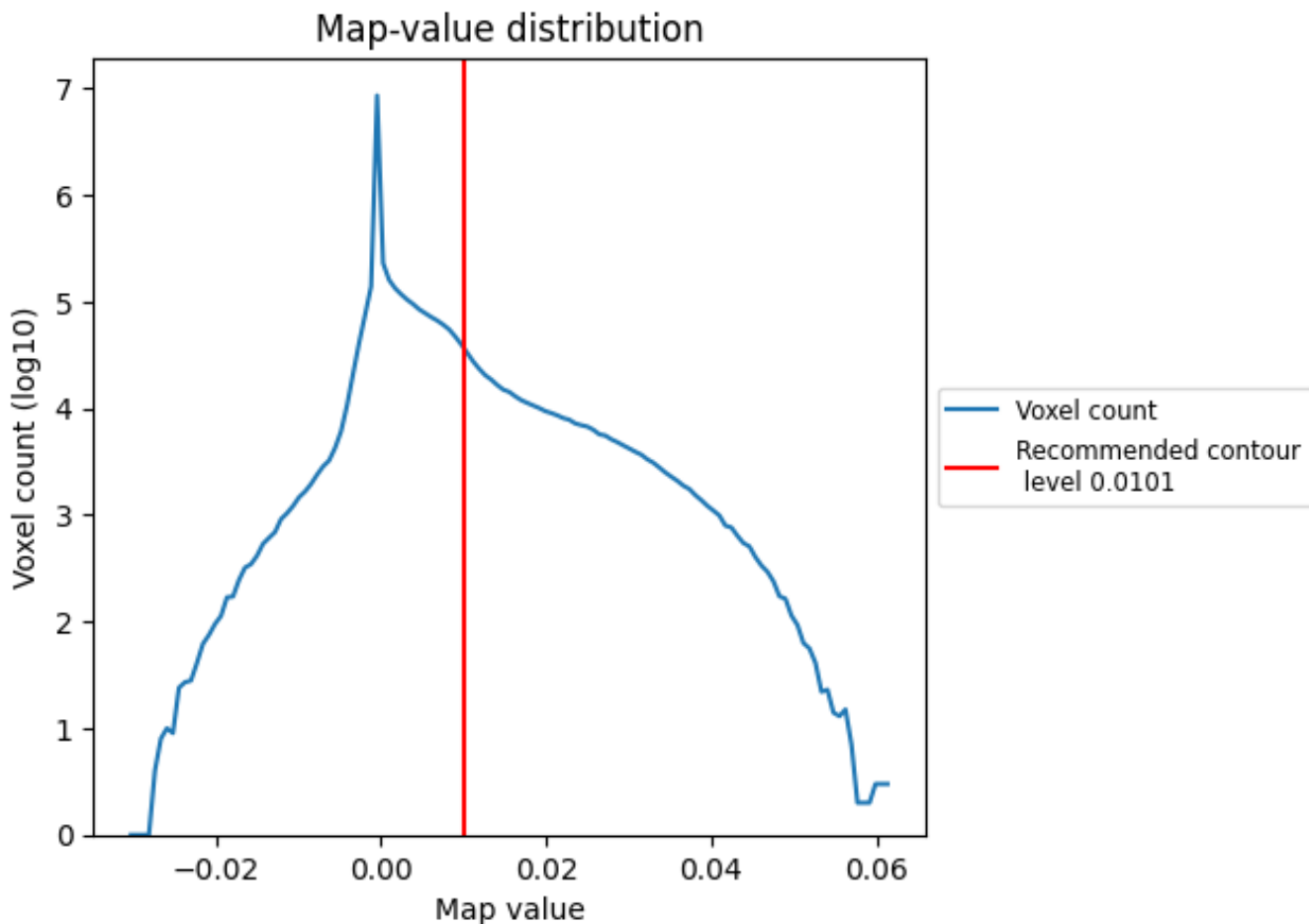
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
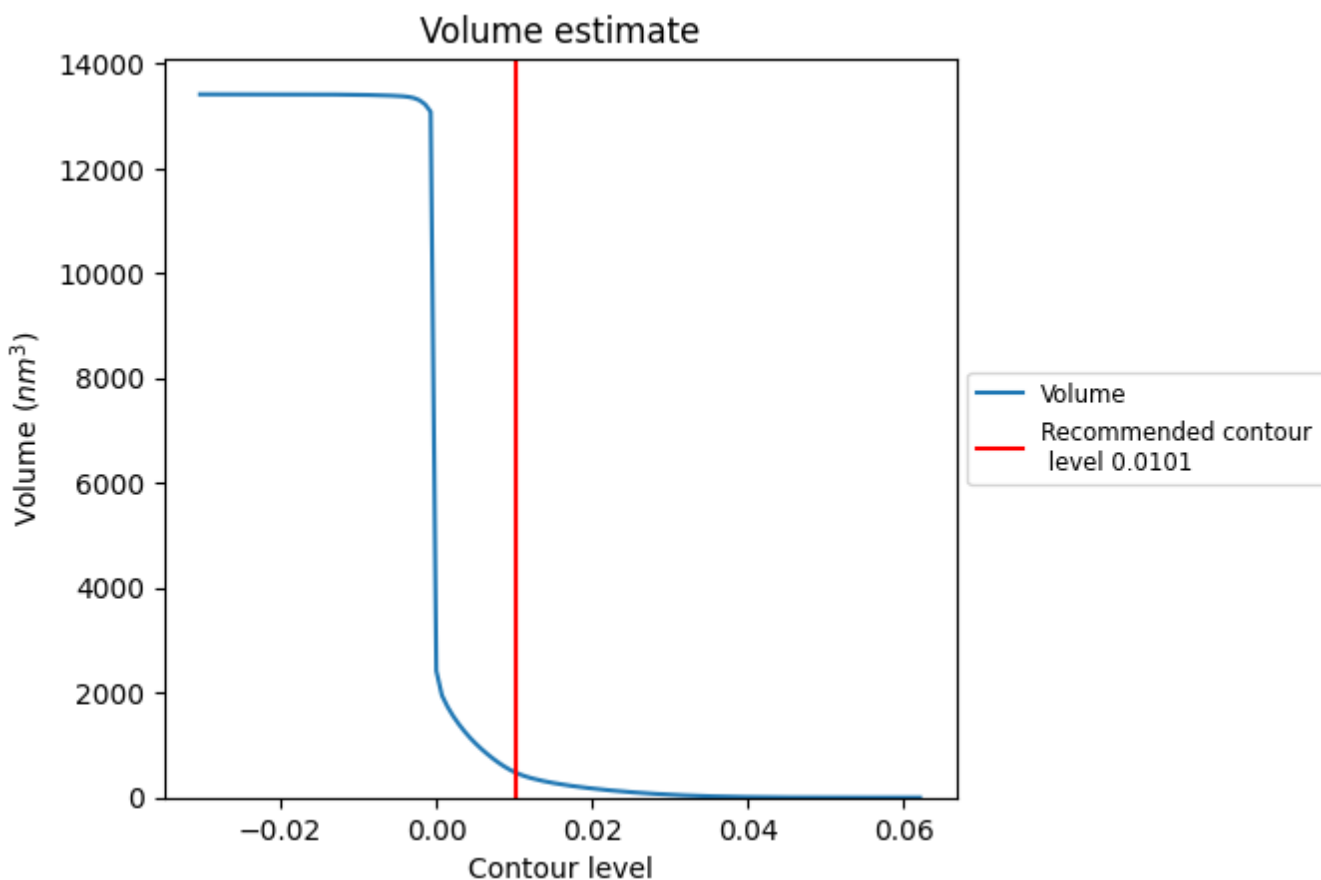
The volume at the recommended contour level is 482 nm^3; this corresponds to an approximate mass of 435 kDa.

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 ⓘ
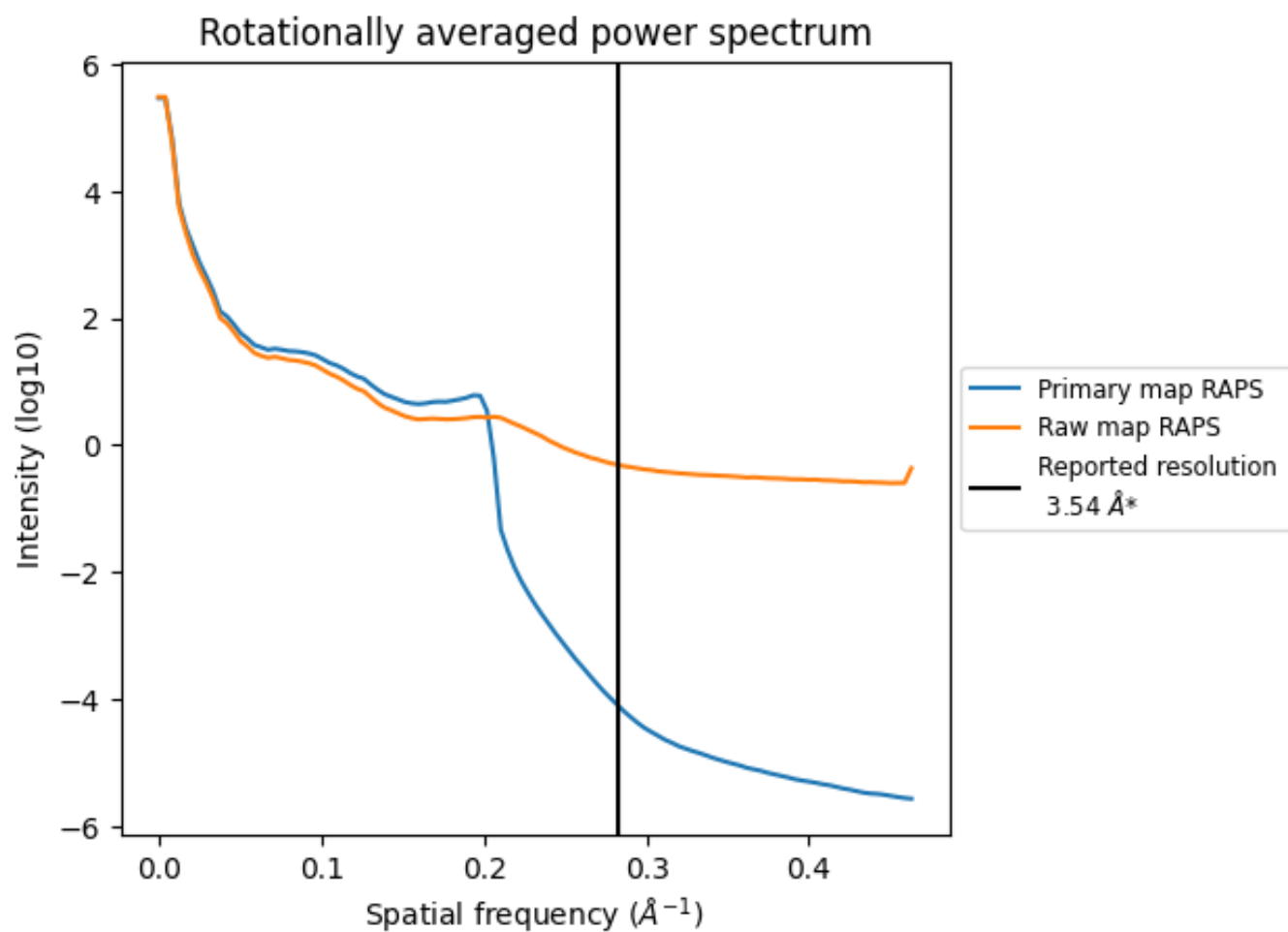
*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

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 ⓘ
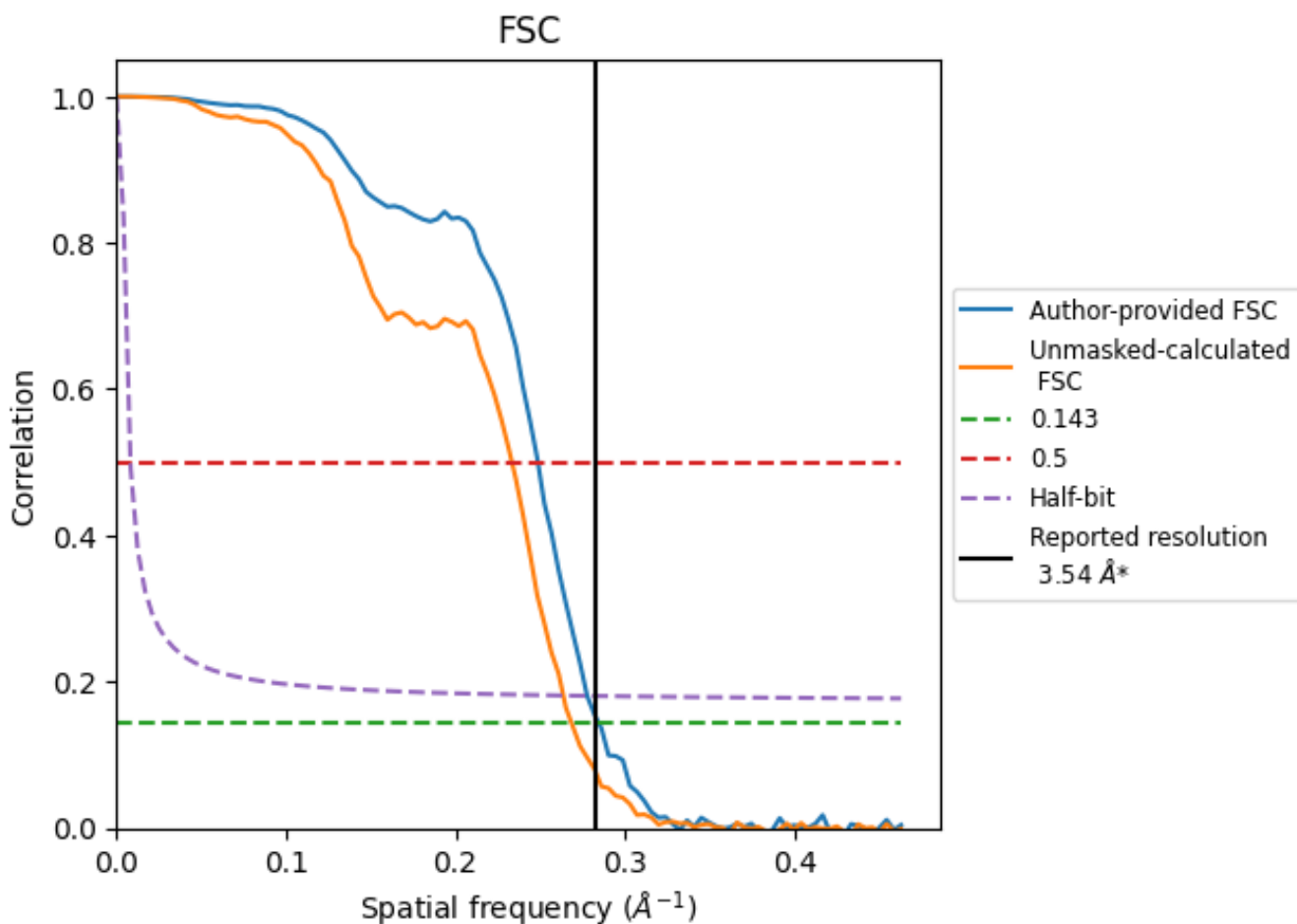
*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

8.2　Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.51	4.02	3.60
Unmasked-calculated*	3.72	4.29	3.79

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-23888 and PDB model 7MKA. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ
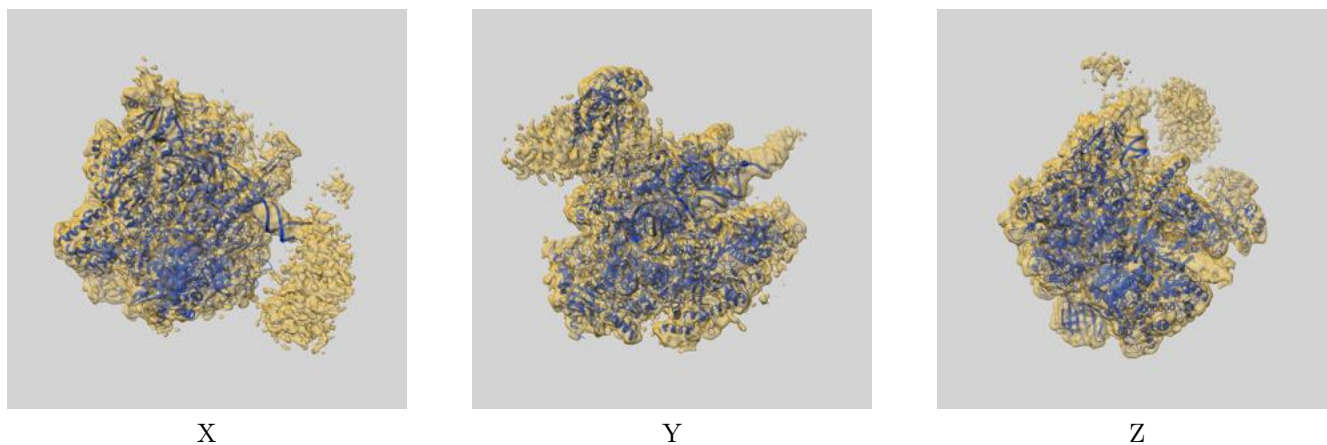
X	Y	Z

The images above show the 3D surface view of the map at the recommended contour level 0.0101 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
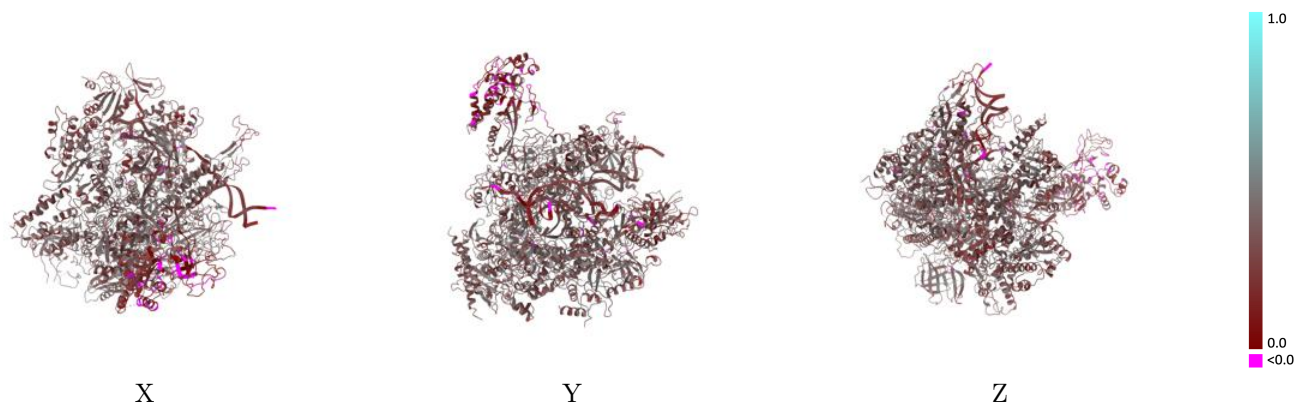
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
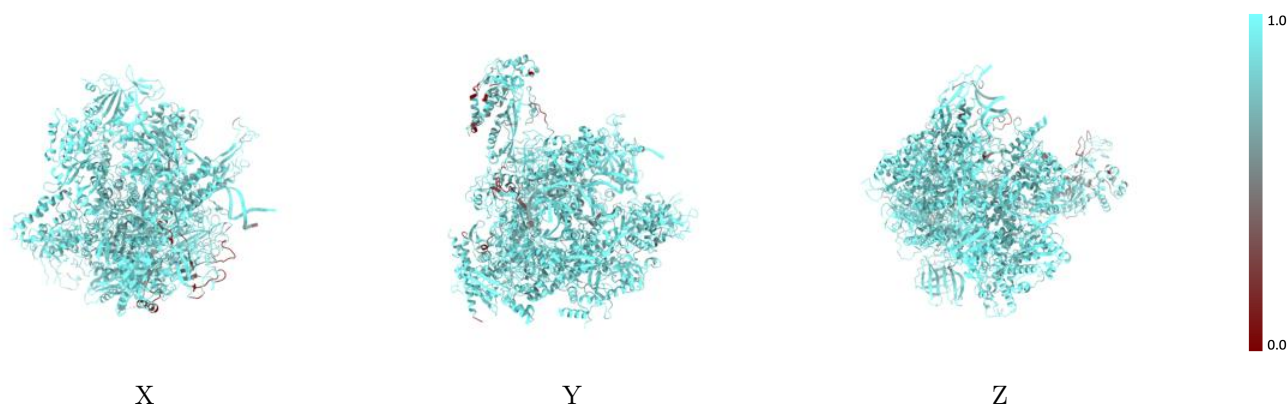
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0101).

9.4 Atom inclusion ⓘ
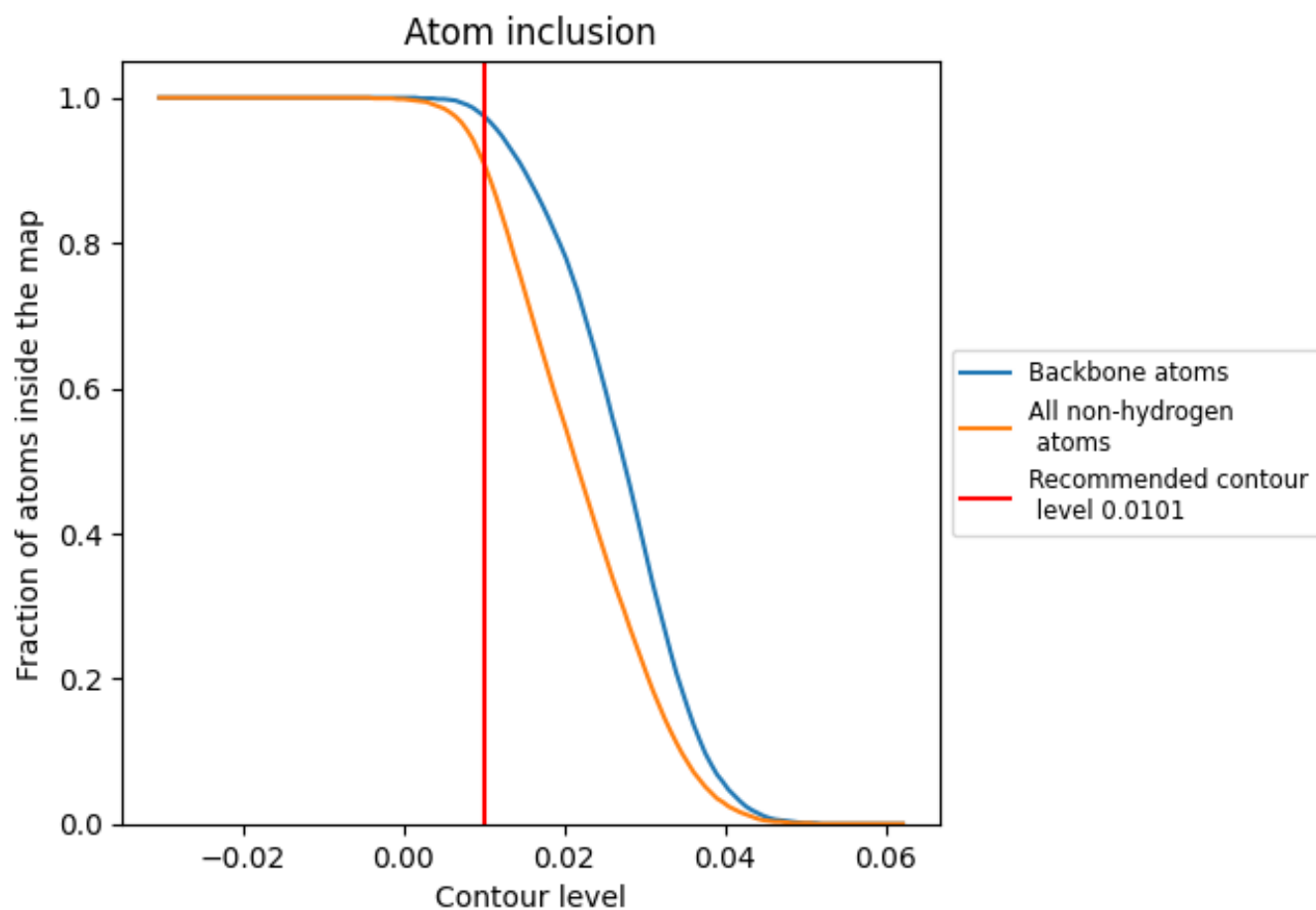
At the recommended contour level, 97% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0101) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9070	0.3320
N	0.8730	0.2180
O	0.9400	0.2870
a	0.9280	0.3500
b	0.9020	0.3530
c	0.9290	0.3660
d	0.7680	0.1610
e	0.9500	0.3510
f	0.9180	0.3540
g	0.8030	0.2110
h	0.9440	0.3470
i	0.9230	0.3220
j	0.9510	0.3650
k	0.8560	0.3400
l	0.9230	0.3510
r	0.8380	0.2540

1.0

0.0
<0.0