



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 07:03 PM EDT

PDB ID : 8UPF
EMDB ID : EMD-42446
Title : Cryo-EM structure of the human nucleosome core particle in complex with RNF168-UbcH5c
Authors : Hu, Q.; Botuyan, M.V.; Zhao, D.; Cui, G.; Mer, G.
Deposited on : 2023-10-22
Resolution : 3.20 Å (reported)
Based on initial models : 5EGG, ., 4GB0

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

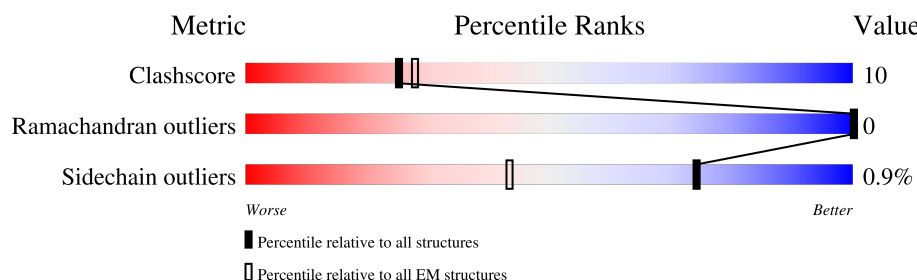
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






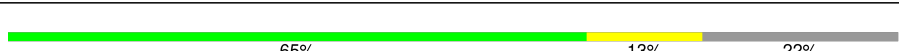

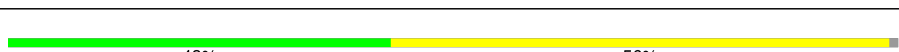
The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	140	
1	E	140	
2	B	107	
2	F	107	
3	D	119	
3	H	119	
4	I	147	
5	J	147	

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Mol	Chain	Length	Quality of chain
6	K	101	<div><div></div><div>29%</div><div>49%</div><div>39%</div><div>13%</div></div>
7	L	174	<div><div></div><div>67%</div><div>47%</div><div>37%</div><div>15%</div></div>
8	C	119	<div><div></div><div>79%</div><div>13%</div><div>8%</div></div>
8	G	119	<div><div></div><div>83%</div><div>9%</div><div>8%</div></div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14012 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	99	Total	C	N	O	S	0	0
			815	514	158	139	4		
1	E	99	Total	C	N	O	S	0	0
			815	514	158	139	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P68431
A	-3	PRO	-	expression tag	UNP P68431
A	-2	GLY	-	expression tag	UNP P68431
A	-1	HIS	-	expression tag	UNP P68431
E	-4	GLY	-	expression tag	UNP P68431
E	-3	PRO	-	expression tag	UNP P68431
E	-2	GLY	-	expression tag	UNP P68431
E	-1	HIS	-	expression tag	UNP P68431

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total	C	N	O	S	0	0
			661	418	129	113	1		
2	F	82	Total	C	N	O	S	0	0
			653	412	127	113	1		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P62805
B	-3	PRO	-	expression tag	UNP P62805
B	-2	GLY	-	expression tag	UNP P62805
B	-1	HIS	-	expression tag	UNP P62805
F	-4	GLY	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	PRO	-	expression tag	UNP P62805
F	-2	GLY	-	expression tag	UNP P62805
F	-1	HIS	-	expression tag	UNP P62805

- Molecule 3 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	95	Total	C	N	O	S	0	0
			751	471	139	139	2		
3	H	93	Total	C	N	O	S	2	0
			743	469	135	137	2		

- Molecule 4 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	147	Total	C	N	O	P	0	0
			2996	1423	545	881	147		

- Molecule 5 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	146	Total	C	N	O	P	0	0
			3010	1425	561	878	146		

- Molecule 6 is a protein called E3 ubiquitin-protein ligase RNF168.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	88	Total	C	N	O	S	1	0
			706	442	130	123	11		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLY	-	expression tag	UNP Q8IYW5
K	0	HIS	-	expression tag	UNP Q8IYW5
K	95	SER	-	expression tag	UNP Q8IYW5
K	96	GLY	-	expression tag	UNP Q8IYW5
K	97	SER	-	expression tag	UNP Q8IYW5
K	98	GLY	-	expression tag	UNP Q8IYW5
K	99	SER	-	expression tag	UNP Q8IYW5

- Molecule 7 is a protein called Ubiquitin-conjugating enzyme E2 D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	148	Total	C	N	O	S	0	0
			1175	751	201	216	7		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	GLY	-	expression tag	UNP P61077
L	-1	SER	-	expression tag	UNP P61077
L	148	GLY	-	expression tag	UNP P61077
L	149	SER	-	expression tag	UNP P61077
L	150	GLY	-	expression tag	UNP P61077
L	151	SER	-	expression tag	UNP P61077
L	152	GLY	-	expression tag	UNP P61077
L	153	SER	-	expression tag	UNP P61077
L	154	GLY	-	expression tag	UNP P61077
L	155	GLY	-	expression tag	UNP P61077
L	156	SER	-	expression tag	UNP P61077
L	157	GLY	-	expression tag	UNP P61077
L	158	GLY	-	expression tag	UNP P61077
L	159	GLY	-	expression tag	UNP P61077
L	160	SER	-	expression tag	UNP P61077
L	161	GLY	-	expression tag	UNP P61077
L	162	GLY	-	expression tag	UNP P61077
L	163	SER	-	expression tag	UNP P61077
L	164	GLY	-	expression tag	UNP P61077
L	165	GLY	-	expression tag	UNP P61077
L	166	SER	-	expression tag	UNP P61077
L	167	GLY	-	expression tag	UNP P61077
L	168	GLY	-	expression tag	UNP P61077
L	169	SER	-	expression tag	UNP P61077
L	170	GLY	-	expression tag	UNP P61077
L	171	SER	-	expression tag	UNP P61077
L	172	GLY	-	expression tag	UNP P61077
L	173	SER	-	expression tag	UNP P61077

- Molecule 8 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	C	109	Total	C	N	O	0	0
			839	529	164	146		

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Mol	Chain	Residues	Atoms				AltConf	Trace
8	G	110	Total	C	N	O	0	0
			846	533	165	148		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	SER	-	expression tag	UNP P04908
G	11	SER	-	expression tag	UNP P04908

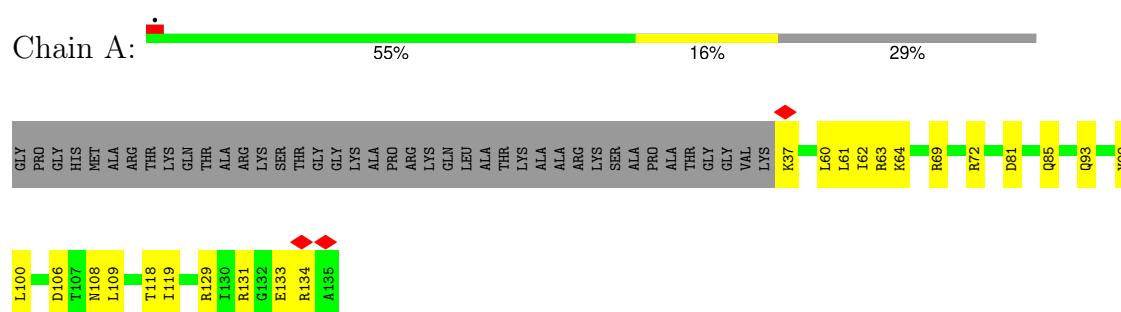
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
9	K	2	Total	Zn	0
			2	2	

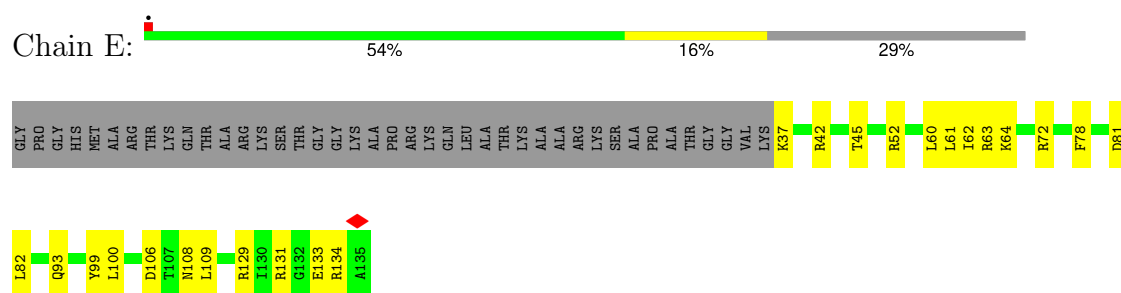
3 Residue-property plots

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.

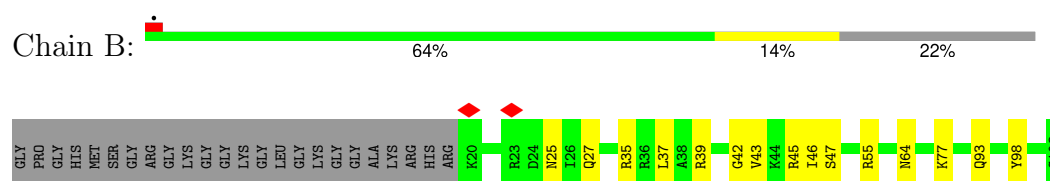
• Molecule 1: Histone H3.1



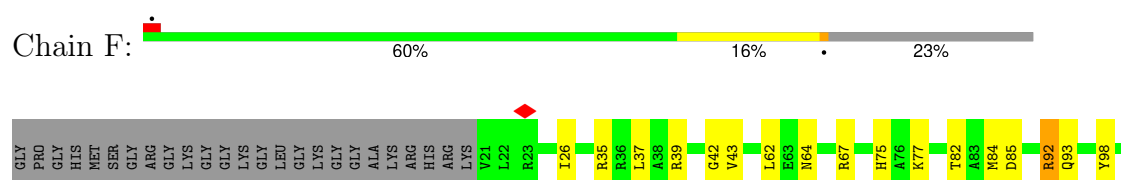
• Molecule 1: Histone H3.1



• Molecule 2: Histone H4



• Molecule 2: Histone H4



◆
G102

• Molecule 3: Histone H2B type 1-J

Chain D: 69% 11% 20%

LYS SER ALA PRO PRO LYS LYS GLY SER SER LYS LYS ALA VAL THR LYS ALA GLN LYS ASP GLY LYS R29 L45 S56 D63 R72 S78 R85 R92 L100 L101 L106 T119 T122 S123

• Molecule 3: Histone H2B type 1-J

Chain H: 65% 13% 22%

LYS SER ALA PRO PRO LYS LYS GLY SER SER LYS LYS ALA VAL THR LYS ALA GLN LYS ASP GLY LYS ARG R31 L39 Y40 V41 H49 P50 D51 T52 D68 I69 T88 I89 T90 S91 R92 E93 L101 K108 K116 S123

• Molecule 4: DNA (147-MER)

Chain I: 50% 50%

A-73 T-72 G-70 C-71 A-69 G-68 A-67 C-63 C-57 C-56 G-55 A-54 T-47 C-46 G-40 T-39 C-38 G-37 G-34 A-33 C-29 T-28 C-27 G-24 C-23 C-22 C-21 G-19 T-17 T-16 A-15 A-14 A-13 C-12 G-11 C-8 G-7 T-6 A-5 G-4 C-3 C0 T1 C4 C5 C6 C7 C8
G9 C10 G11 A17 C18 C19 G20 C21 C22 A23 A24 G25 G26 G27 A29 T30 C35 C36 C37 C45 A46 C49 A50 C51 G52 T53 G54 T55 C56 T64 A65 A72 T73

• Molecule 5: DNA (147-MER)

Chain J: 43% 56%

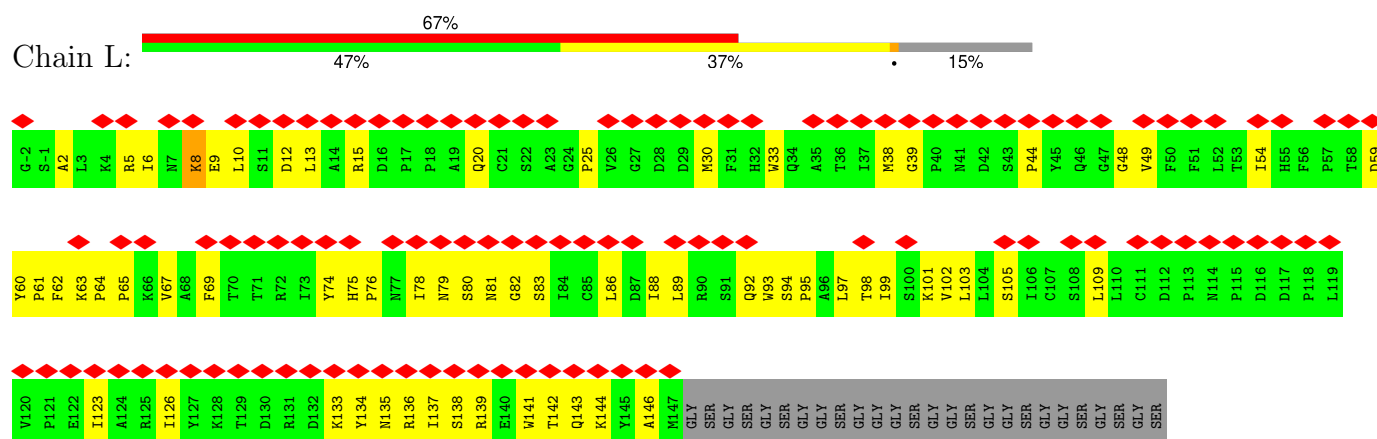
DA T-72 C-71 G-70 G-69 A-68 T-67 G-66 T-61 C-60 A-54 A-53 T-46 G-45 G-44 A-43 G-42 A-41 C-40 G-37 G-36 G-35 A-34 G-33 T-32 A-31 C-26 C-25 T-24 T-23 G-22 G-21 C-20 G-19 G-18 T-17 T-16 A-12 C-11 G-10 G-7 G-6 G-5 A-4 C1 G4 T5 A6 C7 G8
T9 G10 C11 T15 A16 A17 G18 C19 G20 G21 T22 G23 C24 A28 G29 T35 A36 C37 G38 A39 C40 C41 A42 G46 A47 G48 C49 G50 G51 T54 C55 C58 A59 C60 C61 G62 G63 G64 A65 T69 C70 G71 A72 T73

• Molecule 6: E3 ubiquitin-protein ligase RNF168

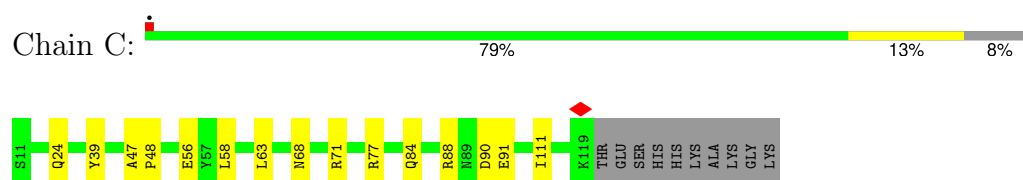
Chain K: 29% 49% 39% 13%

GLY HIS MET ALA LEU PRO LYS ASP A7 I8 P9 S10 L11 S12 E13 C16 G17 I18 C19 N20 E21 I22 L23 V24 E25 P26 C31 L35 C39 E45 K48 A47 S48 L49 C50 C51 R55 R56 R57 V58 S59 T62 R63 Y64 H65 T66 R67 R68 N69 S70 L71 V72
E75 L76 W77 I78 I79 I80 Q81 K82 K83 H84 P85 R86 E87 C88 K89 L90 R91 A92 S93 S94 SER GLY SER GLY SER

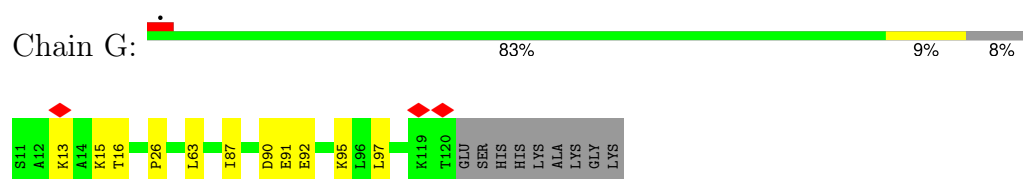
• Molecule 7: Ubiquitin-conjugating enzyme E2 D3



- Molecule 8: Histone H2A type 1-B/E



- Molecule 8: Histone H2A type 1-B/E



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58264	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.652	Depositor
Minimum map value	-1.466	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	263.0656, 263.0656, 263.0656	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0276, 1.0276, 1.0276	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

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	0/827	0.46	0/1109
1	E	0.41	0/827	0.46	0/1109
2	B	0.43	0/668	0.49	0/894
2	F	0.43	0/660	0.47	0/883
3	D	0.41	0/762	0.44	0/1022
3	H	0.41	0/760	0.45	0/1019
4	I	0.74	0/3357	0.92	0/5174
5	J	0.73	0/3379	0.93	0/5218
6	K	0.26	0/725	0.47	0/983
7	L	0.25	0/1210	0.46	0/1650
8	C	0.38	0/849	0.46	0/1144
8	G	0.38	0/856	0.45	0/1154
All	All	0.57	0/14880	0.73	0/21359

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 [i](#)

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	815	0	856	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	815	0	856	18	0
2	B	661	0	709	13	0
2	F	653	0	696	15	0
3	D	751	0	779	11	0
3	H	743	0	779	15	0
4	I	2996	0	1650	53	0
5	J	3010	0	1640	60	0
6	K	706	0	711	30	0
7	L	1175	0	1160	49	0
8	C	839	0	902	10	0
8	G	846	0	909	12	0
9	K	2	0	0	0	0
All	All	14012	0	11647	258	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 258 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)
4:I:21:DC:O2	5:J:-21:DG:N2	2.06	0.86
4:I:21:DC:N3	5:J:-21:DG:N1	2.26	0.77
5:J:72:DA:H2''	5:J:73:DT:H5''	1.71	0.72
1:E:42:ARG:NH1	5:J:71:DG:OP2	2.23	0.71
7:L:61:PRO:O	7:L:93:TRP:NE1	2.22	0.71

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	97/140 (69%)	95 (98%)	2 (2%)	0	100	100
1	E	97/140 (69%)	95 (98%)	2 (2%)	0	100	100
2	B	81/107 (76%)	76 (94%)	5 (6%)	0	100	100
2	F	80/107 (75%)	76 (95%)	4 (5%)	0	100	100
3	D	93/119 (78%)	90 (97%)	3 (3%)	0	100	100
3	H	93/119 (78%)	89 (96%)	4 (4%)	0	100	100
6	K	87/101 (86%)	80 (92%)	7 (8%)	0	100	100
7	L	146/174 (84%)	137 (94%)	9 (6%)	0	100	100
8	C	107/119 (90%)	103 (96%)	4 (4%)	0	100	100
8	G	108/119 (91%)	106 (98%)	2 (2%)	0	100	100
All	All	989/1245 (79%)	947 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/113 (76%)	84 (98%)	2 (2%)	45	72
1	E	86/113 (76%)	84 (98%)	2 (2%)	45	72
2	B	68/81 (84%)	68 (100%)	0	100	100
2	F	67/81 (83%)	66 (98%)	1 (2%)	60	81
3	D	82/100 (82%)	82 (100%)	0	100	100
3	H	82/100 (82%)	81 (99%)	1 (1%)	67	85
6	K	84/92 (91%)	84 (100%)	0	100	100
7	L	132/142 (93%)	131 (99%)	1 (1%)	79	90
8	C	86/94 (92%)	85 (99%)	1 (1%)	67	85
8	G	87/94 (93%)	87 (100%)	0	100	100
All	All	860/1010 (85%)	852 (99%)	8 (1%)	74	89

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	C	84	GLN
7	L	8	LYS
2	F	92	ARG
1	E	134	ARG
3	H	31	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
8	C	112	GLN
8	G	38	ASN
2	F	93	GLN
6	K	81	GLN
6	K	83	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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.

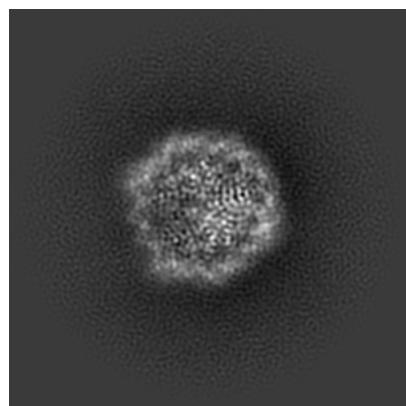
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42446. These allow visual inspection of the internal detail of the map and identification of artifacts.

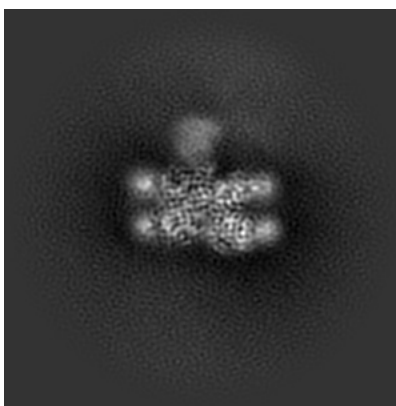
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

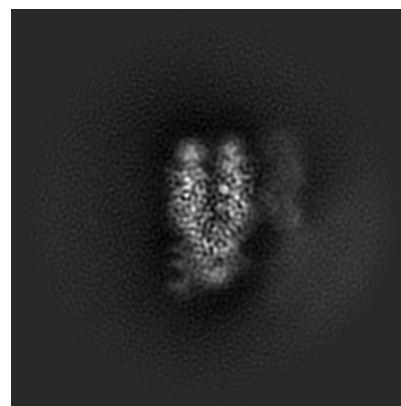
6.1.1 Primary map



X

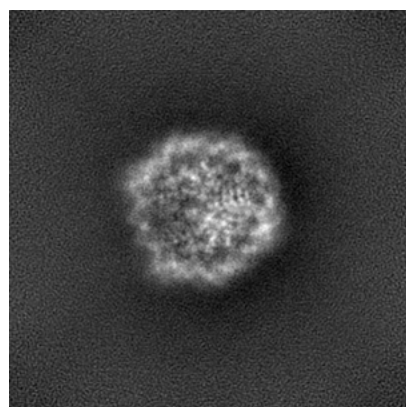


Y

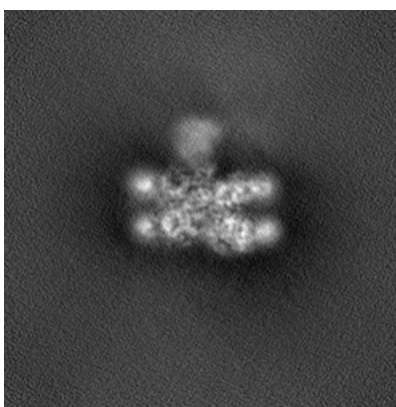


Z

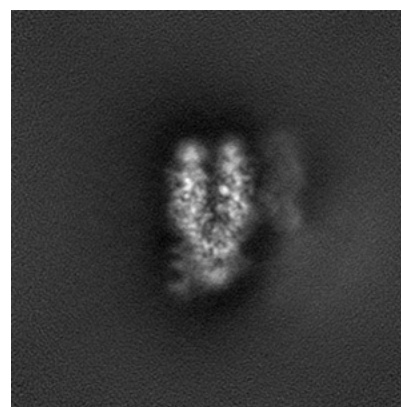
6.1.2 Raw map



X



Y

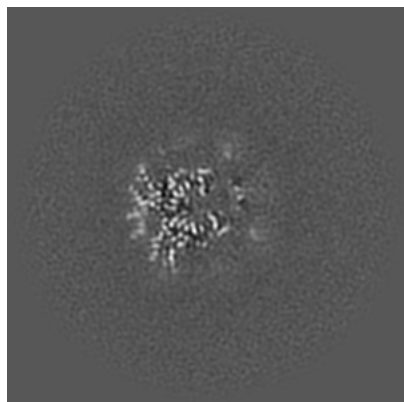


Z

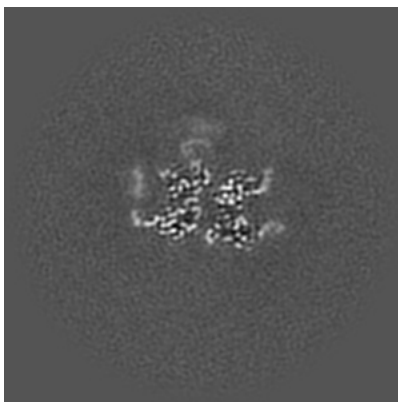
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

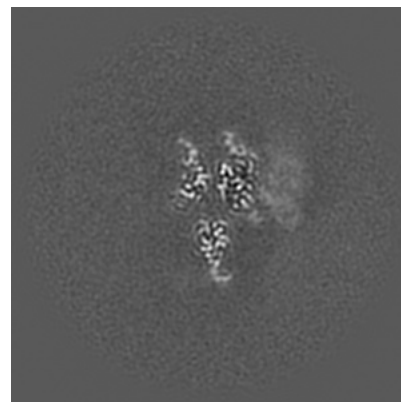
6.2.1 Primary map



X Index: 128

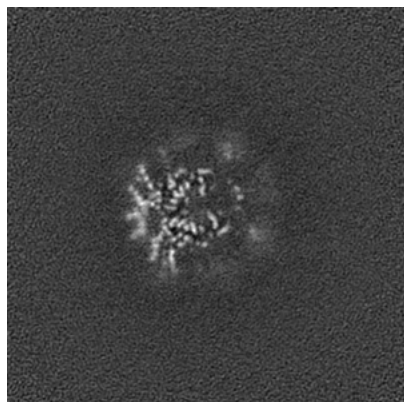


Y Index: 128

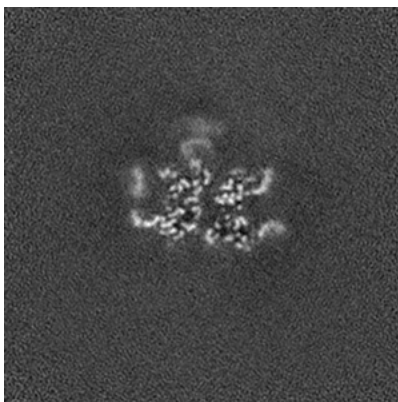


Z Index: 128

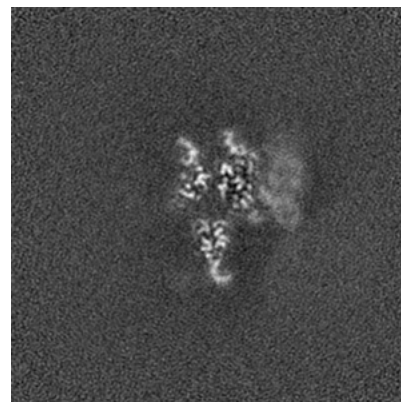
6.2.2 Raw map



X Index: 128



Y Index: 128

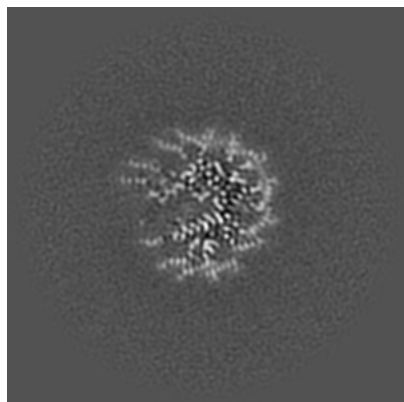


Z Index: 128

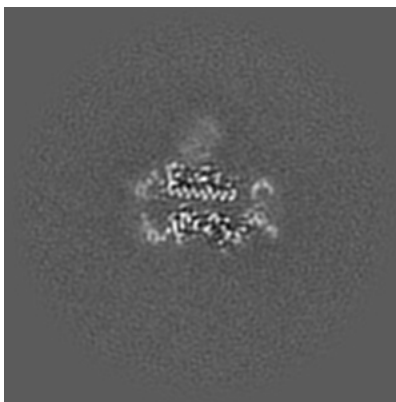
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

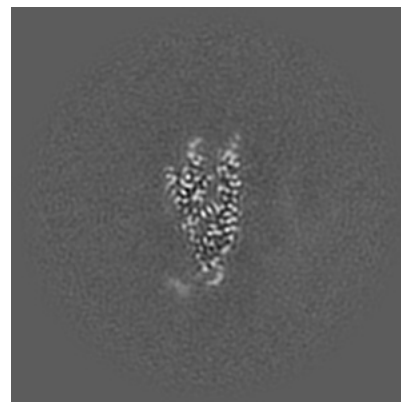
6.3.1 Primary map



X Index: 116

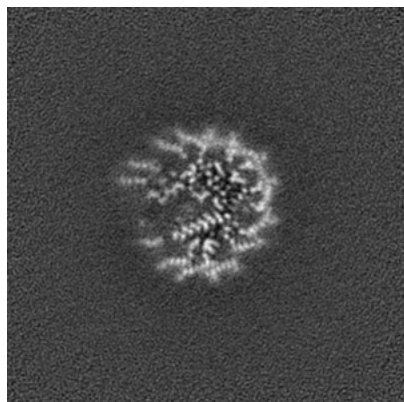


Y Index: 140

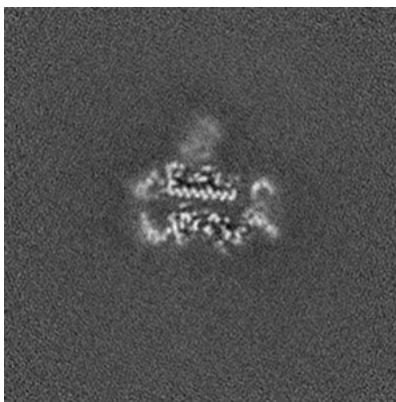


Z Index: 140

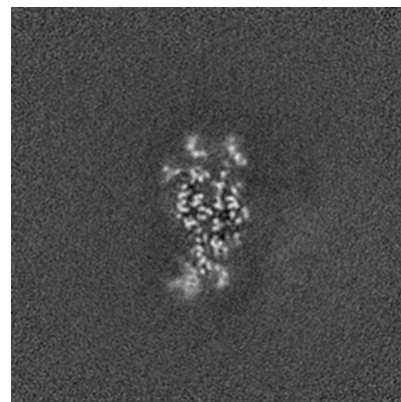
6.3.2 Raw map



X Index: 116



Y Index: 140

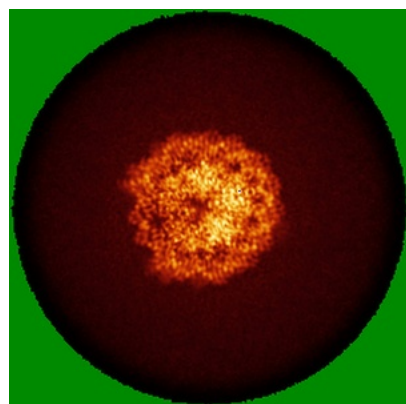


Z Index: 144

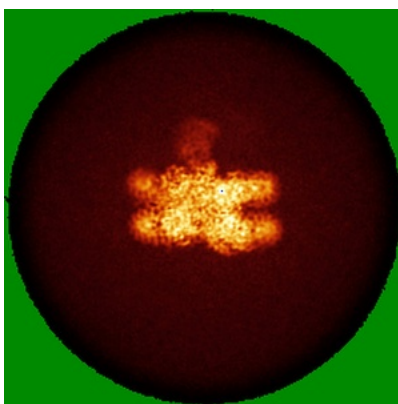
The images above show the largest variance slices of the map in three orthogonal directions.

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

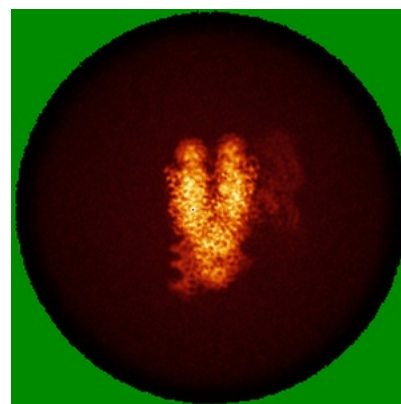
6.4.1 Primary map



X

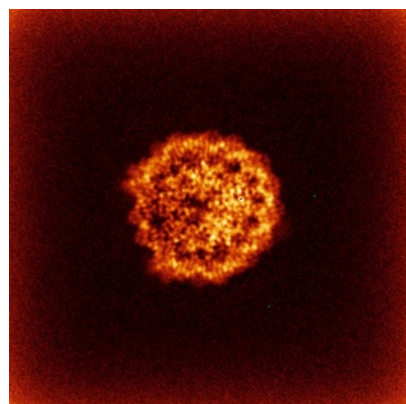


Y

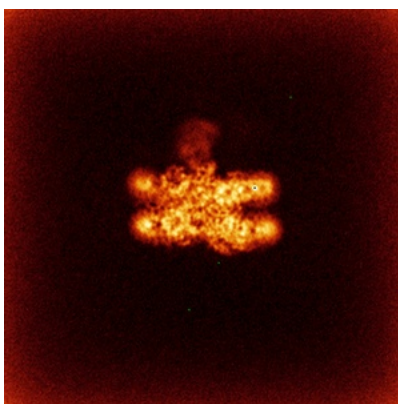


Z

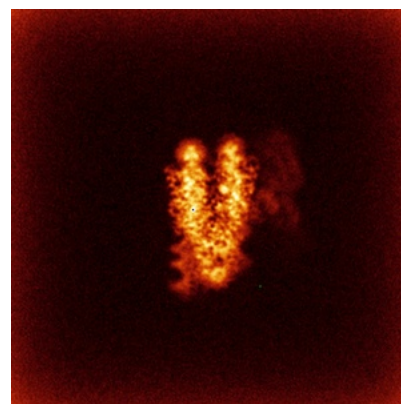
6.4.2 Raw map



X



Y

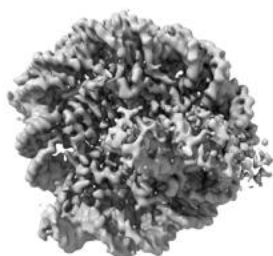


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

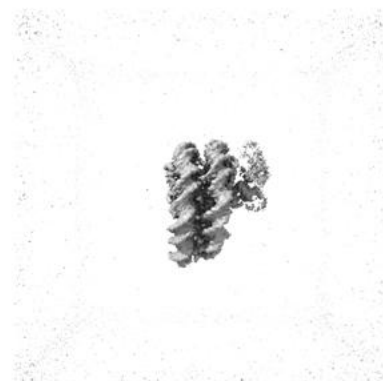
6.5.2 Raw map



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.

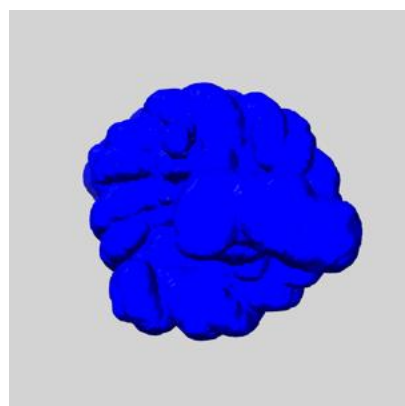
6.6 Mask visualisation [i](#)

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

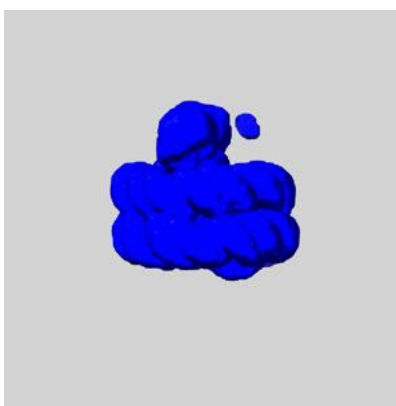
A mask typically either:

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

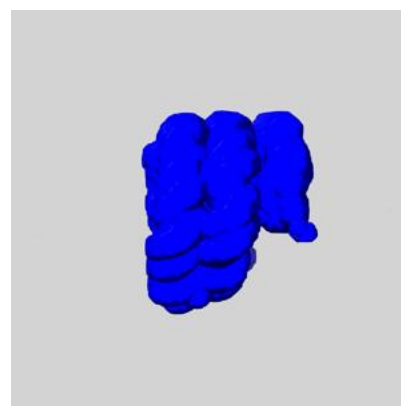
6.6.1 emd_42446_msk_1.map [i](#)



X



Y

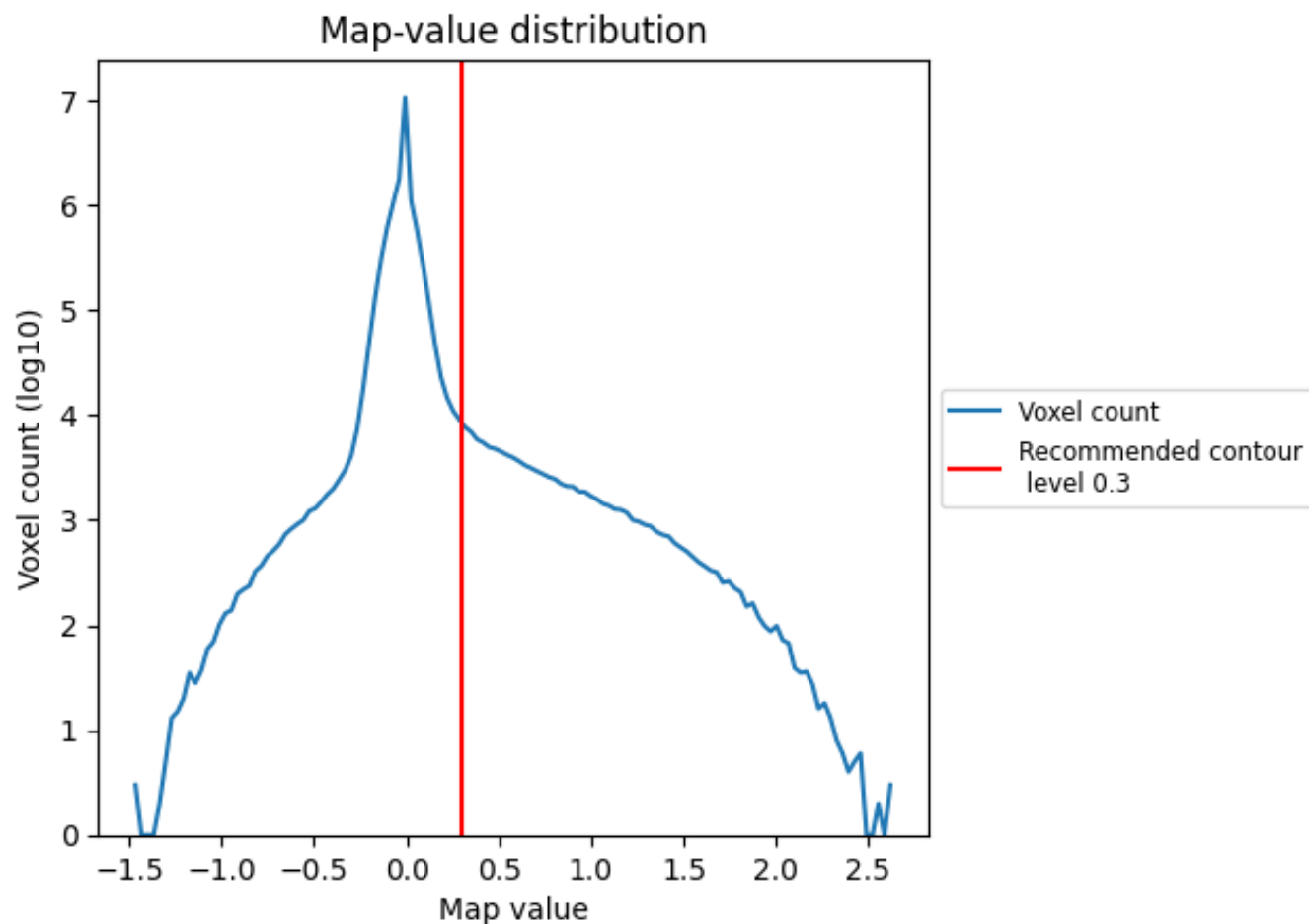


Z

7 Map analysis [i](#)

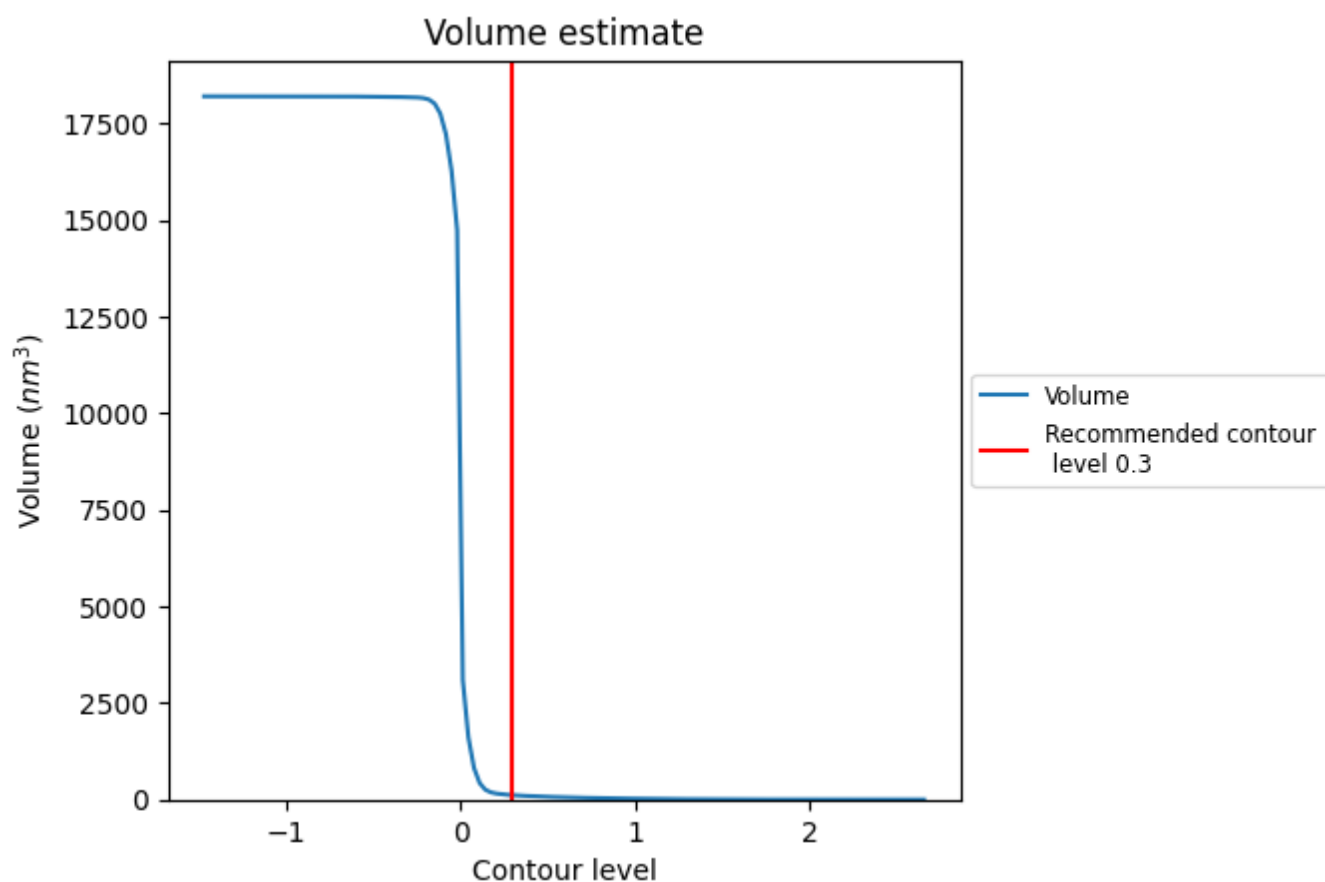
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

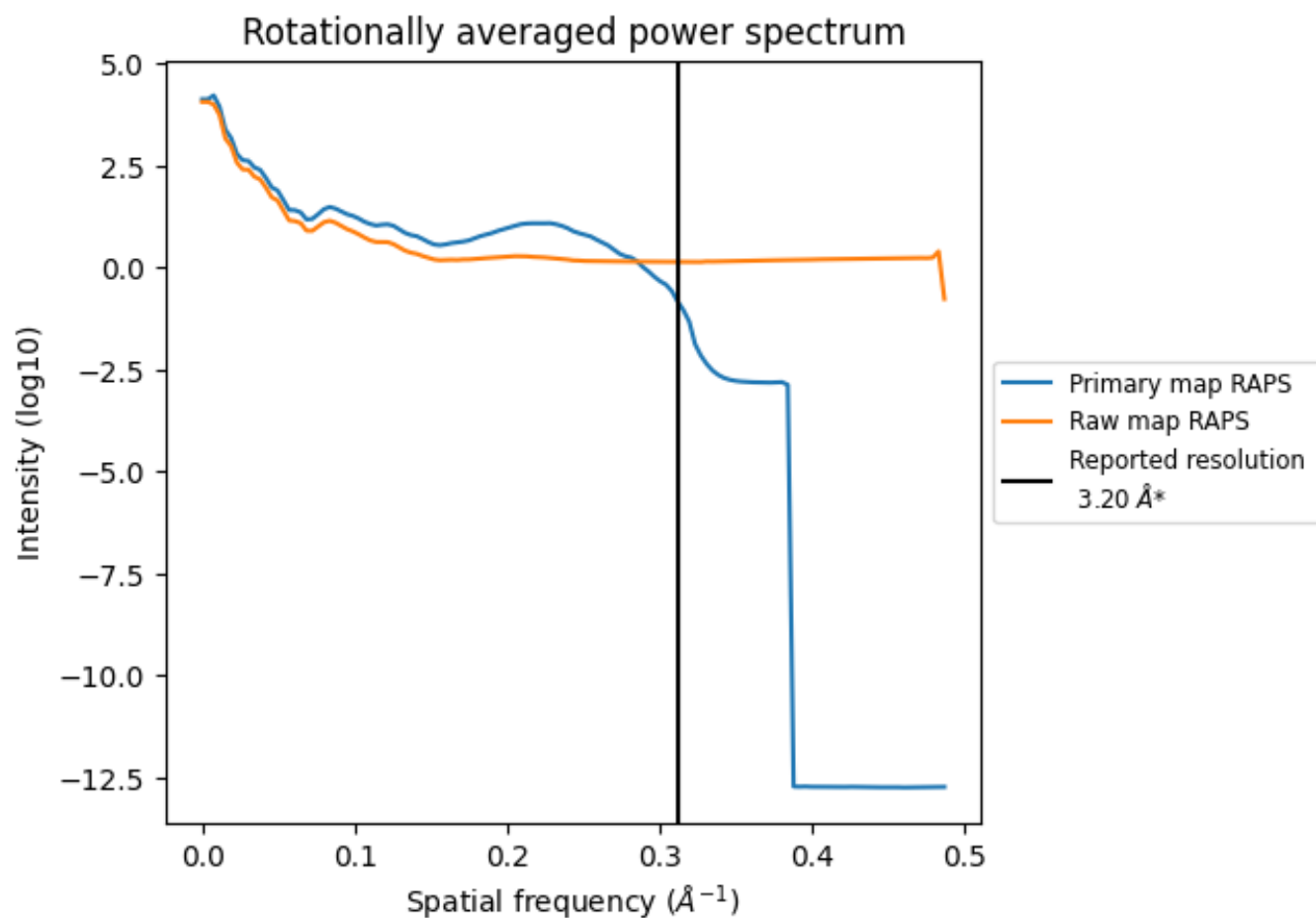
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

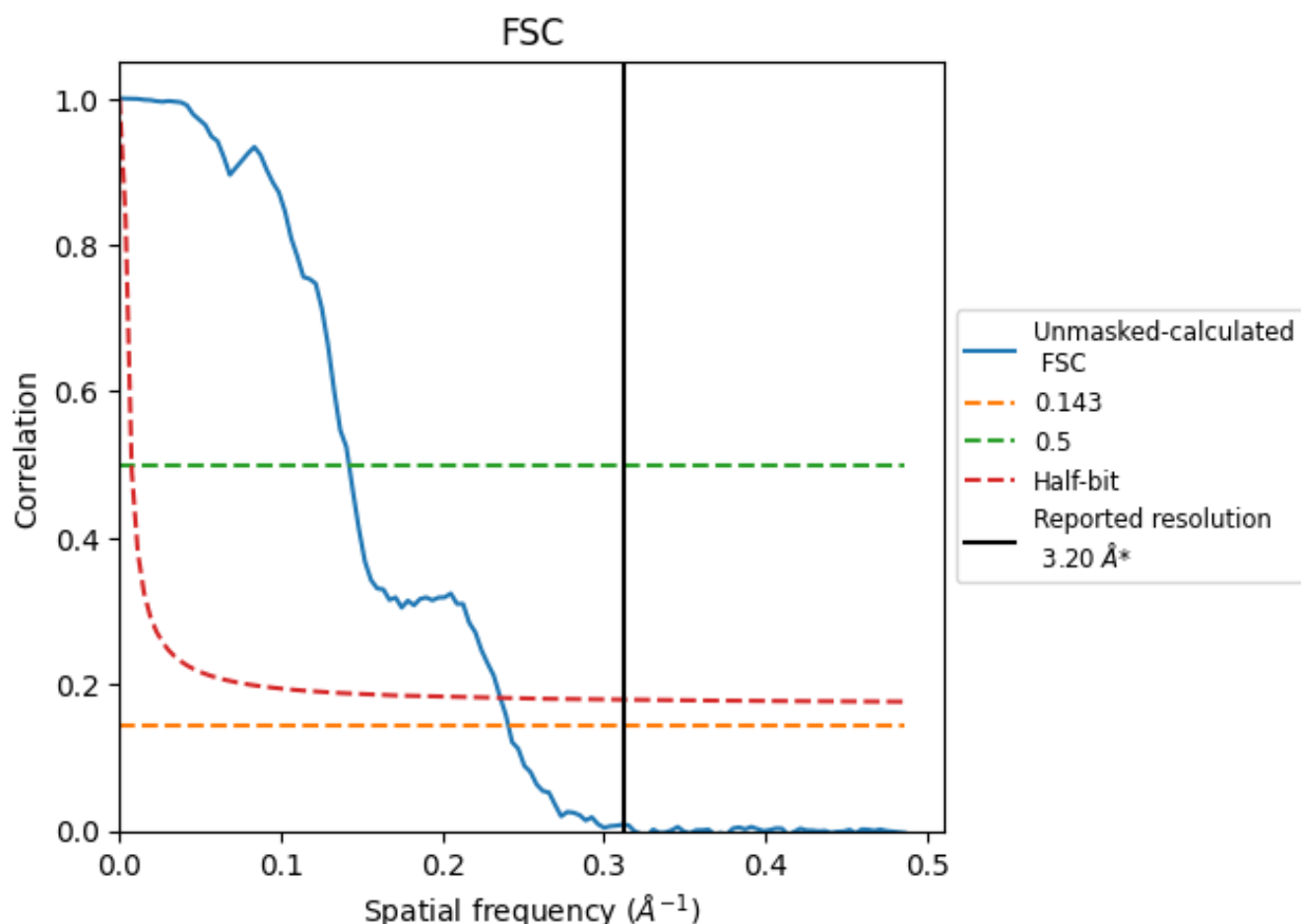


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

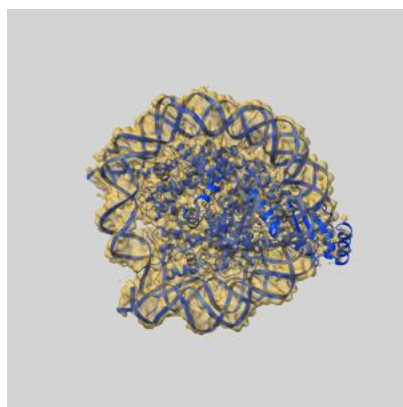
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	7.03	4.24

*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 4.15 differs from the reported value 3.2 by more than 10 %

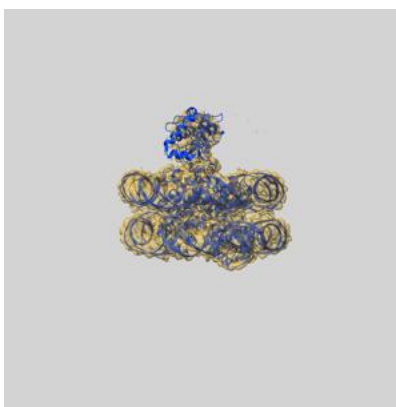
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42446 and PDB model 8UPF. Per-residue inclusion information can be found in section 3 on page 8.

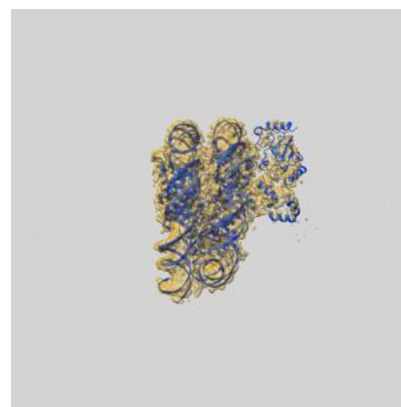
9.1 Map-model overlay [i](#)



X



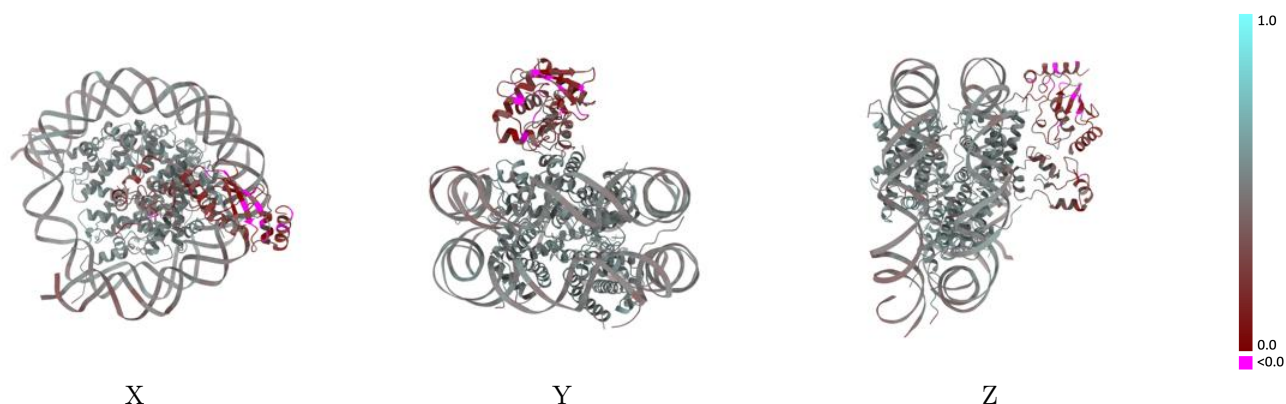
Y



Z

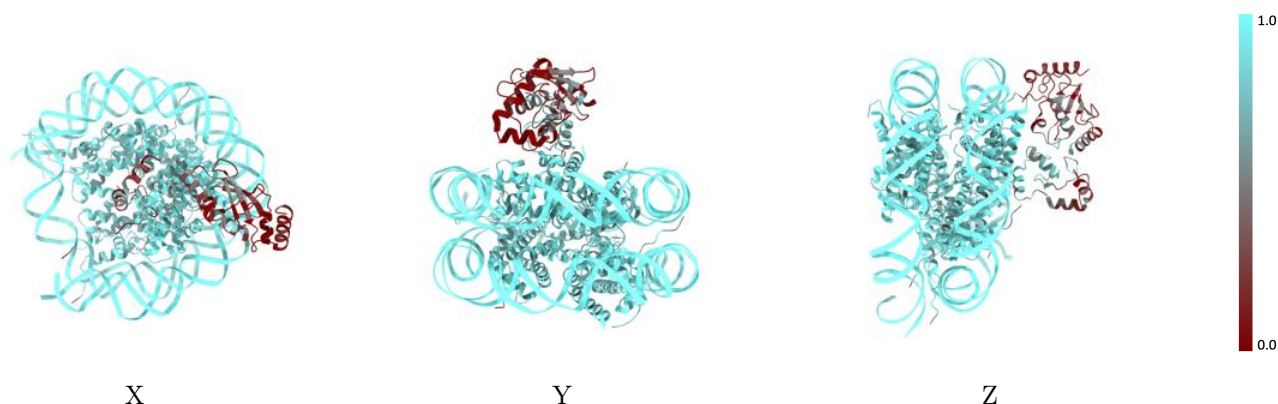
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



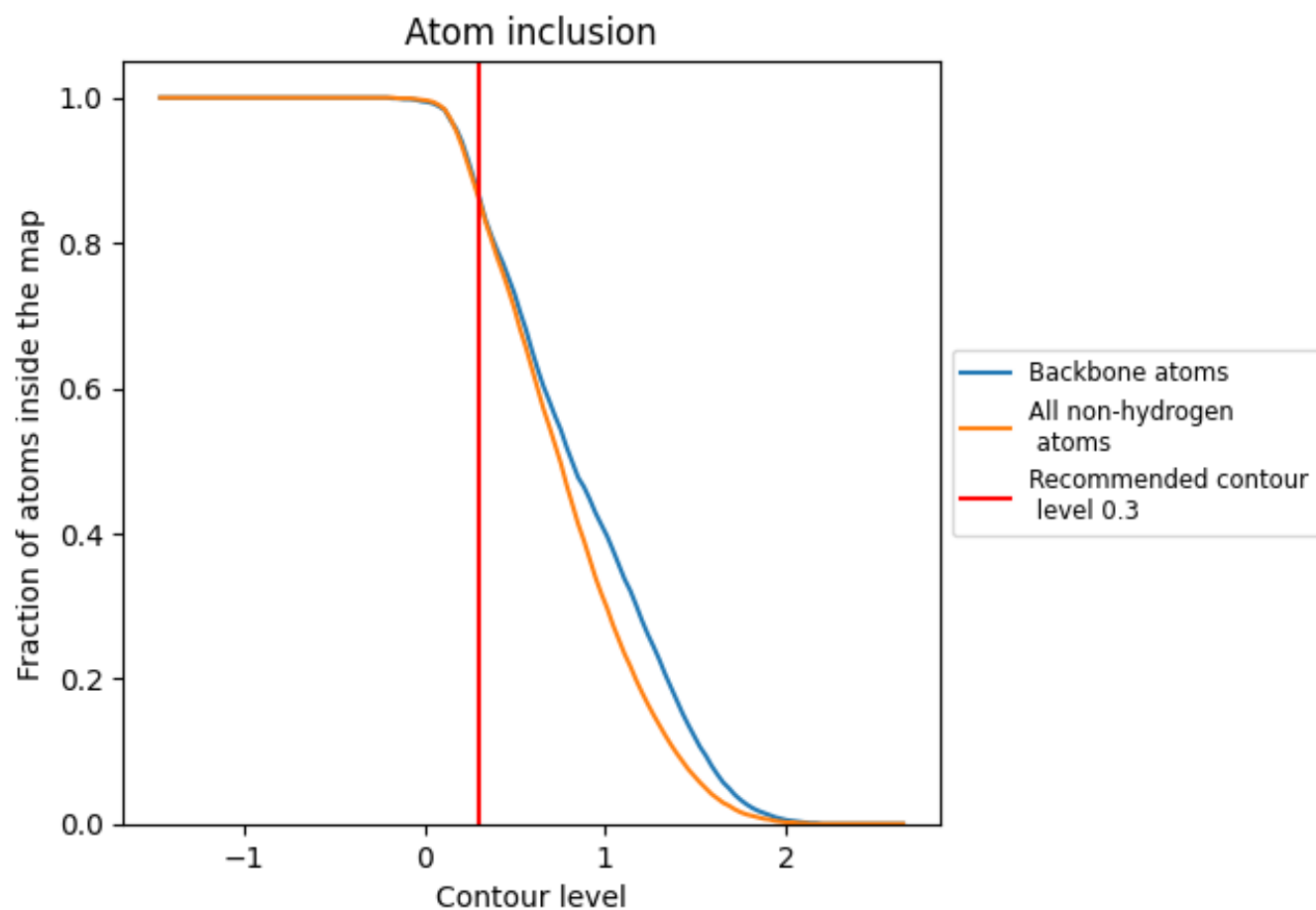
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8610	<div></div> 0.4640
A	<div></div> 0.8860	<div></div> 0.5140
B	<div></div> 0.9050	<div></div> 0.5370
C	<div></div> 0.9030	<div></div> 0.5340
D	<div></div> 0.9160	<div></div> 0.5220
E	<div></div> 0.8890	<div></div> 0.5200
F	<div></div> 0.9110	<div></div> 0.5340
G	<div></div> 0.8980	<div></div> 0.5350
H	<div></div> 0.9060	<div></div> 0.5250
I	<div></div> 0.9730	<div></div> 0.4620
J	<div></div> 0.9780	<div></div> 0.4650
K	<div></div> 0.5800	<div></div> 0.3530
L	<div></div> 0.2170	<div></div> 0.2040

