wwPDB EM Validation Summary Report (i)

Oct 8, 2026 – 01:51 PM EDT

PDB ID	:	9ZSZ / pdb_00009zsz
EMDB ID	:	EMD-74731
Title	:	Nucleosome with an SSB at SHL +5.3 in complex with human PARP2, HPF1 and Olaparib, Class 6
Authors	:	Gregory-Lott, E.; Jayathilake, C.; Virk, R.K.; Kim, T.H.
Deposited on	:	2025-12-22
Resolution	:	2.46 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 (i) 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 (i)) were used in the production of this report:

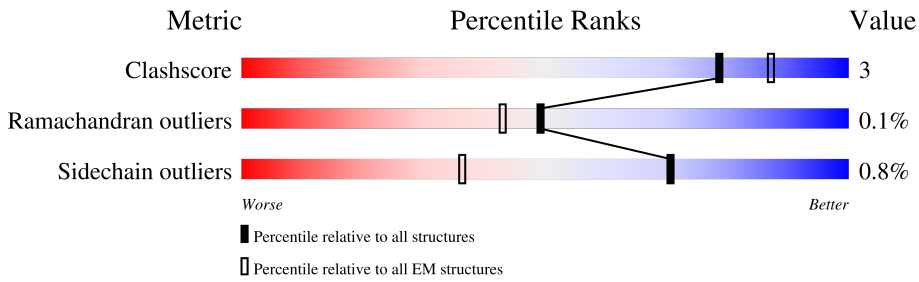
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

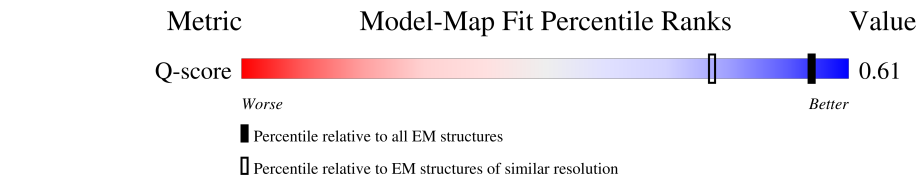
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6014 (1.96 - 2.96)

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	124	82% • • 14%
1	B	124	85% • 14%
2	C	125	71% 6% 22%
2	D	125	71% 5% 24%

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Mol	Chain	Length	Quality of chain
3	E	136	70% 28%
3	F	136	68% 29%
4	G	104	77% 20%
4	H	104	77% 20%
5	K	130	79% 19%
6	M	153	74% 10% 16%
7	I	274	77% 7% 16%
7	J	274	75% 9% 16%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 27776 atoms, of which 12827 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 H2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	107	1701	518	880	160	142	1	0	0
1	B	107	1701	518	880	160	142	1	0	0

- Molecule 2 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C	97	1584	486	813	141	142	2	0	0
2	D	95	1540	474	787	137	140	2	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P02283
C	2	ILE	-	insertion	UNP P02283
D	0	GLY	-	expression tag	UNP P02283
D	2	ILE	-	insertion	UNP P02283

- Molecule 3 is a protein called Histone H3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	98	1662	511	852	157	140	2	0	0
3	F	97	1640	505	839	155	139	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	111	SER	CYS	engineered mutation	UNP P02299

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Chain	Residue	Modelled	Actual	Comment	Reference
F	111	SER	CYS	engineered mutation	UNP P02299

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	G	83	1372	418	710	129	114	1	0	0
4	H	83	1373	418	711	129	114	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2	ILE	-	insertion	UNP P84040
H	2	ILE	-	insertion	UNP P84040

- Molecule 5 is a DNA chain called DNA (130-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
5	K	128	4042	1237	1435	473	769	128	0	0

- Molecule 6 is a DNA chain called DNA (153-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
6	M	128	4076	1248	1435	498	767	128	0	0

- Molecule 7 is a protein called mAb PL2-6 antibody.

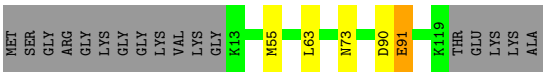
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	I	230	3543	1132	1743	296	363	9	0	0
7	J	230	3542	1132	1742	296	363	9	0	0

3 Residue-property plots (i)

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.

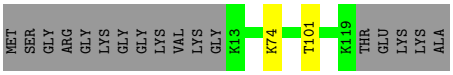
- Molecule 1: Histone H2A

Chain A:



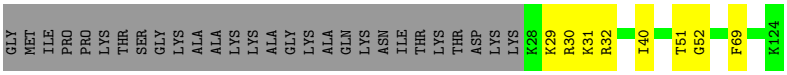
- Molecule 1: Histone H2A

Chain B:



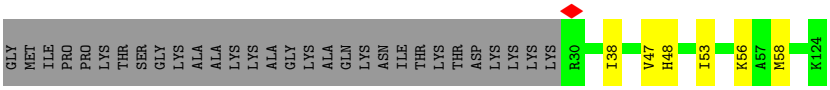
- Molecule 2: Histone H2B

Chain C:



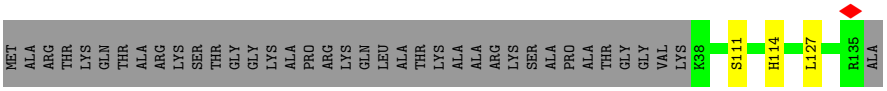
- Molecule 2: Histone H2B

Chain D:



- Molecule 3: Histone H3

Chain E:



- Molecule 3: Histone H3

Chain F: 68% • 29%

MET ALA ARG THR LYS GLN THR ALA ARG LYS SER THR GLY GLY LYS ALA PRO ARG LYS GLN LEU ALA THR LYS ALA ALA ARG LYS SER ALA PRO ALA THR GLY GLY VAL LYS LYS P39 V47 E51 L66 H114 L127 R135 ALA

- Molecule 4: Histone H4

Chain G: • 77% • 20%

MET ILE THR GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG K22 D26 V67 Q95 G104

- Molecule 4: Histone H4

Chain H: • 77% • 20%

MET ILE THR GLY ARG GLY LYS GLY GLY LYS GLY LEU GLY LYS GLY GLY ALA LYS ARG HIS ARG K22 D26 A91 Q95 G104

- Molecule 5: DNA (130-MER)

Chain K: 79% 19% •

A1 T2 C3 C4 T5 G6 C20 C21 T30 C31 T34 T35 T41 A42 C48 T49 C50 T51 A106 T107 T108 C112 C113 C114 T115 T128 DC DC

- Molecule 6: DNA (153-MER)

Chain M: 74% 10% 16%

DA DT DC DA DC DA DG DG DA DT DG DT DA DT DA DT DA DT DC DT DG DA DC DG DG A26 G33 T34 G37 T38 T53 T54 G55 G56 C57 G58 G59 T60 T61 A105 G106 C126 T153

- Molecule 7: mAb PL2-6 antibody

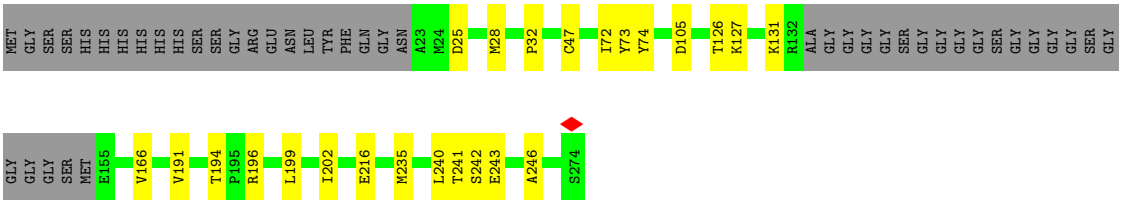
Chain I: 77% 7% 16%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY ASN A23 M24 M28 V43 C47 L57 I72 Y73 Y74 L102 D105 C112 R132 ALA GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY GLY GLY SER

GLY GLY GLY GLY SER MET E155 V156 Q157 V166 M174 K192 I202 Y208 E216 M235 L240 S274

- Molecule 7: mAb PL2-6 antibody

Chain J: 75% 9% 16%


MET
GLY
SER
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HIS
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SER
GLY
ARG
GLU
ASN
LEU
TYR
PHE
GLN
GLY
ASN
A23
M24
D25
M28
P32
C47
I72
Y73
Y74
D105
T126
K127
K131
R132
ALA
GLY
GLY
GLY
GLY
SER
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SER
GLY

GLY
GLY
GLY
SER
MET
E155
V166
V191
T194
P195
R196
L199
I202
E216
M235
L240
T241
S242
E243
A246
S274

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47071	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.682	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0461	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.13	0/831	0.26	0/1119
1	B	0.14	0/831	0.28	0/1119
2	C	0.20	0/782	0.35	0/1046
2	D	0.14	0/764	0.25	0/1024
3	E	0.14	0/822	0.28	0/1102
3	F	0.13	0/813	0.29	0/1090
4	G	0.15	0/669	0.28	0/894
4	H	0.15	0/669	0.29	0/894
5	K	0.74	0/2920	0.87	0/4500
6	M	0.71	0/2966	0.83	0/4580
7	I	0.14	0/1842	0.31	0/2493
7	J	0.15	0/1842	0.31	0/2493
All	All	0.46	0/15751	0.59	0/22354

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	821	880	879	6	0
1	B	821	880	879	1	0
2	C	771	813	811	6	0
2	D	753	787	785	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	810	852	851	3	0
3	F	801	839	839	3	0
4	G	662	710	709	3	0
4	H	662	711	709	3	0
5	K	2607	1435	1436	19	0
6	M	2641	1435	1435	9	0
7	I	1800	1743	1740	11	0
7	J	1800	1742	1740	16	0
All	All	14949	12827	12813	77	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 3.

The worst 5 of 77 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)
7:J:202:ILE:HG21	7:J:235:MET:HE1	1.60	0.82
1:A:73:ASN:O	1:A:73:ASN:ND2	2.19	0.76
5:K:107:DT:H2'	5:K:108:DT:H71	1.78	0.64
7:I:174:MET:HE3	7:I:235:MET:HE3	1.78	0.64
1:A:55:MET:HE3	2:C:69:PHE:HB2	1.81	0.63

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	105/124 (85%)	104 (99%)	1 (1%)	0	100 100
1	B	105/124 (85%)	103 (98%)	2 (2%)	0	100 100
2	C	95/125 (76%)	93 (98%)	1 (1%)	1 (1%)	11 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	93/125 (74%)	93 (100%)	0	0	100	100
3	E	96/136 (71%)	96 (100%)	0	0	100	100
3	F	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
4	G	81/104 (78%)	79 (98%)	2 (2%)	0	100	100
4	H	81/104 (78%)	79 (98%)	2 (2%)	0	100	100
7	I	226/274 (82%)	220 (97%)	6 (3%)	0	100	100
7	J	226/274 (82%)	220 (97%)	6 (3%)	0	100	100
All	All	1203/1526 (79%)	1179 (98%)	23 (2%)	1 (0%)	49	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	30	ARG

5.3.2 Protein sidechains (i)

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	83/94 (88%)	82 (99%)	1 (1%)	63	74
1	B	83/94 (88%)	82 (99%)	1 (1%)	63	74
2	C	84/105 (80%)	83 (99%)	1 (1%)	63	74
2	D	82/105 (78%)	81 (99%)	1 (1%)	63	74
3	E	86/111 (78%)	86 (100%)	0	100	100
3	F	85/111 (77%)	84 (99%)	1 (1%)	63	74
4	G	68/80 (85%)	68 (100%)	0	100	100
4	H	68/80 (85%)	68 (100%)	0	100	100
7	I	202/226 (89%)	200 (99%)	2 (1%)	68	77
7	J	202/226 (89%)	201 (100%)	1 (0%)	81	87
All	All	1043/1232 (85%)	1035 (99%)	8 (1%)	70	83

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

Mol	Chain	Res	Type
7	J	127	LYS
7	I	216	GLU
3	F	66	LEU
2	D	56	LYS
7	I	157	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
7	J	115	HIS
7	I	157	GLN
3	F	86	GLN
2	D	94	GLN
4	G	66	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

There are no ligands in this entry.

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.

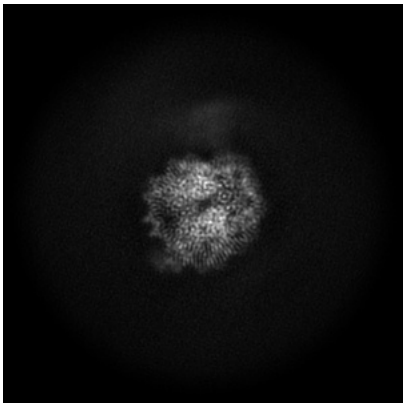
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-74731. These allow visual inspection of the internal detail of the map and identification of artifacts.

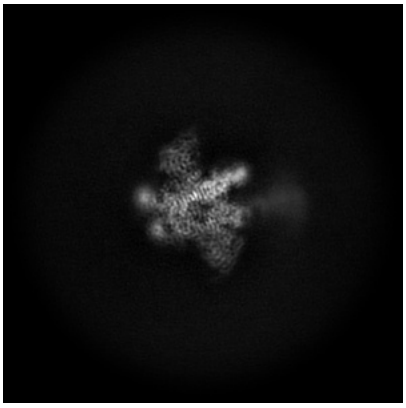
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

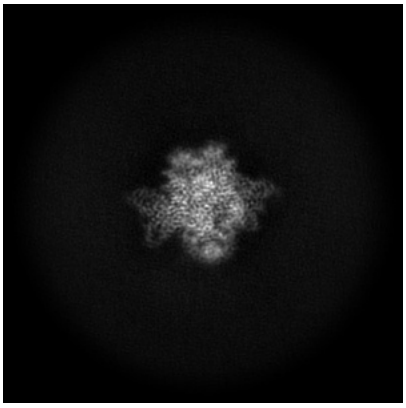
6.1.1 Primary map



X



Y

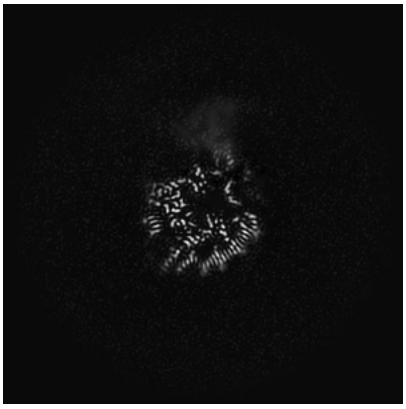


Z

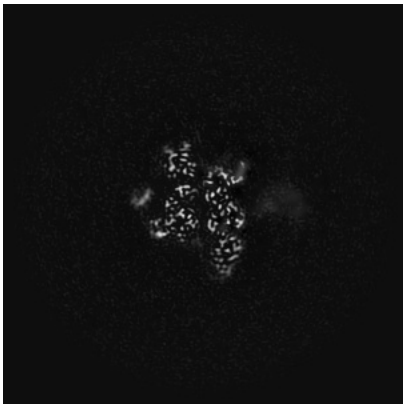
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

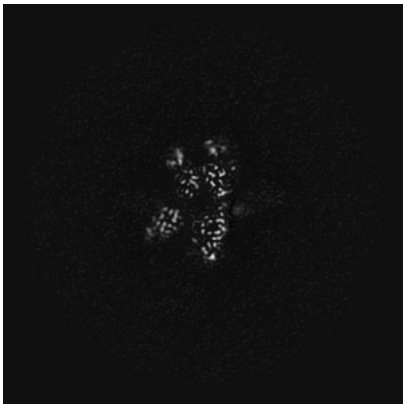
6.2.1 Primary map



X Index: 200



Y Index: 200

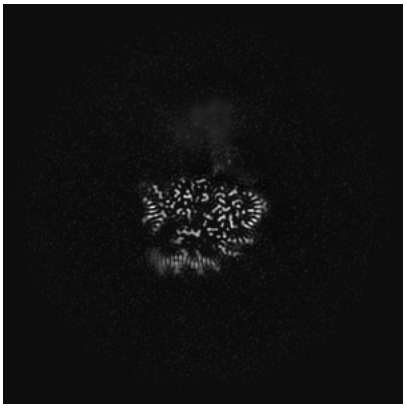


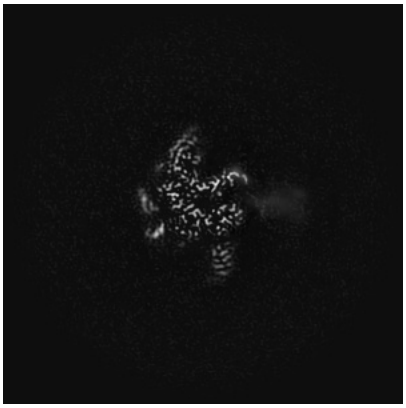
Z Index: 200

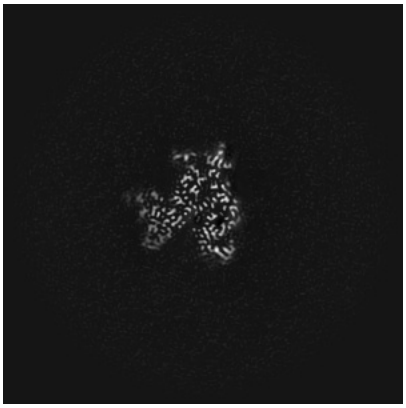
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 207

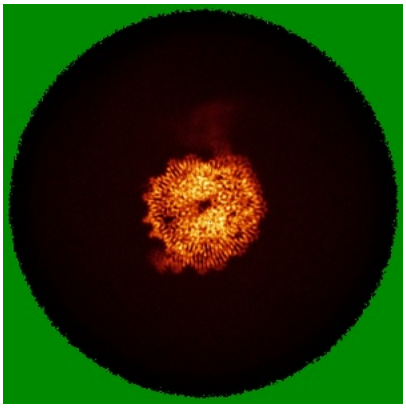

Y Index: 209

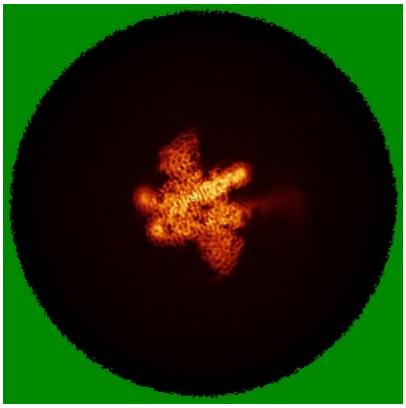

Z Index: 211

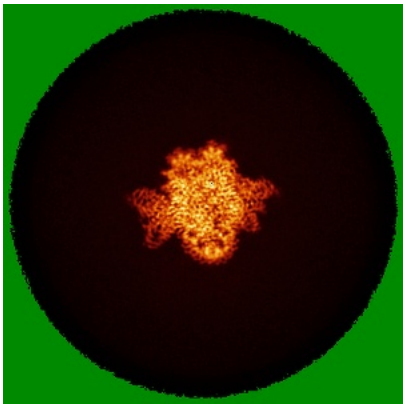
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

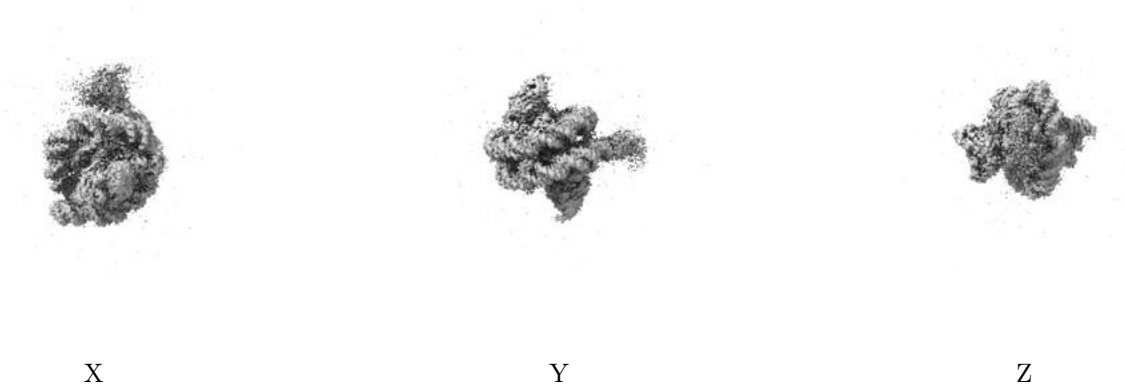

Y


Z

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 0.0461. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

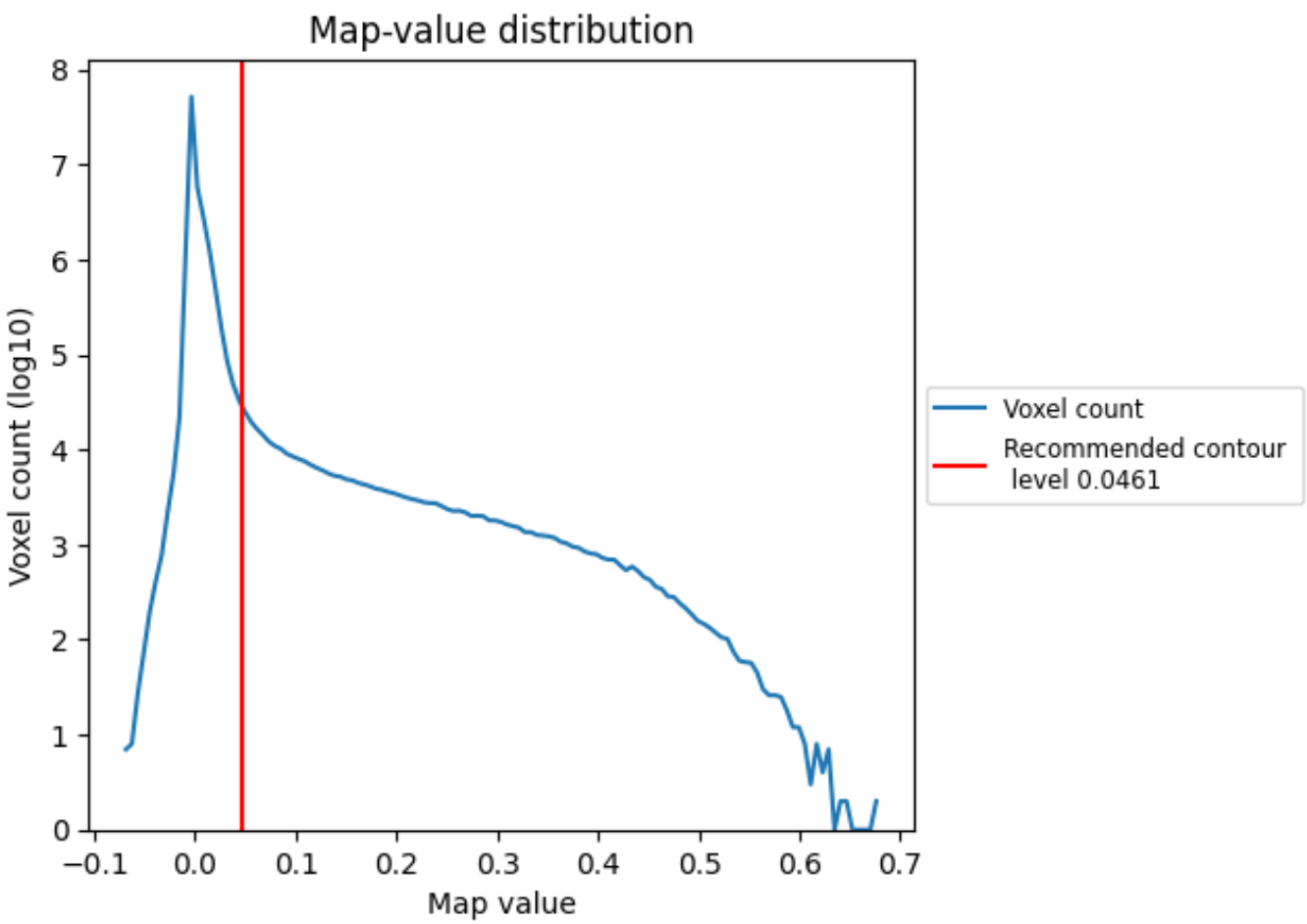
6.6 Mask visualisation (i)

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

7 Map analysis (i)

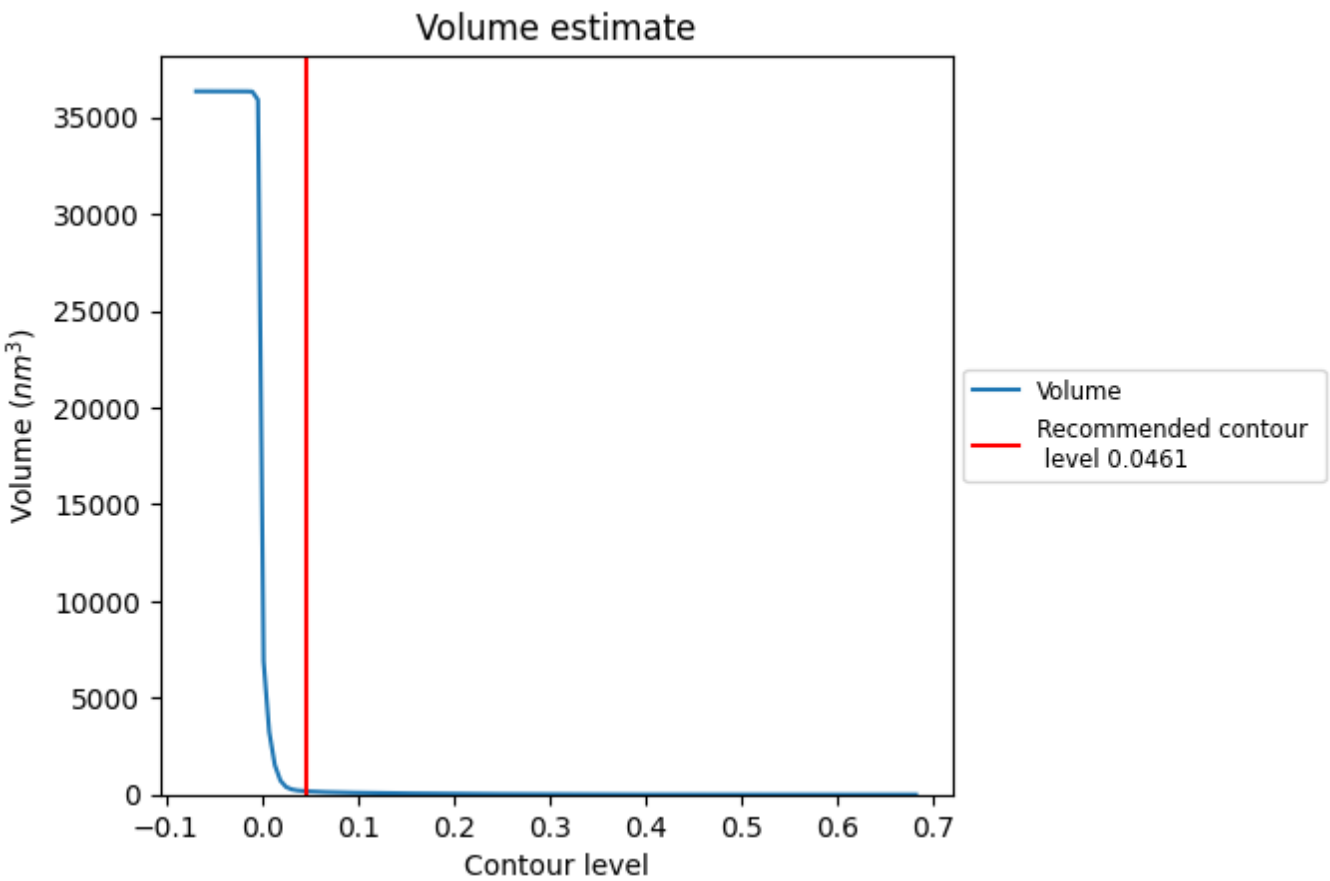
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

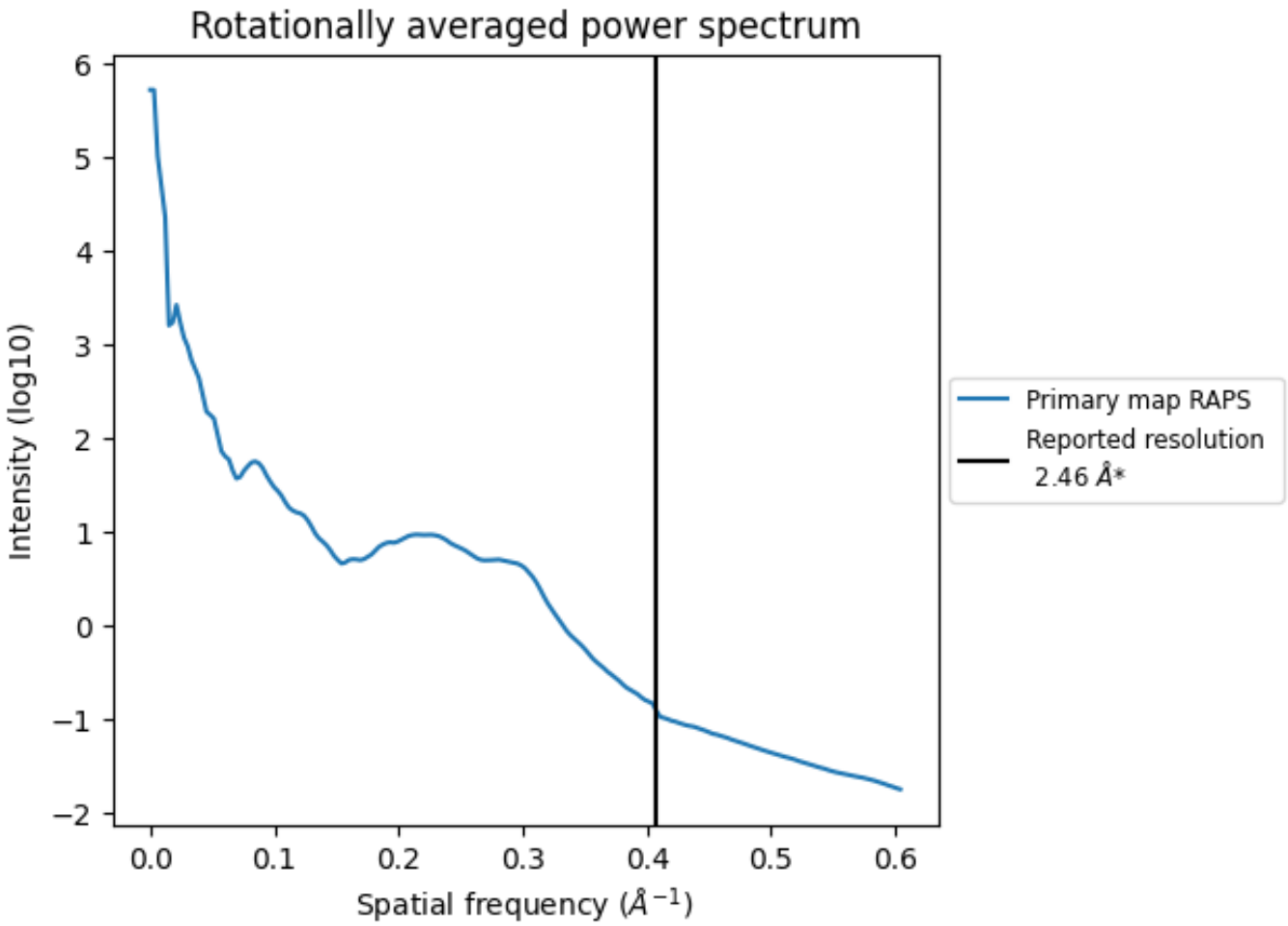
7.2 Volume estimate (i)



The volume at the recommended contour level is 174 nm^3; this corresponds to an approximate mass of 157 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 (i)



*Reported resolution corresponds to spatial frequency of 0.407 Å^{-1}

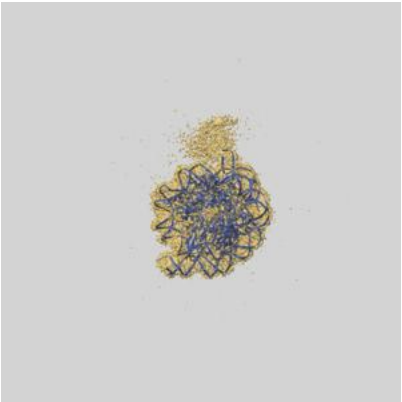
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

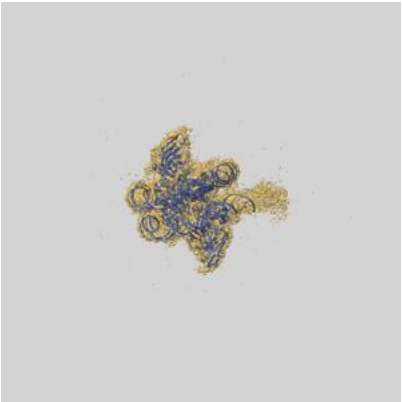
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-74731 and PDB model 9ZSZ. Per-residue inclusion information can be found in section 3 on page 6.

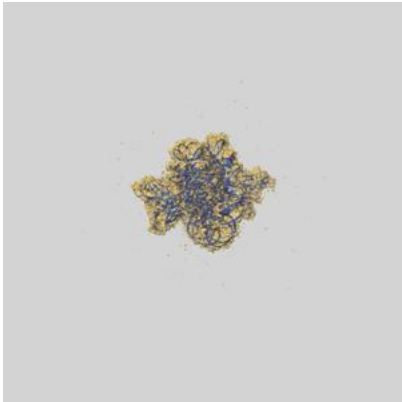
9.1 Map-model overlay (i)



X



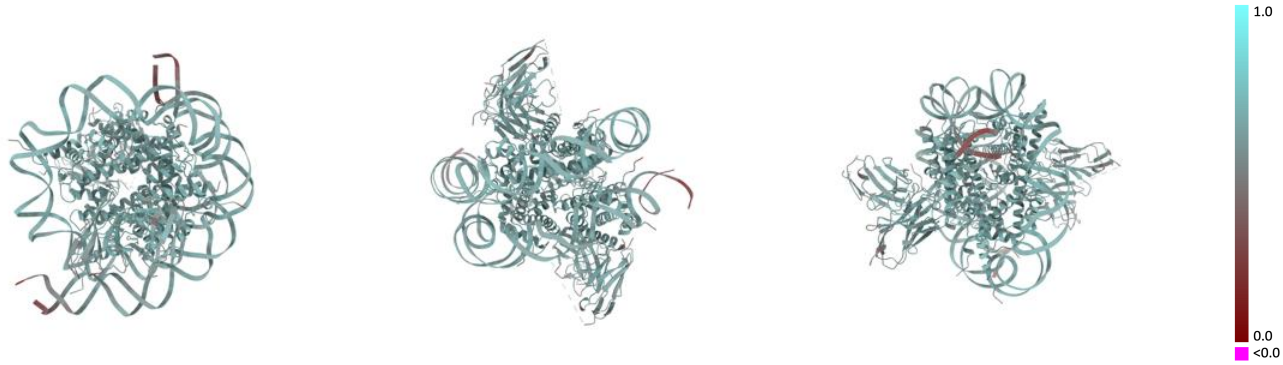
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0461 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.

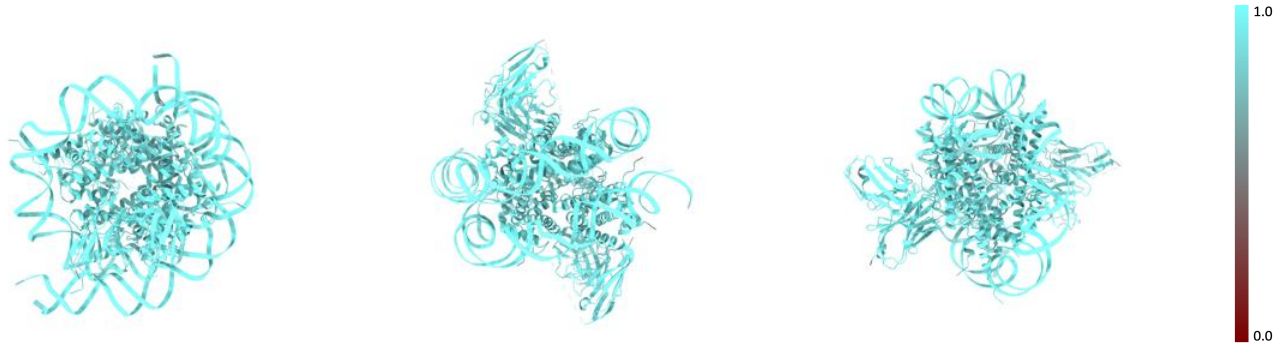
9.2 Q-score mapped to coordinate model (i)



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.

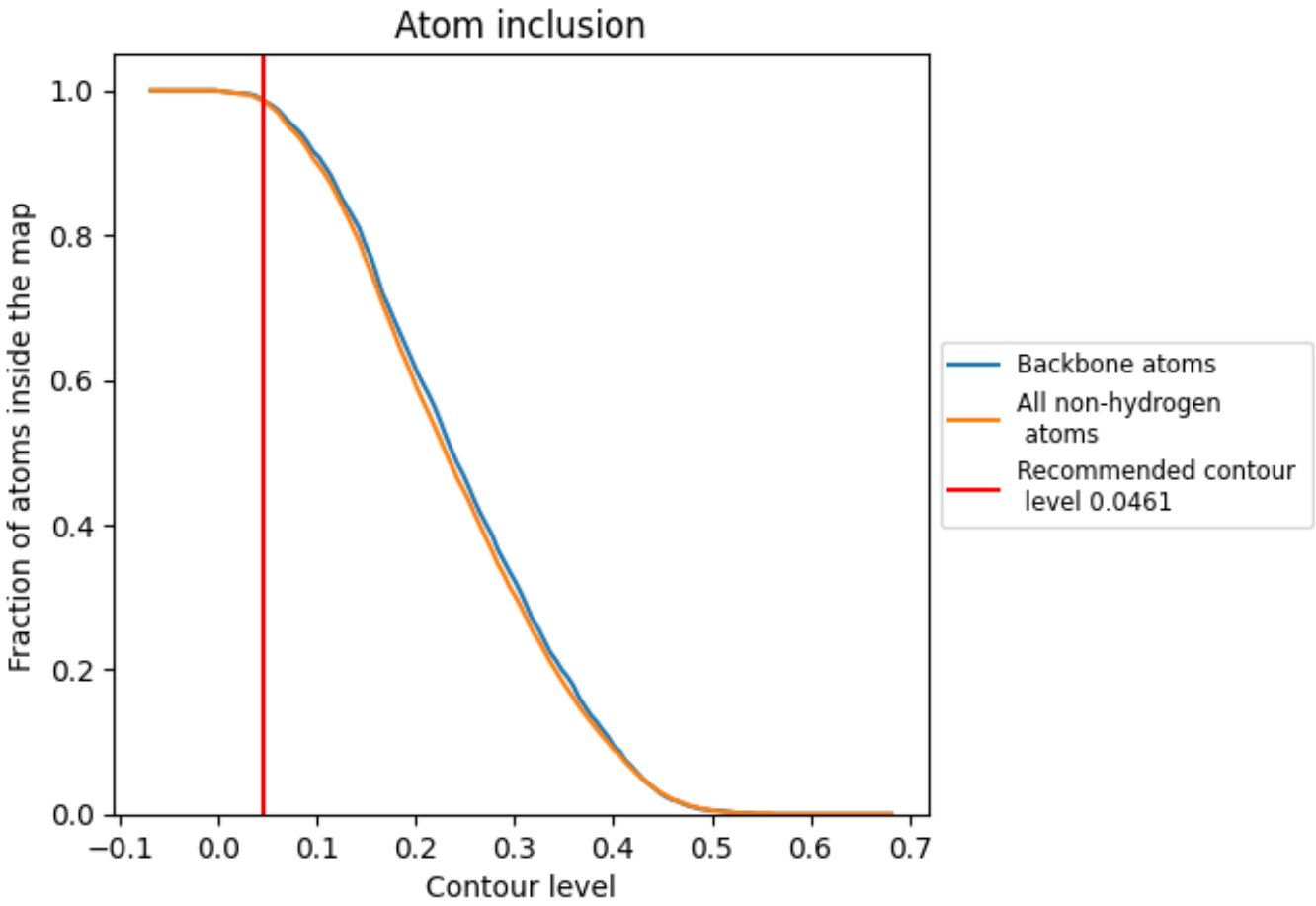
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0461).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0461) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9850	0.6100
A	0.9840	0.6420
B	0.9810	0.6400
C	0.9890	0.6310
D	0.9770	0.6240
E	0.9870	0.6410
F	0.9840	0.6360
G	0.9840	0.6450
H	0.9830	0.6420
I	0.9880	0.5900
J	0.9800	0.5810
K	0.9940	0.5940
M	0.9920	0.5980