



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2024 – 02:21 PM JST

PDB ID : 7D46
EMDB ID : EMD-30571
Title : eIF2B apo
Authors : Kashiwagi, K.; Ito, T.
Deposited on : 2020-09-22
Resolution : 4.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

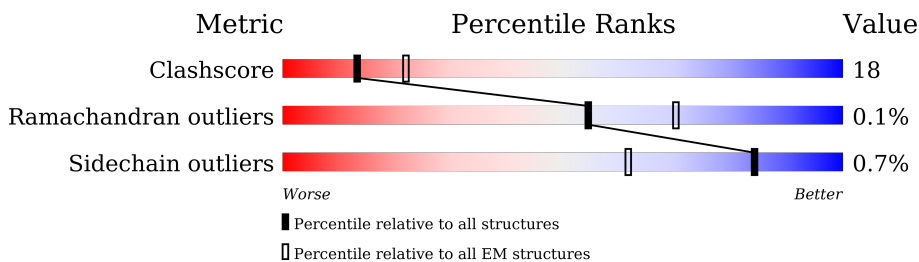
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 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.




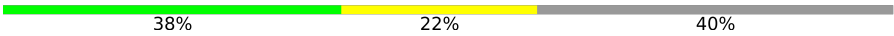
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	305	
1	B	305	
2	C	351	
2	D	351	
3	E	452	
3	F	452	
4	G	523	
4	H	523	

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Mol	Chain	Length	Quality of chain
5	I	721	 32% 26% 41%
5	J	721	 38% 22% 40%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26636 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	293	Total	C	N	O	S	0	0
			2262	1449	377	424	12		
1	B	291	Total	C	N	O	S	0	0
			2249	1442	375	420	12		

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	321	Total	C	N	O	S	0	0
			2489	1571	439	464	15		
2	D	324	Total	C	N	O	S	0	0
			2515	1589	444	467	15		

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	345	Total	C	N	O	S	0	0
			2445	1551	425	454	15		
3	F	345	Total	C	N	O	S	0	0
			2445	1551	425	454	15		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	353	Total	C	N	O	S	0	0
			2750	1740	490	506	14		
4	H	353	Total	C	N	O	S	0	0
			2750	1740	490	506	14		

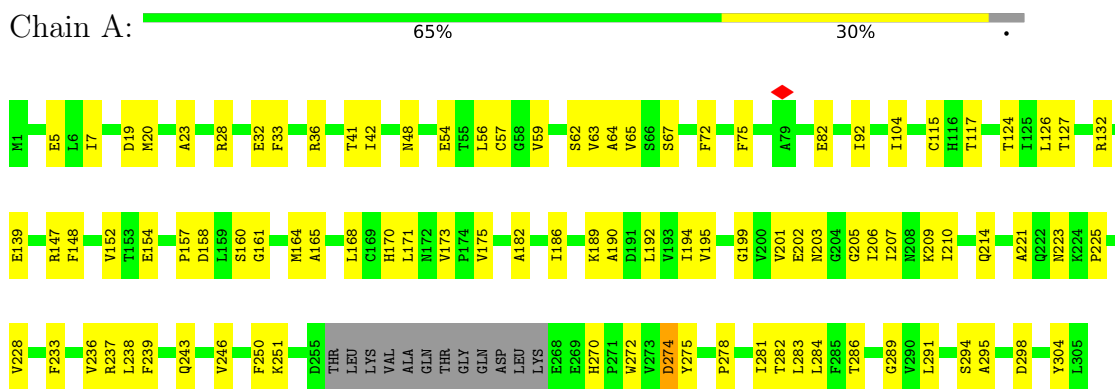
- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	427	3358	2115	591	637	15	0	0
5	J	429	3373	2124	593	641	15	0	0

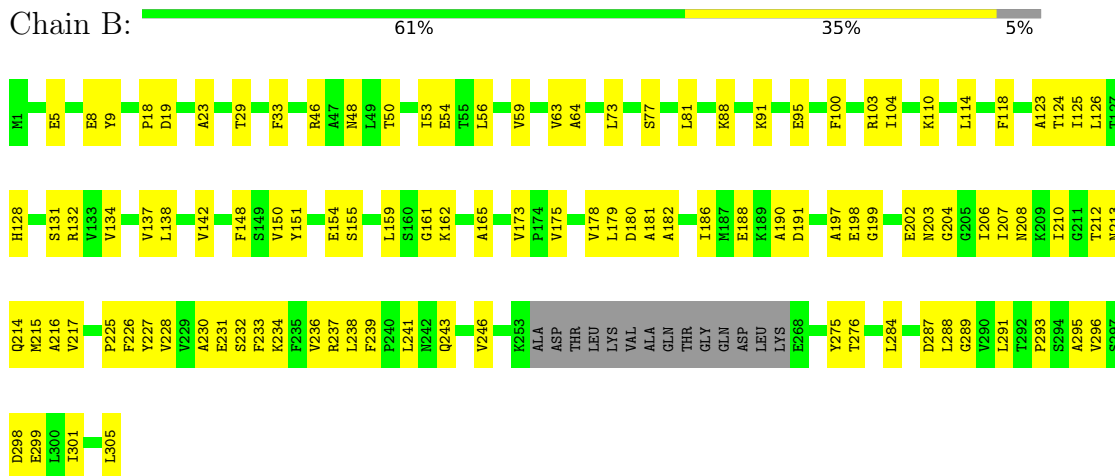
3 Residue-property plots [i](#)

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.

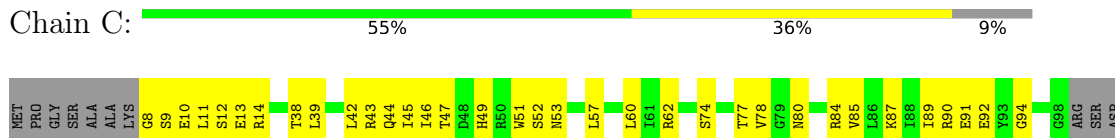
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

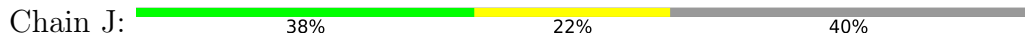


- Molecule 1: Translation initiation factor eIF-2B subunit alpha



- Molecule 2: Translation initiation factor eIF-2B subunit beta





MET	L75	E167	L287	L391	LYS	ARG	LEU	ILE	ASP
ALA	L76	H168	H288	T394	GLY	GLY	GLU	SER	
ALA	L80	R169	H289	T395	TYR	GLY	PHE	MET	
PRO	L170	R170	H290	L396	ASN	SER	PRO	ALA	
VAL	E81	R171	L170	L396	PRO	PRO	LEU	LYS	
VAL	F82	R172	Y296	V400	ALA	GLN	GLN	VAL	
ALA	L83	K173	R299	V401	GLU	MET	GLN	LEU	
PRO	T86	L174	V300	V402	VAL	ASP	MET	LEU	
PRO	G87	T182	S301	A406	GLY	ASP	ASP	ALA	
GLY	V88	M183	C310	Q407	ALA	ILE	SER	ALA	
GLY	V89	K186	I314	T408	LYS	LYS	PRO	TYR	
VAL	E90	S189	R315	H409	GLY	PHE	LEU	GLN	
VAL	F91	P190	R316	L412	TYR	GLN	SER	GLY	
SER	F92	S191	W317	L413	ASN	ASN	ARG	LEU	
ARG	C95	H192	E324	C414	TRP	VAL	VAL	ARG	
ALA	C96	P193	A325	D415	LYS	VAL	GLY	LEU	
ASN	W97	T194	N326	H416	ALA	GLY	LEU	ALA	
LYS	K98	T195	F327	V423	ALA	THR	LEU	THR	
ARG	I102	H197	T328	T424	ALA	LEU	LEU	ILE	
GLY	L106	C196	D329	L425	THR	LEU	LEU	LEU	
ALA	K110	E198	S330	L431	GLY	LYS	LYS	SER	
GLY	V119	D199	T331	T432	GLU	GLU	LYS	THR	
GLY	T124	N200	F332	S433	GLU	GLU	ALA	GLN	
GLY	Y128	V201	Q333	Q434	GLU	GLU	ALA	TRP	
ALA	R129	W202	S334	V435	GLU	GLU	ALA	ASN	
ARG	L131	A204	C335	L441	LEU	GLY	LEU	LYS	
ALA	G132	R211	R339	T442	GLN	ASP	ARG	ASN	
GLU	D133	V212	Y343	L443	ASN	ASP	ARG	ASN	
GLU	V134	L213	E357	L449	LEU	LEU	ASN	LEU	
GLU	L136	K217	F357	H452	GLY	VAL	TYR	VAL	
PRO	R136	F224	N359	P453	LEU	VAL	LEU	VAL	
L43	D137	P227	V360	D455	LEU	VAL	LEU	VAL	
L44	V138	L230	L361	A456	LEU	VAL	LEU	VAL	
A45	V138	F231	L362	A457	LEU	VAL	LEU	VAL	
F46	K141	V238	S364	E458	GLU	VAL	LEU	VAL	
L47	A142	E239	I368	E464	SER	TYR	ALA	ALA	
V48	L143	V240	C372	D468	GLU	ASN	LEU	LEU	
A49	L149	R241	F373	SER	SER	ILE	ALA	ALA	
D50	L150	Y242	F373	GLY	GLY	ALA	ALA	ALA	
S51	V151	D243	L374	ALA	ALA	LEU	LEU	LEU	
R55	V152	L244	T375	ASP	GLN	GLY	ASP	LYS	
F56	G153	S250	R376	SER	SER	VAL	PHE	GLU	
R65	V155	D154	S377	MET	MET	VAL	VAL	VAL	
V66	V155	T251	V378	GLN	GLN	MET	PHE	ALA	
L67	I156	C252	I379	LYS	LYS	GLU	LEU	LEU	
N72	I161	L276	I385	ASP	GLY	LEU	GLY	GLY	
	A164	L277	V389	LYS	VAL	SER	LEU	SER	
		Q286	V390	MET	VAL	VAL	LEU	GLU	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	330601	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.169	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	441.0, 441.0, 441.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.47, 1.47, 1.47	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	0.38	0/2296	0.52	0/3099
1	B	0.38	0/2283	0.51	0/3081
2	C	0.42	0/2534	0.52	0/3428
2	D	0.41	0/2562	0.51	0/3466
3	E	0.34	0/2480	0.52	0/3368
3	F	0.34	0/2480	0.52	0/3368
4	G	0.44	0/2802	0.53	0/3809
4	H	0.44	0/2802	0.53	0/3809
5	I	0.41	0/3427	0.54	1/4662 (0.0%)
5	J	0.40	0/3443	0.53	0/4685
All	All	0.40	0/27109	0.52	1/36775 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	283	LEU	CA-CB-CG	5.95	128.98	115.30

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	2262	0	2333	69	0
1	B	2249	0	2324	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2489	0	2494	112	0
2	D	2515	0	2511	91	0
3	E	2445	0	2216	88	0
3	F	2445	0	2216	83	0
4	G	2750	0	2811	108	0
4	H	2750	0	2811	157	0
5	I	3358	0	3325	138	0
5	J	3373	0	3336	116	0
All	All	26636	0	26377	963	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 18.

The worst 5 of 963 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)
2:D:247:ALA:HB3	2:D:251:THR:HG21	1.59	0.83
3:F:268:LYS:NZ	3:F:271:ASN:O	2.12	0.83
4:H:170:ARG:HH21	4:H:191:SER:HA	1.40	0.83
2:C:247:ALA:HB3	2:C:251:THR:HG21	1.61	0.82
3:E:167:LEU:HD21	3:E:263:ILE:HG12	1.62	0.82

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	289/305 (95%)	249 (86%)	39 (14%)	1 (0%)	41	75
1	B	287/305 (94%)	249 (87%)	38 (13%)	0	100	100
2	C	317/351 (90%)	270 (85%)	47 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	320/351 (91%)	261 (82%)	58 (18%)	1 (0%)	41	75
3	E	335/452 (74%)	256 (76%)	79 (24%)	0	100	100
3	F	335/452 (74%)	261 (78%)	74 (22%)	0	100	100
4	G	351/523 (67%)	305 (87%)	46 (13%)	0	100	100
4	H	351/523 (67%)	299 (85%)	52 (15%)	0	100	100
5	I	425/721 (59%)	343 (81%)	82 (19%)	0	100	100
5	J	427/721 (59%)	340 (80%)	87 (20%)	0	100	100
All	All	3437/4704 (73%)	2833 (82%)	602 (18%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
2	D	127	ALA

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	248/260 (95%)	246 (99%)	2 (1%)	81	89
1	B	247/260 (95%)	246 (100%)	1 (0%)	91	94
2	C	268/298 (90%)	268 (100%)	0	100	100
2	D	270/298 (91%)	270 (100%)	0	100	100
3	E	216/398 (54%)	214 (99%)	2 (1%)	78	88
3	F	216/398 (54%)	213 (99%)	3 (1%)	67	81
4	G	309/444 (70%)	307 (99%)	2 (1%)	86	92
4	H	309/444 (70%)	307 (99%)	2 (1%)	86	92
5	I	381/626 (61%)	377 (99%)	4 (1%)	76	86
5	J	383/626 (61%)	380 (99%)	3 (1%)	81	89
All	All	2847/4052 (70%)	2828 (99%)	19 (1%)	84	90

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	328	THR
5	J	136	ARG
5	J	173	LYS
5	J	55	ARG
4	G	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
4	G	185	GLN
5	J	44	GLN
4	G	275	ASN
5	J	326	ASN
5	I	263	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 monosaccharides 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

There are no chain breaks in this entry.

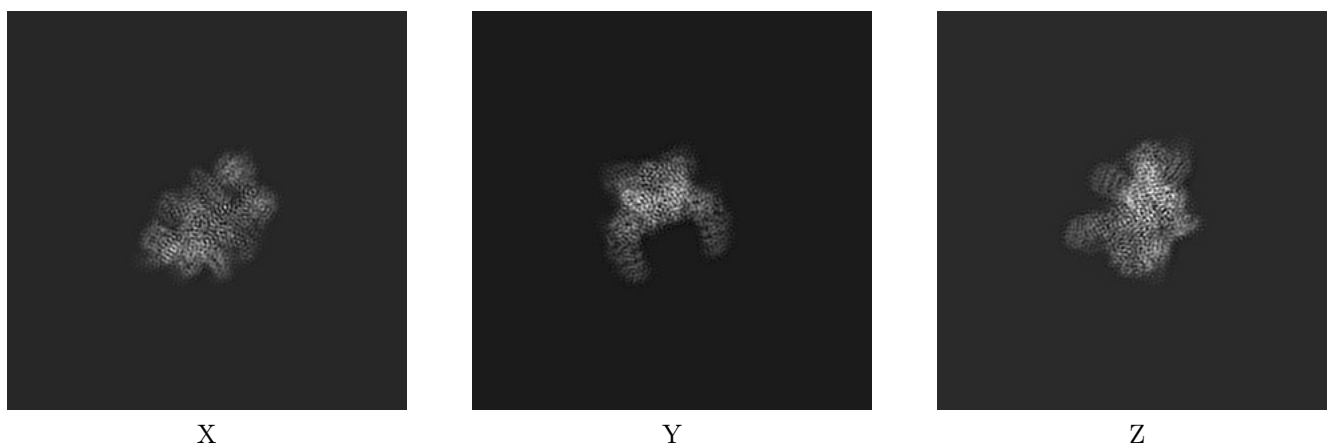
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30571. 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](#)

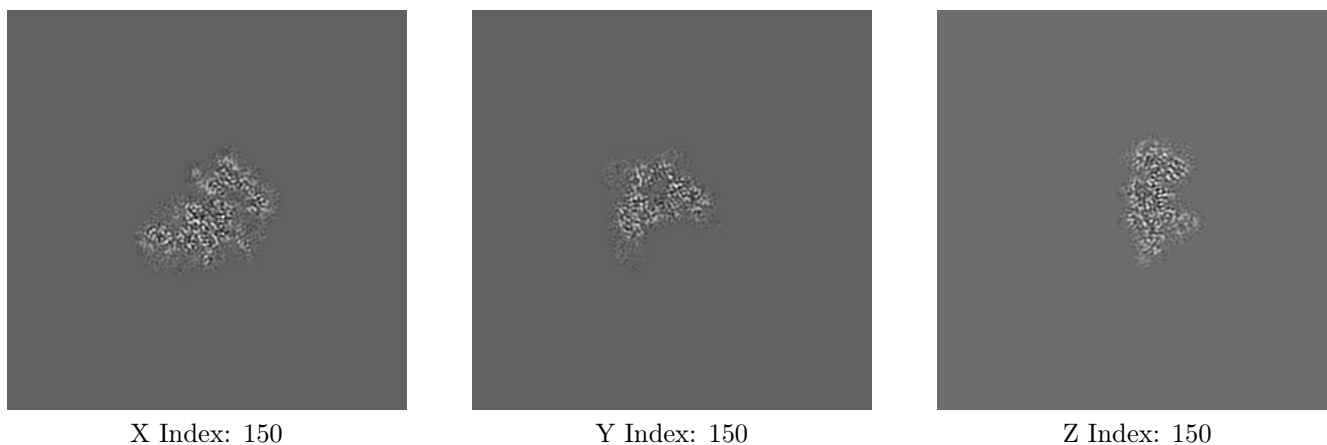
6.1.1 Primary map



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

6.2 Central slices [i](#)

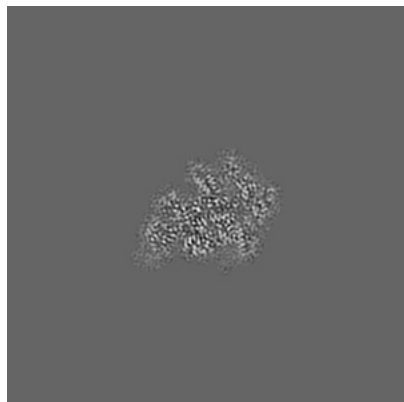
6.2.1 Primary map



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: 158



Y Index: 140

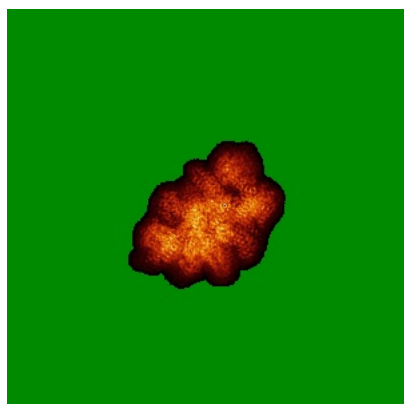


Z Index: 151

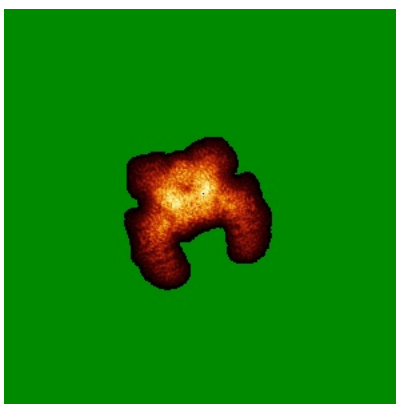
The images above show the largest variance slices of the map in three orthogonal directions.

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

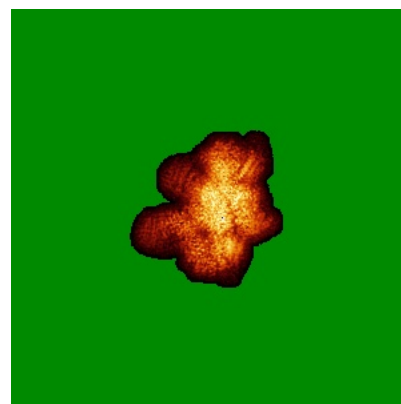
6.4.1 Primary map



X



Y

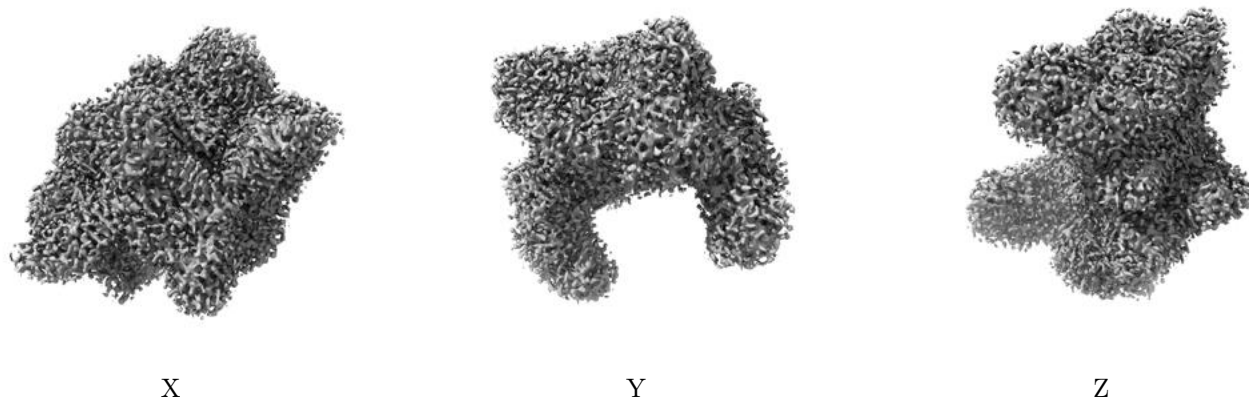


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

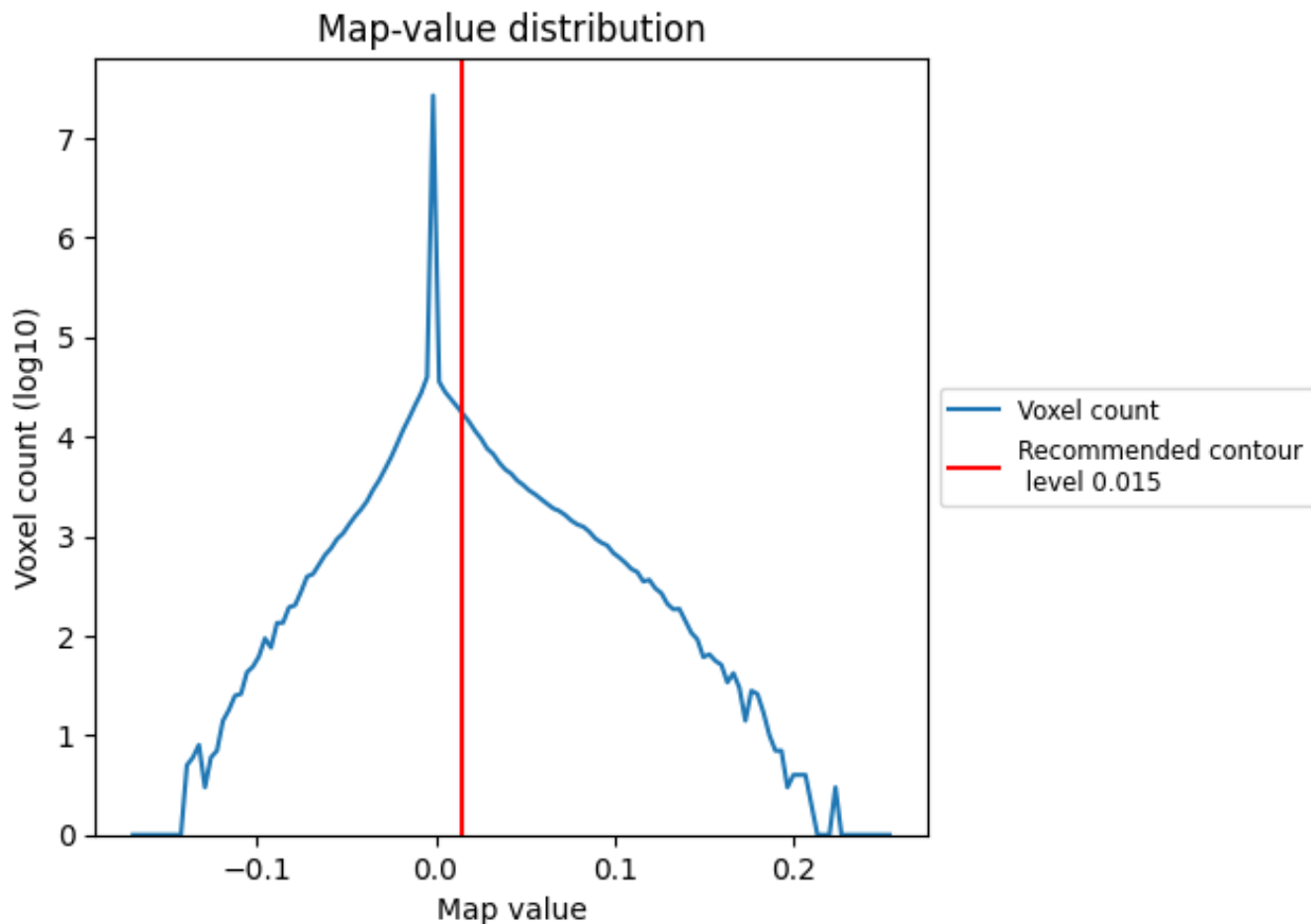
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

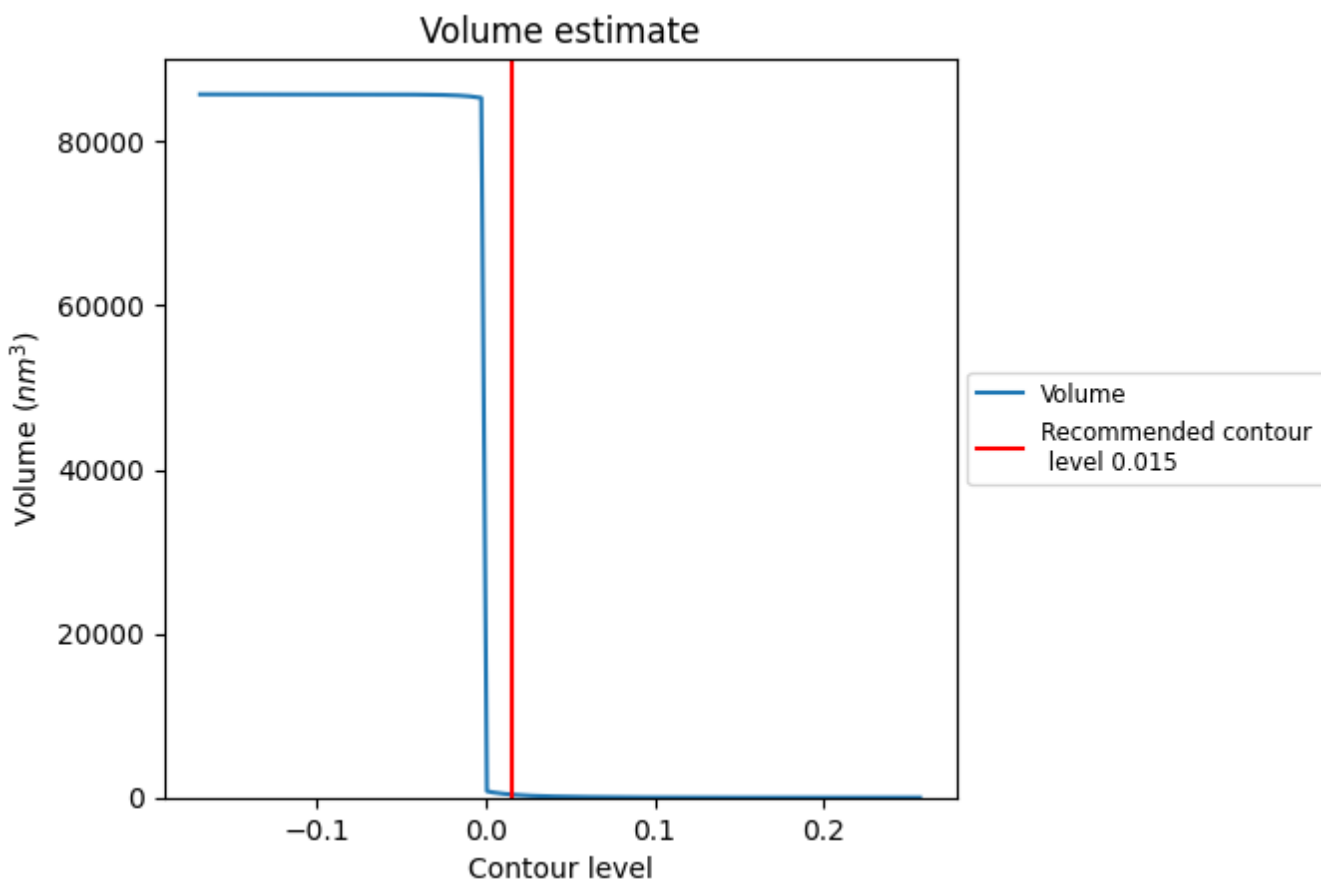
This section contains the results of statistical analysis of the map.

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.

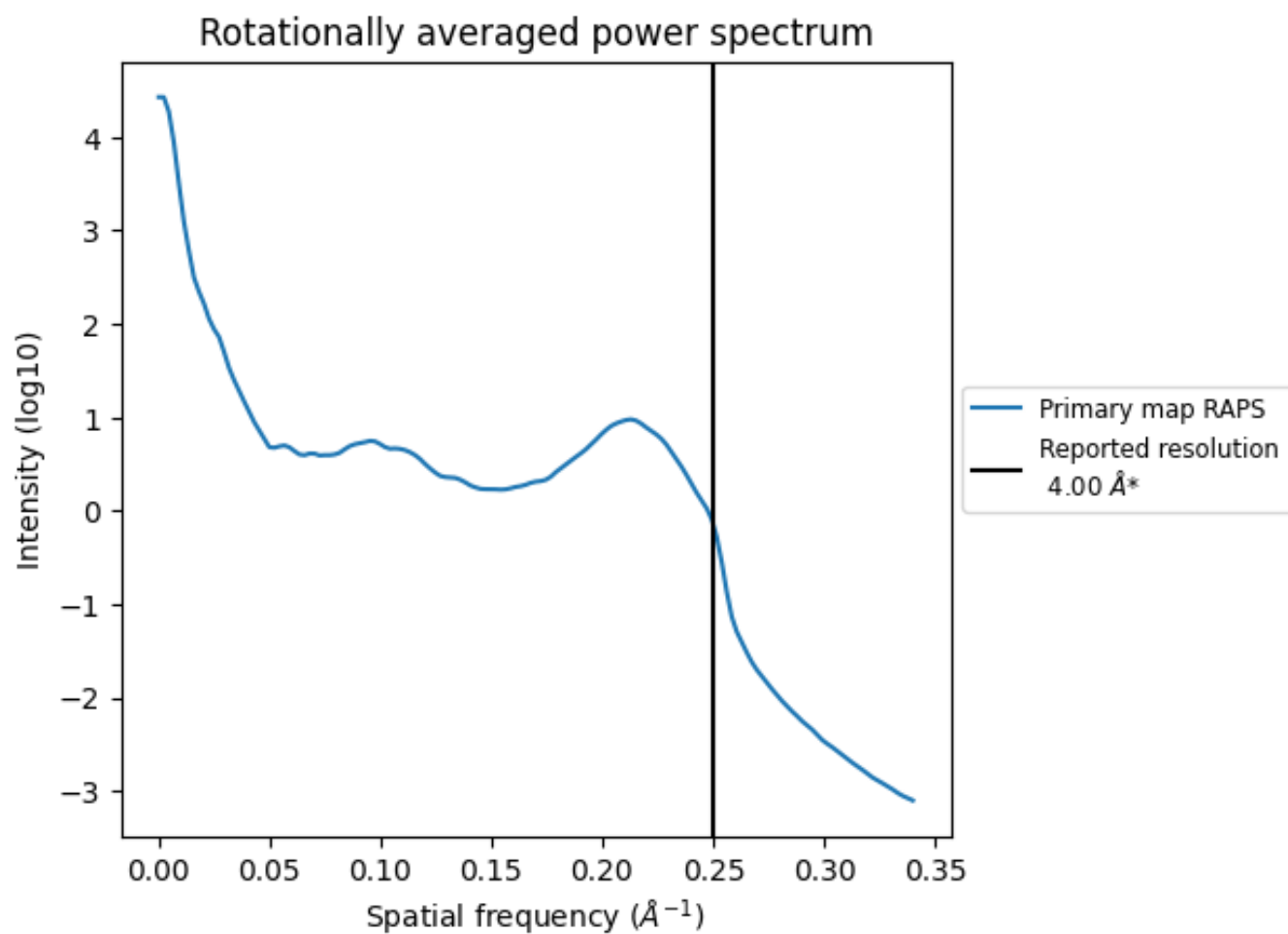
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 375 nm³; this corresponds to an approximate mass of 338 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 0.250 Å⁻¹

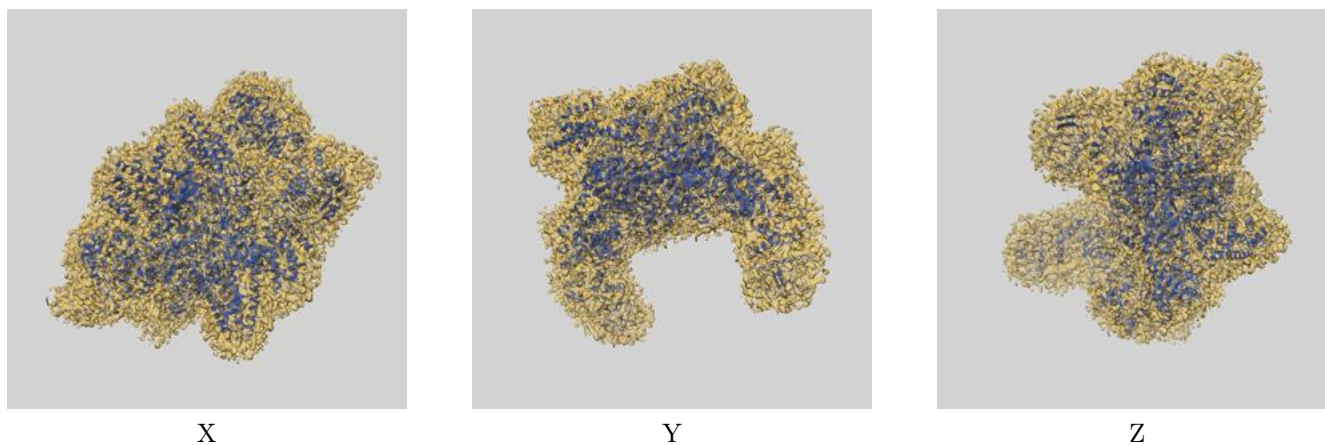
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

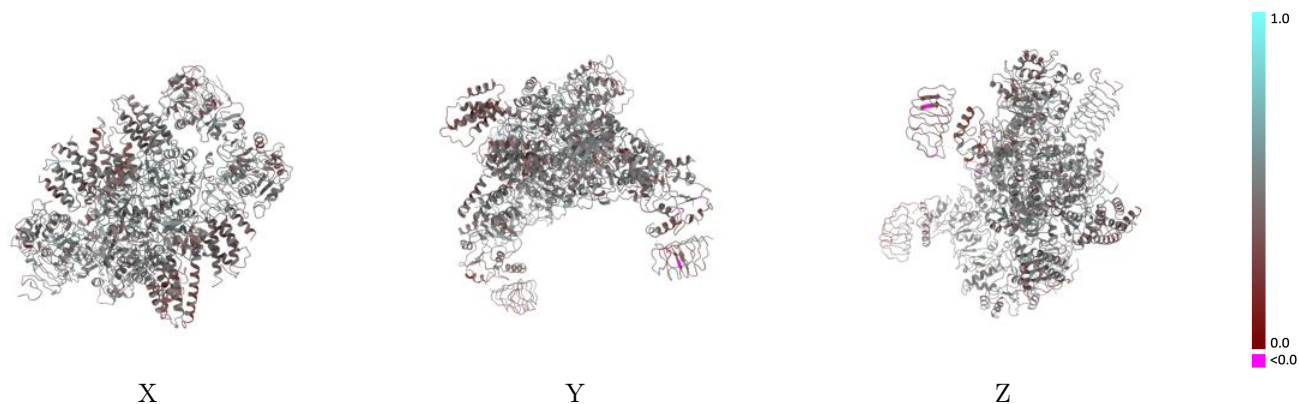
This section contains information regarding the fit between EMDB map EMD-30571 and PDB model 7D46. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



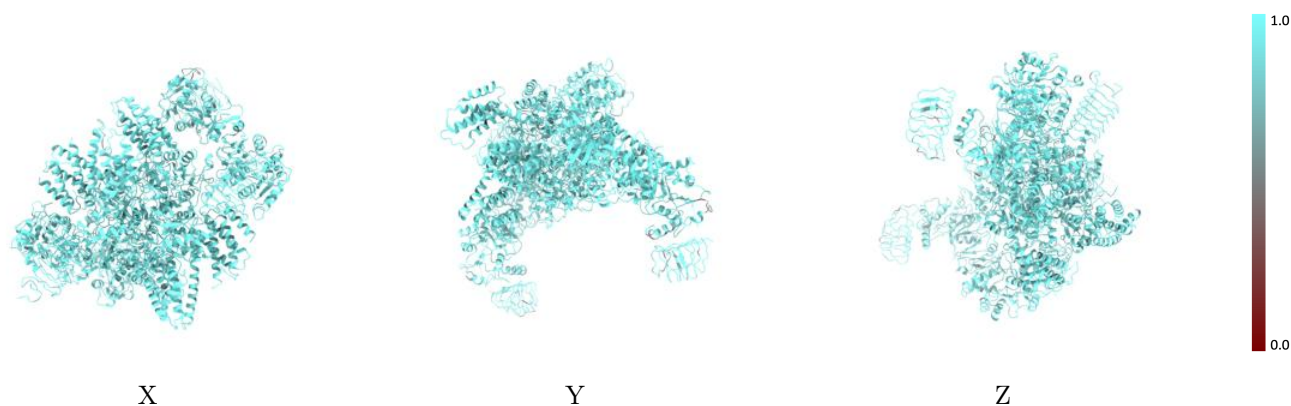
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



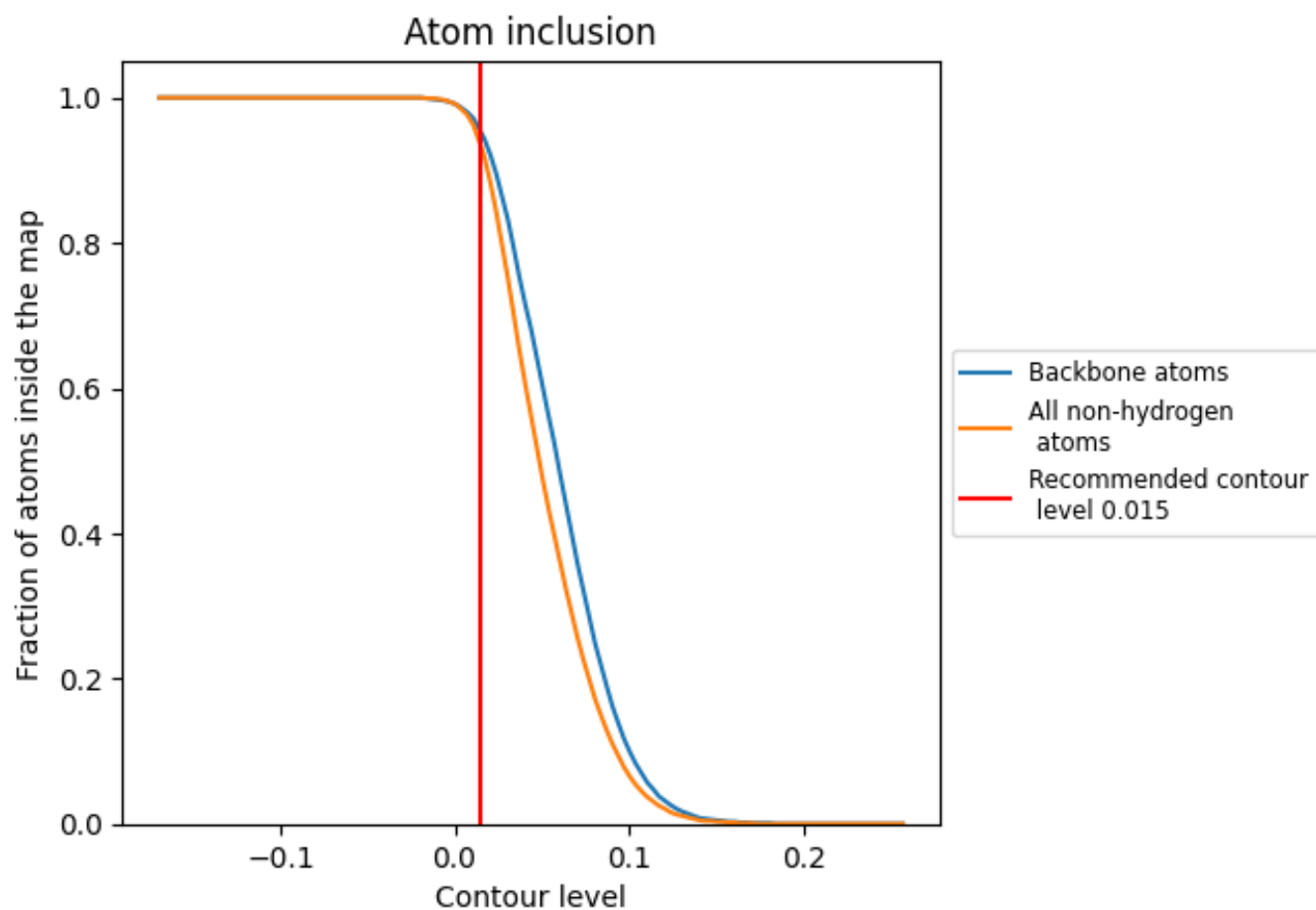
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).























9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.4610
A	 0.9390	 0.4590
B	 0.9350	 0.4420
C	 0.9360	 0.4660
D	 0.9310	 0.4730
E	 0.9150	 0.4180
F	 0.9030	 0.4220
G	 0.9470	 0.4850
H	 0.9430	 0.4840
I	 0.9440	 0.4670
J	 0.9430	 0.4780

