Full wwPDB EM Validation Report (i)

May 12, 2024 – 03:17 am BST

PDB ID	:	6TMJ
EMDB ID	:	EMD-10523
Title	:	Cryo-EM structure of Toxoplasma gondii mitochondrial ATP synthase dimer, rotor-stator model
Authors	:	Muhleip, A.; Kock Flygaard, R.; Amunts, A.
Deposited on	:	2019-12-04
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation 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:

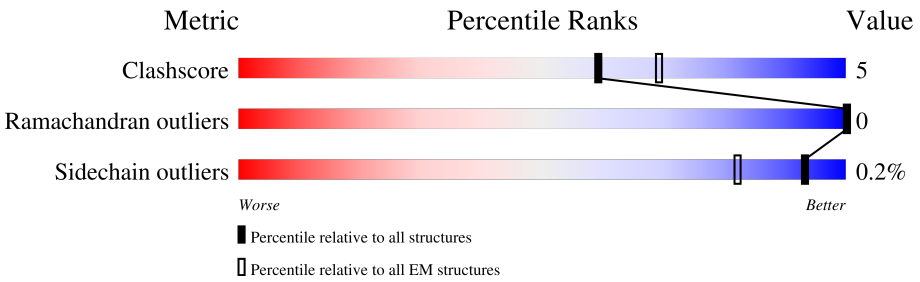
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.50 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 <=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	Q	134	• 9% 91%
2	K	224	12% 27% • 69%
3	g2	314	• 65% 35%
4	d2	183	12% 78% 22%
5	e2	73	15% 89% 11%
6	H2	166	• 39% • 57%
6	I2	166	• 40% • 57%
6	J2	166	• 40% • 57%

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Mol	Chain	Length	Quality of chain
6	K2	166	38% 5% 57%
6	L2	166	37% 6% 57%
6	M2	166	40% 57%
6	N2	166	40% 57%
6	O2	166	37% 5% 57%
6	P2	166	36% 7% 57%
6	Q2	166	39% 57%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18084 atoms, of which 9178 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 ATPTG11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	Q	12	190	66	94	13	17	0	0

- Molecule 2 is a protein called subunit a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	K	69	1159	404	577	81	91	6	0	0

- Molecule 3 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	g2	205	3233	1017	1622	284	299	11	0	0

- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	d2	143	2145	667	1076	181	216	5	0	0

- Molecule 5 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	e2	65	1077	337	539	99	98	4	0	0

- Molecule 6 is a protein called subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	H2	71	1028	328	527	77	92	4	0	0

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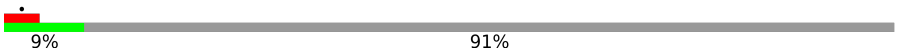
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	I2	71	1028	328	527	77	92	4	0	0
			Total	C	H	N	O	S		
6	J2	71	1028	328	527	77	92	4	0	0
			Total	C	H	N	O	S		
6	K2	71	1028	328	527	77	92	4	0	0
			Total	C	H	N	O	S		
6	M2	71	1028	328	527	77	92	4	0	0
			Total	C	H	N	O	S		
6	N2	71	1028	328	527	77	92	4	0	0
			Total	C	H	N	O	S		
6	O2	71	1028	328	527	77	92	4	0	0
			Total	C	H	N	O	S		
6	P2	71	1028	328	527	77	92	4	0	0
			Total	C	H	N	O	S		
6	Q2	71	1028	328	527	77	92	4	0	0
			Total	C	H	N	O	S		
6	L2	71	1028	328	527	77	92	4	0	0

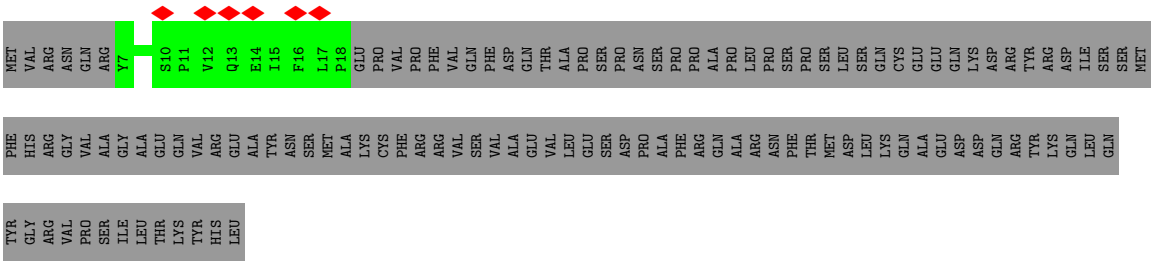
3 Residue-property plots (i)

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: ATPTG11

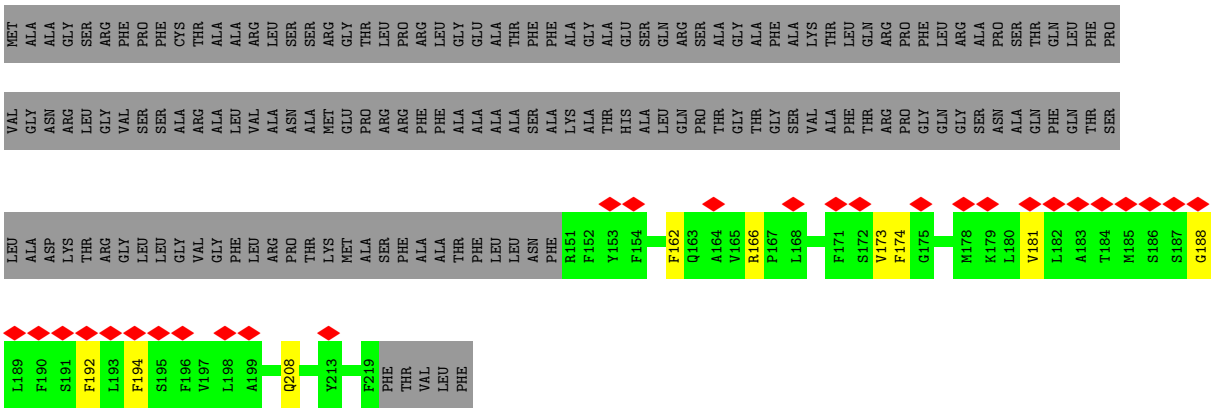
Chain Q:





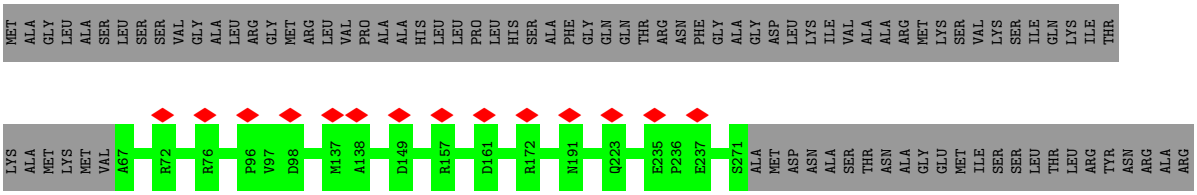
- Molecule 2: subunit a

Chain K:



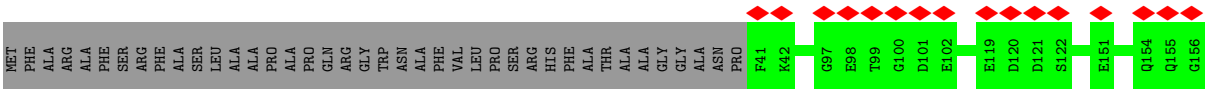
- Molecule 3: ATP synthase subunit gamma

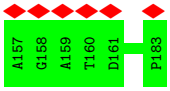
Chain g2:



• Molecule 4: ATP synthase subunit delta

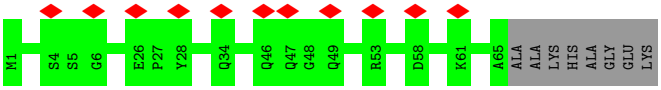
Chain d2:





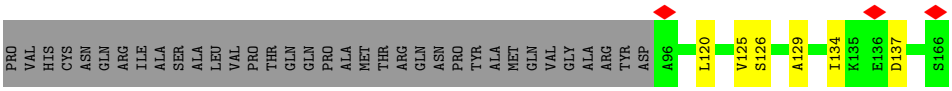
• Molecule 5: ATP synthase subunit epsilon

Chain e2:



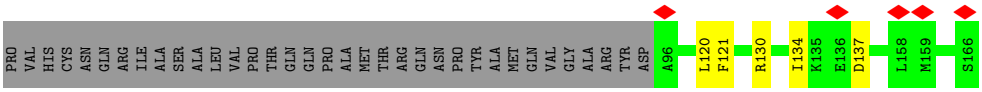
• Molecule 6: subunit c

Chain H2:



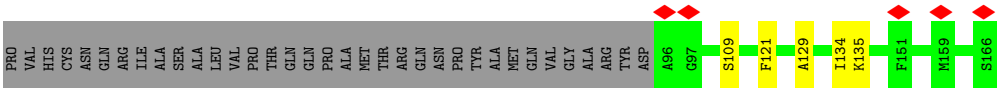
• Molecule 6: subunit c

Chain I2:



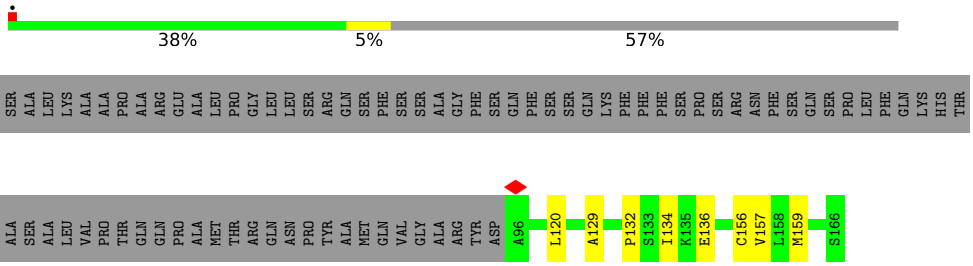
• Molecule 6: subunit c

Chain J2:



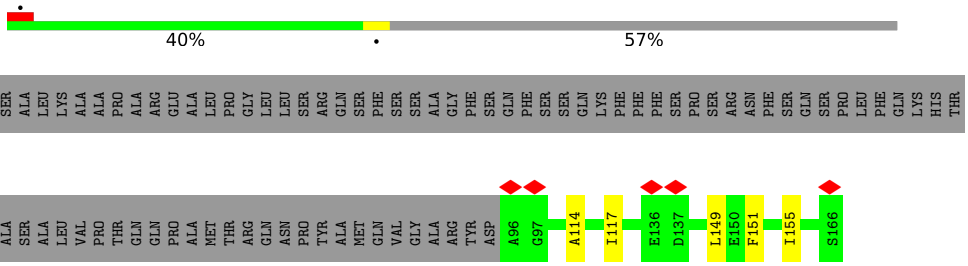
- Molecule 6: subunit c

Chain K2:



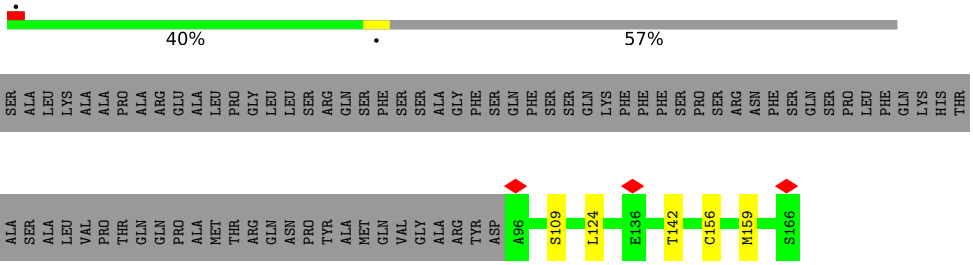
- Molecule 6: subunit c

Chain M2:



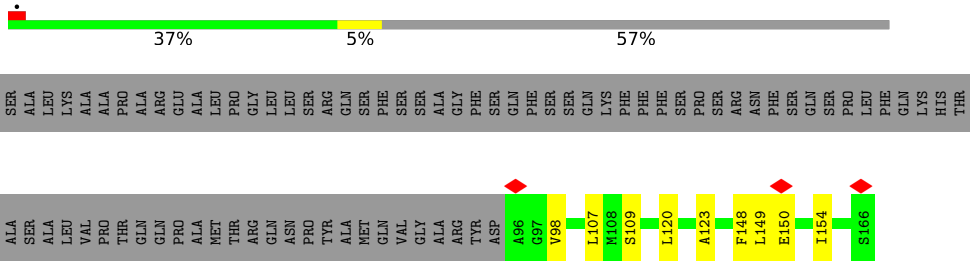
- Molecule 6: subunit c

Chain N2:



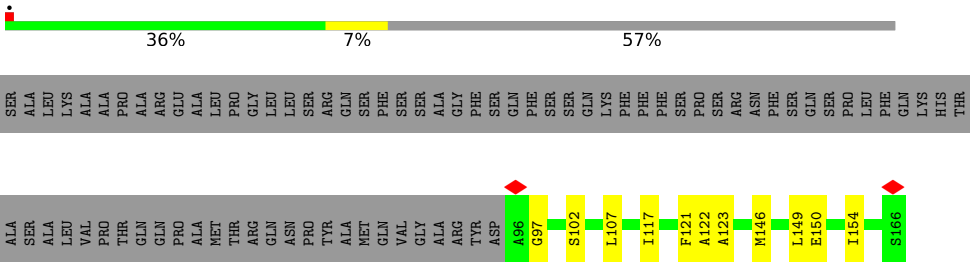
- Molecule 6: subunit c

Chain O2:



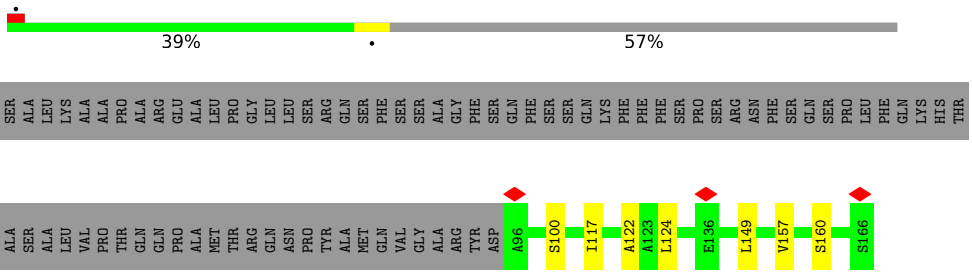
- Molecule 6: subunit c

Chain P2:



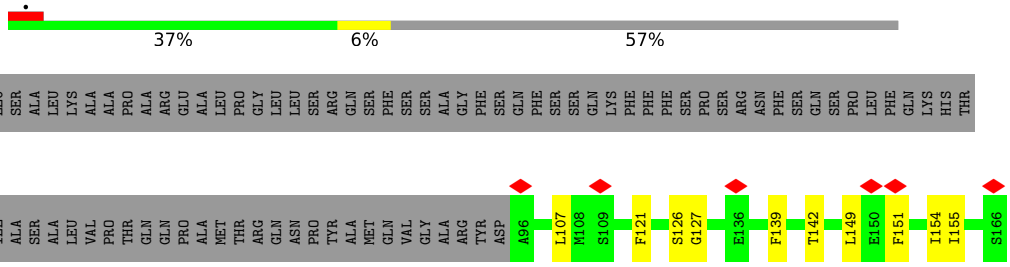
- Molecule 6: subunit c

Chain Q2:



- Molecule 6: subunit c

Chain L2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	203010	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.271	Depositor
Minimum map value	-0.172	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	Q	0.30	0/100	0.40	0/138
2	K	0.35	0/602	0.40	0/811
3	g2	0.37	0/1639	0.47	0/2213
4	d2	0.38	0/1083	0.50	0/1466
5	e2	0.33	0/547	0.47	0/733
6	H2	0.36	0/507	0.41	0/686
6	I2	0.39	0/507	0.49	0/686
6	J2	0.36	0/507	0.44	0/686
6	K2	0.37	0/507	0.44	0/686
6	L2	0.37	0/507	0.42	0/686
6	M2	0.38	0/507	0.44	0/686
6	N2	0.38	0/507	0.49	0/686
6	O2	0.36	0/507	0.43	0/686
6	P2	0.38	0/507	0.47	0/686
6	Q2	0.36	0/507	0.40	0/686
All	All	0.37	0/9041	0.45	0/12221

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	Q	96	94	93	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	582	577	576	8	0
3	g2	1611	1622	1621	0	0
4	d2	1069	1076	1076	0	0
5	e2	538	539	539	0	0
6	H2	501	527	527	4	0
6	I2	501	527	527	4	0
6	J2	501	527	527	6	0
6	K2	501	527	527	7	0
6	L2	501	527	527	7	0
6	M2	501	527	527	3	0
6	N2	501	527	527	3	0
6	O2	501	527	527	10	0
6	P2	501	527	527	10	0
6	Q2	501	527	527	5	0
All	All	8906	9178	9175	44	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 5.

All (44) 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)
6:N2:109:SER:OG	6:O2:107:LEU:O	2.05	0.73
6:J2:134:ILE:HD13	6:K2:132:PRO:HG3	1.69	0.73
6:O2:109:SER:OG	6:P2:107:LEU:O	2.06	0.72
6:I2:137:ASP:OD2	6:J2:135:LYS:NZ	2.25	0.69
6:J2:134:ILE:HD11	6:K2:129:ALA:HA	1.78	0.66
6:L2:139:PHE:O	6:L2:142:THR:OG1	2.14	0.64
6:K2:134:ILE:HG22	6:K2:134:ILE:O	2.00	0.61
2:K:188:GLY:O	2:K:192:PHE:N	2.38	0.56
2:K:162:PHE:CD2	6:P2:154:ILE:HD11	2.41	0.55
6:N2:159:MET:HG2	6:O2:107:LEU:HD11	1.87	0.55
6:Q2:117:ILE:HG13	6:Q2:149:LEU:HD13	1.89	0.55
6:M2:114:ALA:HB1	6:L2:149:LEU:CD2	2.36	0.55
2:K:174:PHE:CZ	6:O2:154:ILE:HD13	2.44	0.52
6:P2:102:SER:OG	6:Q2:100:SER:O	2.25	0.51
6:K2:120:LEU:HD21	6:L2:121:PHE:HB3	1.91	0.51
6:P2:117:ILE:HG13	6:P2:149:LEU:HD23	1.93	0.51
6:O2:98:VAL:HG11	6:P2:97:GLY:O	2.10	0.51
6:O2:123:ALA:HB2	6:P2:122:ALA:HB1	1.93	0.50
6:L2:151:PHE:O	6:L2:155:ILE:HD12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M2:151:PHE:O	6:M2:155:ILE:HG23	2.13	0.48
6:H2:134:ILE:HD11	6:H2:137:ASP:OD2	2.15	0.47
2:K:166:ARG:NH2	6:P2:150:GLU:OE2	2.39	0.46
6:L2:154:ILE:HG13	6:L2:155:ILE:N	2.29	0.46
6:O2:120:LEU:HD21	6:P2:121:PHE:HB2	1.98	0.46
6:J2:109:SER:O	6:J2:109:SER:OG	2.28	0.46
2:K:166:ARG:HD3	2:K:208:GLN:OE1	2.17	0.45
2:K:174:PHE:CZ	6:O2:154:ILE:HG21	2.50	0.45
2:K:173:VAL:HG23	2:K:174:PHE:HD2	1.81	0.45
6:O2:148:PHE:CE1	6:P2:146:MET:SD	3.10	0.45
6:H2:120:LEU:HD21	6:I2:121:PHE:HB2	1.99	0.45
6:N2:124:LEU:HD12	6:N2:142:THR:OG1	2.18	0.44
6:K2:156:CYS:SG	6:K2:157:VAL:N	2.91	0.44
2:K:181:VAL:HG11	2:K:194:PHE:CE2	2.53	0.43
6:K2:136:GLU:OE2	6:K2:136:GLU:N	2.42	0.42
6:H2:125:VAL:HG11	6:Q2:124:LEU:HA	2.00	0.42
6:I2:120:LEU:HD21	6:J2:121:PHE:CB	2.51	0.41
6:Q2:157:VAL:O	6:Q2:160:SER:HB3	2.20	0.41
6:I2:134:ILE:HD11	6:J2:129:ALA:HA	2.03	0.41
6:M2:117:ILE:HG13	6:M2:149:LEU:HD13	2.01	0.41
6:L2:126:SER:OG	6:L2:127:GLY:N	2.54	0.41
6:H2:126:SER:O	6:H2:129:ALA:N	2.54	0.41
6:K2:159:MET:HG3	6:L2:107:LEU:HD11	2.03	0.41
6:O2:149:LEU:O	6:O2:150:GLU:C	2.59	0.41
6:P2:123:ALA:HB2	6:Q2:122:ALA:HB1	2.03	0.40

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	Q	10/134 (8%)	10 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	67/224 (30%)	64 (96%)	3 (4%)	0	100	100
3	g2	203/314 (65%)	187 (92%)	16 (8%)	0	100	100
4	d2	141/183 (77%)	129 (92%)	12 (8%)	0	100	100
5	e2	63/73 (86%)	57 (90%)	6 (10%)	0	100	100
6	H2	69/166 (42%)	61 (88%)	8 (12%)	0	100	100
6	I2	69/166 (42%)	61 (88%)	8 (12%)	0	100	100
6	J2	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
6	K2	69/166 (42%)	58 (84%)	11 (16%)	0	100	100
6	L2	69/166 (42%)	62 (90%)	7 (10%)	0	100	100
6	M2	69/166 (42%)	61 (88%)	8 (12%)	0	100	100
6	N2	69/166 (42%)	67 (97%)	2 (3%)	0	100	100
6	O2	69/166 (42%)	62 (90%)	7 (10%)	0	100	100
6	P2	69/166 (42%)	64 (93%)	5 (7%)	0	100	100
6	Q2	69/166 (42%)	65 (94%)	4 (6%)	0	100	100
All	All	1174/2588 (45%)	1072 (91%)	102 (9%)	0	100	100

There are no Ramachandran outliers to report.

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	Q	11/120 (9%)	11 (100%)	0	100	100
2	K	62/175 (35%)	62 (100%)	0	100	100
3	g2	173/257 (67%)	173 (100%)	0	100	100
4	d2	118/144 (82%)	118 (100%)	0	100	100
5	e2	57/61 (93%)	57 (100%)	0	100	100
6	H2	52/133 (39%)	52 (100%)	0	100	100
6	I2	52/133 (39%)	51 (98%)	1 (2%)	57	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J2	52/133 (39%)	52 (100%)	0	100	100
6	K2	52/133 (39%)	52 (100%)	0	100	100
6	L2	52/133 (39%)	52 (100%)	0	100	100
6	M2	52/133 (39%)	52 (100%)	0	100	100
6	N2	52/133 (39%)	51 (98%)	1 (2%)	57	80
6	O2	52/133 (39%)	52 (100%)	0	100	100
6	P2	52/133 (39%)	52 (100%)	0	100	100
6	Q2	52/133 (39%)	52 (100%)	0	100	100
All	All	941/2087 (45%)	939 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	I2	130	ARG
6	N2	156	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	g2	246	GLN
5	e2	57	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 (i)

There are no chain breaks in this entry.

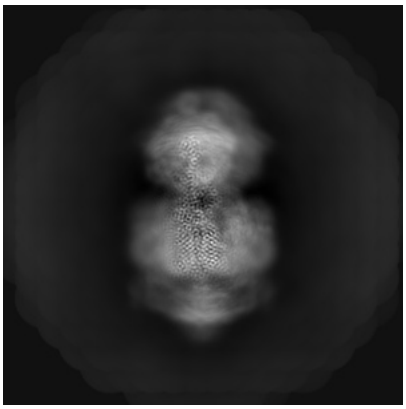
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10523. These allow visual inspection of the internal detail of the map and identification of artifacts.

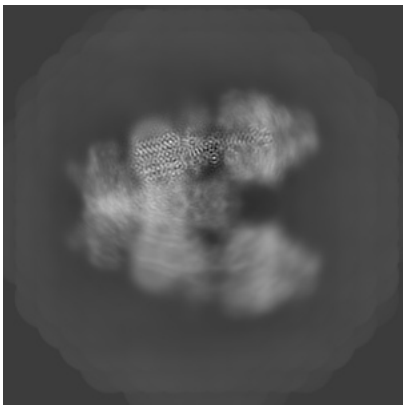
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

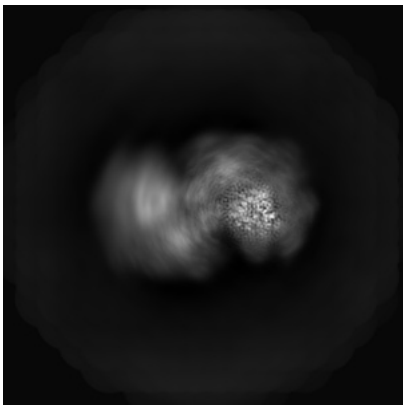
6.1.1 Primary map



X

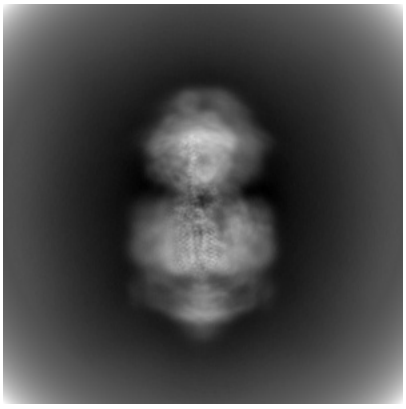


Y

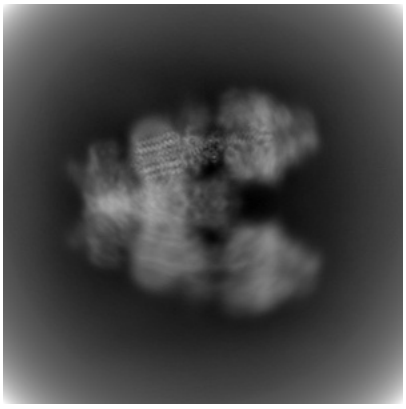


Z

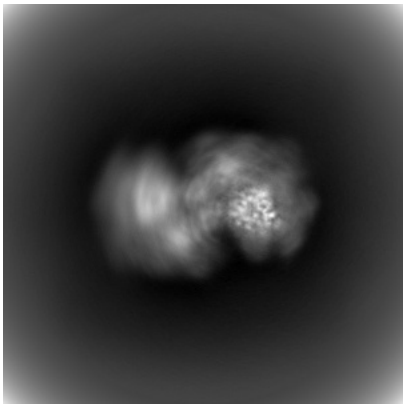
6.1.2 Raw map



X



Y

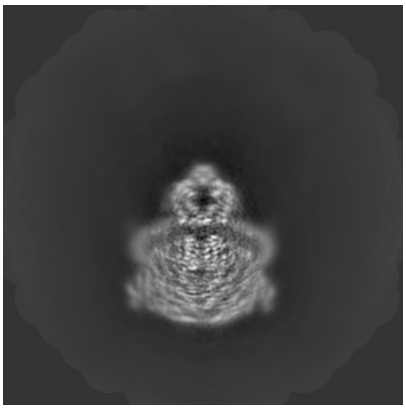


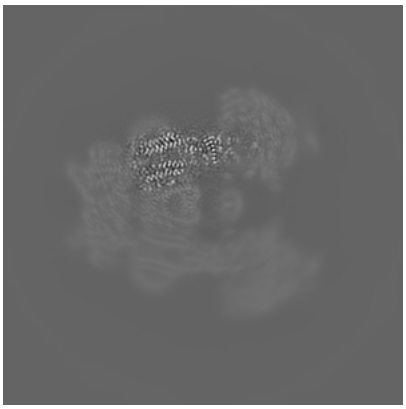
Z

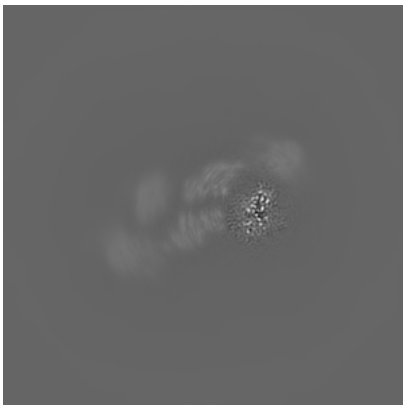
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

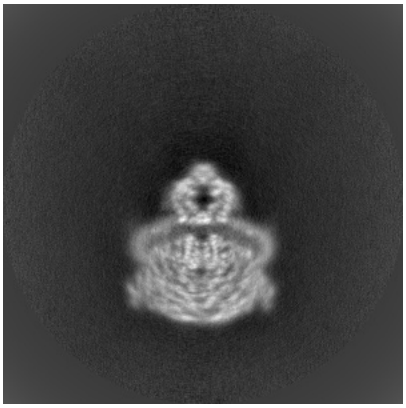
6.2.1 Primary map

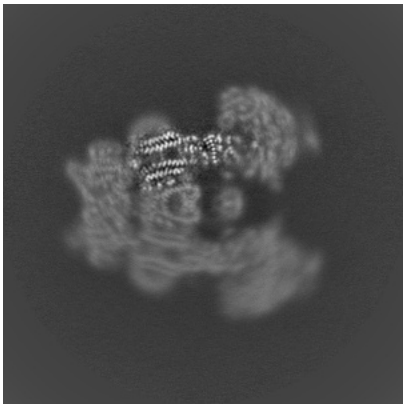

X Index: 280

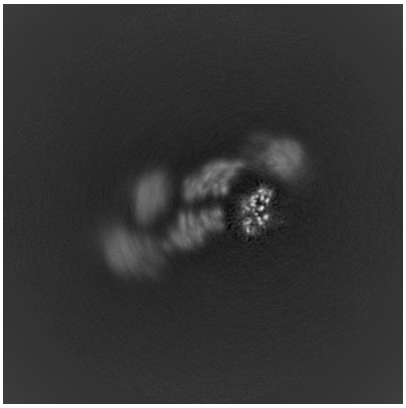

Y Index: 280


Z Index: 280

6.2.2 Raw map


X Index: 280


Y Index: 280

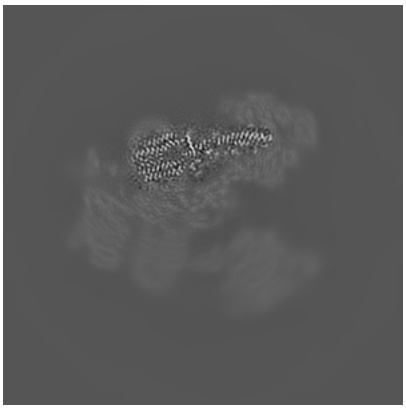

Z Index: 280

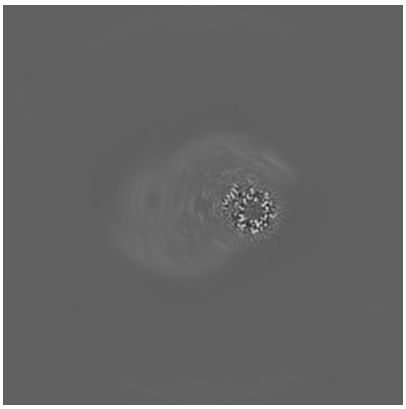
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

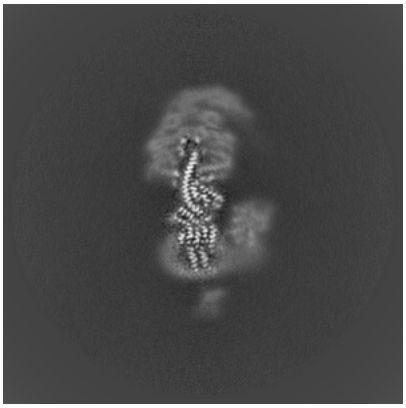
6.3.1 Primary map

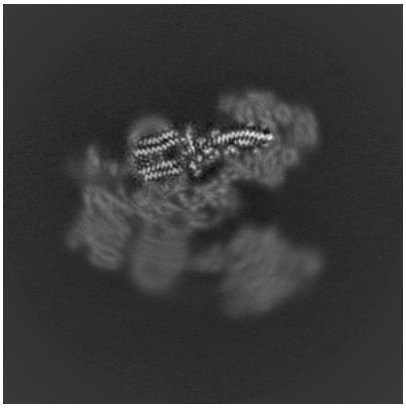
X Index: 357

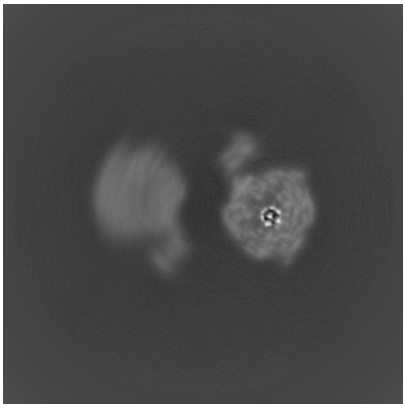

Y Index: 263


Z Index: 235

6.3.2 Raw map


X Index: 367

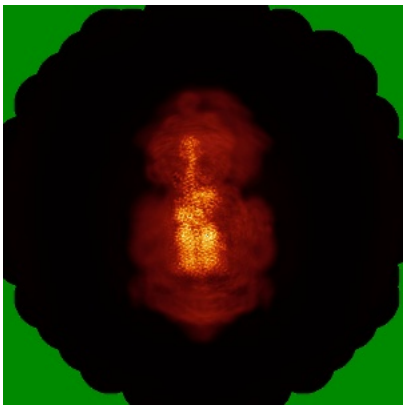

Y Index: 264

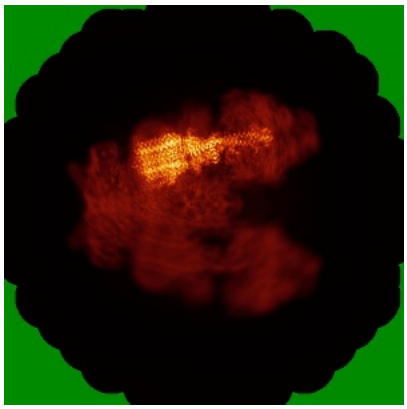

Z Index: 367

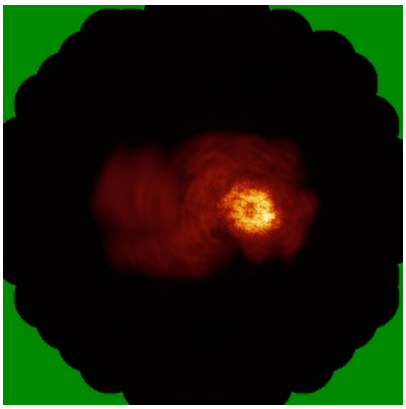
The images above show the largest variance slices of the map in three orthogonal directions.

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

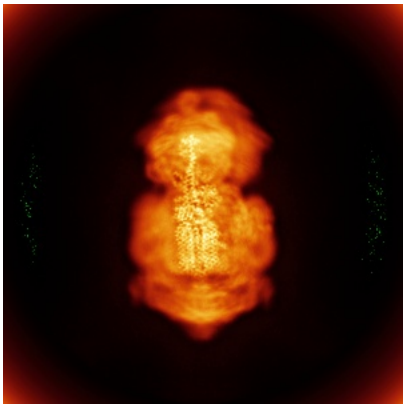
6.4.1 Primary map

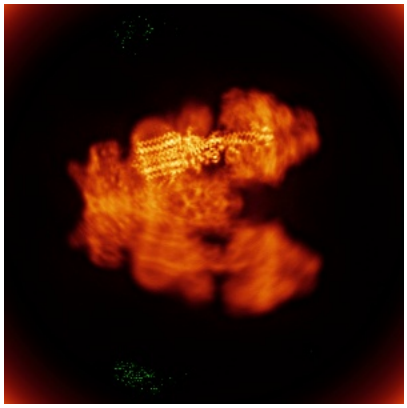

X

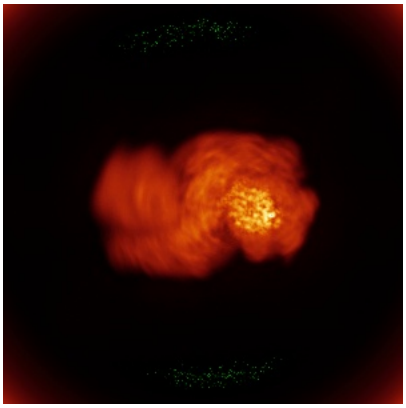

Y


Z

6.4.2 Raw map


X

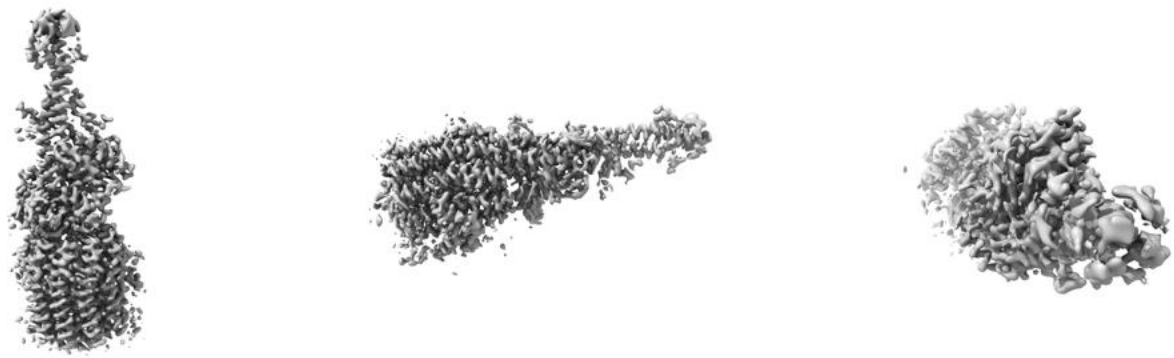

Y


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 0.06. 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.

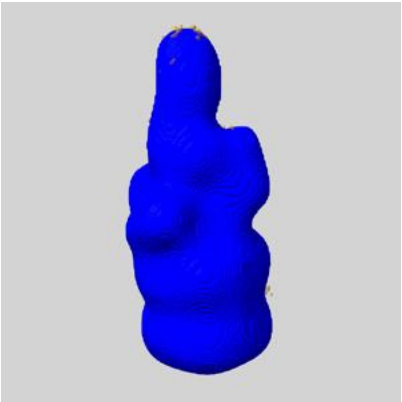
6.6 Mask visualisation (i)

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

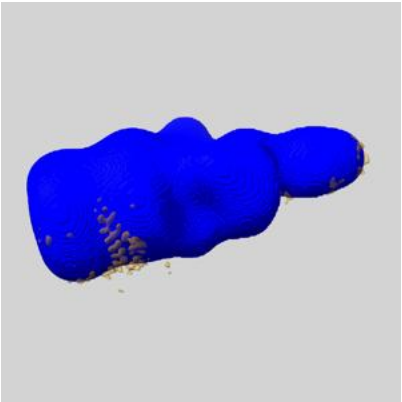
A mask typically either:

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

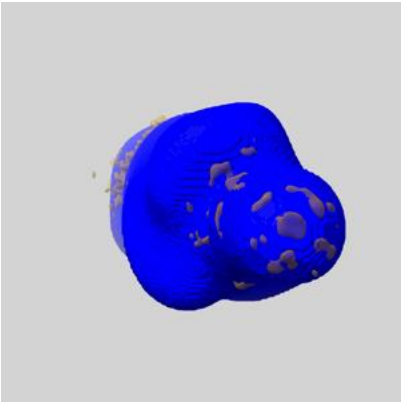
6.6.1 emd_10523_msk_1.map (i)



X



Y

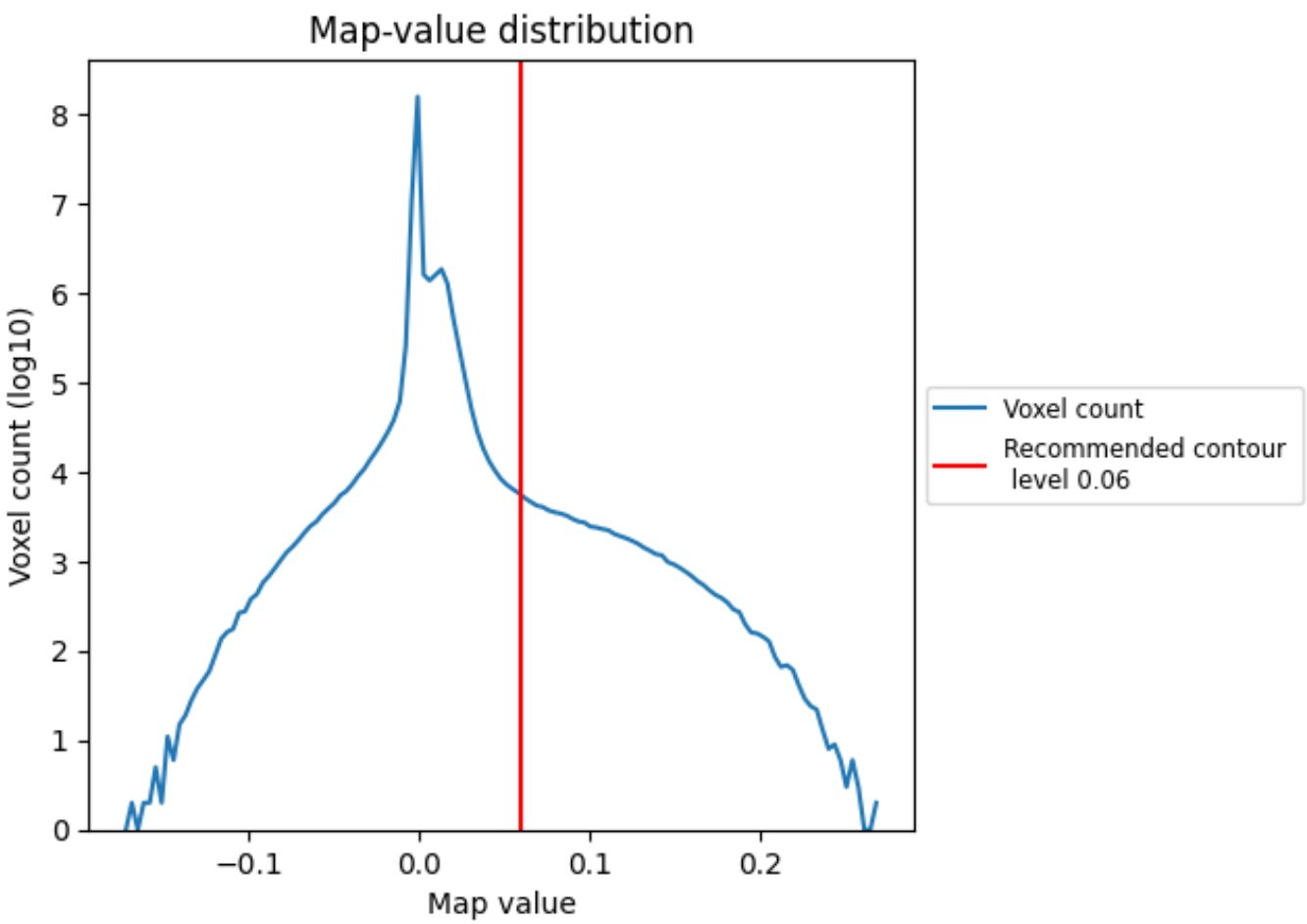


Z

7 Map analysis (i)

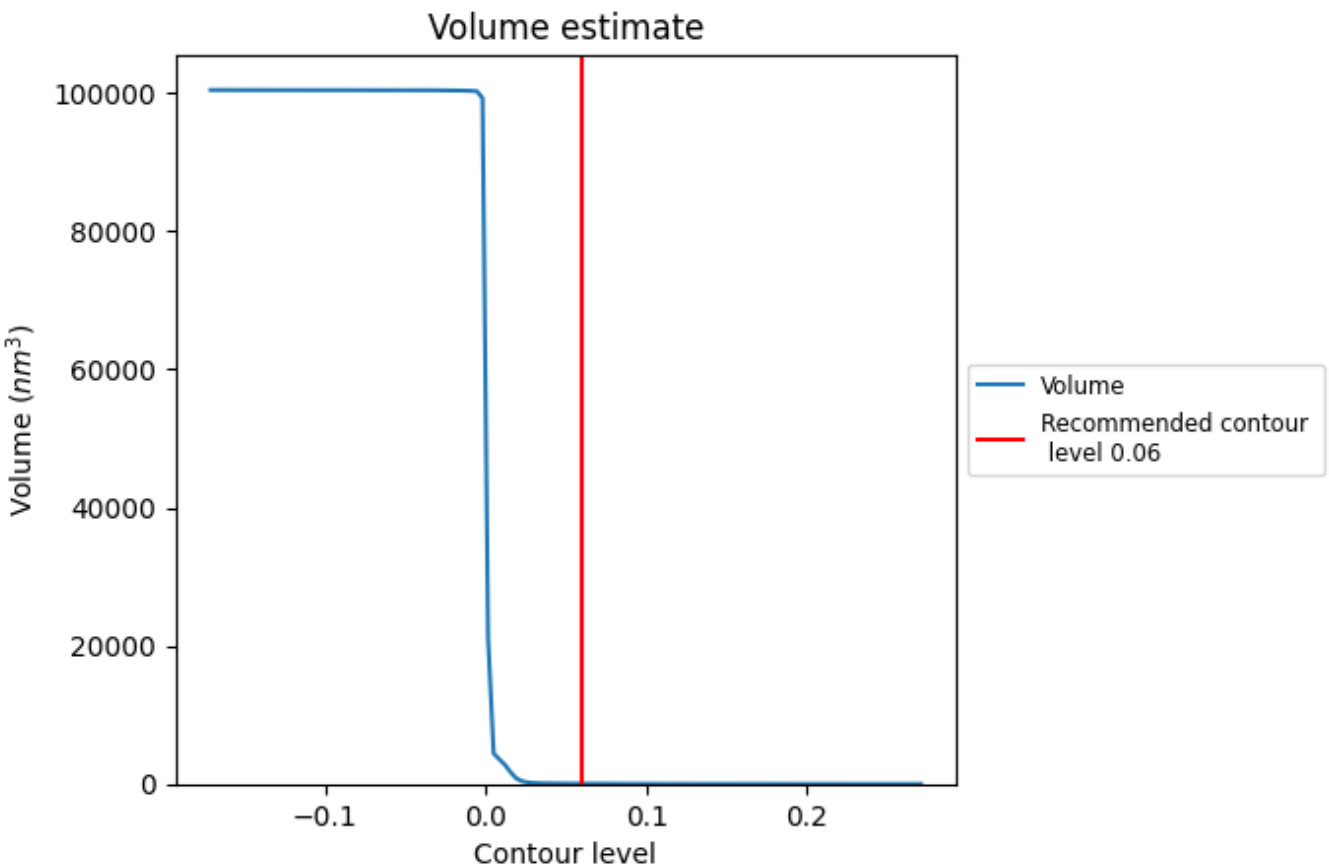
This section contains the results of statistical analysis of the map.

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.

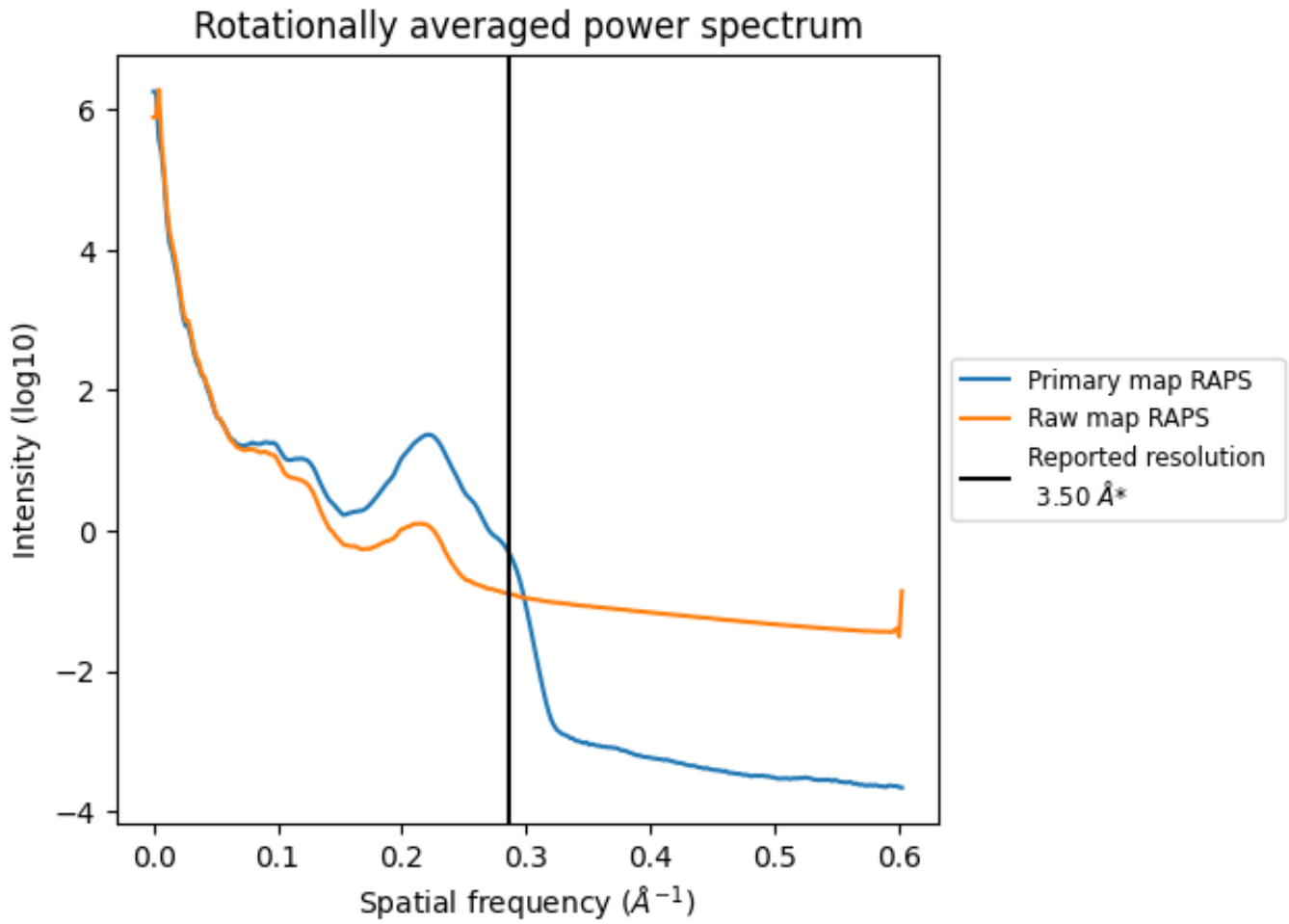
7.2 Volume estimate (i)



The volume at the recommended contour level is 43 nm^3; this corresponds to an approximate mass of 39 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)

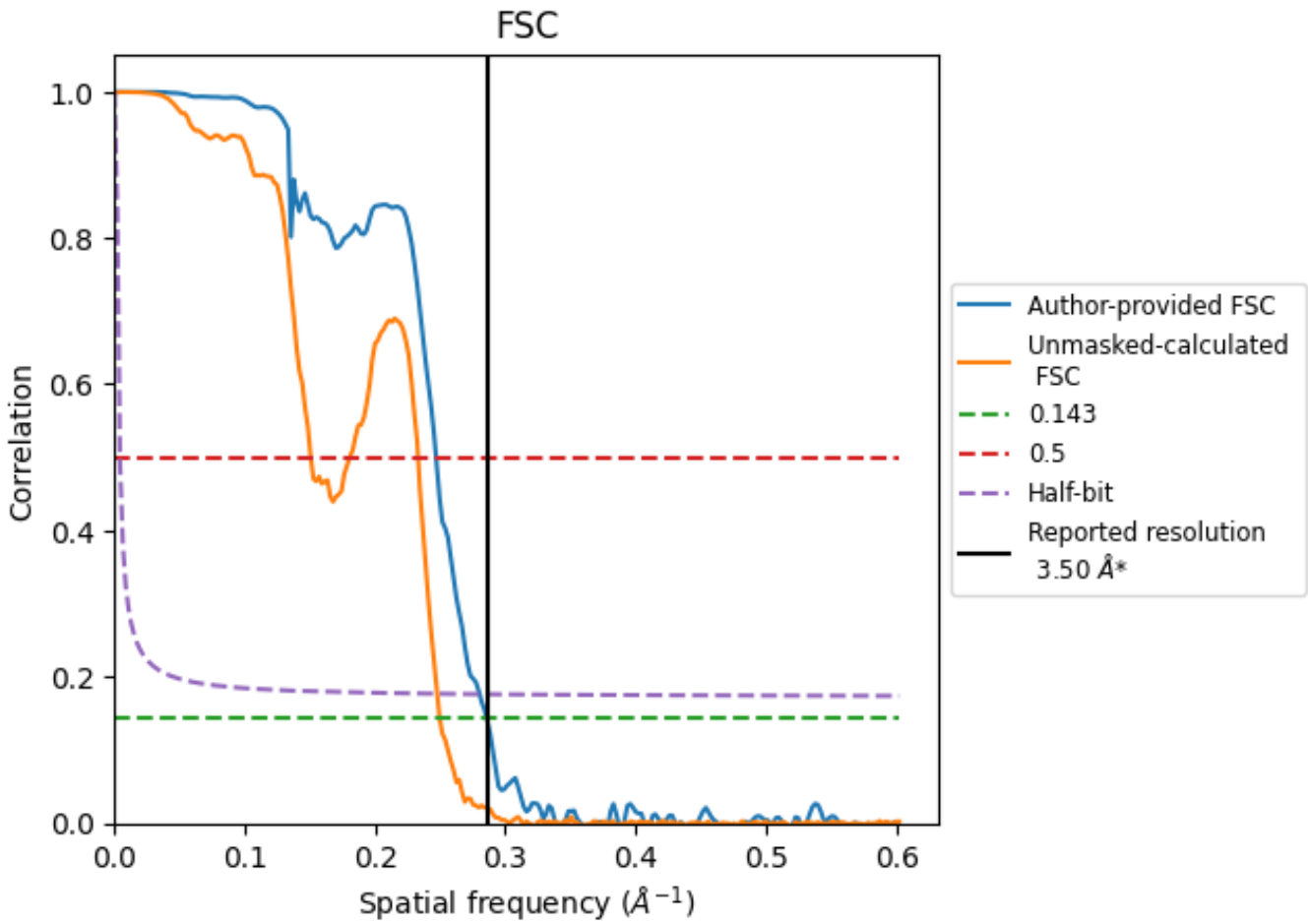


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

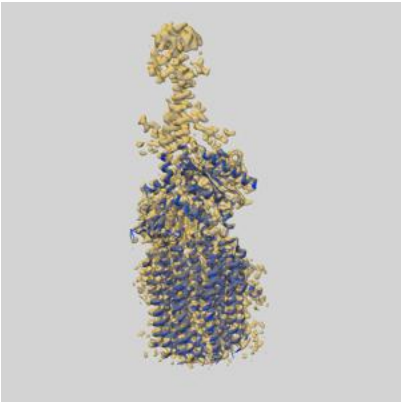
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.05	3.57
Unmasked-calculated*	4.01	6.64	4.04

*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 4.01 differs from the reported value 3.5 by more than 10 %

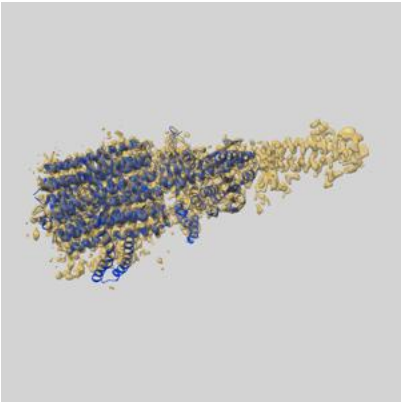
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10523 and PDB model 6TMJ. Per-residue inclusion information can be found in section 3 on page 6.

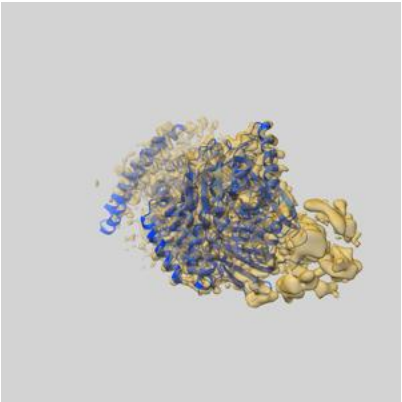
9.1 Map-model overlay (i)



X



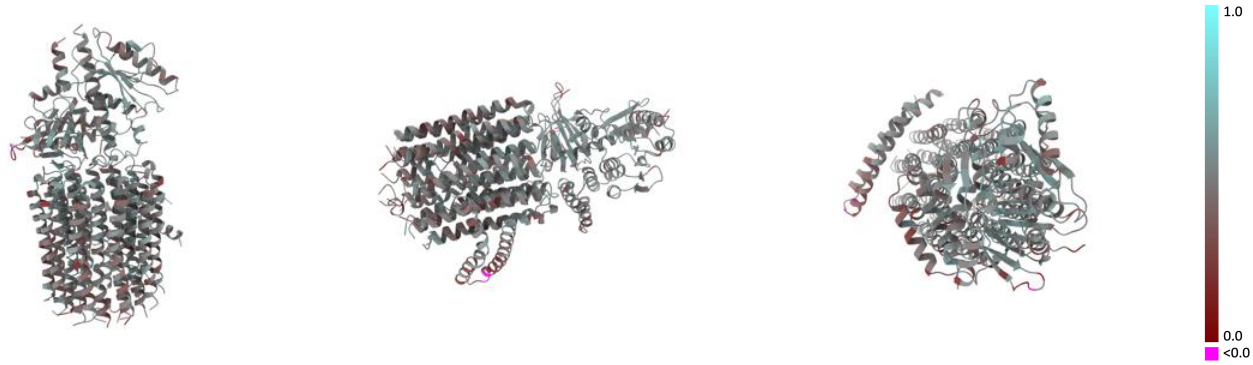
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

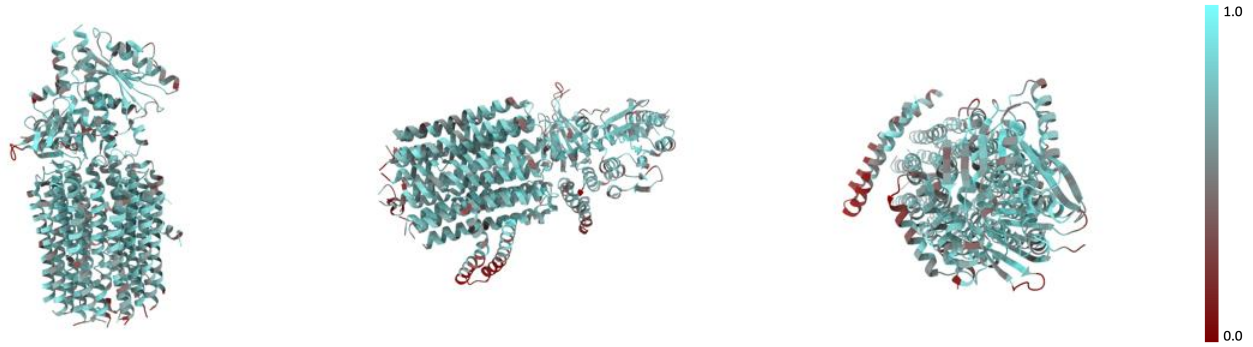
9.2 Q-score mapped to coordinate model (i)



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.

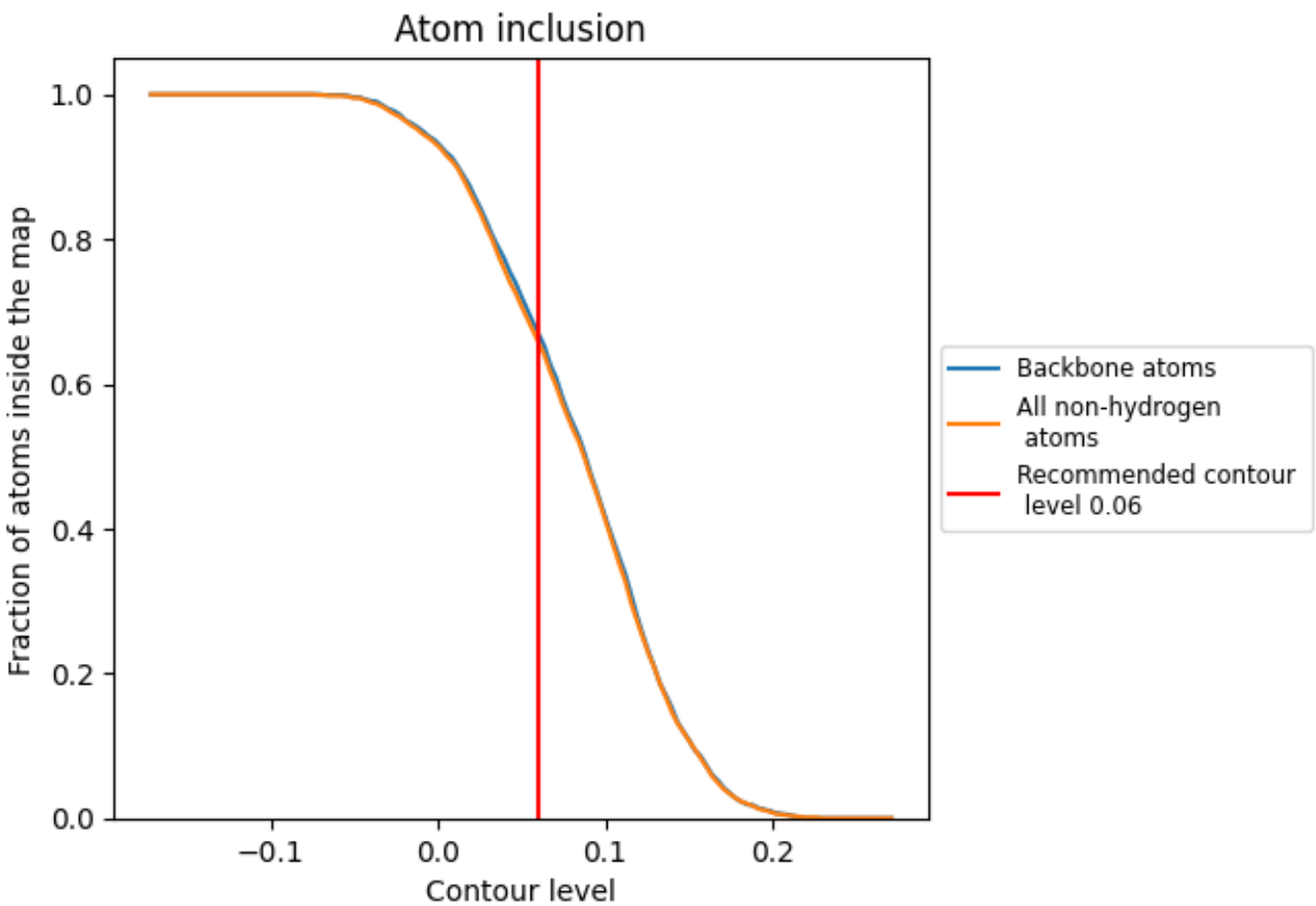
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 66% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6580	0.4730
H2	0.7020	0.4810
I2	0.6800	0.4580
J2	0.6760	0.4570
K	0.4590	0.4080
K2	0.7000	0.4750
L2	0.6960	0.4620
M2	0.7000	0.4690
N2	0.7100	0.4700
O2	0.7000	0.4830
P2	0.7180	0.4700
Q	0.4210	0.4280
Q2	0.6880	0.4810
d2	0.6210	0.4700
e2	0.6260	0.4900
g2	0.6820	0.5010