



Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 04:19 am GMT

PDB ID : 6YKR
EMDB ID : EMD-10830
Title : Structure of a protonation mimic of unplugged C. jejuni MotAB
Authors : Santiveri, M.; Roa-Eguiara, A.; Taylor, N.M.I.
Deposited on : 2020-04-06
Resolution : 3.00 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 ⓘ 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

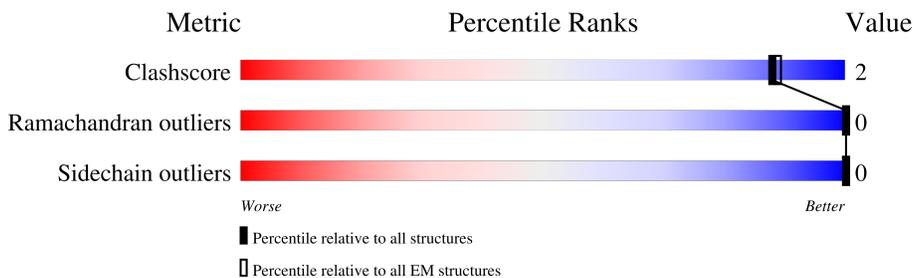
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	258	
1	B	258	
1	C	258	
1	D	258	
1	E	258	
2	F	271	
2	G	271	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 10189 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 Chemotaxis protein MotA, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	255	1954	1260	318	362	14	0	0
1	B	255	1954	1260	318	362	14	0	0
1	C	255	1954	1260	318	362	14	0	0
1	D	255	1954	1260	318	362	14	0	0
1	E	255	1954	1260	318	362	14	0	0

- Molecule 2 is a protein called Chemotaxis protein MotB, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	F	25	203	144	30	29	0	0
2	G	26	210	148	31	31	0	0

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	22	ASN	ASP	engineered mutation	UNP A0A0H3PBX6
F	?	-	ASN	deletion	UNP A0A0H3PBX6
F	?	-	PRO	deletion	UNP A0A0H3PBX6
F	?	-	ALA	deletion	UNP A0A0H3PBX6
F	?	-	LYS	deletion	UNP A0A0H3PBX6
F	?	-	VAL	deletion	UNP A0A0H3PBX6
F	?	-	GLU	deletion	UNP A0A0H3PBX6
F	?	-	ALA	deletion	UNP A0A0H3PBX6
F	?	-	LEU	deletion	UNP A0A0H3PBX6
F	?	-	LYS	deletion	UNP A0A0H3PBX6
F	?	-	THR	deletion	UNP A0A0H3PBX6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLU	deletion	UNP A0A0H3PBX6
F	?	-	PHE	deletion	UNP A0A0H3PBX6
F	?	-	VAL	deletion	UNP A0A0H3PBX6
F	?	-	LYS	deletion	UNP A0A0H3PBX6
F	?	-	ILE	deletion	UNP A0A0H3PBX6
F	?	-	PHE	deletion	UNP A0A0H3PBX6
F	?	-	ASP	deletion	UNP A0A0H3PBX6
F	?	-	TYR	deletion	UNP A0A0H3PBX6
F	?	-	THR	deletion	UNP A0A0H3PBX6
F	?	-	SER	deletion	UNP A0A0H3PBX6
F	228	GLY	-	expression tag	UNP A0A0H3PBX6
F	229	THR	-	expression tag	UNP A0A0H3PBX6
F	230	LEU	-	expression tag	UNP A0A0H3PBX6
F	231	GLU	-	expression tag	UNP A0A0H3PBX6
F	232	VAL	-	expression tag	UNP A0A0H3PBX6
F	233	LEU	-	expression tag	UNP A0A0H3PBX6
F	234	PHE	-	expression tag	UNP A0A0H3PBX6
F	235	GLN	-	expression tag	UNP A0A0H3PBX6
F	236	GLY	-	expression tag	UNP A0A0H3PBX6
F	237	PRO	-	expression tag	UNP A0A0H3PBX6
F	238	GLY	-	expression tag	UNP A0A0H3PBX6
F	239	GLY	-	expression tag	UNP A0A0H3PBX6
F	240	SER	-	expression tag	UNP A0A0H3PBX6
F	241	GLY	-	expression tag	UNP A0A0H3PBX6
F	242	SER	-	expression tag	UNP A0A0H3PBX6
F	243	ALA	-	expression tag	UNP A0A0H3PBX6
F	244	TRP	-	expression tag	UNP A0A0H3PBX6
F	245	SER	-	expression tag	UNP A0A0H3PBX6
F	246	HIS	-	expression tag	UNP A0A0H3PBX6
F	247	PRO	-	expression tag	UNP A0A0H3PBX6
F	248	GLN	-	expression tag	UNP A0A0H3PBX6
F	249	PHE	-	expression tag	UNP A0A0H3PBX6
F	250	GLU	-	expression tag	UNP A0A0H3PBX6
F	251	LYS	-	expression tag	UNP A0A0H3PBX6
F	252	GLY	-	expression tag	UNP A0A0H3PBX6
F	253	GLY	-	expression tag	UNP A0A0H3PBX6
F	254	GLY	-	expression tag	UNP A0A0H3PBX6
F	255	SER	-	expression tag	UNP A0A0H3PBX6
F	256	GLY	-	expression tag	UNP A0A0H3PBX6
F	257	GLY	-	expression tag	UNP A0A0H3PBX6
F	258	GLY	-	expression tag	UNP A0A0H3PBX6
F	259	SER	-	expression tag	UNP A0A0H3PBX6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	260	GLY	-	expression tag	UNP A0A0H3PBX6
F	261	GLY	-	expression tag	UNP A0A0H3PBX6
F	262	SER	-	expression tag	UNP A0A0H3PBX6
F	263	ALA	-	expression tag	UNP A0A0H3PBX6
F	264	TRP	-	expression tag	UNP A0A0H3PBX6
F	265	SER	-	expression tag	UNP A0A0H3PBX6
F	266	HIS	-	expression tag	UNP A0A0H3PBX6
F	267	PRO	-	expression tag	UNP A0A0H3PBX6
F	268	GLN	-	expression tag	UNP A0A0H3PBX6
F	269	PHE	-	expression tag	UNP A0A0H3PBX6
F	270	GLU	-	expression tag	UNP A0A0H3PBX6
F	271	LYS	-	expression tag	UNP A0A0H3PBX6
G	22	ASN	ASP	engineered mutation	UNP A0A0H3PBX6
G	?	-	ASN	deletion	UNP A0A0H3PBX6
G	?	-	PRO	deletion	UNP A0A0H3PBX6
G	?	-	ALA	deletion	UNP A0A0H3PBX6
G	?	-	LYS	deletion	UNP A0A0H3PBX6
G	?	-	VAL	deletion	UNP A0A0H3PBX6
G	?	-	GLU	deletion	UNP A0A0H3PBX6
G	?	-	ALA	deletion	UNP A0A0H3PBX6
G	?	-	LEU	deletion	UNP A0A0H3PBX6
G	?	-	LYS	deletion	UNP A0A0H3PBX6
G	?	-	THR	deletion	UNP A0A0H3PBX6
G	?	-	GLU	deletion	UNP A0A0H3PBX6
G	?	-	PHE	deletion	UNP A0A0H3PBX6
G	?	-	VAL	deletion	UNP A0A0H3PBX6
G	?	-	LYS	deletion	UNP A0A0H3PBX6
G	?	-	ILE	deletion	UNP A0A0H3PBX6
G	?	-	PHE	deletion	UNP A0A0H3PBX6
G	?	-	ASP	deletion	UNP A0A0H3PBX6
G	?	-	TYR	deletion	UNP A0A0H3PBX6
G	?	-	THR	deletion	UNP A0A0H3PBX6
G	?	-	SER	deletion	UNP A0A0H3PBX6
G	228	GLY	-	expression tag	UNP A0A0H3PBX6
G	229	THR	-	expression tag	UNP A0A0H3PBX6
G	230	LEU	-	expression tag	UNP A0A0H3PBX6
G	231	GLU	-	expression tag	UNP A0A0H3PBX6
G	232	VAL	-	expression tag	UNP A0A0H3PBX6
G	233	LEU	-	expression tag	UNP A0A0H3PBX6
G	234	PHE	-	expression tag	UNP A0A0H3PBX6
G	235	GLN	-	expression tag	UNP A0A0H3PBX6
G	236	GLY	-	expression tag	UNP A0A0H3PBX6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	237	PRO	-	expression tag	UNP A0A0H3PBX6
G	238	GLY	-	expression tag	UNP A0A0H3PBX6
G	239	GLY	-	expression tag	UNP A0A0H3PBX6
G	240	SER	-	expression tag	UNP A0A0H3PBX6
G	241	GLY	-	expression tag	UNP A0A0H3PBX6
G	242	SER	-	expression tag	UNP A0A0H3PBX6
G	243	ALA	-	expression tag	UNP A0A0H3PBX6
G	244	TRP	-	expression tag	UNP A0A0H3PBX6
G	245	SER	-	expression tag	UNP A0A0H3PBX6
G	246	HIS	-	expression tag	UNP A0A0H3PBX6
G	247	PRO	-	expression tag	UNP A0A0H3PBX6
G	248	GLN	-	expression tag	UNP A0A0H3PBX6
G	249	PHE	-	expression tag	UNP A0A0H3PBX6
G	250	GLU	-	expression tag	UNP A0A0H3PBX6
G	251	LYS	-	expression tag	UNP A0A0H3PBX6
G	252	GLY	-	expression tag	UNP A0A0H3PBX6
G	253	GLY	-	expression tag	UNP A0A0H3PBX6
G	254	GLY	-	expression tag	UNP A0A0H3PBX6
G	255	SER	-	expression tag	UNP A0A0H3PBX6
G	256	GLY	-	expression tag	UNP A0A0H3PBX6
G	257	GLY	-	expression tag	UNP A0A0H3PBX6
G	258	GLY	-	expression tag	UNP A0A0H3PBX6
G	259	SER	-	expression tag	UNP A0A0H3PBX6
G	260	GLY	-	expression tag	UNP A0A0H3PBX6
G	261	GLY	-	expression tag	UNP A0A0H3PBX6
G	262	SER	-	expression tag	UNP A0A0H3PBX6
G	263	ALA	-	expression tag	UNP A0A0H3PBX6
G	264	TRP	-	expression tag	UNP A0A0H3PBX6
G	265	SER	-	expression tag	UNP A0A0H3PBX6
G	266	HIS	-	expression tag	UNP A0A0H3PBX6
G	267	PRO	-	expression tag	UNP A0A0H3PBX6
G	268	GLN	-	expression tag	UNP A0A0H3PBX6
G	269	PHE	-	expression tag	UNP A0A0H3PBX6
G	270	GLU	-	expression tag	UNP A0A0H3PBX6
G	271	LYS	-	expression tag	UNP A0A0H3PBX6

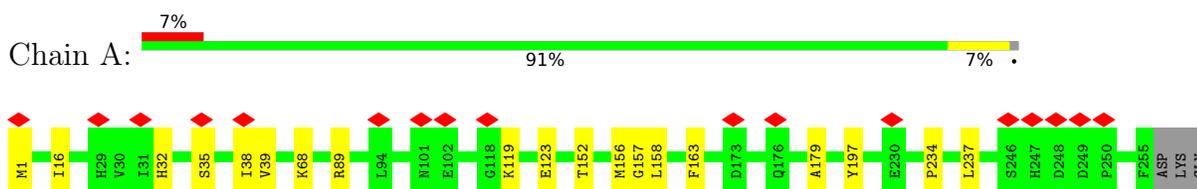
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	AltConf
3	B	3	Total O 3 3	0
3	C	3	Total O 3 3	0

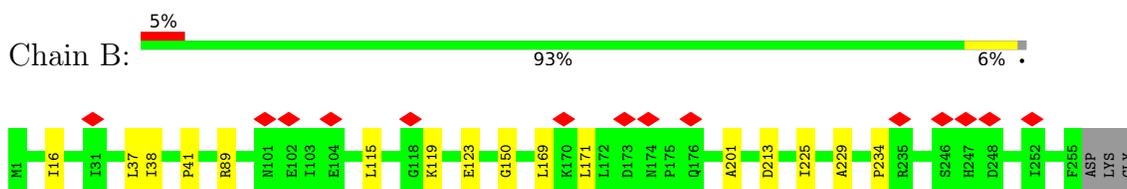
3 Residue-property plots [i](#)

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.

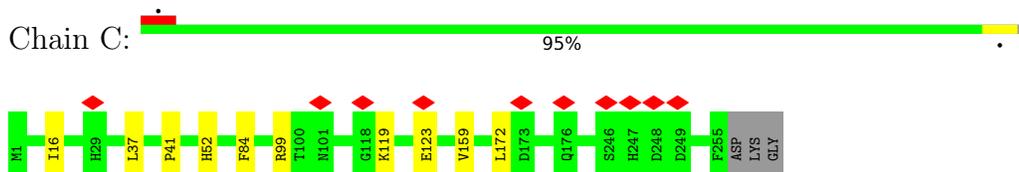
- Molecule 1: Chemotaxis protein MotA, putative



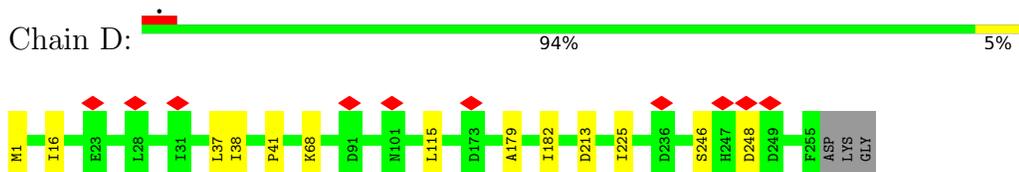
- Molecule 1: Chemotaxis protein MotA, putative



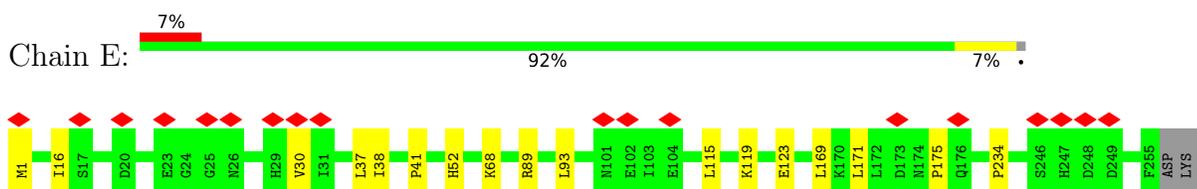
- Molecule 1: Chemotaxis protein MotA, putative



- Molecule 1: Chemotaxis protein MotA, putative

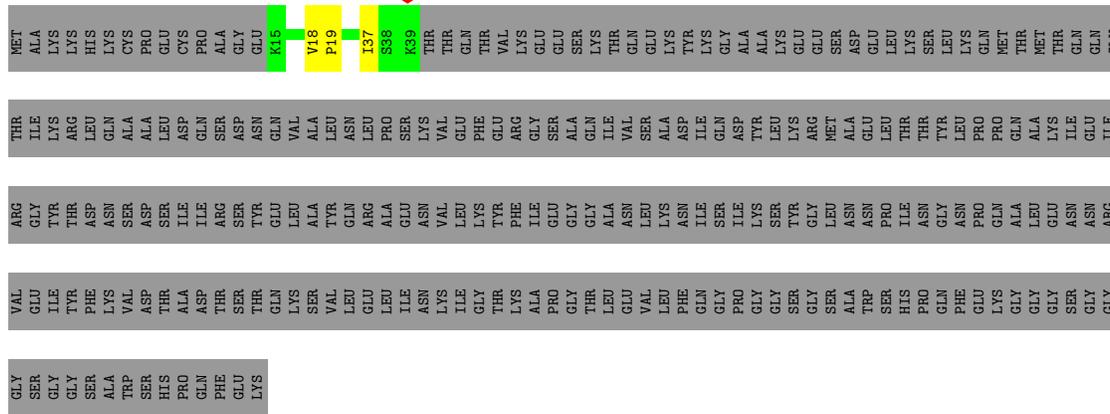


- Molecule 1: Chemotaxis protein MotA, putative



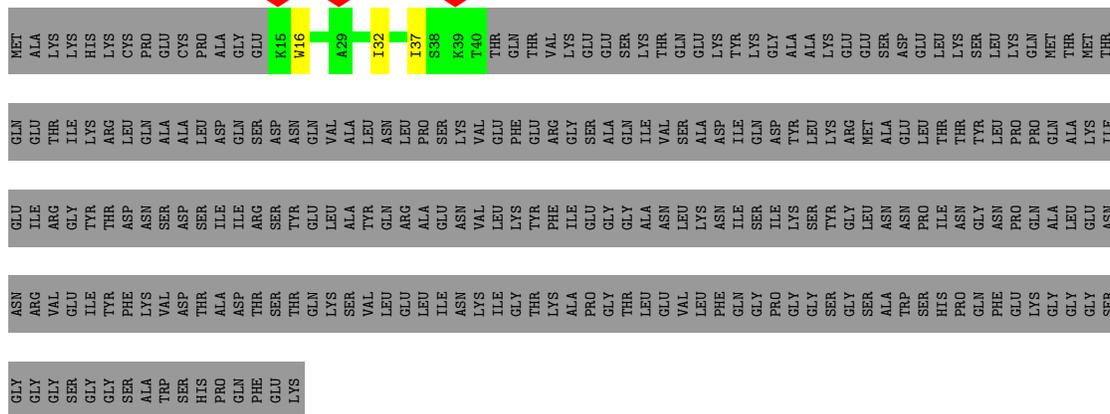
• Molecule 2: Chemotaxis protein MotB, putative

Chain F:  8%  91%



• Molecule 2: Chemotaxis protein MotB, putative

Chain G:  8%  90%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	456384	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 ($e^-/\text{\AA}^2$)	43.44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.387	Depositor
Minimum map value	-0.262	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	212.992, 212.992, 212.992	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.832, 0.832, 0.832	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	0.27	0/1989	0.53	1/2686 (0.0%)
1	B	0.27	0/1989	0.51	1/2686 (0.0%)
1	C	0.27	0/1989	0.51	0/2686
1	D	0.27	0/1989	0.50	0/2686
1	E	0.27	0/1989	0.52	1/2686 (0.0%)
2	F	0.26	0/210	0.44	0/287
2	G	0.28	0/217	0.55	0/297
All	All	0.27	0/10372	0.51	3/14014 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	LEU	CB-CG-CD2	-6.04	100.74	111.00
1	B	171	LEU	CA-CB-CG	5.94	128.97	115.30
1	E	171	LEU	CA-CB-CG	5.24	127.34	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	1954	0	1997	12	0
1	B	1954	0	1997	10	0
1	C	1954	0	1997	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1954	0	1997	9	0
1	E	1954	0	1997	11	0
2	F	203	0	217	2	0
2	G	210	0	224	3	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
All	All	10189	0	10426	40	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 2.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:HH	2:G:16:TRP:HE1	1.39	0.70
1:D:179:ALA:HB1	1:E:169:LEU:HD22	1.84	0.60
1:C:119:LYS:HD2	1:C:123:GLU:HG2	1.87	0.56
1:D:1:MET:HB3	1:D:68:LYS:HA	1.91	0.52
1:A:39:VAL:HG22	1:A:157:GLY:HA2	1.92	0.52
1:B:16:ILE:HD11	1:C:159:VAL:HG11	1.92	0.51
1:E:37:LEU:HD23	1:E:41:PRO:HG2	1.93	0.50
1:A:119:LYS:HD2	1:A:123:GLU:HG2	1.92	0.50
1:D:115:LEU:HD22	1:D:225:ILE:HG23	1.94	0.49
2:F:18:VAL:HG23	2:F:19:PRO:HD3	1.94	0.49
1:B:150:GLY:HA3	1:B:201:ALA:HB2	1.95	0.49
1:E:175:PRO:HB3	2:G:37:ILE:HD13	1.95	0.49
1:D:16:ILE:HG13	1:E:38:ILE:HG23	1.94	0.48
1:A:16:ILE:HG13	1:B:38:ILE:HG23	1.95	0.48
1:E:89:ARG:HH11	1:E:234:PRO:HD2	1.79	0.47
1:A:32:HIS:HB2	1:A:35:SER:HB2	1.97	0.46
1:A:1:MET:HB3	1:A:68:LYS:HA	1.97	0.46
1:A:89:ARG:HH11	1:A:234:PRO:HD2	1.80	0.46
1:D:213:ASP:OD2	1:E:52:HIS:NE2	2.48	0.46
1:B:115:LEU:HD22	1:B:225:ILE:HG23	1.97	0.46
1:C:84:PHE:HE1	1:C:99:ARG:HE	1.63	0.45
1:A:38:ILE:HG23	1:E:16:ILE:HG13	1.98	0.45
1:E:119:LYS:HD2	1:E:123:GLU:HG2	1.99	0.45
1:A:179:ALA:HB1	1:B:169:LEU:HB3	1.99	0.45
1:D:246:SER:OG	1:D:248:ASP:OD1	2.33	0.44
1:B:37:LEU:HD23	1:B:41:PRO:HG2	2.00	0.44
1:E:1:MET:HB3	1:E:68:LYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:OD2	1:C:52:HIS:NE2	2.53	0.42
1:C:16:ILE:HG13	1:D:38:ILE:HG23	2.02	0.42
1:C:172:LEU:HD13	2:F:37:ILE:HD11	2.02	0.42
1:B:119:LYS:HD2	1:B:123:GLU:HG2	2.01	0.42
1:C:37:LEU:HD23	1:C:41:PRO:HG2	2.02	0.41
1:A:152:THR:HG22	1:A:156:MET:HG2	2.01	0.41
1:E:93:LEU:HD11	1:E:115:LEU:HG	2.03	0.41
1:A:163:PHE:HE1	1:E:30:VAL:HG11	1.86	0.41
1:B:115:LEU:HD11	1:B:229:ALA:HB2	2.02	0.41
1:A:234:PRO:HA	1:A:237:LEU:HB3	2.03	0.40
1:D:37:LEU:HD23	1:D:41:PRO:HG2	2.03	0.40
1:B:89:ARG:HH11	1:B:234:PRO:HD2	1.85	0.40
1:D:182:ILE:HD13	2:G:32:ILE:HD13	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	A	253/258 (98%)	247 (98%)	6 (2%)	0	100	100
1	B	253/258 (98%)	246 (97%)	7 (3%)	0	100	100
1	C	253/258 (98%)	246 (97%)	7 (3%)	0	100	100
1	D	253/258 (98%)	248 (98%)	5 (2%)	0	100	100
1	E	253/258 (98%)	246 (97%)	7 (3%)	0	100	100
2	F	23/271 (8%)	22 (96%)	1 (4%)	0	100	100
2	G	24/271 (9%)	23 (96%)	1 (4%)	0	100	100
All	All	1312/1832 (72%)	1278 (97%)	34 (3%)	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	A	208/210 (99%)	208 (100%)	0	100	100
1	B	208/210 (99%)	208 (100%)	0	100	100
1	C	208/210 (99%)	208 (100%)	0	100	100
1	D	208/210 (99%)	208 (100%)	0	100	100
1	E	208/210 (99%)	208 (100%)	0	100	100
2	F	20/225 (9%)	20 (100%)	0	100	100
2	G	21/225 (9%)	21 (100%)	0	100	100
All	All	1081/1500 (72%)	1081 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

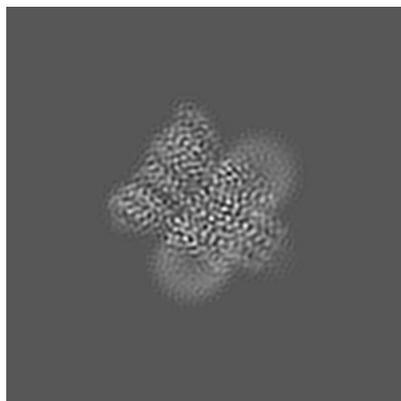
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10830. These allow visual inspection of the internal detail of the map and identification of artifacts.

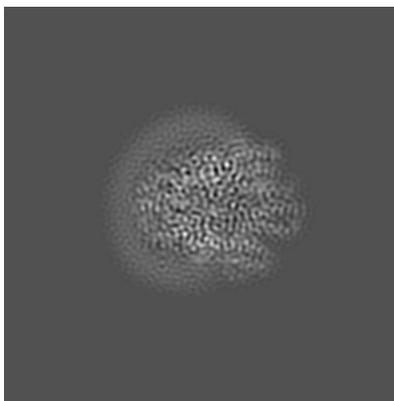
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

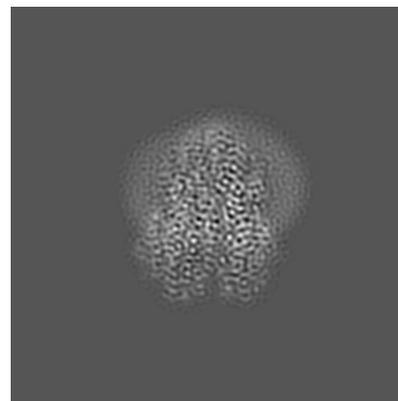
6.1.1 Primary map



X

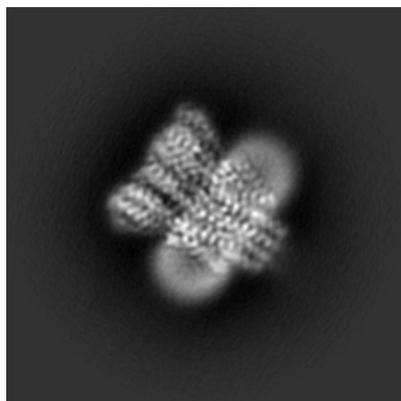


Y

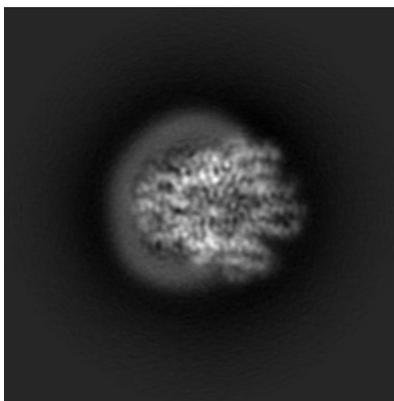


Z

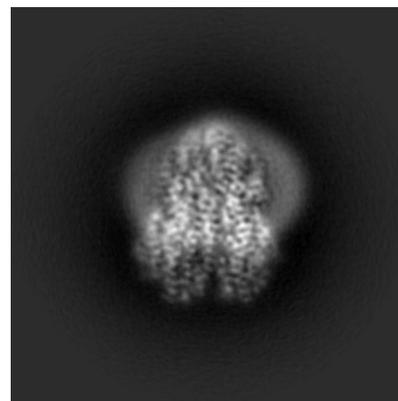
6.1.2 Raw map



X



Y

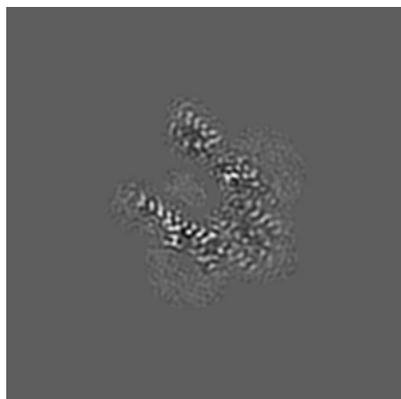


Z

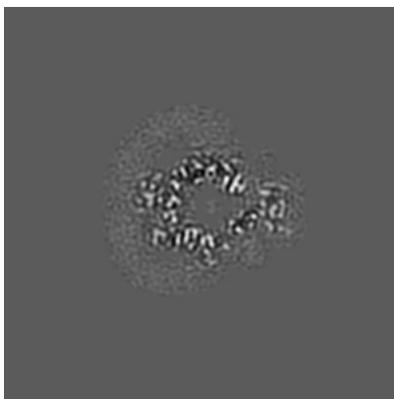
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

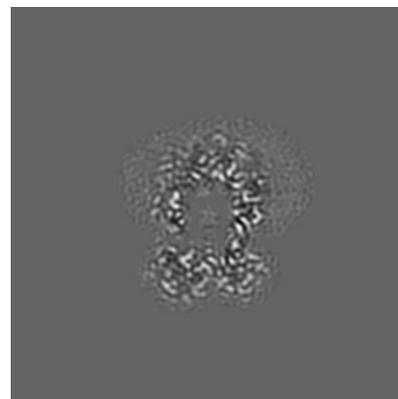
6.2.1 Primary map



X Index: 128

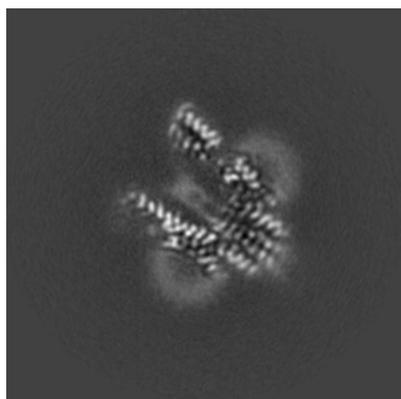


Y Index: 128

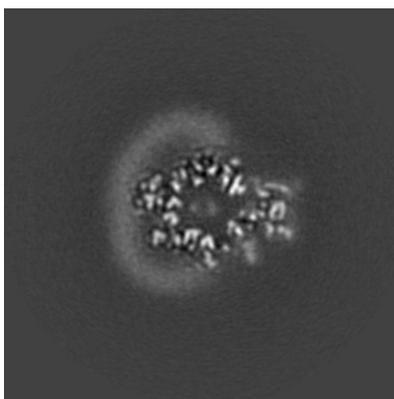


Z Index: 128

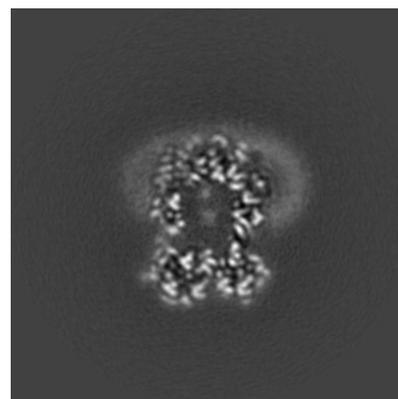
6.2.2 Raw map



X Index: 128



Y Index: 128

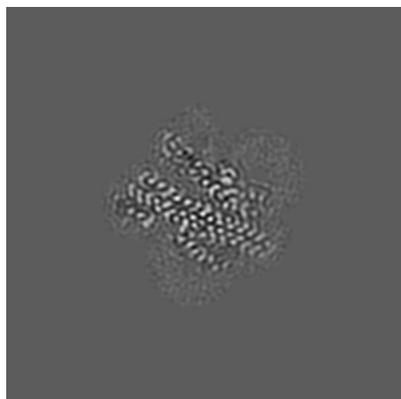


Z Index: 128

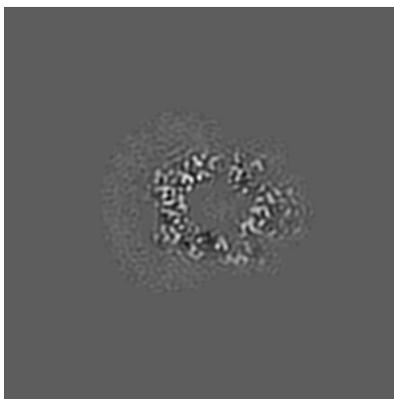
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

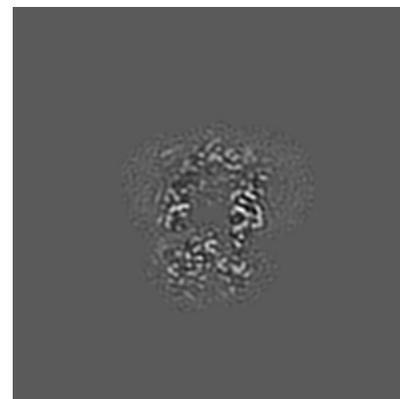
6.3.1 Primary map



X Index: 144

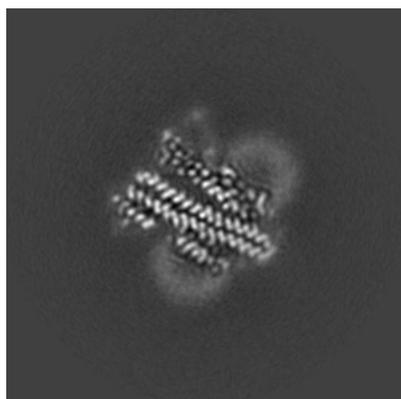


Y Index: 120

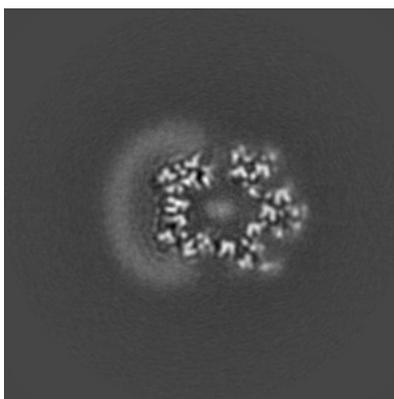


Z Index: 122

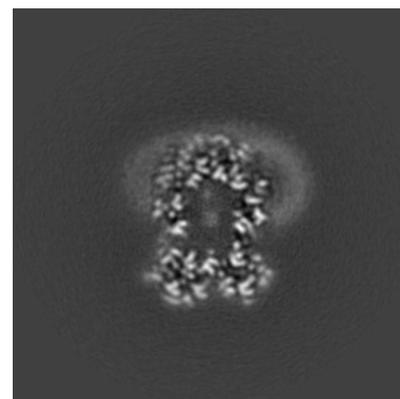
6.3.2 Raw map



X Index: 145



Y Index: 115

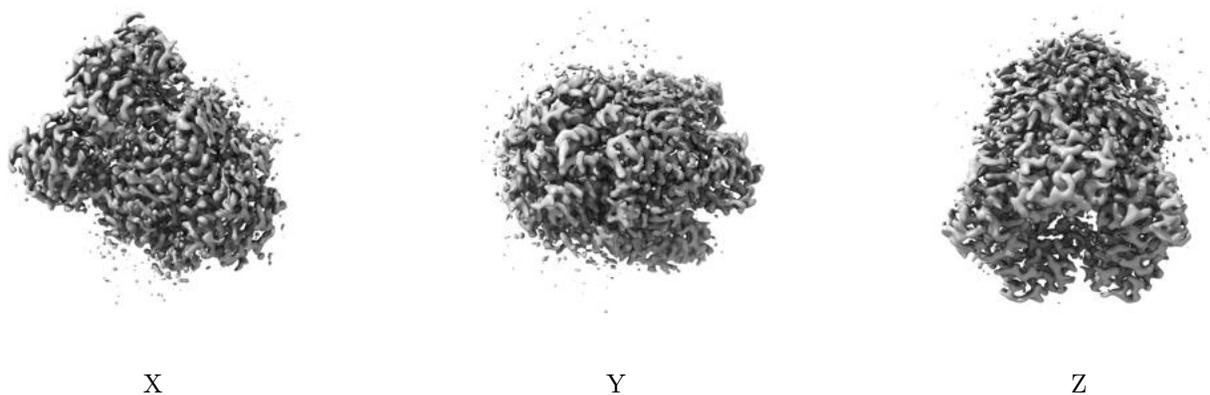


Z Index: 129

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

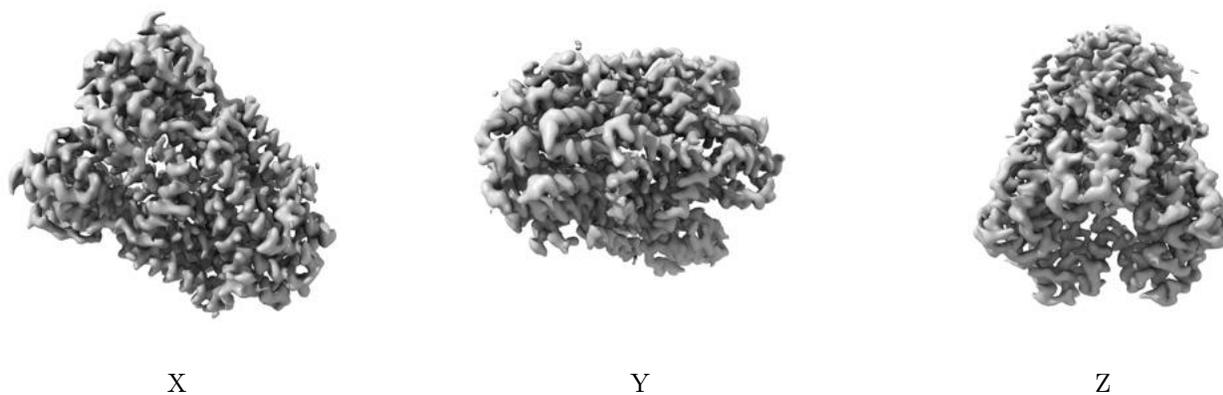
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

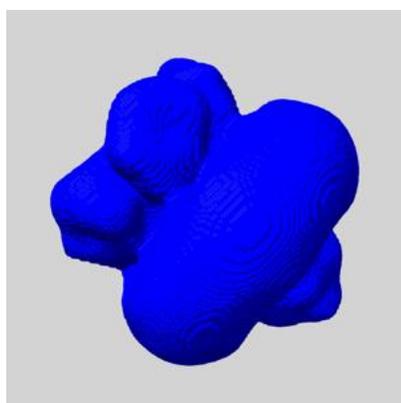
6.5 Mask visualisation [i](#)

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

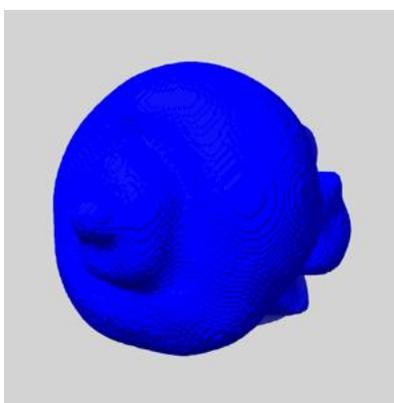
A mask typically either:

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

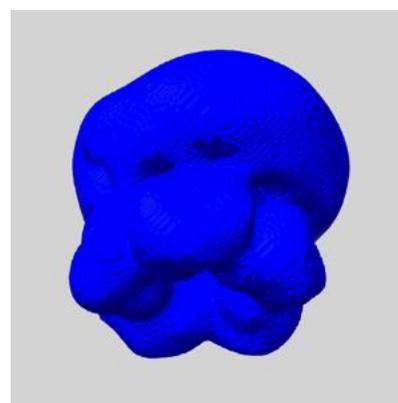
6.5.1 emd_10830_msk_1.map [i](#)



X



Y

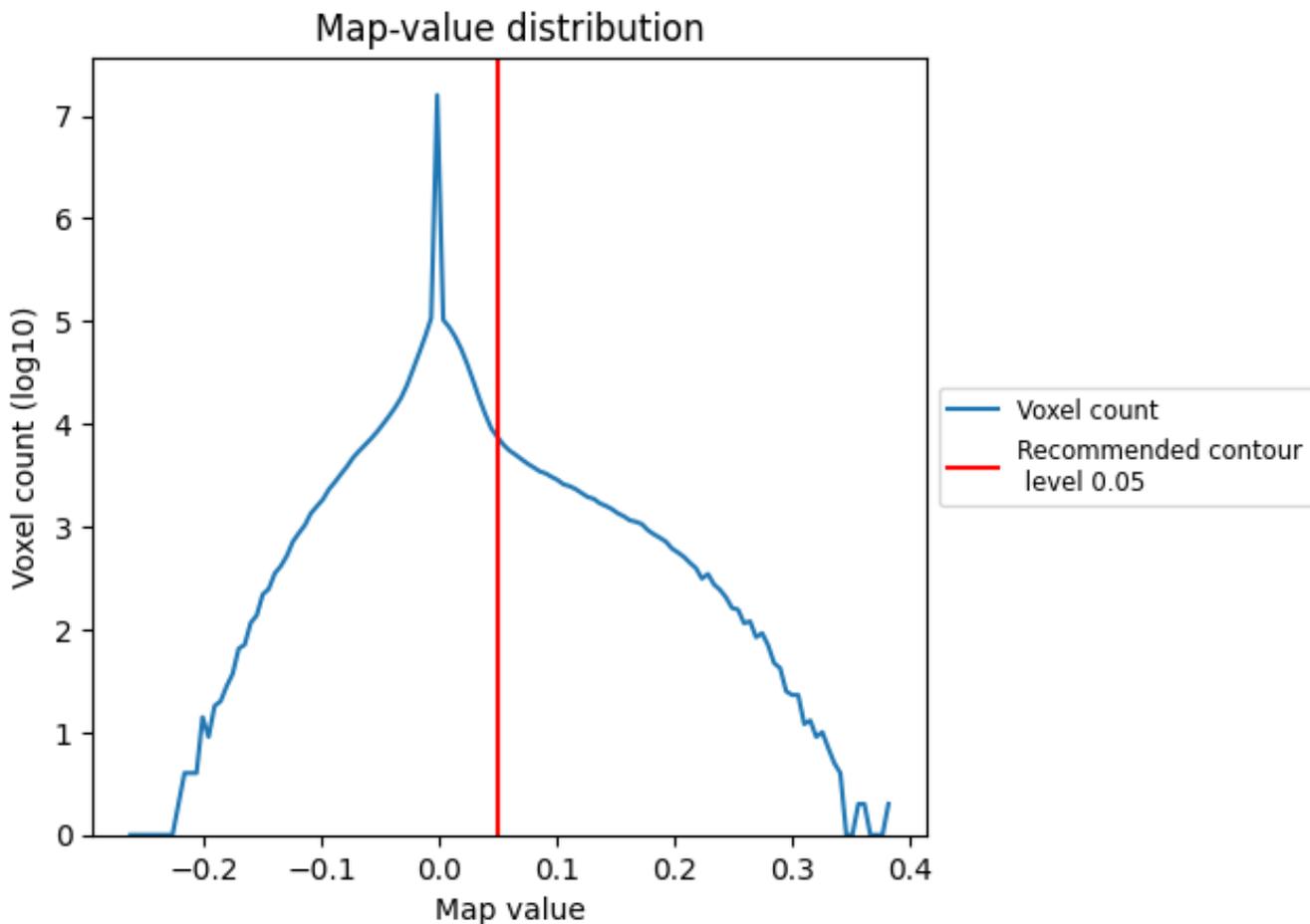


Z

7 Map analysis [i](#)

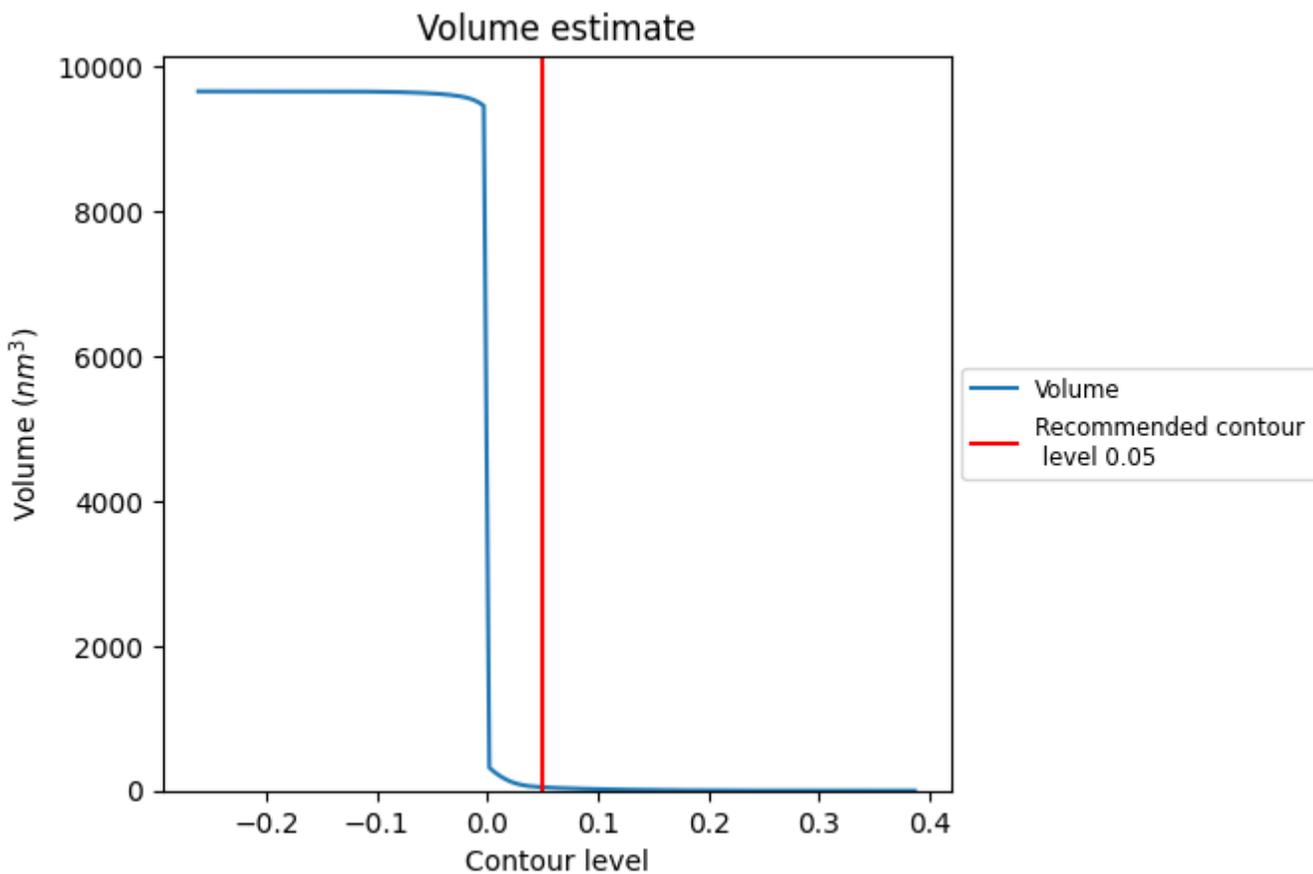
This section contains the results of statistical analysis of the map.

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.

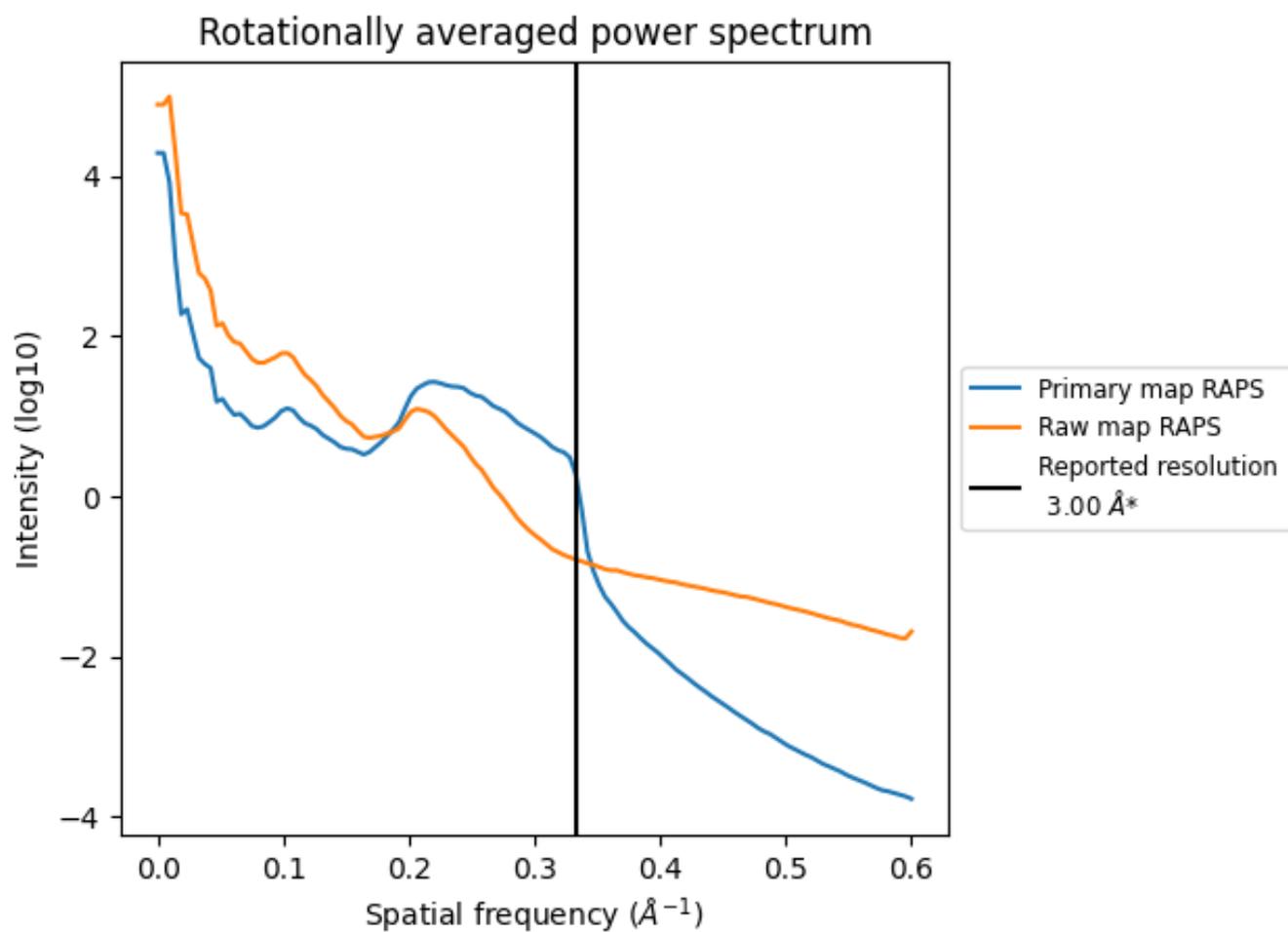
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm³; this corresponds to an approximate mass of 42 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

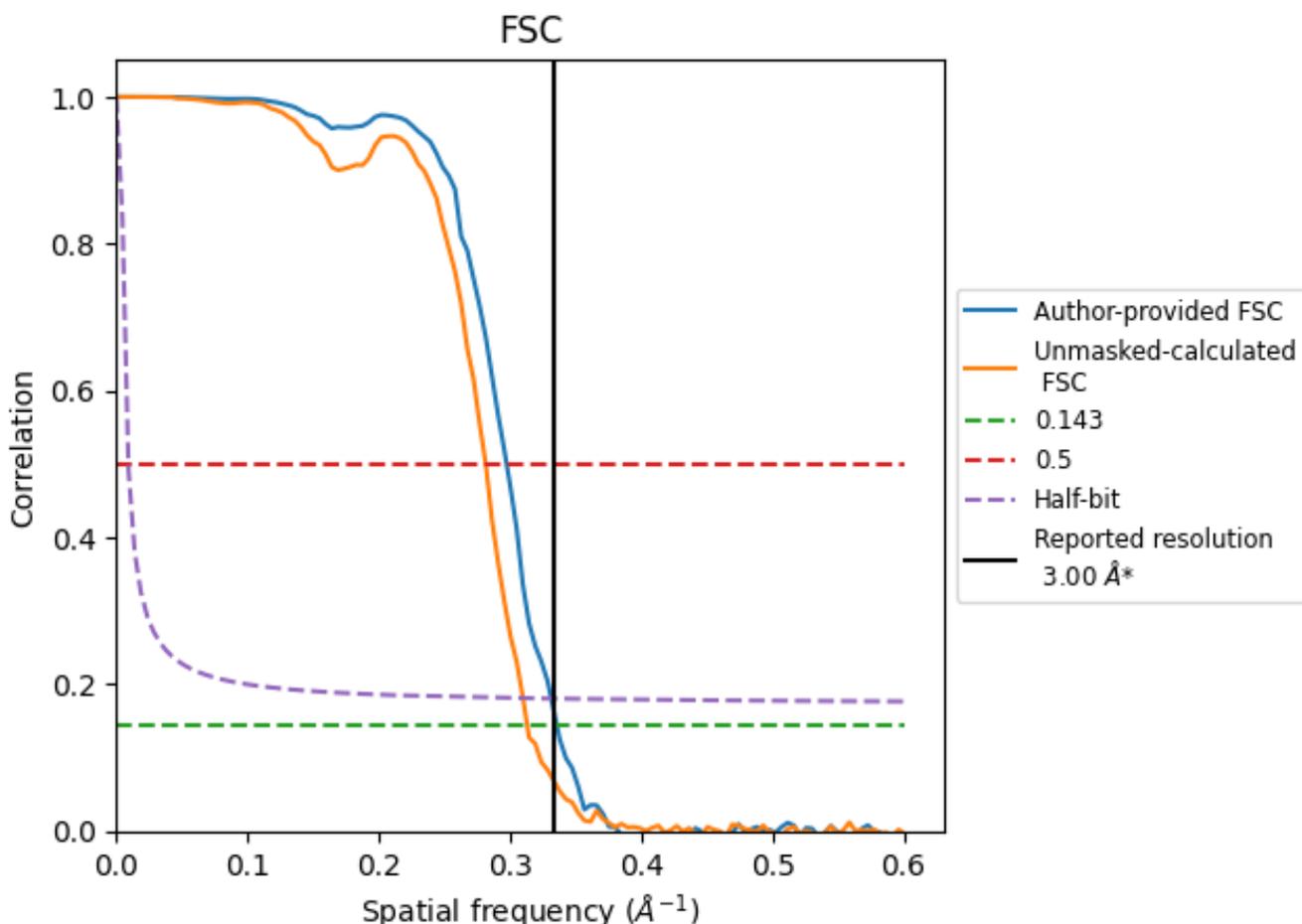


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

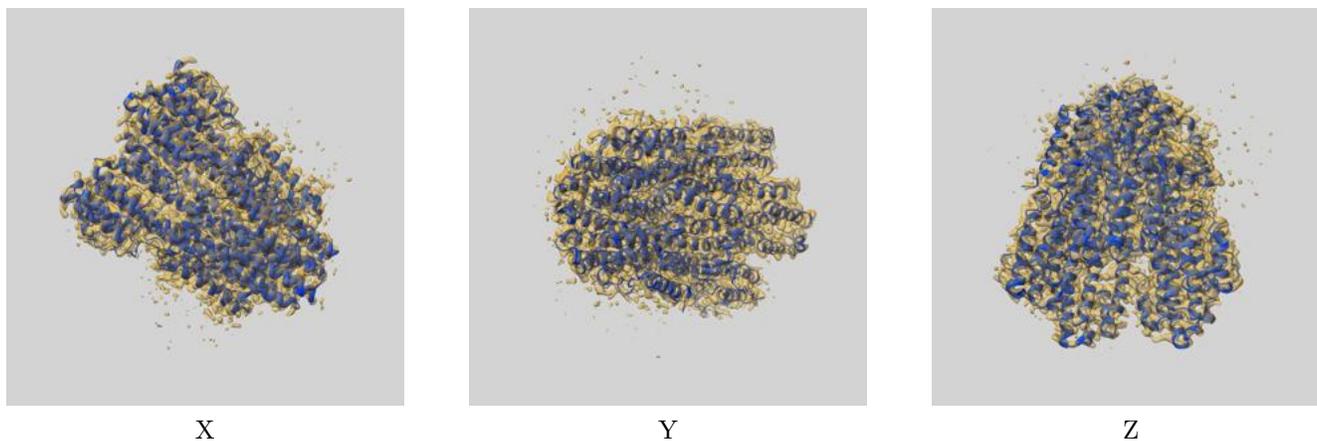
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.36	3.02
Unmasked-calculated*	3.19	3.55	3.23

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

9 Map-model fit [i](#)

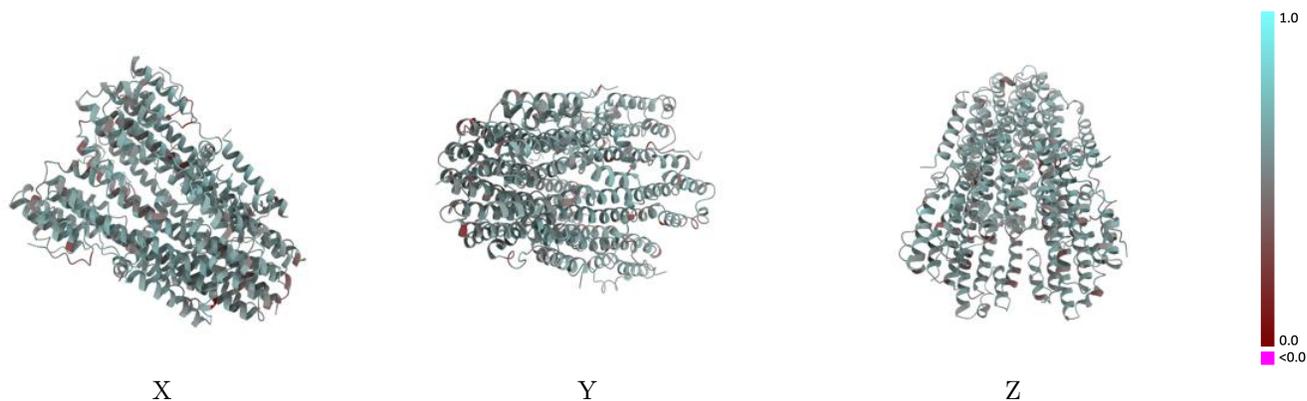
This section contains information regarding the fit between EMDB map EMD-10830 and PDB model 6YKR. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



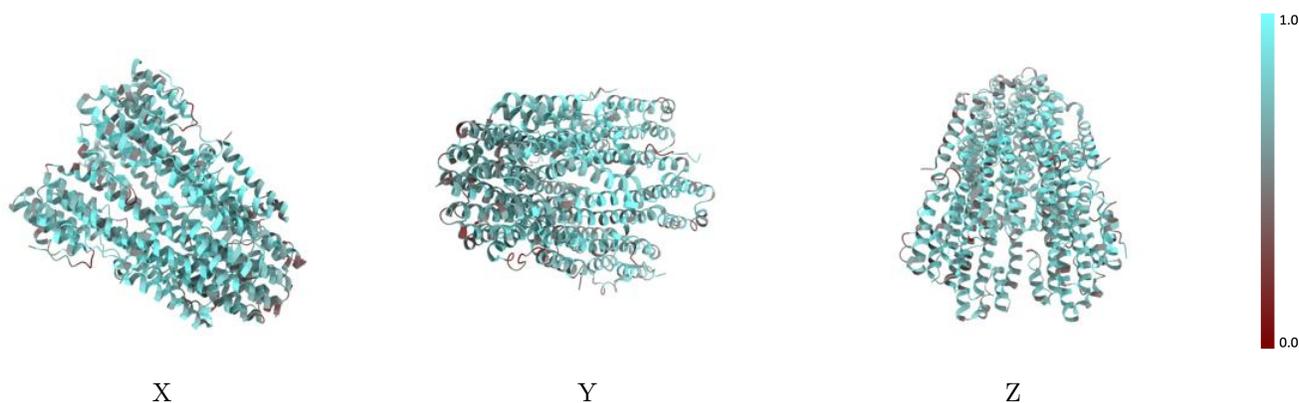
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



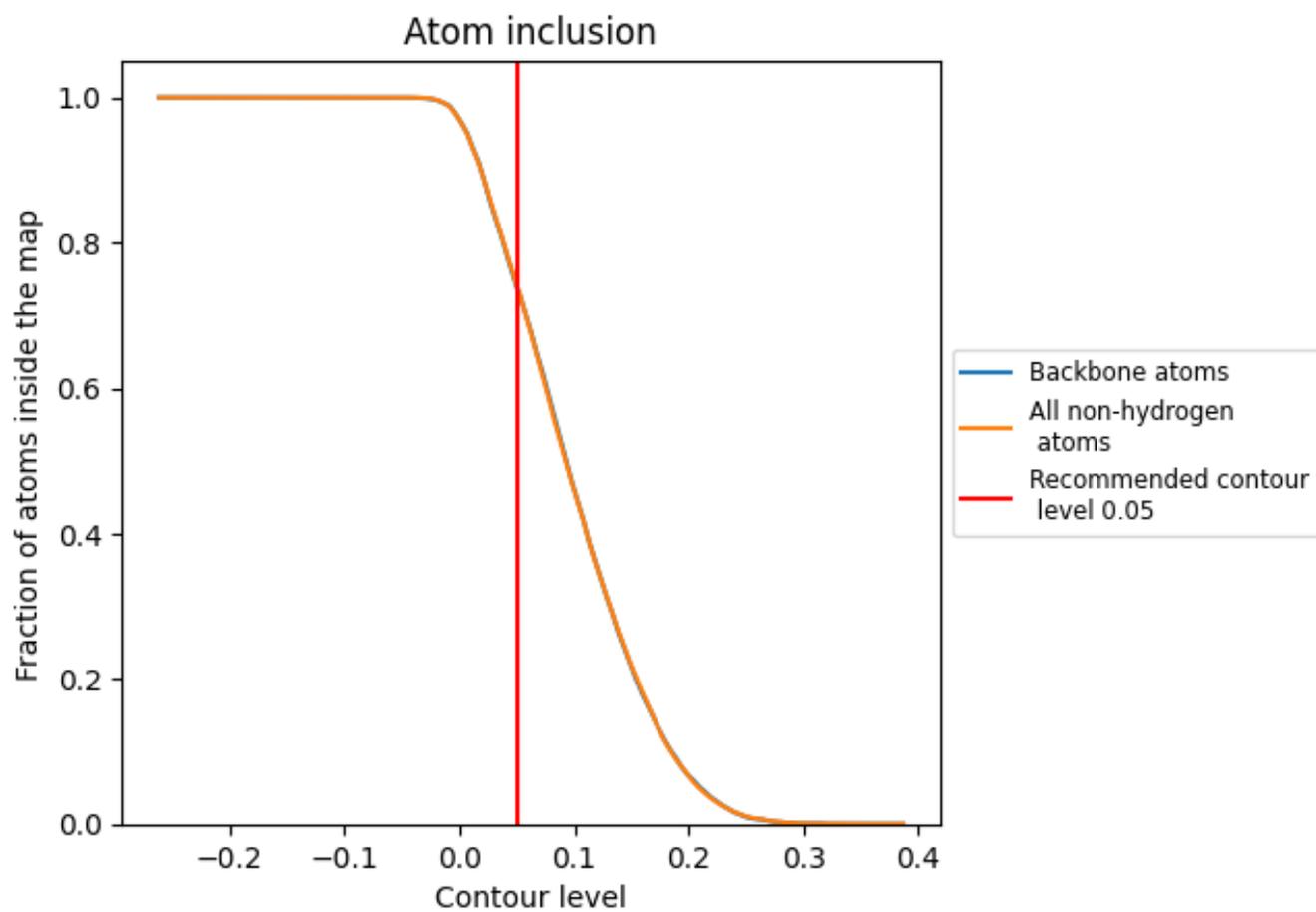
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7397	 0.5510
A	 0.7324	 0.5460
B	 0.7572	 0.5550
C	 0.7577	 0.5520
D	 0.7593	 0.5560
E	 0.7154	 0.5490
F	 0.6950	 0.5360
G	 0.6908	 0.5380

