



## Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 10:27 PM EDT

PDB ID : 9Y3U / pdb\_00009y3u  
EMDB ID : EMD-72467  
Title : Eukaryotic translation initiation factor 2-B (eIF2B) with a truncation in the beta subunit (inactive state)  
Authors : Dalwadi, U.; Croll, T.; Subramanian, A.; Lee, D.J.; Arthur, C.; Walter, P.; Frost, A.  
Deposited on : 2025-09-02  
Resolution : 2.40 Å (reported)  
Based on initial model : 7L7G

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

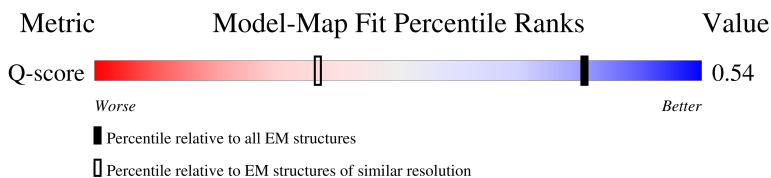
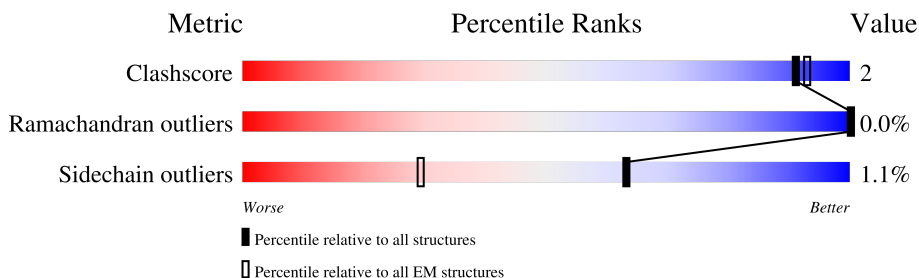
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 2.40 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	5628 ( 1.90 - 2.90 )

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  $\geq 3$ , 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	461	 89% 5% 5%
1	B	461	 87% 8% 5%
2	C	355	 81% 10% 9%
2	D	355	 83% 9% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	523	<div><div></div><div>63%</div><div></div><div>32%</div></div>
3	F	523	<div><div></div><div>62%</div><div>6%</div><div>32%</div></div>
4	G	305	<div><div>6%</div><div></div><div>90%</div><div>6%</div><div></div></div>
4	H	305	<div><div>5%</div><div></div><div>92%</div><div></div><div></div></div>
5	I	452	<div><div>25%</div><div></div><div>86%</div><div></div><div>13%</div></div>
5	J	452	<div><div>29%</div><div></div><div>86%</div><div></div><div>13%</div></div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28169 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 eIF2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	437	Total	C	N	O	S	0	0
			3423	2167	606	635	15		
1	B	437	Total	C	N	O	S	0	0
			3423	2167	606	635	15		

- Molecule 2 is a protein called Translation initiation factor eIF2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	322	Total	C	N	O	S	0	0
			2523	1596	442	470	15		
2	D	327	Total	C	N	O	S	0	0
			2563	1619	451	478	15		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	MET	-	initiating methionine	UNP P49770
C	-15	HIS	-	expression tag	UNP P49770
C	-14	HIS	-	expression tag	UNP P49770
C	-13	HIS	-	expression tag	UNP P49770
C	-12	HIS	-	expression tag	UNP P49770
C	-11	HIS	-	expression tag	UNP P49770
C	-10	HIS	-	expression tag	UNP P49770
C	-9	GLY	-	expression tag	UNP P49770
C	-8	GLY	-	expression tag	UNP P49770
C	-7	GLY	-	expression tag	UNP P49770
C	-6	SER	-	expression tag	UNP P49770
C	-5	GLU	-	expression tag	UNP P49770
C	-4	ASN	-	expression tag	UNP P49770
C	-3	LEU	-	expression tag	UNP P49770
C	-2	TYR	-	expression tag	UNP P49770
C	-1	PHE	-	expression tag	UNP P49770
C	0	GLN	-	expression tag	UNP P49770

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	-	expression tag	UNP P49770
C	113	GLY	SER	linker	UNP P49770
C	114	SER	ASP	linker	UNP P49770
C	115	GLY	GLU	linker	UNP P49770
C	?	-	ASP	deletion	UNP P49770
C	?	-	GLN	deletion	UNP P49770
C	?	-	GLN	deletion	UNP P49770
C	?	-	GLU	deletion	UNP P49770
C	?	-	SER	deletion	UNP P49770
C	?	-	LEU	deletion	UNP P49770
C	?	-	HIS	deletion	UNP P49770
C	?	-	LYS	deletion	UNP P49770
C	?	-	LEU	deletion	UNP P49770
C	?	-	LEU	deletion	UNP P49770
C	?	-	THR	deletion	UNP P49770
C	?	-	SER	deletion	UNP P49770
C	?	-	GLY	deletion	UNP P49770
D	-16	MET	-	initiating methionine	UNP P49770
D	-15	HIS	-	expression tag	UNP P49770
D	-14	HIS	-	expression tag	UNP P49770
D	-13	HIS	-	expression tag	UNP P49770
D	-12	HIS	-	expression tag	UNP P49770
D	-11	HIS	-	expression tag	UNP P49770
D	-10	HIS	-	expression tag	UNP P49770
D	-9	GLY	-	expression tag	UNP P49770
D	-8	GLY	-	expression tag	UNP P49770
D	-7	GLY	-	expression tag	UNP P49770
D	-6	SER	-	expression tag	UNP P49770
D	-5	GLU	-	expression tag	UNP P49770
D	-4	ASN	-	expression tag	UNP P49770
D	-3	LEU	-	expression tag	UNP P49770
D	-2	TYR	-	expression tag	UNP P49770
D	-1	PHE	-	expression tag	UNP P49770
D	0	GLN	-	expression tag	UNP P49770
D	1	SER	-	expression tag	UNP P49770
D	113	GLY	SER	linker	UNP P49770
D	114	SER	ASP	linker	UNP P49770
D	115	GLY	GLU	linker	UNP P49770
D	?	-	ASP	deletion	UNP P49770
D	?	-	GLN	deletion	UNP P49770
D	?	-	GLN	deletion	UNP P49770
D	?	-	GLU	deletion	UNP P49770

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP P49770
D	?	-	LEU	deletion	UNP P49770
D	?	-	HIS	deletion	UNP P49770
D	?	-	LYS	deletion	UNP P49770
D	?	-	LEU	deletion	UNP P49770
D	?	-	LEU	deletion	UNP P49770
D	?	-	THR	deletion	UNP P49770
D	?	-	SER	deletion	UNP P49770
D	?	-	GLY	deletion	UNP P49770

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	356	Total	C	N	O	S	0	0
			2770	1751	493	512	14		
3	F	356	Total	C	N	O	S	0	0
			2770	1751	493	512	14		

- Molecule 4 is a protein called Translation initiation factor eIF2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	296	Total	C	N	O	S	0	0
			2302	1477	381	432	12		
4	H	296	Total	C	N	O	S	0	0
			2302	1477	381	432	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	393	Total	C	N	O	S	0	0
			3040	1929	518	569	24		
5	J	393	Total	C	N	O	S	0	0
			3041	1929	519	569	24		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total	O	P	0
			5	4	1	
6	D	1	Total	O	P	0
			5	4	1	

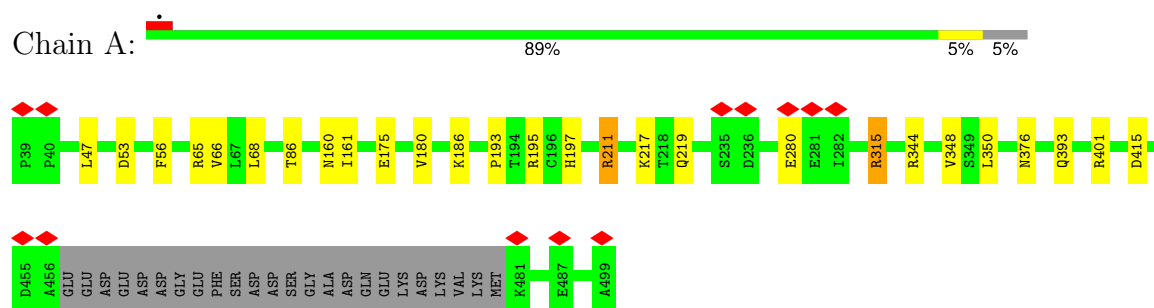
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total	Zn	0
			1	1	
7	F	1	Total	Zn	0
			1	1	

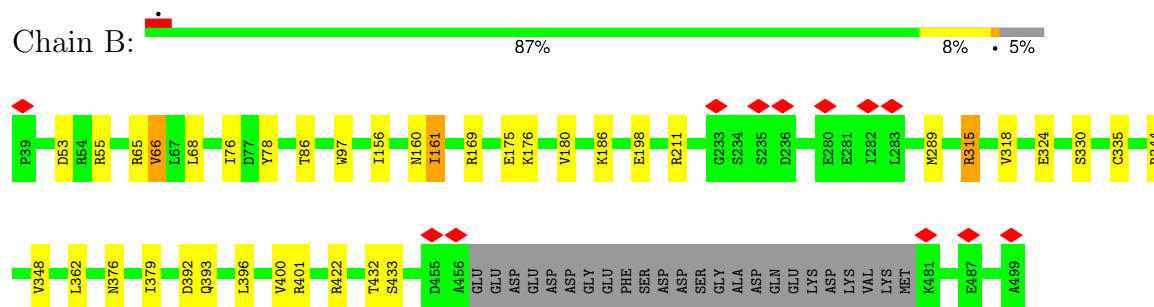
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

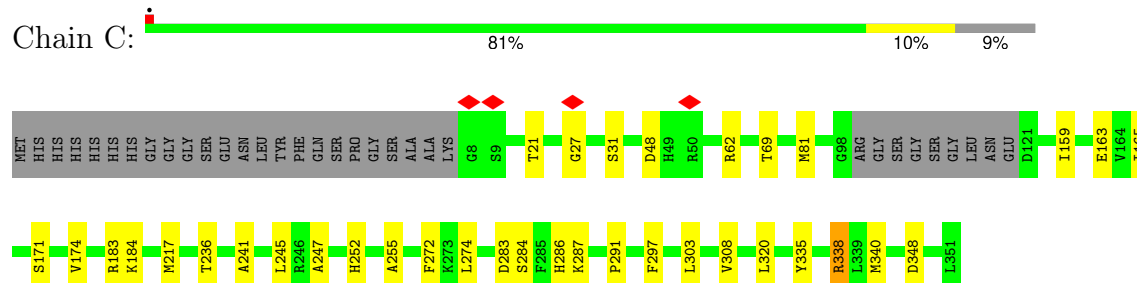
- Molecule 1: Translation initiation factor eIF2B subunit epsilon



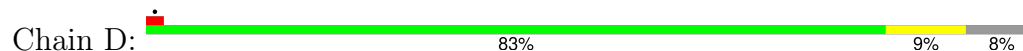
- Molecule 1: Translation initiation factor eIF2B subunit epsilon



- Molecule 2: Translation initiation factor eIF2B subunit beta



- Molecule 2: Translation initiation factor eIF2B subunit beta









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	96151	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.186	Depositor
Minimum map value	-0.075	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size ( $\text{\AA}$ )	371.44, 371.44, 371.44	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.9286, 0.9286, 0.9286	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.67	0/3497	1.08	6/4758 (0.1%)
1	B	0.66	0/3497	1.09	5/4758 (0.1%)
2	C	0.73	2/2572 (0.1%)	1.14	7/3477 (0.2%)
2	D	0.70	0/2612	1.15	8/3530 (0.2%)
3	E	0.68	0/2822	1.09	2/3835 (0.1%)
3	F	0.70	1/2822 (0.0%)	1.10	7/3835 (0.2%)
4	G	0.68	0/2338	1.12	6/3155 (0.2%)
4	H	0.68	0/2338	1.13	3/3155 (0.1%)
5	I	0.55	0/3083	0.97	1/4159 (0.0%)
5	J	0.55	0/3084	0.94	2/4159 (0.0%)
All	All	0.66	3/28665 (0.0%)	1.08	47/38821 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
2	C	0	1
2	D	0	3
3	E	0	2
3	F	0	4
4	G	0	1
4	H	0	2
5	I	0	1
5	J	0	1
All	All	0	24

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	321	ARG	CZ-NH2	9.76	1.46	1.33
2	C	252	HIS	CG-CD2	-5.23	1.30	1.35
2	C	247	ALA	CA-CB	-5.13	1.45	1.54

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	229	VAL	N-CA-CB	-8.68	100.02	111.82
4	G	229	VAL	N-CA-CB	-8.29	101.49	112.10
3	E	490	ASP	CA-CB-CG	7.88	120.48	112.60
3	F	321	ARG	NE-CZ-NH1	-7.21	114.29	121.50
2	D	160	HIS	CA-CB-CG	-6.99	106.81	113.80
3	F	490	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	195	ARG	CA-CB-CG	-6.10	101.89	114.10
1	A	415	ASP	CB-CA-C	6.08	118.96	109.84
1	B	392	ASP	CB-CA-C	6.01	120.17	109.65
4	G	128	HIS	CA-C-N	-5.95	110.19	121.54
4	G	128	HIS	C-N-CA	-5.95	110.19	121.54
1	B	53	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	53	ASP	CA-CB-CG	5.94	118.54	112.60
2	D	287	LYS	CB-CA-C	5.92	119.90	110.19
4	G	274	ASP	CA-CB-CG	5.90	118.50	112.60
2	C	287	LYS	CB-CA-C	5.89	119.47	109.80
3	F	321	ARG	NE-CZ-NH2	5.83	124.44	119.20
1	A	350	LEU	N-CA-CB	-5.81	101.31	110.77
2	C	69	THR	CA-CB-OG1	-5.75	100.97	109.60
2	C	48	ASP	CA-CB-CG	5.74	118.34	112.60
3	F	456	GLU	CB-CA-C	5.70	120.64	109.35
1	B	289	MET	CB-CA-C	-5.70	98.61	109.66
3	F	322	PHE	CB-CA-C	-5.63	102.01	110.90
4	H	268	GLU	CB-CG-CD	5.53	121.99	112.60
2	C	163	GLU	CB-CA-C	-5.49	99.78	109.62
1	A	315	ARG	NE-CZ-NH1	-5.48	116.02	121.50
3	F	310	GLU	CB-CA-C	-5.38	102.67	110.96
2	D	69	THR	CA-CB-OG1	-5.36	101.55	109.60
4	H	192	LEU	N-CA-CB	5.32	120.95	111.69
4	G	192	LEU	N-CA-CB	5.31	120.93	111.69
2	C	283	ASP	CA-CB-CG	5.27	117.87	112.60
5	I	177	ASP	CA-CB-CG	5.26	117.86	112.60
2	C	217	MET	CG-SD-CE	-5.26	89.33	100.90
1	B	175	GLU	CB-CA-C	5.25	119.48	111.76
2	D	286	HIS	CA-C-N	-5.25	115.70	123.05
2	D	286	HIS	C-N-CA	-5.25	115.70	123.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	GLU	N-CA-CB	5.23	117.80	110.12
2	D	197	PHE	CA-CB-CG	-5.18	108.62	113.80
5	J	423	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	68	LEU	CB-CA-C	5.11	116.77	109.26
2	C	274	LEU	N-CA-CB	5.11	117.58	109.71
1	B	68	LEU	CB-CA-C	5.08	116.73	109.26
3	F	450	ASP	CA-CB-CG	5.08	117.68	112.60
3	E	431	ASN	N-CA-CB	-5.07	104.77	112.47
5	J	111	ASP	CA-CB-CG	5.04	117.64	112.60
2	D	294	VAL	N-CA-CB	-5.01	105.04	111.90
4	G	226	PHE	N-CA-CB	-5.00	102.75	110.65

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	GLU	Peptide
1	A	211	ARG	Sidechain
1	A	401	ARG	Sidechain
1	B	169	ARG	Sidechain
1	B	211	ARG	Sidechain
1	B	315	ARG	Sidechain
1	B	401	ARG	Sidechain
1	B	422	ARG	Sidechain
1	B	65	ARG	Sidechain
2	C	338	ARG	Sidechain
2	D	185	ARG	Sidechain
2	D	338	ARG	Sidechain
2	D	63	ARG	Sidechain
3	E	188	ARG	Sidechain
3	E	483	ARG	Sidechain
3	F	344	ARG	Sidechain
3	F	364	ARG	Sidechain
3	F	374	ARG	Sidechain
3	F	483	ARG	Sidechain
4	G	147	ARG	Sidechain
4	H	136	ARG	Sidechain
4	H	237	ARG	Sidechain
5	I	194	ARG	Sidechain
5	J	175	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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	3423	0	3419	10	0
1	B	3423	0	3419	15	0
2	C	2523	0	2527	18	0
2	D	2563	0	2566	14	0
3	E	2770	0	2829	10	0
3	F	2770	0	2829	11	0
4	G	2302	0	2378	12	0
4	H	2302	0	2378	6	0
5	I	3040	0	3160	1	0
5	J	3041	0	3162	2	0
6	C	5	0	0	1	0
6	D	5	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
All	All	28169	0	28667	90	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 (90) 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:C:236:THR:HG21	2:C:245:LEU:HD22	1.46	0.96
2:D:274:LEU:HD22	2:D:340:MET:HE1	1.71	0.73
2:D:274:LEU:HD21	2:D:336:ILE:HG23	1.71	0.73
4:G:192:LEU:HD12	4:G:192:LEU:N	2.06	0.71
4:H:133:VAL:HG22	4:H:229:VAL:CG1	2.25	0.66
2:D:274:LEU:HD22	2:D:340:MET:CE	2.25	0.66
1:B:66:VAL:HG13	1:B:76:ILE:HB	1.79	0.64
3:F:193:THR:HG21	5:J:119:ASP:OD2	1.97	0.64
1:A:344:ARG:NH1	1:A:348:VAL:O	2.33	0.62
3:E:269:LEU:HD22	3:E:273:MET:HE2	1.83	0.60
1:B:86:THR:HG22	1:B:160:ASN:HA	1.84	0.59
2:C:62:ARG:NH1	2:C:348:ASP:OD1	2.35	0.59
2:D:241:ALA:HA	2:D:340:MET:HE3	1.84	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:202:GLU:HA	4:G:300:LEU:HD23	1.86	0.58
1:A:186:LYS:HE3	2:D:297:PHE:CD2	2.40	0.55
3:E:193:THR:HG21	5:I:119:ASP:OD2	2.07	0.55
1:B:344:ARG:NH1	1:B:348:VAL:O	2.40	0.55
4:G:235:PHE:HB3	4:G:300:LEU:HD13	1.89	0.54
4:G:133:VAL:HG13	4:G:229:VAL:HG12	1.90	0.54
2:D:183:ARG:O	2:D:184:LYS:HG3	2.08	0.53
1:B:55:ARG:HH12	1:B:198:GLU:CD	2.17	0.53
1:A:86:THR:HG22	1:A:160:ASN:HA	1.90	0.52
3:E:443:PHE:HB2	3:E:516:LEU:HD23	1.91	0.51
3:F:269:LEU:HD22	3:F:273:MET:HE2	1.91	0.51
1:A:211:ARG:NH1	1:A:280:GLU:OE2	2.44	0.51
1:B:78:TYR:CG	1:B:156:ILE:HD12	2.45	0.51
3:F:344:ARG:NH1	3:F:348:GLU:OE2	2.44	0.51
1:A:56:PHE:CE1	1:A:65:ARG:HD2	2.46	0.51
2:C:284:SER:O	2:C:286:HIS:O	2.28	0.50
4:G:300:LEU:HD12	4:G:304:TYR:CD1	2.46	0.50
1:B:186:LYS:HE3	2:C:297:PHE:CD2	2.46	0.49
4:G:192:LEU:N	4:G:192:LEU:CD1	2.75	0.49
2:D:81:MET:HE2	2:D:81:MET:HA	1.94	0.49
1:A:197:HIS:CE1	1:A:219:GLN:HG3	2.48	0.49
1:A:47:LEU:C	1:A:47:LEU:HD23	2.38	0.48
1:B:432:THR:HG22	1:B:433:SER:H	1.77	0.48
2:D:246:ARG:NH1	2:D:281:GLU:OE1	2.42	0.48
2:C:21:THR:HG22	2:C:27:GLY:HA2	1.96	0.48
1:A:193:PRO:HG3	2:D:304:GLU:HB2	1.95	0.47
2:C:236:THR:CG2	2:C:245:LEU:HD13	2.43	0.47
4:H:192:LEU:HD12	4:H:192:LEU:N	2.28	0.47
3:E:180:PHE:CZ	3:E:452:PHE:CE2	3.02	0.47
3:F:178:SER:HA	3:F:181:SER:HB3	1.96	0.47
3:E:227:ILE:HD11	3:E:312:ILE:HG21	1.96	0.47
2:C:241:ALA:HA	2:C:340:MET:HE3	1.97	0.47
4:G:186:ILE:HD13	4:G:186:ILE:HA	1.78	0.47
3:F:388:ILE:N	3:F:389:PRO:CD	2.78	0.46
2:D:271:MET:HA	2:D:271:MET:HE2	1.96	0.46
4:H:178:VAL:HG11	4:H:186:ILE:HG13	1.96	0.46
1:B:186:LYS:HE3	2:C:297:PHE:CG	2.51	0.46
4:H:119:ILE:O	4:H:146:LYS:HD3	2.16	0.46
2:C:81:MET:HE3	2:C:272:PHE:HB2	1.96	0.46
1:B:396:LEU:HG	1:B:400:VAL:HG11	1.98	0.45
3:E:167:VAL:HG22	3:E:202:VAL:HG11	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:ARG:NH2	2:D:351:LEU:O	2.48	0.44
1:B:362:LEU:CD2	1:B:379:ILE:HD12	2.48	0.44
1:B:376:ASN:O	1:B:393:GLN:HA	2.18	0.43
2:C:236:THR:HG21	2:C:245:LEU:CD2	2.34	0.43
3:F:183:LEU:HD22	3:F:455:ASN:O	2.18	0.43
4:G:198:GLU:HG2	4:G:208:ASN:HA	2.00	0.43
3:E:188:ARG:HH11	3:E:458:ASP:CG	2.26	0.43
4:G:300:LEU:HD12	4:G:304:TYR:HD1	1.84	0.43
3:E:320:SER:HA	3:E:345:ILE:HG12	2.01	0.43
2:C:335:TYR:CE1	2:C:338:ARG:HD3	2.53	0.43
2:D:223:PHE:CD1	3:E:425:LEU:HD22	2.55	0.42
1:A:315:ARG:NH1	2:D:303:LEU:O	2.32	0.42
1:B:161:ILE:HD13	1:B:161:ILE:HA	1.86	0.42
2:C:171:SER:OG	2:C:174:VAL:HG23	2.19	0.42
4:G:70:GLU:OE2	4:G:237:ARG:NH1	2.52	0.42
4:G:75:PHE:O	4:G:96:ARG:NH2	2.48	0.42
3:F:338:CYS:HB2	3:F:368:GLU:HB3	2.02	0.42
1:B:315:ARG:NH1	2:C:303:LEU:O	2.50	0.41
4:H:186:ILE:HD13	4:H:186:ILE:HA	1.80	0.41
2:D:21:THR:HG22	2:D:27:GLY:HA2	2.02	0.41
2:C:255:ALA:HB1	2:C:320:LEU:HB3	2.02	0.41
5:J:391:LEU:C	5:J:391:LEU:HD13	2.46	0.41
1:B:324:GLU:HA	1:B:335:CYS:SG	2.60	0.41
3:F:395:LEU:CD1	3:F:426:VAL:HG12	2.51	0.41
3:F:322:PHE:CZ	3:F:505:GLY:HA2	2.56	0.41
3:F:443:PHE:HB2	3:F:516:LEU:HD23	2.02	0.41
4:H:191:ASP:C	4:H:192:LEU:HD12	2.46	0.41
2:C:159:ILE:HG23	2:C:165:ILE:HD11	2.02	0.41
1:A:376:ASN:O	1:A:393:GLN:HA	2.20	0.41
2:C:31:SER:OG	6:C:1000:PO4:O1	2.36	0.41
3:E:435:LEU:N	3:E:435:LEU:HD12	2.35	0.41
4:G:133:VAL:HG13	4:G:229:VAL:CG1	2.51	0.41
1:B:97:TRP:O	1:B:97:TRP:CE3	2.74	0.41
2:C:291:PRO:HB3	2:C:308:VAL:HB	2.03	0.41
2:C:183:ARG:O	2:C:184:LYS:HG2	2.21	0.40
3:F:257:LYS:HB2	3:F:258:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	433/461 (94%)	420 (97%)	13 (3%)	0	100	100
1	B	433/461 (94%)	413 (95%)	19 (4%)	1 (0%)	43	58
2	C	318/355 (90%)	313 (98%)	5 (2%)	0	100	100
2	D	323/355 (91%)	316 (98%)	7 (2%)	0	100	100
3	E	354/523 (68%)	349 (99%)	5 (1%)	0	100	100
3	F	354/523 (68%)	351 (99%)	3 (1%)	0	100	100
4	G	292/305 (96%)	286 (98%)	6 (2%)	0	100	100
4	H	292/305 (96%)	283 (97%)	9 (3%)	0	100	100
5	I	387/452 (86%)	369 (95%)	18 (5%)	0	100	100
5	J	387/452 (86%)	367 (95%)	20 (5%)	0	100	100
All	All	3573/4192 (85%)	3467 (97%)	105 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	176	LYS

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/405 (95%)	380 (99%)	4 (1%)	68	84
1	B	384/405 (95%)	379 (99%)	5 (1%)	61	80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	274/298 (92%)	274 (100%)	0	100	100
2	D	278/298 (93%)	274 (99%)	4 (1%)	59	79
3	E	312/444 (70%)	308 (99%)	4 (1%)	61	80
3	F	312/444 (70%)	310 (99%)	2 (1%)	78	89
4	G	253/260 (97%)	246 (97%)	7 (3%)	38	60
4	H	253/260 (97%)	245 (97%)	8 (3%)	34	56
5	I	347/398 (87%)	345 (99%)	2 (1%)	78	89
5	J	347/398 (87%)	347 (100%)	0	100	100
All	All	3144/3610 (87%)	3108 (99%)	36 (1%)	63	82

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	161	ILE
1	A	180	VAL
1	A	217	LYS
1	B	66	VAL
1	B	161	ILE
1	B	180	VAL
1	B	318	VAL
1	B	330	SER
2	D	148	MET
2	D	163	GLU
2	D	175	GLU
2	D	328	ILE
3	E	246	GLU
3	E	282	LYS
3	E	328	SER
3	E	462	ASP
3	F	431	ASN
3	F	454	SER
4	G	24	VAL
4	G	160	SER
4	G	186	ILE
4	G	192	LEU
4	G	229	VAL
4	G	268	GLU
4	G	279	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	H	24	VAL
4	H	186	ILE
4	H	192	LEU
4	H	229	VAL
4	H	245	ASP
4	H	255	ASP
4	H	279	SER
4	H	297	SER
5	I	177	ASP
5	I	185	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	HIS
1	A	216	GLN
1	A	341	ASN
1	A	359	ASN
1	A	376	ASN
1	B	101	GLN
1	B	216	GLN
2	C	132	ASN
2	D	72	GLN
2	D	132	ASN
2	D	260	HIS
3	E	309	GLN
3	E	411	ASN
3	E	470	HIS
3	F	190	ASN
3	F	411	ASN
3	F	470	HIS
4	G	208	ASN
4	G	270	HIS
4	H	208	ASN
4	H	213	ASN
4	H	270	HIS
5	I	154	GLN
5	I	303	HIS
5	I	363	GLN
5	I	405	GLN
5	J	115	HIS
5	J	303	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	J	363	GLN

### 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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	PO4	D	1000	-	4,4,4	0.39	0	6,6,6	0.82	0
6	PO4	C	1000	-	4,4,4	1.02	0	6,6,6	0.76	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1000	PO4	1	0

## 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.

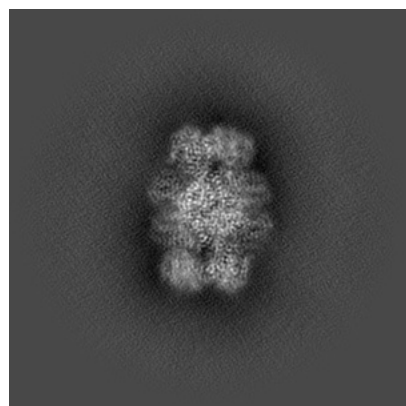
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72467. These allow visual inspection of the internal detail of the map and identification of artifacts.

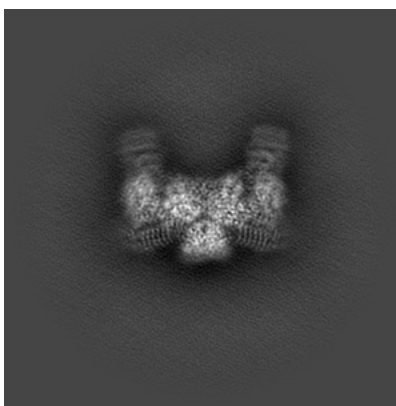
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

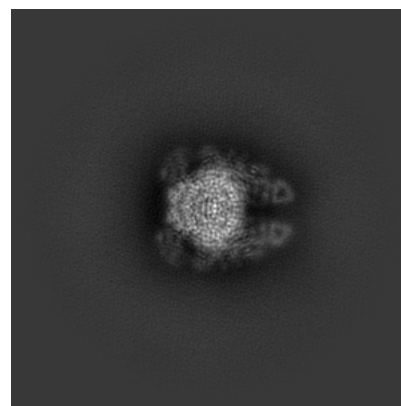
#### 6.1.1 Primary map



X

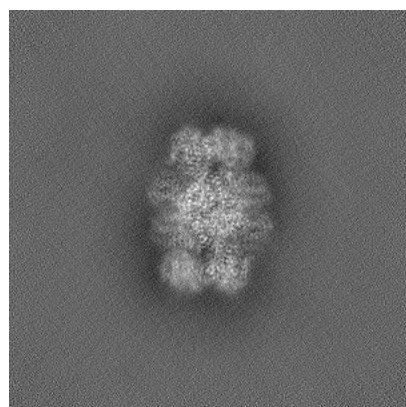


Y

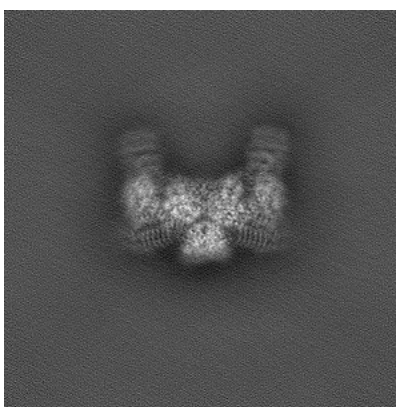


Z

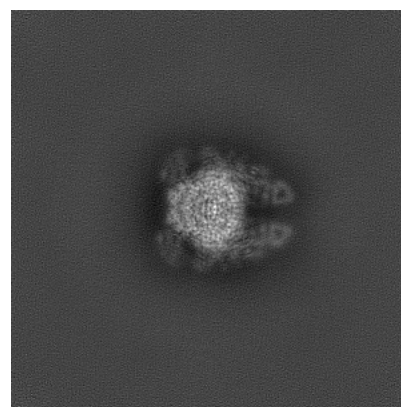
#### 6.1.2 Raw map



X



Y



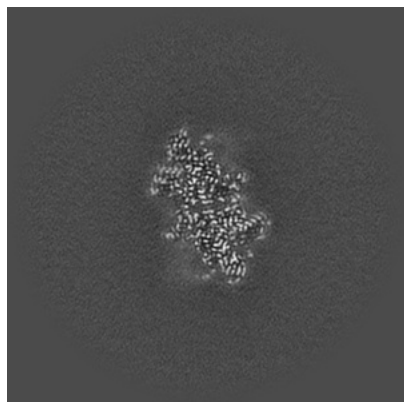
Z

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

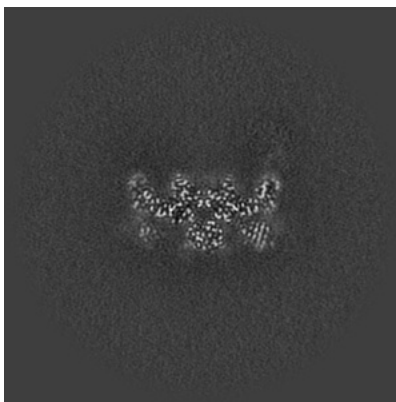


## 6.2 Central slices [i](#)

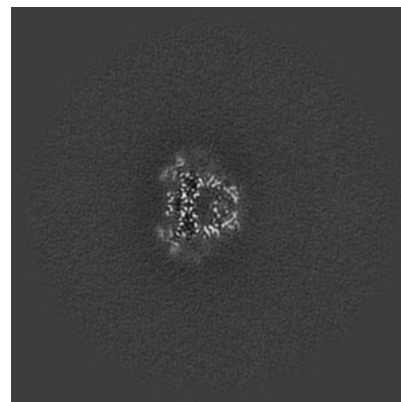
### 6.2.1 Primary map



X Index: 200

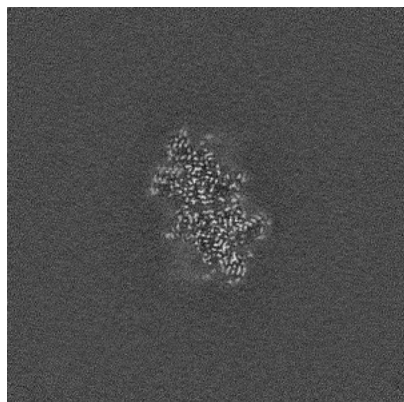


Y Index: 200

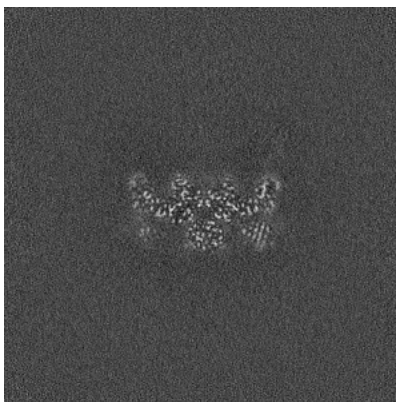


Z Index: 200

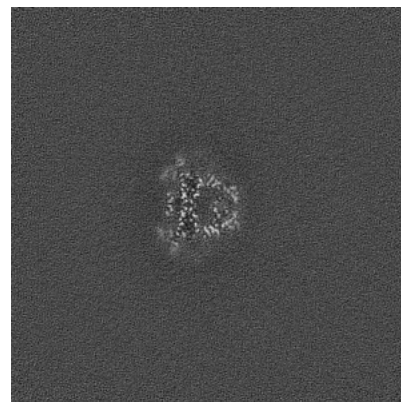
### 6.2.2 Raw map



X Index: 200



Y Index: 200



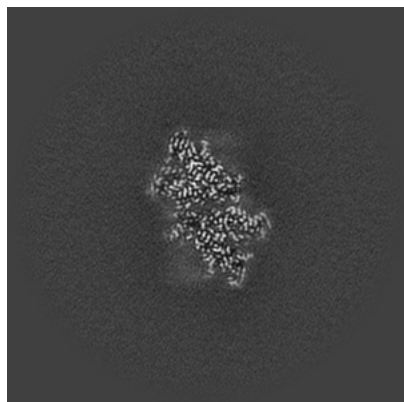
Z Index: 200

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

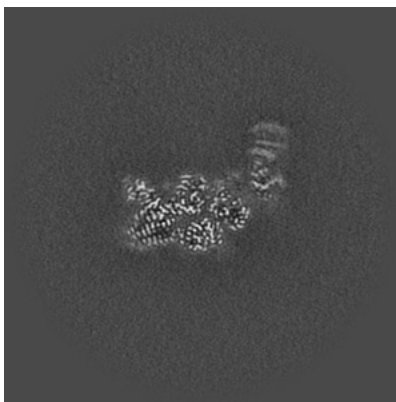


## 6.3 Largest variance slices [i](#)

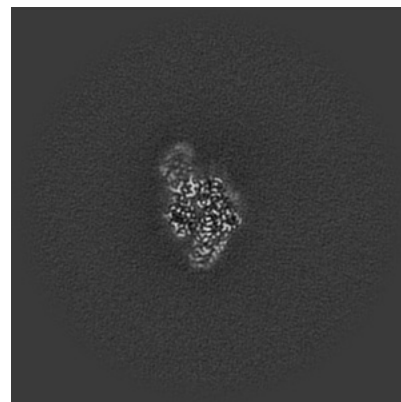
### 6.3.1 Primary map



X Index: 198

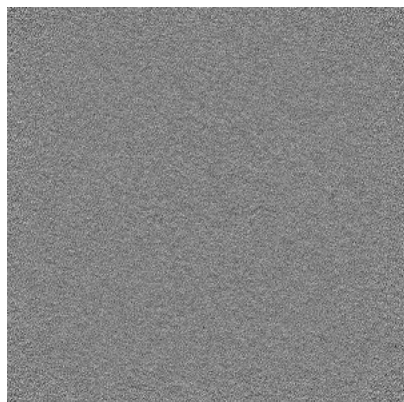


Y Index: 213

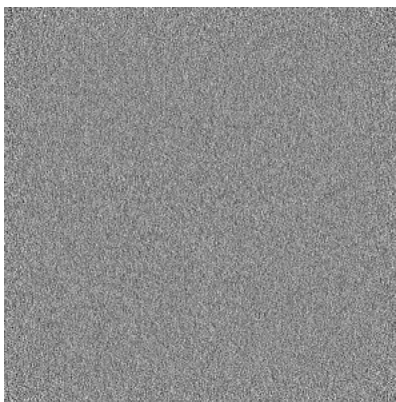


Z Index: 213

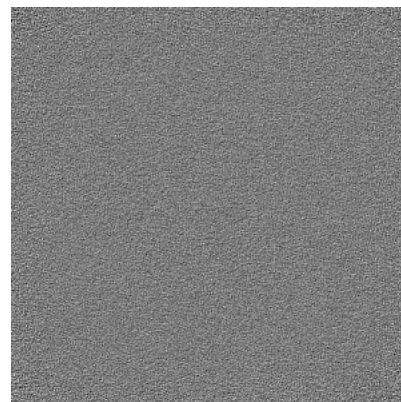
### 6.3.2 Raw map



X Index: 0



Y Index: 0

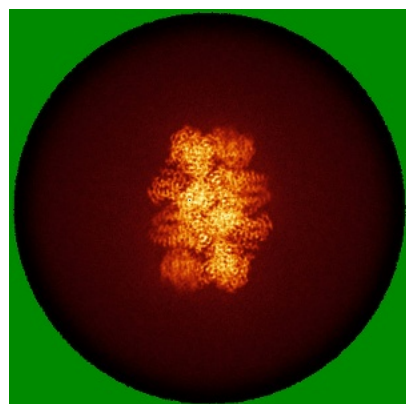


Z Index: 0

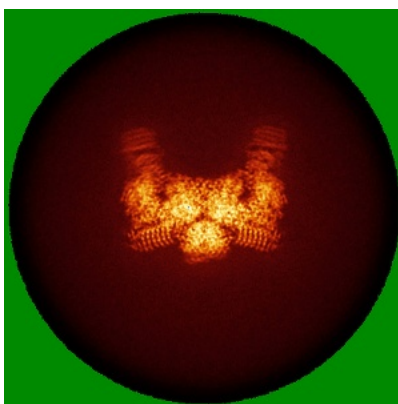
The images above show the largest variance slices of the map in three orthogonal directions.

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

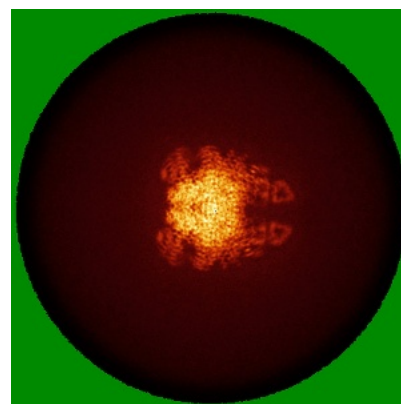
### 6.4.1 Primary map



X

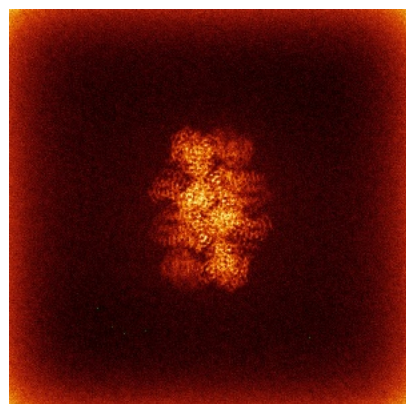


Y

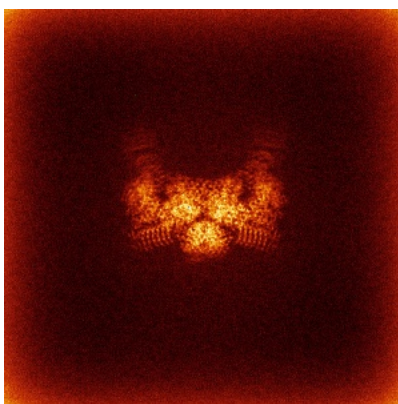


Z

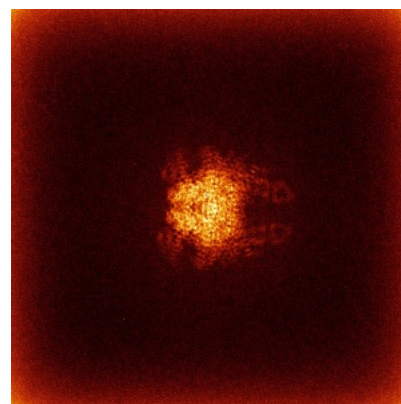
### 6.4.2 Raw map



X



Y

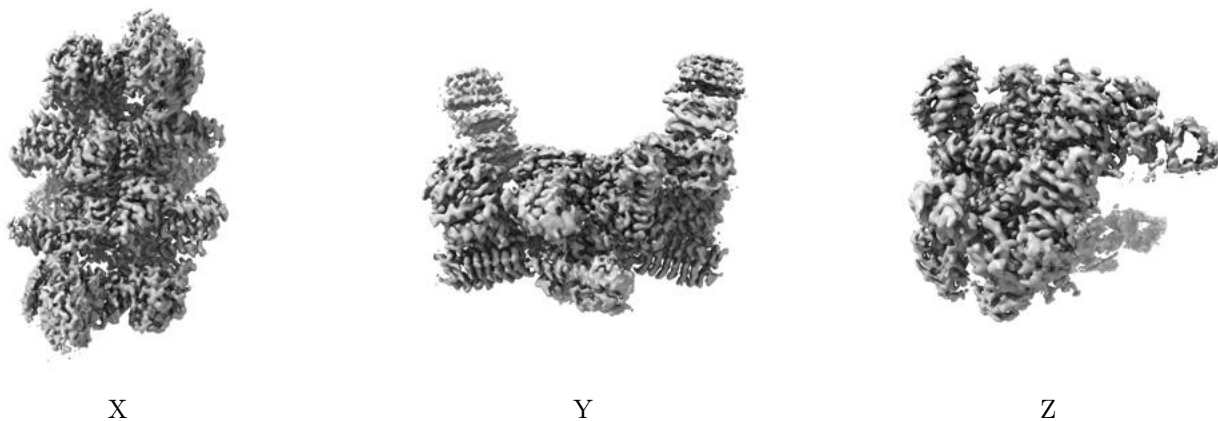


Z

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.

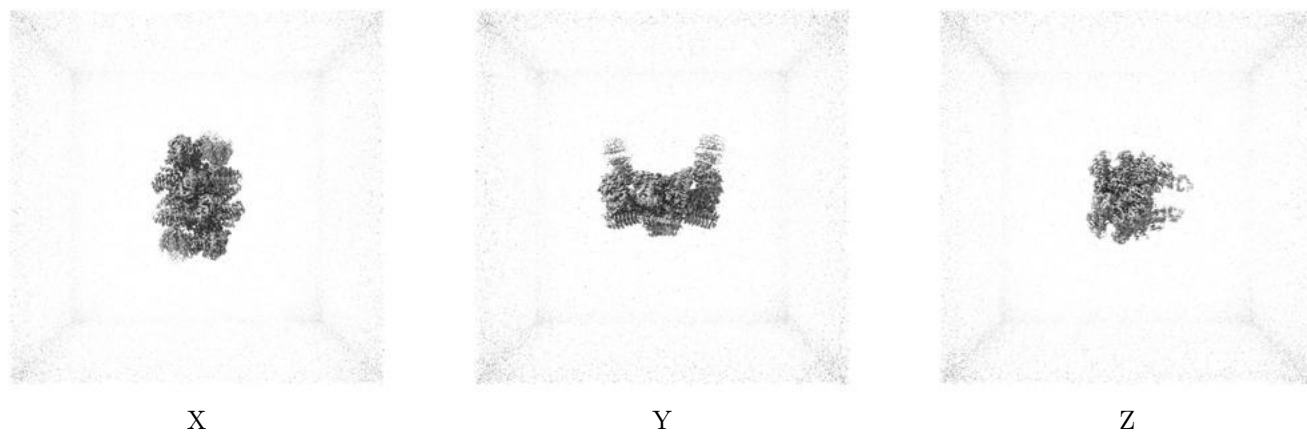
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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



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.

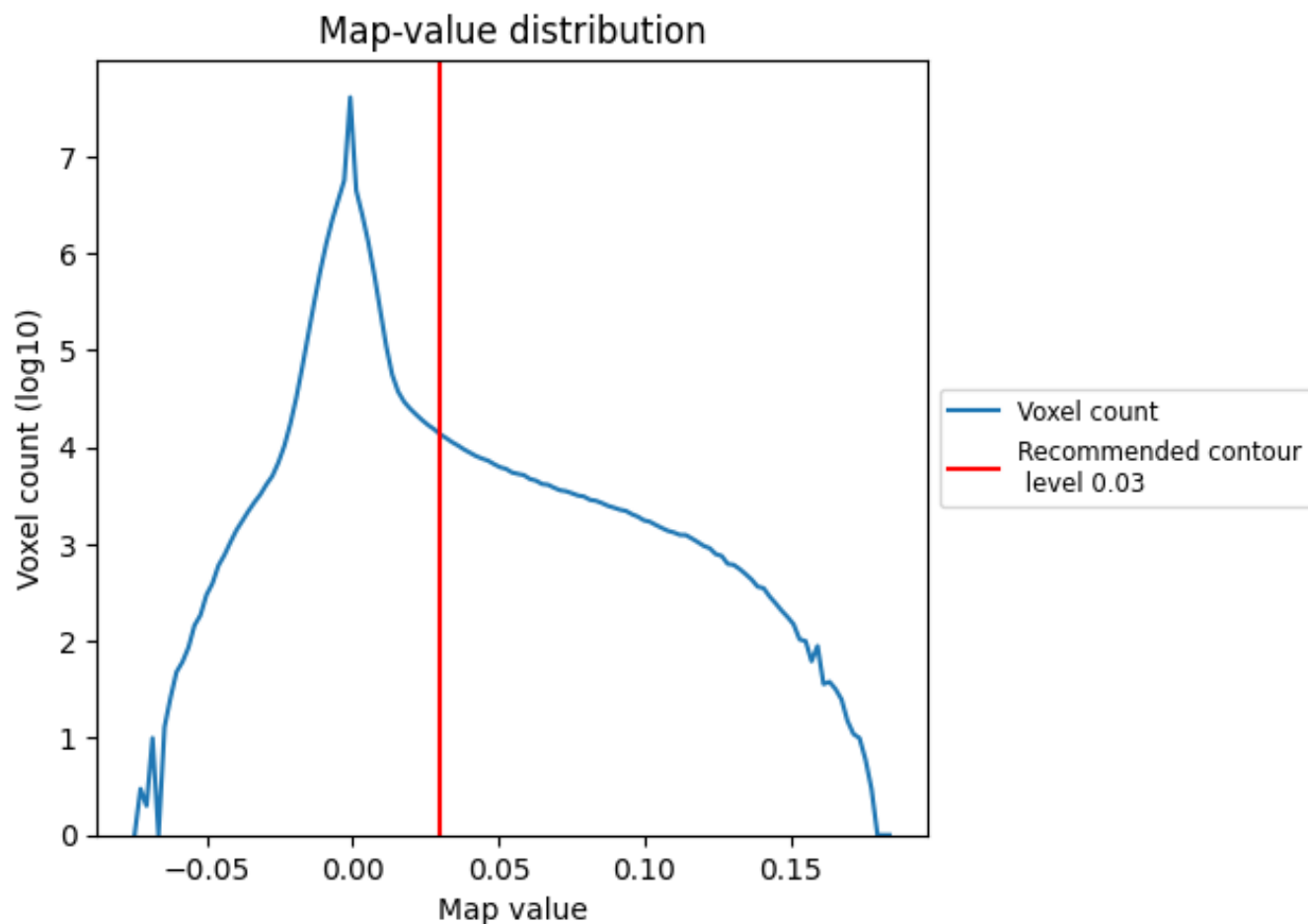
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

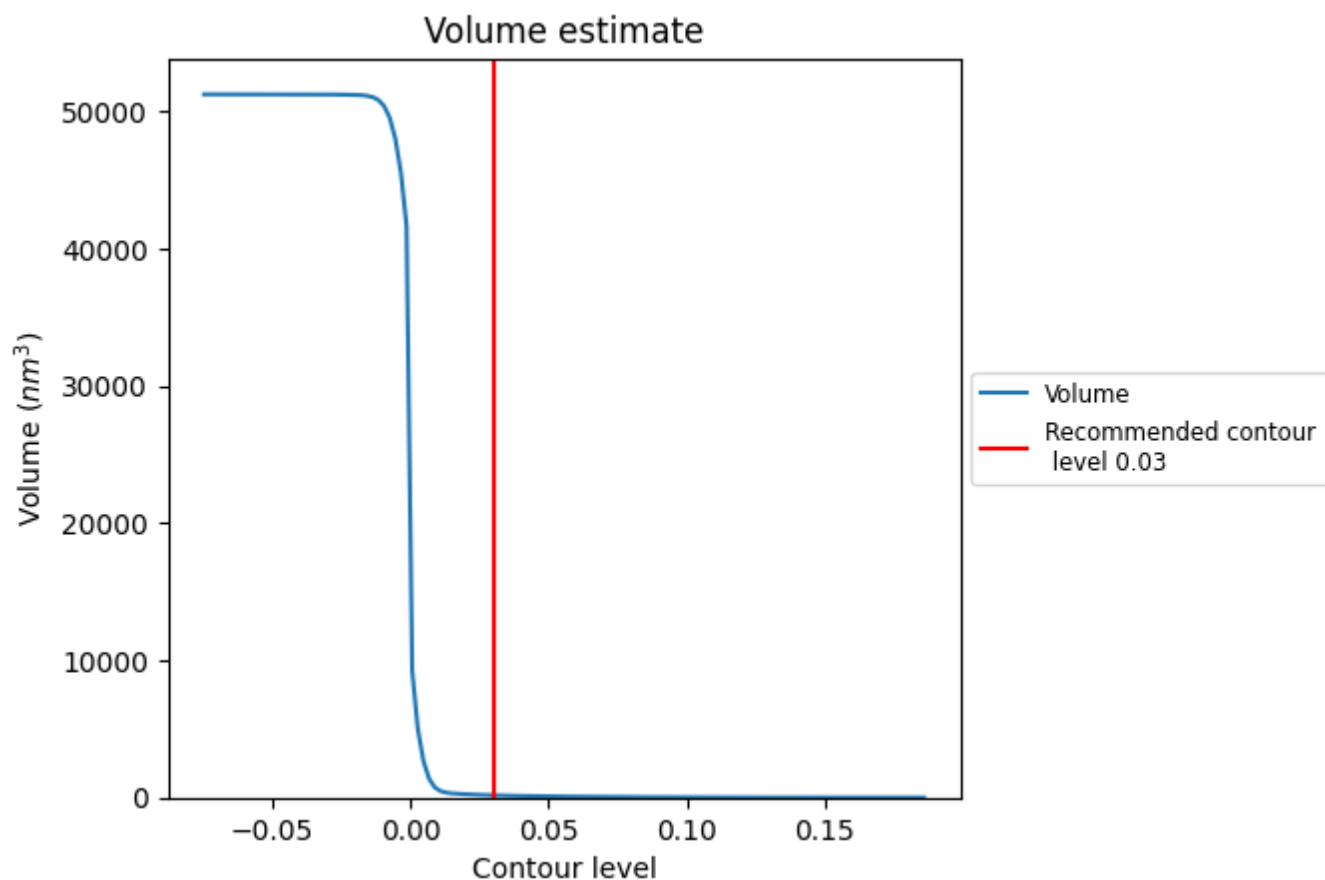
This section contains the results of statistical analysis of the map.

### 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.

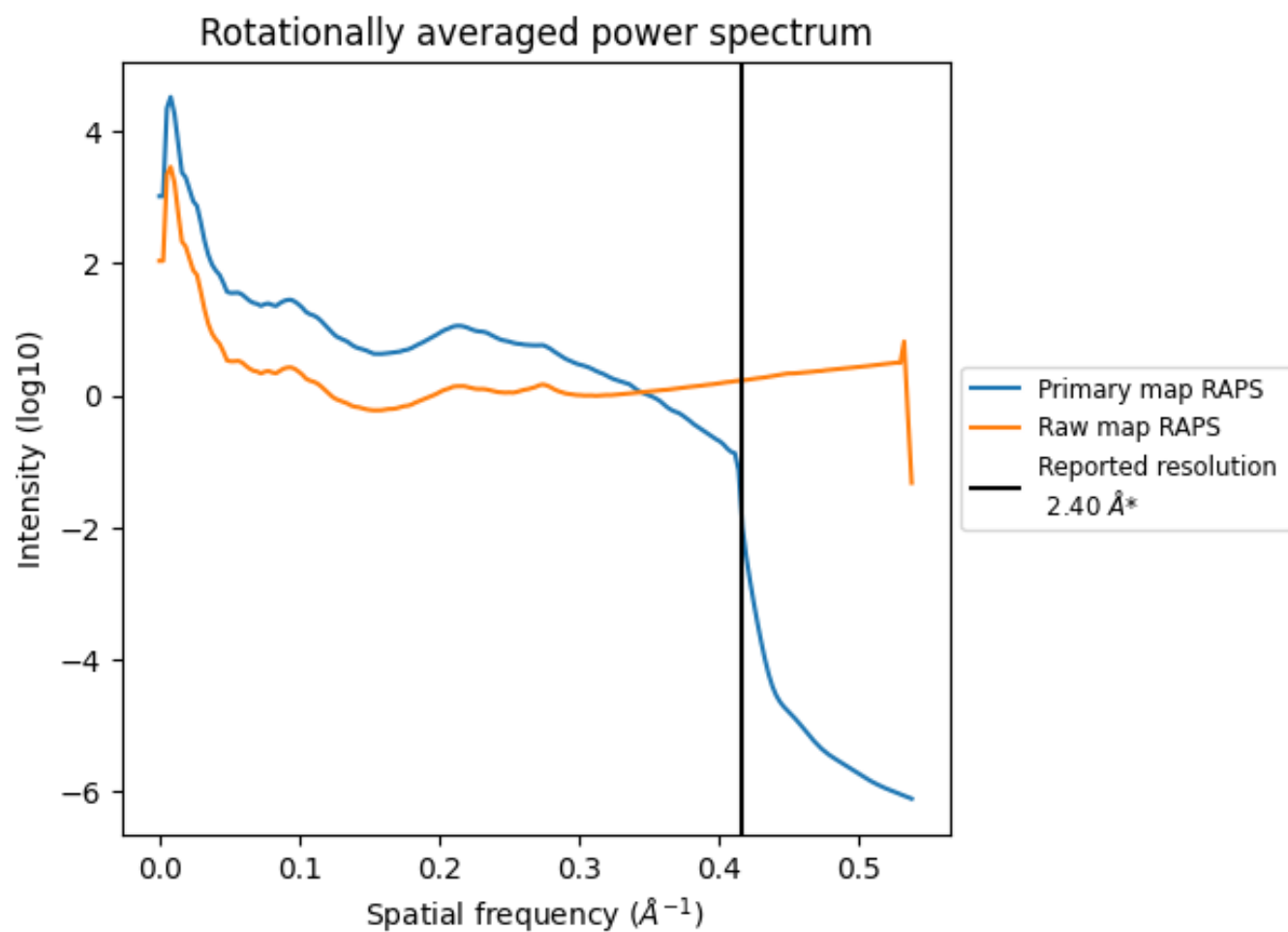
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm<sup>3</sup>; this corresponds to an approximate mass of 149 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



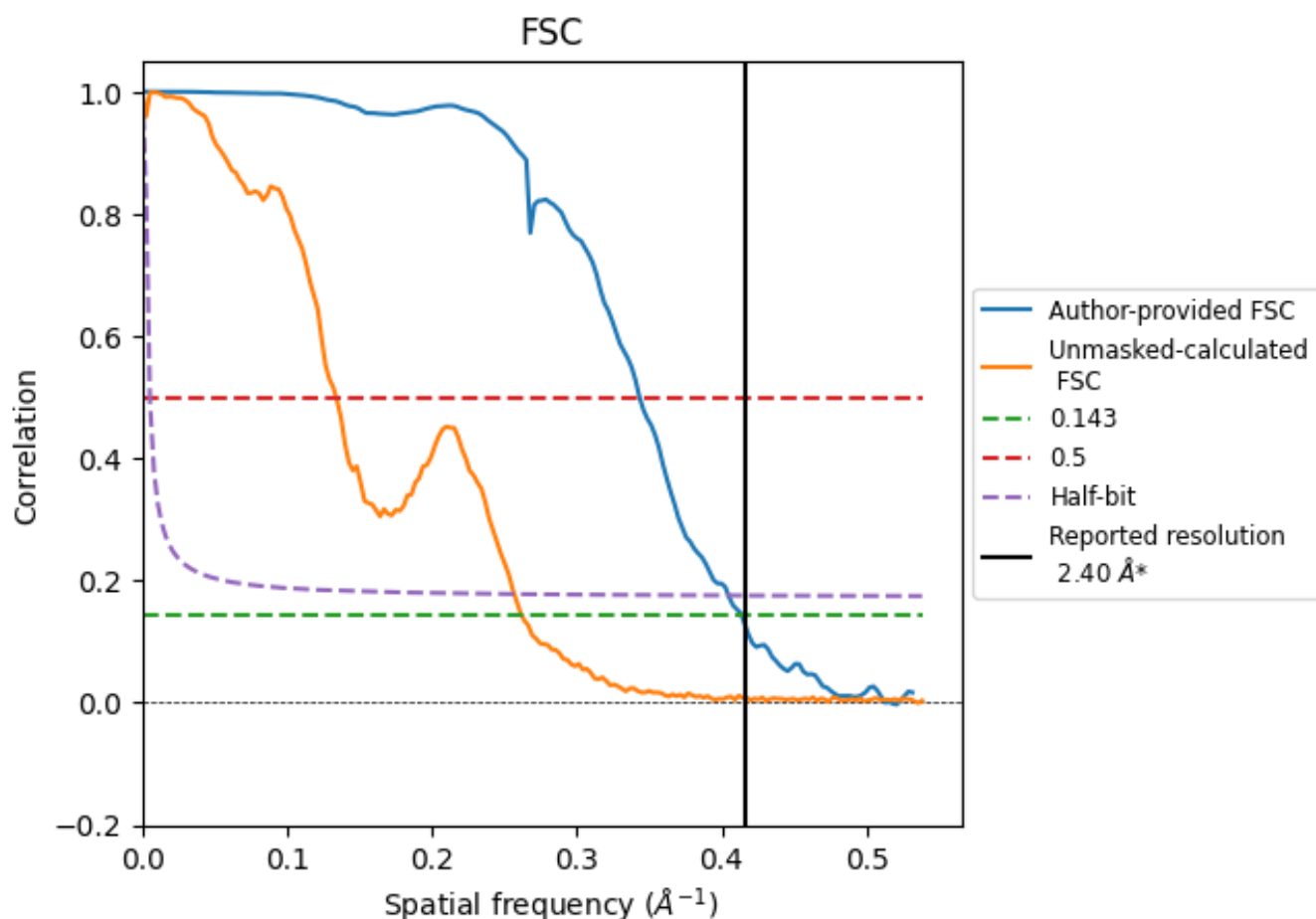
\*Reported resolution corresponds to spatial frequency of 0.417 Å<sup>-1</sup>



## 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  $0.417 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.42	2.91	2.47
Unmasked-calculated*	3.82	7.47	3.89

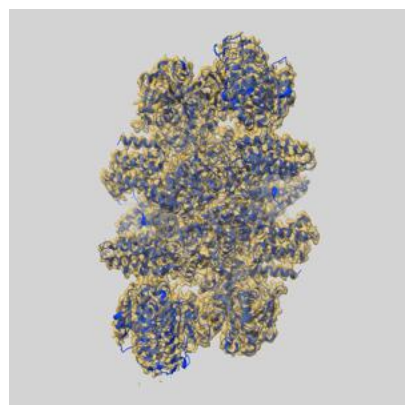
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 2.4 by more than 10 %



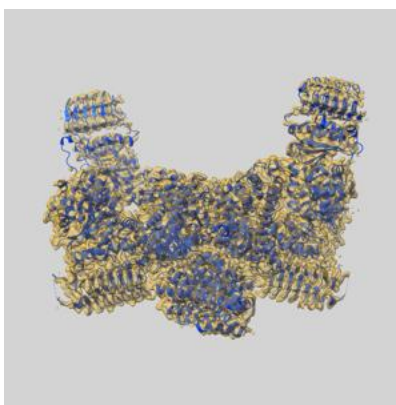
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72467 and PDB model 9Y3U. Per-residue inclusion information can be found in section [3](#) on page [8](#).

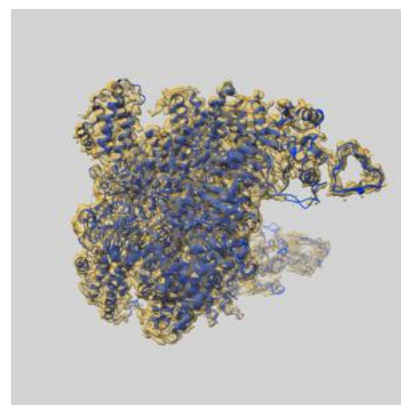
### 9.1 Map-model overlay [i](#)



X



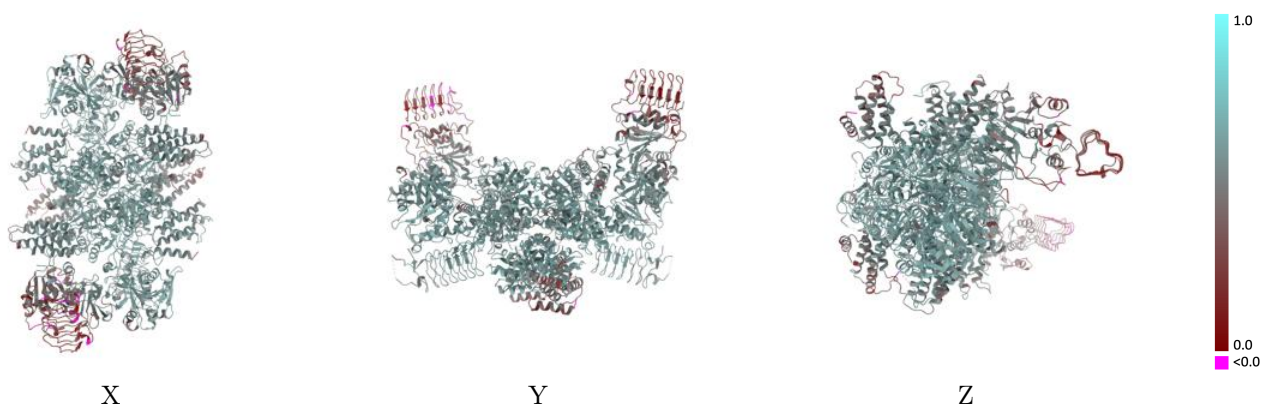
Y



Z

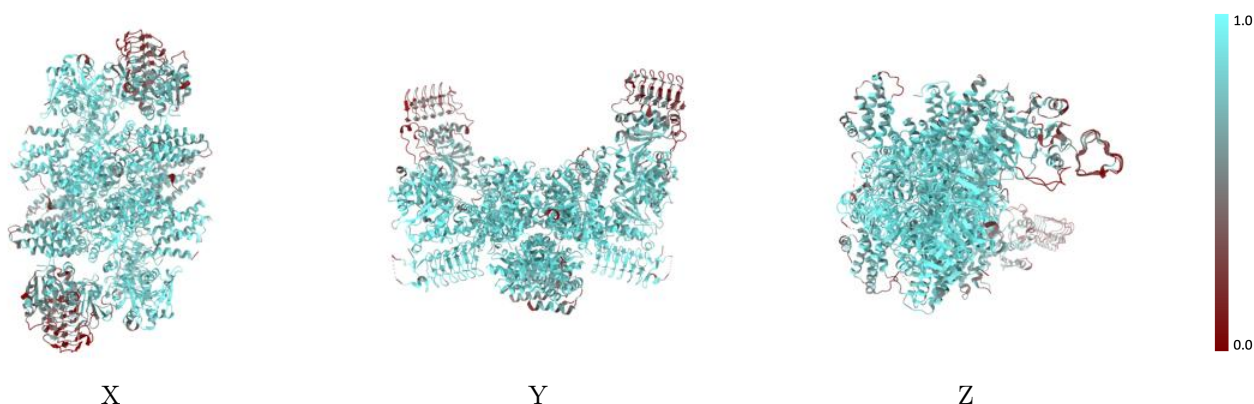
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



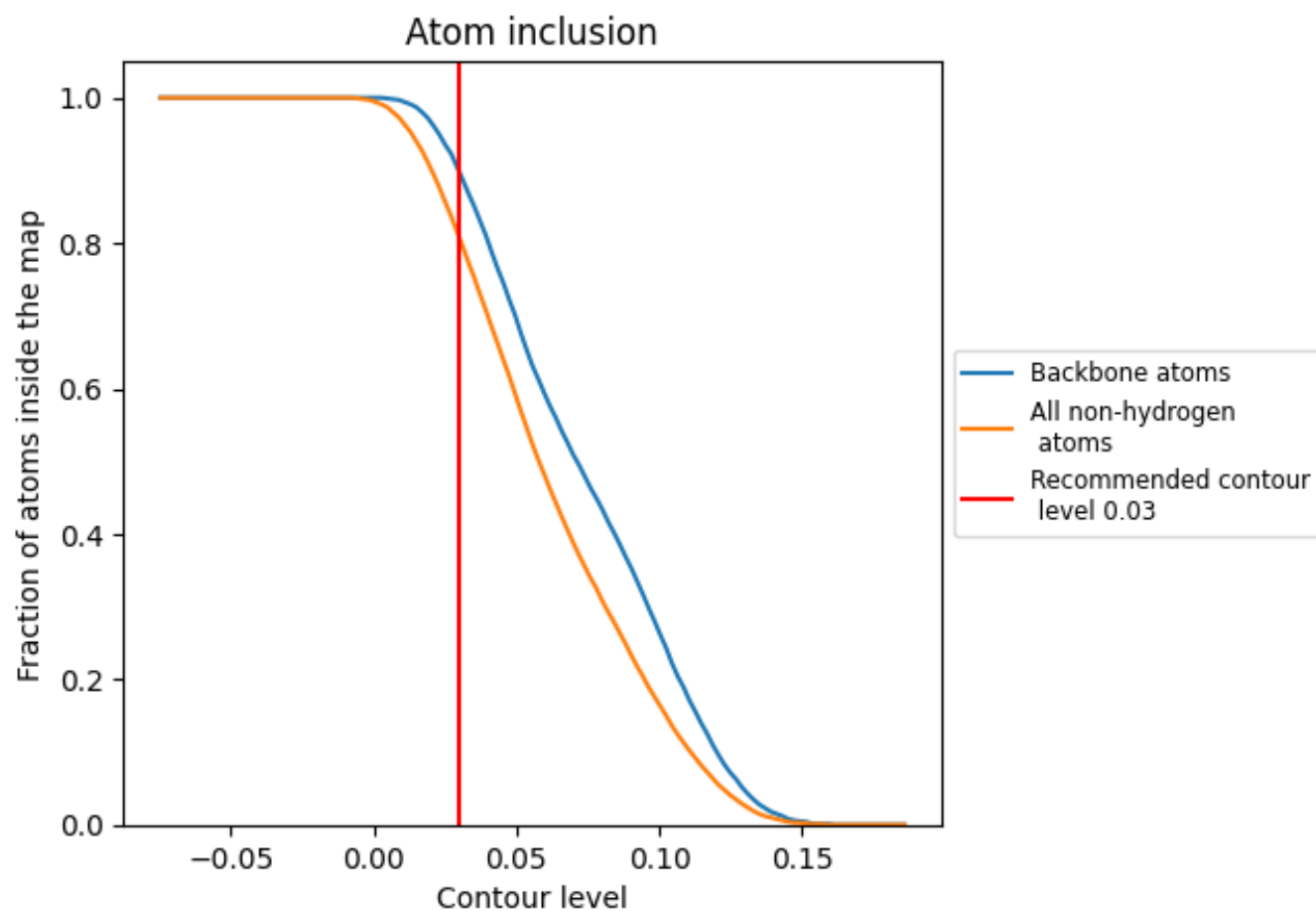
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8080	<div></div> 0.5400
A	<div></div> 0.8870	<div></div> 0.5910
B	<div></div> 0.8950	<div></div> 0.5870
C	<div></div> 0.9100	<div></div> 0.5960
D	<div></div> 0.8960	<div></div> 0.5920
E	<div></div> 0.8560	<div></div> 0.5810
F	<div></div> 0.8660	<div></div> 0.5890
G	<div></div> 0.8370	<div></div> 0.5480
H	<div></div> 0.8440	<div></div> 0.5490
I	<div></div> 0.5810	<div></div> 0.4170
J	<div></div> 0.5420	<div></div> 0.3650

1.0

0.0

<0.0