



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 01:44 PM UTC

PDB ID : 7TKL / pdb\_00007tkl  
EMDB ID : EMD-25973  
Title : Yeast ATP synthase State 3binding(a) with 10 mM ATP backbone model  
Authors : Guo, H.; Rubinstein, J.L.  
Deposited on : 2022-01-17  
Resolution : 6.40 Å (reported)  
Based on initial model : 2HLD

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>.

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

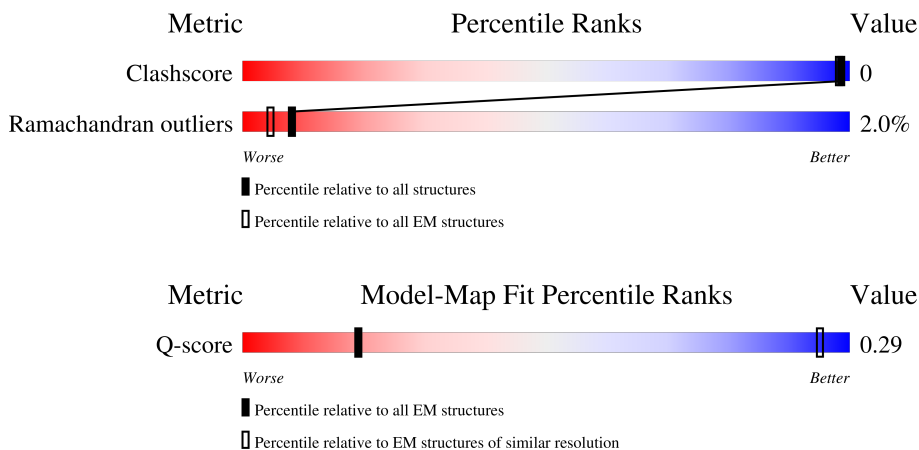
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 6.40 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	-
Q-score	-	25397	544 ( 5.90 - 6.90 )

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	0	76	8% 95% ..
1	1	76	7% 92% 7% ..
1	2	76	7% 96% ..
1	3	76	11% 93% ...
1	4	76	14% 89% 9% ..

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Mol	Chain	Length	Quality of chain
1	5	76	18% 92% 7%
1	6	76	22% 89% 8%
1	7	76	11% 89% 7%
1	8	76	8% 93% ..
1	9	76	13% 91% 7%
2	A	510	89% 9%
2	B	510	92% 8%
2	C	510	90% 7%
3	D	478	89% 9%
3	E	478	90% 7%
3	F	478	89% 9%
4	G	278	89% 6% 5%
5	H	138	80% 7% 13%
6	I	61	77% 21%
7	O	195	84% 12%
8	T	249	6% 86% 10%
9	U	209	73% 26%
10	V	173	19% 86% 13%
11	W	95	18% 77% 11% 11%
12	X	92	18% 57% 11% 33%
13	Y	59	8% 56% 7% 37%
14	Z	48	6% 98%

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 20227 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 ATP synthase subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	75	Total 300	C 150	N 75	O 75	0	0
1	1	75	Total 300	C 150	N 75	O 75	0	0
1	2	75	Total 300	C 150	N 75	O 75	0	0
1	3	74	Total 296	C 148	N 74	O 74	0	0
1	4	75	Total 300	C 150	N 75	O 75	0	0
1	5	75	Total 300	C 150	N 75	O 75	0	0
1	6	74	Total 296	C 148	N 74	O 74	0	0
1	7	73	Total 292	C 146	N 73	O 73	0	0
1	8	75	Total 300	C 150	N 75	O 75	0	0
1	9	74	Total 296	C 148	N 74	O 74	0	0

- Molecule 2 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	A	499	Total 1996	C 998	N 499	O 499	0	0
2	B	507	Total 2028	C 1014	N 507	O 507	0	0
2	C	496	Total 1984	C 992	N 496	O 496	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	468	Total	C	N	O	0	0
			1872	936	468	468		
3	E	469	Total	C	N	O	0	0
			1876	938	469	469		
3	F	470	Total	C	N	O	0	0
			1880	940	470	470		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	265	Total	C	N	O	0	0
			1059	530	265	264		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	120	Total	C	N	O	0	0
			480	240	120	120		

- Molecule 6 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	I	48	Total	C	N	O	0	0
			193	96	48	49		

- Molecule 7 is a protein called ATP synthase subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	187	Total	C	N	O	0	0
			748	374	187	187		

- Molecule 8 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	T	224	Total	C	N	O	0	0
			897	448	224	225		

- Molecule 9 is a protein called ATP synthase subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	U	155	Total	C	N	O	0	0
			620	310	155	155		

- Molecule 10 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	V	171	685	342	171	172	0	0

- Molecule 11 is a protein called ATP synthase subunit f.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	W	85	340	170	85	85	0	0

- Molecule 12 is a protein called ATP synthase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	X	62	248	124	62	62	0	0

- Molecule 13 is a protein called ATP synthase subunit J.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	Y	37	148	74	37	37	0	0

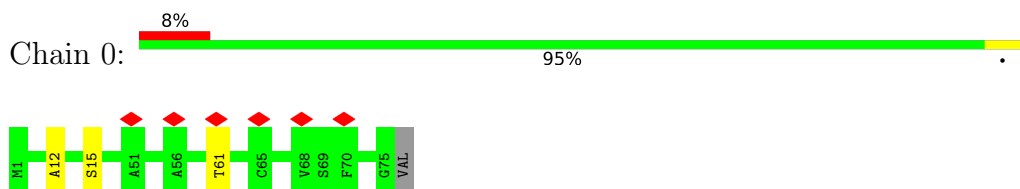
- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	Z	48	193	96	48	49	0	0

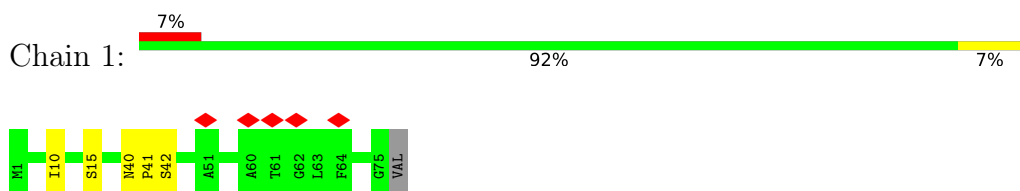
### 3 Residue-property plots [i](#)

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.

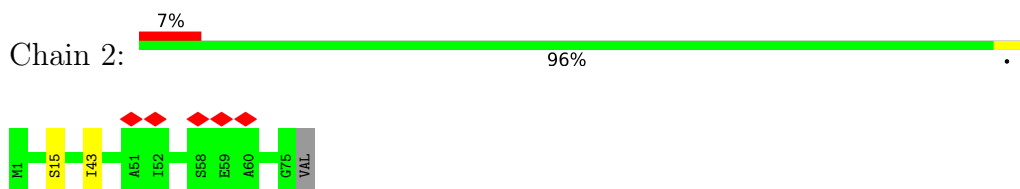
- Molecule 1: ATP synthase subunit 9



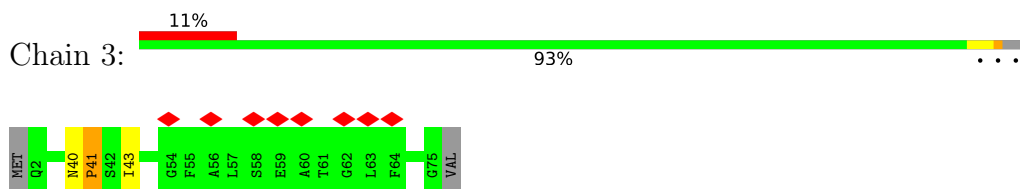
- Molecule 1: ATP synthase subunit 9



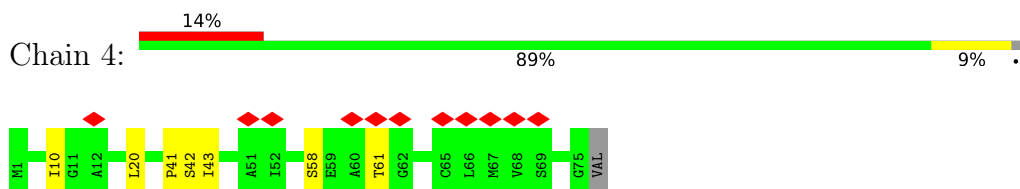
- Molecule 1: ATP synthase subunit 9



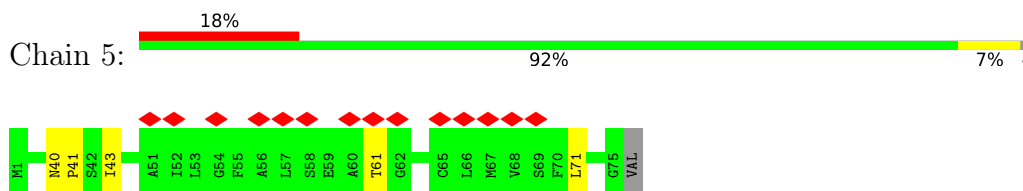
- Molecule 1: ATP synthase subunit 9



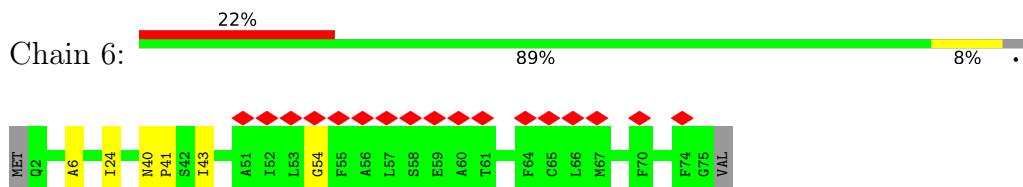
- Molecule 1: ATP synthase subunit 9



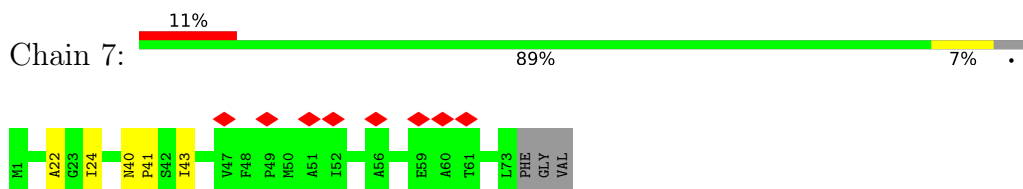
- Molecule 1: ATP synthase subunit 9



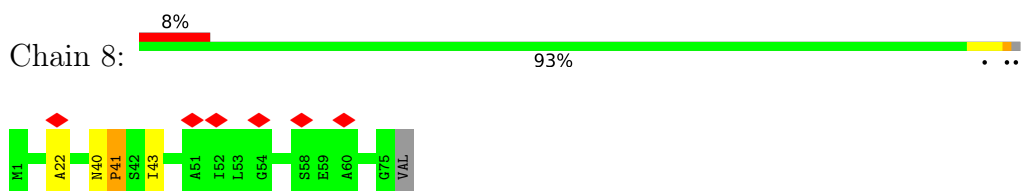
- Molecule 1: ATP synthase subunit 9



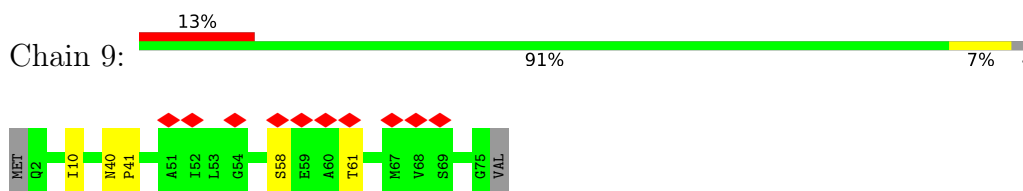
- Molecule 1: ATP synthase subunit 9



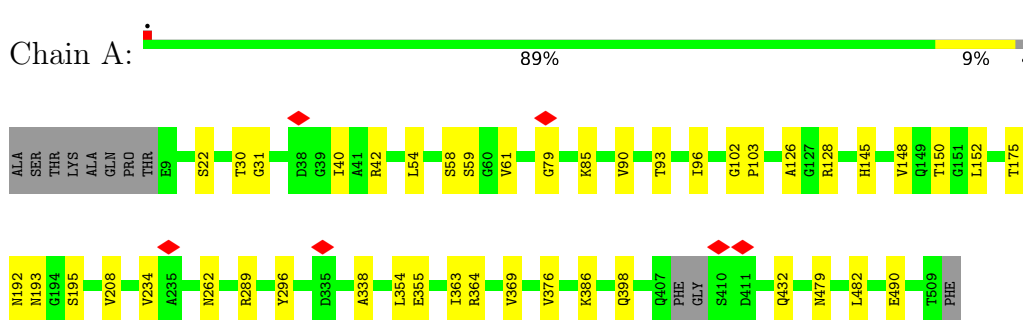
- Molecule 1: ATP synthase subunit 9




- Molecule 1: ATP synthase subunit 9

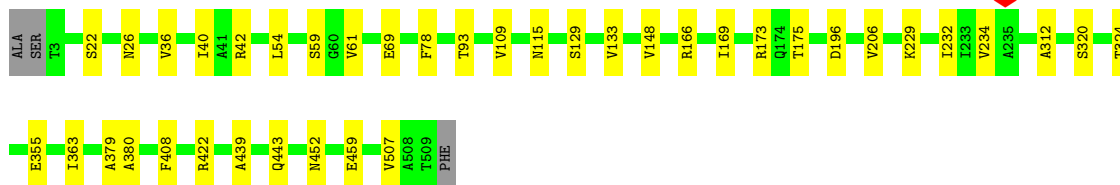


- Molecule 2: ATP synthase subunit alpha




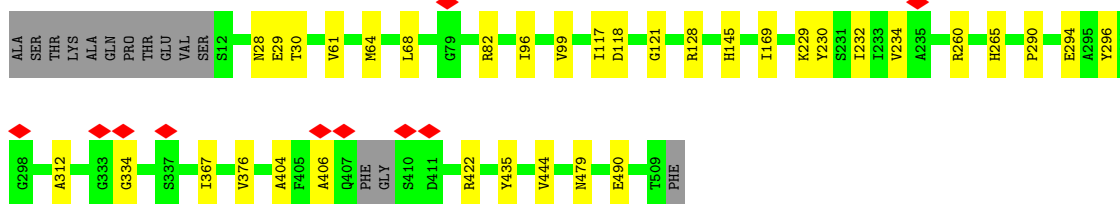
- Molecule 2: ATP synthase subunit alpha

Chain B:  92% 8%




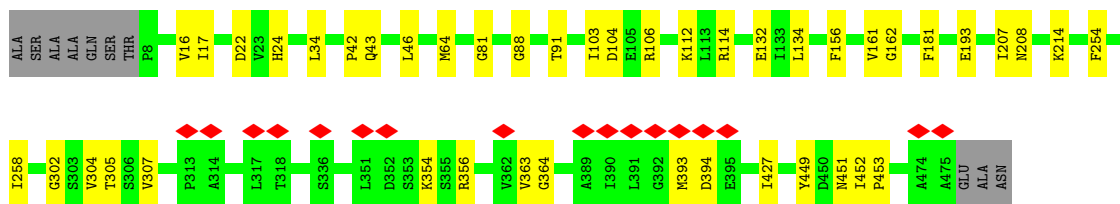
- Molecule 2: ATP synthase subunit alpha

Chain C:  90% 7%




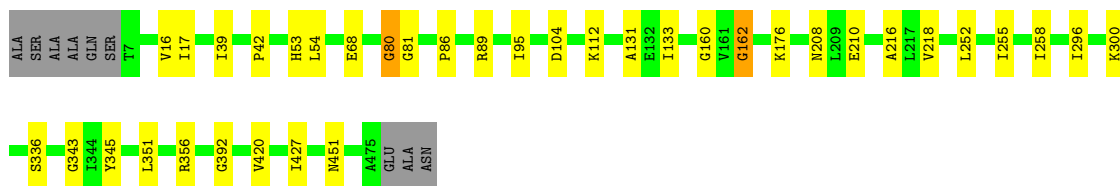
- Molecule 3: ATP synthase subunit beta

Chain D:  89% 9%




- Molecule 3: ATP synthase subunit beta

Chain E:  90% 7%



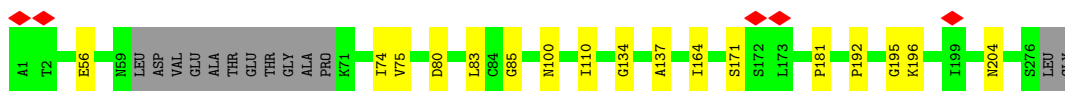
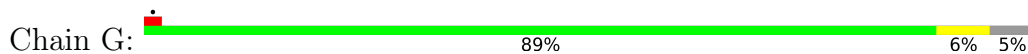
- Molecule 3: ATP synthase subunit beta

Chain F:  89% 9%

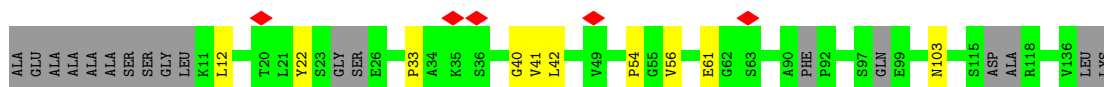
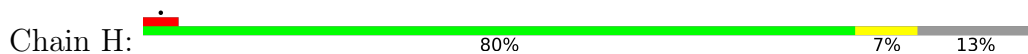




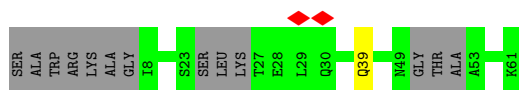
- Molecule 4: ATP synthase subunit gamma



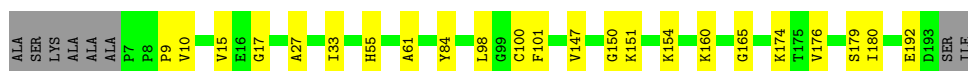
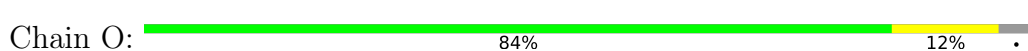
- Molecule 5: ATP synthase subunit delta



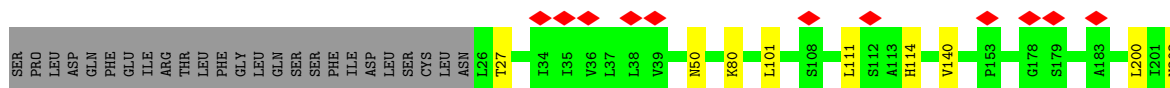
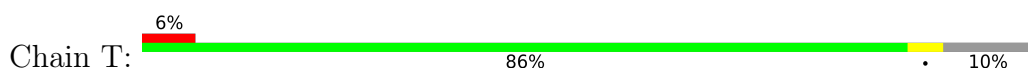
- Molecule 6: ATP synthase subunit epsilon



- Molecule 7: ATP synthase subunit 5

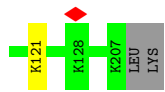
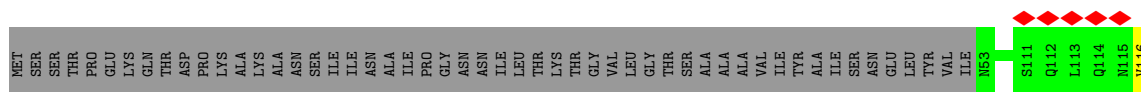


- Molecule 8: ATP synthase subunit a

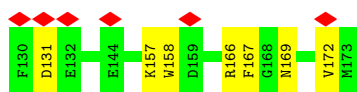
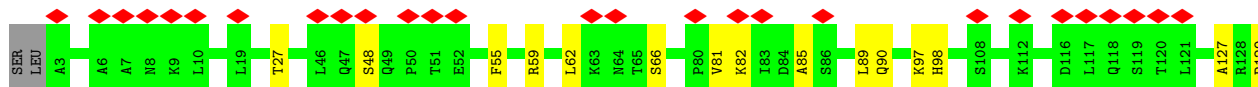
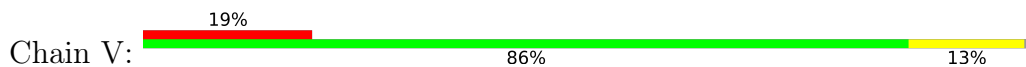


- Molecule 9: ATP synthase subunit 4

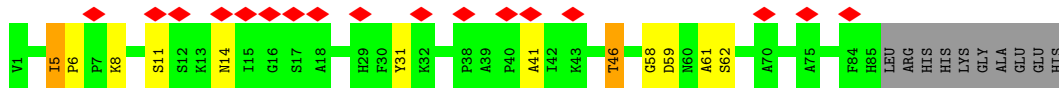
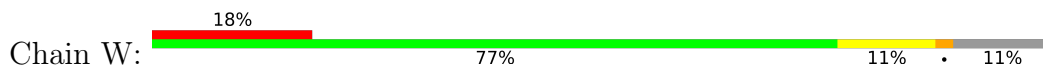




• Molecule 10: ATP synthase subunit d



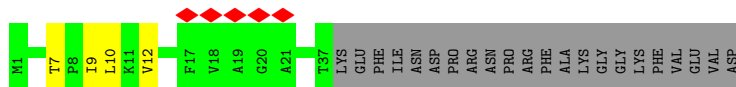
• Molecule 11: ATP synthase subunit f



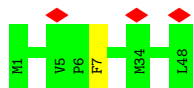
• Molecule 12: ATP synthase subunit H



• Molecule 13: ATP synthase subunit J



• Molecule 14: ATP synthase protein 8



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12214	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	103896	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.988	Depositor
Minimum map value	-0.606	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.6	Depositor
Map size ( $\text{\AA}$ )	344.96, 344.96, 344.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3475, 1.3475, 1.3475	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	0	1.23	0/299	2.14	6/372 (1.6%)
1	1	1.23	0/299	2.04	4/372 (1.1%)
1	2	1.23	0/299	2.10	4/372 (1.1%)
1	3	1.24	0/295	1.98	3/367 (0.8%)
1	4	1.24	0/299	2.13	10/372 (2.7%)
1	5	1.20	0/299	2.10	6/372 (1.6%)
1	6	1.21	0/295	2.21	8/367 (2.2%)
1	7	1.24	0/291	2.18	6/362 (1.7%)
1	8	1.20	0/299	2.17	5/372 (1.3%)
1	9	1.21	0/295	2.07	6/367 (1.6%)
2	A	1.55	0/1994	1.82	40/2489 (1.6%)
2	B	1.56	0/2027	1.75	35/2532 (1.4%)
2	C	1.57	0/1982	1.80	30/2474 (1.2%)
3	D	1.57	0/1871	1.85	46/2337 (2.0%)
3	E	1.57	0/1875	1.80	32/2342 (1.4%)
3	F	1.57	1/1879 (0.1%)	1.83	41/2347 (1.7%)
4	G	1.37	0/1057	1.99	16/1318 (1.2%)
5	H	1.50	0/475	1.78	7/585 (1.2%)
6	I	1.40	0/190	1.75	0/231
7	O	1.60	0/747	1.88	15/932 (1.6%)
8	T	1.31	0/896	1.62	9/1117 (0.8%)
9	U	1.31	0/619	1.83	4/772 (0.5%)
10	V	1.34	0/684	1.92	15/852 (1.8%)
11	W	1.31	0/339	1.92	7/422 (1.7%)
12	X	1.36	0/247	2.13	10/307 (3.3%)
13	Y	1.16	0/147	1.70	2/182 (1.1%)
14	Z	1.30	0/192	1.76	3/237 (1.3%)
All	All	1.47	1/20191 (0.0%)	1.87	370/25171 (1.5%)

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	1	0	1
1	3	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
3	E	0	1
3	F	0	1
5	H	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	312	VAL	N-CA	-5.27	1.42	1.46

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	172	VAL	N-CA-C	-11.22	102.70	112.12
4	G	204	ASN	CA-C-N	9.99	126.53	120.24
4	G	204	ASN	C-N-CA	9.99	126.53	120.24
4	G	85	GLY	N-CA-C	-9.62	101.21	111.21
2	C	376	VAL	N-CA-C	-9.21	104.38	112.12
2	C	29	GLU	CA-C-N	8.82	137.57	121.70
2	C	29	GLU	C-N-CA	8.82	137.57	121.70
3	E	420	VAL	N-CA-C	-8.71	104.85	111.90
2	B	507	VAL	N-CA-C	-8.69	104.23	112.83
7	O	176	VAL	N-CA-C	-8.67	95.63	108.12
7	O	180	ILE	N-CA-C	-8.39	104.59	111.81
3	D	161	VAL	N-CA-C	-8.33	104.58	112.83
2	B	234	VAL	N-CA-C	-8.08	96.85	108.17
11	W	6	PRO	N-CA-C	8.03	120.50	110.70
3	E	258	ILE	N-CA-C	-8.02	104.89	112.83
3	F	103	ILE	N-CA-C	-7.99	104.07	113.42
10	V	59	ARG	N-CA-C	-7.94	103.42	113.43
3	D	356	ARG	N-CA-C	-7.90	101.41	113.89
3	E	162	GLY	N-CA-C	-7.74	104.03	115.72
2	A	398	GLN	N-CA-C	-7.71	104.01	113.41
5	H	61	GLU	N-CA-C	-7.69	95.72	108.34
3	F	392	GLY	N-CA-C	-7.65	104.68	111.95
3	D	258	ILE	N-CA-C	-7.57	103.92	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	84	TYR	N-CA-C	-7.57	101.93	112.45
2	C	99	VAL	N-CA-C	-7.54	103.01	109.19
3	D	106	ARG	N-CA-C	-7.54	104.05	112.57
7	O	192	GLU	N-CA-C	-7.53	104.23	113.50
4	G	137	ALA	N-CA-C	-7.49	100.63	110.07
2	C	128	ARG	N-CA-C	-7.37	96.89	108.90
2	A	192	ASN	N-CA-C	-7.34	102.92	112.68
7	O	33	ILE	N-CA-C	-7.21	106.06	111.90
2	B	93	THR	N-CA-C	-7.16	103.55	111.36
4	G	100	ASN	N-CA-C	-7.14	104.72	113.50
3	D	363	VAL	N-CA-C	-7.08	105.92	112.43
8	T	140	VAL	N-CA-C	-7.08	105.83	112.83
10	V	167	PHE	N-CA-C	-7.07	98.71	109.95
2	C	479	ASN	N-CA-C	-7.05	104.67	113.28
3	D	208	ASN	N-CA-C	-7.04	95.36	107.61
2	C	296	TYR	N-CA-C	-7.00	100.39	110.40
3	D	305	THR	N-CA-C	-6.98	98.04	108.99
11	W	59	ASP	N-CA-C	-6.93	103.50	113.21
2	A	54	LEU	N-CA-C	-6.91	97.97	109.24
2	B	206	VAL	N-CA-C	-6.84	98.53	108.11
3	E	53	HIS	N-CA-C	-6.82	98.09	109.07
2	A	190	ARG	N-CA-C	-6.79	105.02	113.38
8	T	80	LYS	N-CA-C	-6.79	103.43	113.61
3	D	103	ILE	N-CA-C	-6.77	106.54	113.10
3	F	208	ASN	N-CA-C	-6.75	97.06	108.26
7	O	101	PHE	N-CA-C	-6.69	104.04	112.93
1	8	43	ILE	CA-C-N	6.68	129.54	120.38
1	8	43	ILE	C-N-CA	6.68	129.54	120.38
2	A	479	ASN	N-CA-C	-6.67	104.88	113.16
3	D	304	VAL	N-CA-C	-6.67	102.78	110.05
5	H	56	VAL	N-CA-C	-6.65	98.79	108.11
12	X	39	LEU	N-CA-C	-6.63	98.97	109.04
3	D	207	ILE	N-CA-C	-6.55	99.05	108.48
2	A	96	ILE	N-CA-C	-6.55	102.81	110.21
3	E	218	VAL	N-CA-C	-6.51	98.74	108.12
1	4	61	THR	CA-C-N	6.50	127.19	119.98
1	4	61	THR	C-N-CA	6.50	127.19	119.98
3	E	300	LYS	N-CA-C	-6.47	105.14	113.16
3	E	39	ILE	N-CA-C	-6.39	99.22	108.36
3	D	449	TYR	N-CA-C	-6.38	104.74	113.30
2	A	31	GLY	N-CA-C	-6.38	101.83	111.14
1	4	43	ILE	CA-C-N	6.37	129.68	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	43	ILE	C-N-CA	6.37	129.68	120.38
2	A	193	ASN	N-CA-C	-6.35	105.28	113.16
2	B	169	ILE	N-CA-C	-6.35	98.71	107.99
2	C	232	ILE	N-CA-C	-6.32	99.10	108.45
2	A	42	ARG	N-CA-C	-6.30	98.01	108.34
1	6	43	ILE	CA-C-N	6.29	128.99	120.38
1	6	43	ILE	C-N-CA	6.29	128.99	120.38
2	A	234	VAL	N-CA-C	-6.28	99.35	108.89
4	G	164	ILE	N-CA-C	-6.25	99.15	108.46
2	A	262	ASN	N-CA-C	-6.24	105.31	113.17
5	H	41	VAL	N-CA-C	-6.22	99.17	108.12
2	B	232	ILE	N-CA-C	-6.21	99.53	108.48
7	O	150	GLY	N-CA-C	-6.20	107.15	115.21
2	B	109	VAL	N-CA-C	-6.18	99.50	108.71
3	D	42	PRO	N-CA-C	-6.16	108.27	114.68
3	D	91	THR	N-CA-C	-6.14	105.83	113.38
1	3	43	ILE	CA-C-N	6.13	129.34	120.38
1	3	43	ILE	C-N-CA	6.13	129.34	120.38
3	D	114	ARG	N-CA-C	-6.13	100.01	109.52
3	F	299	THR	N-CA-C	-6.11	100.11	109.65
1	7	43	ILE	CA-C-N	6.11	128.74	120.38
1	7	43	ILE	C-N-CA	6.11	128.74	120.38
3	D	43	GLN	N-CA-C	-6.10	105.15	112.59
3	F	120	ASP	CA-C-N	6.08	124.10	119.66
3	F	120	ASP	C-N-CA	6.08	124.10	119.66
2	B	408	PHE	N-CA-C	-6.08	105.62	113.16
3	E	17	ILE	N-CA-C	-6.06	98.41	107.37
3	E	252	LEU	N-CA-C	-6.06	99.86	109.07
3	E	104	ASP	N-CA-C	-6.05	105.90	113.28
2	A	296	TYR	N-CA-C	-6.05	100.20	109.64
7	O	154	LYS	N-CA-C	-6.04	99.55	109.40
8	T	101	LEU	N-CA-C	-6.04	104.90	112.93
7	O	179	SER	N-CA-C	-6.03	101.07	110.17
10	V	55	PHE	N-CA-C	-6.03	104.74	114.09
2	C	234	VAL	N-CA-C	-6.02	99.91	108.58
3	E	95	ILE	N-CA-C	-6.02	99.69	108.11
3	F	422	GLU	N-CA-C	-6.00	105.04	112.90
2	A	150	THR	N-CA-C	-6.00	106.60	114.04
10	V	90	GLN	N-CA-C	-6.00	106.00	113.55
2	A	128	ARG	N-CA-C	-5.98	100.05	109.50
1	0	12	ALA	CA-C-N	5.98	126.58	119.94
1	0	12	ALA	C-N-CA	5.98	126.58	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	64	MET	N-CA-C	-5.96	106.62	114.31
3	D	88	GLY	N-CA-C	-5.94	103.90	110.96
8	T	27	THR	CA-C-N	5.93	128.23	120.28
8	T	27	THR	C-N-CA	5.93	128.23	120.28
2	A	175	THR	N-CA-C	-5.93	105.63	112.92
2	A	296	TYR	CA-C-N	5.92	127.24	119.84
2	A	296	TYR	C-N-CA	5.92	127.24	119.84
10	V	82	LYS	N-CA-C	-5.92	101.69	108.49
2	A	79	GLY	CA-C-N	5.90	129.09	120.71
2	A	79	GLY	C-N-CA	5.90	129.09	120.71
3	D	394	ASP	N-CA-C	-5.89	106.10	113.28
3	F	23	VAL	N-CA-C	-5.89	99.23	108.95
2	B	69	GLU	N-CA-C	-5.88	103.25	110.31
3	F	53	HIS	N-CA-C	-5.86	99.84	109.40
2	B	22	SER	CA-C-N	5.85	128.43	120.54
2	B	22	SER	C-N-CA	5.85	128.43	120.54
3	E	255	ILE	N-CA-C	-5.84	99.64	108.17
5	H	42	LEU	N-CA-C	-5.84	98.08	108.13
2	A	85	LYS	N-CA-C	-5.83	100.44	109.24
2	C	334	GLY	N-CA-C	-5.82	106.42	115.67
1	6	54	GLY	CA-C-N	5.82	128.00	120.44
1	6	54	GLY	C-N-CA	5.82	128.00	120.44
4	G	110	ILE	N-CA-C	-5.81	98.05	106.88
3	D	134	LEU	N-CA-C	-5.78	97.90	108.02
3	F	114	ARG	N-CA-C	-5.77	100.58	109.52
3	F	65	ASP	CA-C-N	5.76	125.45	119.92
3	F	65	ASP	C-N-CA	5.76	125.45	119.92
2	A	40	ILE	N-CA-C	-5.76	99.48	108.81
14	Z	7	PHE	N-CA-C	-5.74	104.83	113.89
2	C	82	ARG	N-CA-C	-5.73	98.60	110.80
3	F	307	VAL	N-CA-C	-5.71	99.42	107.75
4	G	74	ILE	N-CA-C	-5.70	99.92	108.12
1	5	61	THR	CA-C-N	5.70	126.30	119.98
1	5	61	THR	C-N-CA	5.70	126.30	119.98
7	O	151	LYS	N-CA-C	-5.69	98.06	108.02
2	C	169	ILE	N-CA-C	-5.69	97.51	109.34
3	F	22	ASP	N-CA-C	-5.67	100.93	109.95
1	5	71	LEU	CA-C-N	5.67	127.88	120.28
1	5	71	LEU	C-N-CA	5.67	127.88	120.28
3	D	46	LEU	N-CA-C	-5.67	99.66	108.90
3	F	251	VAL	N-CA-C	-5.66	101.62	108.53
3	F	106	ARG	N-CA-C	-5.65	106.98	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8	22	ALA	CA-C-N	5.65	126.21	119.94
1	8	22	ALA	C-N-CA	5.65	126.21	119.94
3	D	132	GLU	CA-C-N	5.64	128.20	120.35
3	D	132	GLU	C-N-CA	5.64	128.20	120.35
2	A	355	GLU	CA-C-N	5.64	127.84	120.28
2	A	355	GLU	C-N-CA	5.64	127.84	120.28
4	G	83	LEU	CA-C-N	5.64	128.40	120.28
4	G	83	LEU	C-N-CA	5.64	128.40	120.28
3	F	95	ILE	N-CA-C	-5.64	100.28	108.17
2	C	64	MET	N-CA-C	-5.63	100.85	109.41
3	D	181	PHE	N-CA-C	-5.63	100.92	108.86
3	F	214	LYS	N-CA-C	-5.63	105.76	113.30
2	C	444	VAL	CA-C-O	-5.62	114.08	118.85
3	D	307	VAL	N-CA-C	-5.61	100.32	108.17
8	T	200	LEU	N-CA-C	-5.60	106.12	113.12
11	W	62	SER	N-CA-C	-5.59	100.29	109.40
3	F	311	TYR	N-CA-C	-5.59	99.80	108.90
1	0	15	SER	CA-C-N	5.57	128.30	120.28
1	0	15	SER	C-N-CA	5.57	128.30	120.28
7	O	174	LYS	N-CA-C	-5.57	99.34	108.76
3	D	22	ASP	N-CA-C	-5.57	100.62	109.59
2	B	422	ARG	CA-C-N	5.57	126.16	119.98
2	B	422	ARG	C-N-CA	5.57	126.16	119.98
3	F	206	VAL	N-CA-C	-5.56	105.10	110.72
2	A	90	VAL	N-CA-C	-5.56	100.39	108.17
3	D	112	LYS	N-CA-C	-5.56	105.54	112.93
3	E	216	ALA	N-CA-C	-5.55	100.91	109.52
10	V	127	ALA	N-CA-C	-5.55	101.94	109.54
2	B	54	LEU	N-CA-C	-5.53	100.17	109.07
3	E	176	LYS	N-CA-C	-5.53	105.90	113.30
3	F	360	ALA	N-CA-C	-5.51	106.06	112.89
2	C	61	VAL	N-CA-C	-5.51	104.05	110.05
3	E	336	SER	CA-C-N	5.50	128.21	120.28
3	E	336	SER	C-N-CA	5.50	128.21	120.28
4	G	75	VAL	N-CA-C	-5.49	99.91	108.86
4	G	195	GLY	N-CA-C	-5.49	108.13	115.32
3	F	207	ILE	N-CA-C	-5.48	99.99	107.99
1	6	6	ALA	CA-C-N	5.47	127.61	120.28
1	6	6	ALA	C-N-CA	5.47	127.61	120.28
1	5	43	ILE	CA-C-N	5.47	128.36	120.38
1	5	43	ILE	C-N-CA	5.47	128.36	120.38
2	A	386	LYS	N-CA-C	-5.46	106.29	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	166	ARG	N-CA-C	-5.46	99.51	108.41
2	A	369	VAL	N-CA-C	-5.46	107.66	112.90
2	B	26	ASN	N-CA-C	-5.45	106.00	113.30
10	V	158	TRP	N-CA-C	-5.45	105.64	114.09
2	B	355	GLU	CA-C-N	5.44	127.57	120.28
2	B	355	GLU	C-N-CA	5.44	127.57	120.28
3	F	112	LYS	N-CA-C	-5.44	99.22	110.80
3	E	89	ARG	N-CA-C	-5.42	106.44	113.16
3	E	296	ILE	N-CA-C	-5.42	107.47	112.83
3	F	312	VAL	N-CA-C	-5.41	101.81	107.60
2	A	490	GLU	N-CA-C	-5.41	99.50	108.75
3	D	81	GLY	CA-C-N	5.38	125.39	119.90
3	D	81	GLY	C-N-CA	5.38	125.39	119.90
3	F	121	PRO	CA-C-O	-5.38	117.03	120.90
3	D	393	MET	N-CA-C	-5.38	106.50	113.16
14	Z	7	PHE	CA-C-N	5.37	131.42	122.66
14	Z	7	PHE	C-N-CA	5.37	131.42	122.66
2	B	78	PHE	N-CA-C	-5.37	105.54	112.68
3	D	427	ILE	CA-C-N	5.37	125.38	119.90
3	D	427	ILE	C-N-CA	5.37	125.38	119.90
3	E	356	ARG	N-CA-C	-5.36	106.51	113.16
5	H	40	GLY	N-CA-C	-5.36	102.08	111.46
5	H	103	ASN	CA-C-N	5.36	127.46	120.28
5	H	103	ASN	C-N-CA	5.36	127.46	120.28
3	F	421	ALA	N-CA-C	-5.35	104.03	110.88
1	7	22	ALA	CA-C-N	5.35	125.92	119.98
1	7	22	ALA	C-N-CA	5.35	125.92	119.98
3	D	17	ILE	N-CA-C	-5.35	100.18	107.99
4	G	196	LYS	N-CA-C	-5.35	106.94	112.93
3	D	104	ASP	N-CA-C	-5.35	106.26	112.89
1	3	41	PRO	N-CA-C	5.34	123.48	112.47
1	1	15	SER	CA-C-N	5.34	127.97	120.28
1	1	15	SER	C-N-CA	5.34	127.97	120.28
3	F	163	LYS	N-CA-C	-5.34	105.54	111.36
2	B	452	ASN	N-CA-C	-5.34	106.95	112.93
3	D	364	GLY	CA-C-N	5.33	127.86	120.29
3	D	364	GLY	C-N-CA	5.33	127.86	120.29
12	X	61	ALA	N-CA-C	-5.33	99.72	108.41
2	B	42	ARG	N-CA-C	-5.33	98.89	108.48
3	F	416	GLN	N-CA-C	-5.33	99.60	108.23
10	V	55	PHE	CA-C-N	5.33	127.42	120.28
10	V	55	PHE	C-N-CA	5.33	127.42	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	58	GLY	CA-C-N	5.32	128.29	119.35
11	W	58	GLY	C-N-CA	5.32	128.29	119.35
1	6	24	ILE	CA-C-N	5.31	125.84	119.94
1	6	24	ILE	C-N-CA	5.31	125.84	119.94
2	B	363	ILE	N-CA-C	-5.31	100.69	108.54
7	O	27	ALA	N-CA-C	-5.29	106.82	113.28
2	A	364	ARG	N-CA-C	-5.29	98.90	108.85
7	O	100	CYS	N-CA-C	-5.29	103.98	110.65
2	A	354	LEU	N-CA-C	-5.29	101.25	109.72
1	4	10	ILE	CA-C-N	5.29	125.85	119.98
1	4	10	ILE	C-N-CA	5.29	125.85	119.98
1	9	10	ILE	CA-C-N	5.28	125.84	119.98
1	9	10	ILE	C-N-CA	5.28	125.84	119.98
7	O	147	VAL	N-CA-C	-5.27	99.66	107.51
1	9	61	THR	CA-C-N	5.27	125.83	119.98
1	9	61	THR	C-N-CA	5.27	125.83	119.98
3	F	162	GLY	N-CA-C	-5.27	105.73	114.48
4	G	137	ALA	CA-C-N	5.26	126.41	119.84
4	G	137	ALA	C-N-CA	5.26	126.41	119.84
3	E	351	LEU	N-CA-C	-5.25	106.55	113.17
2	A	177	LYS	CA-C-N	5.25	127.84	120.28
2	A	177	LYS	C-N-CA	5.25	127.84	120.28
10	V	98	HIS	CA-C-N	5.25	127.27	120.44
10	V	98	HIS	C-N-CA	5.25	127.27	120.44
3	F	12	LYS	N-CA-C	-5.25	100.34	108.90
3	F	21	VAL	N-CA-C	-5.25	100.51	108.17
1	7	24	ILE	CA-C-N	5.24	125.76	119.94
1	7	24	ILE	C-N-CA	5.24	125.76	119.94
3	D	156	PHE	N-CA-C	-5.24	101.32	109.24
3	E	112	LYS	N-CA-C	-5.24	105.95	112.93
2	B	133	VAL	N-CA-C	-5.24	99.98	107.78
3	D	452	ILE	CA-C-N	5.24	126.39	119.84
3	D	452	ILE	C-N-CA	5.24	126.39	119.84
1	8	41	PRO	N-CA-C	5.24	123.25	112.47
3	F	457	PHE	N-CA-C	-5.23	107.02	113.41
3	E	427	ILE	N-CA-C	-5.23	102.19	107.89
10	V	27	THR	N-CA-C	-5.23	105.66	111.36
2	C	260	ARG	CA-C-N	5.23	127.71	120.29
2	C	260	ARG	C-N-CA	5.23	127.71	120.29
3	D	354	LYS	N-CA-C	-5.22	101.14	109.23
2	B	59	SER	N-CA-C	-5.22	106.67	112.57
3	D	254	PHE	N-CA-C	-5.22	102.02	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	61	VAL	N-CA-C	-5.22	100.34	108.95
2	A	58	SER	N-CA-C	-5.21	100.02	108.41
2	B	324	THR	N-CA-C	-5.21	101.67	109.95
2	C	117	ILE	N-CA-C	-5.21	107.68	112.83
12	X	55	GLU	CA-C-N	5.21	127.25	120.28
12	X	55	GLU	C-N-CA	5.21	127.25	120.28
8	T	111	LEU	N-CA-C	-5.20	106.88	113.43
2	C	68	LEU	N-CA-C	-5.20	97.25	107.69
3	F	255	ILE	N-CA-C	-5.20	100.39	108.86
3	F	256	ASP	N-CA-C	-5.19	101.18	109.07
2	B	443	GLN	N-CA-C	-5.19	107.50	113.88
11	W	5	ILE	O-C-N	-5.19	115.19	121.10
3	F	88	GLY	N-CA-C	-5.18	103.72	110.45
12	X	17	ALA	CA-C-N	5.17	125.11	119.78
12	X	17	ALA	C-N-CA	5.17	125.11	119.78
12	X	6	LEU	CA-C-N	5.17	127.16	120.44
12	X	6	LEU	C-N-CA	5.17	127.16	120.44
1	1	10	ILE	CA-C-N	5.17	126.60	120.14
1	1	10	ILE	C-N-CA	5.17	126.60	120.14
2	C	118	ASP	N-CA-C	-5.16	106.76	113.16
4	G	171	SER	N-CA-C	-5.16	101.27	108.96
3	E	16	VAL	N-CA-C	-5.15	98.62	109.34
3	F	451	ASN	N-CA-C	-5.15	106.23	112.88
1	4	20	LEU	CA-C-N	5.15	125.67	120.00
1	4	20	LEU	C-N-CA	5.15	125.67	120.00
1	2	15	SER	CA-C-N	5.14	127.69	120.28
1	2	15	SER	C-N-CA	5.14	127.69	120.28
3	E	54	LEU	N-CA-C	-5.14	106.69	113.17
3	F	17	ILE	N-CA-C	-5.14	98.64	109.34
2	B	115	ASN	N-CA-C	-5.14	99.19	108.85
2	C	265	HIS	N-CA-C	-5.14	101.56	109.52
10	V	97	LYS	CA-C-N	5.13	127.16	120.28
10	V	97	LYS	C-N-CA	5.13	127.16	120.28
2	A	152	LEU	N-CA-C	-5.13	100.16	108.52
2	C	422	ARG	CA-C-N	5.13	125.67	119.98
2	C	422	ARG	C-N-CA	5.13	125.67	119.98
7	O	160	LYS	N-CA-C	-5.13	98.47	109.81
3	E	80	GLY	CA-C-N	5.12	129.91	121.87
3	E	80	GLY	C-N-CA	5.12	129.91	121.87
3	F	11	GLY	N-CA-C	-5.12	103.03	111.38
9	U	116	VAL	CA-C-N	5.12	127.14	120.28
9	U	116	VAL	C-N-CA	5.12	127.14	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	459	GLU	CA-C-N	5.12	127.14	120.28
2	B	459	GLU	C-N-CA	5.12	127.14	120.28
2	C	294	GLU	CA-C-N	5.12	129.60	122.08
2	C	294	GLU	C-N-CA	5.12	129.60	122.08
3	D	193	GLU	CA-C-N	5.12	125.66	119.98
3	D	193	GLU	C-N-CA	5.12	125.66	119.98
2	C	96	ILE	N-CA-C	-5.11	103.00	109.80
8	T	114	HIS	CA-C-N	5.11	128.08	120.31
8	T	114	HIS	C-N-CA	5.11	128.08	120.31
3	E	343	GLY	N-CA-C	-5.11	108.61	114.69
2	B	148	VAL	N-CA-C	-5.11	101.27	108.27
2	A	289	ARG	N-CA-C	-5.11	103.64	110.07
3	D	302	GLY	N-CA-C	-5.11	103.79	111.19
3	E	42	PRO	N-CA-C	-5.11	107.48	113.86
3	E	210	GLU	N-CA-C	-5.11	106.74	113.12
1	0	61	THR	CA-C-N	5.10	125.65	119.98
1	0	61	THR	C-N-CA	5.10	125.65	119.98
3	F	289	MET	CA-C-N	5.10	125.64	119.98
3	F	289	MET	C-N-CA	5.10	125.64	119.98
2	A	148	VAL	N-CA-C	-5.10	100.97	108.11
1	9	58	SER	CA-C-N	5.09	127.11	120.28
1	9	58	SER	C-N-CA	5.09	127.11	120.28
2	A	93	THR	N-CA-C	-5.09	105.81	111.36
2	C	290	PRO	N-CA-C	5.09	115.35	110.47
3	F	450	ASP	N-CA-C	-5.08	106.32	112.88
3	E	208	ASN	N-CA-C	-5.08	100.89	109.07
13	Y	7	THR	CA-C-N	5.08	125.08	119.90
13	Y	7	THR	C-N-CA	5.08	125.08	119.90
3	D	214	LYS	N-CA-C	-5.08	104.80	111.96
3	D	24	HIS	N-CA-C	-5.08	100.90	109.07
1	2	43	ILE	CA-C-N	5.07	127.33	120.38
1	2	43	ILE	C-N-CA	5.07	127.33	120.38
12	X	7	TYR	CA-C-N	5.07	127.03	120.44
12	X	7	TYR	C-N-CA	5.07	127.03	120.44
2	A	482	LEU	CA-C-N	5.06	127.06	120.28
2	A	482	LEU	C-N-CA	5.06	127.06	120.28
9	U	121	LYS	CA-C-N	5.05	126.93	120.56
9	U	121	LYS	C-N-CA	5.05	126.93	120.56
2	C	121	GLY	CA-C-N	5.05	126.15	119.84
2	C	121	GLY	C-N-CA	5.05	126.15	119.84
2	C	490	GLU	N-CA-C	-5.04	100.14	108.75
3	D	162	GLY	N-CA-C	-5.03	106.84	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	439	ALA	CA-C-N	5.02	127.01	120.28
2	B	439	ALA	C-N-CA	5.02	127.01	120.28
11	W	46	THR	N-CA-C	-5.01	100.12	110.80
2	B	129	SER	N-CA-C	-5.01	101.80	108.86
2	B	312	ALA	CA-C-N	5.01	129.06	122.30
2	B	312	ALA	C-N-CA	5.01	129.06	122.30
1	4	58	SER	CA-C-N	5.00	126.99	120.28
1	4	58	SER	C-N-CA	5.00	126.99	120.28
3	E	392	GLY	CA-C-N	5.00	126.99	120.28
3	E	392	GLY	C-N-CA	5.00	126.99	120.28
2	A	208	VAL	N-CA-C	-5.00	101.28	108.48

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	40	ASN	Peptide
1	3	40	ASN	Peptide
1	5	40	ASN	Peptide
1	6	40	ASN	Peptide
1	7	40	ASN	Peptide
1	8	40	ASN	Peptide
1	9	40	ASN	Peptide
3	E	345	TYR	Peptide
3	F	256	ASP	Peptide
5	H	54	PRO	Peptide

## 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	0	300	0	95	0	0
1	1	300	0	95	0	0
1	2	300	0	95	0	0
1	3	296	0	91	0	0
1	4	300	0	95	0	0
1	5	300	0	95	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	296	0	91	0	0
1	7	292	0	91	0	0
1	8	300	0	95	0	0
1	9	296	0	91	0	0
2	A	1996	0	570	1	0
2	B	2028	0	580	1	0
2	C	1984	0	567	0	0
3	D	1872	0	537	0	0
3	E	1876	0	537	1	0
3	F	1880	0	538	0	0
4	G	1059	0	277	1	0
5	H	480	0	122	0	0
6	I	193	0	43	0	0
7	O	748	0	205	1	0
8	T	897	0	248	0	0
9	U	620	0	158	0	0
10	V	685	0	173	0	0
11	W	340	0	92	0	0
12	X	248	0	61	0	0
13	Y	148	0	40	0	0
14	Z	193	0	49	0	0
All	All	20227	0	5731	5	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 0.

All (5) 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:A:102:GLY:HA3	2:A:126:ALA:H	1.78	0.49
7:O:15:VAL:C	7:O:17:GLY:H	2.23	0.46
3:E:160:GLY:C	3:E:162:GLY:H	2.24	0.46
4:G:80:ASP:H	4:G:134:GLY:HA3	1.82	0.45
2:B:173:ARG:C	2:B:175:THR:H	2.30	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	0	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	4	25
1	2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	3	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	9	40
1	4	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	4	25
1	5	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	6	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	9	40
1	7	71/76 (93%)	69 (97%)	1 (1%)	1 (1%)	9	40
1	8	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	9	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	9	40
2	A	495/510 (97%)	468 (94%)	16 (3%)	11 (2%)	5	29
2	B	505/510 (99%)	477 (94%)	20 (4%)	8 (2%)	7	37
2	C	492/510 (96%)	469 (95%)	13 (3%)	10 (2%)	6	31
3	D	466/478 (98%)	441 (95%)	21 (4%)	4 (1%)	14	50
3	E	467/478 (98%)	433 (93%)	27 (6%)	7 (2%)	8	39
3	F	468/478 (98%)	435 (93%)	26 (6%)	7 (2%)	8	39
4	G	261/278 (94%)	249 (95%)	9 (3%)	3 (1%)	11	46
5	H	110/138 (80%)	104 (94%)	3 (3%)	3 (3%)	4	25
6	I	42/61 (69%)	38 (90%)	3 (7%)	1 (2%)	4	27
7	O	185/195 (95%)	162 (88%)	17 (9%)	6 (3%)	3	21
8	T	222/249 (89%)	214 (96%)	6 (3%)	2 (1%)	14	50
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	150 (89%)	8 (5%)	11 (6%)	1	12
11	W	83/95 (87%)	66 (80%)	9 (11%)	8 (10%)	0	7
12	X	60/92 (65%)	50 (83%)	6 (10%)	4 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Y	35/59 (59%)	31 (89%)	1 (3%)	3 (9%)	0	8
14	Z	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
All	All	4984/5321 (94%)	4686 (94%)	200 (4%)	98 (2%)	8	31

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	41	PRO
1	3	41	PRO
1	4	41	PRO
1	5	41	PRO
1	6	41	PRO
1	7	41	PRO
1	8	41	PRO
1	9	41	PRO
2	A	30	THR
2	A	59	SER
2	A	338	ALA
2	A	363	ILE
2	B	36	VAL
2	B	379	ALA
2	C	229	LYS
2	C	404	ALA
3	E	131	ALA
3	E	451	ASN
3	F	131	ALA
3	F	358	LEU
3	F	462	GLY
10	V	62	LEU
11	W	8	LYS
11	W	41	ALA
11	W	46	THR
2	A	22	SER
2	A	195	SER
2	B	61	VAL
2	B	196	ASP
2	B	229	LYS
2	B	320	SER
3	D	451	ASN
3	E	81	GLY
7	O	10	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	O	61	ALA
7	O	165	GLY
11	W	14	ASN
11	W	31	TYR
12	X	58	VAL
12	X	60	THR
3	E	68	GLU
3	E	86	PRO
3	F	34	LEU
5	H	22	TYR
5	H	33	PRO
7	O	55	HIS
8	T	202	ASN
10	V	48	SER
10	V	85	ALA
10	V	89	LEU
10	V	131	ASP
10	V	157	LYS
10	V	166	ARG
10	V	169	ASN
1	1	42	SER
2	A	432	GLN
2	B	380	ALA
2	C	312	ALA
3	D	34	LEU
3	F	277	SER
11	W	61	ALA
12	X	16	LEU
13	Y	10	LEU
2	A	103	PRO
2	A	189	LYS
2	B	40	ILE
2	C	28	ASN
2	C	30	THR
2	C	230	TYR
2	C	367	ILE
2	C	406	ALA
2	C	435	TYR
3	D	16	VAL
4	G	56	GLU
5	H	12	LEU
6	I	39	GLN

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Mol	Chain	Res	Type
7	O	98	LEU
10	V	66	SER
11	W	11	SER
1	4	42	SER
2	A	145	HIS
2	C	145	HIS
4	G	192	PRO
8	T	50	ASN
10	V	81	VAL
10	V	129	PRO
12	X	36	LYS
13	Y	12	VAL
3	D	453	PRO
3	F	31	PRO
4	G	181	PRO
13	Y	9	ILE
2	A	376	VAL
3	E	133	ILE
3	F	86	PRO
11	W	5	ILE
3	E	80	GLY
7	O	9	PRO

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

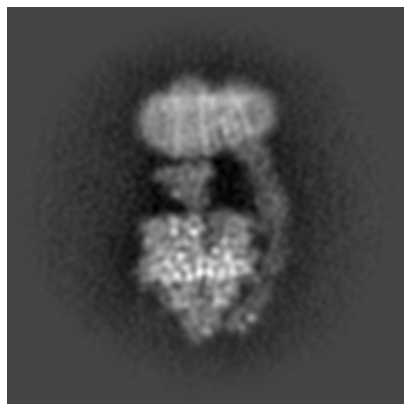
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25973. These allow visual inspection of the internal detail of the map and identification of artifacts.

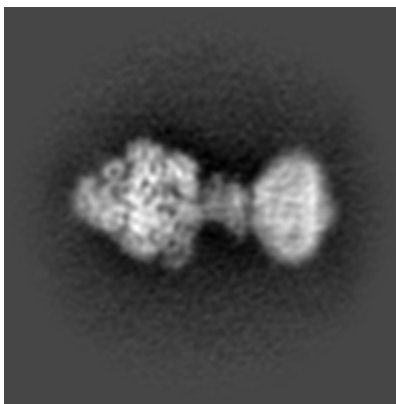
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

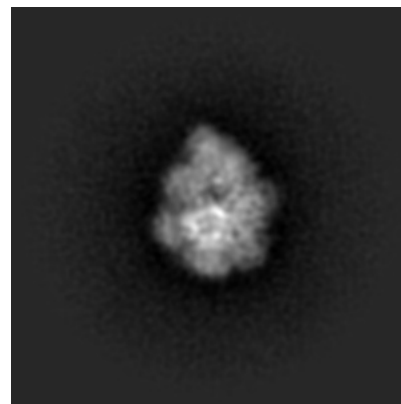
#### 6.1.1 Primary map



X

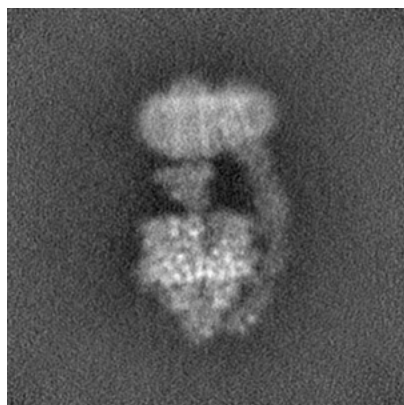


Y

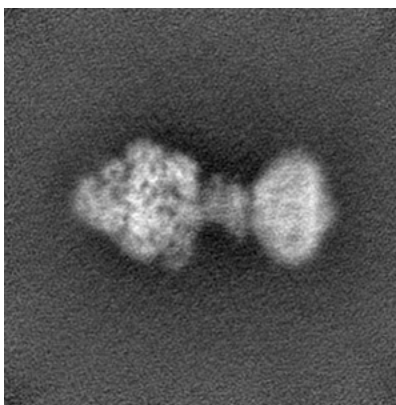


Z

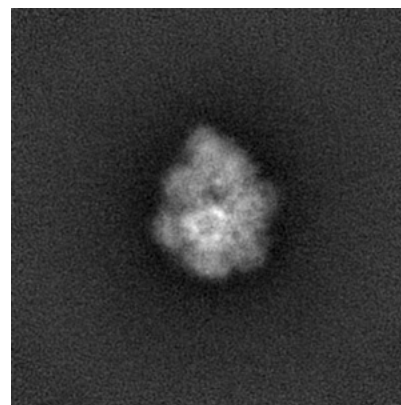
#### 6.1.2 Raw map



X



Y

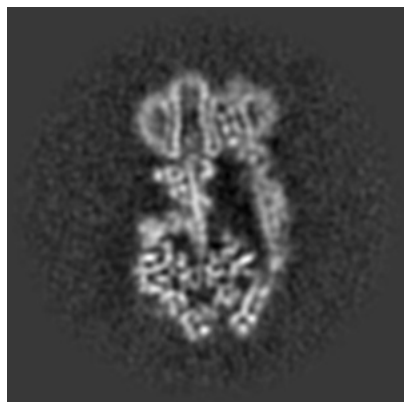


Z

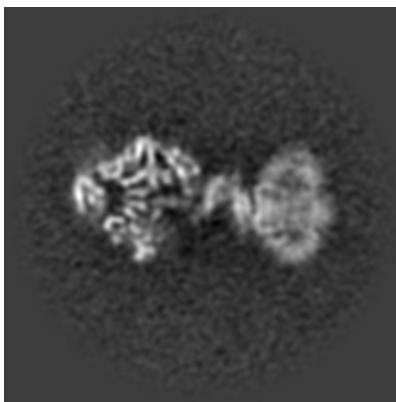
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

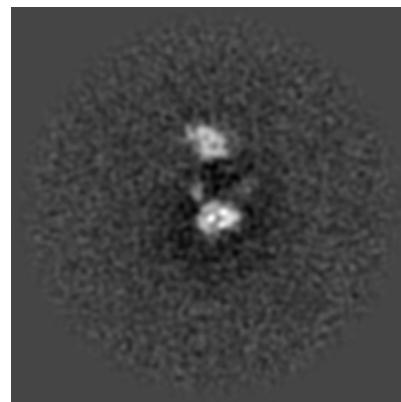
### 6.2.1 Primary map



X Index: 128

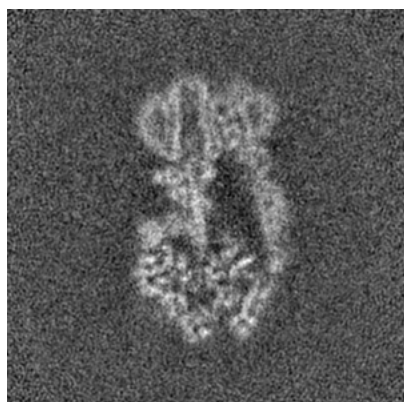


Y Index: 128

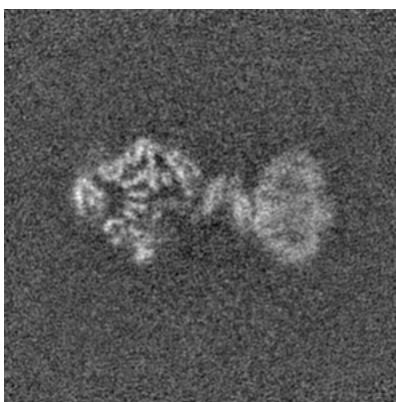


Z Index: 128

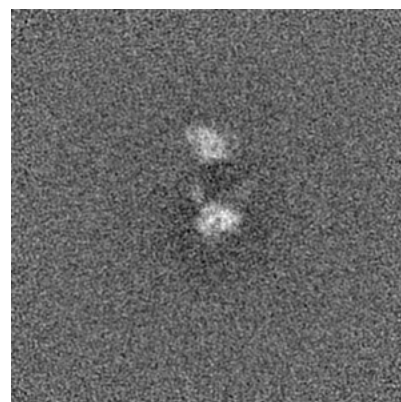
### 6.2.2 Raw map



X Index: 128



Y Index: 128

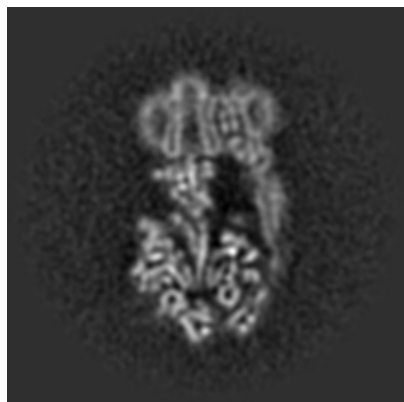


Z Index: 128

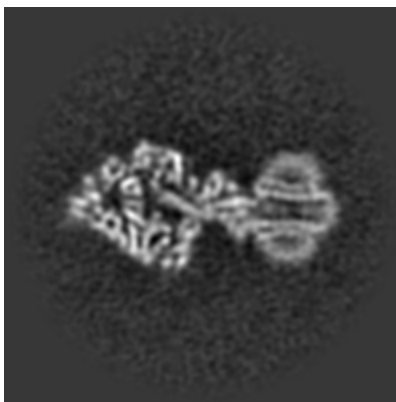
The images above show central slices of the map in three orthogonal directions.

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

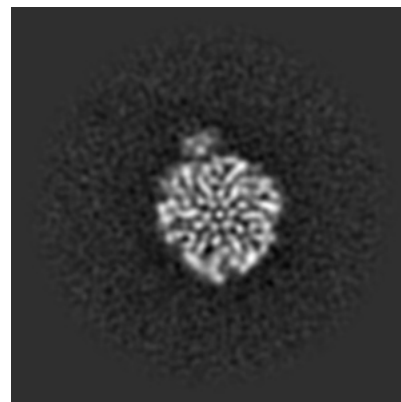
### 6.3.1 Primary map



X Index: 131

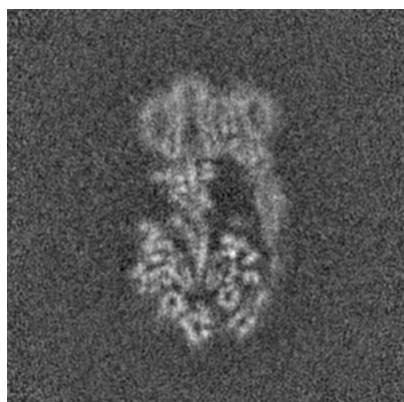


Y Index: 117

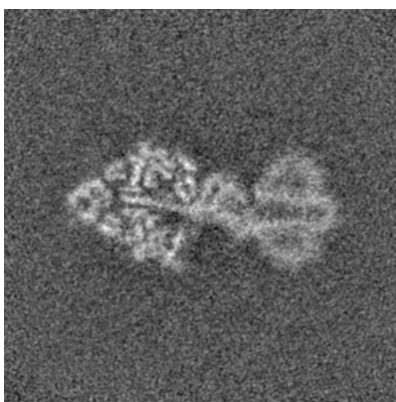


Z Index: 86

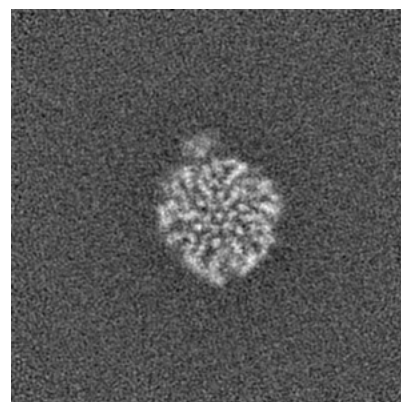
### 6.3.2 Raw map



X Index: 131



Y Index: 122

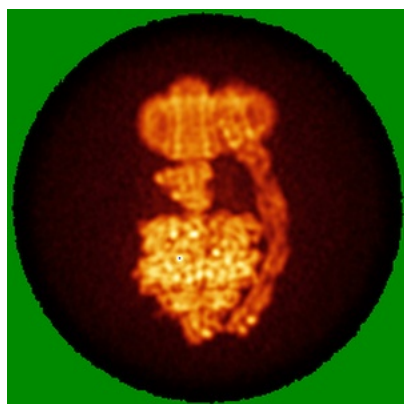


Z Index: 86

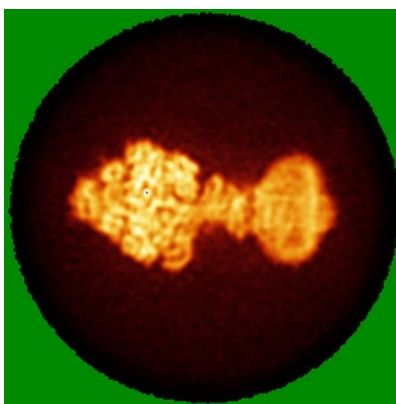
The images above show the largest variance slices of the map in three orthogonal directions.

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

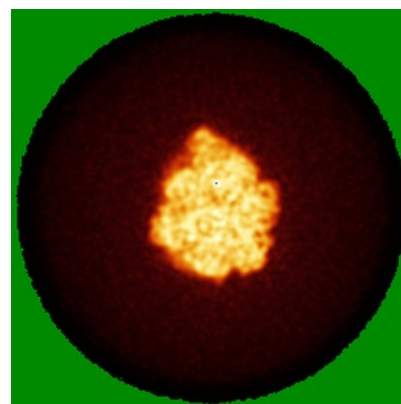
### 6.4.1 Primary map



X

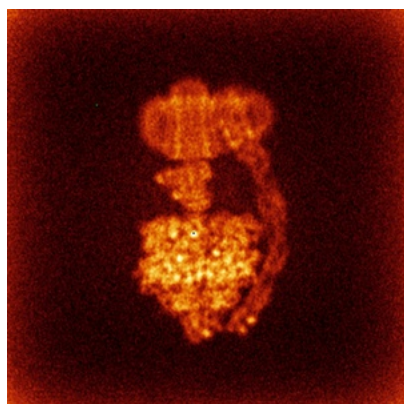


Y

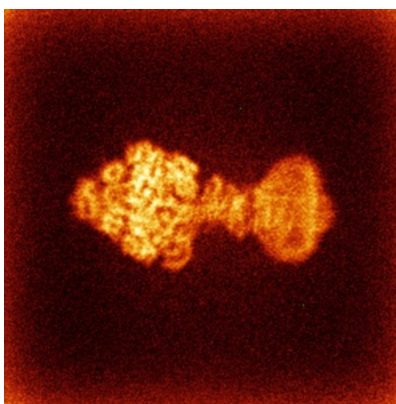


Z

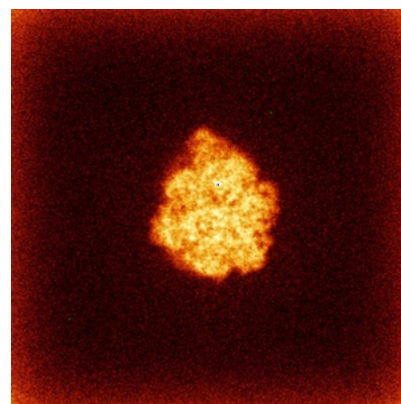
### 6.4.2 Raw map



X



Y



Z

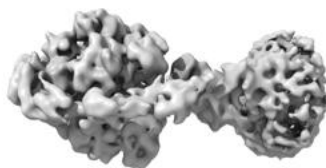
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

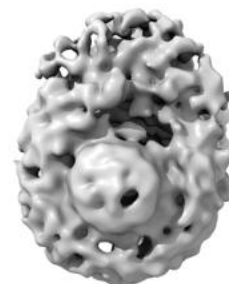
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

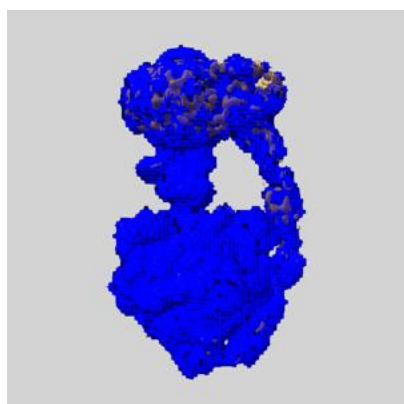
## 6.6 Mask visualisation [i](#)

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

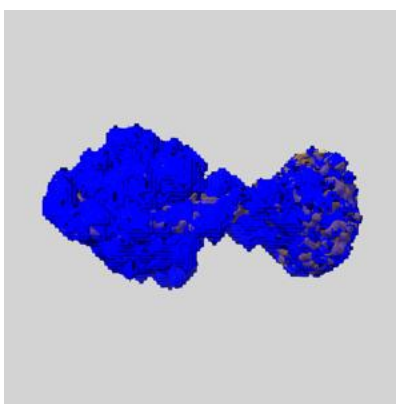
A mask typically either:

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

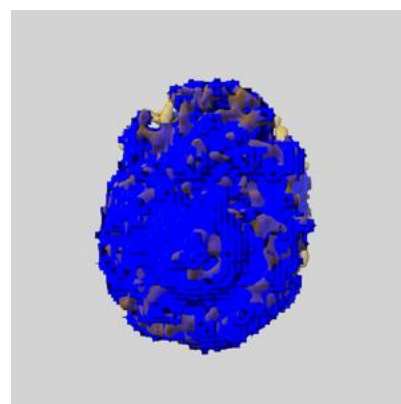
### 6.6.1 emd\_25973\_msk\_1.map [i](#)



X



Y

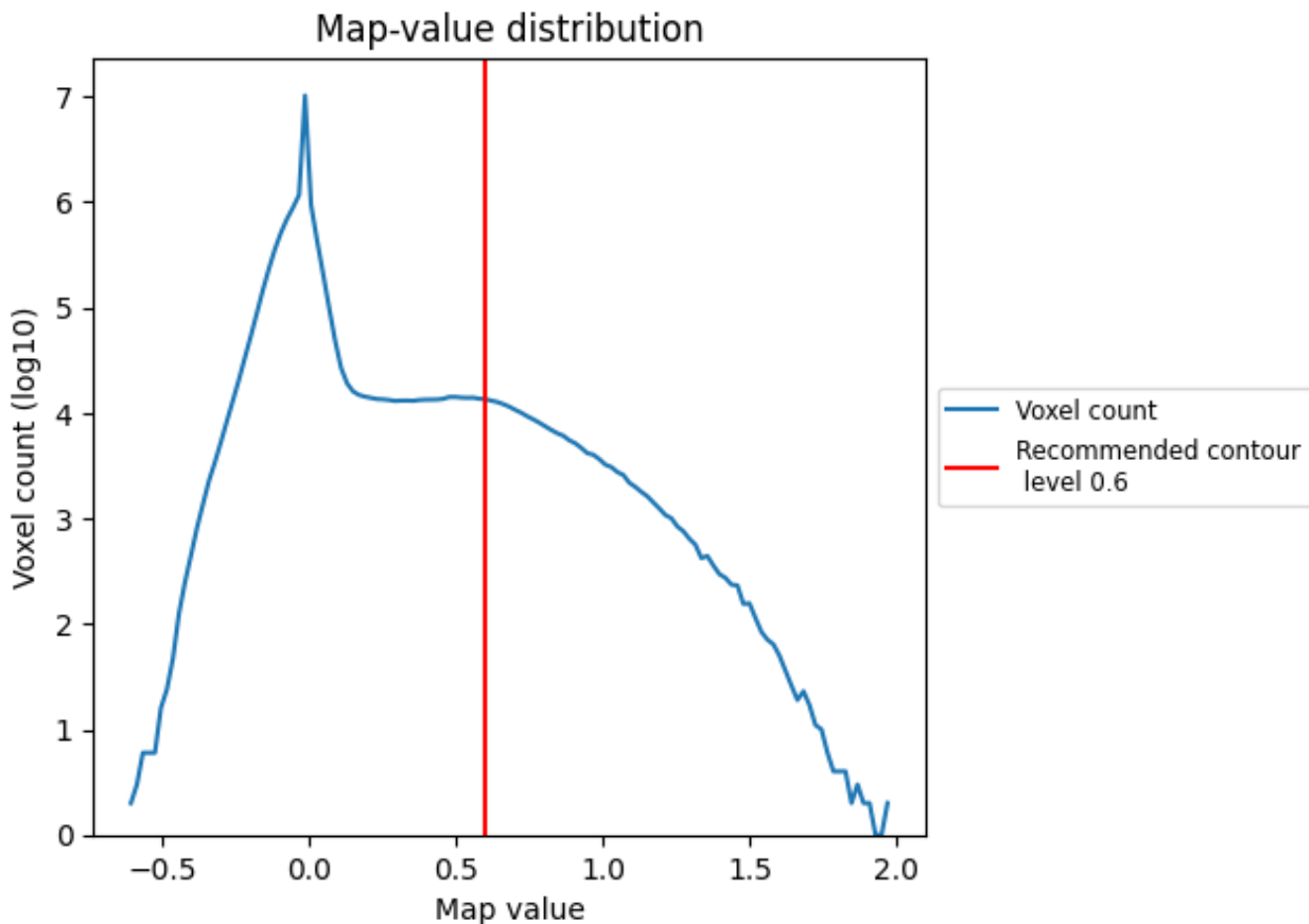


Z

## 7 Map analysis [i](#)

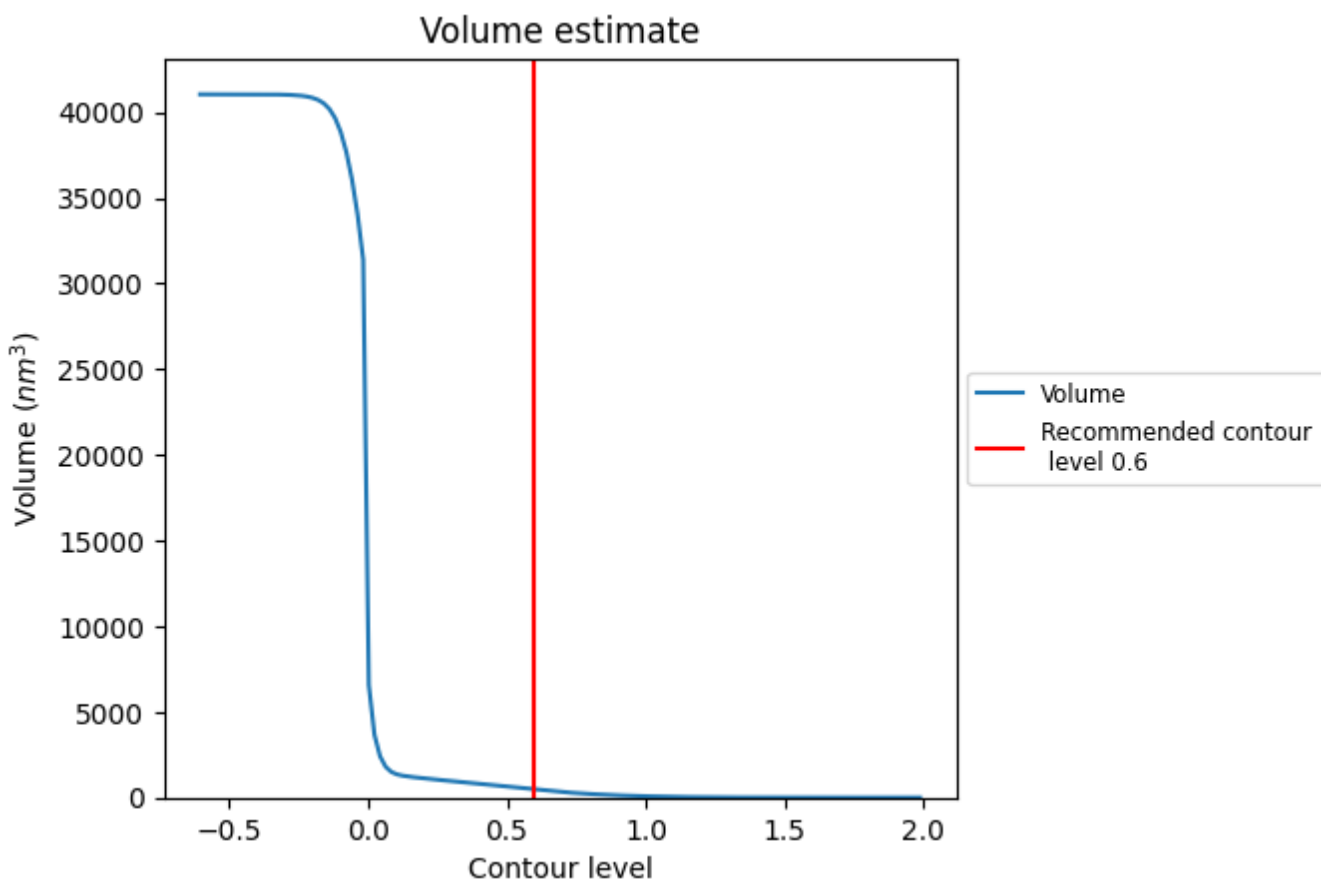
This section contains the results of statistical analysis of the map.

### 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.

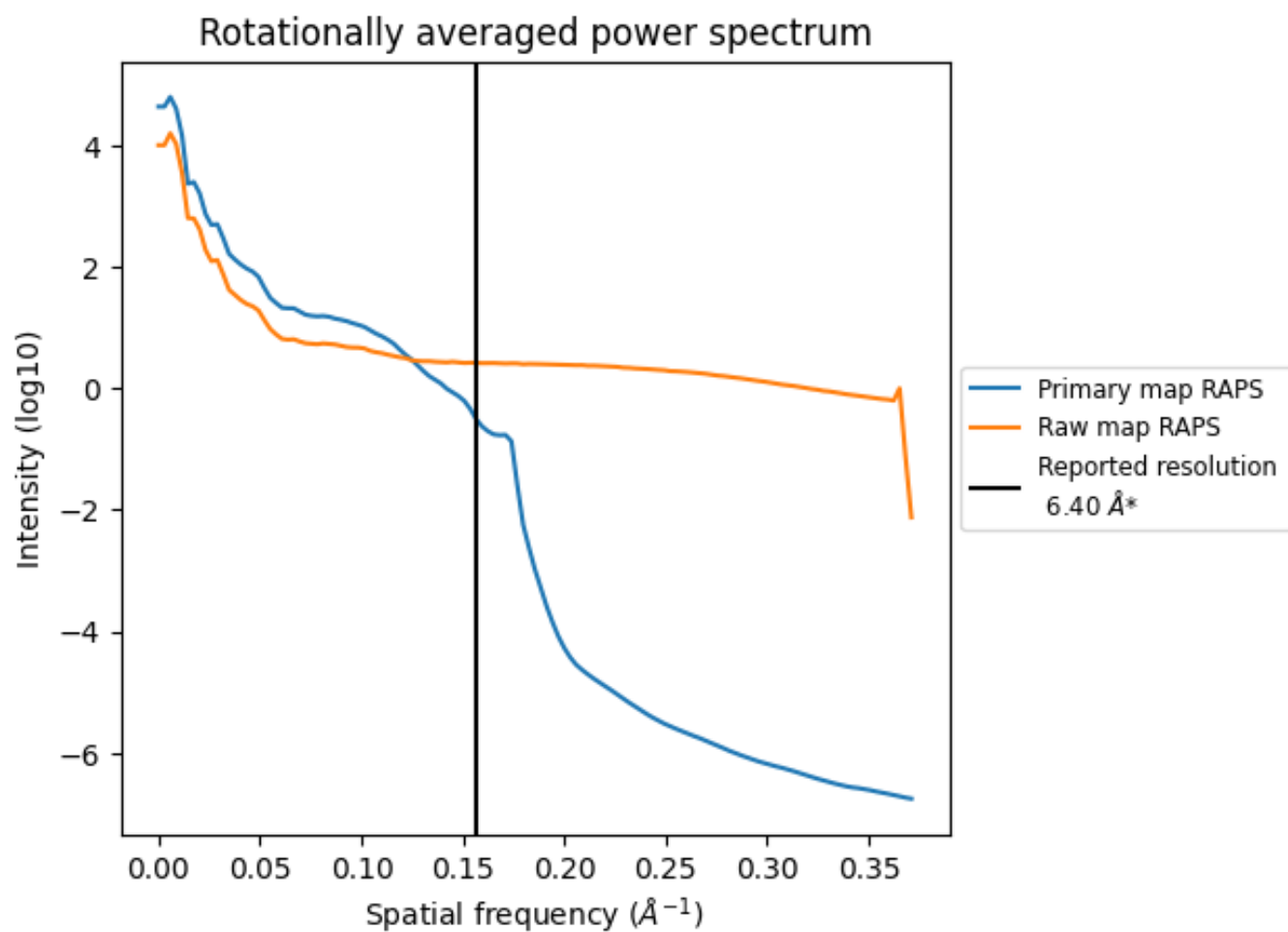
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 474 nm<sup>3</sup>; this corresponds to an approximate mass of 428 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 [\(i\)](#)

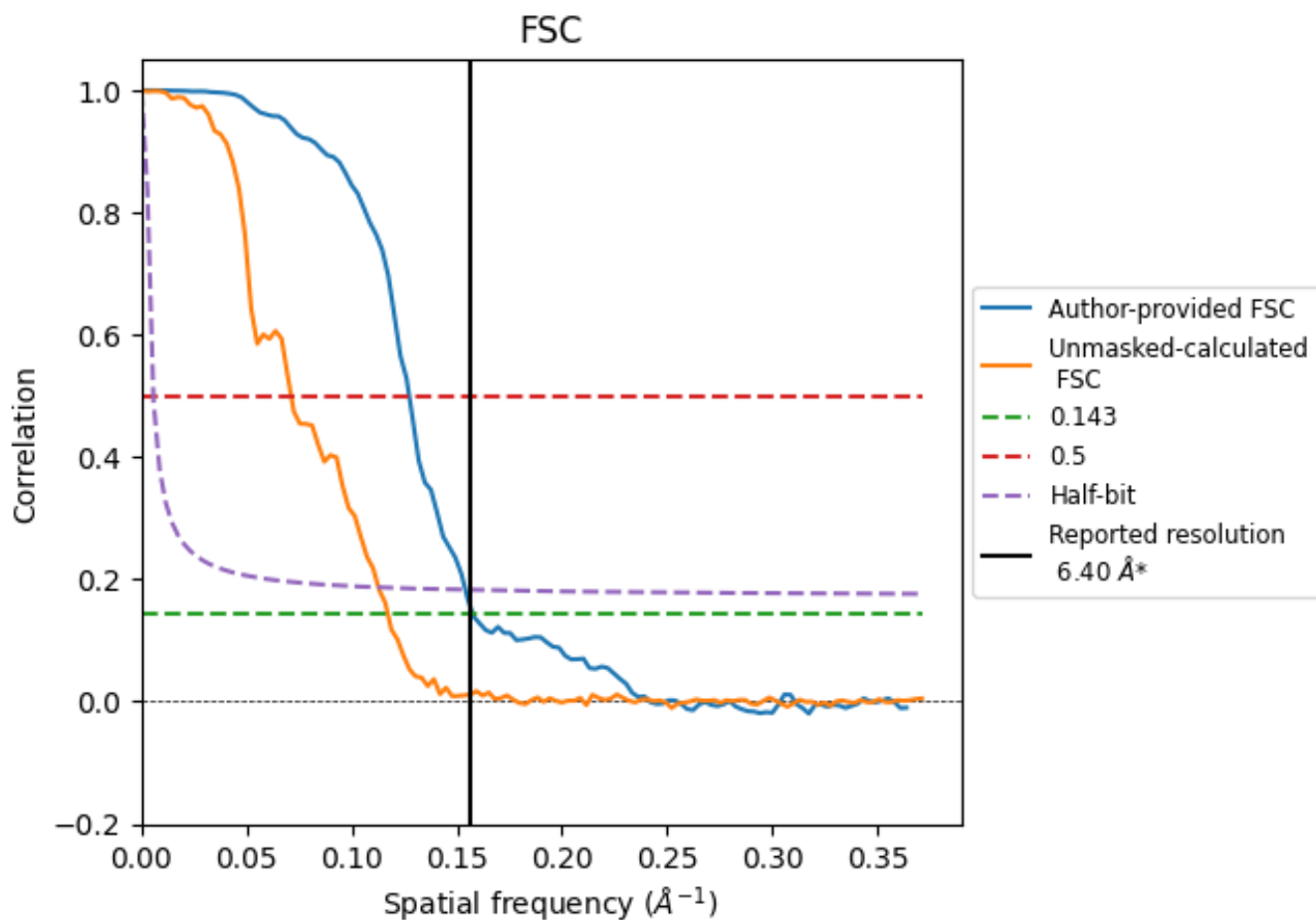


\*Reported resolution corresponds to spatial frequency of 0.156 Å<sup>-1</sup>

## 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 0.156 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

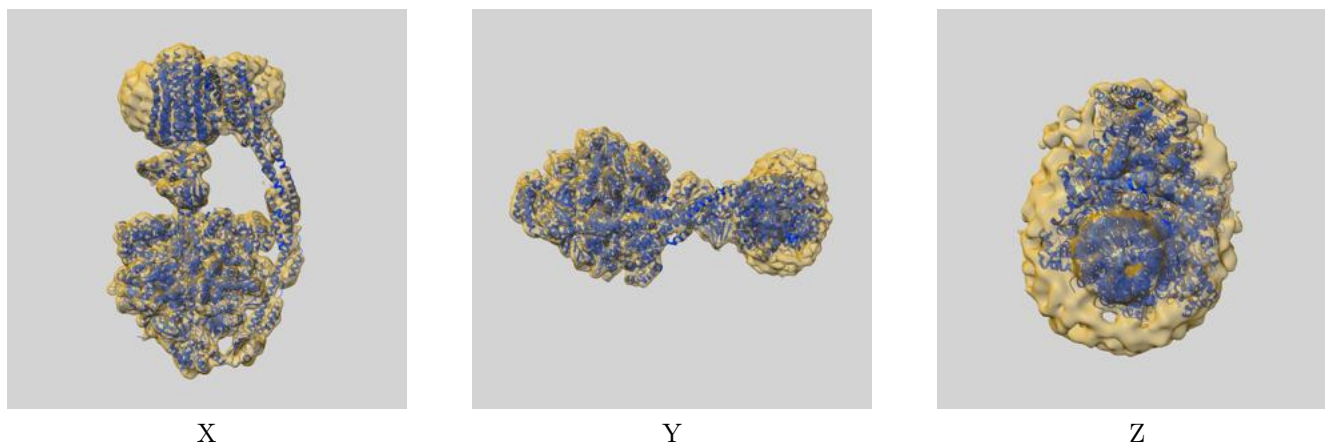
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	6.35	7.85	6.49
Unmasked-calculated*	8.53	14.04	8.87

\*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 8.53 differs from the reported value 6.4 by more than 10 %

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

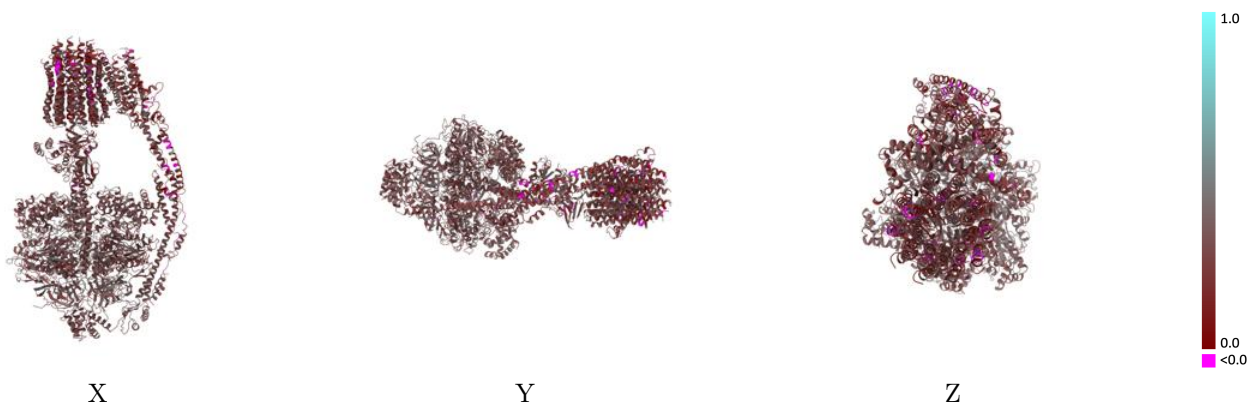
This section contains information regarding the fit between EMDB map EMD-25973 and PDB model 7TKL. Per-residue inclusion information can be found in section 3 on page 7.

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



The images above show the 3D surface view of the map at the recommended contour level 0.6 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 [\(i\)](#)

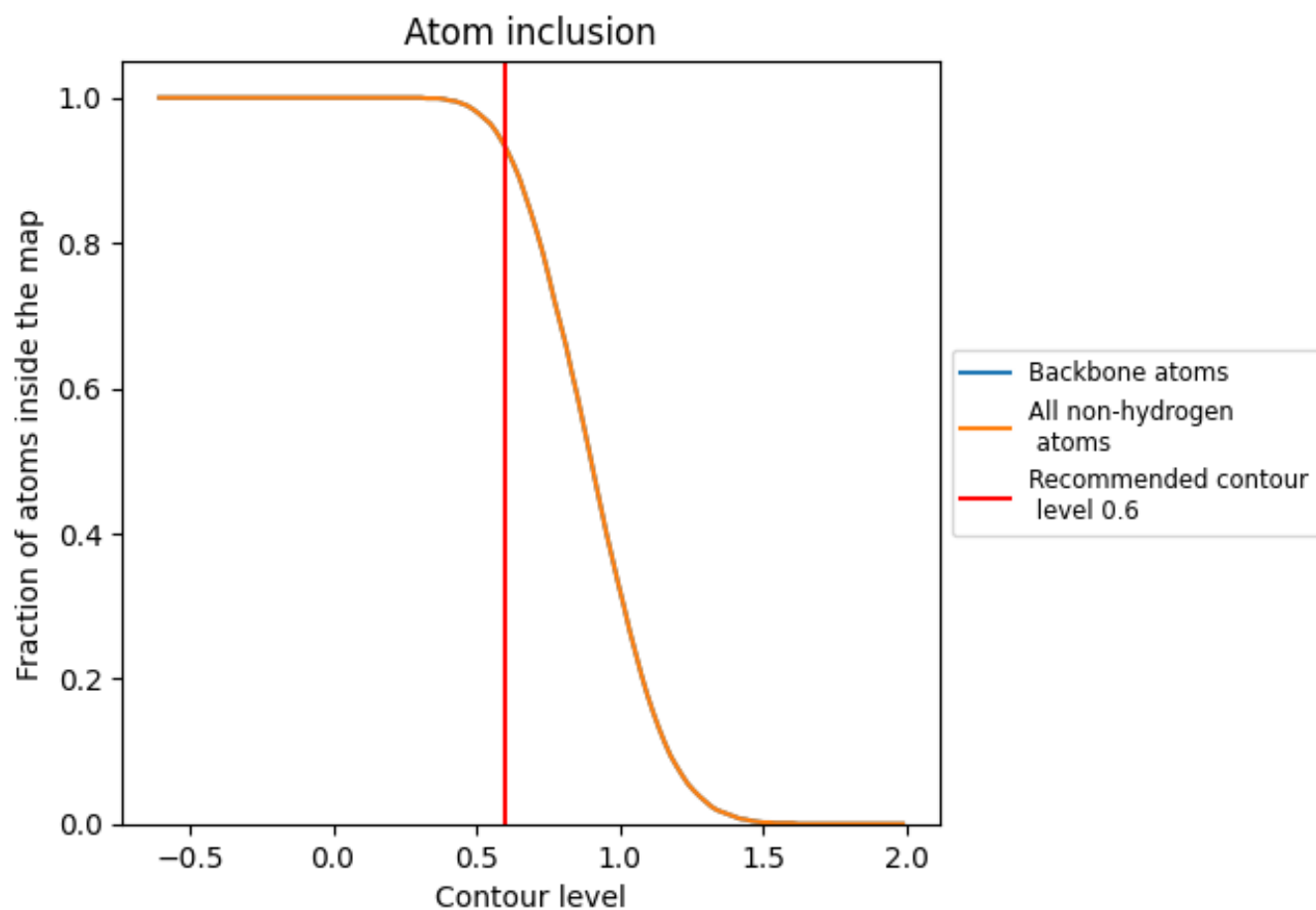


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.2900
0	 0.8970	 0.2280
1	 0.8870	 0.2470
2	 0.8900	 0.2400
3	 0.8650	 0.2430
4	 0.8300	 0.1990
5	 0.7730	 0.1910
6	 0.7500	 0.1970
7	 0.8120	 0.2230
8	 0.8400	 0.2250
9	 0.8070	 0.1950
A	 0.9700	 0.3250
B	 0.9830	 0.3270
C	 0.9730	 0.3200
D	 0.9550	 0.3160
E	 0.9920	 0.3350
F	 0.9850	 0.3240
G	 0.9580	 0.2860
H	 0.9250	 0.2340
I	 0.9480	 0.2710
O	 0.9920	 0.3140
T	 0.9010	 0.2570
U	 0.9500	 0.2660
V	 0.7560	 0.2150
W	 0.7500	 0.1850
X	 0.6770	 0.2390
Y	 0.8380	 0.2090
Z	 0.9220	 0.2380

