



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:03 PM UTC

PDB ID : 7TKF / pdb_00007tkf
EMDB ID : EMD-25967
Title : Yeast ATP synthase State 2binding(b) with 10 mM ATP backbone model
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2022-01-17
Resolution : 7.10 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

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:

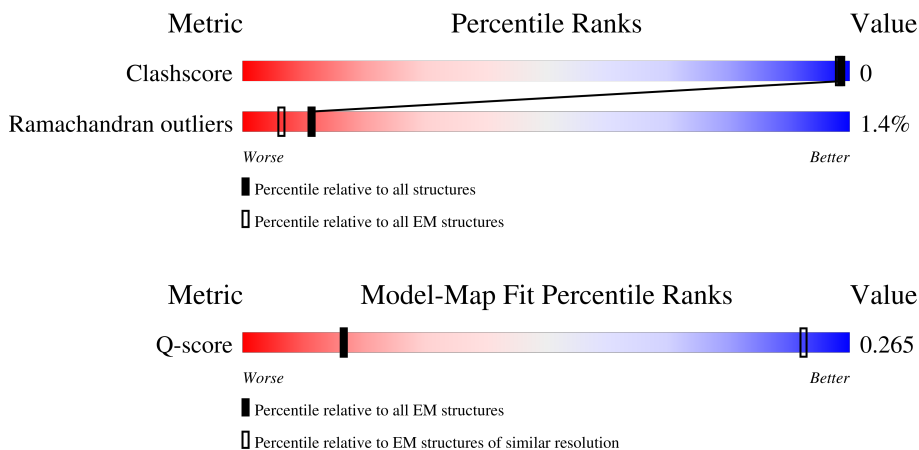
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.10 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	464 (6.60 - 7.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	76	92% 7% .
1	1	76	5% 92% 7% .
1	2	76	5% 92% 7% .
1	3	76	12% 91% 7% .
1	4	76	9% 95% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	5	76	91% 7% ..
1	6	76	11% 89% 8% .
1	7	76	88% 8% .
1	8	76	92% 7% .
1	9	76	9% 87% 11% .
2	A	510	90% 8% .
2	B	510	90% 9% .
2	C	510	89% 8% .
3	D	478	88% 10% .
3	E	478	87% 10% .
3	F	478	87% 11% .
4	G	278	89% 6% 5%
5	H	138	80% 7% 13%
6	I	61	79% 21%
7	O	195	87% 9% ..
8	T	249	85% 5% 10%
9	U	209	74% 26%
10	V	173	8% 92% 7% .
11	W	95	8% 80% 8% . 11%
12	X	92	7% 65% . 33%
13	Y	59	10% 61% . 37%
14	Z	48	100%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 20228 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
1	0	75	Total	C	N	O	0	0
			300	150	75	75		
1	1	75	Total	C	N	O	0	0
			300	150	75	75		
1	2	75	Total	C	N	O	0	0
			300	150	75	75		
1	3	74	Total	C	N	O	0	0
			296	148	74	74		
1	4	75	Total	C	N	O	0	0
			300	150	75	75		
1	5	75	Total	C	N	O	0	0
			300	150	75	75		
1	6	74	Total	C	N	O	0	0
			296	148	74	74		
1	7	73	Total	C	N	O	0	0
			292	146	73	73		
1	8	75	Total	C	N	O	0	0
			300	150	75	75		
1	9	74	Total	C	N	O	0	0
			296	148	74	74		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	501	Total	C	N	O	0	0
			2004	1002	501	501		
2	B	505	Total	C	N	O	0	0
			2020	1010	505	505		
2	C	496	Total	C	N	O	0	0
			1984	992	496	496		

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

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

- 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
			1060	530	265	265		

- 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

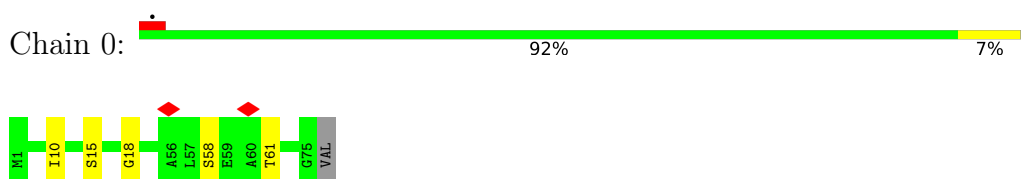
- Molecule 14 is a protein called ATP synthase protein 8.

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

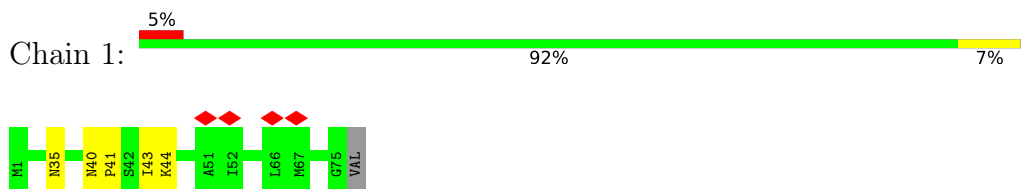
3 Residue-property plots [i](#)

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.

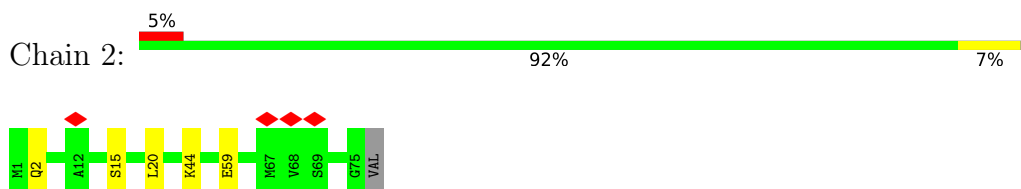
- Molecule 1: ATP synthase subunit 9



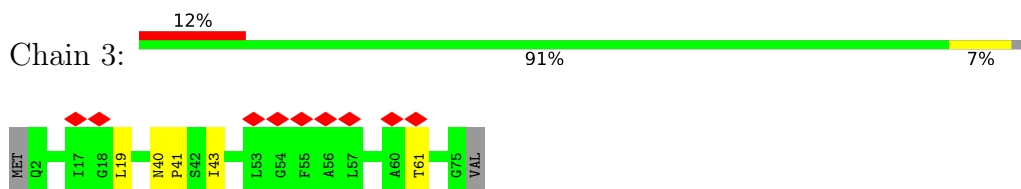
- Molecule 1: ATP synthase subunit 9



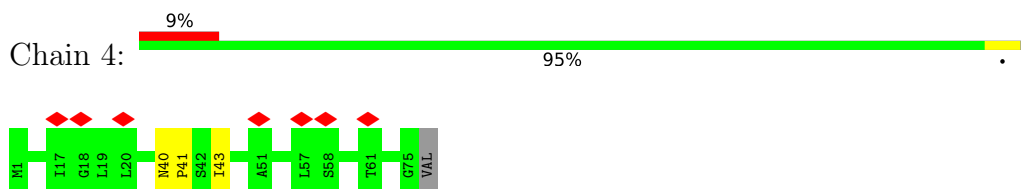
- Molecule 1: ATP synthase subunit 9




- Molecule 1: ATP synthase subunit 9

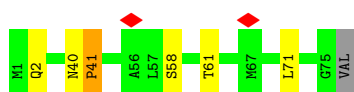


- Molecule 1: ATP synthase subunit 9




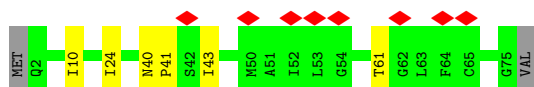
- Molecule 1: ATP synthase subunit 9

Chain 5:  91% 7% ..




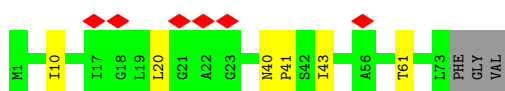
- Molecule 1: ATP synthase subunit 9

Chain 6:  11% 89% 8% .




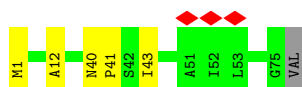
- Molecule 1: ATP synthase subunit 9

Chain 7:  8% 88% 8% .




- Molecule 1: ATP synthase subunit 9

Chain 8:  92% 7% .




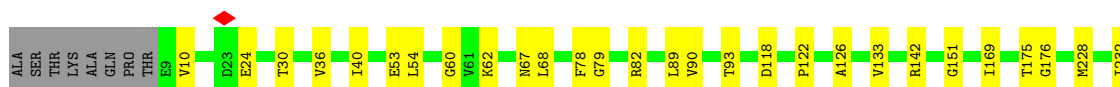
- Molecule 1: ATP synthase subunit 9

Chain 9:  9% 87% 11% .

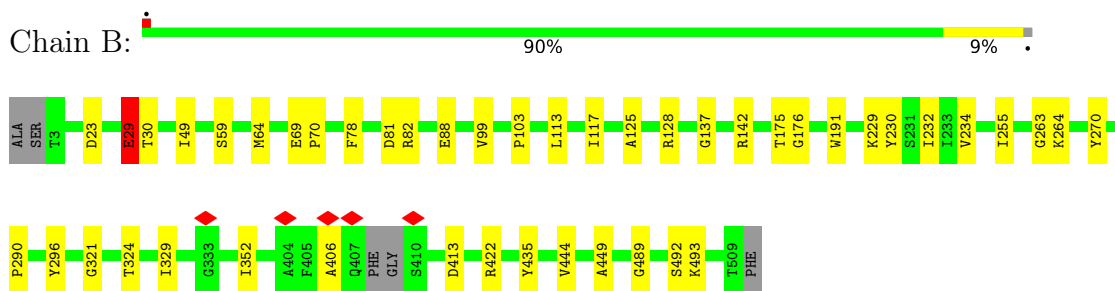


- Molecule 2: ATP synthase subunit alpha

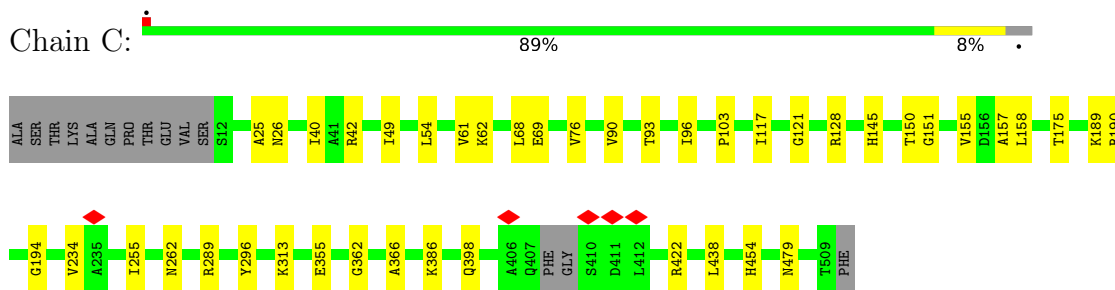
Chain A:  90% 8% .



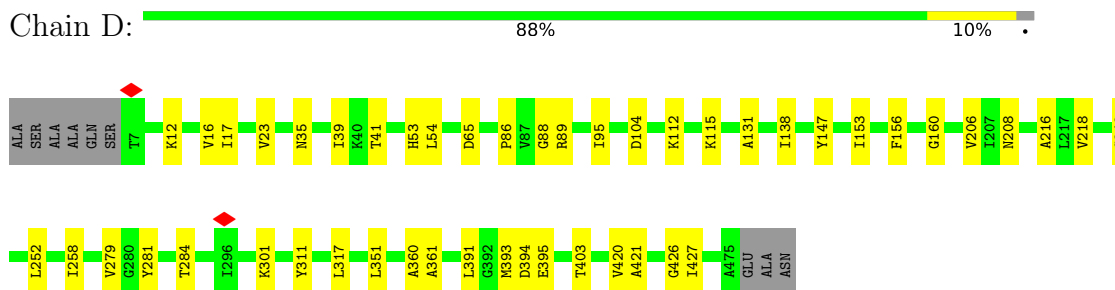
- Molecule 2: ATP synthase subunit alpha



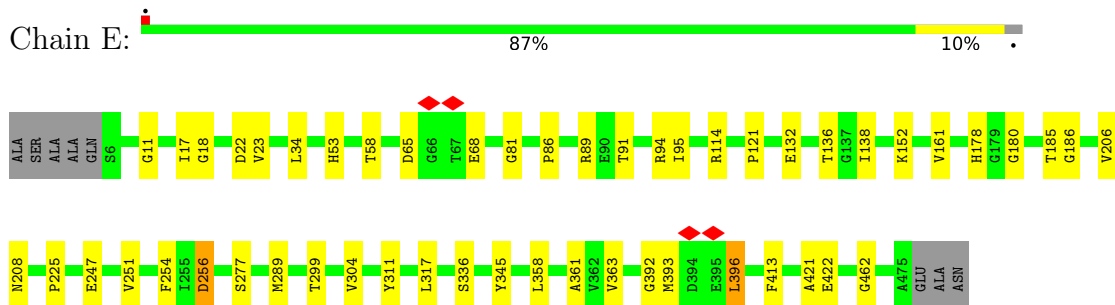
- Molecule 2: ATP synthase subunit alpha



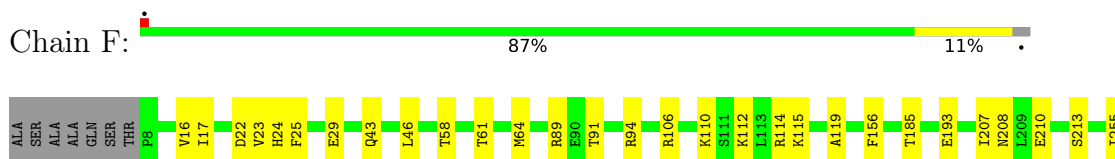
- Molecule 3: ATP synthase subunit beta

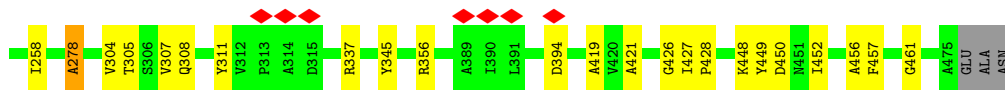


- Molecule 3: ATP synthase subunit beta

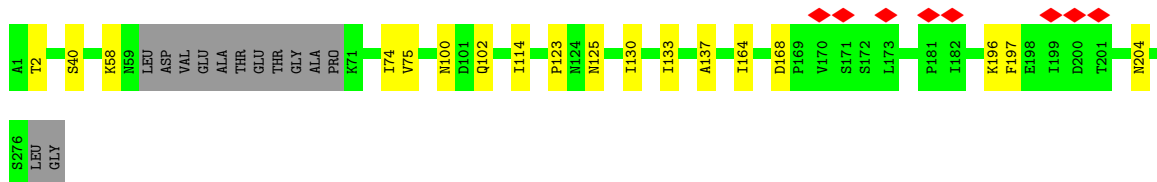
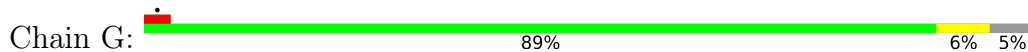


- Molecule 3: ATP synthase subunit beta

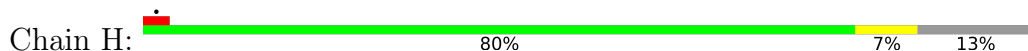




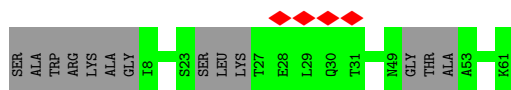
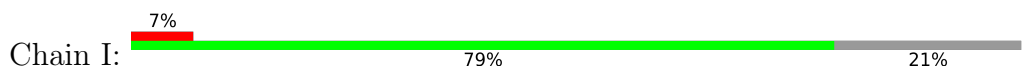
• Molecule 4: ATP synthase subunit gamma



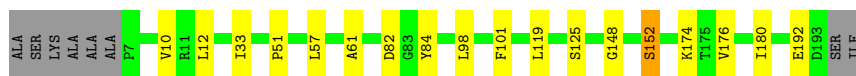
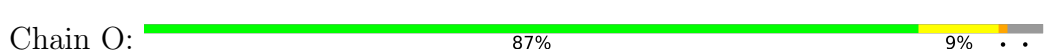
• Molecule 5: ATP synthase subunit delta



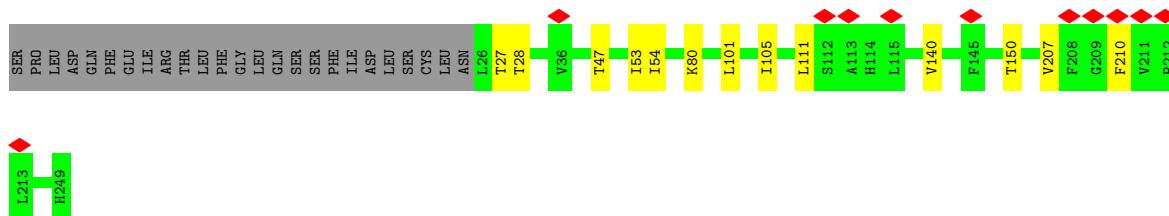
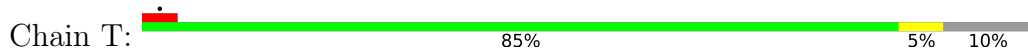
• Molecule 6: ATP synthase subunit epsilon



• Molecule 7: ATP synthase subunit 5

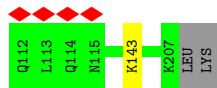
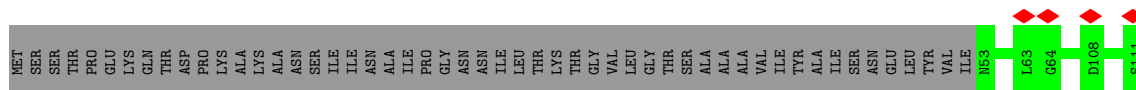


• Molecule 8: ATP synthase subunit a



• Molecule 9: ATP synthase subunit 4

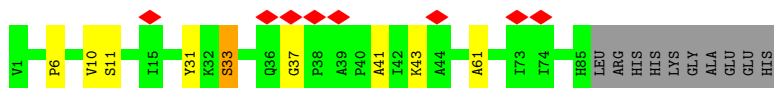
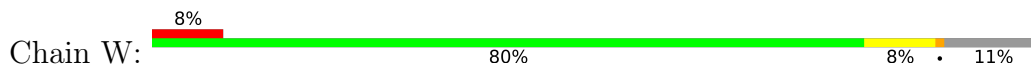




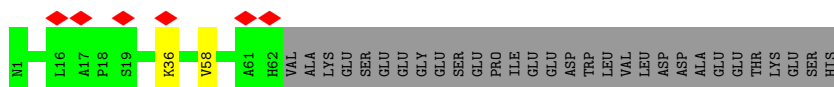
• Molecule 10: ATP synthase subunit d



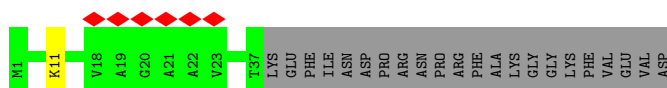
• Molecule 11: ATP synthase subunit f



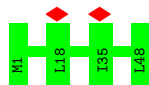
• Molecule 12: ATP synthase subunit H



• 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	9157	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	1.773	Depositor
Minimum map value	-0.514	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	344.96, 344.96, 344.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	1.21	0/299	2.14	10/372 (2.7%)
1	1	1.19	0/299	2.04	5/372 (1.3%)
1	2	1.22	0/299	2.22	9/372 (2.4%)
1	3	1.16	0/295	2.10	6/367 (1.6%)
1	4	1.20	0/299	2.23	2/372 (0.5%)
1	5	1.25	0/299	2.26	8/372 (2.2%)
1	6	1.24	0/295	2.15	8/367 (2.2%)
1	7	1.20	0/291	2.23	8/362 (2.2%)
1	8	1.21	0/299	2.20	6/372 (1.6%)
1	9	1.24	0/295	2.25	11/367 (3.0%)
2	A	1.54	0/2003	1.82	41/2502 (1.6%)
2	B	1.56	0/2018	1.89	39/2519 (1.5%)
2	C	1.53	0/1982	1.91	40/2474 (1.6%)
3	D	1.55	1/1875 (0.1%)	1.89	45/2342 (1.9%)
3	E	1.57	1/1879 (0.1%)	1.94	51/2347 (2.2%)
3	F	1.57	0/1871	1.94	56/2337 (2.4%)
4	G	1.43	0/1058	2.03	21/1319 (1.6%)
5	H	1.47	0/475	1.84	9/585 (1.5%)
6	I	1.33	0/190	1.73	0/231
7	O	1.53	0/747	1.86	14/932 (1.5%)
8	T	1.27	0/896	1.73	16/1117 (1.4%)
9	U	1.31	0/619	1.85	2/772 (0.3%)
10	V	1.39	0/684	1.93	8/852 (0.9%)
11	W	1.25	0/339	1.96	8/422 (1.9%)
12	X	1.38	0/247	2.21	0/307
13	Y	1.19	0/147	1.67	0/182
14	Z	1.26	0/192	1.85	0/237
All	All	1.46	2/20192 (0.0%)	1.94	423/25172 (1.7%)

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	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
2	B	0	1
3	E	0	1
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	391	LEU	CA-C	-6.84	1.49	1.53
3	E	11	GLY	CA-C	-5.02	1.47	1.51

All (423) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	204	ASN	CA-C-N	13.59	128.80	120.24
4	G	204	ASN	C-N-CA	13.59	128.80	120.24
3	D	361	ALA	N-CA-C	-9.69	103.57	114.62
2	C	190	ARG	N-CA-C	-9.33	101.90	113.38
3	E	161	VAL	N-CA-C	-8.99	102.46	112.80
8	T	54	ILE	N-CA-C	-8.83	104.64	111.62
2	B	99	VAL	N-CA-C	-8.67	102.08	109.19
2	C	398	GLN	N-CA-C	-8.66	102.84	113.41
7	O	101	PHE	N-CA-C	-8.53	101.59	112.93
3	D	160	GLY	N-CA-C	-8.42	103.76	114.37
8	T	105	ILE	N-CA-C	-8.32	101.47	108.63
10	V	172	VAL	N-CA-C	-8.31	103.72	111.45
8	T	80	LYS	N-CA-C	-8.09	102.98	113.17
8	T	140	VAL	N-CA-C	-7.79	103.84	112.80
2	C	96	ILE	N-CA-C	-7.68	101.53	110.21
3	E	132	GLU	N-CA-C	-7.63	97.72	109.24
2	A	232	ILE	N-CA-C	-7.62	97.50	108.48
4	G	100	ASN	N-CA-C	-7.60	104.04	113.38
3	D	112	LYS	N-CA-C	-7.56	99.53	111.02
2	C	145	HIS	N-CA-C	-7.55	105.24	114.75
8	T	53	ILE	N-CA-C	-7.53	105.50	112.43
3	F	304	VAL	N-CA-C	-7.46	101.92	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	311	TYR	N-CA-C	-7.44	96.60	108.73
3	D	95	ILE	N-CA-C	-7.42	97.73	108.11
3	F	29	GLU	N-CA-C	-7.40	98.36	109.83
8	T	47	THR	N-CA-C	-7.30	104.52	113.50
1	7	10	ILE	CA-C-N	7.29	128.07	119.98
1	7	10	ILE	C-N-CA	7.29	128.07	119.98
2	C	93	THR	N-CA-C	-7.28	103.43	111.36
3	E	363	VAL	N-CA-C	-7.27	105.92	112.90
2	C	40	ILE	N-CA-C	-7.20	97.15	108.81
7	O	174	LYS	N-CA-C	-7.20	96.60	108.76
7	O	180	ILE	N-CA-C	-7.14	105.67	111.81
2	A	60	GLY	N-CA-C	-7.11	106.02	114.48
7	O	152	SER	CA-C-N	7.09	129.79	120.28
7	O	152	SER	C-N-CA	7.09	129.79	120.28
3	F	305	THR	N-CA-C	-7.09	97.86	108.99
5	H	41	VAL	N-CA-C	-7.09	97.92	108.12
11	W	10	VAL	N-CA-C	-7.08	97.90	108.46
2	B	296	TYR	N-CA-C	-7.07	100.29	110.40
3	D	39	ILE	N-CA-C	-7.04	98.29	108.36
3	D	17	ILE	N-CA-C	-7.03	96.96	107.37
3	F	345	TYR	N-CA-C	-7.01	95.66	108.85
2	B	352	ILE	N-CA-C	-7.01	98.03	108.12
3	F	110	LYS	N-CA-C	-6.99	97.82	109.07
3	F	419	ALA	N-CA-C	6.96	118.52	111.07
2	C	289	ARG	N-CA-C	-6.96	101.02	109.72
3	F	207	ILE	N-CA-C	-6.95	97.08	107.37
1	4	43	ILE	CA-C-N	6.93	130.50	120.38
1	4	43	ILE	C-N-CA	6.93	130.50	120.38
2	B	290	PRO	N-CA-C	6.90	117.09	110.47
3	F	43	GLN	N-CA-C	-6.89	104.86	112.72
3	F	46	LEU	N-CA-C	-6.88	97.68	108.90
5	H	61	GLU	N-CA-C	-6.88	97.06	108.34
3	E	17	ILE	N-CA-C	-6.88	95.04	109.34
3	F	64	MET	N-CA-C	-6.85	103.82	112.93
3	F	156	PHE	N-CA-C	-6.85	98.90	109.24
5	H	56	VAL	N-CA-C	-6.74	98.68	108.11
3	F	17	ILE	N-CA-C	-6.73	98.17	107.99
3	E	299	THR	N-CA-C	-6.71	100.03	109.69
2	B	176	GLY	N-CA-C	-6.71	103.35	114.48
3	E	317	LEU	N-CA-C	-6.69	105.02	113.72
3	F	114	ARG	N-CA-C	-6.68	99.17	109.52
2	A	118	ASP	N-CA-C	-6.68	105.13	113.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	386	LYS	N-CA-C	-6.68	104.78	113.12
2	B	255	ILE	CA-C-N	6.67	127.39	119.98
2	B	255	ILE	C-N-CA	6.67	127.39	119.98
2	A	323	LEU	N-CA-C	-6.64	98.44	109.46
2	A	234	VAL	N-CA-C	-6.61	98.91	108.17
3	E	58	THR	N-CA-C	-6.60	97.52	108.34
1	8	43	ILE	CA-C-N	6.59	129.41	120.38
1	8	43	ILE	C-N-CA	6.59	129.41	120.38
3	E	392	GLY	N-CA-C	-6.58	105.43	112.08
7	O	176	VAL	N-CA-C	-6.58	98.65	108.12
2	C	479	ASN	N-CA-C	-6.55	105.04	113.16
2	C	234	VAL	N-CA-C	-6.53	99.07	108.53
3	E	89	ARG	N-CA-C	-6.52	105.08	113.16
2	A	68	LEU	N-CA-C	-6.50	98.30	108.90
3	F	91	THR	N-CA-C	-6.50	105.27	113.72
2	C	42	ARG	N-CA-C	-6.50	97.78	108.76
7	O	192	GLU	N-CA-C	-6.50	105.39	113.38
4	G	164	ILE	N-CA-C	-6.50	98.27	108.86
2	B	232	ILE	N-CA-C	-6.48	98.86	108.45
11	W	6	PRO	N-CA-C	6.46	118.59	110.70
3	F	22	ASP	N-CA-C	-6.46	99.19	109.59
3	D	420	VAL	N-CA-C	-6.44	106.46	112.83
1	6	10	ILE	CA-C-N	6.41	127.09	119.98
1	6	10	ILE	C-N-CA	6.41	127.09	119.98
2	C	128	ARG	N-CA-C	-6.37	99.43	109.50
1	0	18	GLY	CA-C-N	6.36	129.43	120.28
1	0	18	GLY	C-N-CA	6.36	129.43	120.28
2	A	40	ILE	N-CA-C	-6.34	99.07	108.45
2	C	68	LEU	N-CA-C	-6.34	98.40	108.73
2	C	313	LYS	N-CA-C	-6.32	96.81	107.99
2	B	422	ARG	CA-C-N	6.30	126.93	120.00
2	B	422	ARG	C-N-CA	6.30	126.93	120.00
3	F	428	PRO	CA-C-N	6.27	125.94	119.92
3	F	428	PRO	C-N-CA	6.27	125.94	119.92
1	5	61	THR	CA-C-N	6.27	126.94	119.98
1	5	61	THR	C-N-CA	6.27	126.94	119.98
2	A	355	GLU	CA-C-N	6.27	129.20	120.29
2	A	355	GLU	C-N-CA	6.27	129.20	120.29
3	F	457	PHE	N-CA-C	-6.27	105.29	114.39
4	G	75	VAL	N-CA-C	-6.26	98.65	108.86
4	G	133	ILE	N-CA-C	-6.25	106.71	112.96
10	V	163	TYR	N-CA-C	-6.25	105.31	113.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9	10	ILE	CA-C-N	6.25	126.91	119.98
1	9	10	ILE	C-N-CA	6.25	126.91	119.98
8	T	27	THR	CA-C-N	6.23	128.63	120.28
8	T	27	THR	C-N-CA	6.23	128.63	120.28
10	V	63	LYS	N-CA-C	-6.21	105.64	113.72
11	W	41	ALA	CA-C-N	6.20	128.96	120.46
11	W	41	ALA	C-N-CA	6.20	128.96	120.46
1	5	2	GLN	N-CA-C	-6.20	104.45	111.14
4	G	204	ASN	N-CA-C	-6.18	105.02	113.30
3	D	252	LEU	N-CA-C	-6.18	99.68	109.07
3	D	65	ASP	CA-C-N	6.17	125.85	119.92
3	D	65	ASP	C-N-CA	6.17	125.85	119.92
9	U	143	LYS	CA-C-N	6.16	128.32	120.56
9	U	143	LYS	C-N-CA	6.16	128.32	120.56
10	V	64	ASN	N-CA-C	-6.14	102.91	110.65
2	A	329	ILE	N-CA-C	-6.12	99.31	108.12
3	D	88	GLY	N-CA-C	-6.12	102.50	110.45
3	E	22	ASP	N-CA-C	-6.11	100.23	109.95
2	A	443	GLN	CA-C-N	6.11	124.09	120.24
2	A	443	GLN	C-N-CA	6.11	124.09	120.24
3	F	89	ARG	N-CA-C	-6.11	105.59	113.16
1	0	10	ILE	CA-C-N	6.10	127.76	120.14
1	0	10	ILE	C-N-CA	6.10	127.76	120.14
3	D	421	ALA	N-CA-C	-6.10	104.48	112.41
2	A	175	THR	N-CA-C	-6.08	104.45	112.72
2	B	30	THR	CA-C-N	6.07	127.91	121.48
2	B	30	THR	C-N-CA	6.07	127.91	121.48
2	C	150	THR	N-CA-C	-6.06	106.50	114.31
3	E	422	GLU	N-CA-C	-6.05	105.72	113.23
3	F	106	ARG	N-CA-C	-6.05	101.41	110.06
3	F	394	ASP	N-CA-C	-6.04	105.56	113.17
7	O	125	SER	N-CA-C	-6.03	100.43	108.74
1	5	58	SER	CA-C-N	6.00	128.32	120.28
1	5	58	SER	C-N-CA	6.00	128.32	120.28
2	B	64	MET	N-CA-C	-6.00	100.29	109.41
1	1	44	LYS	N-CA-C	5.99	119.42	111.75
3	E	114	ARG	N-CA-C	-5.99	100.38	109.85
2	A	176	GLY	N-CA-C	-5.99	103.62	114.46
2	C	366	ALA	CA-C-N	5.98	128.58	120.63
2	C	366	ALA	C-N-CA	5.98	128.58	120.63
3	E	251	VAL	N-CA-C	-5.98	99.64	108.85
3	F	452	ILE	CA-C-N	5.97	125.99	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	452	ILE	C-N-CA	5.97	125.99	119.90
8	T	150	THR	N-CA-C	-5.95	102.77	108.07
2	A	142	ARG	N-CA-C	-5.95	99.20	108.90
3	F	25	PHE	N-CA-C	-5.94	100.46	109.85
1	3	43	ILE	CA-C-N	5.93	129.04	120.38
1	3	43	ILE	C-N-CA	5.93	129.04	120.38
2	B	69	GLU	N-CA-C	-5.93	101.33	110.58
3	D	104	ASP	N-CA-C	-5.91	105.72	113.17
2	A	82	ARG	N-CA-C	-5.90	105.84	113.16
2	B	489	GLY	N-CA-C	-5.89	107.11	115.30
1	2	20	LEU	CA-C-N	5.89	126.52	119.98
1	2	20	LEU	C-N-CA	5.89	126.52	119.98
2	C	194	GLY	N-CA-C	-5.88	104.08	112.55
1	7	20	LEU	CA-C-N	5.87	126.50	119.98
1	7	20	LEU	C-N-CA	5.87	126.50	119.98
3	F	24	HIS	N-CA-C	-5.87	99.62	109.07
1	6	24	ILE	CA-C-N	5.87	126.45	119.94
1	6	24	ILE	C-N-CA	5.87	126.45	119.94
8	T	207	VAL	N-CA-C	-5.86	99.91	108.11
3	F	427	ILE	N-CA-C	-5.85	101.52	107.89
3	D	206	VAL	N-CA-C	-5.84	104.66	110.62
3	F	421	ALA	N-CA-C	-5.84	106.06	112.72
3	E	311	TYR	N-CA-C	-5.84	99.39	108.90
3	D	138	ILE	N-CA-C	-5.82	100.19	108.58
3	E	152	LYS	CA-C-N	5.82	128.44	120.35
3	E	152	LYS	C-N-CA	5.82	128.44	120.35
2	B	117	ILE	N-CA-C	-5.82	107.07	112.83
2	B	128	ARG	N-CA-C	-5.81	99.43	108.90
7	O	98	LEU	N-CA-C	-5.80	104.76	112.94
3	E	91	THR	N-CA-C	-5.79	106.26	113.38
1	2	59	GLU	CA-C-N	5.78	128.02	120.28
1	2	59	GLU	C-N-CA	5.78	128.02	120.28
3	E	206	VAL	N-CA-C	-5.78	104.47	112.50
3	E	208	ASN	N-CA-C	-5.78	99.77	109.07
1	6	43	ILE	CA-C-N	5.78	128.29	120.38
1	6	43	ILE	C-N-CA	5.78	128.29	120.38
2	A	78	PHE	N-CA-C	-5.78	106.40	113.50
3	D	54	LEU	N-CA-C	-5.76	105.91	113.17
2	B	444	VAL	CA-C-O	-5.76	113.95	118.85
2	C	175	THR	N-CA-C	-5.76	103.52	111.81
2	C	117	ILE	N-CA-C	-5.76	107.13	112.83
11	W	43	LYS	N-CA-C	-5.74	99.54	108.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	449	TYR	N-CA-C	-5.73	105.19	113.21
7	O	84	TYR	N-CA-C	-5.73	104.64	111.69
1	5	41	PRO	N-CA-C	5.73	124.27	112.47
3	D	12	LYS	N-CA-C	-5.73	100.64	109.52
2	C	158	LEU	N-CA-C	-5.72	106.47	113.50
2	A	30	THR	N-CA-C	-5.71	100.74	109.65
5	H	78	GLN	N-CA-C	-5.71	102.41	110.29
3	D	393	MET	N-CA-C	-5.69	106.38	113.38
3	D	23	VAL	N-CA-C	-5.67	100.15	108.99
10	V	90	GLN	N-CA-C	-5.66	106.92	113.88
3	E	18	GLY	CA-C-N	5.65	127.85	120.28
3	E	18	GLY	C-N-CA	5.65	127.85	120.28
3	E	65	ASP	N-CA-C	-5.65	100.15	108.79
3	F	61	THR	N-CA-C	-5.65	100.83	109.41
1	9	43	ILE	CA-C-N	5.64	127.84	120.28
1	9	43	ILE	C-N-CA	5.64	127.84	120.28
3	E	23	VAL	N-CA-C	-5.64	99.65	108.95
10	V	158	TRP	N-CA-C	-5.64	106.07	113.17
3	E	421	ALA	N-CA-C	-5.63	103.67	110.88
4	G	123	PRO	N-CA-C	-5.62	106.37	114.18
8	T	210	PHE	CA-C-N	5.62	123.78	120.24
8	T	210	PHE	C-N-CA	5.62	123.78	120.24
3	F	307	VAL	N-CA-C	-5.61	100.31	108.17
2	B	137	GLY	CA-C-N	5.61	127.62	120.56
2	B	137	GLY	C-N-CA	5.61	127.62	120.56
3	D	258	ILE	N-CA-C	-5.60	106.36	112.80
3	E	136	THR	N-CA-C	-5.60	105.57	112.90
3	F	208	ASN	N-CA-C	-5.59	99.62	108.73
8	T	101	LEU	N-CA-C	-5.58	106.39	113.43
2	C	155	VAL	N-CA-C	-5.58	107.30	112.83
1	0	15	SER	CA-C-N	5.58	128.32	120.28
1	0	15	SER	C-N-CA	5.58	128.32	120.28
2	B	324	THR	N-CA-C	-5.58	102.63	110.50
2	C	90	VAL	N-CA-C	-5.58	100.36	108.17
2	A	53	GLU	N-CA-C	-5.57	103.34	110.53
3	D	35	ASN	N-CA-C	-5.56	103.35	110.53
3	E	95	ILE	N-CA-C	-5.56	99.74	107.80
2	C	26	ASN	N-CA-C	-5.54	106.19	113.17
2	A	287	LEU	N-CA-C	-5.54	106.19	113.17
3	E	304	VAL	N-CA-C	-5.54	100.68	108.27
3	F	210	GLU	N-CA-C	-5.53	101.26	110.17
8	T	111	LEU	N-CA-C	-5.53	106.58	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	317	LEU	N-CA-C	-5.53	106.38	113.23
3	F	112	LYS	N-CA-C	-5.53	102.62	111.02
1	9	44	LYS	N-CA-C	5.52	117.30	111.28
3	E	121	PRO	CA-C-N	5.52	126.74	119.84
3	E	121	PRO	C-N-CA	5.52	126.74	119.84
3	D	395	GLU	N-CA-C	-5.52	105.76	112.88
2	A	228	MET	N-CA-C	-5.52	106.40	113.02
2	C	121	GLY	CA-C-N	5.51	126.73	119.84
2	C	121	GLY	C-N-CA	5.51	126.73	119.84
3	D	216	ALA	N-CA-C	-5.51	100.98	109.52
1	2	44	LYS	N-CA-C	5.50	117.99	111.33
2	B	449	ALA	CA-C-N	5.50	126.05	120.00
2	B	449	ALA	C-N-CA	5.50	126.05	120.00
3	E	138	ILE	N-CA-C	-5.50	99.73	107.75
1	2	2	GLN	CA-C-N	5.49	127.63	120.28
1	2	2	GLN	C-N-CA	5.49	127.63	120.28
1	9	15	SER	CA-C-N	5.49	128.18	120.28
1	9	15	SER	C-N-CA	5.49	128.18	120.28
2	B	264	LYS	N-CA-C	-5.47	102.65	110.59
3	E	186	GLY	N-CA-C	-5.47	100.21	113.18
3	F	356	ARG	N-CA-C	-5.46	105.83	112.88
1	7	43	ILE	CA-C-N	5.46	127.86	120.38
1	7	43	ILE	C-N-CA	5.46	127.86	120.38
2	A	507	VAL	N-CA-C	-5.46	105.02	113.16
3	E	81	GLY	CA-C-N	5.46	125.47	119.90
3	E	81	GLY	C-N-CA	5.46	125.47	119.90
2	C	54	LEU	N-CA-C	-5.43	100.39	109.24
7	O	57	LEU	N-CA-C	-5.43	106.78	113.41
2	A	122	PRO	N-CA-C	-5.43	102.71	111.77
2	C	422	ARG	CA-C-N	5.42	125.95	119.94
2	C	422	ARG	C-N-CA	5.42	125.95	119.94
3	D	41	THR	N-CA-C	-5.41	101.82	110.10
4	G	40	SER	CA-C-N	5.41	127.47	120.44
4	G	40	SER	C-N-CA	5.41	127.47	120.44
3	E	393	MET	N-CA-C	-5.40	106.53	113.23
2	B	82	ARG	N-CA-C	-5.40	106.19	112.89
2	A	422	ARG	CA-C-N	5.39	125.96	119.98
2	A	422	ARG	C-N-CA	5.39	125.96	119.98
2	B	29	GLU	N-CA-C	-5.38	99.33	110.80
2	B	142	ARG	N-CA-C	-5.38	101.11	109.72
1	7	61	THR	CA-C-N	5.38	125.95	119.98
1	7	61	THR	C-N-CA	5.38	125.95	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	191	TRP	CA-C-N	5.38	127.48	120.28
2	B	191	TRP	C-N-CA	5.38	127.48	120.28
1	0	61	THR	CA-C-N	5.37	125.94	119.98
1	0	61	THR	C-N-CA	5.37	125.94	119.98
3	D	89	ARG	N-CA-C	-5.37	106.31	112.92
7	O	82	ASP	N-CA-C	-5.37	105.87	112.90
1	1	43	ILE	CA-C-N	5.36	128.21	120.38
1	1	43	ILE	C-N-CA	5.36	128.21	120.38
4	G	114	ILE	CA-C-N	5.36	127.46	120.28
4	G	114	ILE	C-N-CA	5.36	127.46	120.28
2	C	262	ASN	N-CA-C	-5.36	106.52	113.16
3	D	394	ASP	N-CA-C	-5.36	106.52	113.16
2	A	133	VAL	N-CA-C	-5.36	100.35	108.17
3	F	308	GLN	N-CA-C	-5.35	101.23	109.52
3	F	193	GLU	CA-C-N	5.35	125.91	119.98
3	F	193	GLU	C-N-CA	5.35	125.91	119.98
3	D	53	HIS	N-CA-C	-5.34	100.47	109.07
2	B	234	VAL	N-CA-C	-5.34	100.89	108.58
5	H	92	PRO	CA-C-N	5.33	127.43	120.28
5	H	92	PRO	C-N-CA	5.33	127.43	120.28
4	G	74	ILE	N-CA-C	-5.33	100.44	108.12
2	B	81	ASP	N-CA-C	-5.33	106.46	113.17
3	F	456	ALA	N-CA-C	-5.33	106.37	112.92
2	C	355	GLU	CA-C-N	5.32	127.41	120.28
2	C	355	GLU	C-N-CA	5.32	127.41	120.28
3	E	289	MET	CA-C-N	5.32	125.88	119.98
3	E	289	MET	C-N-CA	5.32	125.88	119.98
4	G	197	PHE	N-CA-C	-5.32	101.40	108.74
2	A	62	LYS	N-CA-C	-5.31	100.75	109.40
3	F	427	ILE	CA-C-N	5.30	126.46	119.84
3	F	427	ILE	C-N-CA	5.30	126.46	119.84
8	T	28	THR	CA-C-N	5.29	127.38	120.28
8	T	28	THR	C-N-CA	5.29	127.38	120.28
2	B	270	TYR	N-CA-C	-5.29	100.10	108.73
1	2	15	SER	CA-C-N	5.29	127.90	120.28
1	2	15	SER	C-N-CA	5.29	127.90	120.28
3	F	337	ARG	N-CA-C	-5.29	106.67	113.23
3	D	208	ASN	N-CA-C	-5.28	99.80	108.41
1	9	12	ALA	CA-C-N	5.28	125.80	119.94
1	9	12	ALA	C-N-CA	5.28	125.80	119.94
2	C	62	LYS	N-CA-C	-5.27	101.35	109.52
1	8	12	ALA	CA-C-N	5.27	125.79	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8	12	ALA	C-N-CA	5.27	125.79	119.94
3	E	225	PRO	CA-C-N	5.27	125.08	119.28
3	E	225	PRO	C-N-CA	5.27	125.08	119.28
1	0	58	SER	CA-C-N	5.26	127.32	120.28
1	0	58	SER	C-N-CA	5.26	127.32	120.28
3	D	16	VAL	N-CA-C	-5.25	98.42	109.34
2	C	255	ILE	CA-C-N	5.24	125.80	119.98
2	C	255	ILE	C-N-CA	5.24	125.80	119.98
3	F	23	VAL	N-CA-C	-5.24	100.65	108.46
3	E	178	HIS	CA-C-N	5.24	125.31	120.34
3	E	178	HIS	C-N-CA	5.24	125.31	120.34
2	A	449	ALA	CA-C-N	5.23	125.64	119.94
2	A	449	ALA	C-N-CA	5.23	125.64	119.94
2	A	89	LEU	N-CA-C	-5.22	101.76	110.17
3	D	248	GLY	CA-C-N	5.22	128.50	120.82
3	D	248	GLY	C-N-CA	5.22	128.50	120.82
3	F	461	GLY	N-CA-C	-5.22	105.13	112.13
4	G	168	ASP	N-CA-C	-5.22	103.08	109.65
3	D	218	VAL	N-CA-C	-5.21	100.61	108.12
3	E	256	ASP	N-CA-C	-5.21	101.15	109.07
4	G	137	ALA	CA-C-N	5.20	126.34	119.84
4	G	137	ALA	C-N-CA	5.20	126.34	119.84
2	A	90	VAL	N-CA-C	-5.20	100.71	108.46
2	C	76	VAL	N-CA-C	-5.20	100.83	108.11
2	B	113	LEU	N-CA-C	-5.19	106.34	113.30
3	F	278	ALA	N-CA-C	-5.19	99.74	110.80
3	E	345	TYR	N-CA-C	-5.18	98.07	109.11
4	G	2	THR	N-CA-C	-5.18	105.55	111.14
3	E	247	GLU	N-CA-C	-5.18	106.36	113.30
3	D	351	LEU	N-CA-C	-5.17	106.65	113.17
4	G	196	LYS	N-CA-C	-5.17	106.97	113.28
1	3	61	THR	CA-C-N	5.17	125.71	119.98
1	3	61	THR	C-N-CA	5.17	125.71	119.98
2	A	169	ILE	N-CA-C	-5.17	100.45	107.99
3	F	213	SER	N-CA-C	-5.17	98.98	108.02
11	W	33	SER	N-CA-C	-5.16	99.80	110.80
2	A	452	ASN	N-CA-C	-5.16	107.15	112.93
2	B	493	LYS	CA-C-N	5.16	127.19	120.28
2	B	493	LYS	C-N-CA	5.16	127.19	120.28
3	E	180	GLY	N-CA-C	-5.16	105.95	112.65
2	A	479	ASN	N-CA-C	-5.15	106.84	113.23
3	F	448	LYS	N-CA-C	-5.15	106.59	112.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	492	SER	N-CA-C	-5.14	103.14	110.59
2	A	10	VAL	CA-C-N	5.13	127.16	120.28
2	A	10	VAL	C-N-CA	5.13	127.16	120.28
3	D	115	LYS	CA-C-N	5.13	125.04	119.76
3	D	115	LYS	C-N-CA	5.13	125.04	119.76
3	D	426	GLY	N-CA-C	-5.13	108.04	115.27
3	E	53	HIS	N-CA-C	-5.12	101.05	109.40
3	F	185	THR	N-CA-C	-5.12	100.83	109.07
3	F	426	GLY	N-CA-C	-5.12	108.05	115.27
11	W	37	GLY	CA-C-N	5.12	125.84	120.11
11	W	37	GLY	C-N-CA	5.12	125.84	120.11
1	5	71	LEU	CA-C-N	5.12	127.55	120.29
1	5	71	LEU	C-N-CA	5.12	127.55	120.29
1	8	1	MET	CA-C-N	5.11	127.13	120.28
1	8	1	MET	C-N-CA	5.11	127.13	120.28
3	D	156	PHE	N-CA-C	-5.11	100.15	109.56
3	E	336	SER	CA-C-N	5.11	127.13	120.28
3	E	336	SER	C-N-CA	5.11	127.13	120.28
2	A	93	THR	N-CA-C	-5.11	105.79	111.36
1	6	61	THR	CA-C-N	5.10	125.64	119.98
1	6	61	THR	C-N-CA	5.10	125.64	119.98
3	E	185	THR	N-CA-C	-5.10	101.08	109.40
1	3	19	LEU	CA-C-N	5.10	127.42	120.54
1	3	19	LEU	C-N-CA	5.10	127.42	120.54
1	9	2	GLN	CA-C-N	5.10	127.11	120.28
1	9	2	GLN	C-N-CA	5.10	127.11	120.28
2	C	296	TYR	N-CA-C	-5.09	102.24	109.62
1	1	35	ASN	CA-C-N	5.09	125.63	119.98
1	1	35	ASN	C-N-CA	5.09	125.63	119.98
2	A	67	ASN	N-CA-C	-5.08	100.17	108.76
3	F	311	TYR	N-CA-C	-5.08	100.44	108.73
2	C	61	VAL	N-CA-C	-5.08	102.53	109.55
3	F	58	THR	N-CA-C	-5.08	101.65	109.52
10	V	135	VAL	CA-C-N	5.08	127.50	120.29
10	V	135	VAL	C-N-CA	5.08	127.50	120.29
2	A	54	LEU	N-CA-C	-5.08	100.90	109.07
7	O	148	GLY	N-CA-C	-5.07	106.70	112.79
2	A	79	GLY	CA-C-N	5.07	128.40	120.75
2	A	79	GLY	C-N-CA	5.07	128.40	120.75
2	B	329	ILE	N-CA-C	-5.07	100.91	108.46
3	F	258	ILE	N-CA-C	-5.06	106.99	113.22
5	H	69	PHE	N-CA-C	-5.06	100.65	108.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	450	ASP	N-CA-C	-5.06	106.88	113.16
4	G	125	ASN	N-CA-C	5.06	116.80	111.28
3	D	284	THR	N-CA-C	-5.06	107.27	112.93
3	E	254	PHE	N-CA-C	-5.05	100.47	109.06
3	E	413	PHE	N-CA-C	-5.05	105.87	112.23
5	H	121	ALA	CA-C-N	5.05	127.00	120.44
5	H	121	ALA	C-N-CA	5.05	127.00	120.44
3	F	115	LYS	CA-C-N	5.05	124.98	119.78
3	F	115	LYS	C-N-CA	5.05	124.98	119.78
2	C	454	HIS	N-CA-C	-5.05	106.90	113.16
3	D	153	ILE	N-CA-C	-5.04	101.22	108.89
2	C	69	GLU	N-CA-C	-5.04	100.32	109.09
3	D	427	ILE	CA-C-N	5.04	124.97	119.78
3	D	427	ILE	C-N-CA	5.04	124.97	119.78
3	F	94	ARG	N-CA-C	-5.03	101.20	109.40
3	F	255	ILE	N-CA-C	-5.03	100.65	108.86
2	B	175	THR	N-CA-C	-5.03	103.69	110.68
2	B	78	PHE	N-CA-C	-5.03	102.33	110.32
3	D	403	THR	CA-C-N	5.02	127.34	120.46
3	D	403	THR	C-N-CA	5.02	127.34	120.46
4	G	130	ILE	N-CA-C	-5.02	100.34	107.77
3	E	396	LEU	N-CA-C	-5.01	100.12	110.80
7	O	33	ILE	N-CA-C	-5.00	107.85	111.90

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	4	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
2	B	29	GLU	Peptide
3	E	256	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	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
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	2004	0	575	1	0
2	B	2020	0	575	1	0
2	C	1984	0	567	1	0
3	D	1876	0	537	0	0
3	E	1880	0	538	0	0
3	F	1872	0	537	0	0
4	G	1060	0	277	0	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	20228	0	5731	4	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 (4) 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:B:263:GLY:HA2	2:B:321:GLY:H	1.72	0.55
2:C:151:GLY:HA3	2:C:438:LEU:H	1.83	0.43
7:O:119:LEU:H	7:O:152:SER:H	1.68	0.41
2:A:151:GLY:HA3	2:A:438:LEU:H	1.86	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	9	40
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%)	2 (3%)	1 (1%)	9	40
1	5	73/76 (96%)	70 (96%)	2 (3%)	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%)	69 (96%)	2 (3%)	1 (1%)	9	40
2	A	499/510 (98%)	476 (95%)	20 (4%)	3 (1%)	21	59
2	B	501/510 (98%)	464 (93%)	24 (5%)	13 (3%)	4	25
2	C	492/510 (96%)	463 (94%)	23 (5%)	6 (1%)	10	44
3	D	467/478 (98%)	430 (92%)	30 (6%)	7 (2%)	8	40
3	E	468/478 (98%)	439 (94%)	20 (4%)	9 (2%)	6	32
3	F	466/478 (98%)	441 (95%)	22 (5%)	3 (1%)	21	59
4	G	261/278 (94%)	254 (97%)	5 (2%)	2 (1%)	16	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	110/138 (80%)	100 (91%)	7 (6%)	3 (3%)	4	25
6	I	42/61 (69%)	39 (93%)	3 (7%)	0	100	100
7	O	185/195 (95%)	175 (95%)	6 (3%)	4 (2%)	5	29
8	T	222/249 (89%)	212 (96%)	10 (4%)	0	100	100
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	150 (89%)	14 (8%)	5 (3%)	3	22
11	W	83/95 (87%)	71 (86%)	8 (10%)	4 (5%)	2	16
12	X	60/92 (65%)	53 (88%)	5 (8%)	2 (3%)	3	21
13	Y	35/59 (59%)	30 (86%)	4 (11%)	1 (3%)	3	23
14	Z	46/48 (96%)	42 (91%)	4 (9%)	0	100	100
All	All	4984/5321 (94%)	4694 (94%)	220 (4%)	70 (1%)	11	40

All (70) 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	24	GLU
2	B	29	GLU
2	B	59	SER
2	B	229	LYS
2	C	25	ALA
3	D	360	ALA
3	E	68	GLU
3	E	94	ARG
3	E	358	LEU
3	F	278	ALA
7	O	61	ALA
10	V	83	ILE
11	W	33	SER
12	X	58	VAL
13	Y	11	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	126	ALA
2	B	49	ILE
2	B	103	PRO
2	B	125	ALA
2	B	406	ALA
2	B	435	TYR
2	C	49	ILE
3	E	34	LEU
3	E	396	LEU
4	G	58	LYS
5	H	22	TYR
10	V	84	ASP
11	W	31	TYR
2	B	88	GLU
3	D	86	PRO
3	D	281	TYR
3	E	462	GLY
3	F	119	ALA
5	H	33	PRO
7	O	10	VAL
11	W	11	SER
11	W	61	ALA
2	A	36	VAL
2	B	23	ASP
2	B	413	ASP
2	C	103	PRO
2	C	157	ALA
2	C	189	LYS
3	D	301	LYS
3	E	277	SER
3	E	361	ALA
3	F	16	VAL
7	O	12	LEU
10	V	55	PHE
10	V	89	LEU
12	X	36	LYS
2	B	230	TYR
3	D	131	ALA
3	D	147	TYR
2	C	362	GLY
10	V	128	ARG
2	B	70	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	86	PRO
4	G	102	GLN
3	D	279	VAL
7	O	51	PRO
5	H	17	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.

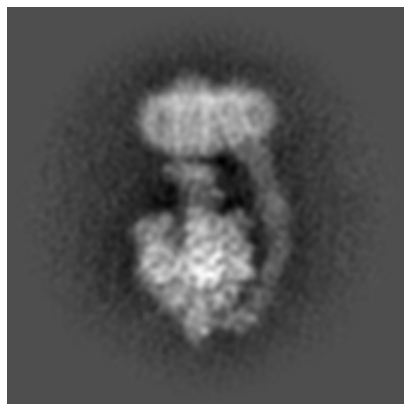
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25967. These allow visual inspection of the internal detail of the map and identification of artifacts.

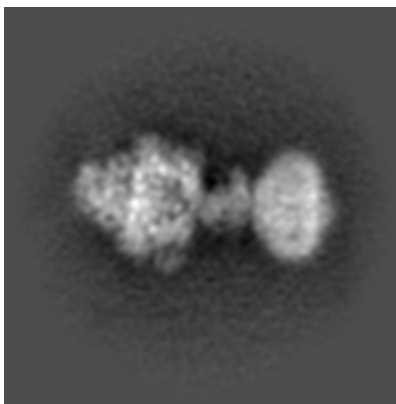
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

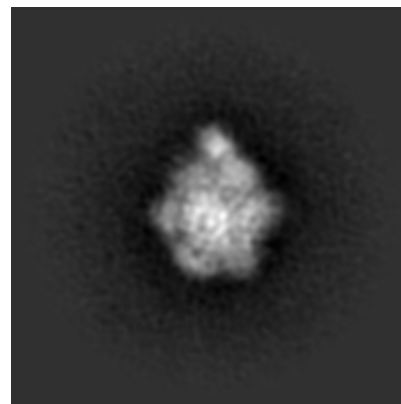
6.1.1 Primary map



X

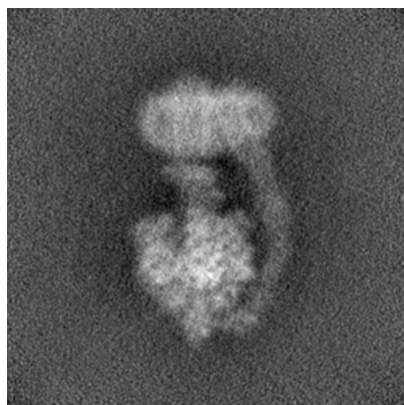


Y

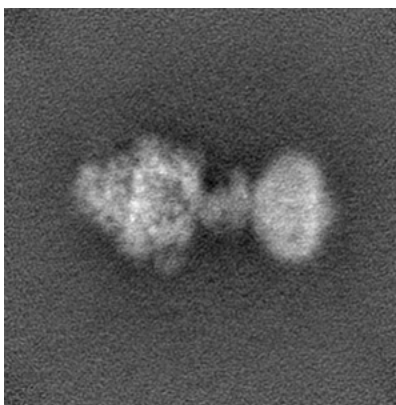


Z

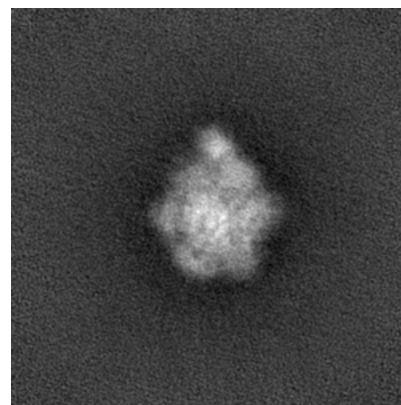
6.1.2 Raw map



X



Y

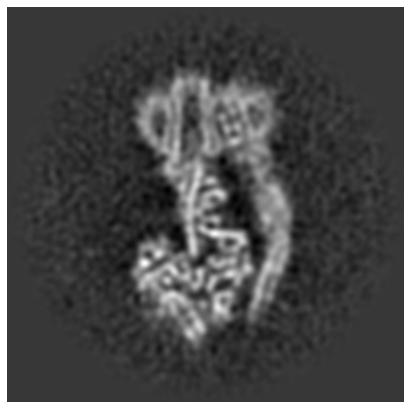


Z

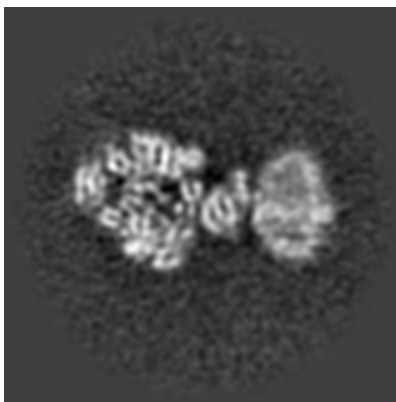
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

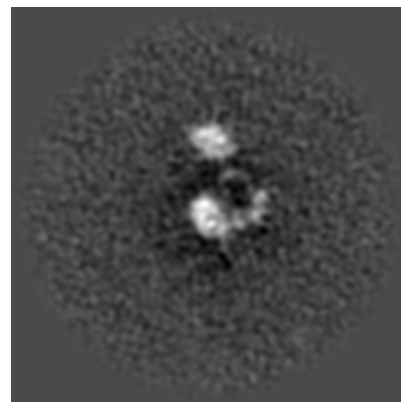
6.2.1 Primary map



X Index: 128

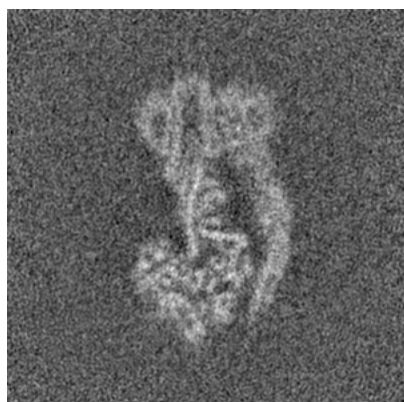


Y Index: 128

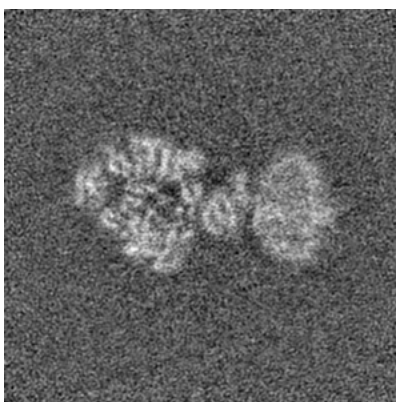


Z Index: 128

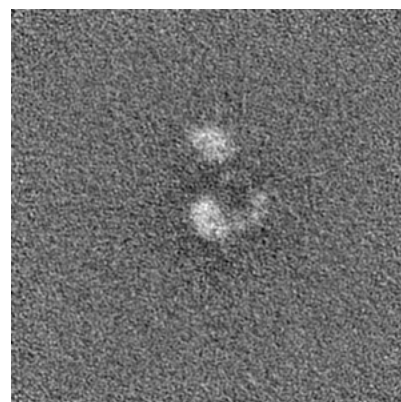
6.2.2 Raw map



X Index: 128



Y Index: 128

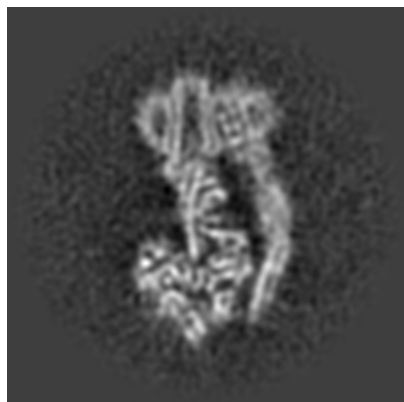


Z Index: 128

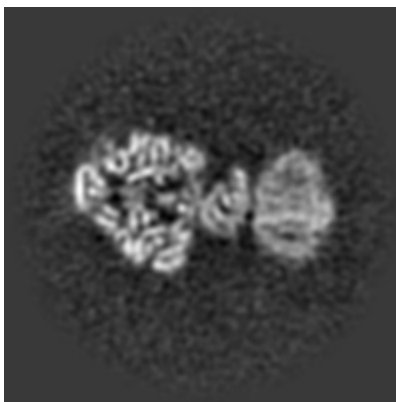
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

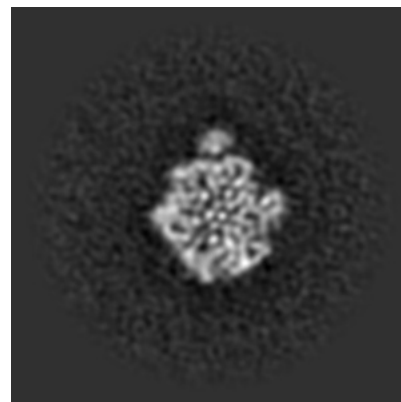
6.3.1 Primary map



X Index: 129

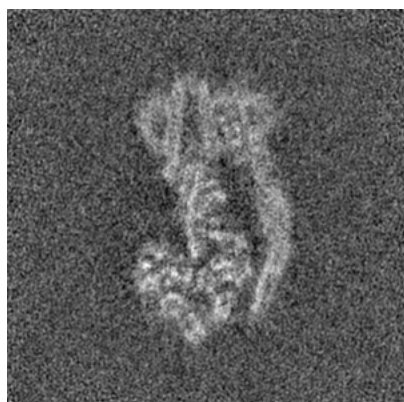


Y Index: 125

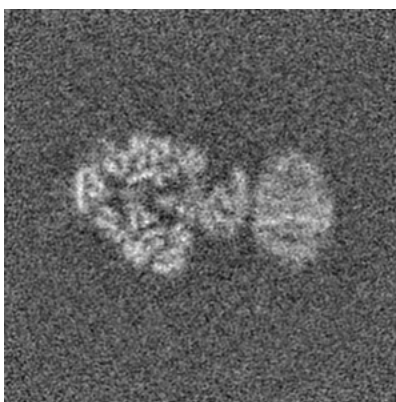


Z Index: 86

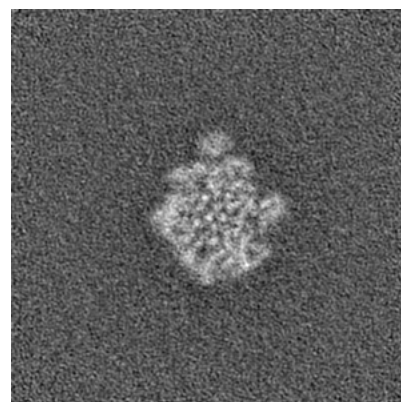
6.3.2 Raw map



X Index: 129



Y Index: 125

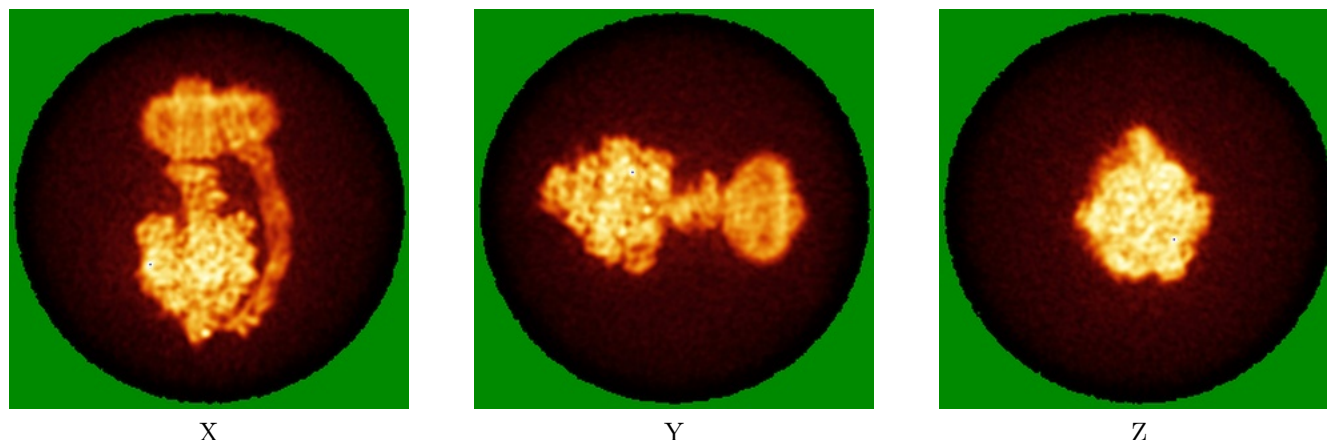


Z Index: 85

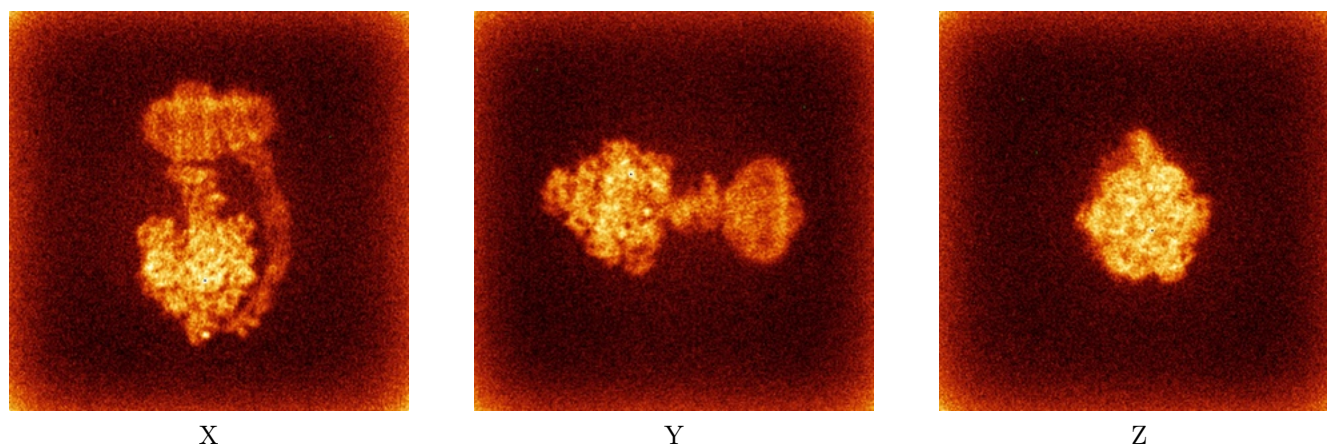
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



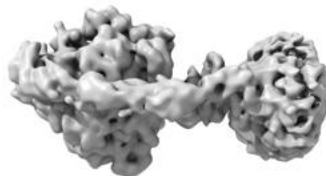
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

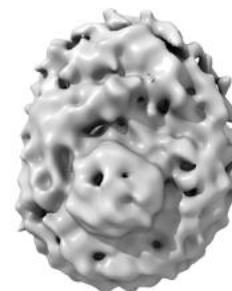
6.5.1 Primary map



X



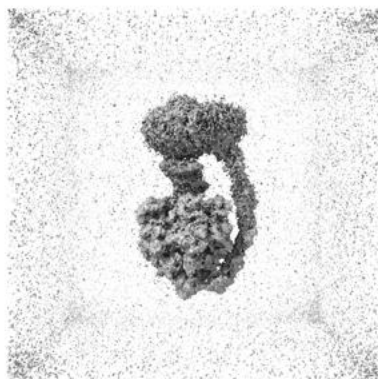
Y



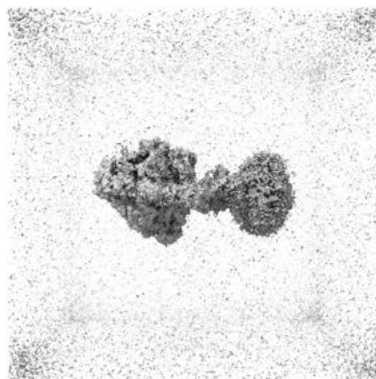
Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

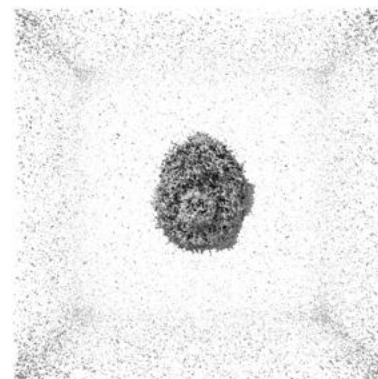
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

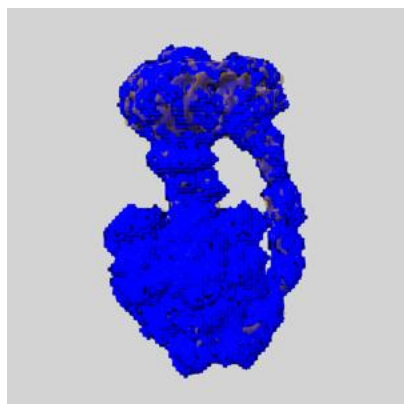
6.6 Mask visualisation [i](#)

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

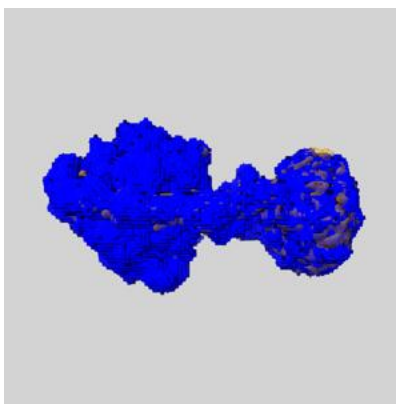
A mask typically either:

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

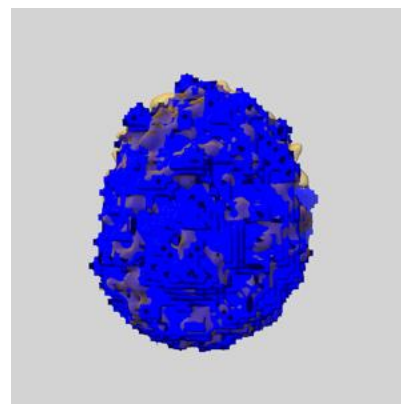
6.6.1 emd_25967_msk_1.map [i](#)



X



Y

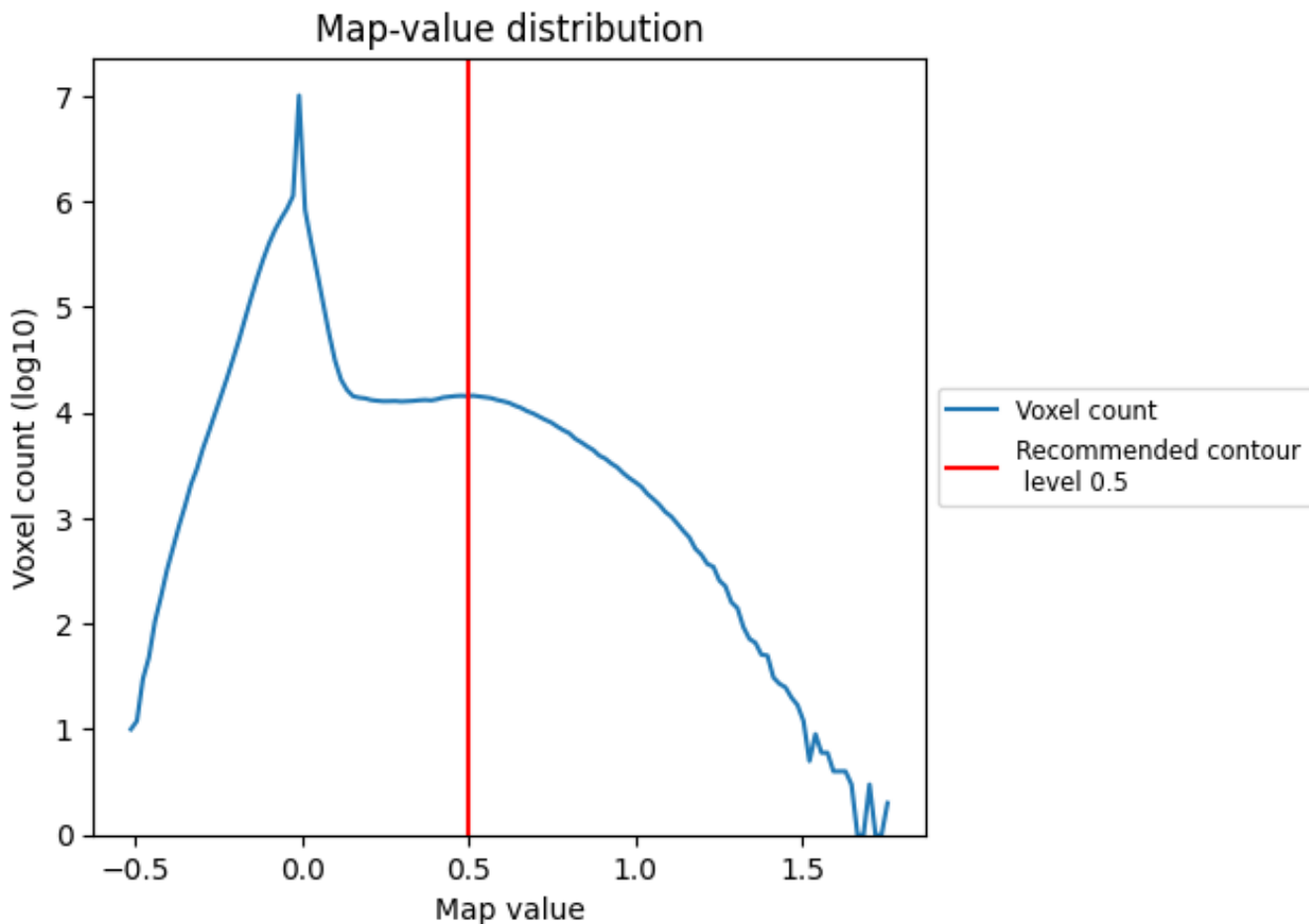


Z

7 Map analysis [i](#)

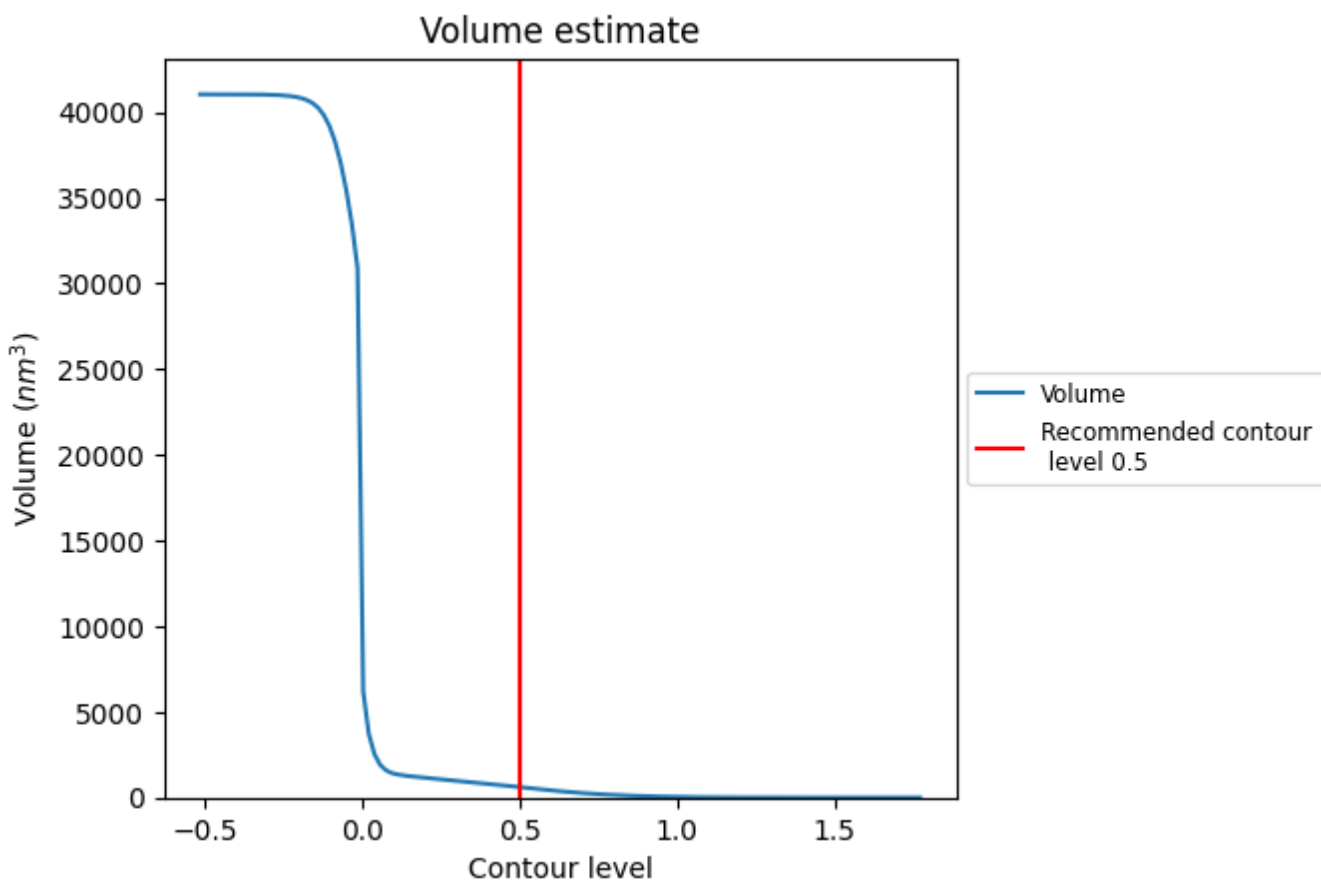
This section contains the results of statistical analysis of the map.

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.

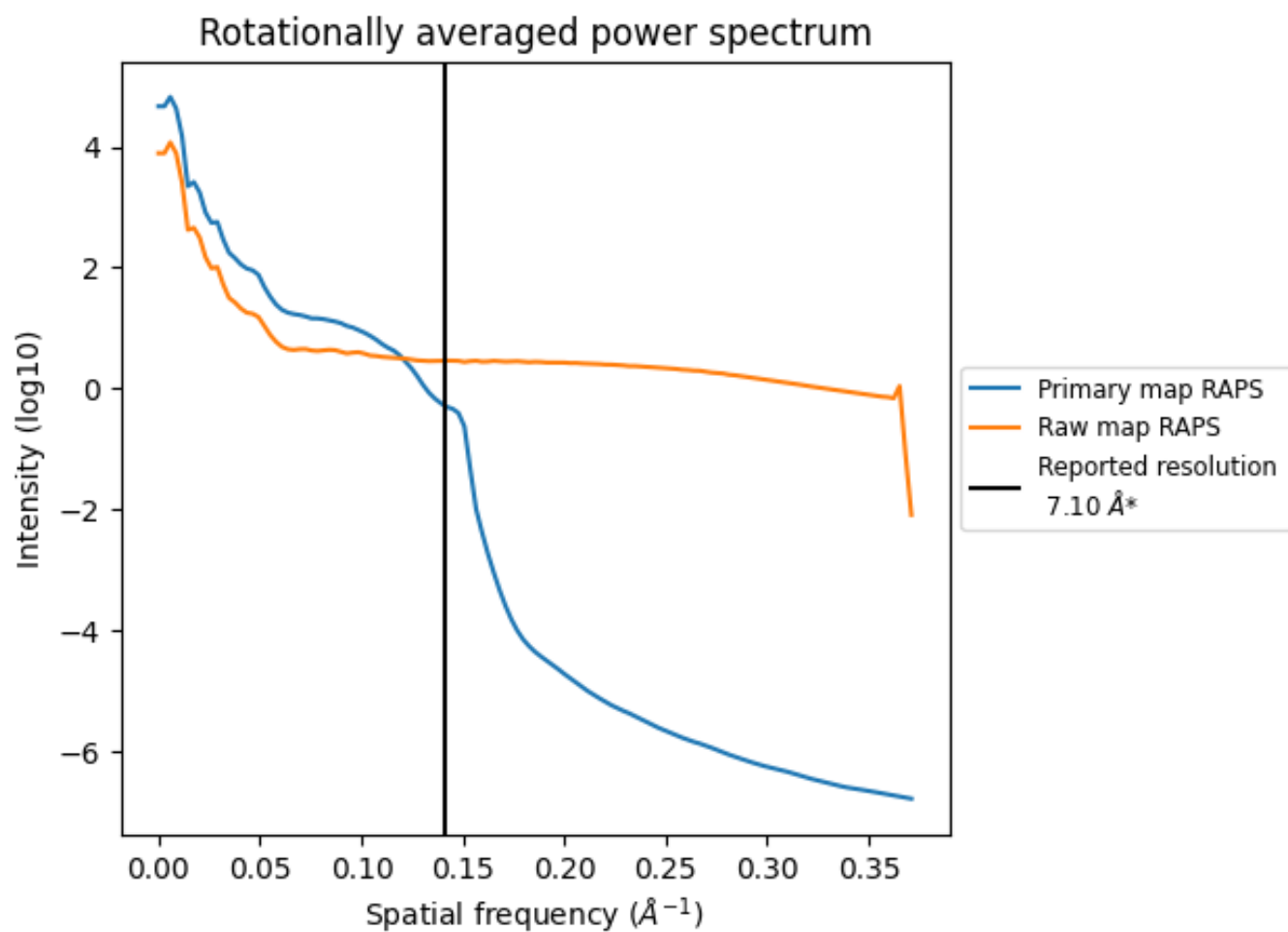
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 610 nm³; this corresponds to an approximate mass of 551 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](#)

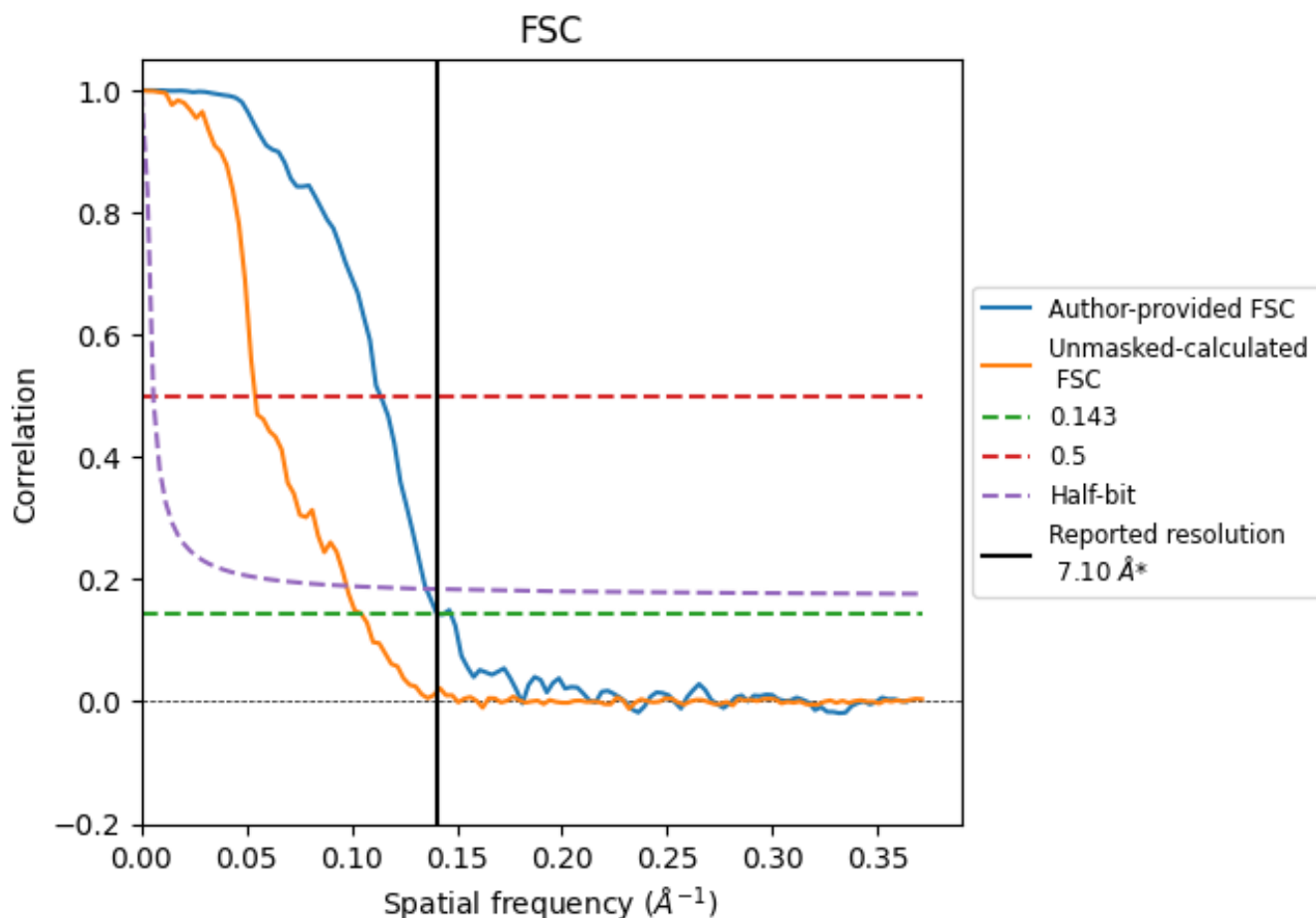


*Reported resolution corresponds to spatial frequency of 0.141 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.141 Å⁻¹

8.2 Resolution estimates [i](#)

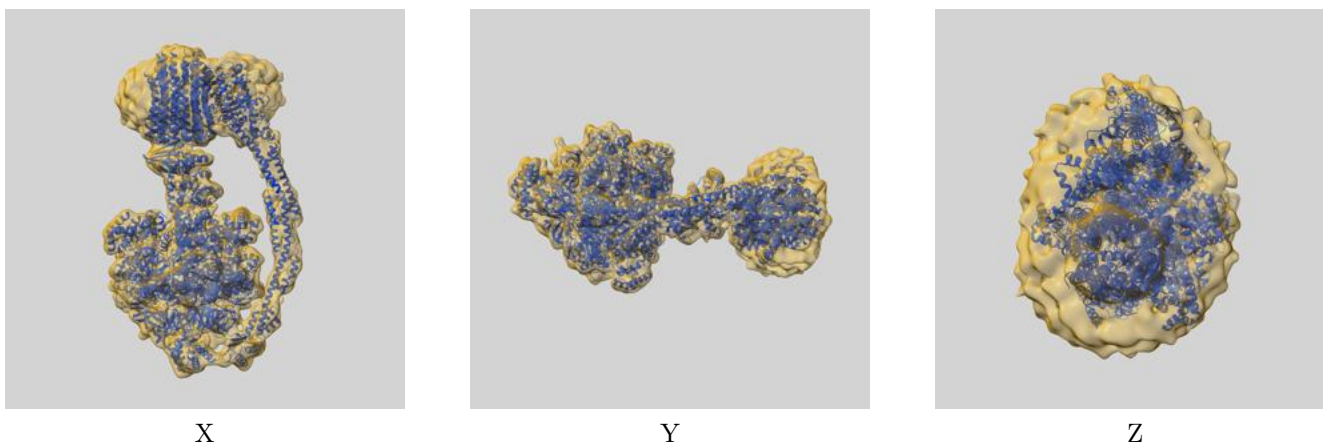
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.10	-	-
Author-provided FSC curve	7.11	8.80	7.38
Unmasked-calculated*	9.56	18.48	10.26

*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 9.56 differs from the reported value 7.1 by more than 10 %

9 Map-model fit [i](#)

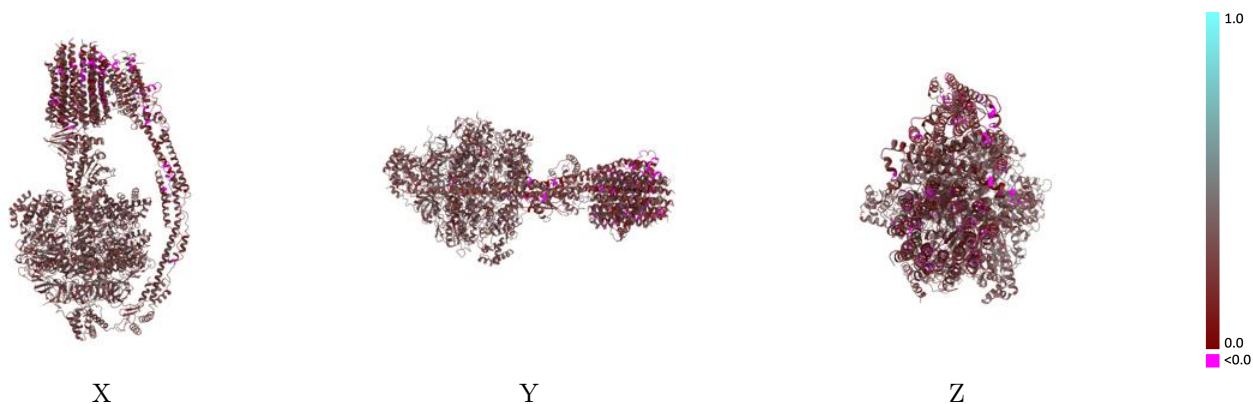
This section contains information regarding the fit between EMDB map EMD-25967 and PDB model 7TKF. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



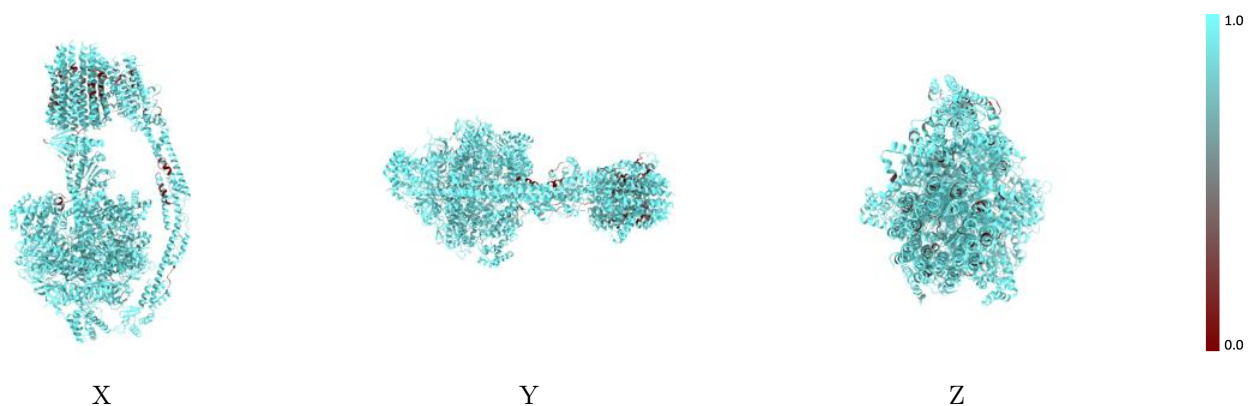
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



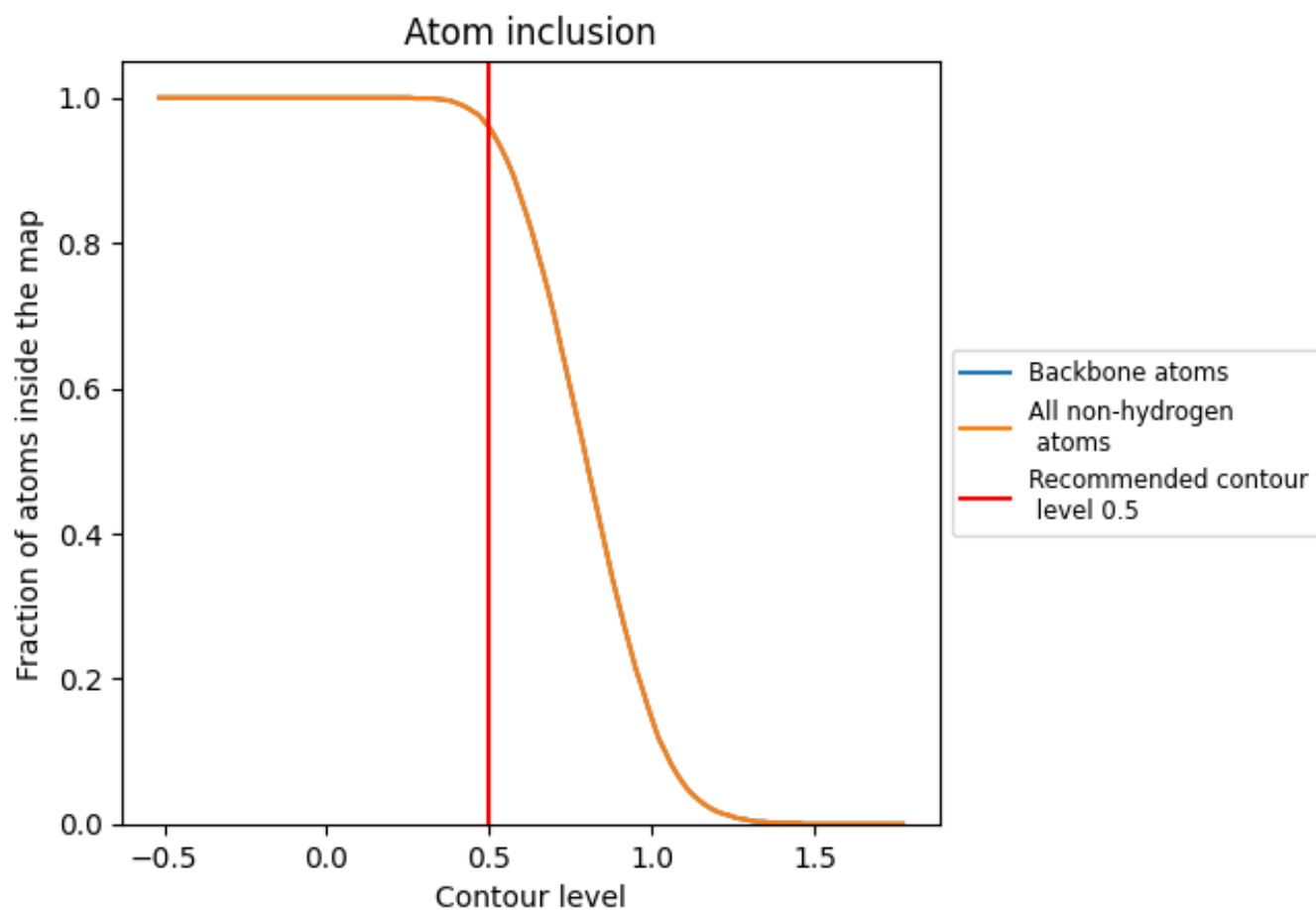
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.2650
0	 0.9300	 0.2220
1	 0.9300	 0.2070
2	 0.9170	 0.1860
3	 0.8510	 0.1780
4	 0.8530	 0.1890
5	 0.9470	 0.1710
6	 0.8850	 0.2210
7	 0.8970	 0.1760
8	 0.9500	 0.2330
9	 0.8880	 0.1610
A	 0.9900	 0.3030
B	 0.9870	 0.2980
C	 0.9830	 0.2890
D	 0.9940	 0.2980
E	 0.9840	 0.3020
F	 0.9760	 0.2830
G	 0.9640	 0.2730
H	 0.9400	 0.2380
I	 0.9020	 0.2640
O	 1.0000	 0.2930
T	 0.9310	 0.2150
U	 0.9320	 0.2470
V	 0.8990	 0.2150
W	 0.8590	 0.1380
X	 0.8430	 0.2310
Y	 0.8650	 0.1830
Z	 0.9430	 0.1790

