



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 12:40 AM UTC

PDB ID : 7TK9 / pdb_00007tk9
EMDB ID : EMD-25961
Title : Yeast ATP synthase State 1catalytic(d) with 10 mM ATP backbone model
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2022-01-17
Resolution : 6.00 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:

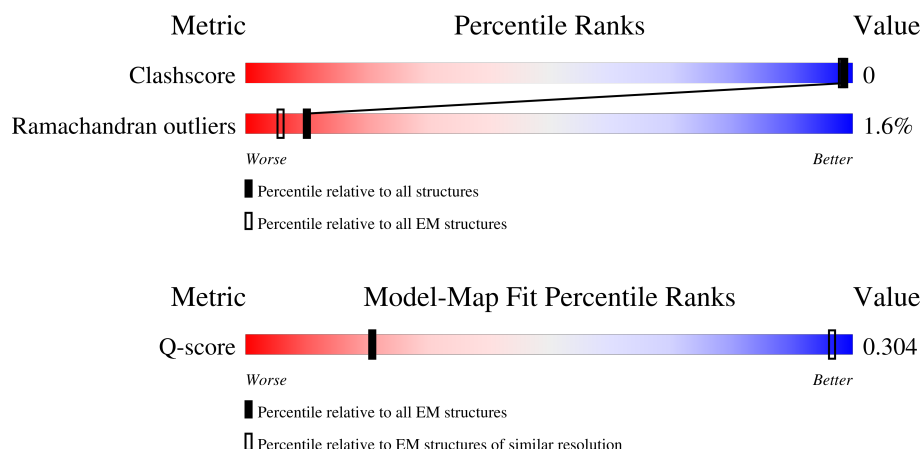
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	525 (5.50 - 6.50)

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	14% 95% ..
1	1	76	13% 95% ..
1	2	76	8% 92% 7% .
1	3	76	28% 92% 5% .
1	4	76	21% 92% 7% .

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Mol	Chain	Length	Quality of chain
1	5	76	
1	6	76	
1	7	76	
1	8	76	
1	9	76	
2	A	510	
2	B	510	
2	C	510	
3	D	478	
3	E	478	
3	F	478	
4	G	278	
5	H	138	
6	I	61	
7	O	195	
8	T	249	
9	U	209	
10	V	173	
11	W	95	
12	X	92	
13	Y	59	
14	Z	48	

2 Entry composition

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, mitochondrial.

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	499	Total	C	N	O	0	0
			1996	998	499	499		
2	B	505	Total	C	N	O	0	0
			2020	1010	505	505		
2	C	498	Total	C	N	O	0	0
			1992	996	498	498		

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

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

- 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
10	V	171	Total	C	N	O	0	0
			685	342	171	172		

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

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

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

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

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

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

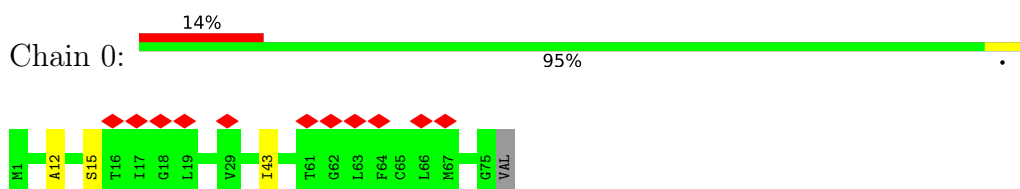
- Molecule 14 is a protein called ATP synthase protein 8.

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

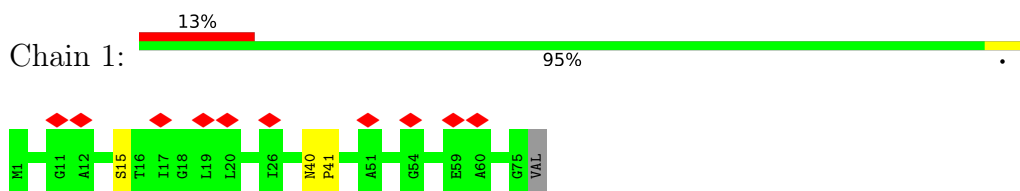
3 Residue-property plots [i](#)

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.

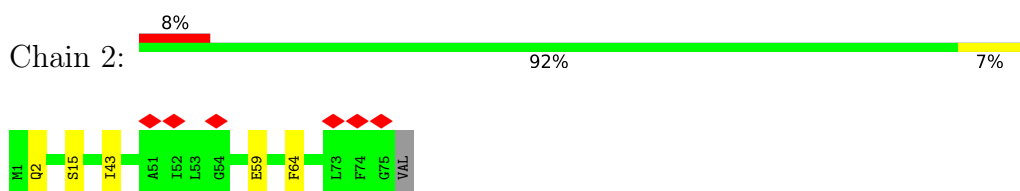
- Molecule 1: ATP synthase subunit 9, mitochondrial



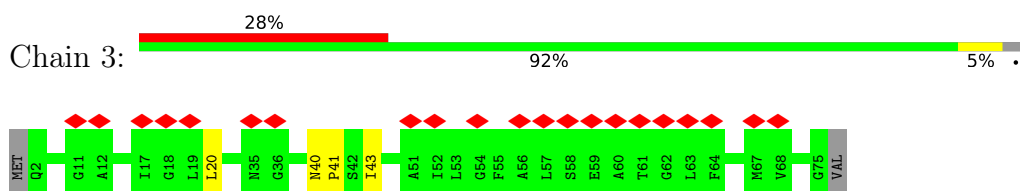
- Molecule 1: ATP synthase subunit 9, mitochondrial



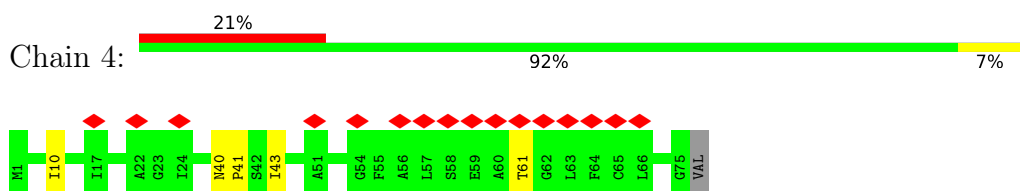
- Molecule 1: ATP synthase subunit 9, mitochondrial



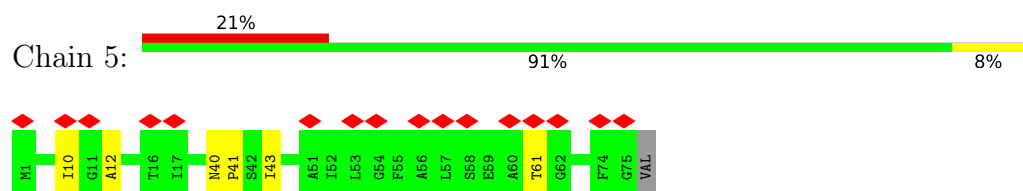
- Molecule 1: ATP synthase subunit 9, mitochondrial



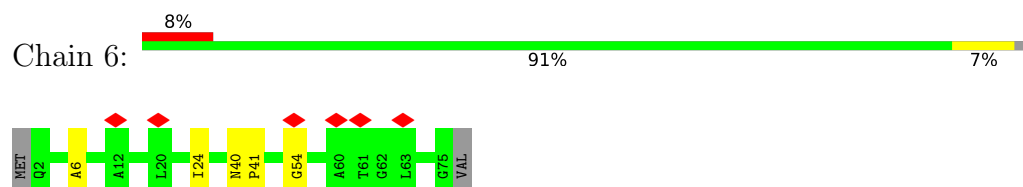
- Molecule 1: ATP synthase subunit 9, mitochondrial



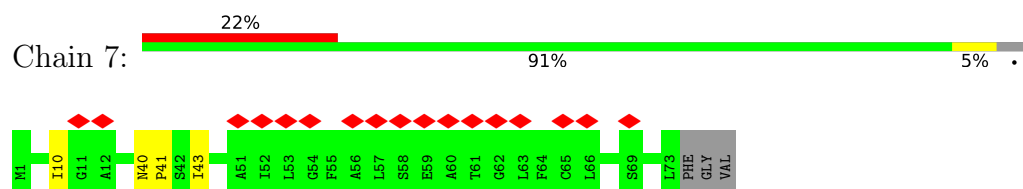
- Molecule 1: ATP synthase subunit 9, mitochondrial



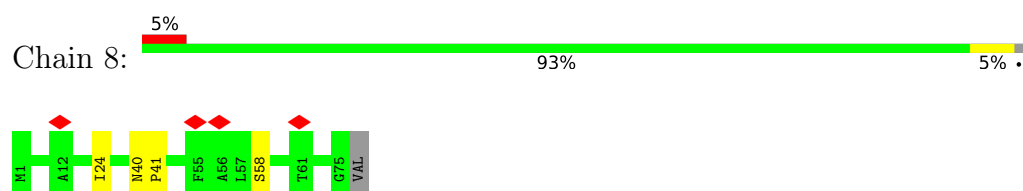
- Molecule 1: ATP synthase subunit 9, mitochondrial



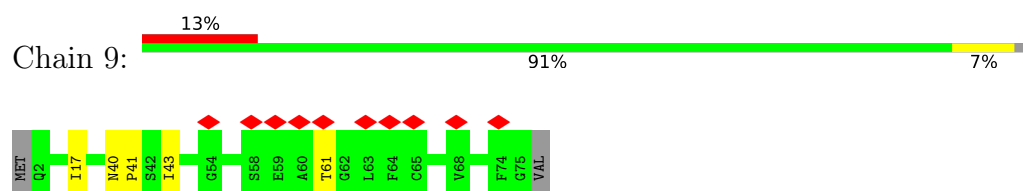
- Molecule 1: ATP synthase subunit 9, mitochondrial



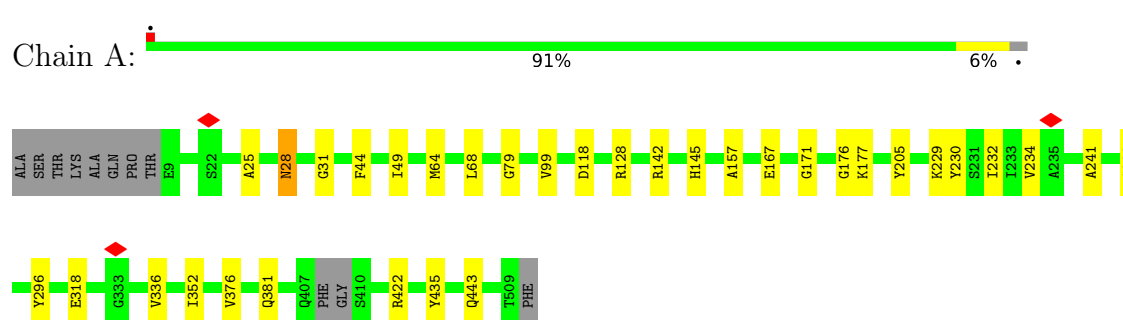
- Molecule 1: ATP synthase subunit 9, mitochondrial



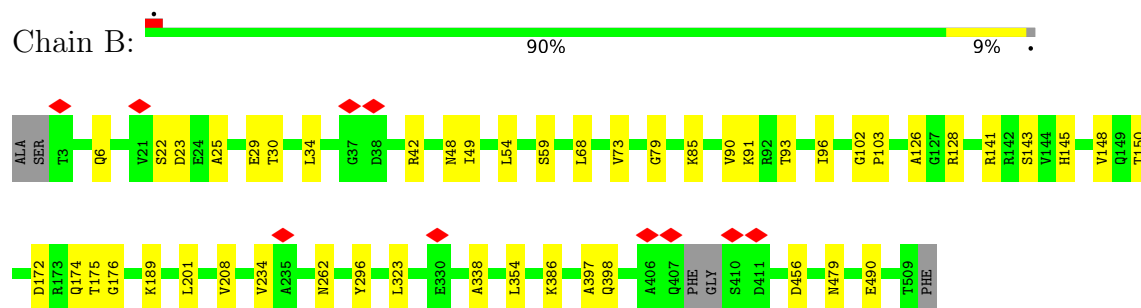
- Molecule 1: ATP synthase subunit 9, mitochondrial



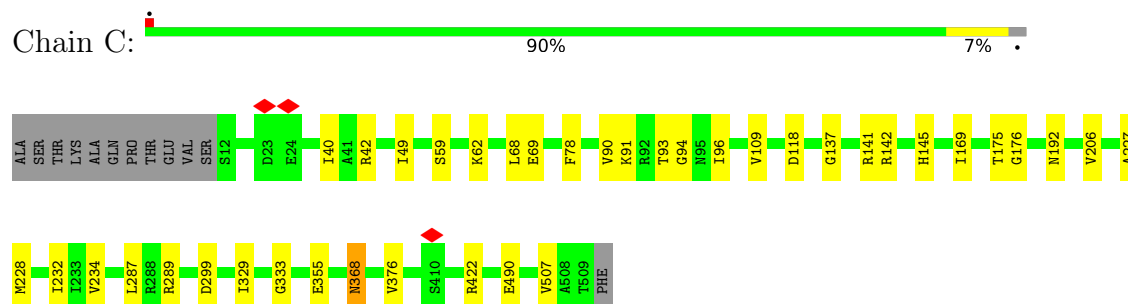
- Molecule 2: ATP synthase subunit alpha



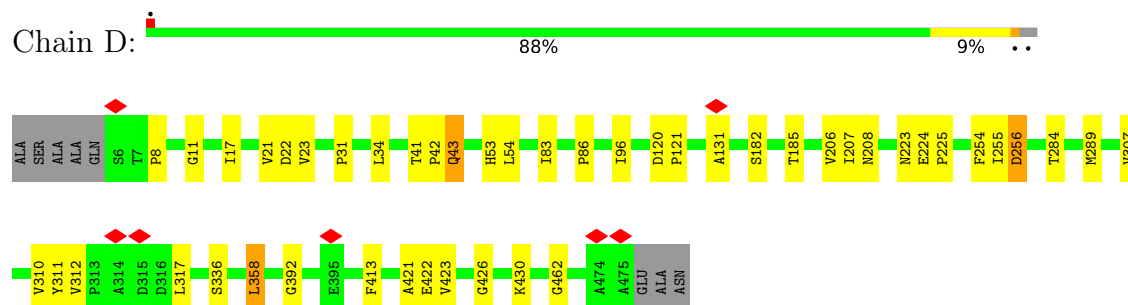
- Molecule 2: ATP synthase subunit alpha



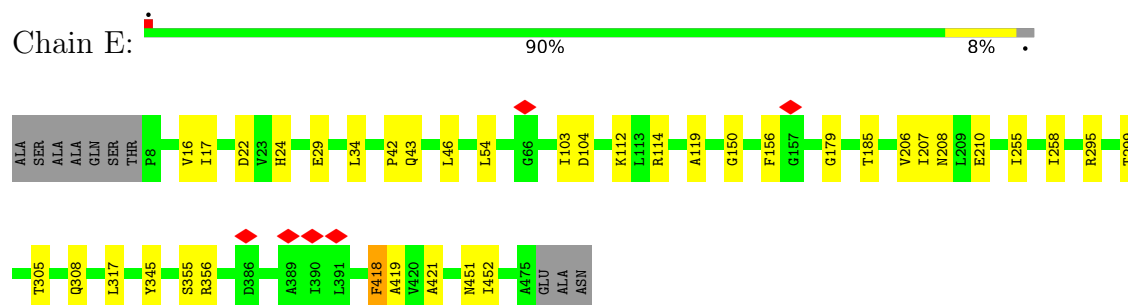
- Molecule 2: ATP synthase subunit alpha



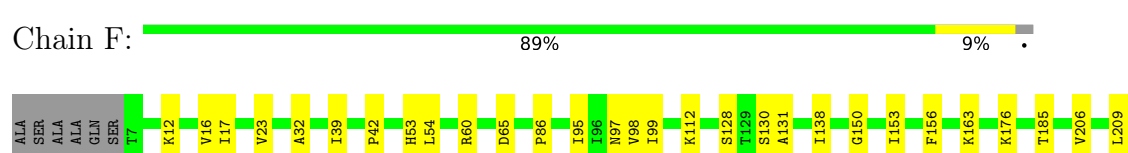
- Molecule 3: ATP synthase subunit beta



- Molecule 3: ATP synthase subunit beta



- Molecule 3: ATP synthase subunit beta





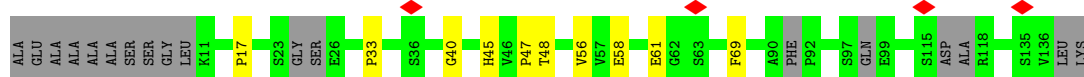
- Molecule 4: ATP synthase subunit gamma

Chain G: 88% 7% 5%



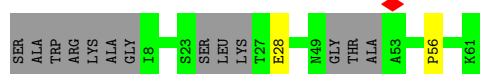
- Molecule 5: ATP synthase subunit delta

Chain H: 80% 7% 13%



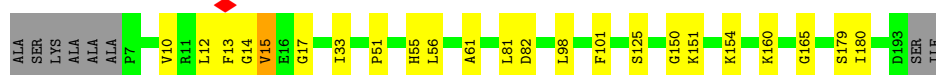
- Molecule 6: ATP synthase subunit epsilon

Chain I: 75% 21%



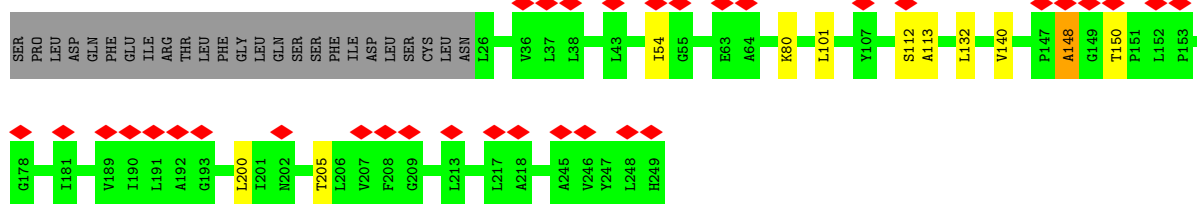
- Molecule 7: ATP synthase subunit 5

Chain O: 84% 11%



- Molecule 8: ATP synthase subunit a

Chain T: 86% 10%

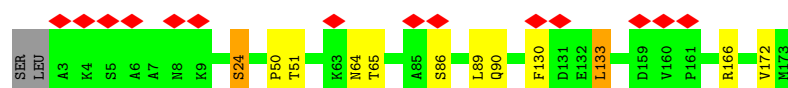


- Molecule 9: ATP synthase subunit 4

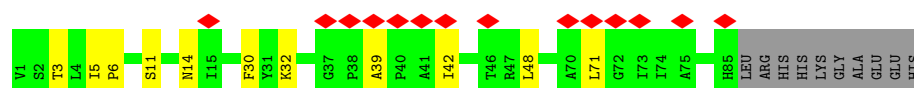
Chain U: 73% 26%



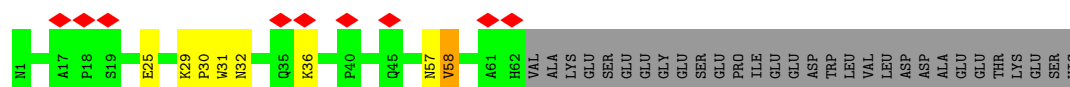
Chain V: 8% 92% 6%



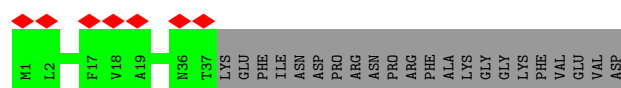
Chain W: 15% 78% 12% 11%



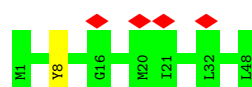
Chain X: 10% 59% 8% 23%



Chain Y:



Chain Z: 8% 98%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7185	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	2.207	Depositor
Minimum map value	-0.661	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.123	Depositor
Recommended contour level	0.67	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

5.1 Standard geometry

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	2.04	6/372 (1.6%)
1	1	1.20	0/299	2.02	2/372 (0.5%)
1	2	1.26	0/299	2.06	10/372 (2.7%)
1	3	1.25	0/295	1.93	4/367 (1.1%)
1	4	1.22	0/299	2.08	6/372 (1.6%)
1	5	1.24	0/299	2.09	8/372 (2.2%)
1	6	1.24	0/295	2.15	6/367 (1.6%)
1	7	1.21	0/291	2.16	4/362 (1.1%)
1	8	1.25	0/299	2.14	4/372 (1.1%)
1	9	1.25	0/295	2.11	6/367 (1.6%)
2	A	1.58	1/1994 (0.1%)	1.80	34/2489 (1.4%)
2	B	1.59	1/2018 (0.0%)	1.83	37/2519 (1.5%)
2	C	1.58	1/1991 (0.1%)	1.80	36/2487 (1.4%)
3	D	1.59	1/1879 (0.1%)	1.86	42/2347 (1.8%)
3	E	1.57	0/1871	1.84	38/2337 (1.6%)
3	F	1.60	0/1875	1.82	43/2342 (1.8%)
4	G	1.49	0/1058	1.83	19/1319 (1.4%)
5	H	1.52	0/475	1.75	9/585 (1.5%)
6	I	1.41	0/190	1.80	3/231 (1.3%)
7	O	1.51	0/747	1.87	17/932 (1.8%)
8	T	1.31	0/896	1.74	13/1117 (1.2%)
9	U	1.30	0/619	1.80	4/772 (0.5%)
10	V	1.36	0/684	1.75	7/852 (0.8%)
11	W	1.23	0/339	1.97	11/422 (2.6%)
12	X	1.40	0/247	2.14	7/307 (2.3%)
13	Y	1.27	0/147	1.66	0/182
14	Z	1.30	0/192	1.67	1/237 (0.4%)
All	All	1.49	4/20192 (0.0%)	1.86	377/25172 (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	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
3	D	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	34	LEU	CA-C	-6.61	1.50	1.53
3	D	11	GLY	CA-C	-6.21	1.47	1.52
2	C	227	ALA	CA-C	-5.29	1.47	1.53
2	A	157	ALA	CA-C	-5.16	1.48	1.52

All (377) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	6	PRO	N-CA-C	10.04	122.95	110.70
4	G	204	ASN	CA-C-N	9.52	126.24	120.24
4	G	204	ASN	C-N-CA	9.52	126.24	120.24
2	A	376	VAL	N-CA-C	-8.93	104.62	112.12
8	T	80	LYS	N-CA-C	-8.64	102.75	113.38
3	F	225	PRO	CA-C-O	-8.43	114.83	120.90
3	F	99	ILE	N-CA-C	-8.36	104.43	112.29
2	B	398	GLN	N-CA-C	-8.32	103.26	113.41
2	B	96	ILE	N-CA-C	-8.27	100.87	110.21
3	F	95	ILE	N-CA-C	-8.25	96.62	108.17
2	B	189	LYS	N-CA-C	-8.18	102.25	112.72
3	F	209	LEU	N-CA-C	-8.16	103.27	113.55
5	H	56	VAL	N-CA-C	-8.01	96.90	108.11
2	A	128	ARG	N-CA-C	-7.98	95.90	108.90
2	B	479	ASN	N-CA-C	-7.95	103.58	113.28
3	E	208	ASN	N-CA-C	-7.68	95.89	108.41
2	A	232	ILE	N-CA-C	-7.63	97.16	108.45
7	O	55	HIS	N-CA-C	-7.54	105.25	114.75
2	C	90	VAL	N-CA-C	-7.46	97.34	108.46
3	D	225	PRO	CA-C-O	-7.46	115.53	120.90
7	O	13	PHE	N-CA-C	-7.45	102.70	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	43	GLN	N-CA-C	-7.40	103.56	112.59
2	B	93	THR	N-CA-C	-7.39	103.30	111.36
4	G	2	THR	N-CA-C	-7.37	103.18	111.14
3	D	358	LEU	N-CA-C	-7.34	95.17	110.80
3	F	218	VAL	N-CA-C	-7.33	97.56	108.12
5	H	61	GLU	N-CA-C	-7.28	96.40	108.34
3	E	258	ILE	N-CA-C	-7.27	104.28	113.22
2	C	93	THR	N-CA-C	-7.27	103.44	111.36
10	V	90	GLN	N-CA-C	-7.27	104.39	113.55
3	F	39	ILE	N-CA-C	-7.26	97.98	108.36
1	4	43	ILE	CA-C-N	7.22	130.92	120.38
1	4	43	ILE	C-N-CA	7.22	130.92	120.38
2	B	386	LYS	N-CA-C	-7.22	104.09	113.12
2	A	44	PHE	N-CA-C	-7.18	96.81	108.52
2	B	175	THR	N-CA-C	-7.18	102.96	112.72
2	A	31	GLY	N-CA-C	-7.15	100.66	111.10
2	C	234	VAL	N-CA-C	-7.10	98.23	108.17
8	T	54	ILE	N-CA-C	-7.10	106.15	111.90
3	E	103	ILE	N-CA-C	-7.06	106.25	113.10
8	T	140	VAL	N-CA-C	-7.02	105.66	111.91
7	O	180	ILE	N-CA-C	-7.01	104.15	111.58
2	C	376	VAL	N-CA-C	-7.01	105.67	111.91
3	E	17	ILE	N-CA-C	-6.97	97.82	107.99
3	D	311	TYR	N-CA-C	-6.96	97.55	108.90
6	I	28	GLU	N-CA-C	-6.95	106.00	114.75
2	C	169	ILE	N-CA-C	-6.94	97.86	107.99
7	O	14	GLY	CA-C-N	6.93	134.44	121.97
7	O	14	GLY	C-N-CA	6.93	134.44	121.97
2	B	234	VAL	N-CA-C	-6.91	98.51	108.53
2	B	42	ARG	N-CA-C	-6.84	97.13	108.34
3	D	121	PRO	CA-C-O	-6.80	116.00	120.90
3	D	317	LEU	N-CA-C	-6.76	105.07	113.38
3	E	179	GLY	N-CA-C	-6.75	104.94	115.67
3	D	312	VAL	N-CA-C	-6.72	100.41	107.60
2	C	287	LEU	N-CA-C	-6.72	104.70	113.17
5	H	45	HIS	N-CA-C	-6.72	99.09	109.24
2	A	64	MET	N-CA-C	-6.69	99.24	109.41
2	B	323	LEU	N-CA-C	-6.66	96.62	110.80
2	B	148	VAL	N-CA-C	-6.65	98.05	107.75
10	V	133	LEU	N-CA-C	-6.62	96.70	110.80
4	G	74	ILE	N-CA-C	-6.61	98.60	108.12
3	E	207	ILE	N-CA-C	-6.59	98.63	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	112	LYS	N-CA-C	-6.58	103.92	112.68
3	F	17	ILE	N-CA-C	-6.58	97.63	107.37
2	A	177	LYS	N-CA-C	-6.58	104.19	111.36
7	O	33	ILE	N-CA-C	-6.57	106.58	111.90
2	C	329	ILE	N-CA-C	-6.56	98.67	108.12
3	D	254	PHE	N-CA-C	-6.56	97.90	109.06
4	G	86	SER	N-CA-C	-6.51	105.21	112.57
3	E	452	ILE	N-CA-C	-6.51	100.31	107.73
2	C	69	GLU	N-CA-C	-6.50	100.15	110.10
2	B	262	ASN	N-CA-C	-6.50	105.35	113.28
2	B	490	GLU	N-CA-C	-6.48	99.35	109.72
3	E	112	LYS	N-CA-C	-6.45	104.10	112.68
2	C	490	GLU	N-CA-C	-6.44	98.58	108.76
3	E	150	GLY	CA-C-N	6.41	127.43	120.44
3	E	150	GLY	C-N-CA	6.41	127.43	120.44
2	B	128	ARG	N-CA-C	-6.40	99.39	109.50
2	A	296	TYR	N-CA-C	-6.39	99.18	109.40
8	T	101	LEU	N-CA-C	-6.36	105.42	113.43
7	O	179	SER	N-CA-C	-6.35	101.07	110.46
3	F	138	ILE	N-CA-C	-6.33	99.31	108.17
2	A	99	VAL	N-CA-C	-6.33	104.00	109.19
2	A	422	ARG	CA-C-N	6.31	126.98	119.98
2	A	422	ARG	C-N-CA	6.31	126.98	119.98
5	H	69	PHE	N-CA-C	-6.31	98.62	108.90
3	F	53	HIS	N-CA-C	-6.29	98.94	109.07
3	D	426	GLY	N-CA-C	-6.27	107.23	114.69
3	F	295	ARG	N-CA-C	-6.27	105.39	113.16
2	A	142	ARG	N-CA-C	-6.23	99.86	109.52
3	D	422	GLU	N-CA-C	-6.23	105.71	113.38
1	6	54	GLY	CA-C-N	6.23	128.53	120.44
1	6	54	GLY	C-N-CA	6.23	128.53	120.44
11	W	5	ILE	CA-C-N	6.22	126.78	120.38
11	W	5	ILE	C-N-CA	6.22	126.78	120.38
3	E	42	PRO	N-CA-C	-6.21	108.22	114.68
2	B	54	LEU	N-CA-C	-6.20	99.14	109.24
2	C	142	ARG	N-CA-C	-6.19	99.63	109.23
3	D	53	HIS	N-CA-C	-6.17	99.34	109.40
2	B	48	ASN	N-CA-C	-6.13	99.19	109.07
12	X	29	LYS	N-CA-C	-6.10	102.38	110.07
3	E	22	ASP	N-CA-C	-6.08	99.80	109.59
3	F	163	LYS	N-CA-C	-6.06	104.67	111.28
2	B	456	ASP	N-CA-C	-6.05	104.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	252	LEU	N-CA-C	-6.05	99.88	109.07
4	G	133	ILE	N-CA-C	-6.05	107.04	112.12
3	F	452	ILE	CA-C-N	6.04	126.05	119.89
3	F	452	ILE	C-N-CA	6.04	126.05	119.89
3	D	256	ASP	N-CA-C	-6.04	99.89	109.07
3	D	392	GLY	N-CA-C	-6.02	106.23	111.95
2	C	78	PHE	N-CA-C	-6.02	106.09	113.50
3	D	22	ASP	N-CA-C	-6.02	100.38	109.95
3	F	153	ILE	N-CA-C	-6.02	99.74	108.89
8	T	200	LEU	N-CA-C	-6.01	105.77	113.23
3	E	185	THR	N-CA-C	-6.01	99.39	109.07
2	C	42	ARG	N-CA-C	-6.01	97.66	108.48
2	B	150	THR	N-CA-C	-6.00	106.00	113.38
11	W	48	LEU	N-CA-C	-6.00	105.53	114.64
3	E	114	ARG	N-CA-C	-5.97	100.27	109.52
4	G	137	ALA	CA-C-N	5.95	125.97	119.90
4	G	137	ALA	C-N-CA	5.95	125.97	119.90
3	D	421	ALA	N-CA-C	-5.95	102.80	111.30
2	A	49	ILE	N-CA-C	-5.94	100.51	108.35
3	E	24	HIS	N-CA-C	-5.93	99.53	109.07
2	A	68	LEU	N-CA-C	-5.92	97.66	108.02
1	4	61	THR	CA-C-N	5.91	126.54	119.98
1	4	61	THR	C-N-CA	5.91	126.54	119.98
3	F	258	ILE	N-CA-C	-5.91	106.98	112.83
2	A	336	VAL	N-CA-C	-5.88	107.40	113.10
2	A	234	VAL	N-CA-C	-5.87	100.13	108.58
7	O	125	SER	N-CA-C	-5.87	100.64	108.74
1	7	10	ILE	CA-C-N	5.86	126.49	119.98
1	7	10	ILE	C-N-CA	5.86	126.49	119.98
3	D	284	THR	N-CA-C	-5.85	106.05	112.72
3	E	156	PHE	N-CA-C	-5.85	100.40	109.24
11	W	3	THR	N-CA-C	-5.83	105.82	113.17
3	E	355	SER	N-CA-C	-5.81	100.47	109.24
7	O	101	PHE	N-CA-C	-5.80	105.22	112.93
3	F	65	ASP	CA-C-N	5.79	125.60	120.10
3	F	65	ASP	C-N-CA	5.79	125.60	120.10
3	E	418	PHE	CA-C-N	5.78	128.03	120.28
3	E	418	PHE	C-N-CA	5.78	128.03	120.28
12	X	25	GLU	CA-C-N	5.78	126.39	119.98
12	X	25	GLU	C-N-CA	5.78	126.39	119.98
3	D	255	ILE	N-CA-C	-5.76	99.47	108.86
2	A	292	GLY	CA-C-N	5.75	128.92	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	292	GLY	C-N-CA	5.75	128.92	120.82
3	E	419	ALA	N-CA-C	5.74	117.54	111.28
2	B	296	TYR	N-CA-C	-5.74	102.55	109.72
3	D	23	VAL	N-CA-C	-5.74	99.48	108.95
3	D	43	GLN	N-CA-C	-5.73	101.69	109.54
2	C	62	LYS	N-CA-C	-5.73	100.06	109.40
12	X	57	ASN	CA-C-N	5.73	132.29	121.97
12	X	57	ASN	C-N-CA	5.73	132.29	121.97
1	3	43	ILE	CA-C-N	5.72	128.74	120.38
1	3	43	ILE	C-N-CA	5.72	128.74	120.38
3	E	104	ASP	N-CA-C	-5.72	106.14	113.23
3	E	29	GLU	N-CA-C	-5.71	104.89	112.94
2	C	289	ARG	N-CA-C	-5.71	102.43	110.31
4	G	100	ASN	N-CA-C	-5.70	105.05	112.23
10	V	51	THR	N-CA-C	-5.69	105.44	112.90
3	F	336	SER	CA-C-N	5.69	127.90	120.28
3	F	336	SER	C-N-CA	5.69	127.90	120.28
3	D	96	ILE	N-CA-C	-5.68	100.15	108.11
11	W	71	LEU	CA-C-N	5.68	126.29	119.98
11	W	71	LEU	C-N-CA	5.68	126.29	119.98
8	T	132	LEU	CA-C-N	5.68	126.25	120.00
8	T	132	LEU	C-N-CA	5.68	126.25	120.00
3	E	54	LEU	N-CA-C	-5.68	106.12	113.16
2	B	397	ALA	N-CA-C	-5.67	105.56	112.88
2	C	232	ILE	N-CA-C	-5.67	100.32	108.48
8	T	112	SER	N-CA-C	-5.67	106.37	113.28
9	U	143	LYS	CA-C-N	5.66	127.70	120.56
9	U	143	LYS	C-N-CA	5.66	127.70	120.56
3	F	42	PRO	N-CA-C	-5.66	108.79	114.68
3	D	182	SER	N-CA-C	-5.66	100.70	109.24
7	O	56	LEU	N-CA-C	-5.65	106.05	113.17
4	G	78	THR	N-CA-C	-5.65	100.75	108.38
3	F	206	VAL	N-CA-C	-5.65	105.01	110.72
8	T	148	ALA	CA-C-N	5.64	125.46	120.10
8	T	148	ALA	C-N-CA	5.64	125.46	120.10
2	C	355	GLU	CA-C-N	5.64	127.84	120.28
2	C	355	GLU	C-N-CA	5.64	127.84	120.28
4	G	99	LEU	N-CA-C	-5.64	106.44	113.38
1	6	6	ALA	CA-C-N	5.63	127.82	120.28
1	6	6	ALA	C-N-CA	5.63	127.82	120.28
3	E	317	LEU	CA-C-N	5.62	127.82	120.28
3	E	317	LEU	C-N-CA	5.62	127.82	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	2	GLN	CA-C-N	5.62	127.81	120.28
1	2	2	GLN	C-N-CA	5.62	127.81	120.28
3	D	208	ASN	N-CA-C	-5.62	99.25	108.41
3	F	185	THR	N-CA-C	-5.62	99.13	108.34
1	9	61	THR	CA-C-N	5.60	126.19	119.98
1	9	61	THR	C-N-CA	5.60	126.19	119.98
3	D	21	VAL	N-CA-C	-5.60	99.99	108.17
3	F	224	GLU	CA-C-N	5.60	123.75	119.66
3	F	224	GLU	C-N-CA	5.60	123.75	119.66
2	B	354	LEU	N-CA-C	-5.58	100.31	109.40
2	C	94	GLY	N-CA-C	-5.58	107.56	115.43
8	T	150	THR	N-CA-C	-5.57	103.11	108.07
2	B	6	GLN	N-CA-C	-5.57	103.11	110.40
4	G	180	LYS	N-CA-C	-5.57	103.21	108.22
5	H	58	GLU	N-CA-C	-5.56	99.96	109.24
3	F	396	LEU	CA-C-N	5.55	129.59	121.31
3	F	396	LEU	C-N-CA	5.55	129.59	121.31
3	E	345	TYR	N-CA-C	-5.55	98.42	108.85
3	E	255	ILE	N-CA-C	-5.55	99.82	108.86
2	C	137	GLY	CA-C-N	5.54	128.05	120.46
2	C	137	GLY	C-N-CA	5.54	128.05	120.46
3	E	295	ARG	N-CA-C	-5.53	106.31	113.16
2	C	422	ARG	CA-C-N	5.52	126.11	119.98
2	C	422	ARG	C-N-CA	5.52	126.11	119.98
14	Z	8	TYR	N-CA-C	-5.52	106.75	112.93
2	C	91	LYS	N-CA-C	-5.51	99.91	108.90
3	D	224	GLU	CA-C-N	5.51	123.68	119.66
3	D	224	GLU	C-N-CA	5.51	123.68	119.66
3	D	17	ILE	N-CA-C	-5.51	97.88	109.34
3	F	216	ALA	N-CA-C	-5.51	100.98	109.52
2	C	118	ASP	N-CA-C	-5.50	106.07	112.89
2	C	206	VAL	N-CA-C	-5.50	100.42	108.11
4	G	75	VAL	N-CA-C	-5.49	99.91	108.86
6	I	56	PRO	CA-C-N	5.49	128.99	120.60
6	I	56	PRO	C-N-CA	5.49	128.99	120.60
8	T	113	ALA	N-CA-C	-5.48	106.59	113.28
1	7	43	ILE	CA-C-N	5.48	127.89	120.38
1	7	43	ILE	C-N-CA	5.48	127.89	120.38
3	D	423	VAL	N-CA-C	-5.48	106.48	113.22
3	D	310	VAL	N-CA-C	-5.48	100.34	108.45
2	C	368	ASN	N-CA-C	-5.47	99.15	110.80
2	A	241	ALA	CA-C-N	5.47	126.57	120.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	241	ALA	C-N-CA	5.47	126.57	120.06
1	2	64	PHE	CA-C-N	5.46	127.54	120.44
1	2	64	PHE	C-N-CA	5.46	127.54	120.44
3	F	247	GLU	N-CA-C	-5.46	106.62	113.72
3	D	42	PRO	N-CA-C	-5.45	109.02	114.68
2	B	25	ALA	CA-C-N	5.44	128.12	120.28
2	B	25	ALA	C-N-CA	5.44	128.12	120.28
3	D	307	VAL	N-CA-C	-5.43	99.73	107.77
1	6	24	ILE	CA-C-N	5.43	125.97	119.94
1	6	24	ILE	C-N-CA	5.43	125.97	119.94
2	A	318	GLU	N-CA-C	-5.43	106.53	112.72
7	O	98	LEU	N-CA-C	-5.42	104.94	113.02
2	B	68	LEU	N-CA-C	-5.42	99.90	108.73
3	F	16	VAL	N-CA-C	-5.42	98.07	109.34
4	G	168	ASP	N-CA-C	-5.42	102.82	109.65
2	B	208	VAL	N-CA-C	-5.41	100.69	108.48
2	C	176	GLY	N-CA-C	-5.41	103.34	114.16
11	W	30	PHE	CA-C-N	5.41	130.25	122.40
11	W	30	PHE	C-N-CA	5.41	130.25	122.40
7	O	150	GLY	N-CA-C	-5.41	107.46	113.79
2	A	205	TYR	N-CA-C	-5.40	100.38	109.07
3	D	120	ASP	CA-C-N	5.39	123.60	119.66
3	D	120	ASP	C-N-CA	5.39	123.60	119.66
3	F	54	LEU	N-CA-C	-5.39	106.08	113.30
2	B	30	THR	N-CA-C	-5.39	101.17	109.52
3	D	430	LYS	N-CA-C	-5.38	99.92	109.06
7	O	154	LYS	N-CA-C	-5.37	100.14	108.90
2	C	175	THR	N-CA-C	-5.36	105.43	112.72
2	C	68	LEU	N-CA-C	-5.36	98.65	108.02
2	C	96	ILE	N-CA-C	-5.36	102.68	109.80
9	U	116	VAL	CA-C-N	5.36	127.46	120.28
9	U	116	VAL	C-N-CA	5.36	127.46	120.28
1	2	59	GLU	CA-C-N	5.35	127.45	120.28
1	2	59	GLU	C-N-CA	5.35	127.45	120.28
7	O	12	LEU	CA-C-N	5.35	130.16	122.40
7	O	12	LEU	C-N-CA	5.35	130.16	122.40
3	D	54	LEU	N-CA-C	-5.34	106.14	113.30
12	X	58	VAL	N-CA-C	-5.33	98.25	109.34
3	D	185	THR	N-CA-C	-5.33	99.76	108.76
2	B	90	VAL	N-CA-C	-5.32	100.72	108.17
3	E	206	VAL	N-CA-C	-5.32	105.83	113.07
1	0	15	SER	CA-C-N	5.31	128.13	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	15	SER	C-N-CA	5.31	128.13	120.38
2	A	352	ILE	N-CA-C	-5.30	100.49	108.12
3	D	207	ILE	N-CA-C	-5.30	100.26	107.99
10	V	24	SER	CA-C-N	5.30	127.38	120.28
10	V	24	SER	C-N-CA	5.30	127.38	120.28
2	A	79	GLY	CA-C-N	5.29	128.74	120.75
2	A	79	GLY	C-N-CA	5.29	128.74	120.75
4	G	130	ILE	N-CA-C	-5.29	100.62	108.45
3	E	305	THR	N-CA-C	-5.29	101.66	110.17
1	5	43	ILE	CA-C-N	5.27	128.08	120.38
1	5	43	ILE	C-N-CA	5.27	128.08	120.38
3	E	46	LEU	N-CA-C	-5.27	100.31	108.90
2	B	79	GLY	CA-C-N	5.26	128.69	120.75
2	B	79	GLY	C-N-CA	5.26	128.69	120.75
2	C	109	VAL	N-CA-C	-5.25	100.88	108.71
3	D	413	PHE	N-CA-C	-5.25	106.87	113.28
4	G	171	SER	N-CA-C	-5.25	101.14	108.96
2	A	171	GLY	CA-C-N	5.24	128.15	120.71
2	A	171	GLY	C-N-CA	5.24	128.15	120.71
2	A	296	TYR	CA-C-N	5.23	126.38	119.84
2	A	296	TYR	C-N-CA	5.23	126.38	119.84
1	5	61	THR	CA-C-N	5.23	125.74	119.94
1	5	61	THR	C-N-CA	5.23	125.74	119.94
1	8	58	SER	CA-C-N	5.22	127.28	120.28
1	8	58	SER	C-N-CA	5.22	127.28	120.28
11	W	6	PRO	CA-C-O	-5.22	112.99	120.56
3	D	336	SER	CA-C-N	5.22	127.27	120.28
3	D	336	SER	C-N-CA	5.22	127.27	120.28
3	E	356	ARG	N-CA-C	-5.22	106.60	113.17
2	C	192	ASN	CA-C-N	5.20	127.68	120.29
2	C	192	ASN	C-N-CA	5.20	127.68	120.29
3	F	156	PHE	N-CA-C	-5.20	102.41	109.54
5	H	40	GLY	N-CA-C	-5.20	102.37	111.46
3	F	335	LEU	N-CA-C	-5.18	100.45	108.90
8	T	205	THR	N-CA-C	-5.18	106.81	113.23
3	E	421	ALA	N-CA-C	-5.18	106.81	112.72
4	G	162	ILE	N-CA-C	-5.18	100.42	108.86
11	W	14	ASN	N-CA-C	-5.16	106.66	113.17
2	A	28	ASN	N-CA-C	-5.15	99.83	110.80
1	9	17	ILE	CA-C-N	5.15	126.62	120.13
1	9	17	ILE	C-N-CA	5.15	126.62	120.13
3	F	311	TYR	N-CA-C	-5.15	100.34	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	60	ARG	N-CA-C	-5.14	100.06	108.76
1	4	10	ILE	CA-C-N	5.14	125.69	119.98
1	4	10	ILE	C-N-CA	5.14	125.69	119.98
3	F	150	GLY	CA-C-N	5.13	126.03	120.44
3	F	150	GLY	C-N-CA	5.13	126.03	120.44
3	E	299	THR	N-CA-C	-5.12	102.43	110.17
1	2	15	SER	CA-C-N	5.12	127.66	120.28
1	2	15	SER	C-N-CA	5.12	127.66	120.28
2	A	443	GLN	CA-C-N	5.12	123.47	120.24
2	A	443	GLN	C-N-CA	5.12	123.47	120.24
2	B	172	ASP	CA-C-N	5.12	129.55	121.56
2	B	172	ASP	C-N-CA	5.12	129.55	121.56
3	D	289	MET	CA-C-N	5.12	125.66	119.98
3	D	289	MET	C-N-CA	5.12	125.66	119.98
1	0	12	ALA	CA-C-N	5.11	125.61	119.94
1	0	12	ALA	C-N-CA	5.11	125.61	119.94
1	0	43	ILE	CA-C-N	5.11	127.13	120.28
1	0	43	ILE	C-N-CA	5.11	127.13	120.28
3	E	210	GLU	N-CA-C	-5.11	101.38	109.96
3	F	176	LYS	N-CA-C	-5.11	107.10	113.38
3	D	206	VAL	N-CA-C	-5.10	105.57	110.72
1	8	24	ILE	CA-C-N	5.09	125.59	119.94
1	8	24	ILE	C-N-CA	5.09	125.59	119.94
1	2	43	ILE	CA-C-N	5.09	127.35	120.38
1	2	43	ILE	C-N-CA	5.09	127.35	120.38
3	F	23	VAL	N-CA-C	-5.08	101.07	108.99
2	C	507	VAL	N-CA-C	-5.08	104.64	111.44
3	F	255	ILE	N-CA-C	-5.07	100.77	108.17
1	3	20	LEU	CA-C-N	5.07	125.58	120.00
1	3	20	LEU	C-N-CA	5.07	125.58	120.00
3	E	317	LEU	N-CA-C	-5.06	106.61	112.89
1	9	43	ILE	CA-C-N	5.06	127.06	120.28
1	9	43	ILE	C-N-CA	5.06	127.06	120.28
10	V	64	ASN	N-CA-C	-5.06	105.86	112.23
5	H	47	PRO	CA-C-N	5.06	131.20	121.54
5	H	47	PRO	C-N-CA	5.06	131.20	121.54
1	5	12	ALA	CA-C-N	5.05	125.55	119.94
1	5	12	ALA	C-N-CA	5.05	125.55	119.94
2	B	338	ALA	N-CA-C	-5.05	101.05	108.99
10	V	172	VAL	N-CA-C	-5.05	100.25	107.78
2	B	201	LEU	N-CA-C	-5.05	102.29	110.32
3	D	8	PRO	N-CA-C	-5.05	108.14	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	193	SER	CA-C-N	5.04	127.54	120.28
4	G	193	SER	C-N-CA	5.04	127.54	120.28
2	B	73	VAL	N-CA-C	-5.04	100.95	108.46
2	A	176	GLY	N-CA-C	-5.04	101.24	113.18
1	1	15	SER	CA-C-N	5.03	127.53	120.28
1	1	15	SER	C-N-CA	5.03	127.53	120.28
12	X	32	ASN	N-CA-C	-5.03	102.40	110.10
2	B	91	LYS	N-CA-C	-5.03	101.20	109.40
1	5	10	ILE	CA-C-N	5.03	125.56	119.98
1	5	10	ILE	C-N-CA	5.03	125.56	119.98
2	B	85	LYS	N-CA-C	-5.03	101.10	108.99
2	C	40	ILE	N-CA-C	-5.02	100.34	107.77
7	O	160	LYS	N-CA-C	-5.02	98.72	109.81
7	O	151	LYS	N-CA-C	-5.02	99.24	108.02
2	A	118	ASP	N-CA-C	-5.01	106.85	113.17
2	C	141	ARG	N-CA-C	-5.01	100.84	108.76
3	F	12	LYS	N-CA-C	-5.01	101.75	109.52
3	E	308	GLN	N-CA-C	-5.01	101.76	109.52
5	H	17	PRO	N-CA-C	-5.00	106.69	113.40
3	F	128	SER	N-CA-C	-5.00	99.95	108.26

There are no chirality outliers.

All (9) 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
3	D	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	1996	0	570	0	0
2	B	2020	0	575	2	0
2	C	1992	0	572	0	0
3	D	1880	0	538	1	0
3	E	1872	0	537	0	0
3	F	1876	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)
7:O:15:VAL:C	7:O:17:GLY:H	2.22	0.46
3:D:41:THR:C	3:D:43:GLN:H	2.25	0.45
2:B:102:GLY:HA3	2:B:126:ALA:H	1.84	0.42
2:B:174:GLN:C	2:B:176:GLY:H	2.29	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%)	72 (99%)	1 (1%)	0	100	100
1	1	73/76 (96%)	70 (96%)	2 (3%)	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%)	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%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	9	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	9	40
2	A	495/510 (97%)	470 (95%)	17 (3%)	8 (2%)	7	37
2	B	501/510 (98%)	470 (94%)	22 (4%)	9 (2%)	6	34
2	C	496/510 (97%)	472 (95%)	17 (3%)	7 (1%)	9	40
3	D	468/478 (98%)	434 (93%)	26 (6%)	8 (2%)	7	36
3	E	466/478 (98%)	444 (95%)	17 (4%)	5 (1%)	11	46
3	F	467/478 (98%)	424 (91%)	35 (8%)	8 (2%)	7	36
4	G	261/278 (94%)	249 (95%)	9 (3%)	3 (1%)	11	46
5	H	110/138 (80%)	102 (93%)	6 (6%)	2 (2%)	6	34
6	I	42/61 (69%)	38 (90%)	4 (10%)	0	100	100
7	O	185/195 (95%)	164 (89%)	14 (8%)	7 (4%)	2	19
8	T	222/249 (89%)	209 (94%)	12 (5%)	1 (0%)	24	63
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	150 (89%)	11 (6%)	8 (5%)	2	16
11	W	83/95 (87%)	69 (83%)	10 (12%)	4 (5%)	2	16
12	X	60/92 (65%)	54 (90%)	2 (3%)	4 (7%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Y	35/59 (59%)	32 (91%)	3 (9%)	0	100	100
14	Z	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
All	All	4984/5321 (94%)	4682 (94%)	220 (4%)	82 (2%)	10	37

All (82) 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	229	LYS
2	A	381	GLN
2	B	59	SER
2	B	141	ARG
2	C	59	SER
2	C	299	ASP
3	D	223	ASN
3	D	358	LEU
3	E	418	PHE
3	F	278	ALA
7	O	51	PRO
7	O	61	ALA
10	V	65	THR
10	V	86	SER
10	V	89	LEU
11	W	11	SER
12	X	58	VAL
2	A	25	ALA
2	A	167	GLU
2	B	49	ILE
2	C	49	ILE
3	D	462	GLY
3	F	32	ALA
3	F	97	ASN
3	F	98	VAL
3	F	131	ALA

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Mol	Chain	Res	Type
3	F	301	LYS
4	G	56	GLU
5	H	48	THR
7	O	10	VAL
7	O	81	LEU
8	T	148	ALA
10	V	133	LEU
11	W	42	ILE
2	A	145	HIS
2	B	23	ASP
2	B	29	GLU
2	B	103	PRO
2	C	145	HIS
2	C	333	GLY
2	C	368	ASN
3	D	131	ALA
3	E	451	ASN
3	F	86	PRO
5	H	33	PRO
10	V	24	SER
10	V	50	PRO
10	V	130	PHE
2	A	28	ASN
2	B	145	HIS
2	C	228	MET
3	D	31	PRO
3	E	16	VAL
3	E	34	LEU
3	E	119	ALA
3	F	130	SER
7	O	82	ASP
11	W	32	LYS
12	X	30	PRO
12	X	36	LYS
2	A	230	TYR
2	A	435	TYR
2	B	143	SER
3	D	34	LEU
3	D	83	ILE
12	X	31	TRP
2	B	22	SER
7	O	15	VAL

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Mol	Chain	Res	Type
10	V	166	ARG
4	G	181	PRO
3	D	86	PRO
4	G	123	PRO
7	O	165	GLY
11	W	39	ALA

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.

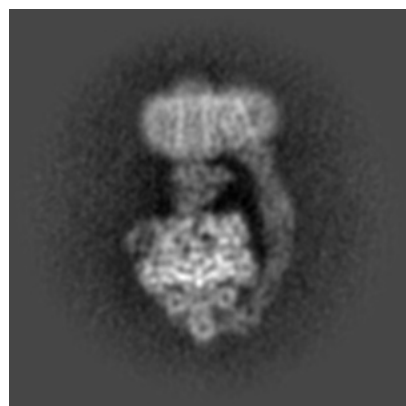
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25961. These allow visual inspection of the internal detail of the map and identification of artifacts.

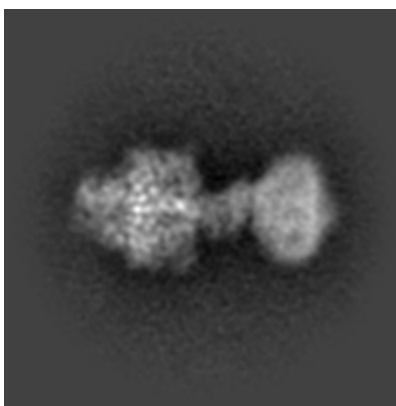
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

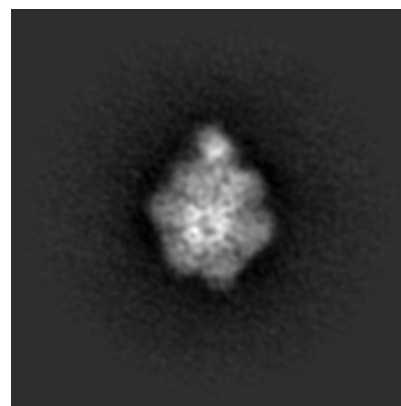
6.1.1 Primary map



X

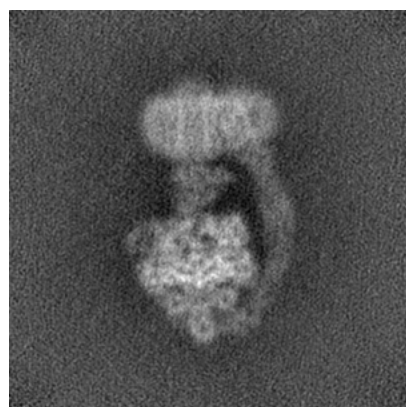


Y

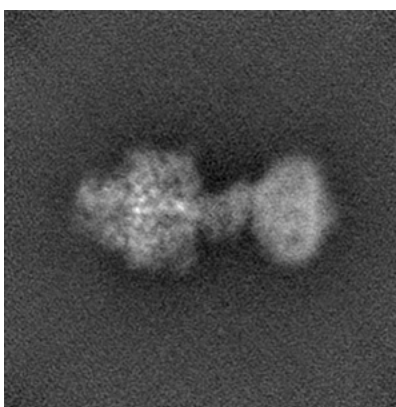


Z

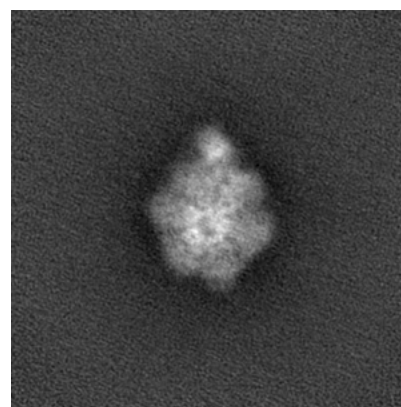
6.1.2 Raw map



X



Y

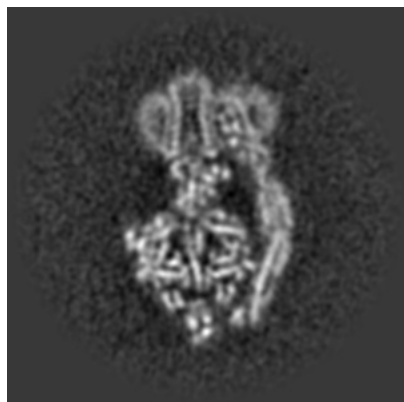


Z

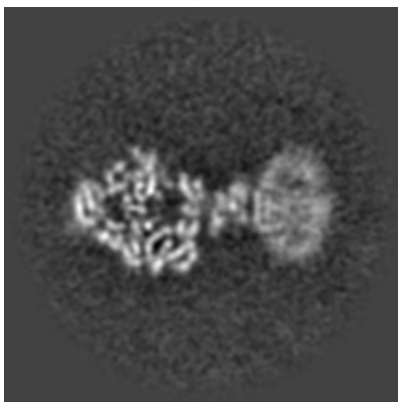
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

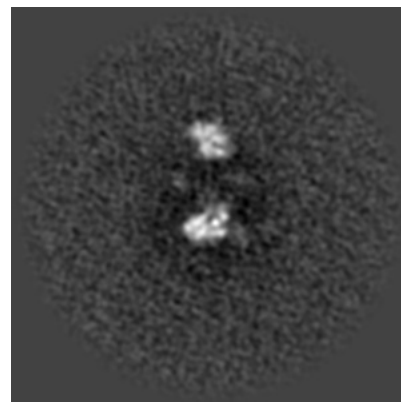
6.2.1 Primary map



X Index: 128

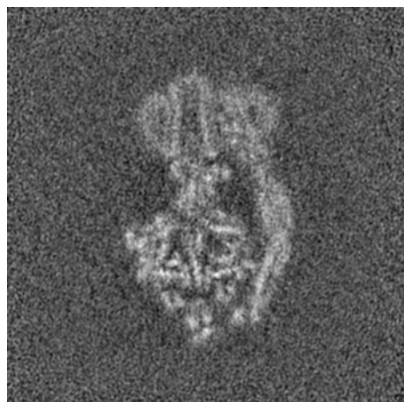


Y Index: 128

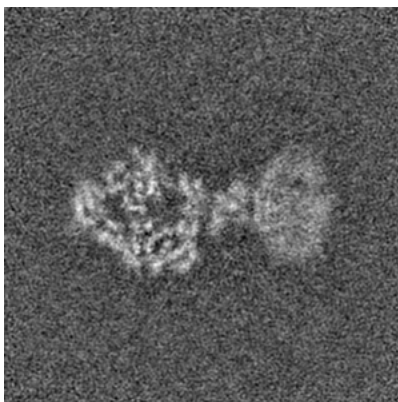


Z Index: 128

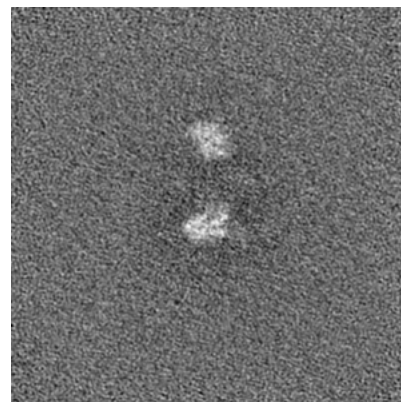
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

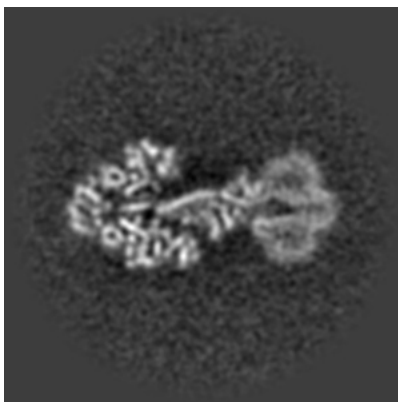
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

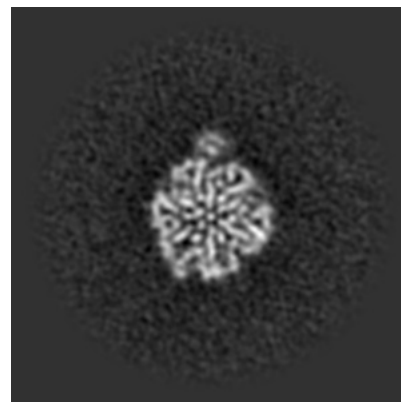
6.3.1 Primary map



X Index: 134

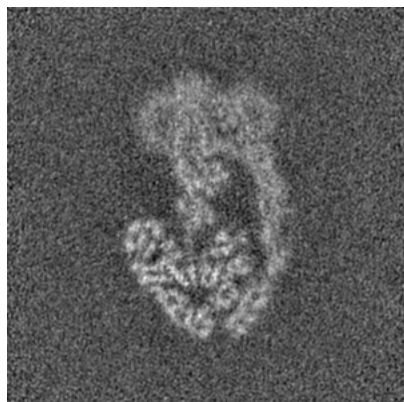


Y Index: 122

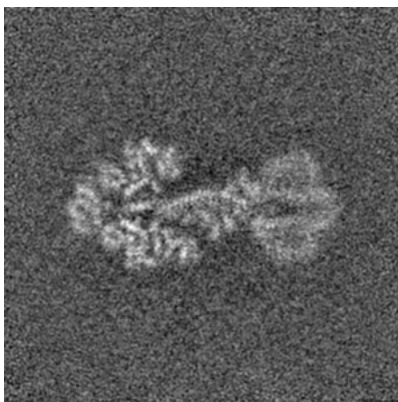


Z Index: 85

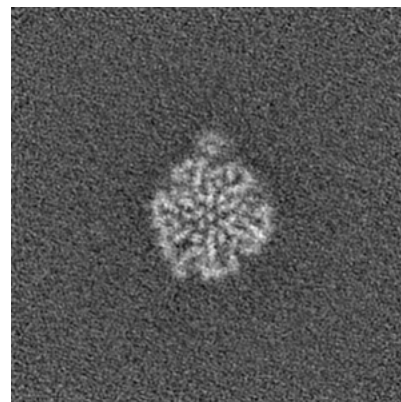
6.3.2 Raw map



X Index: 134



Y Index: 121

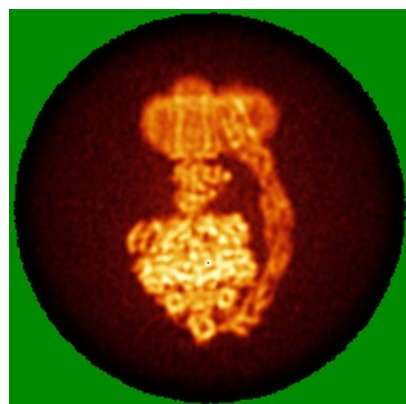


Z Index: 85

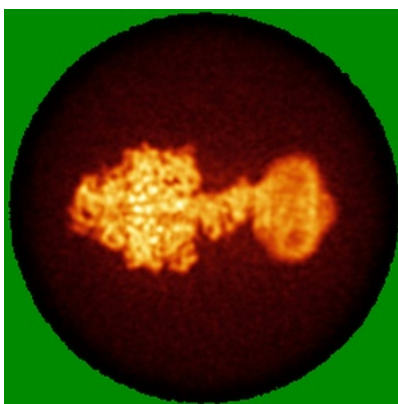
The images above show the largest variance slices of the map in three orthogonal directions.

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

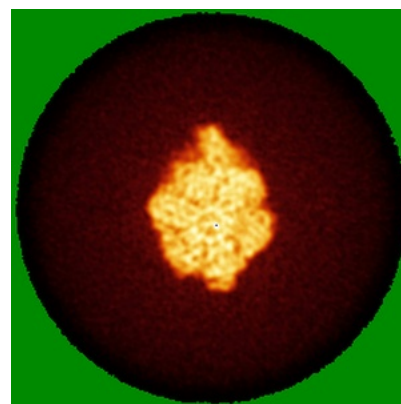
6.4.1 Primary map



X

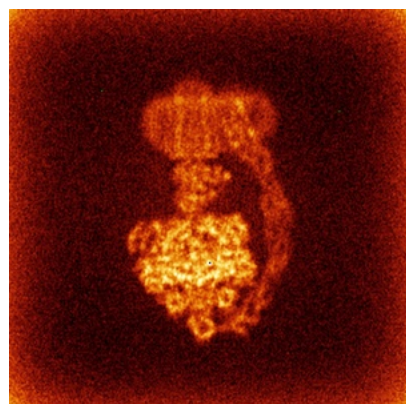


Y

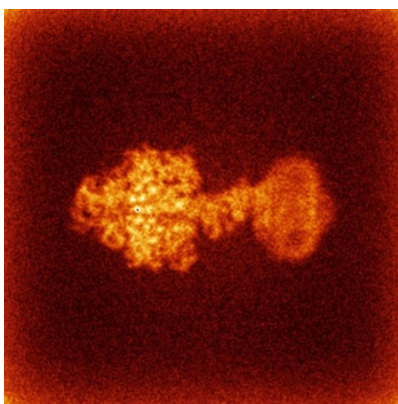


Z

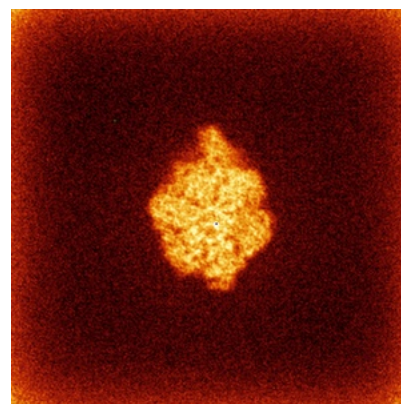
6.4.2 Raw map



X



Y



Z

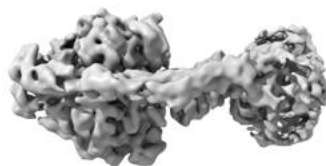
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

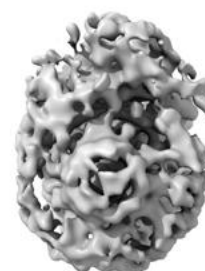
6.5.1 Primary map



X



Y



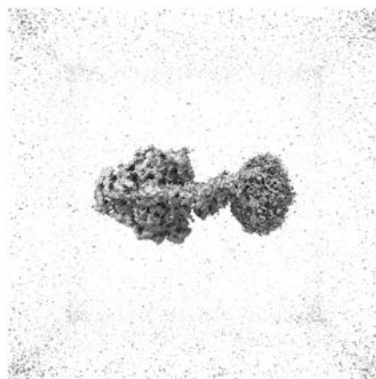
Z

The images above show the 3D surface view of the map at the recommended contour level 0.67. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

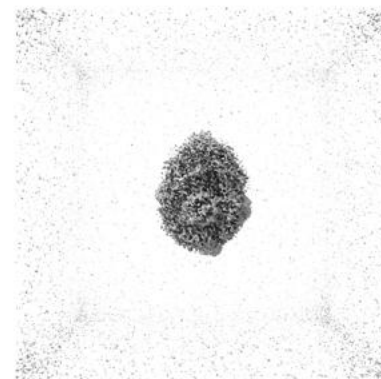
6.5.2 Raw map



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.

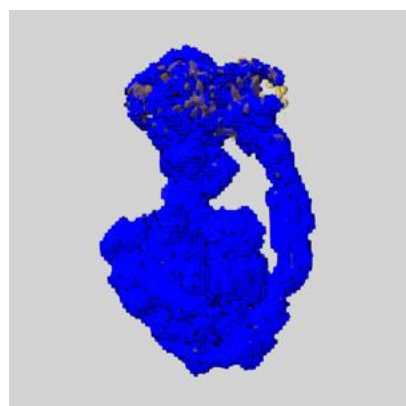
6.6 Mask visualisation [i](#)

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

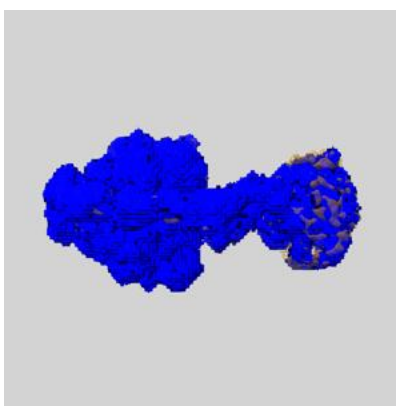
A mask typically either:

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

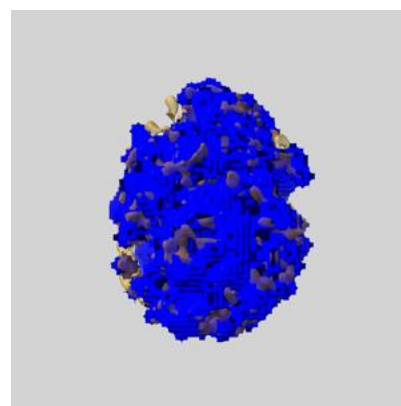
6.6.1 emd_25961_msk_1.map [i](#)



X



Y

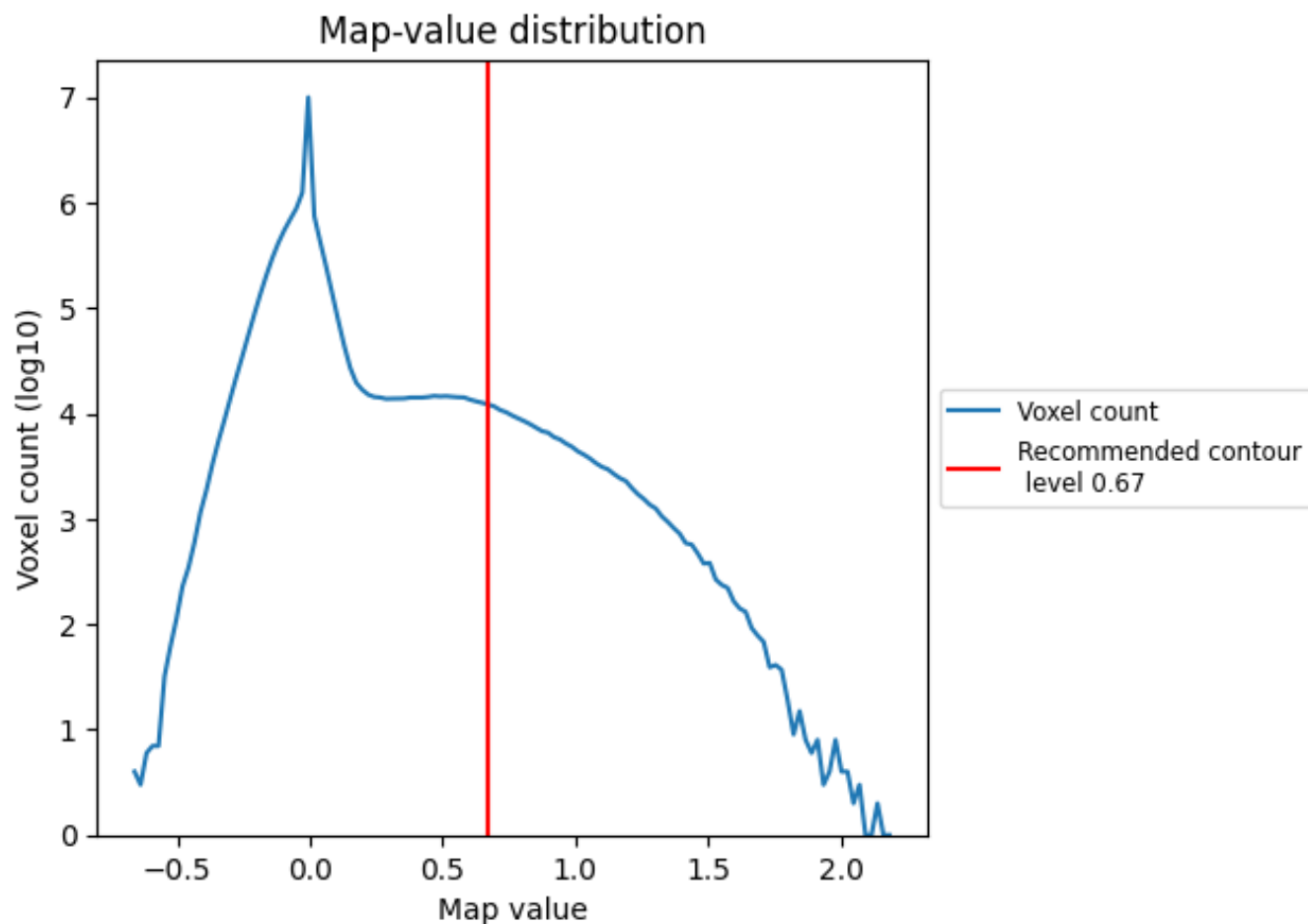


Z

7 Map analysis [i](#)

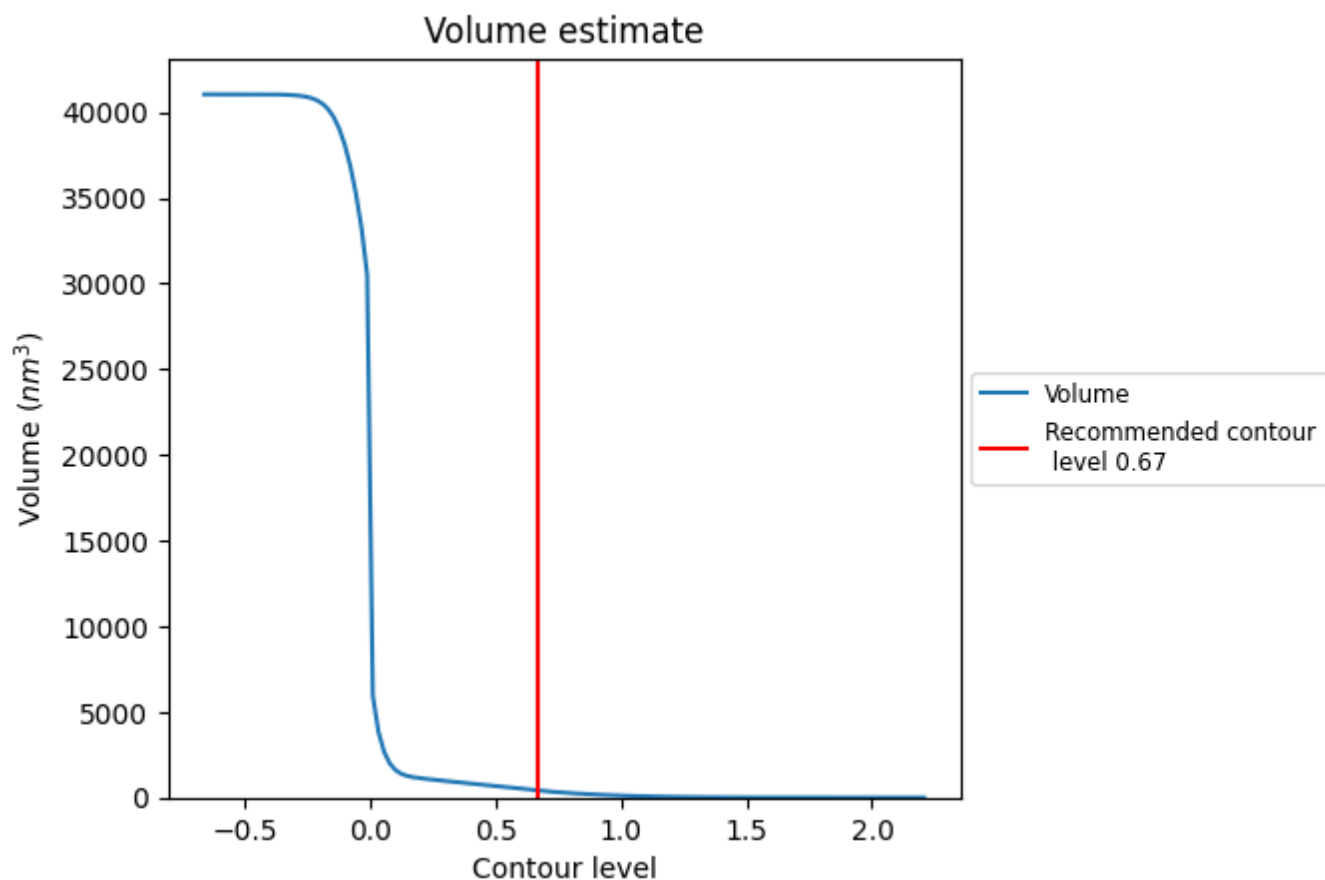
This section contains the results of statistical analysis of the map.

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.

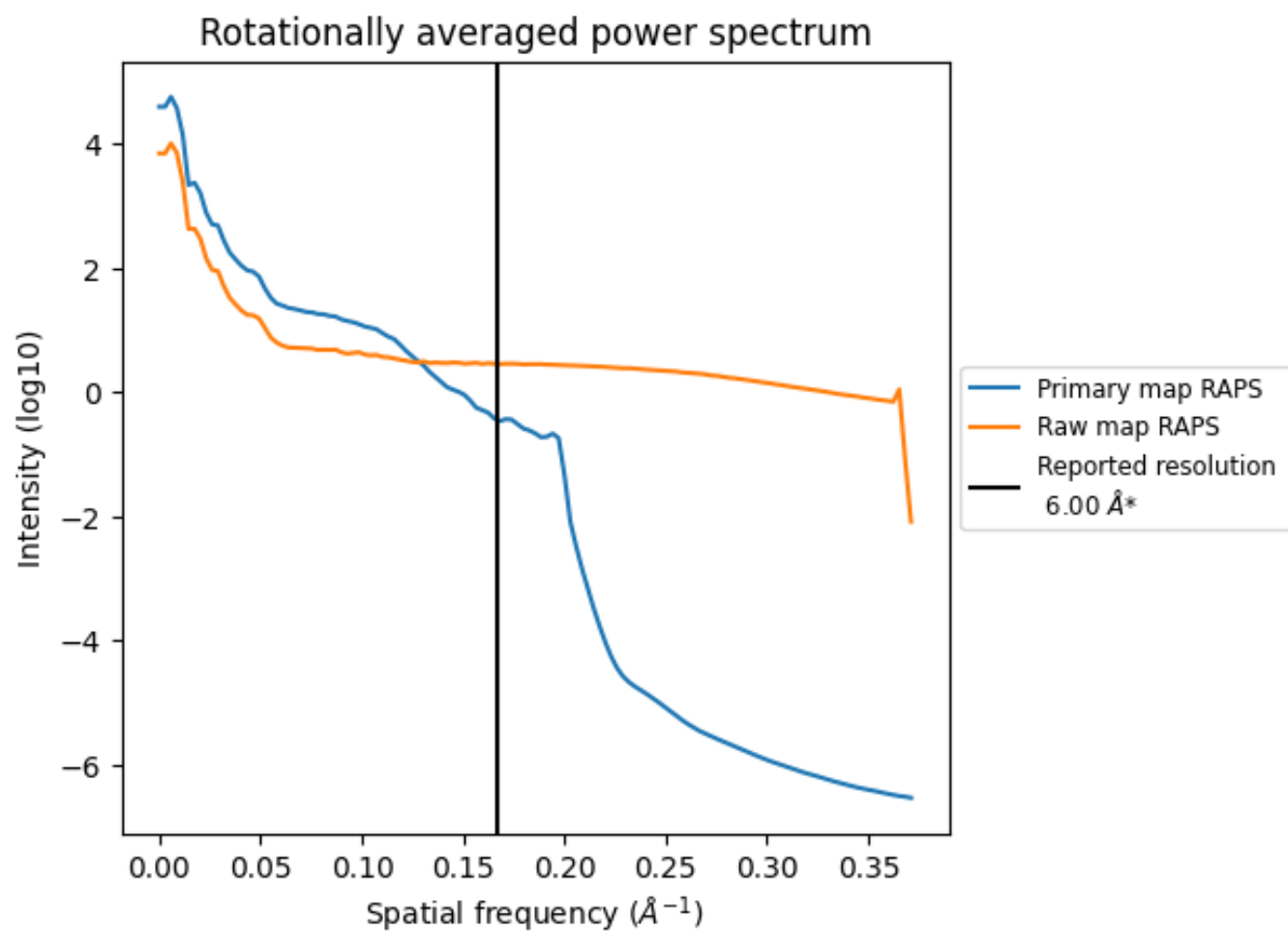
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 409 nm³; this corresponds to an approximate mass of 369 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

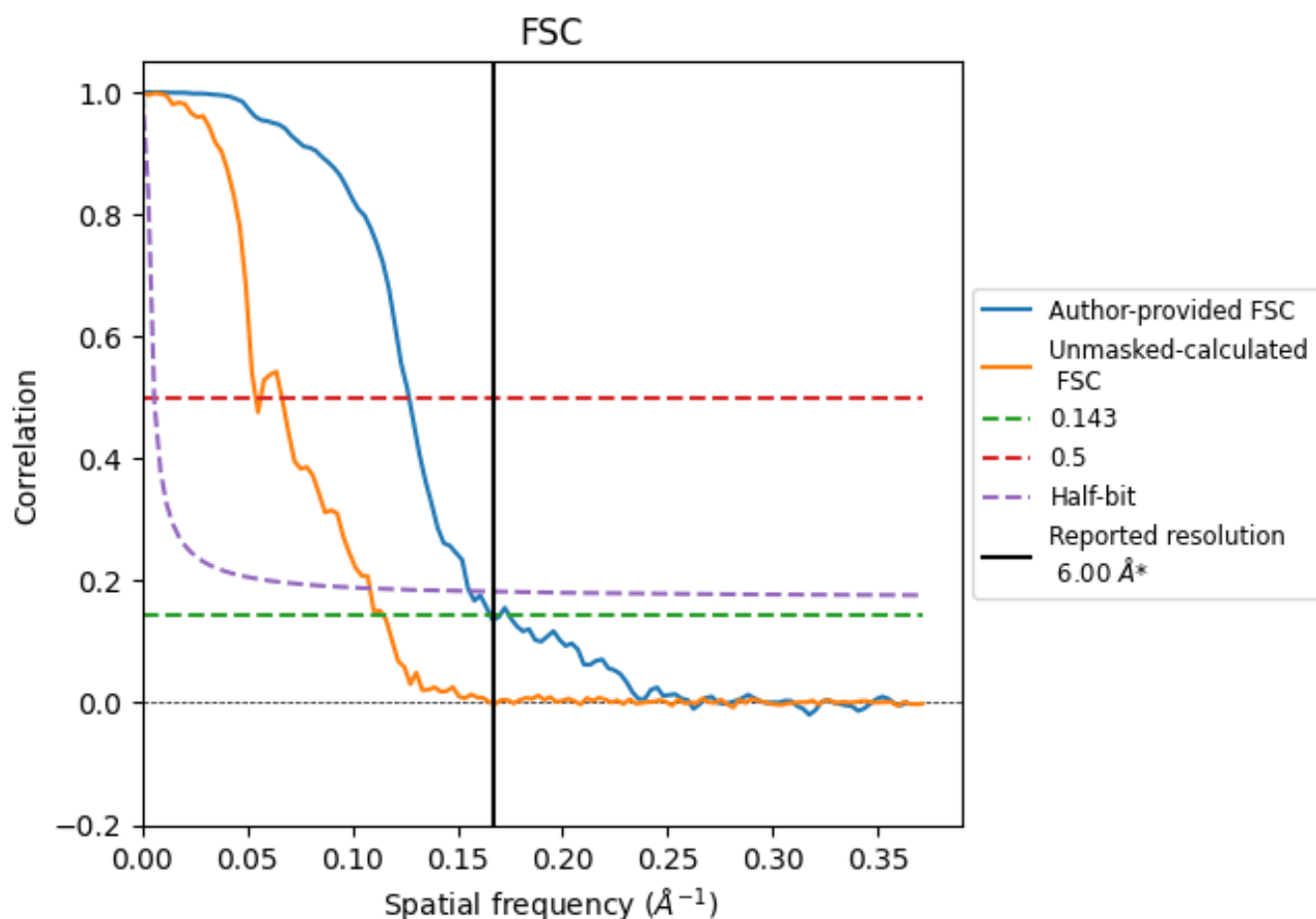


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

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 $0.167 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

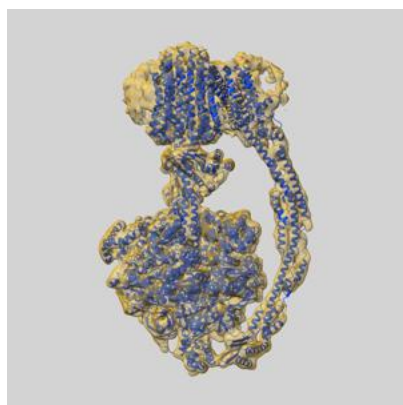
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	6.04	7.88	6.42
Unmasked-calculated*	8.73	18.52	9.23

*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 8.73 differs from the reported value 6.0 by more than 10 %

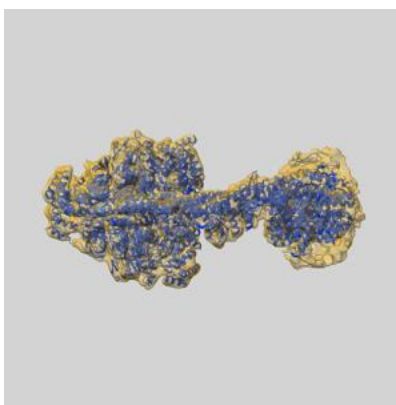
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25961 and PDB model 7TK9. Per-residue inclusion information can be found in section [3](#) on page [7](#).

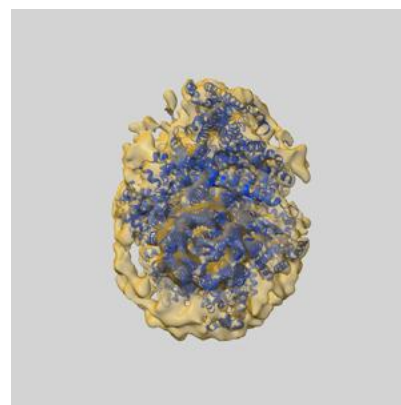
9.1 Map-model overlay [i](#)



X



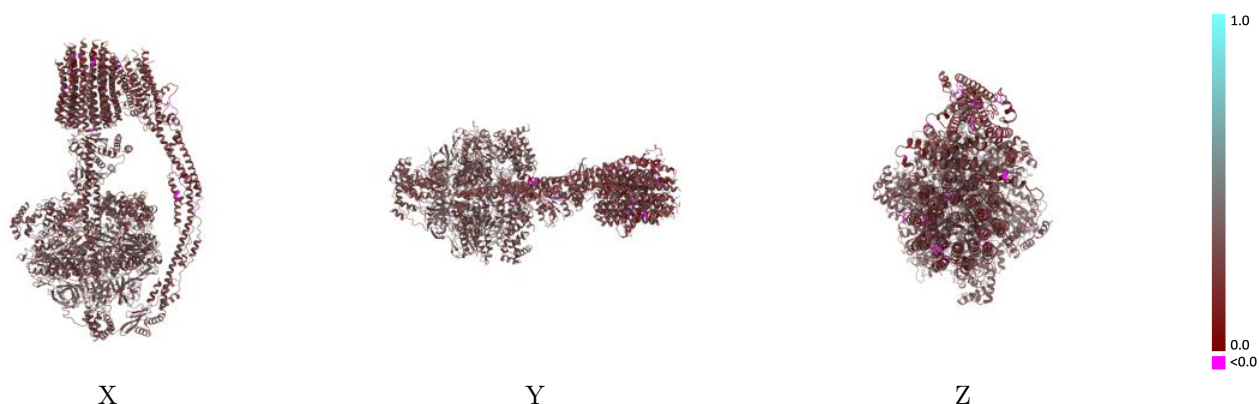
Y



Z

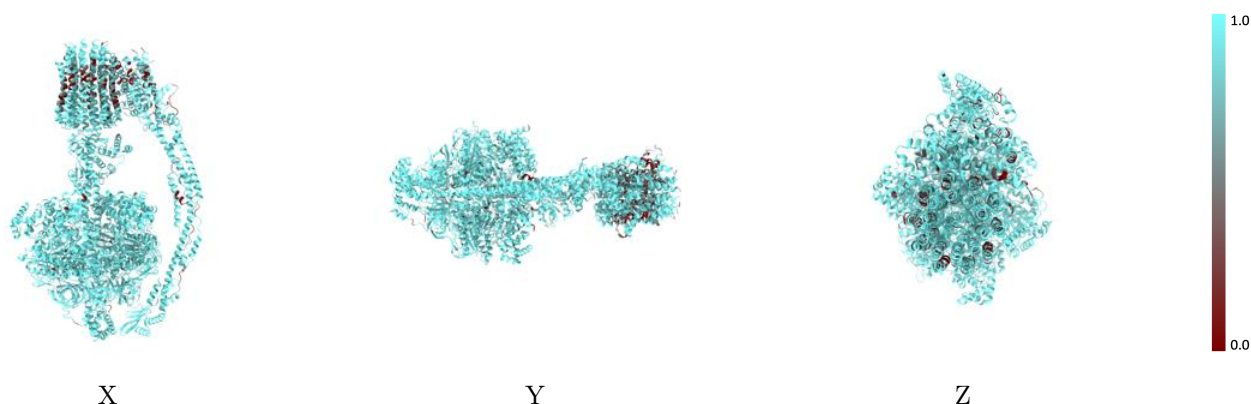
The images above show the 3D surface view of the map at the recommended contour level 0.67 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



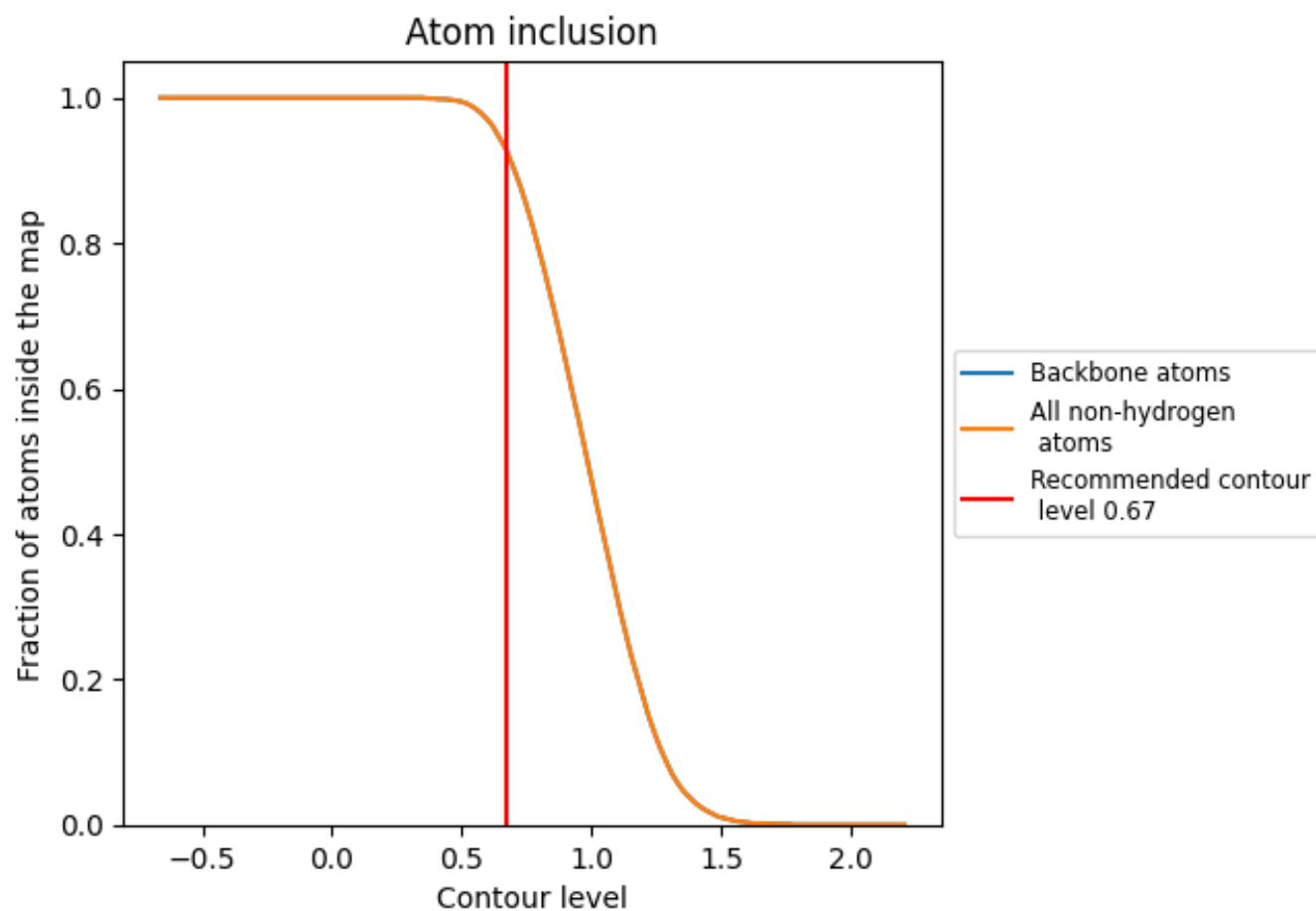
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.67).

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 (0.67) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.3040
0	 0.8430	 0.2560
1	 0.8000	 0.2540
2	 0.8270	 0.2610
3	 0.7030	 0.2410
4	 0.7130	 0.2410
5	 0.7670	 0.2380
6	 0.8280	 0.2470
7	 0.7230	 0.2190
8	 0.8800	 0.2610
9	 0.8310	 0.2570
A	 0.9780	 0.3330
B	 0.9680	 0.3310
C	 0.9760	 0.3290
D	 0.9710	 0.3370
E	 0.9810	 0.3300
F	 0.9860	 0.3410
G	 0.9770	 0.3040
H	 0.9310	 0.3100
I	 0.9640	 0.3190
O	 0.9870	 0.3190
T	 0.8090	 0.2440
U	 0.9450	 0.2770
V	 0.8890	 0.2450
W	 0.7910	 0.1870
X	 0.7940	 0.2590
Y	 0.7700	 0.2260
Z	 0.8860	 0.2510

