Full wwPDB EM Validation Report ⓘ

Feb 14, 2024 – 06:58 AM EST

PDB ID	:	7TK1
EMDB ID	:	EMD-25949
Title	:	Yeast ATP synthase State 1catalytic(d) without exogenous 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:

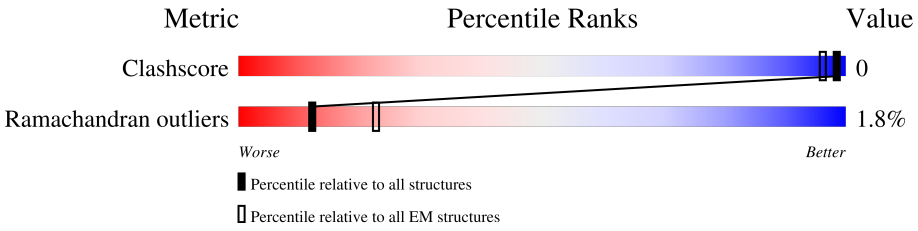
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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 <=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	17% 99%
1	1	76	22% 95%
1	2	76	13% 99%
1	3	76	16% 95%
1	4	76	17% 96%
1	5	76	13% 96%
1	6	76	13% 95%
1	7	76	30% 93%
1	8	76	14% 97%

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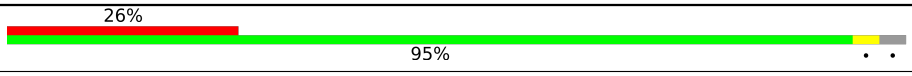
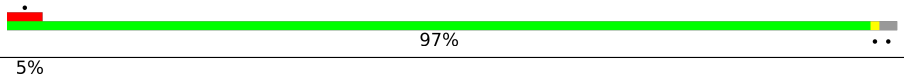
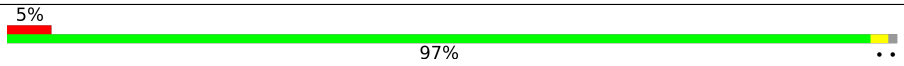
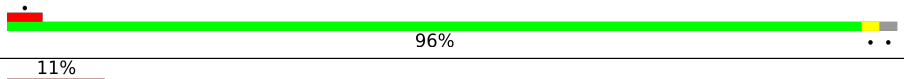
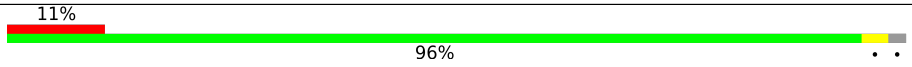
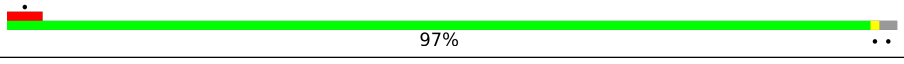
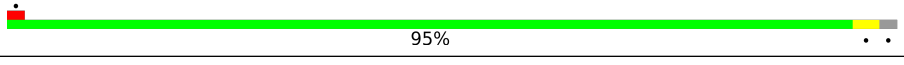
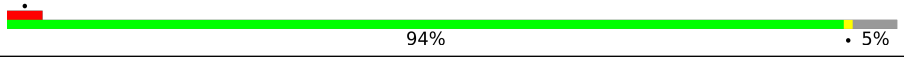
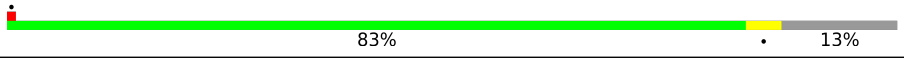
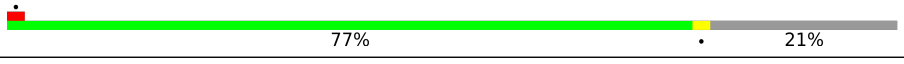
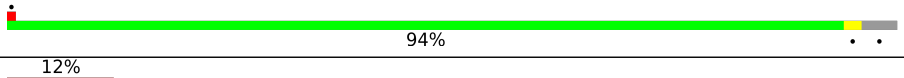
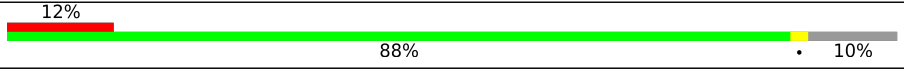
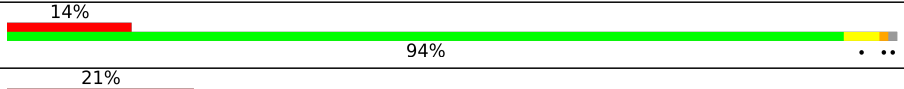
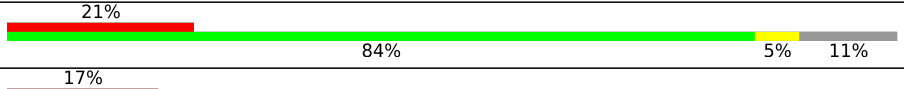
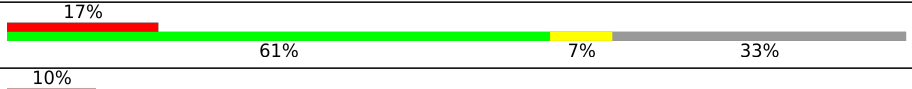
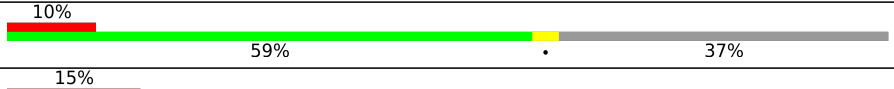
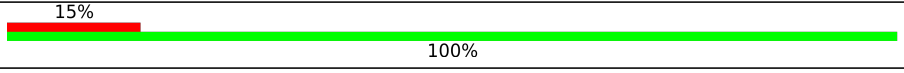
Mol	Chain	Length	Quality of chain
1	9	76	
2	A	510	
2	B	510	
2	C	510	
3	D	478	
3	E	478	
3	F	478	
4	G	278	
5	H	138	
6	I	61	
7	O	195	
8	T	249	
9	U	209	
10	V	173	
11	W	95	
12	X	92	
13	Y	59	
14	Z	48	

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.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	499	Total 1996	C 998	N 499	O 499	0	0
2	B	505	Total 2020	C 1010	N 505	O 505	0	0
2	C	498	Total 1992	C 996	N 498	O 498	0	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	265	Total 1060	C 530	N 265	O 265	0	0

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

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

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

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

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

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

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

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

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

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

- 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.

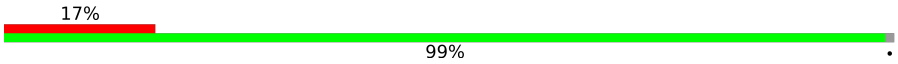
Mol	Chain	Residues	Atoms				AltConf	Trace
14	Z	48	Total	C	N	O	0	0
			193	96	48	49		

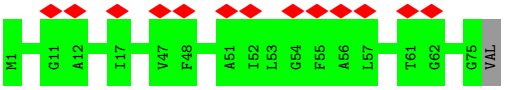
3 Residue-property plots (i)

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

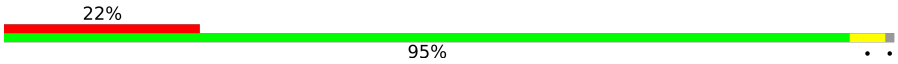
Chain 0:

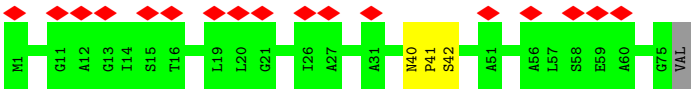




• Molecule 1: ATP synthase subunit 9

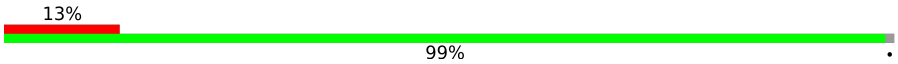
Chain 1:

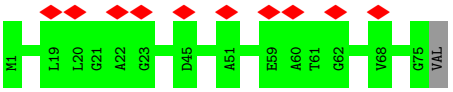




• Molecule 1: ATP synthase subunit 9

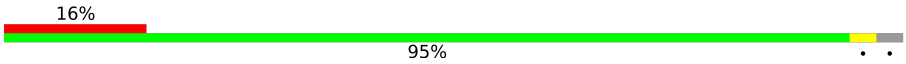
Chain 2:

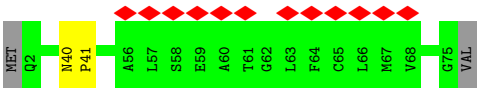




• Molecule 1: ATP synthase subunit 9

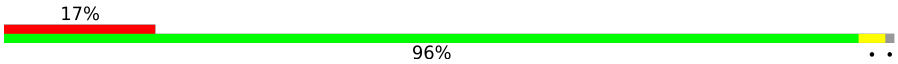
Chain 3:

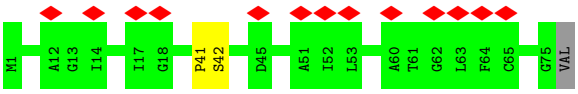




• Molecule 1: ATP synthase subunit 9

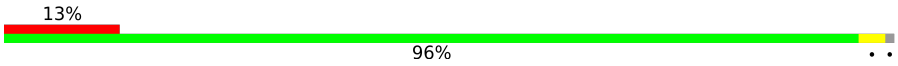
Chain 4:

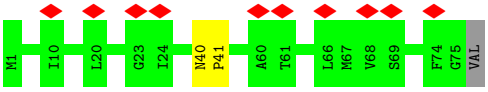




• Molecule 1: ATP synthase subunit 9

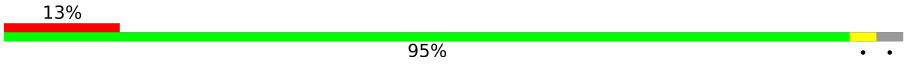
Chain 5:

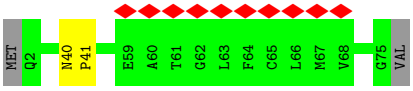




• Molecule 1: ATP synthase subunit 9

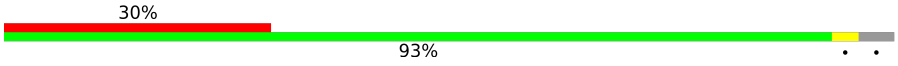
Chain 6:

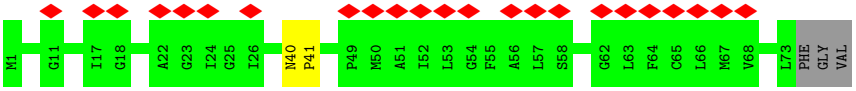




• Molecule 1: ATP synthase subunit 9

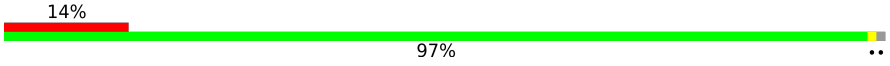
Chain 7:

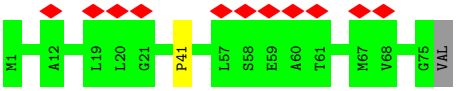




• Molecule 1: ATP synthase subunit 9

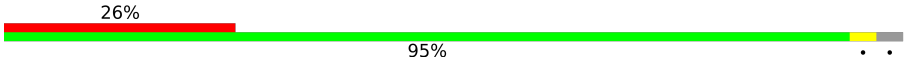
Chain 8:

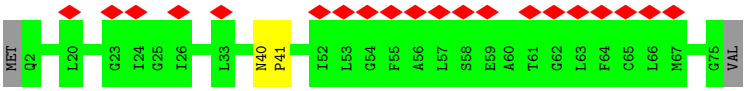




• Molecule 1: ATP synthase subunit 9

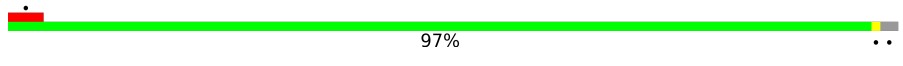
Chain 9:

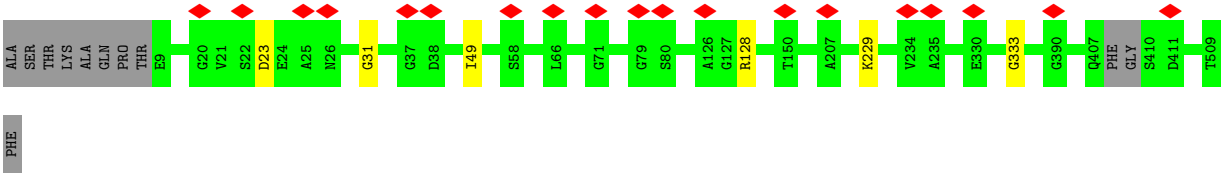




• Molecule 2: ATP synthase subunit alpha

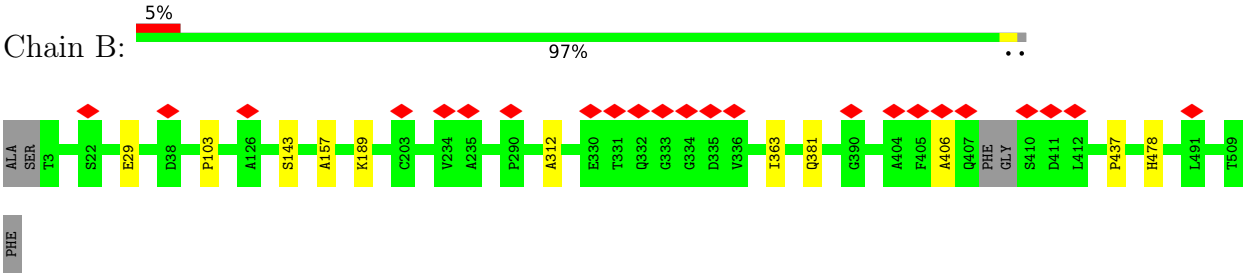
Chain A:





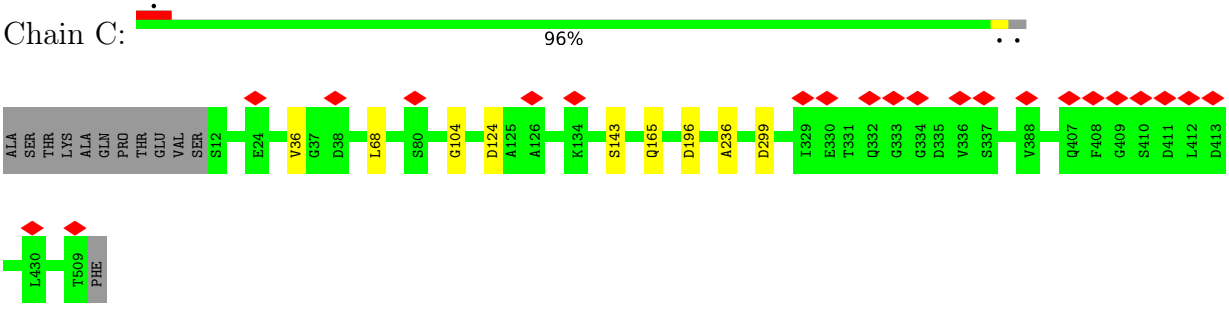
• Molecule 2: ATP synthase subunit alpha

Chain B:



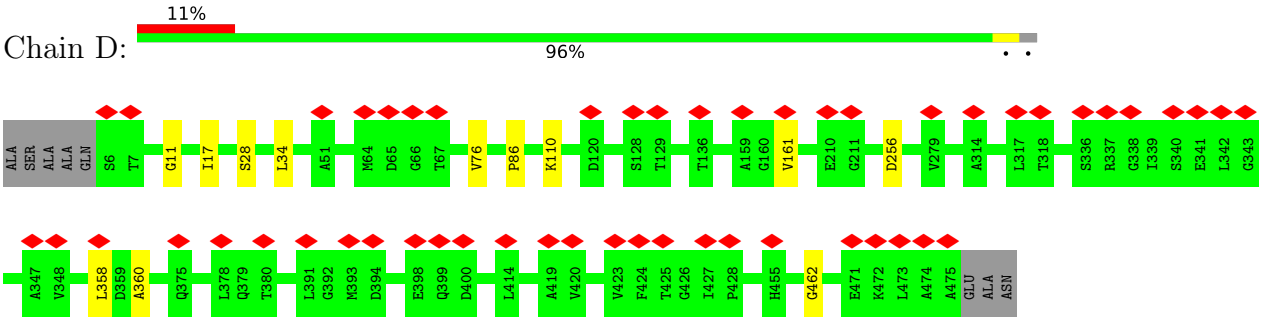
• Molecule 2: ATP synthase subunit alpha

Chain C:



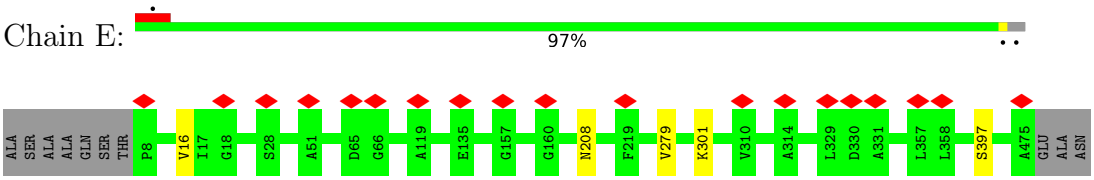
• Molecule 3: ATP synthase subunit beta

Chain D:



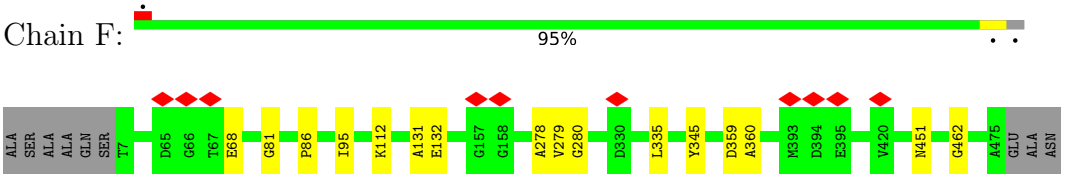
• Molecule 3: ATP synthase subunit beta

Chain E:



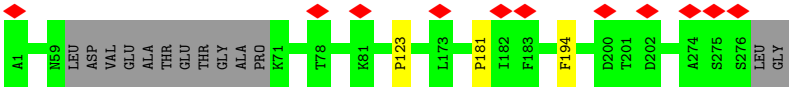
• Molecule 3: ATP synthase subunit beta

Chain F:

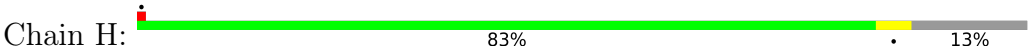


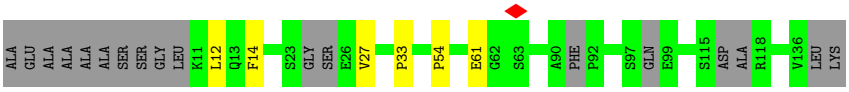
• Molecule 4: ATP synthase subunit gamma

Chain G:

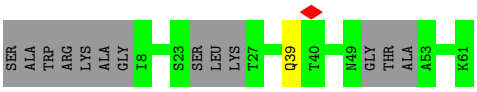


• Molecule 5: ATP synthase subunit delta

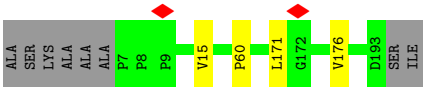




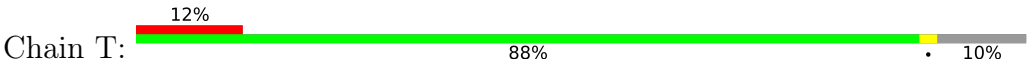
• Molecule 6: ATP synthase subunit epsilon

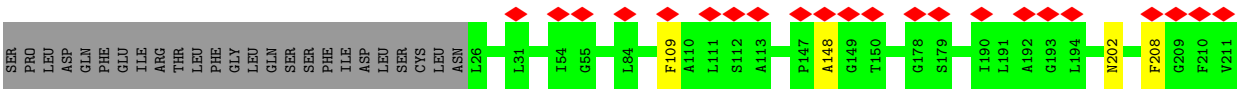


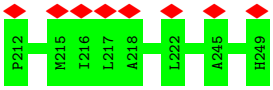
• Molecule 7: ATP synthase subunit 5



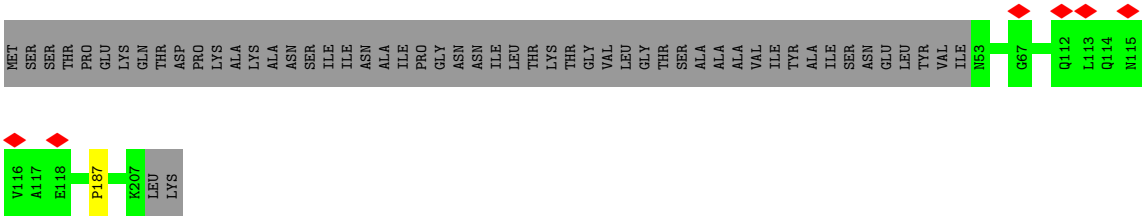
• Molecule 8: ATP synthase subunit a





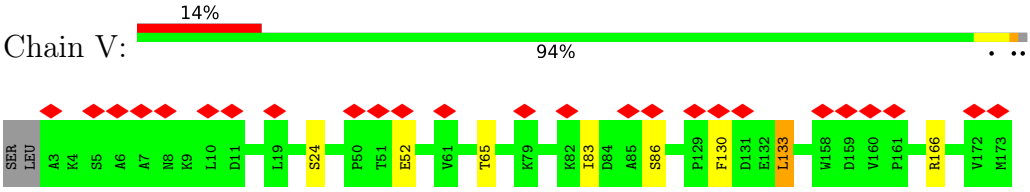


• Molecule 9: ATP synthase subunit 4



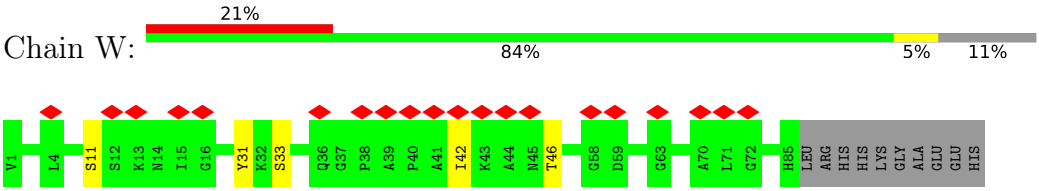
• Molecule 10: ATP synthase subunit d

Chain V:



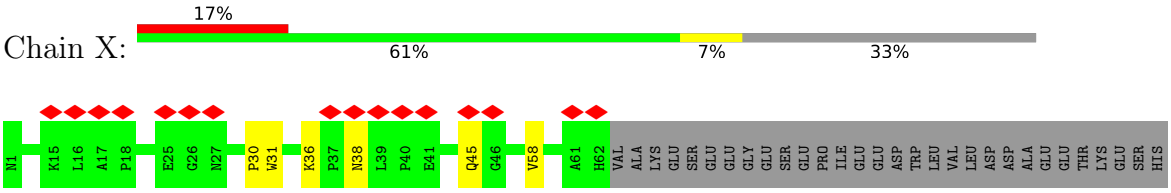
• Molecule 11: ATP synthase subunit f

Chain W:



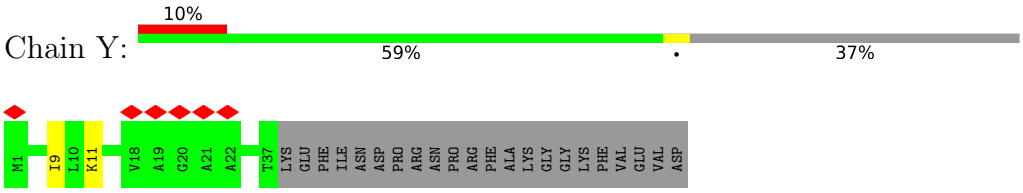
• Molecule 12: ATP synthase subunit H

Chain X:



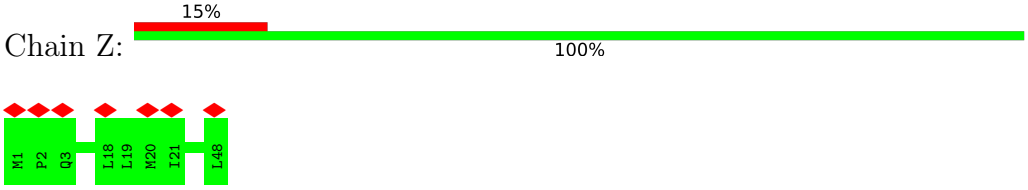
• Molecule 13: ATP synthase subunit J

Chain Y:



• Molecule 14: ATP synthase protein 8

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1984	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 ($e^-/Å^2$)	39	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	133843	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.648	Depositor
Minimum map value	-0.486	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.6	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	0.75	0/299	0.76	0/372
1	1	0.73	0/299	0.77	0/372
1	2	0.75	0/299	0.74	0/372
1	3	0.75	0/295	0.77	0/367
1	4	0.74	0/299	0.79	0/372
1	5	0.75	0/299	0.78	0/372
1	6	0.74	0/295	0.76	0/367
1	7	0.72	0/291	0.72	0/362
1	8	0.75	0/299	0.81	0/372
1	9	0.73	0/295	0.80	0/367
2	A	0.90	0/1994	0.95	2/2489 (0.1%)
2	B	0.90	0/2018	0.98	0/2519
2	C	0.89	0/1991	0.97	2/2487 (0.1%)
3	D	0.89	0/1879	1.02	1/2347 (0.0%)
3	E	0.91	0/1871	1.01	1/2337 (0.0%)
3	F	0.91	0/1875	1.02	3/2342 (0.1%)
4	G	0.82	0/1058	0.86	0/1319
5	H	0.91	0/475	1.17	2/585 (0.3%)
6	I	0.84	0/190	0.94	0/231
7	O	0.90	0/747	1.01	1/932 (0.1%)
8	T	0.75	0/896	0.74	0/1117
9	U	0.72	0/619	0.62	0/772
10	V	0.79	0/684	0.91	1/852 (0.1%)
11	W	0.76	0/339	1.09	0/422
12	X	0.77	0/247	1.03	0/307
13	Y	0.76	0/147	0.75	0/182
14	Z	0.74	0/192	0.65	0/237
All	All	0.85	0/20192	0.94	13/25172 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	3	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	9	0	1
3	D	0	1
3	F	0	1
5	H	0	1
9	U	0	1
All	All	0	10

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	176	VAL	N-CA-C	-5.85	95.20	111.00
5	H	61	GLU	N-CA-C	-5.84	95.24	111.00
2	C	68	LEU	N-CA-C	-5.78	95.39	111.00
3	D	17	ILE	N-CA-C	-5.71	95.60	111.00
2	A	128	ARG	N-CA-C	-5.47	96.22	111.00
3	F	95	ILE	N-CA-C	-5.28	96.74	111.00
2	A	31	GLY	N-CA-C	-5.27	99.93	113.10
3	F	112	LYS	N-CA-C	-5.26	96.81	111.00
5	H	14	PHE	N-CA-C	-5.18	97.01	111.00
3	F	335	LEU	N-CA-C	-5.16	97.08	111.00
3	E	208	ASN	N-CA-C	-5.15	97.09	111.00
10	V	133	LEU	N-CA-C	-5.13	97.14	111.00
2	C	236	ALA	N-CA-C	-5.08	97.27	111.00

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	40	ASN	Peptide
1	3	40	ASN	Peptide
1	5	40	ASN	Peptide
1	6	40	ASN	Peptide
1	7	40	ASN	Peptide
1	9	40	ASN	Peptide
3	D	256	ASP	Peptide
3	F	345	TYR	Peptide

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Mol	Chain	Res	Type	Group
5	H	54	PRO	Peptide
9	U	187	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	300	0	95	0	0
1	1	300	0	95	0	0
1	2	300	0	95	0	0
1	3	296	0	91	0	0
1	4	300	0	95	0	0
1	5	300	0	95	0	0
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	0	0
2	C	1992	0	572	1	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	0	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	2	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 (2) 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)
3:D:11:GLY:H	3:D:76:VAL:H	1.59	0.50
2:C:104:GLY:HA3	2:C:124:ASP:H	1.78	0.49

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%)	72 (99%)	1 (1%)	0	100 100
1	1	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	5 31
1	2	73/76 (96%)	72 (99%)	1 (1%)	0	100 100
1	3	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	11 46
1	4	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	5 31
1	5	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	11 46
1	6	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	11 46
1	7	71/76 (93%)	69 (97%)	1 (1%)	1 (1%)	11 46
1	8	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	11 46
1	9	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	11 46
2	A	495/510 (97%)	474 (96%)	17 (3%)	4 (1%)	19 60
2	B	501/510 (98%)	469 (94%)	21 (4%)	11 (2%)	6 35
2	C	496/510 (97%)	463 (93%)	28 (6%)	5 (1%)	15 54
3	D	468/478 (98%)	437 (93%)	23 (5%)	8 (2%)	9 42
3	E	466/478 (98%)	440 (94%)	22 (5%)	4 (1%)	17 57
3	F	467/478 (98%)	425 (91%)	30 (6%)	12 (3%)	5 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	G	261/278 (94%)	250 (96%)	8 (3%)	3 (1%)	14 52
5	H	110/138 (80%)	103 (94%)	4 (4%)	3 (3%)	5 31
6	I	42/61 (69%)	37 (88%)	4 (10%)	1 (2%)	6 33
7	O	185/195 (95%)	169 (91%)	13 (7%)	3 (2%)	9 44
8	T	222/249 (89%)	211 (95%)	7 (3%)	4 (2%)	8 40
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100 100
10	V	169/173 (98%)	148 (88%)	13 (8%)	8 (5%)	2 21
11	W	83/95 (87%)	71 (86%)	7 (8%)	5 (6%)	1 17
12	X	60/92 (65%)	50 (83%)	4 (7%)	6 (10%)	0 9
13	Y	35/59 (59%)	31 (89%)	2 (6%)	2 (6%)	1 18
14	Z	46/48 (96%)	43 (94%)	3 (6%)	0	100 100
All	All	4984/5321 (94%)	4673 (94%)	222 (4%)	89 (2%)	12 40

All (89) 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	49	ILE
2	C	299	ASP
3	D	28	SER
3	D	110	LYS
3	D	358	LEU
3	F	360	ALA
8	T	109	PHE
10	V	24	SER
10	V	52	GLU
10	V	83	ILE
10	V	133	LEU
11	W	31	TYR
11	W	33	SER
12	X	31	TRP

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Mol	Chain	Res	Type
12	X	58	VAL
2	B	103	PRO
2	B	437	PRO
2	C	36	VAL
2	C	143	SER
2	C	165	GLN
3	D	360	ALA
3	E	279	VAL
3	E	301	LYS
3	F	68	GLU
3	F	359	ASP
3	F	451	ASN
3	F	462	GLY
5	H	33	PRO
8	T	148	ALA
10	V	65	THR
10	V	130	PHE
11	W	11	SER
11	W	42	ILE
12	X	38	ASN
12	X	45	GLN
2	A	23	ASP
2	A	229	LYS
2	A	333	GLY
2	B	29	GLU
2	B	312	ALA
2	B	381	GLN
2	B	406	ALA
3	F	86	PRO
3	F	132	GLU
3	F	278	ALA
3	F	280	GLY
4	G	123	PRO
4	G	194	PHE
6	I	39	GLN
8	T	202	ASN
12	X	30	PRO
13	Y	11	LYS
1	1	42	SER
2	B	143	SER
2	B	478	HIS
3	E	397	SER

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Mol	Chain	Res	Type
7	O	171	LEU
8	T	208	PHE
10	V	166	ARG
12	X	36	LYS
13	Y	9	ILE
1	4	42	SER
2	B	189	LYS
2	B	363	ILE
2	C	196	ASP
3	D	34	LEU
3	D	86	PRO
3	D	462	GLY
3	E	16	VAL
3	F	131	ALA
5	H	12	LEU
10	V	86	SER
11	W	46	THR
2	B	157	ALA
3	F	81	GLY
4	G	181	PRO
3	F	279	VAL
5	H	27	VAL
3	D	161	VAL
7	O	15	VAL
7	O	60	PRO

5.3.2 Protein sidechains

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

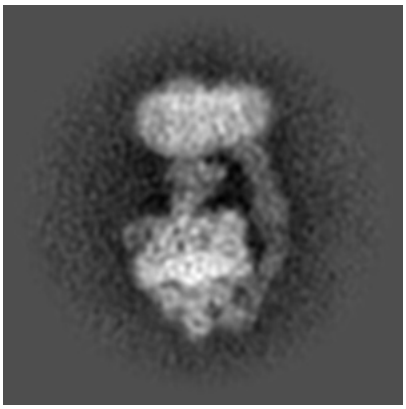
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25949. These allow visual inspection of the internal detail of the map and identification of artifacts.

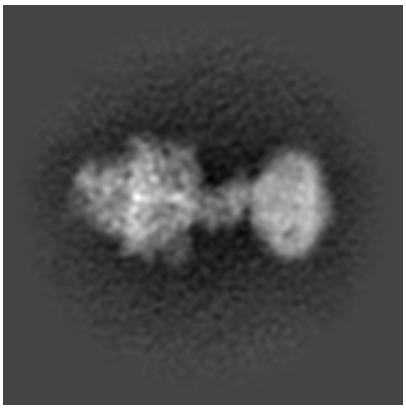
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

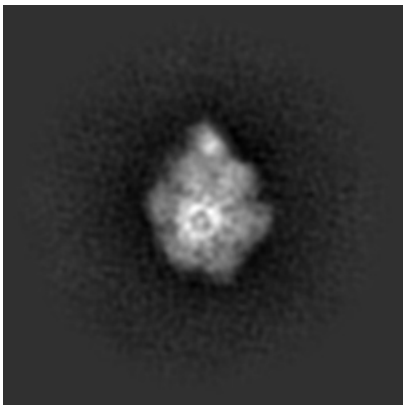
6.1.1 Primary map



X

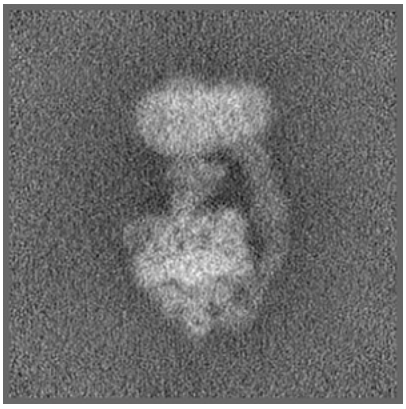


Y

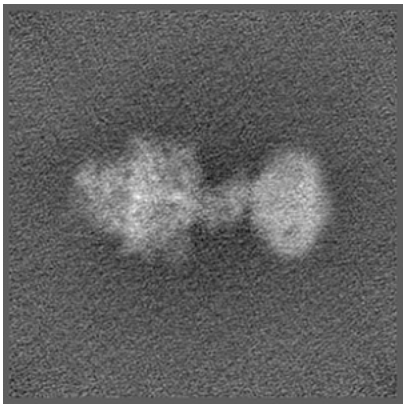


Z

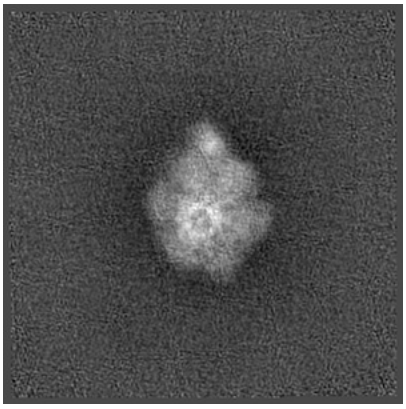
6.1.2 Raw map



X



Y

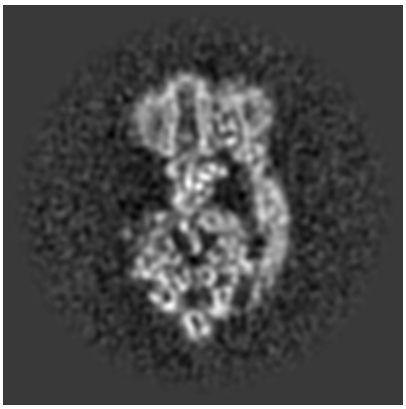


Z

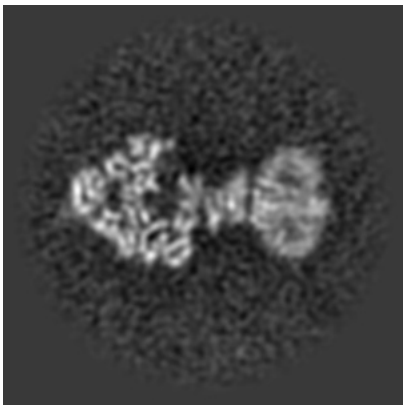
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

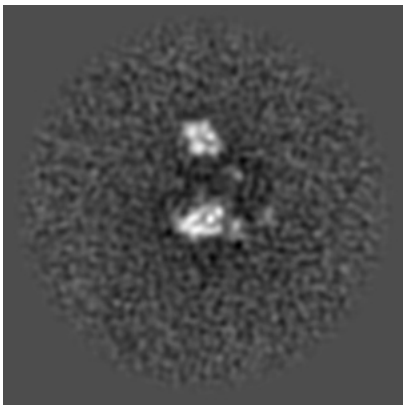
6.2.1 Primary map



X Index: 128

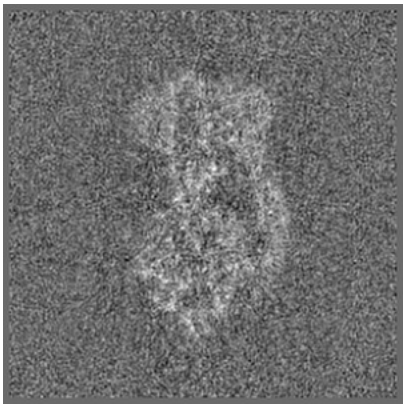


Y Index: 128

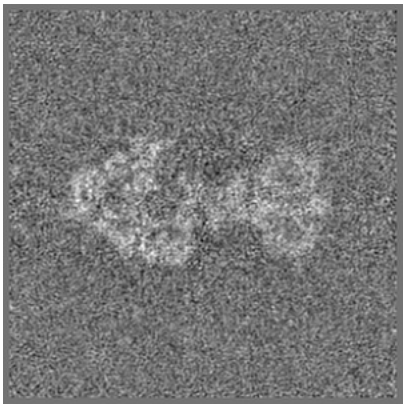


Z Index: 128

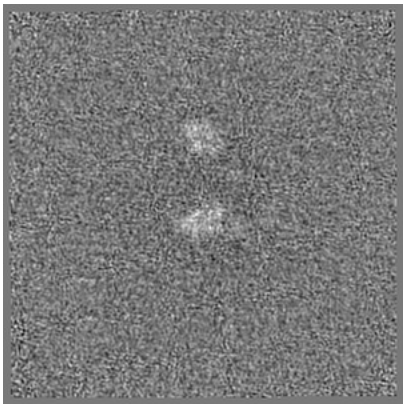
6.2.2 Raw map



X Index: 128



Y Index: 128

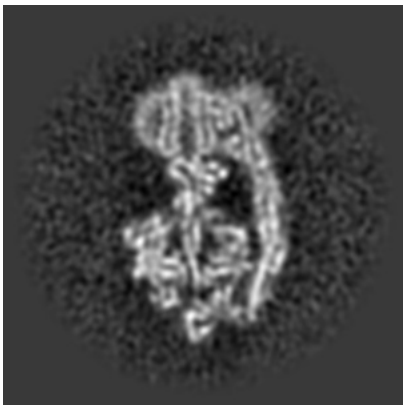


Z Index: 128

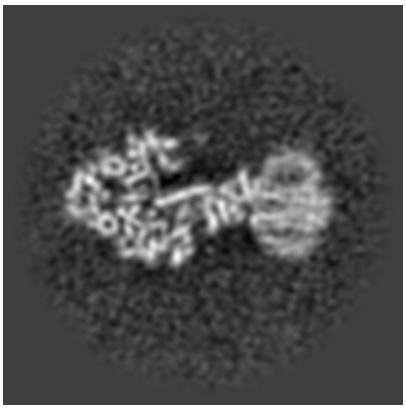
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

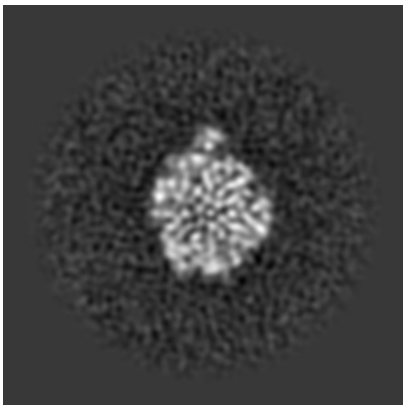
6.3.1 Primary map



X Index: 132

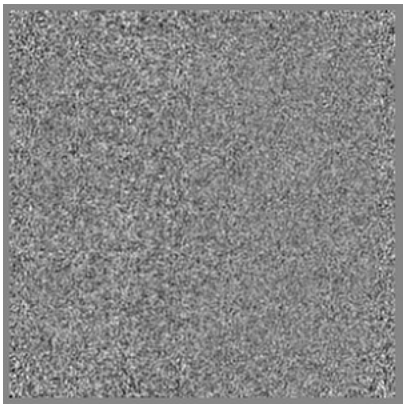


Y Index: 124

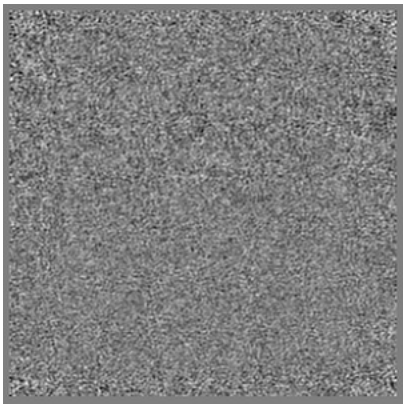


Z Index: 86

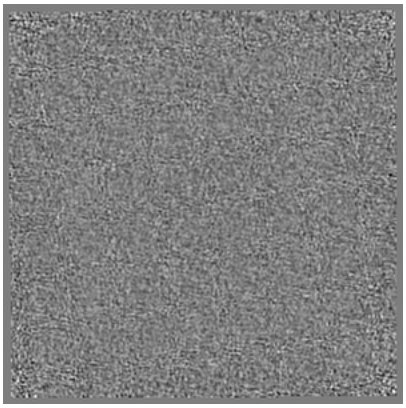
6.3.2 Raw map



X Index: 5



Y Index: 5

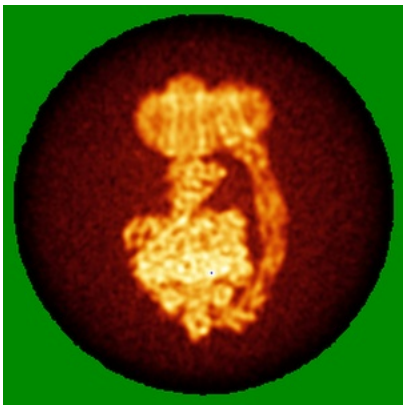


Z Index: 251

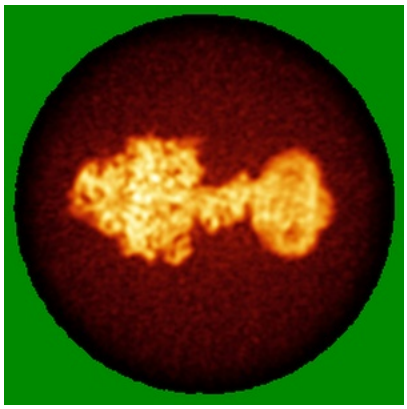
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

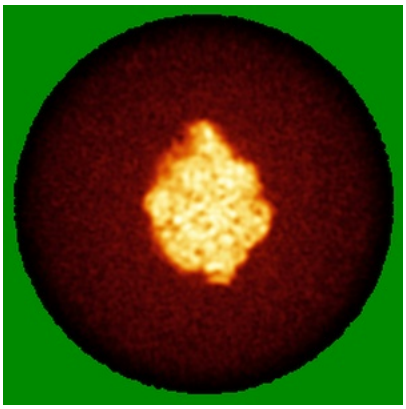
6.4.1 Primary map



X

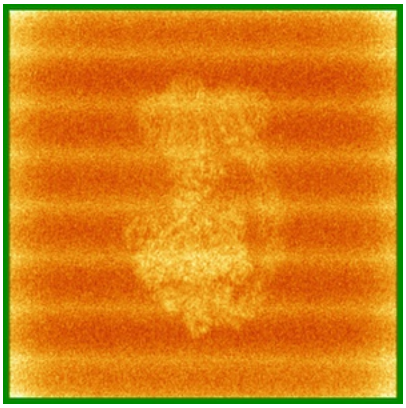


Y

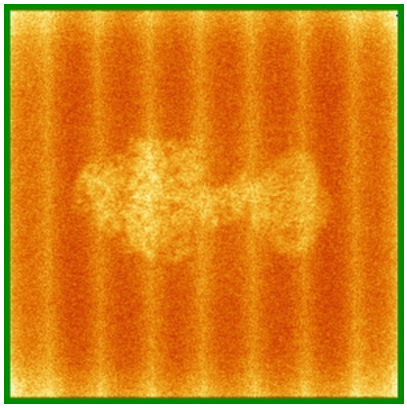


Z

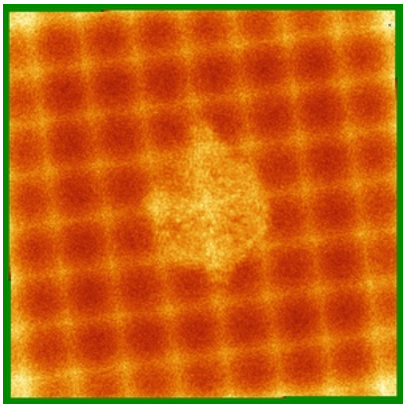
6.4.2 Raw map



X



Y

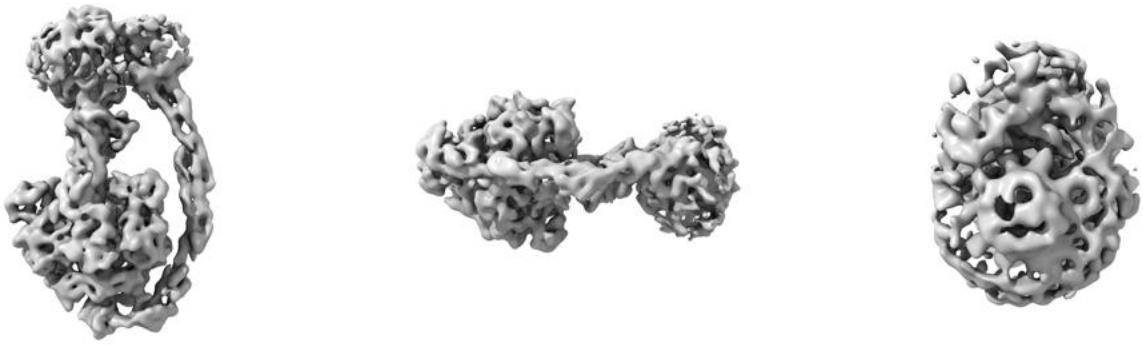


Z

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

6.5 Orthogonal surface views (i)

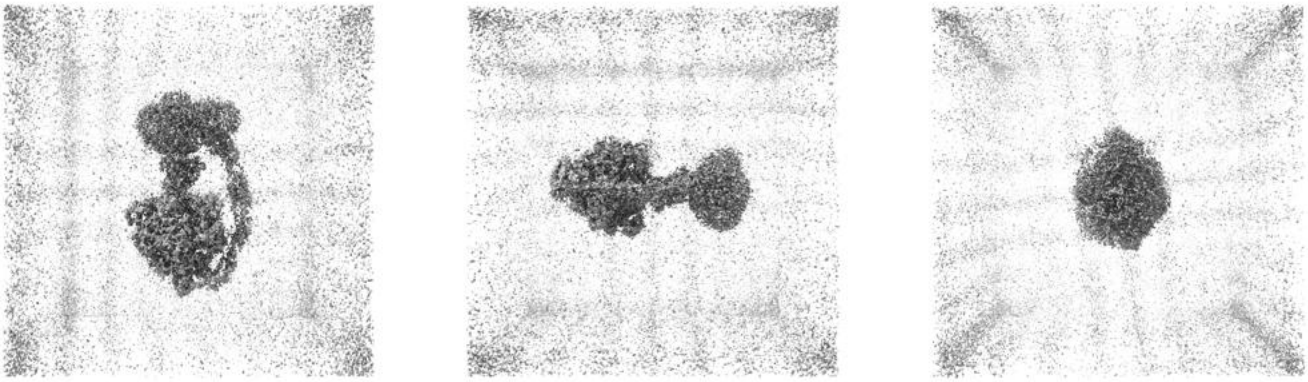
6.5.1 Primary map



X Y Z

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

6.5.2 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.

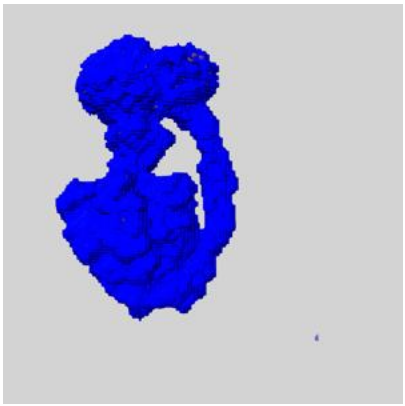
6.6 Mask visualisation (i)

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

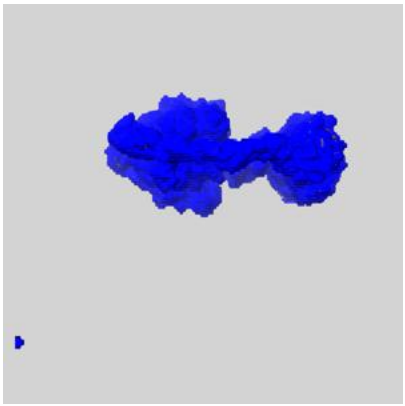
A mask typically either:

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

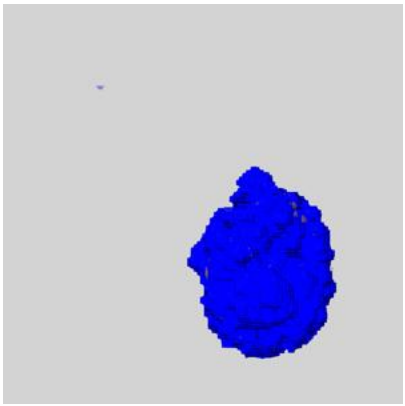
6.6.1 emd_25949_msk_1.map (i)



X



Y

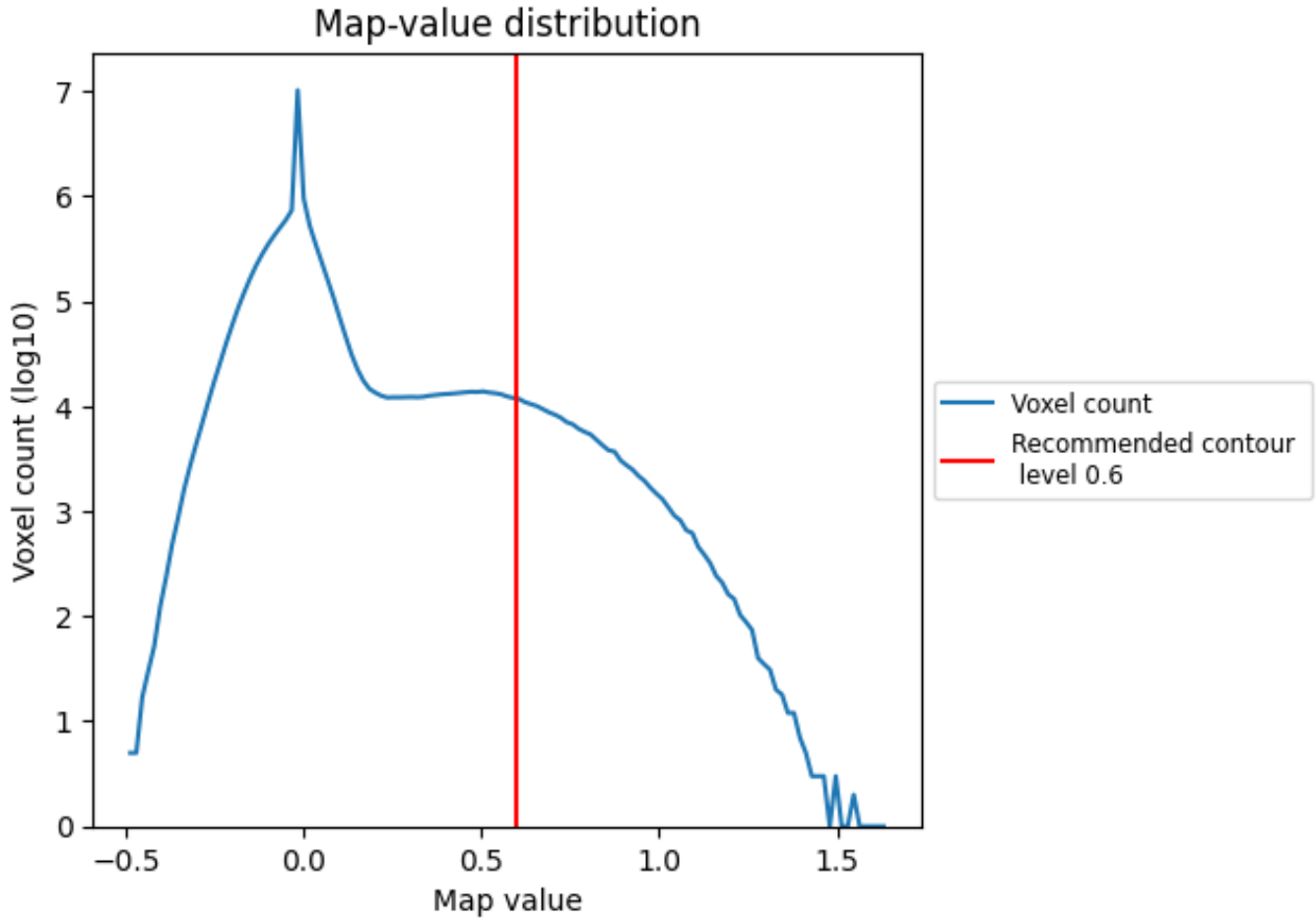


Z

7 Map analysis

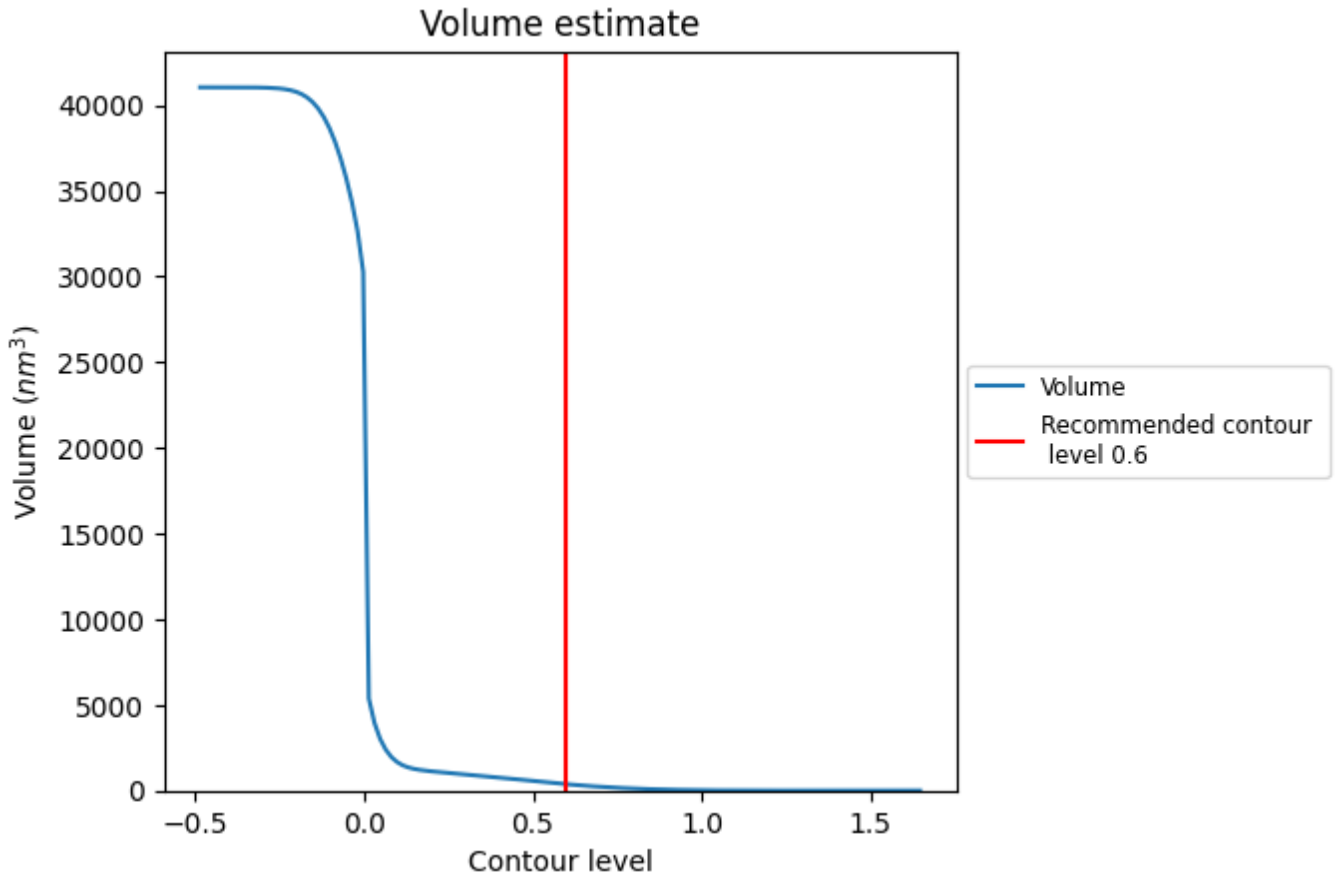
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

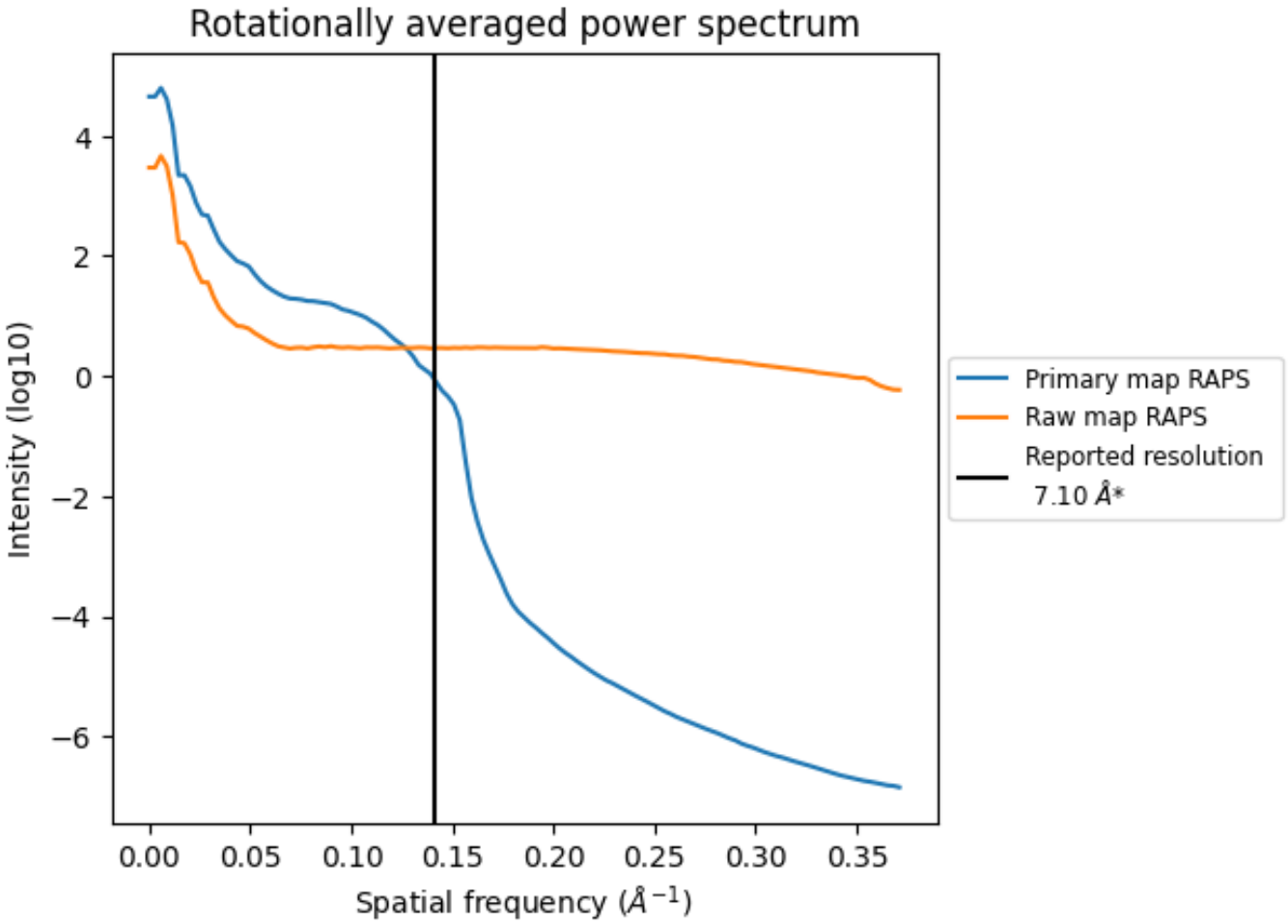
7.2 Volume estimate



The volume at the recommended contour level is 372 nm^3; this corresponds to an approximate mass of 336 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)

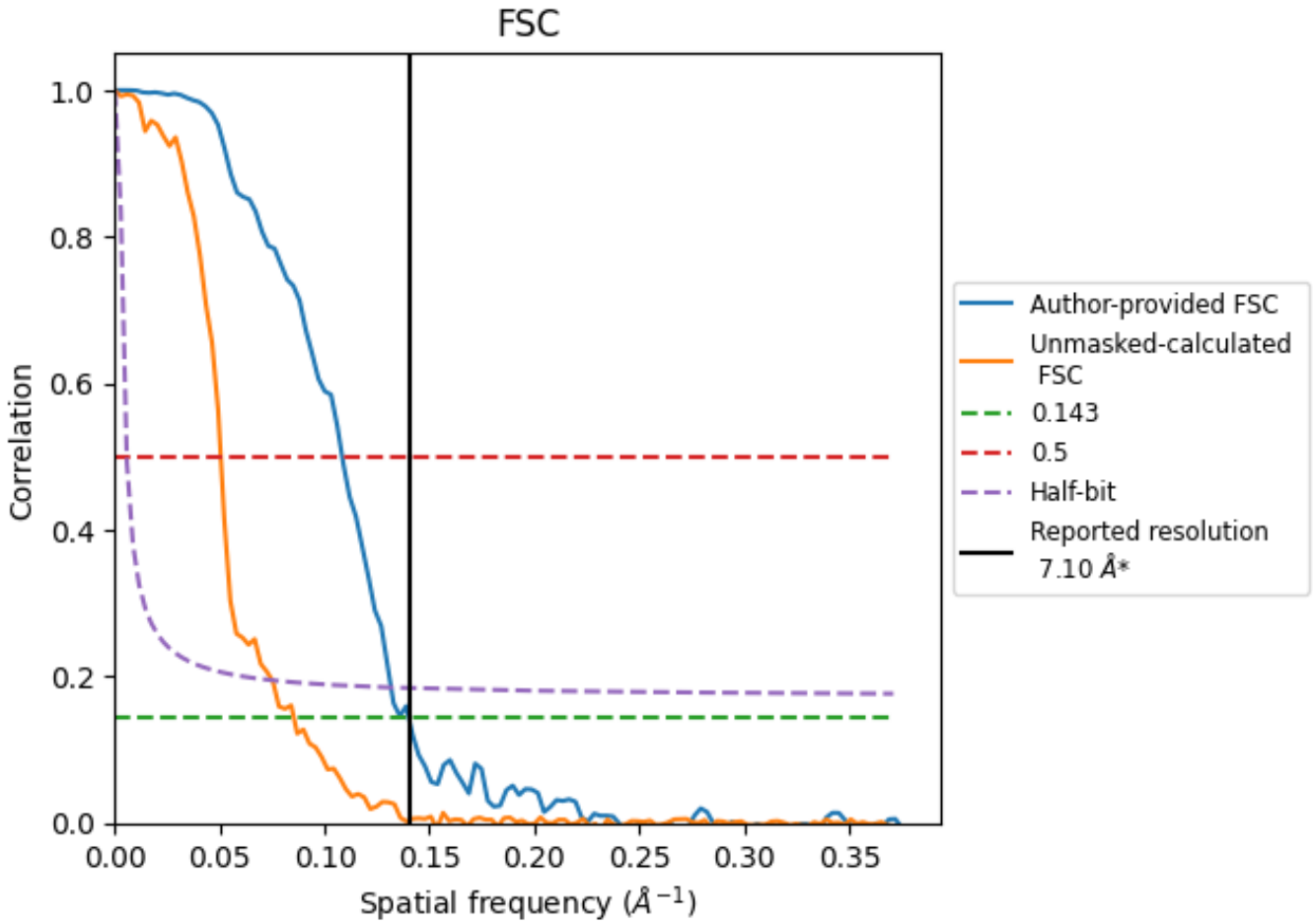


*Reported resolution corresponds to spatial frequency of 0.141 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.141 Å^{-1}

8.2 Resolution estimates (i)

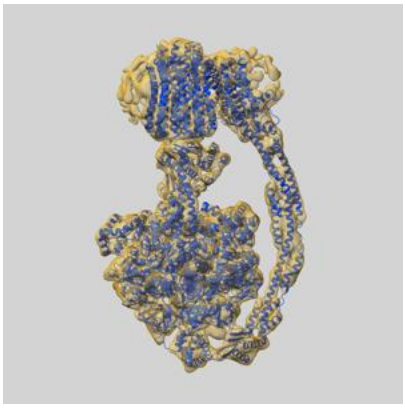
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.10	-	-
Author-provided FSC curve	7.13	9.23	7.59
Unmasked-calculated*	11.71	19.80	13.32

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

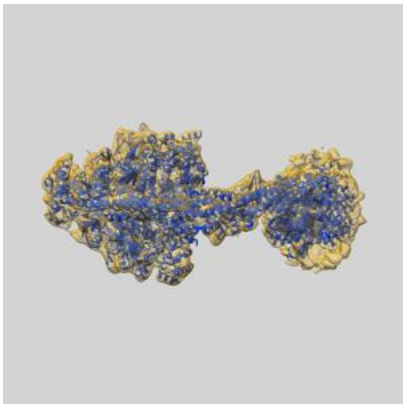
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25949 and PDB model 7TK1. Per-residue inclusion information can be found in section 3 on page 7.

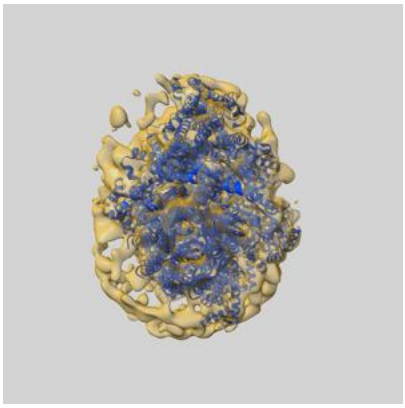
9.1 Map-model overlay



X



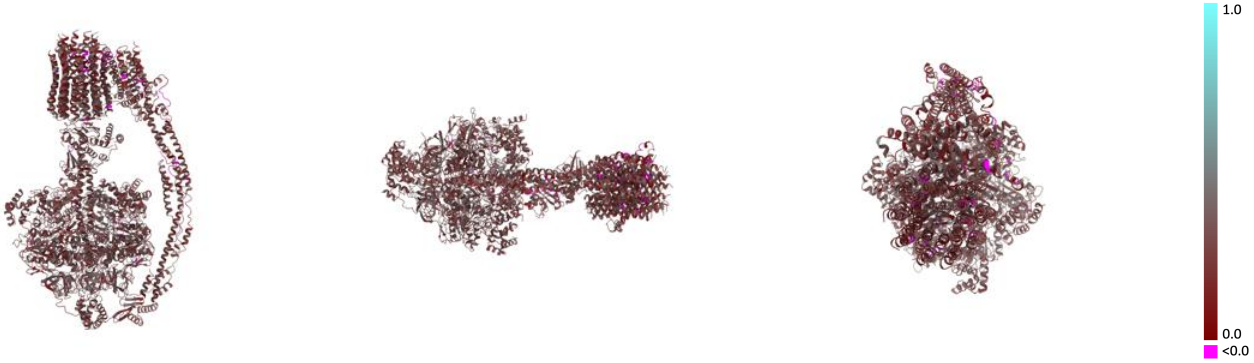
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

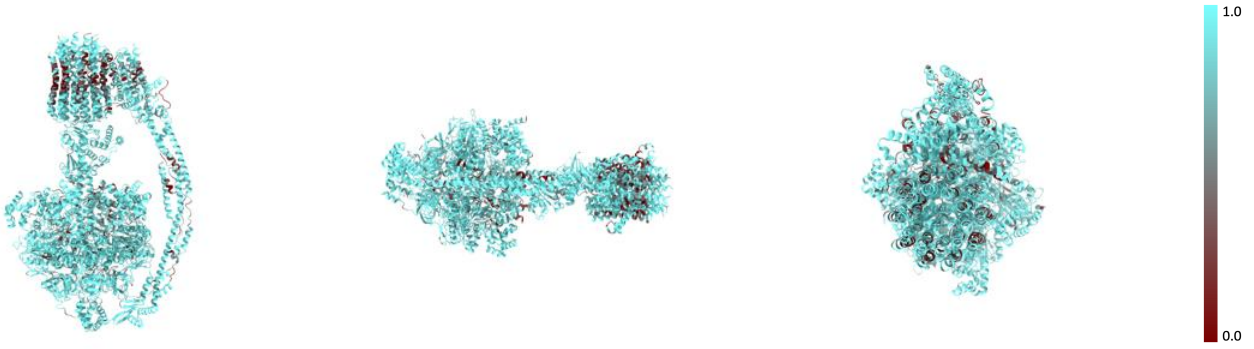
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

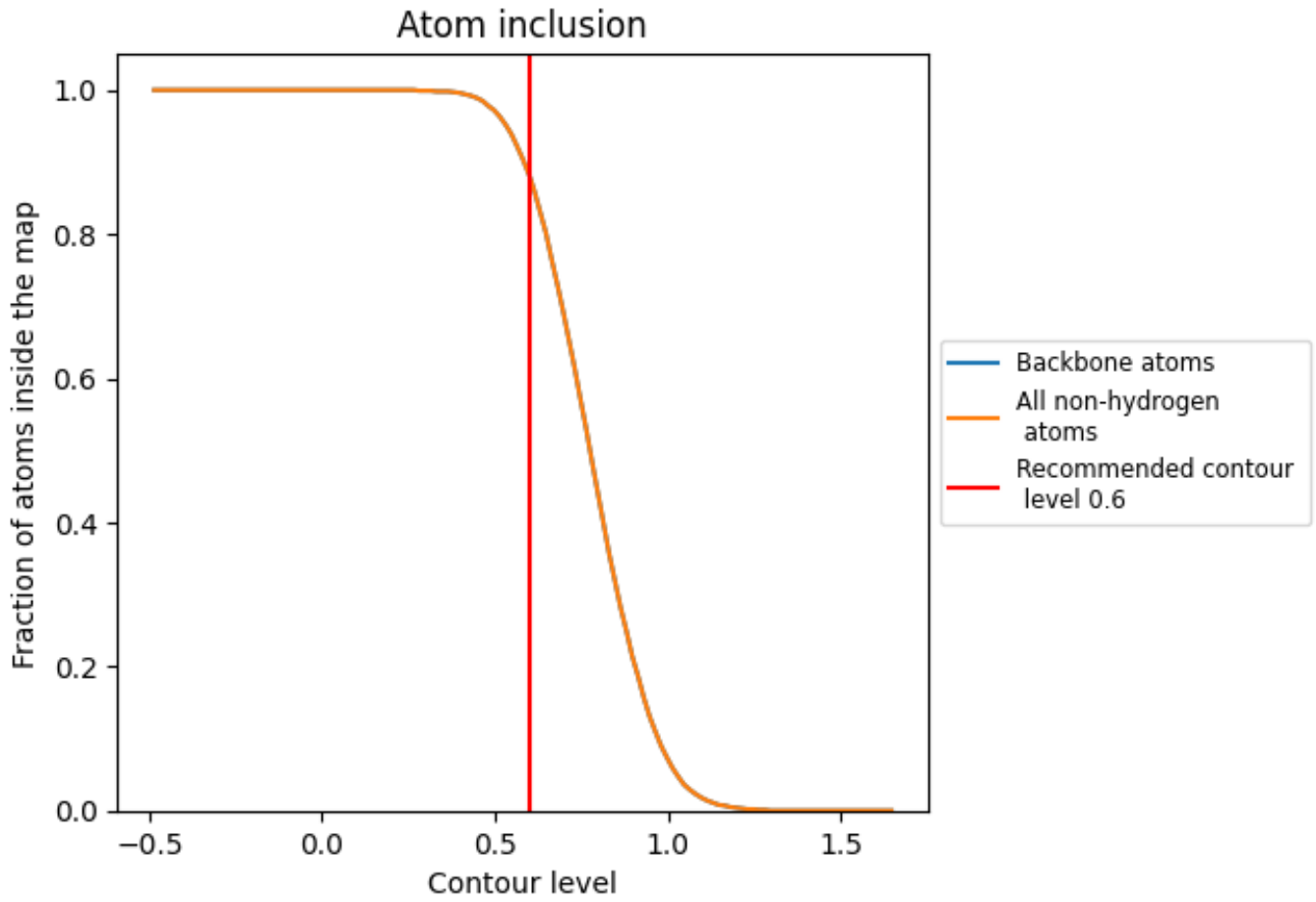
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.2790
0	0.7800	0.2220
1	0.7370	0.2220
2	0.7970	0.2530
3	0.7900	0.2500
4	0.7370	0.2480
5	0.8230	0.2250
6	0.8010	0.2140
7	0.6610	0.2380
8	0.7900	0.2430
9	0.7300	0.2280
A	0.9220	0.3010
B	0.9250	0.2960
C	0.9280	0.2970
D	0.8480	0.2890
E	0.9250	0.2960
F	0.9460	0.3010
G	0.9260	0.2930
H	0.9520	0.2980
I	0.9640	0.2990
O	0.9710	0.2980
T	0.7980	0.2470
U	0.9350	0.2740
V	0.8180	0.2470
W	0.7030	0.1620
X	0.6610	0.2420
Y	0.8110	0.2540
Z	0.8390	0.2440