



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:25 AM UTC

PDB ID : 7TK3 / pdb_00007tk3
EMDB ID : EMD-25955
Title : Yeast ATP synthase State 1binding(b) with 10 mM ATP backbone model
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2022-01-17
Resolution : 6.30 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:

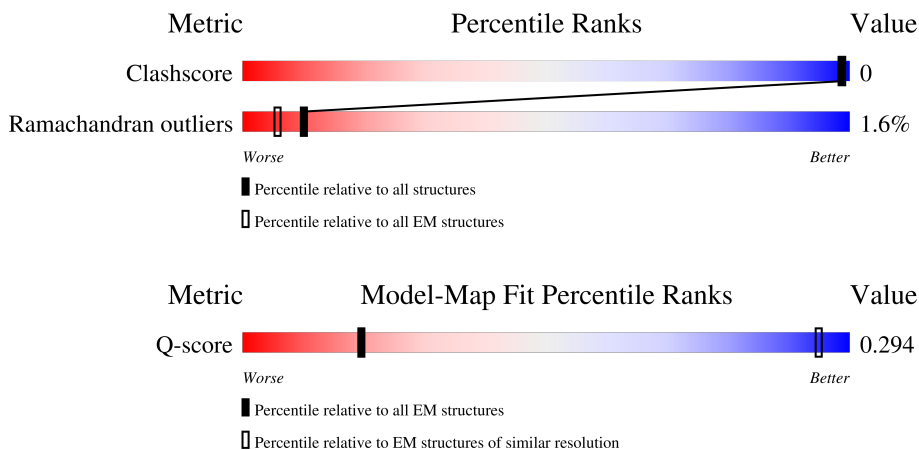
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.30 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	550 (5.80 - 6.80)

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	 41% 91% 8% .
1	1	76	 28% 93% 5% .
1	2	76	 32% 95% . .
1	3	76	 26% 91% 5% . .
1	4	76	 16% 93% 5% .

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Mol	Chain	Length	Quality of chain
1	5	76	25% 91% 8%
1	6	76	16% 91% 7%
1	7	76	17% 87% 9%
1	8	76	18% 91% 8%
1	9	76	30% 87% 11%
2	A	510	89% 9%
2	B	510	90% 8%
2	C	510	90% 7%
3	D	478	90% 8%
3	E	478	88% 10%
3	F	478	88% 10%
4	G	278	86% 10% 5%
5	H	138	13% 74% 12% 13%
6	I	61	11% 79% 21%
7	O	195	85% 11%
8	T	249	5% 86% 10%
9	U	209	74% 26%
10	V	173	6% 90% 9%
11	W	95	12% 76% 14% 11%
12	X	92	18% 65% 33%
13	Y	59	7% 59% 37%
14	Z	48	8% 96%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 20228 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit 9, mitochondrial.

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

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

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

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

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

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

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

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

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

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

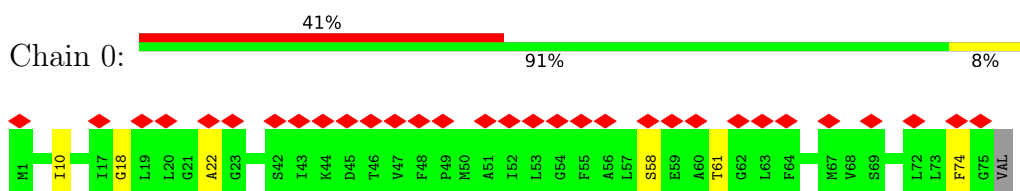
- Molecule 14 is a protein called ATP synthase protein 8.

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

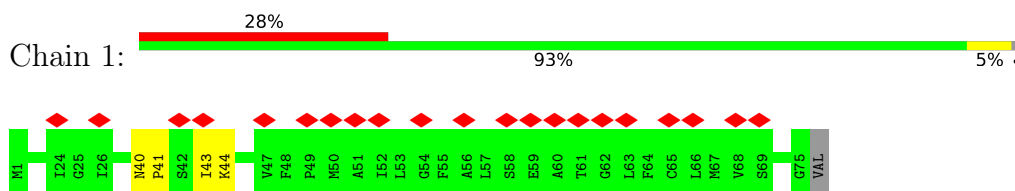
3 Residue-property plots [i](#)

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

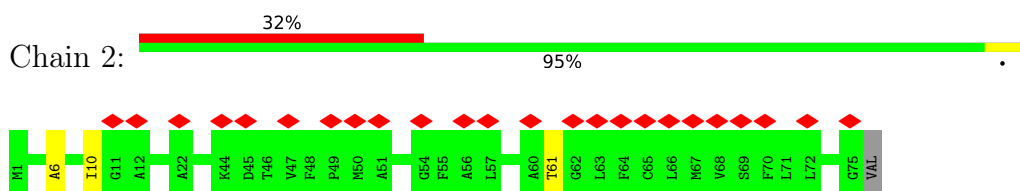
- Molecule 1: ATP synthase subunit 9, mitochondrial



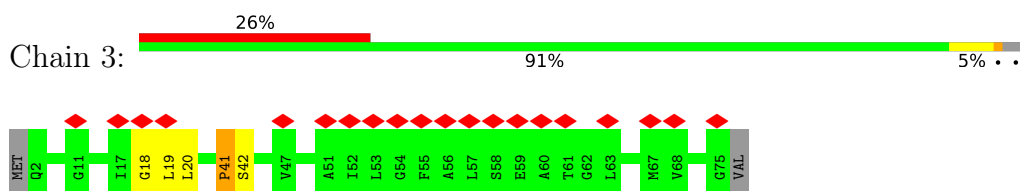
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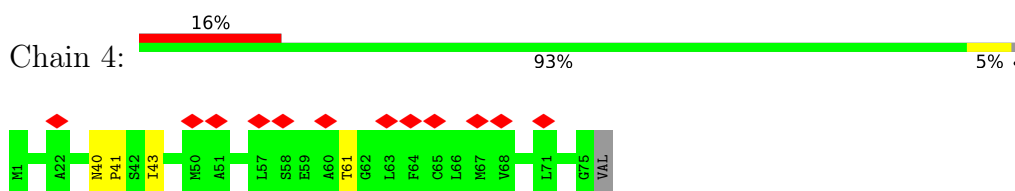
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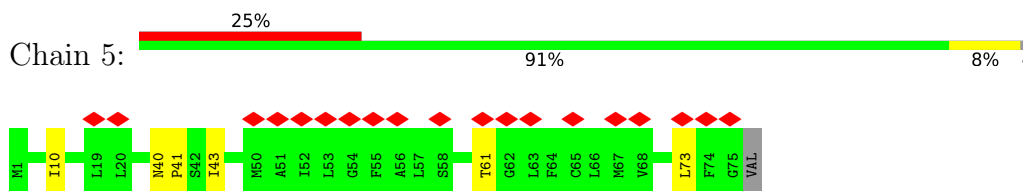
- Molecule 1: ATP synthase subunit 9, mitochondrial



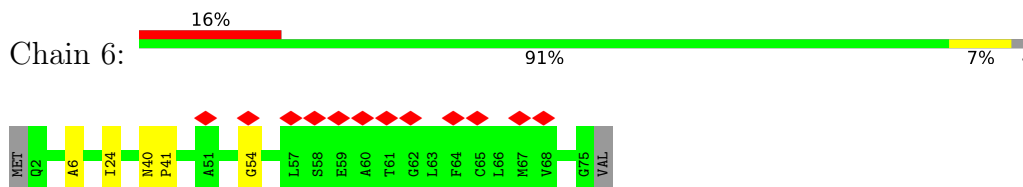
- Molecule 1: ATP synthase subunit 9, mitochondrial



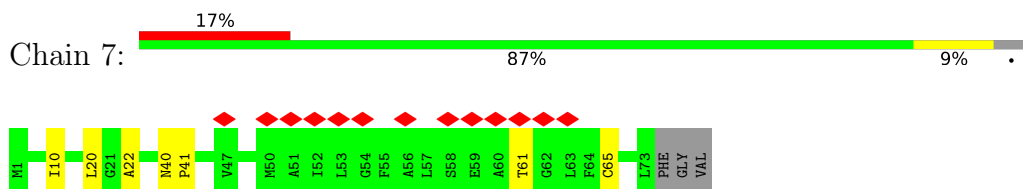
- Molecule 1: ATP synthase subunit 9, mitochondrial



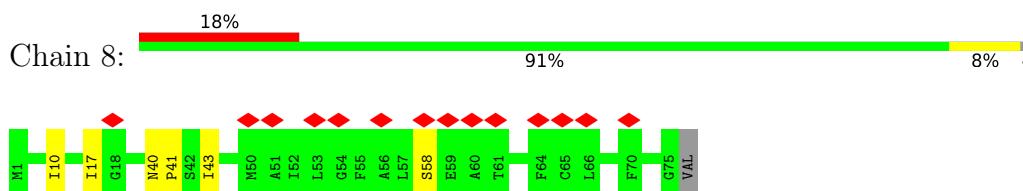
- Molecule 1: ATP synthase subunit 9, mitochondrial



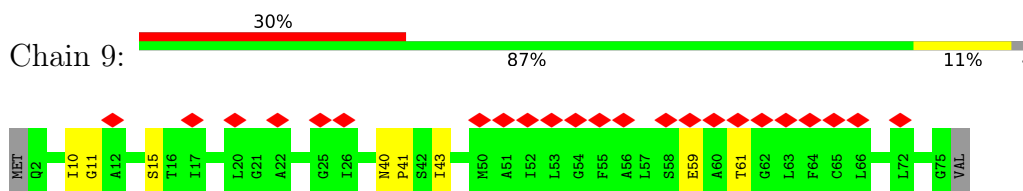
- Molecule 1: ATP synthase subunit 9, mitochondrial



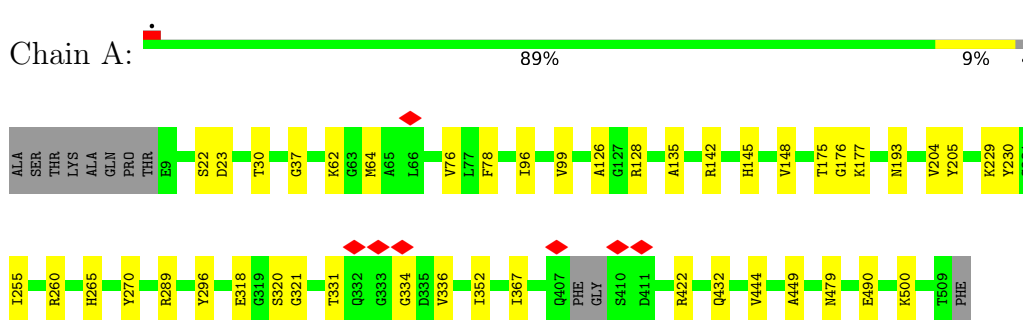
- Molecule 1: ATP synthase subunit 9, mitochondrial



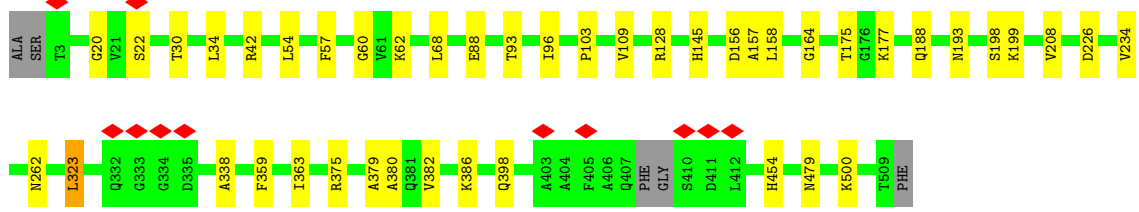
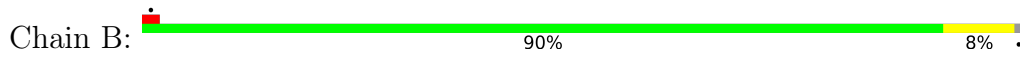
- Molecule 1: ATP synthase subunit 9, mitochondrial



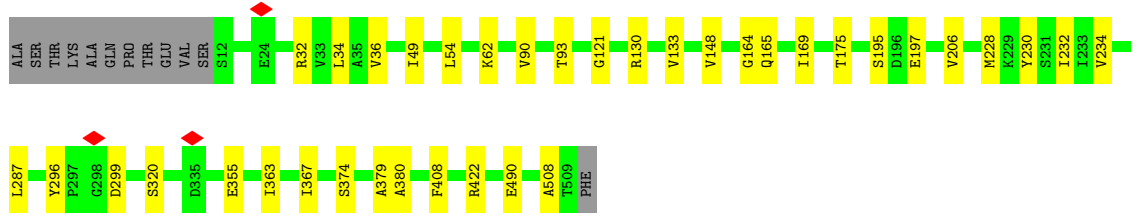
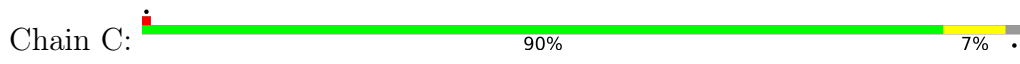
- Molecule 2: ATP synthase subunit alpha



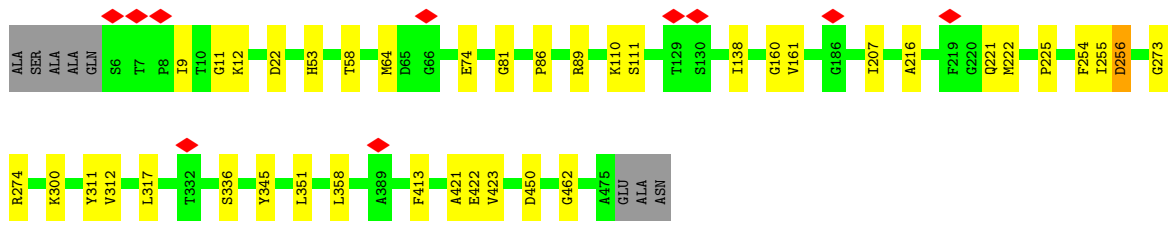
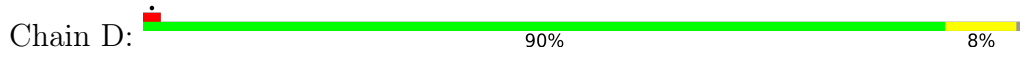
- Molecule 2: ATP synthase subunit alpha



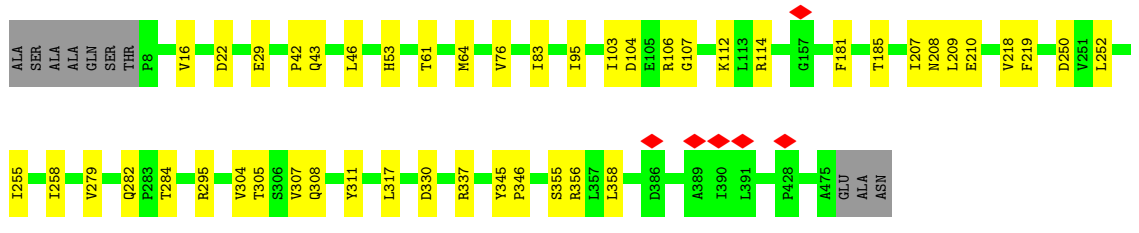
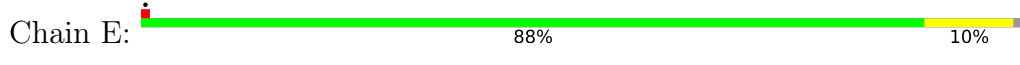
• Molecule 2: ATP synthase subunit alpha



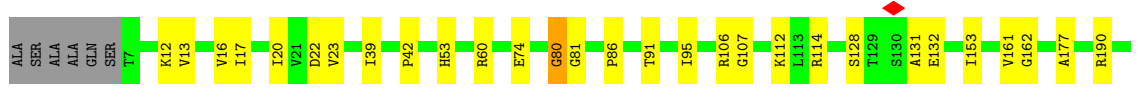
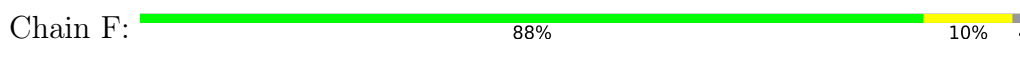
• Molecule 3: ATP synthase subunit beta



• Molecule 3: ATP synthase subunit beta

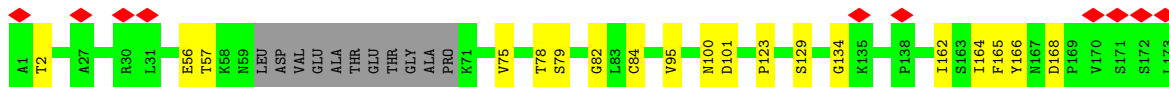
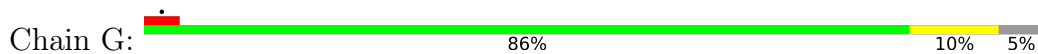


• Molecule 3: ATP synthase subunit beta

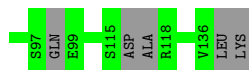
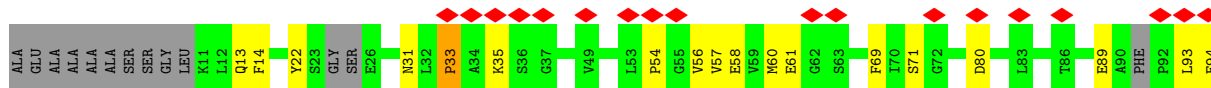
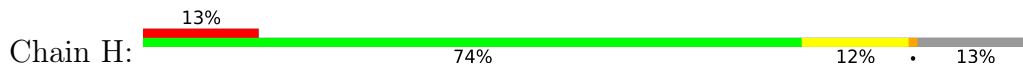




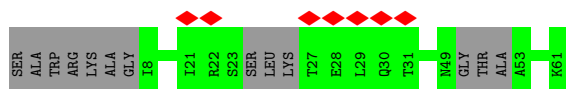
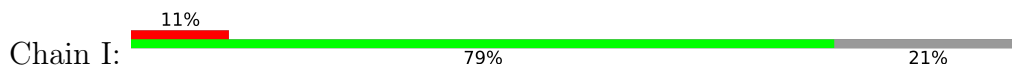
• Molecule 4: ATP synthase subunit gamma



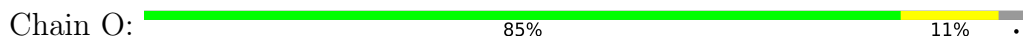
• Molecule 5: ATP synthase subunit delta



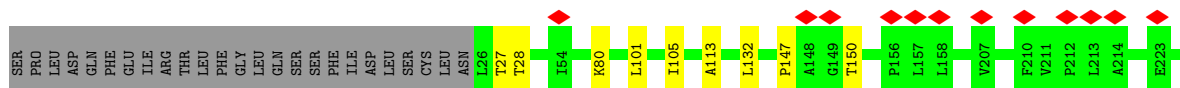
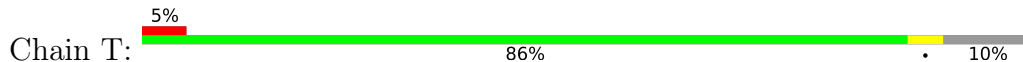
• Molecule 6: ATP synthase subunit epsilon



• Molecule 7: ATP synthase subunit 5

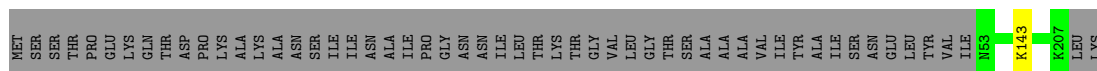


• Molecule 8: ATP synthase subunit a




- Molecule 9: ATP synthase subunit 4

Chain U:  74% 26%




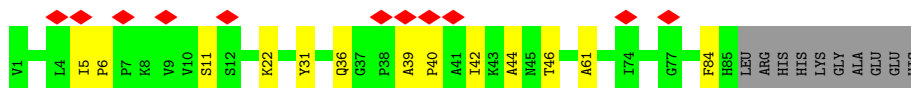
- Molecule 10: ATP synthase subunit d

Chain V:  6% 90% 9%



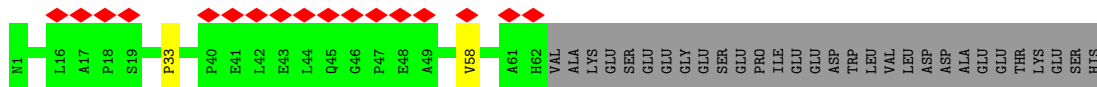
- Molecule 11: ATP synthase subunit f

Chain W:  12% 76% 14% 11%



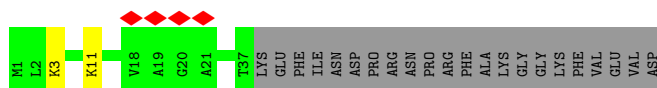
- Molecule 12: ATP synthase subunit H

Chain X:  18% 65% 33%



- Molecule 13: ATP synthase subunit J

Chain Y:  7% 59% 37%



- Molecule 14: ATP synthase protein 8

Chain Z:  8% 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8184	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	2.152	Depositor
Minimum map value	-0.664	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.666	Depositor
Map size (\AA)	344.96, 344.96, 344.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3475, 1.3475, 1.3475	Depositor

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	1.20	0/299	2.24	11/372 (3.0%)
1	1	1.21	0/299	2.01	3/372 (0.8%)
1	2	1.20	0/299	2.15	6/372 (1.6%)
1	3	1.23	0/295	2.06	7/367 (1.9%)
1	4	1.23	0/299	2.07	4/372 (1.1%)
1	5	1.23	0/299	2.16	7/372 (1.9%)
1	6	1.22	0/295	2.19	6/367 (1.6%)
1	7	1.24	0/291	2.17	10/362 (2.8%)
1	8	1.20	0/299	2.16	8/372 (2.2%)
1	9	1.19	0/295	2.19	12/367 (3.3%)
2	A	1.57	1/1994 (0.1%)	1.85	51/2489 (2.0%)
2	B	1.56	1/2018 (0.0%)	1.83	36/2519 (1.4%)
2	C	1.57	0/1991	1.79	34/2487 (1.4%)
3	D	1.56	1/1879 (0.1%)	1.84	37/2347 (1.6%)
3	E	1.59	0/1871	1.85	42/2337 (1.8%)
3	F	1.59	0/1875	1.86	49/2342 (2.1%)
4	G	1.47	0/1058	2.00	27/1319 (2.0%)
5	H	1.53	0/475	1.87	16/585 (2.7%)
6	I	1.37	0/190	1.89	0/231
7	O	1.58	0/747	1.88	22/932 (2.4%)
8	T	1.32	0/896	1.66	11/1117 (1.0%)
9	U	1.33	0/619	1.73	2/772 (0.3%)
10	V	1.40	0/684	1.91	14/852 (1.6%)
11	W	1.29	0/339	1.87	5/422 (1.2%)
12	X	1.37	0/247	2.03	3/307 (1.0%)
13	Y	1.30	0/147	1.60	0/182
14	Z	1.28	0/192	1.71	2/237 (0.8%)
All	All	1.48	3/20192 (0.0%)	1.89	425/25172 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	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
3	F	0	1
5	H	0	1
All	All	0	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	34	LEU	CA-C	-6.75	1.49	1.53
3	D	11	GLY	CA-C	-5.72	1.47	1.52
2	A	321	GLY	CA-C	-5.64	1.46	1.52

All (425) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	162	GLY	N-CA-C	-9.26	102.21	115.27
4	G	204	ASN	CA-C-N	9.24	126.06	120.24
4	G	204	ASN	C-N-CA	9.24	126.06	120.24
11	W	6	PRO	N-CA-C	9.14	121.85	110.70
3	F	161	VAL	N-CA-C	-9.10	102.31	111.77
7	O	55	HIS	N-CA-C	-8.91	102.20	113.43
2	A	148	VAL	N-CA-C	-8.90	96.60	108.35
3	F	95	ILE	N-CA-C	-8.85	95.79	108.17
7	O	180	ILE	N-CA-C	-8.43	102.65	111.58
5	H	61	GLU	N-CA-C	-8.31	94.71	108.34
7	O	176	VAL	N-CA-C	-8.07	95.83	107.77
3	E	210	GLU	N-CA-C	-8.00	102.58	113.30
2	B	175	THR	N-CA-C	-7.96	104.01	112.93
2	A	296	TYR	N-CA-C	-7.96	96.67	109.40
8	T	80	LYS	N-CA-C	-7.87	103.49	113.72
2	B	193	ASN	N-CA-C	-7.73	103.85	113.28
3	F	17	ILE	N-CA-C	-7.71	95.97	107.37
3	E	103	ILE	N-CA-C	-7.70	105.35	112.43
2	A	99	VAL	N-CA-C	-7.67	102.90	109.19
2	A	230	TYR	N-CA-C	-7.55	104.97	114.56
5	H	56	VAL	N-CA-C	-7.52	97.58	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	305	THR	N-CA-C	-7.50	97.22	108.99
2	B	158	LEU	N-CA-C	-7.41	105.15	114.56
10	V	164	LYS	N-CA-C	-7.31	104.61	113.97
2	C	374	SER	N-CA-C	-7.27	95.07	108.02
1	4	43	ILE	CA-C-N	7.23	130.94	120.38
1	4	43	ILE	C-N-CA	7.23	130.94	120.38
3	D	312	VAL	N-CA-C	-7.18	99.92	107.60
3	E	43	GLN	N-CA-C	-7.17	104.55	112.72
2	B	479	ASN	N-CA-C	-7.14	104.30	113.16
2	C	175	THR	N-CA-C	-7.14	104.93	112.93
2	C	408	PHE	N-CA-C	-7.13	104.05	112.89
2	A	479	ASN	N-CA-C	-7.12	104.60	113.28
2	C	234	VAL	N-CA-C	-7.11	98.22	108.17
2	A	175	THR	N-CA-C	-7.05	105.03	112.93
12	X	58	VAL	N-CA-C	-7.04	106.14	112.90
3	E	304	VAL	N-CA-C	-7.01	102.41	110.05
7	O	164	LYS	N-CA-C	-6.96	97.55	108.90
2	C	422	ARG	CA-C-N	6.96	127.70	119.98
2	C	422	ARG	C-N-CA	6.96	127.70	119.98
3	F	255	ILE	N-CA-C	-6.81	98.23	108.17
2	B	398	GLN	N-CA-C	-6.79	105.13	113.41
1	2	10	ILE	CA-C-N	6.79	127.51	119.98
1	2	10	ILE	C-N-CA	6.79	127.51	119.98
2	B	96	ILE	N-CA-C	-6.78	102.55	110.21
3	D	423	VAL	N-CA-C	-6.77	106.89	113.53
3	F	53	HIS	N-CA-C	-6.77	98.18	109.07
2	A	232	ILE	N-CA-C	-6.75	98.45	108.45
7	O	101	PHE	N-CA-C	-6.73	103.98	112.93
2	B	42	ARG	N-CA-C	-6.72	97.41	108.76
4	G	197	PHE	N-CA-C	-6.72	98.82	109.23
2	B	386	LYS	N-CA-C	-6.71	104.74	113.12
4	G	180	LYS	N-CA-C	-6.70	102.19	108.22
2	C	93	THR	N-CA-C	-6.69	104.06	111.36
10	V	163	TYR	N-CA-C	-6.69	104.87	113.16
2	A	422	ARG	CA-C-N	6.68	127.39	119.98
2	A	422	ARG	C-N-CA	6.68	127.39	119.98
3	E	356	ARG	N-CA-C	-6.66	105.31	113.50
3	D	317	LEU	N-CA-C	-6.62	104.82	113.17
2	A	177	LYS	N-CA-C	-6.62	104.14	111.36
1	7	10	ILE	CA-C-N	6.61	127.32	119.98
1	7	10	ILE	C-N-CA	6.61	127.32	119.98
1	1	43	ILE	CA-C-N	6.60	130.01	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	43	ILE	C-N-CA	6.60	130.01	120.38
2	A	30	THR	N-CA-C	-6.58	100.21	109.69
7	O	192	GLU	N-CA-C	-6.58	104.85	114.39
3	E	42	PRO	N-CA-C	-6.57	107.85	114.68
4	G	84	CYS	N-CA-C	-6.55	105.17	112.57
3	D	58	THR	N-CA-C	-6.53	97.63	108.34
3	F	207	ILE	N-CA-C	-6.50	99.07	108.17
2	C	232	ILE	N-CA-C	-6.44	99.21	108.48
3	E	208	ASN	N-CA-C	-6.43	97.07	108.13
3	E	307	VAL	N-CA-C	-6.42	99.18	108.17
2	B	20	GLY	N-CA-C	-6.41	98.00	113.18
3	E	308	GLN	N-CA-C	-6.40	99.61	109.52
3	E	258	ILE	N-CA-C	-6.39	105.36	113.22
3	F	91	THR	N-CA-C	-6.38	105.66	113.50
4	G	75	VAL	N-CA-C	-6.36	98.49	108.86
2	C	287	LEU	N-CA-C	-6.36	104.78	113.30
3	D	89	ARG	N-CA-C	-6.36	105.16	113.17
7	O	58	LEU	N-CA-C	-6.34	105.12	112.92
2	B	62	LYS	N-CA-C	-6.32	99.51	109.50
7	O	84	TYR	N-CA-C	-6.30	104.29	112.23
3	E	207	ILE	N-CA-C	-6.26	99.35	108.11
1	6	54	GLY	CA-C-N	6.25	128.57	120.44
1	6	54	GLY	C-N-CA	6.25	128.57	120.44
14	Z	3	GLN	N-CA-C	-6.24	105.61	113.72
2	B	359	PHE	CA-C-N	6.22	129.13	120.29
2	B	359	PHE	C-N-CA	6.22	129.13	120.29
2	C	296	TYR	N-CA-C	-6.21	101.95	109.72
2	C	508	ALA	N-CA-C	-6.21	100.20	109.83
3	E	64	MET	N-CA-C	-6.20	104.68	112.93
8	T	105	ILE	N-CA-C	-6.20	100.24	107.61
2	B	60	GLY	N-CA-C	-6.19	107.32	114.69
7	O	120	LYS	N-CA-C	-6.17	100.38	109.81
2	B	177	LYS	CA-C-N	6.15	129.14	120.28
2	B	177	LYS	C-N-CA	6.15	129.14	120.28
2	B	93	THR	N-CA-C	-6.13	104.68	111.36
2	A	193	ASN	CA-C-N	6.10	125.78	119.92
2	A	193	ASN	C-N-CA	6.10	125.78	119.92
2	C	133	VAL	N-CA-C	-6.10	99.43	108.45
1	0	10	ILE	CA-C-N	6.09	127.75	120.14
1	0	10	ILE	C-N-CA	6.09	127.75	120.14
3	E	46	LEU	N-CA-C	-6.09	98.46	108.76
10	V	47	GLN	N-CA-C	-6.08	106.53	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	154	LYS	N-CA-C	-6.06	99.53	109.40
3	F	336	SER	CA-C-N	6.05	128.39	120.28
3	F	336	SER	C-N-CA	6.05	128.39	120.28
2	A	78	PHE	N-CA-C	-6.05	104.25	111.69
8	T	150	THR	N-CA-C	-6.04	101.20	108.14
3	F	106	ARG	N-CA-C	-6.04	106.17	112.93
2	B	54	LEU	N-CA-C	-6.03	99.41	109.24
3	D	53	HIS	N-CA-C	-6.00	99.61	109.40
3	D	311	TYR	N-CA-C	-5.99	99.14	108.90
3	E	218	VAL	N-CA-C	-5.98	98.92	107.77
3	E	345	TYR	N-CA-C	-5.97	95.49	108.74
2	B	234	VAL	N-CA-C	-5.96	99.84	108.89
3	E	95	ILE	N-CA-C	-5.95	100.01	108.58
2	C	169	ILE	N-CA-C	-5.94	99.32	107.99
2	C	363	ILE	N-CA-C	-5.92	98.50	107.73
3	D	12	LYS	N-CA-C	-5.91	99.27	108.90
3	E	250	ASP	N-CA-C	-5.91	99.56	109.07
4	G	100	ASN	N-CA-C	-5.91	106.11	113.38
11	W	61	ALA	N-CA-C	-5.89	105.75	113.17
2	A	352	ILE	N-CA-C	-5.88	99.65	108.12
2	A	296	TYR	CA-C-N	5.88	125.89	119.89
2	A	296	TYR	C-N-CA	5.88	125.89	119.89
7	O	167	LEU	N-CA-C	-5.86	100.16	109.07
1	5	10	ILE	CA-C-N	5.86	126.49	119.98
1	5	10	ILE	C-N-CA	5.86	126.49	119.98
2	B	128	ARG	N-CA-C	-5.83	100.28	109.50
3	E	29	GLU	N-CA-C	-5.83	101.55	109.54
3	F	39	ILE	N-CA-C	-5.83	100.00	108.17
5	H	71	SER	CA-C-N	5.83	129.90	121.44
5	H	71	SER	C-N-CA	5.83	129.90	121.44
3	F	23	VAL	N-CA-C	-5.83	99.89	108.99
5	H	57	VAL	N-CA-C	-5.83	99.36	108.86
2	C	148	VAL	N-CA-C	-5.82	99.67	108.17
1	0	18	GLY	CA-C-N	5.82	128.66	120.28
1	0	18	GLY	C-N-CA	5.82	128.66	120.28
2	B	57	PHE	N-CA-C	-5.80	101.93	110.52
7	O	83	GLY	N-CA-C	-5.80	106.71	114.25
3	F	353	SER	N-CA-C	-5.79	99.90	108.99
1	4	61	THR	CA-C-N	5.78	126.40	119.98
1	4	61	THR	C-N-CA	5.78	126.40	119.98
2	C	367	ILE	N-CA-C	-5.78	100.08	108.17
1	3	19	LEU	CA-C-N	5.77	128.28	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	19	LEU	C-N-CA	5.77	128.28	120.38
4	G	57	THR	N-CA-C	-5.77	106.00	113.16
3	D	254	PHE	N-CA-C	-5.77	99.26	109.06
1	5	73	LEU	N-CA-C	5.76	117.37	111.14
3	E	337	ARG	N-CA-C	-5.76	106.09	113.23
1	8	43	ILE	CA-C-N	5.76	128.27	120.38
1	8	43	ILE	C-N-CA	5.76	128.27	120.38
2	B	88	GLU	N-CA-C	-5.75	101.50	110.42
3	D	207	ILE	N-CA-C	-5.75	98.35	107.15
9	U	143	LYS	CA-C-N	5.75	127.81	120.56
9	U	143	LYS	C-N-CA	5.75	127.81	120.56
3	D	81	GLY	CA-C-N	5.75	125.76	119.90
3	D	81	GLY	C-N-CA	5.75	125.76	119.90
3	D	413	PHE	N-CA-C	-5.75	106.27	113.28
5	H	14	PHE	N-CA-C	-5.74	98.92	108.34
3	E	209	LEU	N-CA-C	-5.74	105.61	113.30
3	E	106	ARG	N-CA-C	-5.73	106.09	112.57
3	D	422	GLU	N-CA-C	-5.73	106.06	113.16
2	B	198	SER	N-CA-C	-5.72	105.96	113.17
1	7	20	LEU	CA-C-N	5.70	126.31	119.98
1	7	20	LEU	C-N-CA	5.70	126.31	119.98
2	A	334	GLY	N-CA-C	-5.69	107.34	115.64
4	G	101	ASP	N-CA-C	-5.68	106.39	113.38
3	F	420	VAL	N-CA-C	-5.67	107.45	112.90
2	A	62	LYS	N-CA-C	-5.67	100.93	109.95
2	A	336	VAL	N-CA-C	-5.67	105.30	113.07
2	C	90	VAL	N-CA-C	-5.67	100.01	108.46
2	A	289	ARG	N-CA-C	-5.65	102.94	110.07
3	E	114	ARG	N-CA-C	-5.65	100.57	109.50
1	9	10	ILE	CA-C-N	5.65	126.25	119.98
1	9	10	ILE	C-N-CA	5.65	126.25	119.98
4	G	185	ALA	CA-C-N	5.65	127.85	120.28
4	G	185	ALA	C-N-CA	5.65	127.85	120.28
10	V	18	SER	CA-C-N	5.63	128.10	120.38
10	V	18	SER	C-N-CA	5.63	128.10	120.38
3	E	317	LEU	N-CA-C	-5.63	106.41	113.28
2	B	500	LYS	CA-C-N	5.62	127.75	120.44
2	B	500	LYS	C-N-CA	5.62	127.75	120.44
1	6	6	ALA	CA-C-N	5.62	127.81	120.28
1	6	6	ALA	C-N-CA	5.62	127.81	120.28
2	C	206	VAL	N-CA-C	-5.62	100.24	108.11
2	A	318	GLU	N-CA-C	-5.61	106.24	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	114	ARG	N-CA-C	-5.61	100.05	109.07
1	0	58	SER	CA-C-N	5.60	127.78	120.28
1	0	58	SER	C-N-CA	5.60	127.78	120.28
2	A	331	THR	CA-C-N	5.59	127.77	120.28
2	A	331	THR	C-N-CA	5.59	127.77	120.28
2	A	64	MET	N-CA-C	-5.58	100.87	109.52
2	A	444	VAL	CA-C-O	-5.58	114.11	118.85
7	O	8	PRO	CA-C-N	5.58	126.81	119.84
7	O	8	PRO	C-N-CA	5.58	126.81	119.84
3	F	12	LYS	N-CA-C	-5.57	100.88	109.52
1	3	20	LEU	CA-C-N	5.57	126.13	120.00
1	3	20	LEU	C-N-CA	5.57	126.13	120.00
8	T	28	THR	CA-C-N	5.57	127.74	120.28
8	T	28	THR	C-N-CA	5.57	127.74	120.28
2	A	321	GLY	N-CA-C	-5.56	102.84	111.12
2	B	30	THR	N-CA-C	-5.55	100.91	109.52
8	T	113	ALA	N-CA-C	-5.55	105.86	113.30
1	2	61	THR	CA-C-N	5.55	126.10	120.00
1	2	61	THR	C-N-CA	5.55	126.10	120.00
2	A	265	HIS	N-CA-C	-5.55	101.08	109.85
2	B	363	ILE	N-CA-C	-5.55	99.56	107.77
3	D	274	ARG	N-CA-C	-5.55	99.48	108.41
2	B	68	LEU	N-CA-C	-5.55	99.69	108.73
1	9	43	ILE	CA-C-N	5.54	127.71	120.28
1	9	43	ILE	C-N-CA	5.54	127.71	120.28
3	F	190	ARG	N-CA-C	-5.54	100.16	108.96
4	G	164	ILE	N-CA-C	-5.54	99.84	108.86
2	C	380	ALA	N-CA-C	-5.53	103.70	110.61
8	T	101	LEU	N-CA-C	-5.53	105.65	112.72
3	F	218	VAL	N-CA-C	-5.52	100.17	108.12
4	G	129	SER	N-CA-C	-5.51	100.69	109.07
3	D	421	ALA	N-CA-C	-5.51	103.83	110.88
4	G	201	THR	N-CA-C	-5.51	104.41	113.50
1	1	44	LYS	N-CA-C	5.50	118.79	111.75
1	5	61	THR	CA-C-N	5.50	126.09	119.98
1	5	61	THR	C-N-CA	5.50	126.09	119.98
2	A	449	ALA	CA-C-N	5.49	126.04	120.00
2	A	449	ALA	C-N-CA	5.49	126.04	120.00
1	8	10	ILE	CA-C-N	5.49	126.08	119.98
1	8	10	ILE	C-N-CA	5.49	126.08	119.98
4	G	2	THR	N-CA-C	-5.49	105.21	111.14
10	V	81	VAL	N-CA-C	-5.48	97.93	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	13	PHE	CA-C-N	5.48	125.18	119.92
7	O	13	PHE	C-N-CA	5.48	125.18	119.92
1	0	74	PHE	N-CA-C	-5.47	104.86	112.30
2	C	355	GLU	CA-C-N	5.47	127.61	120.28
2	C	355	GLU	C-N-CA	5.47	127.61	120.28
1	6	24	ILE	CA-C-N	5.47	126.01	119.94
1	6	24	ILE	C-N-CA	5.47	126.01	119.94
3	F	205	GLY	CA-C-N	5.46	127.94	120.46
3	F	205	GLY	C-N-CA	5.46	127.94	120.46
3	E	185	THR	N-CA-C	-5.46	100.28	109.07
10	V	167	PHE	N-CA-C	-5.46	101.06	109.52
2	B	188	GLN	N-CA-C	-5.45	106.41	112.57
2	C	62	LYS	N-CA-C	-5.45	100.52	109.40
2	A	490	GLU	N-CA-C	-5.44	101.02	109.24
3	D	138	ILE	N-CA-C	-5.44	99.32	107.37
2	A	270	TYR	N-CA-C	-5.44	99.87	108.73
2	C	197	GLU	N-CA-C	-5.44	99.22	110.80
8	T	132	LEU	CA-C-N	5.44	125.98	120.00
8	T	132	LEU	C-N-CA	5.44	125.98	120.00
10	V	35	ARG	CA-C-N	5.43	127.50	120.44
10	V	35	ARG	C-N-CA	5.43	127.50	120.44
1	7	61	THR	CA-C-N	5.42	126.00	119.98
1	7	61	THR	C-N-CA	5.42	126.00	119.98
3	F	258	ILE	N-CA-C	-5.42	107.47	112.83
11	W	84	PHE	N-CA-C	-5.42	106.04	113.30
3	F	213	SER	N-CA-C	-5.41	99.62	108.76
2	B	34	LEU	N-CA-C	-5.41	103.56	108.75
3	E	255	ILE	N-CA-C	-5.40	100.05	108.86
3	D	74	GLU	CA-C-N	5.40	128.38	120.71
3	D	74	GLU	C-N-CA	5.40	128.38	120.71
4	G	166	TYR	N-CA-C	-5.40	100.27	107.88
3	F	252	LEU	N-CA-C	-5.40	102.05	110.42
2	C	490	GLU	N-CA-C	-5.40	100.52	108.99
1	0	61	THR	CA-C-N	5.38	125.95	119.98
1	0	61	THR	C-N-CA	5.38	125.95	119.98
3	D	255	ILE	N-CA-C	-5.37	100.10	108.86
2	A	76	VAL	N-CA-C	-5.36	100.03	107.80
5	H	60	MET	N-CA-C	-5.36	99.71	108.76
1	9	15	SER	CA-C-N	5.36	127.99	120.28
1	9	15	SER	C-N-CA	5.36	127.99	120.28
2	B	375	ARG	N-CA-C	-5.35	106.62	112.72
3	E	284	THR	N-CA-C	-5.35	106.53	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	355	SER	N-CA-C	-5.34	101.17	109.24
2	B	323	LEU	N-CA-C	-5.34	99.43	110.80
4	G	165	PHE	N-CA-C	-5.33	101.08	109.50
3	F	452	ILE	CA-C-N	5.33	125.32	119.89
3	F	452	ILE	C-N-CA	5.33	125.32	119.89
3	F	296	ILE	N-CA-C	-5.33	106.24	111.88
10	V	52	GLU	CA-C-N	5.32	127.74	120.35
10	V	52	GLU	C-N-CA	5.32	127.74	120.35
3	F	221	GLN	N-CA-C	-5.31	102.19	110.42
3	E	107	GLY	CA-C-N	5.31	126.48	119.84
3	E	107	GLY	C-N-CA	5.31	126.48	119.84
3	F	355	SER	N-CA-C	-5.30	100.66	108.99
3	F	20	ILE	CA-C-N	5.29	128.47	120.75
3	F	20	ILE	C-N-CA	5.29	128.47	120.75
4	G	134	GLY	CA-C-N	5.29	127.37	120.28
4	G	134	GLY	C-N-CA	5.29	127.37	120.28
3	D	256	ASP	N-CA-C	-5.29	101.03	109.07
3	F	16	VAL	N-CA-C	-5.28	98.35	109.34
1	9	11	GLY	CA-C-N	5.28	127.36	120.28
1	9	11	GLY	C-N-CA	5.28	127.36	120.28
10	V	26	ALA	N-CA-C	-5.28	105.91	114.09
2	C	130	ARG	N-CA-C	-5.27	101.29	109.72
3	F	387	ILE	CA-C-N	5.27	127.68	120.46
3	F	387	ILE	C-N-CA	5.27	127.68	120.46
7	O	180	ILE	CA-C-N	5.27	127.65	120.54
7	O	180	ILE	C-N-CA	5.27	127.65	120.54
2	A	96	ILE	N-CA-C	-5.27	104.26	110.21
2	A	204	VAL	N-CA-C	-5.26	100.54	108.12
3	D	221	GLN	N-CA-C	-5.26	101.30	109.72
4	G	162	ILE	N-CA-C	-5.26	100.75	108.85
5	H	13	GLN	N-CA-C	-5.26	98.82	108.02
2	C	121	GLY	CA-C-N	5.26	126.41	119.84
2	C	121	GLY	C-N-CA	5.26	126.41	119.84
7	O	175	THR	N-CA-C	-5.26	101.30	109.24
3	E	330	ASP	N-CA-C	-5.25	106.55	113.12
5	H	69	PHE	N-CA-C	-5.25	100.35	108.90
5	H	35	LYS	N-CA-C	-5.25	106.72	113.02
3	E	76	VAL	N-CA-C	-5.24	100.30	108.95
3	F	60	ARG	N-CA-C	-5.24	99.90	108.76
3	E	252	LEU	N-CA-C	-5.24	99.56	108.26
1	2	6	ALA	CA-C-N	5.24	127.30	120.28
1	2	6	ALA	C-N-CA	5.24	127.30	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	347	ALA	CA-C-N	5.23	127.58	120.63
3	F	347	ALA	C-N-CA	5.23	127.58	120.63
3	D	345	TYR	N-CA-C	-5.22	97.45	108.73
3	F	351	LEU	N-CA-C	-5.22	106.59	113.17
3	F	132	GLU	CA-C-N	5.22	127.57	120.63
3	F	132	GLU	C-N-CA	5.22	127.57	120.63
1	3	18	GLY	CA-C-N	5.21	127.79	120.28
1	3	18	GLY	C-N-CA	5.21	127.79	120.28
3	D	22	ASP	N-CA-C	-5.21	101.66	109.95
5	H	58	GLU	N-CA-C	-5.21	100.53	109.24
2	A	37	GLY	N-CA-C	-5.21	100.83	113.18
3	D	351	LEU	N-CA-C	-5.21	106.70	113.16
1	3	41	PRO	N-CA-C	5.20	123.17	112.47
1	9	59	GLU	CA-C-N	5.19	127.23	120.28
1	9	59	GLU	C-N-CA	5.19	127.23	120.28
3	E	181	PHE	N-CA-C	-5.18	101.55	108.86
4	G	82	GLY	N-CA-C	-5.18	105.66	112.81
3	F	153	ILE	N-CA-C	-5.18	101.02	108.89
3	E	112	LYS	N-CA-C	-5.18	103.15	111.02
1	5	43	ILE	CA-C-N	5.17	127.93	120.38
1	5	43	ILE	C-N-CA	5.17	127.93	120.38
2	A	260	ARG	CA-C-N	5.17	127.63	120.29
2	A	260	ARG	C-N-CA	5.17	127.63	120.29
2	C	164	GLY	CA-C-N	5.17	131.41	121.54
2	C	164	GLY	C-N-CA	5.17	131.41	121.54
10	V	87	LYS	N-CA-C	-5.17	105.72	113.89
3	F	128	SER	N-CA-C	-5.16	98.83	108.02
2	A	234	VAL	N-CA-C	-5.16	101.15	108.58
1	7	22	ALA	CA-C-N	5.16	125.70	119.98
1	7	22	ALA	C-N-CA	5.16	125.70	119.98
1	8	17	ILE	CA-C-N	5.16	125.81	120.03
1	8	17	ILE	C-N-CA	5.16	125.81	120.03
2	A	126	ALA	N-CA-C	5.15	116.90	111.28
7	O	8	PRO	N-CA-C	5.15	116.99	110.70
3	E	219	PHE	N-CA-C	-5.15	100.51	108.90
7	O	63	SER	N-CA-C	-5.15	102.00	109.31
2	B	109	VAL	N-CA-C	-5.14	100.97	108.17
5	H	80	ASP	N-CA-C	-5.14	106.32	112.59
3	F	80	GLY	CA-C-N	5.14	129.94	121.87
3	F	80	GLY	C-N-CA	5.14	129.94	121.87
2	A	176	GLY	N-CA-C	-5.13	101.01	113.18
3	D	216	ALA	N-CA-C	-5.13	101.74	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	111	SER	N-CA-C	-5.13	99.88	110.80
2	B	208	VAL	N-CA-C	-5.12	101.10	108.48
5	H	31	ASN	N-CA-C	-5.12	100.10	108.76
2	B	262	ASN	N-CA-C	-5.12	106.81	113.16
3	D	273	GLY	N-CA-C	-5.12	108.05	115.27
3	E	311	TYR	N-CA-C	-5.12	100.18	108.52
2	B	199	LYS	N-CA-C	-5.12	107.07	113.72
3	E	22	ASP	N-CA-C	-5.12	101.35	109.59
4	G	95	VAL	CA-C-N	5.12	127.14	120.28
4	G	95	VAL	C-N-CA	5.12	127.14	120.28
2	C	195	SER	N-CA-C	-5.11	106.82	113.16
3	D	300	LYS	N-CA-C	-5.11	107.04	113.28
2	C	54	LEU	N-CA-C	-5.11	100.84	109.07
4	G	168	ASP	N-CA-C	-5.11	103.22	109.65
3	D	222	MET	CA-C-N	5.10	127.12	120.28
3	D	222	MET	C-N-CA	5.10	127.12	120.28
2	A	135	ALA	CA-C-N	5.10	125.04	119.78
2	A	135	ALA	C-N-CA	5.10	125.04	119.78
8	T	27	THR	CA-C-N	5.10	127.12	120.28
8	T	27	THR	C-N-CA	5.10	127.12	120.28
3	D	64	MET	N-CA-C	-5.10	104.77	111.96
3	F	42	PRO	N-CA-C	-5.09	106.90	113.57
2	B	454	HIS	N-CA-C	-5.09	106.85	113.16
10	V	169	ASN	N-CA-C	-5.09	106.32	112.88
3	E	104	ASP	N-CA-C	-5.08	106.59	112.89
3	F	22	ASP	N-CA-C	-5.08	100.76	109.24
3	D	336	SER	CA-C-N	5.07	127.08	120.28
3	D	336	SER	C-N-CA	5.07	127.08	120.28
1	7	65	CYS	CA-C-N	5.07	127.07	120.28
1	7	65	CYS	C-N-CA	5.07	127.07	120.28
3	F	107	GLY	CA-C-N	5.07	125.07	119.90
3	F	107	GLY	C-N-CA	5.07	125.07	119.90
2	A	500	LYS	CA-C-N	5.06	127.06	120.28
2	A	500	LYS	C-N-CA	5.06	127.06	120.28
7	O	179	SER	N-CA-C	-5.06	101.37	109.07
1	0	22	ALA	CA-C-N	5.06	125.60	119.98
1	0	22	ALA	C-N-CA	5.06	125.60	119.98
1	8	58	SER	CA-C-N	5.06	127.06	120.28
1	8	58	SER	C-N-CA	5.06	127.06	120.28
1	9	61	THR	CA-C-N	5.05	125.59	119.98
1	9	61	THR	C-N-CA	5.05	125.59	119.98
2	C	32	ARG	CA-C-N	5.05	127.38	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	32	ARG	C-N-CA	5.05	127.38	120.35
4	G	78	THR	CA-C-N	5.05	131.18	121.54
4	G	78	THR	C-N-CA	5.05	131.18	121.54
3	E	61	THR	N-CA-C	-5.04	101.74	109.41
5	H	33	PRO	N-CA-C	-5.04	102.08	112.47
2	C	34	LEU	N-CA-C	-5.03	108.41	114.75
4	G	195	GLY	N-CA-C	-5.03	108.74	115.32
2	A	205	TYR	N-CA-C	-5.02	100.72	108.90
3	E	295	ARG	N-CA-C	-5.01	106.85	113.17
3	F	112	LYS	N-CA-C	-5.01	103.89	111.56
2	A	255	ILE	CA-C-N	5.01	125.54	119.98
2	A	255	ILE	C-N-CA	5.01	125.54	119.98
2	A	128	ARG	N-CA-C	-5.01	100.73	108.90
2	A	142	ARG	N-CA-C	-5.01	101.47	109.23
3	D	225	PRO	CA-C-N	5.01	124.79	119.28
3	D	225	PRO	C-N-CA	5.01	124.79	119.28
14	Z	7	PHE	N-CA-C	-5.00	105.90	112.41
2	A	432	GLN	N-CA-C	-5.00	99.53	108.13
3	D	450	ASP	N-CA-C	-5.00	106.87	113.17
3	E	53	HIS	N-CA-C	-5.00	100.26	108.41
5	H	94	GLU	CA-C-N	5.00	126.98	120.28
5	H	94	GLU	C-N-CA	5.00	126.98	120.28
11	W	22	LYS	CA-C-N	5.00	126.94	120.44
11	W	22	LYS	C-N-CA	5.00	126.94	120.44
12	X	33	PRO	CA-C-N	5.00	126.09	119.84
12	X	33	PRO	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	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
3	F	345	TYR	Peptide
5	H	54	PRO	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	1	0
2	C	1992	0	572	0	0
3	D	1880	0	538	0	0
3	E	1872	0	537	0	0
3	F	1876	0	537	1	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:F:13:VAL:H	3:F:74:GLU:H	1.55	0.54
2:B:164:GLY:HA2	2:B:323:LEU:H	1.84	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	73/76 (96%)	73 (100%)	0	0	100	100
1	1	73/76 (96%)	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%)	1 (1%)	2 (3%)	4	24
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%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	9	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	9	40
2	A	495/510 (97%)	470 (95%)	19 (4%)	6 (1%)	10	43
2	B	501/510 (98%)	471 (94%)	20 (4%)	10 (2%)	6	31
2	C	496/510 (97%)	472 (95%)	16 (3%)	8 (2%)	7	37
3	D	468/478 (98%)	439 (94%)	22 (5%)	7 (2%)	8	39
3	E	466/478 (98%)	442 (95%)	18 (4%)	6 (1%)	9	42
3	F	467/478 (98%)	435 (93%)	26 (6%)	6 (1%)	9	42
4	G	261/278 (94%)	245 (94%)	11 (4%)	5 (2%)	6	32
5	H	110/138 (80%)	102 (93%)	4 (4%)	4 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	I	42/61 (69%)	40 (95%)	2 (5%)	0	100	100
7	O	185/195 (95%)	167 (90%)	14 (8%)	4 (2%)	5	29
8	T	222/249 (89%)	208 (94%)	13 (6%)	1 (0%)	24	63
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	155 (92%)	9 (5%)	5 (3%)	3	22
11	W	83/95 (87%)	68 (82%)	6 (7%)	9 (11%)	0	6
12	X	60/92 (65%)	54 (90%)	6 (10%)	0	100	100
13	Y	35/59 (59%)	32 (91%)	1 (3%)	2 (6%)	1	13
14	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
All	All	4984/5321 (94%)	4699 (94%)	203 (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	B	22	SER
2	B	380	ALA
2	C	228	MET
2	C	299	ASP
2	C	320	SER
3	D	110	LYS
3	F	177	ALA
4	G	79	SER
10	V	130	PHE
11	W	40	PRO
11	W	42	ILE
11	W	44	ALA
11	W	46	THR
2	A	22	SER
2	A	320	SER
2	B	338	ALA

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Mol	Chain	Res	Type
2	C	36	VAL
2	C	49	ILE
2	C	165	GLN
2	C	379	ALA
3	D	160	GLY
3	D	358	LEU
3	D	462	GLY
5	H	89	GLU
10	V	170	LEU
11	W	11	SER
11	W	31	TYR
2	A	23	ASP
2	B	145	HIS
2	B	156	ASP
2	B	157	ALA
3	E	358	LEU
3	F	81	GLY
3	F	86	PRO
3	F	131	ALA
3	F	280	GLY
5	H	22	TYR
5	H	33	PRO
7	O	51	PRO
7	O	61	ALA
7	O	118	LEU
8	T	147	PRO
10	V	132	GLU
10	V	133	LEU
11	W	36	GLN
1	3	42	SER
2	A	367	ILE
2	B	103	PRO
2	C	230	TYR
3	E	346	PRO
2	B	379	ALA
3	E	16	VAL
4	G	56	GLU
4	G	123	PRO
7	O	10	VAL
13	Y	3	LYS
13	Y	11	LYS
2	A	145	HIS

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Mol	Chain	Res	Type
2	B	226	ASP
3	D	161	VAL
5	H	93	LEU
3	E	282	GLN
11	W	39	ALA
2	B	382	VAL
3	D	9	ILE
3	E	279	VAL
10	V	50	PRO
3	E	83	ILE
4	G	181	PRO
3	F	80	GLY
4	G	192	PRO
3	D	86	PRO
11	W	5	ILE

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

There are no chain breaks in this entry.

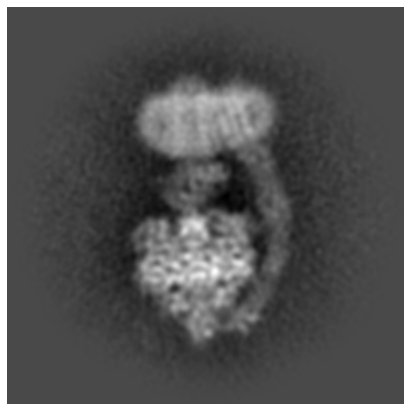
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25955. These allow visual inspection of the internal detail of the map and identification of artifacts.

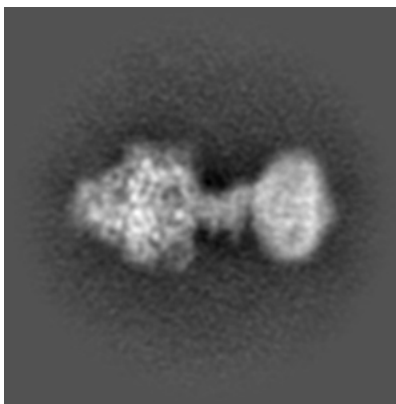
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

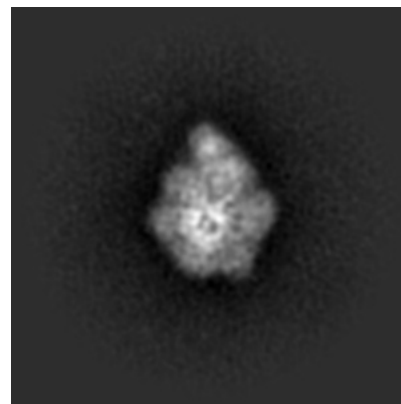
6.1.1 Primary map



X

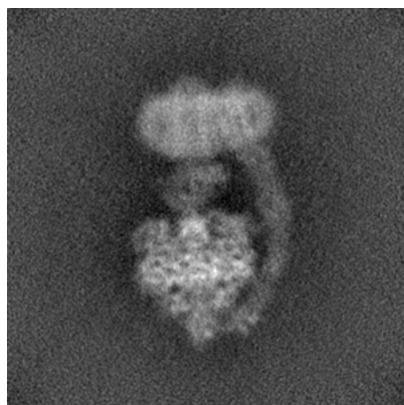


Y

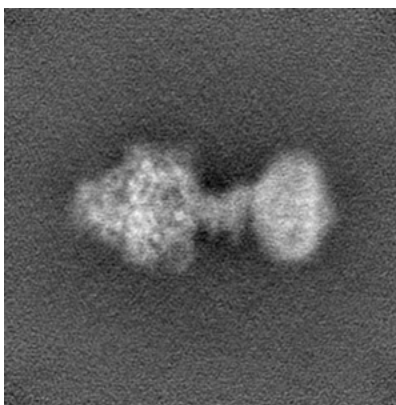


Z

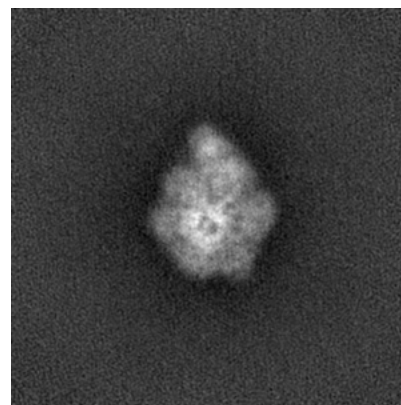
6.1.2 Raw map



X



Y

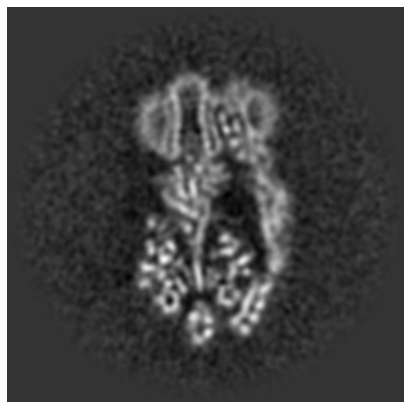


Z

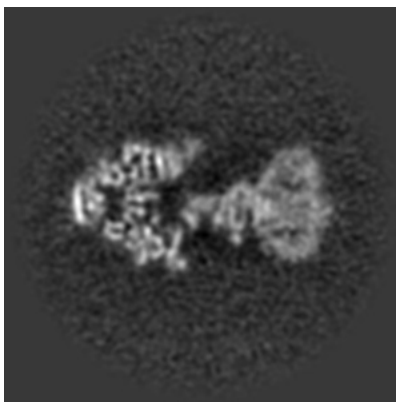
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

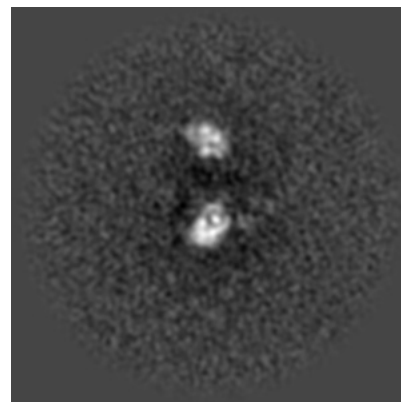
6.2.1 Primary map



X Index: 128

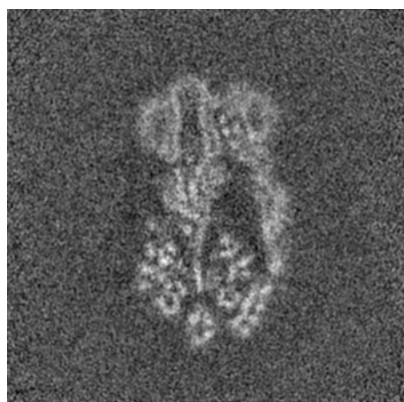


Y Index: 128

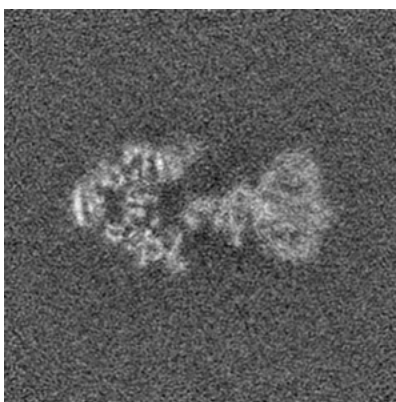


Z Index: 128

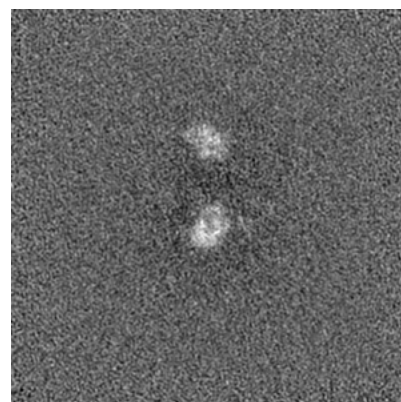
6.2.2 Raw map



X Index: 128



Y Index: 128

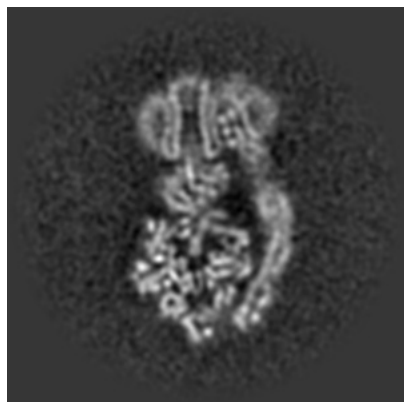


Z Index: 128

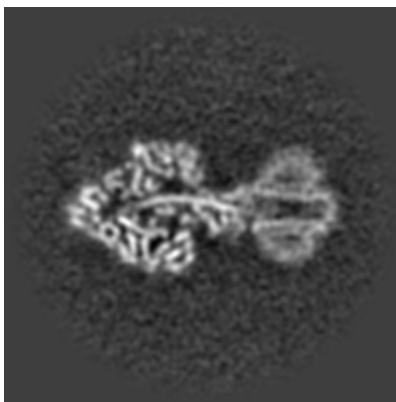
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

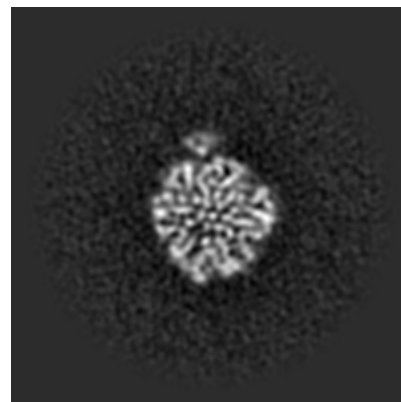
6.3.1 Primary map



X Index: 124

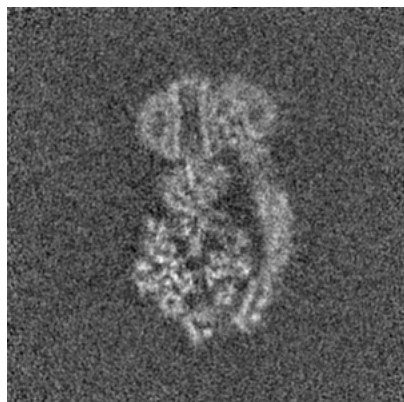


Y Index: 119

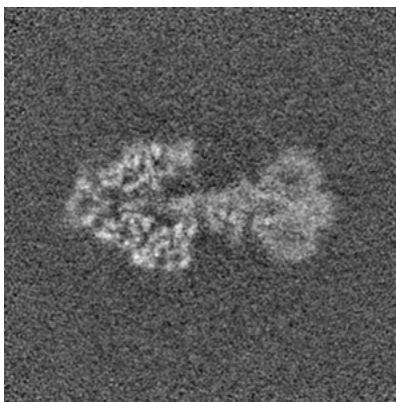


Z Index: 85

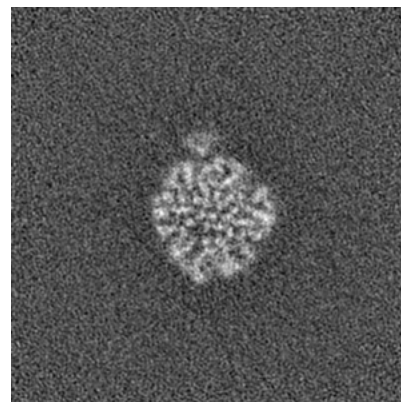
6.3.2 Raw map



X Index: 125



Y Index: 124

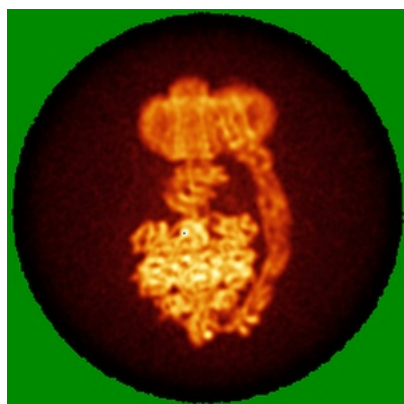


Z Index: 85

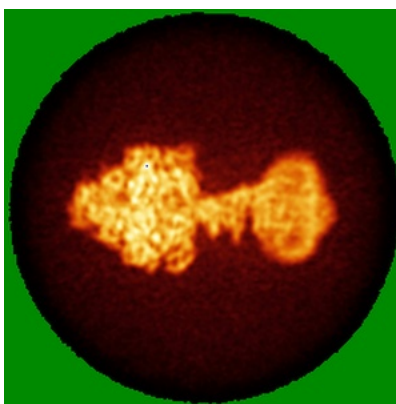
The images above show the largest variance slices of the map in three orthogonal directions.

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

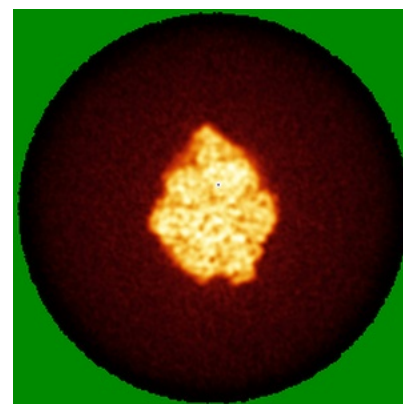
6.4.1 Primary map



X

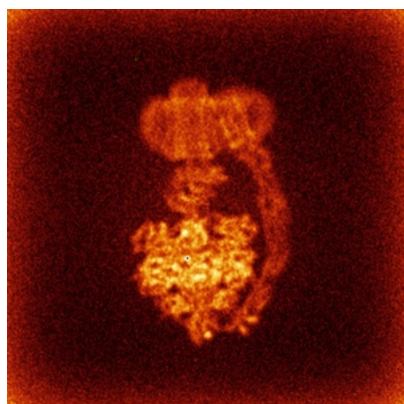


Y

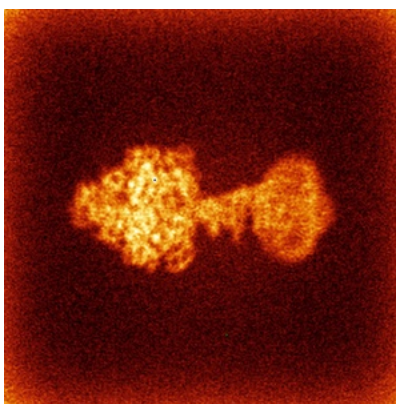


Z

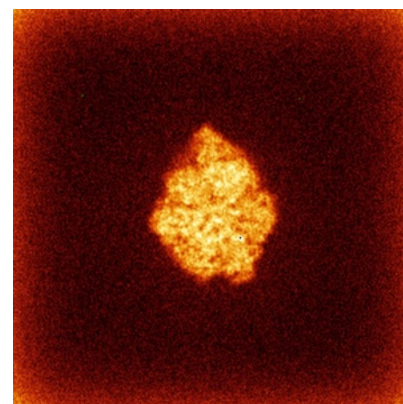
6.4.2 Raw map



X



Y

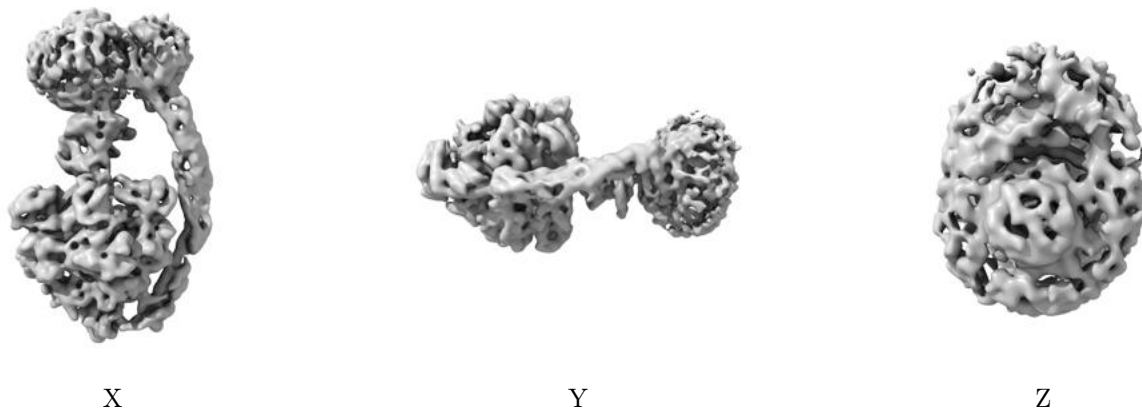


Z

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.

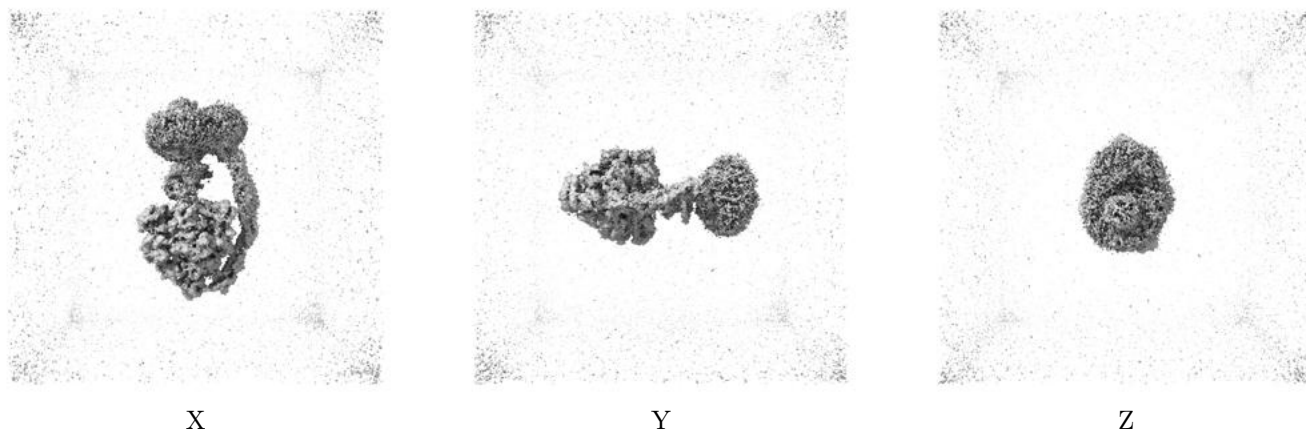
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.666. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

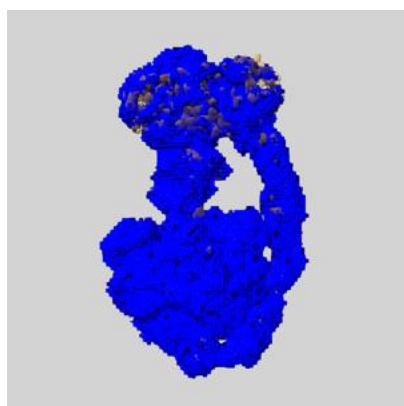
6.6 Mask visualisation [i](#)

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

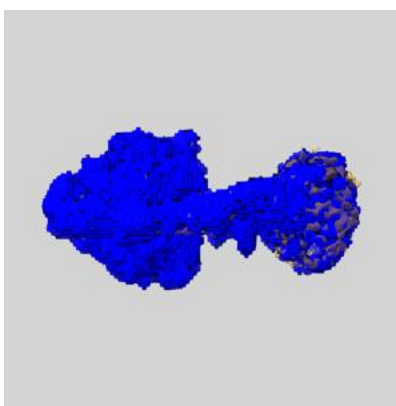
A mask typically either:

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

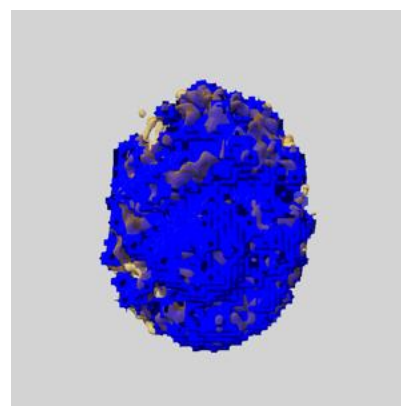
6.6.1 emd_25955_msk_1.map [i](#)



X



Y

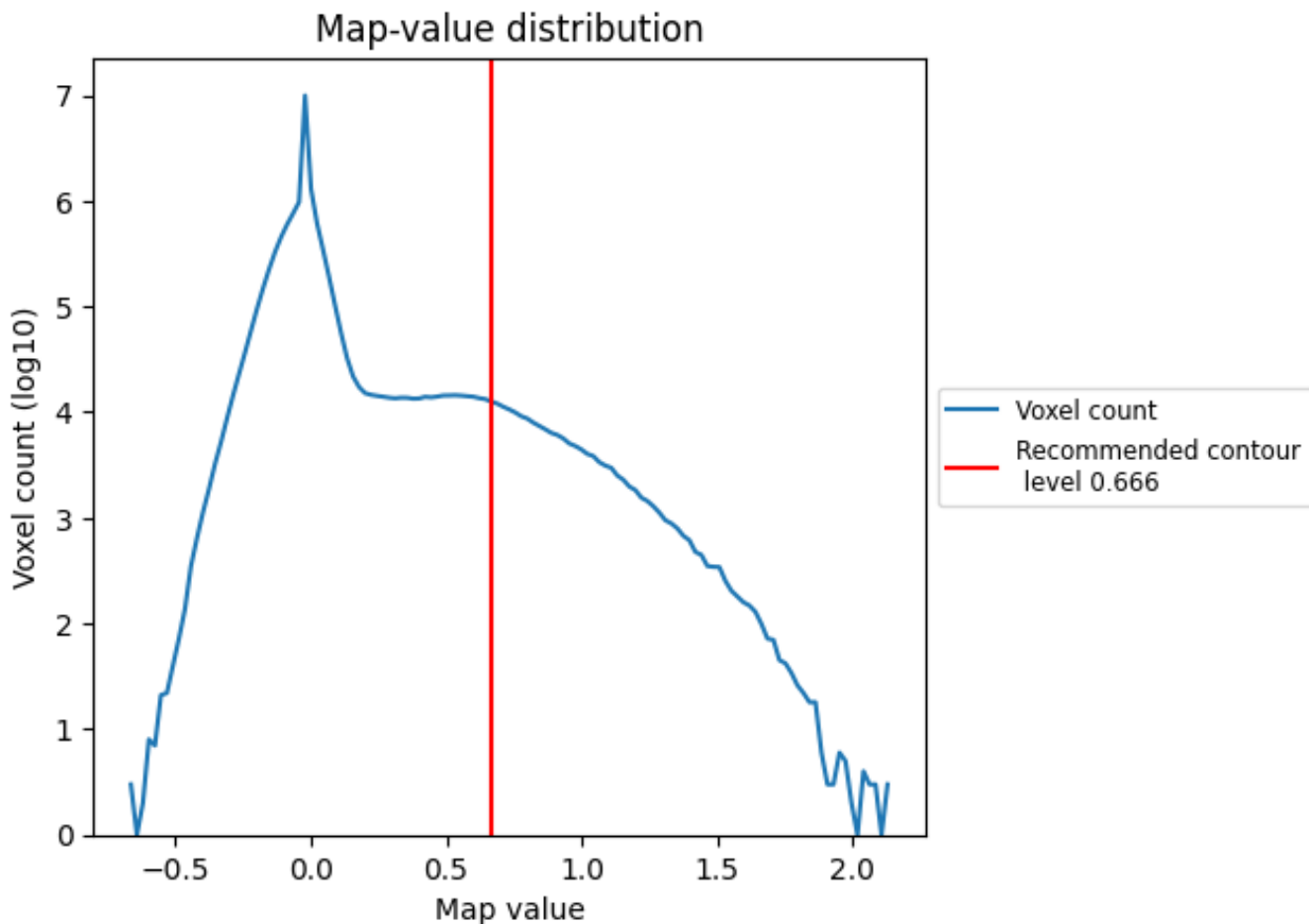


Z

7 Map analysis [i](#)

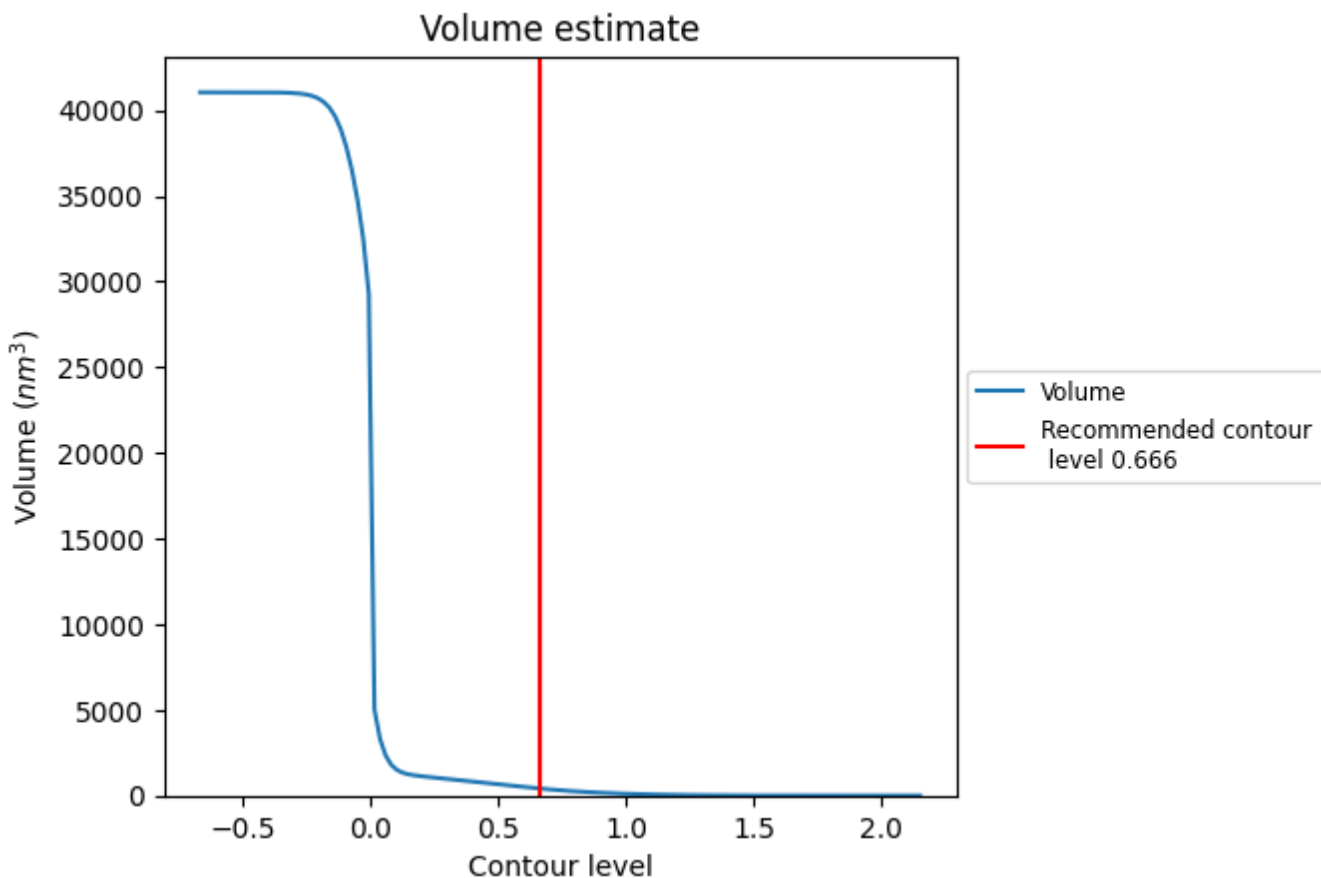
This section contains the results of statistical analysis of the map.

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.

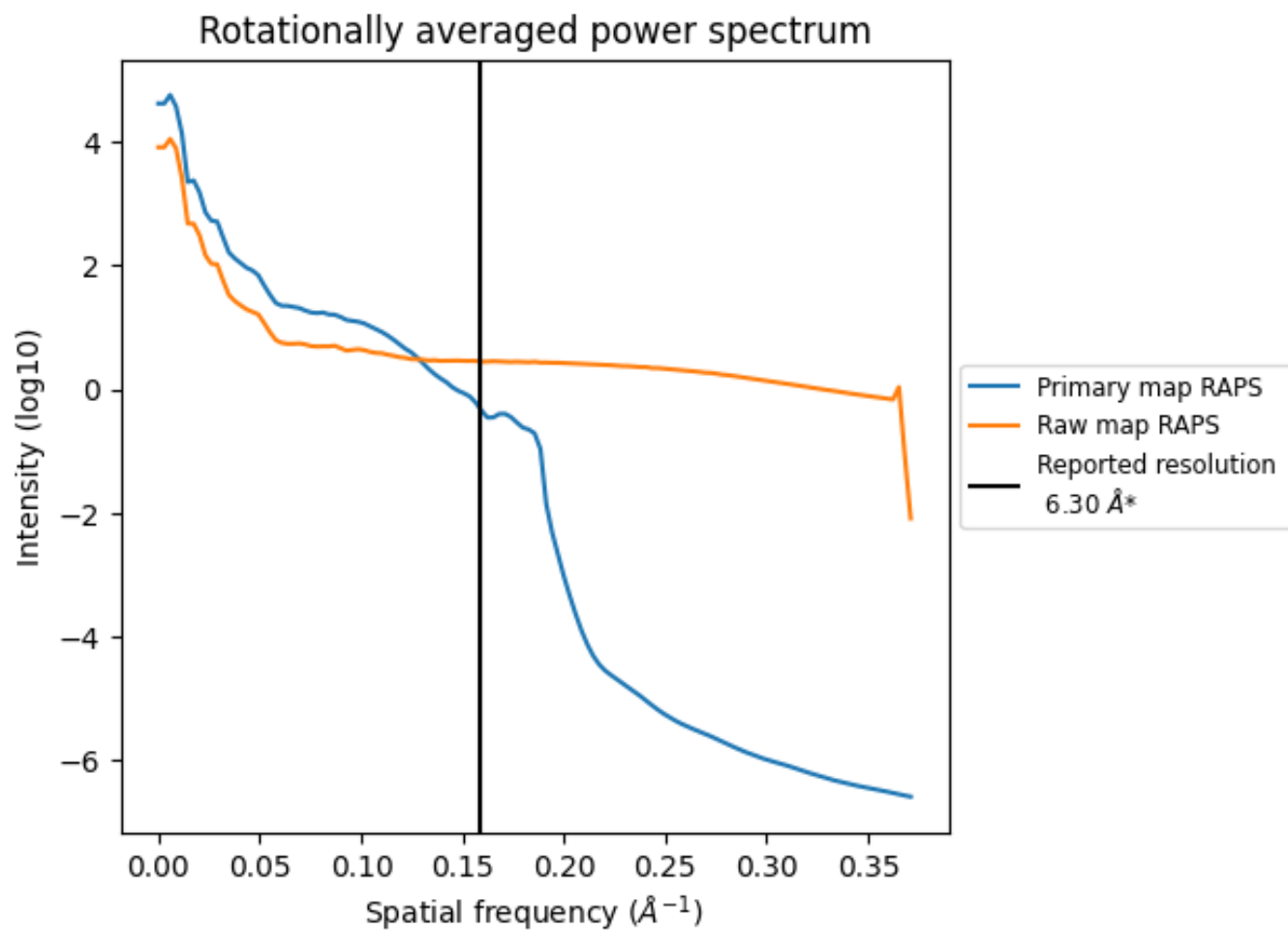
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 411 nm³; this corresponds to an approximate mass of 371 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](#)

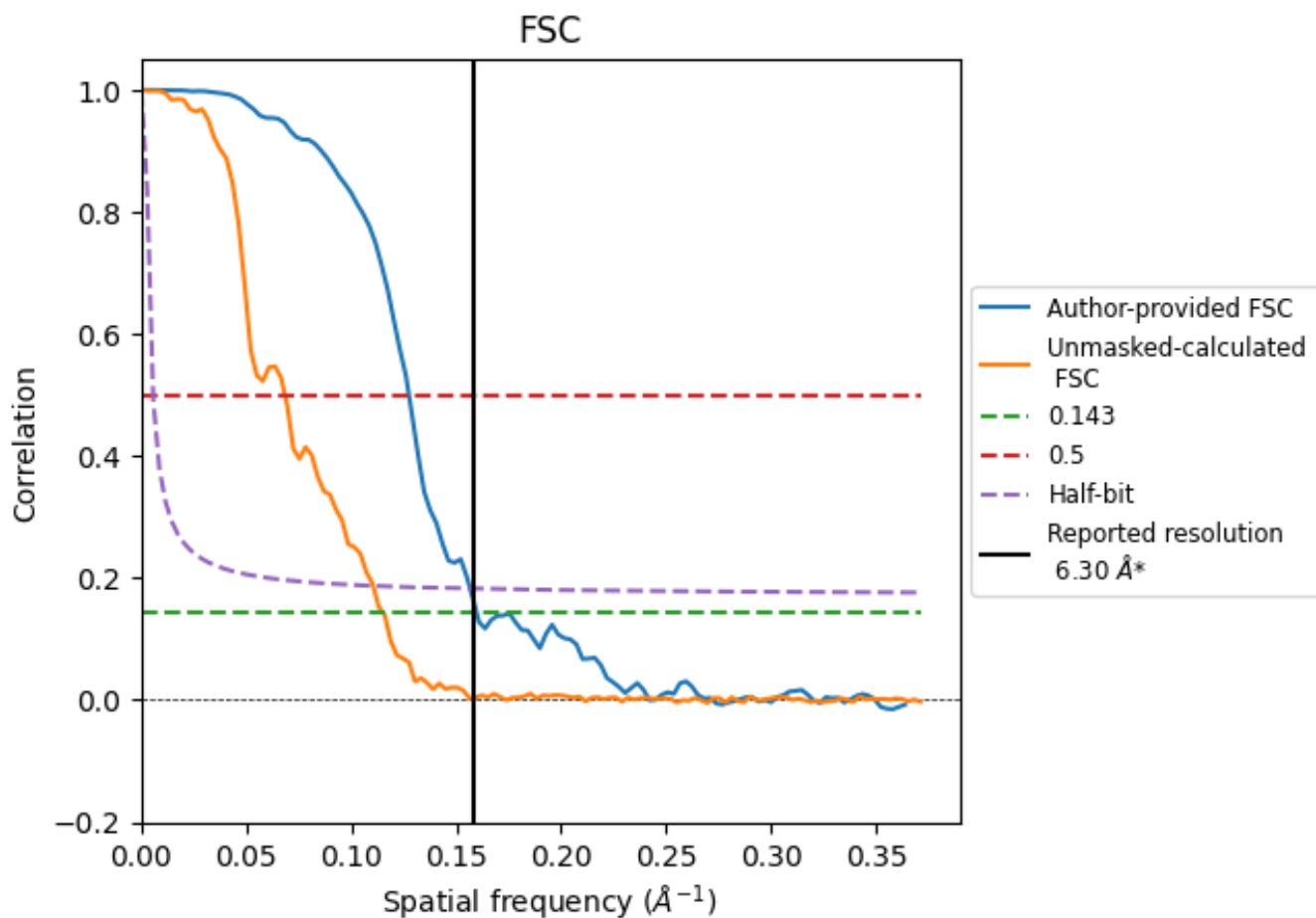


*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

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 0.159 Å⁻¹

8.2 Resolution estimates [i](#)

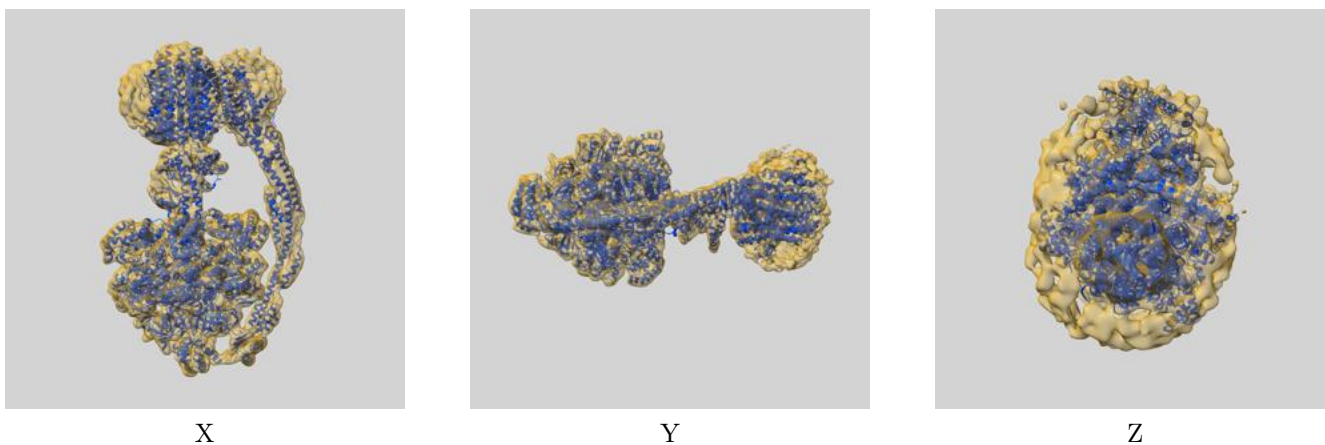
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.26	7.84	6.38
Unmasked-calculated*	8.69	14.62	9.06

*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 8.69 differs from the reported value 6.3 by more than 10 %

9 Map-model fit [i](#)

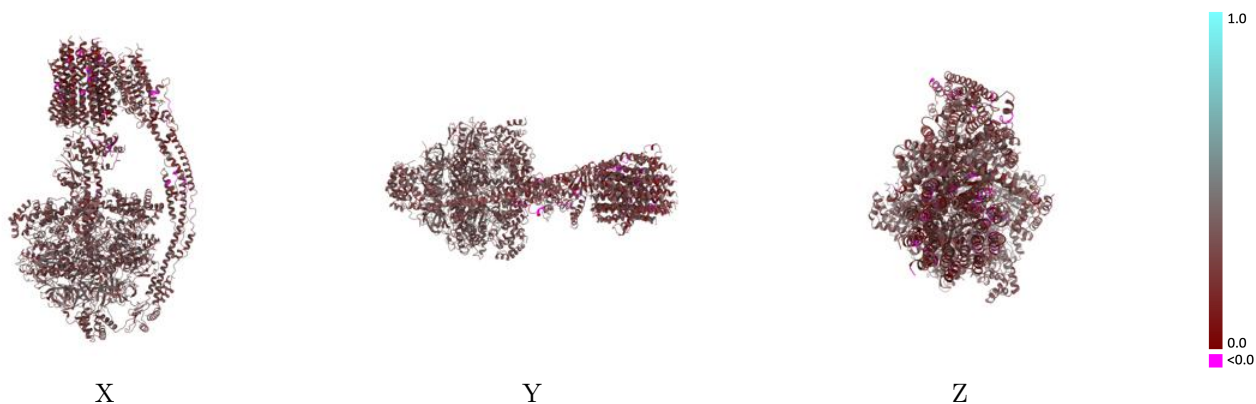
This section contains information regarding the fit between EMDB map EMD-25955 and PDB model 7TK3. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



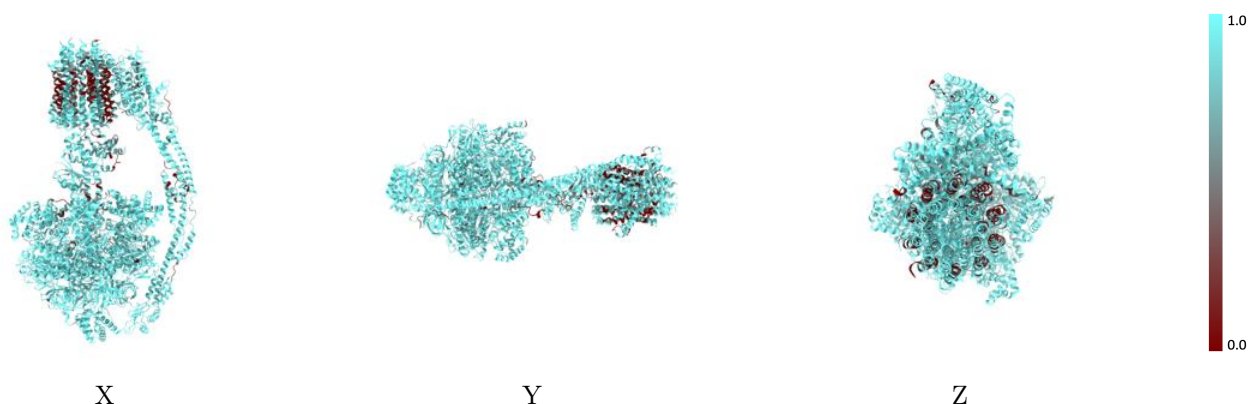
The images above show the 3D surface view of the map at the recommended contour level 0.666 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



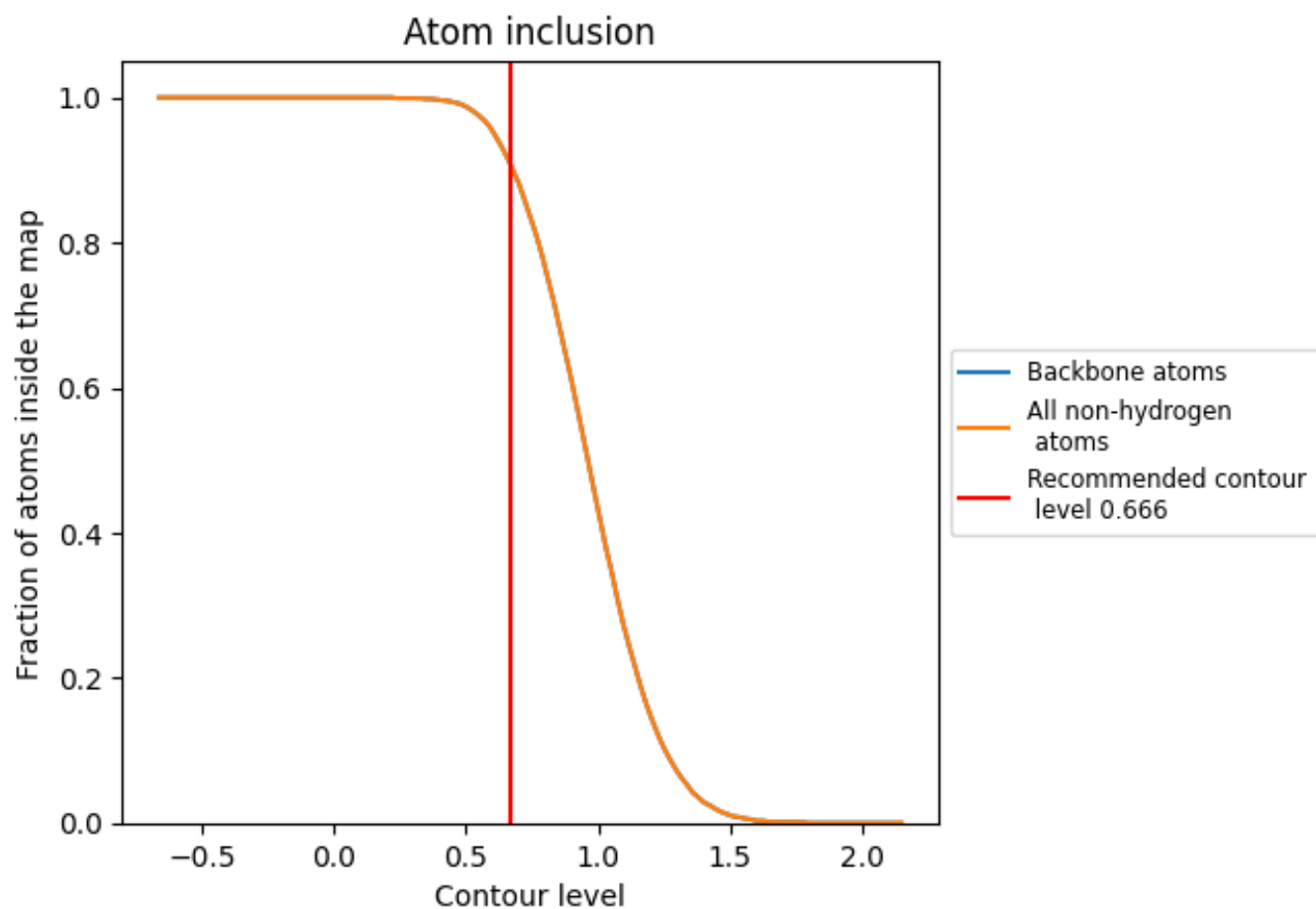
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.666).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.666) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9100	 0.2940
0	 0.5430	 0.1930
1	 0.6930	 0.2290
2	 0.6500	 0.2130
3	 0.6650	 0.2210
4	 0.7900	 0.1980
5	 0.7030	 0.2180
6	 0.8210	 0.2280
7	 0.7700	 0.2310
8	 0.7130	 0.1970
9	 0.6350	 0.2150
A	 0.9690	 0.3270
B	 0.9620	 0.3280
C	 0.9830	 0.3330
D	 0.9540	 0.3210
E	 0.9620	 0.3210
F	 0.9880	 0.3390
G	 0.9370	 0.2800
H	 0.8020	 0.2220
I	 0.8140	 0.2540
O	 0.9920	 0.3160
T	 0.8820	 0.2620
U	 0.9920	 0.2860
V	 0.9040	 0.2590
W	 0.8380	 0.2080
X	 0.6530	 0.2210
Y	 0.8450	 0.2690
Z	 0.8650	 0.2570

