



## Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 12:10 PM UTC

PDB ID : 7TK7 / pdb\_00007tk7  
EMDB ID : EMD-25959  
Title : Yeast ATP synthase State 1catalytic(b) with 10 mM ATP backbone model  
Authors : Guo, H.; Rubinstein, J.L.  
Deposited on : 2022-01-17  
Resolution : 6.70 Å (reported)  
Based on initial model : 2HLD

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

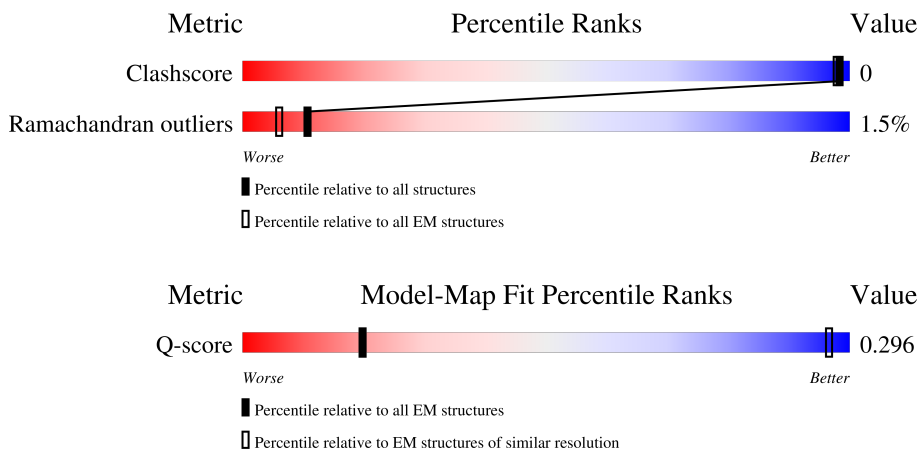
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 6.70 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	523 ( 6.20 - 7.20 )

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

Mol	Chain	Length	Quality of chain
1	0	76	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 38%, orange 38%, yellow 95%, green 95%, grey 95%);"></span> 38% 95% . .
1	1	76	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 46%, orange 46%, yellow 91%, green 91%, grey 91%);"></span> 46% 91% 8% .
1	2	76	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 38%, orange 38%, yellow 93%, green 93%, grey 93%);"></span> 38% 93% 5% .
1	3	76	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 38%, orange 38%, yellow 91%, green 91%, grey 91%);"></span> 38% 91% 7% .
1	4	76	<span style="display: inline-block; width: 100%; height: 15px; background: linear-gradient(to right, red 37%, orange 37%, yellow 91%, green 91%, grey 91%);"></span> 37% 91% 8% .

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Mol	Chain	Length	Quality of chain
1	5	76	38% 92% 7%
1	6	76	22% 88% 9%
1	7	76	32% 87% 9%
1	8	76	29% 87% 12%
1	9	76	21% 89% 8%
2	A	510	5% 90% 7%
2	B	510	• 90% 9%
2	C	510	• 89% 8%
3	D	478	• 88% 10%
3	E	478	6% 89% 8%
3	F	478	• 88% 10%
4	G	278	5% 88% 8% 5%
5	H	138	11% 78% 9% 13%
6	I	61	5% 77% • 21%
7	O	195	• 86% 10%
8	T	249	18% 82% 8% 10%
9	U	209	5% 73% • 26%
10	V	173	10% 88% 10% ••
11	W	95	28% 79% 11% 11%
12	X	92	26% 61% 5% • 33%
13	Y	59	17% 63% 37%
14	Z	48	12% 100%

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 20227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP synthase subunit 9, 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
			479	240	120	119		

- 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

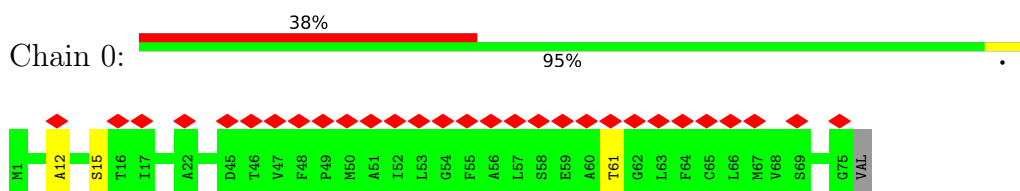
- Molecule 14 is a protein called ATP synthase protein 8.

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

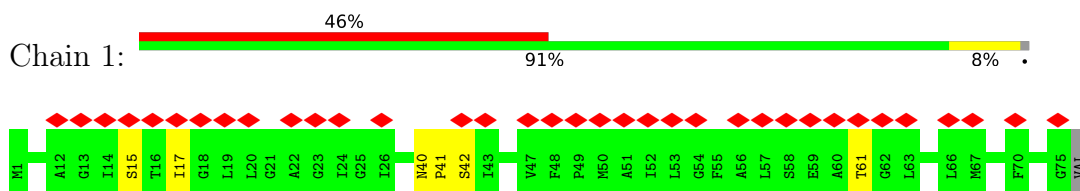
### 3 Residue-property plots

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

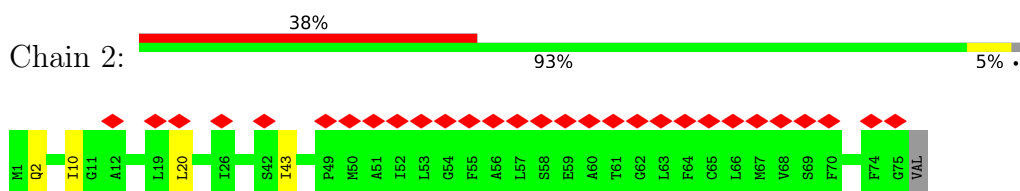
- Molecule 1: ATP synthase subunit 9, mitochondrial



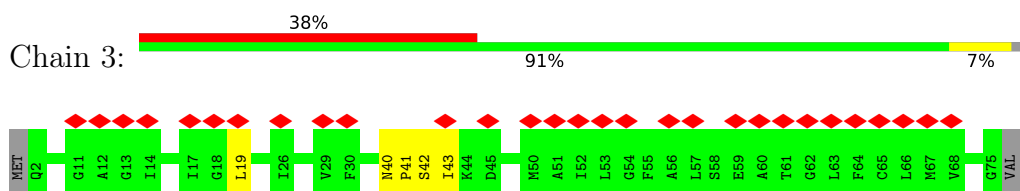
- Molecule 1: ATP synthase subunit 9, mitochondrial



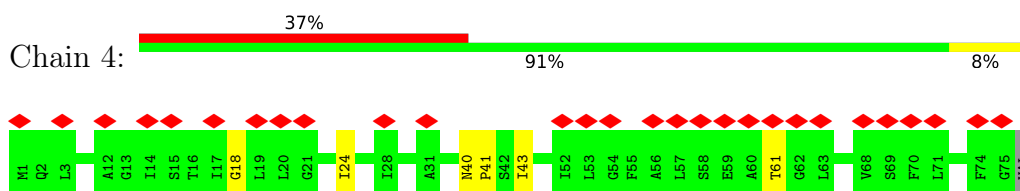
- Molecule 1: ATP synthase subunit 9, mitochondrial



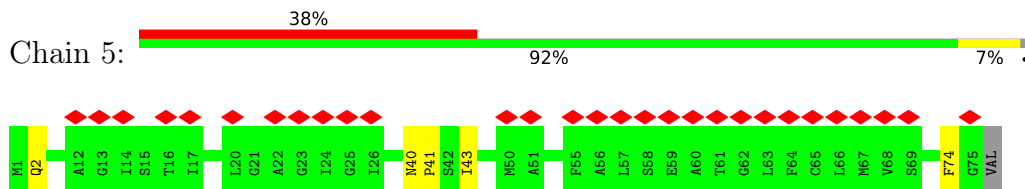
- Molecule 1: ATP synthase subunit 9, mitochondrial



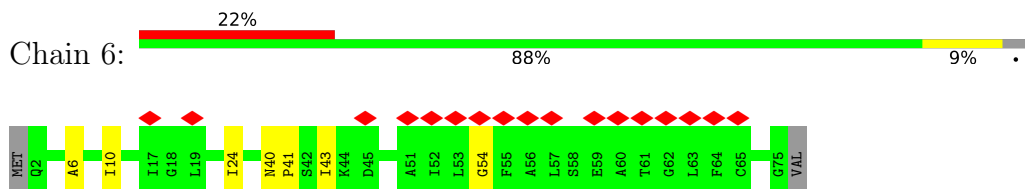
- Molecule 1: ATP synthase subunit 9, mitochondrial



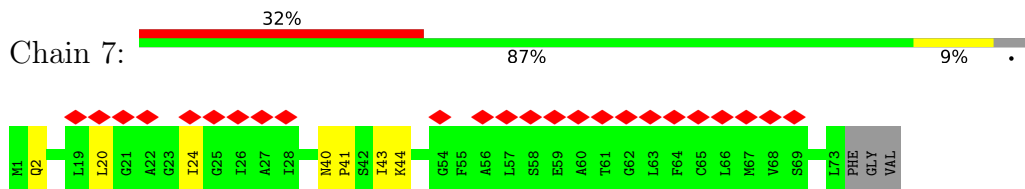
• Molecule 1: ATP synthase subunit 9, mitochondrial



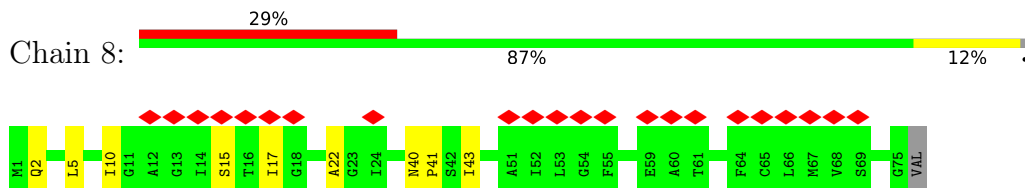
• Molecule 1: ATP synthase subunit 9, mitochondrial



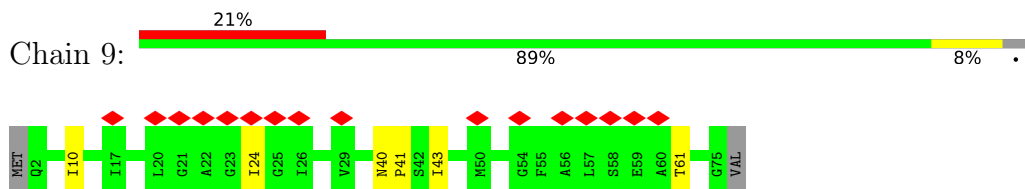
• Molecule 1: ATP synthase subunit 9, mitochondrial



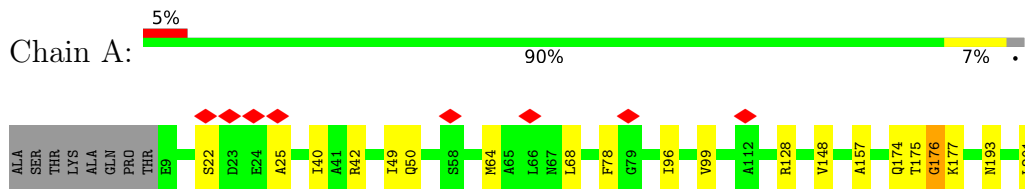
• Molecule 1: ATP synthase subunit 9, mitochondrial



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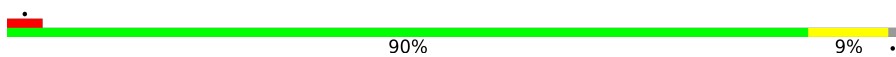


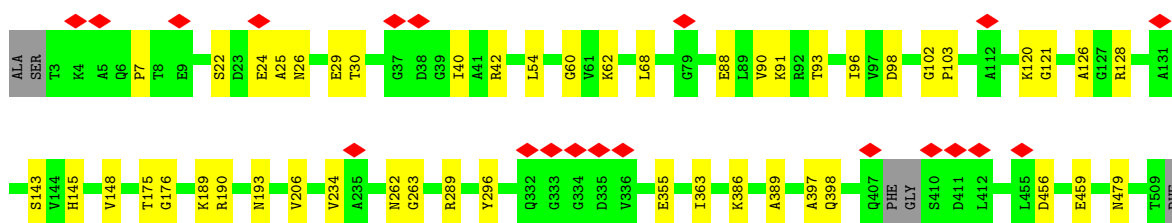
• Molecule 2: ATP synthase subunit alpha




• Molecule 2: ATP synthase subunit alpha

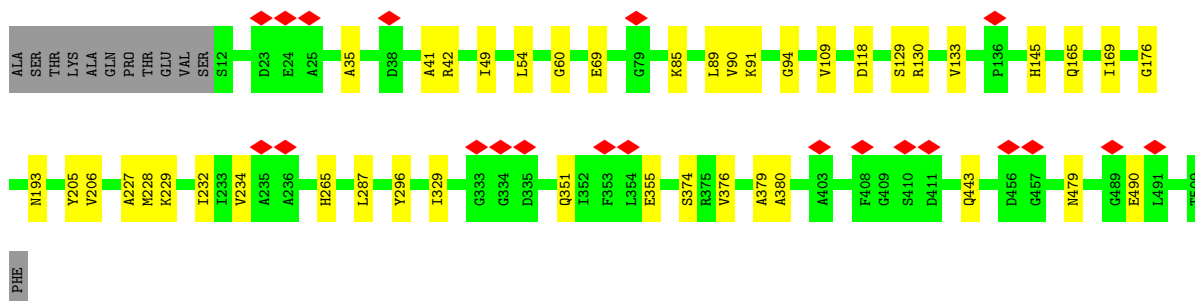


Chain B:  90% 9%




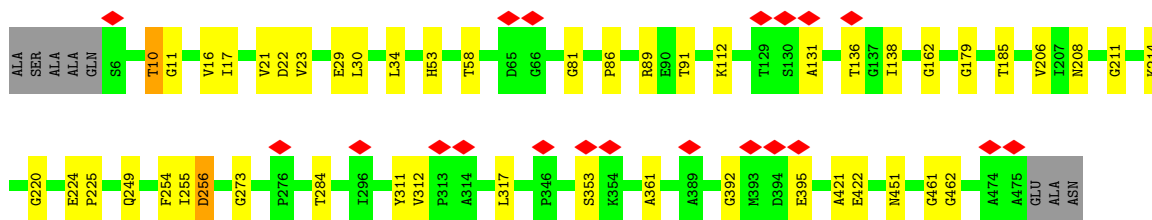
• Molecule 2: ATP synthase subunit alpha

Chain C:  89% 8%




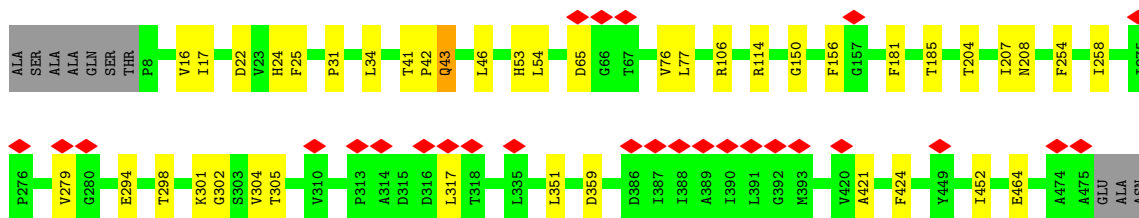
• Molecule 3: ATP synthase subunit beta

Chain D:  88% 10%




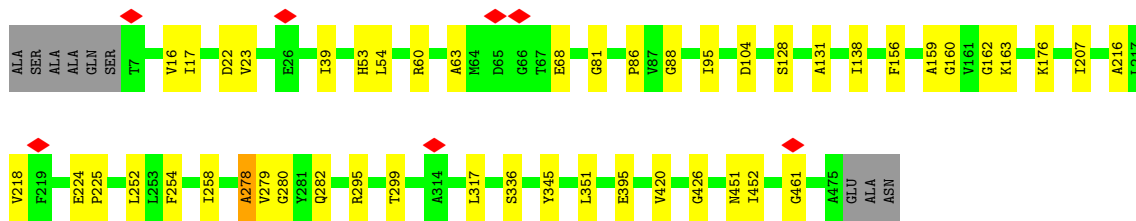
• Molecule 3: ATP synthase subunit beta

Chain E:  89% 6% 8%

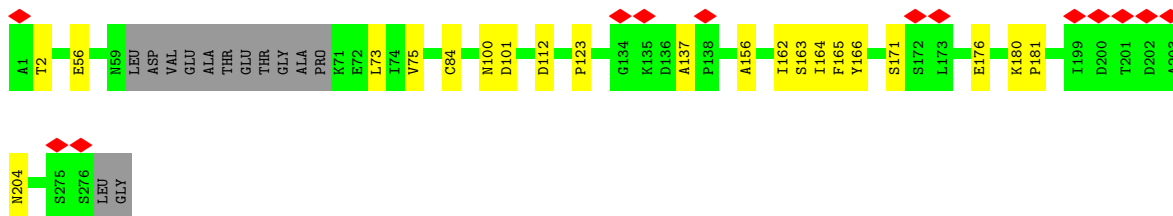
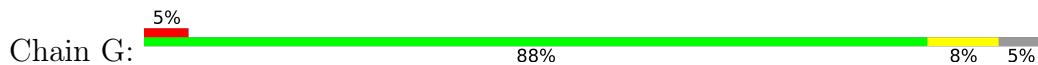


• Molecule 3: ATP synthase subunit beta

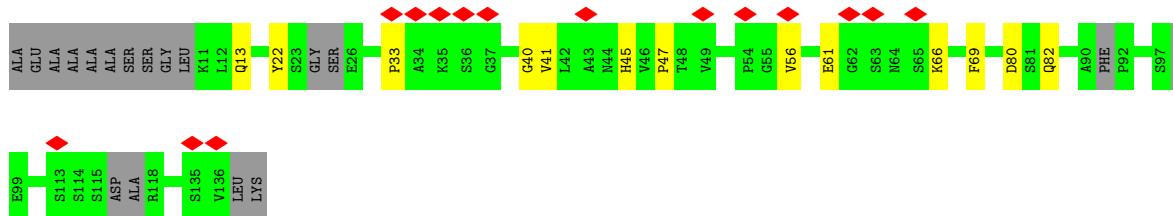
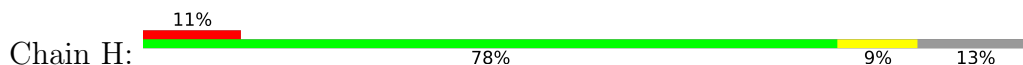
Chain F:  88% 10%



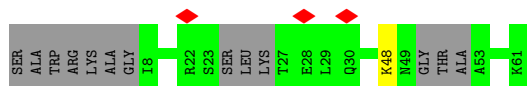
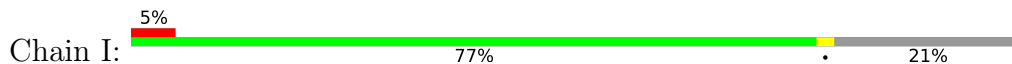
• Molecule 4: ATP synthase subunit gamma



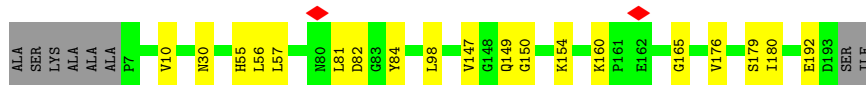
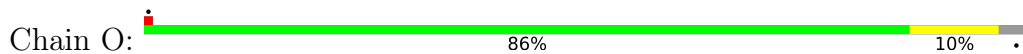
• Molecule 5: ATP synthase subunit delta



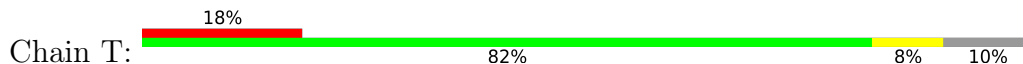
• Molecule 6: ATP synthase subunit epsilon

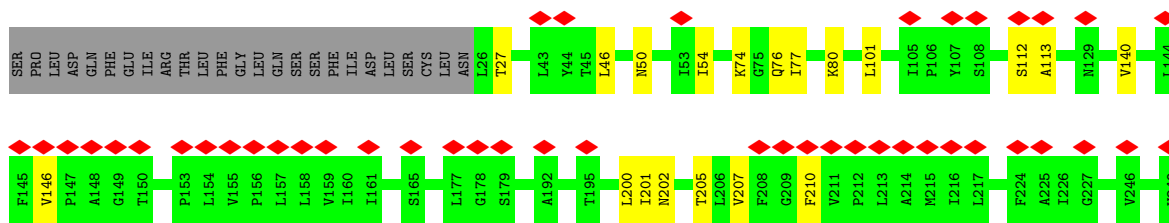


• Molecule 7: ATP synthase subunit 5

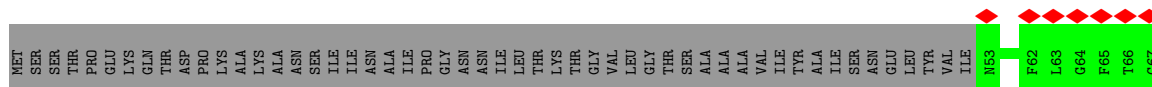
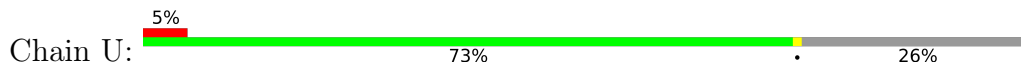


• Molecule 8: ATP synthase subunit a

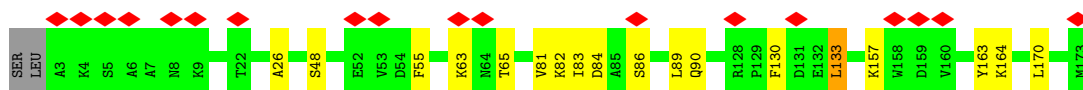
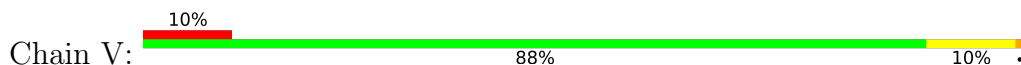




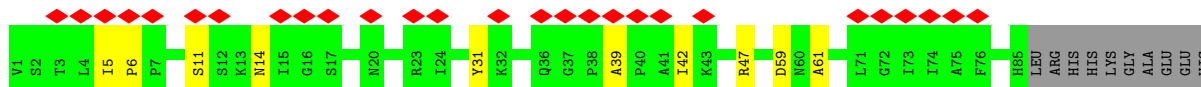
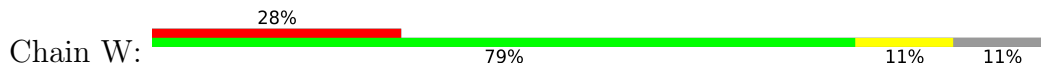
• Molecule 9: ATP synthase subunit 4



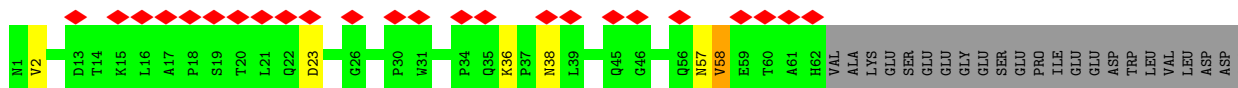
• Molecule 10: ATP synthase subunit d



• Molecule 11: ATP synthase subunit f



• Molecule 12: ATP synthase subunit H

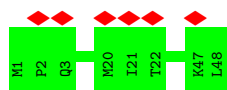


• Molecule 13: ATP synthase subunit J



- Molecule 14: ATP synthase protein 8

Chain Z:  12% 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7581	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	103896	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.857	Depositor
Minimum map value	-0.624	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	344.96, 344.96, 344.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3475, 1.3475, 1.3475	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	0	1.27	0/299	2.11	6/372 (1.6%)
1	1	1.24	0/299	2.04	7/372 (1.9%)
1	2	1.25	0/299	2.08	8/372 (2.2%)
1	3	1.22	0/295	1.95	4/367 (1.1%)
1	4	1.23	0/299	2.14	8/372 (2.2%)
1	5	1.24	0/299	2.15	4/372 (1.1%)
1	6	1.24	0/295	2.16	10/367 (2.7%)
1	7	1.25	0/291	2.18	9/362 (2.5%)
1	8	1.25	0/299	2.23	14/372 (3.8%)
1	9	1.24	0/295	2.09	8/367 (2.2%)
2	A	1.60	3/1994 (0.2%)	1.83	31/2489 (1.2%)
2	B	1.58	0/2018	1.90	45/2519 (1.8%)
2	C	1.62	1/1991 (0.1%)	1.84	38/2487 (1.5%)
3	D	1.58	1/1879 (0.1%)	1.88	42/2347 (1.8%)
3	E	1.61	0/1871	1.88	40/2337 (1.7%)
3	F	1.60	0/1875	1.84	40/2342 (1.7%)
4	G	1.51	0/1058	1.92	20/1319 (1.5%)
5	H	1.45	0/474	1.74	10/584 (1.7%)
6	I	1.37	0/190	1.72	1/231 (0.4%)
7	O	1.57	0/747	1.92	15/932 (1.6%)
8	T	1.34	0/896	1.70	20/1117 (1.8%)
9	U	1.35	0/619	1.74	4/772 (0.5%)
10	V	1.40	0/684	1.82	11/852 (1.3%)
11	W	1.27	0/339	1.94	8/422 (1.9%)
12	X	1.40	0/247	2.15	7/307 (2.3%)
13	Y	1.29	0/147	1.67	0/182
14	Z	1.33	0/192	1.67	0/237
All	All	1.50	5/20191 (0.0%)	1.89	410/25171 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	3	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
3	D	0	1
3	F	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	145	HIS	CA-C	-5.70	1.49	1.52
2	A	321	GLY	CA-C	-5.55	1.46	1.52
2	A	40	ILE	CA-C	-5.52	1.48	1.53
2	A	157	ALA	CA-C	-5.43	1.48	1.52
3	D	11	GLY	CA-C	-5.18	1.47	1.51

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	ARG	N-CA-C	-11.32	98.97	113.12
4	G	204	ASN	CA-C-N	10.30	126.73	120.24
4	G	204	ASN	C-N-CA	10.30	126.73	120.24
2	C	376	VAL	N-CA-C	-10.18	103.65	111.90
7	O	55	HIS	N-CA-C	-9.62	103.66	114.62
3	F	95	ILE	N-CA-C	-8.89	95.66	108.11
2	C	232	ILE	N-CA-C	-8.82	95.78	108.48
11	W	6	PRO	N-CA-C	8.80	121.43	110.70
2	B	398	GLN	N-CA-C	-8.60	102.92	113.41
7	O	180	ILE	N-CA-C	-8.43	102.64	111.58
3	E	258	ILE	N-CA-C	-8.39	102.90	113.22
2	A	479	ASN	N-CA-C	-8.20	103.28	113.28
4	G	171	SER	N-CA-C	-8.20	96.93	109.14
8	T	140	VAL	N-CA-C	-8.05	104.72	112.29
2	B	479	ASN	N-CA-C	-8.02	103.50	113.28
2	B	193	ASN	N-CA-C	-7.80	102.27	112.41
8	T	80	LYS	N-CA-C	-7.78	102.29	112.41
3	E	106	ARG	N-CA-C	-7.78	103.78	112.57
7	O	98	LEU	N-CA-C	-7.78	102.33	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	90	VAL	N-CA-C	-7.77	96.88	108.46
3	D	312	VAL	N-CA-C	-7.73	99.90	107.55
2	A	177	LYS	N-CA-C	-7.72	102.94	111.36
3	F	39	ILE	N-CA-C	-7.67	97.39	108.36
4	G	137	ALA	N-CA-C	-7.57	100.53	110.07
2	C	69	GLU	N-CA-C	-7.55	97.28	109.58
3	F	225	PRO	CA-C-O	-7.50	115.50	120.90
2	B	30	THR	N-CA-C	-7.48	97.93	109.52
2	B	42	ARG	N-CA-C	-7.46	96.11	108.34
8	T	101	LEU	N-CA-C	-7.46	104.03	113.43
7	O	179	SER	N-CA-C	-7.40	99.50	110.46
10	V	164	LYS	N-CA-C	-7.37	105.21	114.56
3	D	29	GLU	N-CA-C	-7.36	103.89	114.12
2	B	96	ILE	N-CA-C	-7.35	101.90	110.21
10	V	63	LYS	N-CA-C	-7.33	104.59	113.97
3	F	17	ILE	N-CA-C	-7.27	96.61	107.37
4	G	100	ASN	N-CA-C	-7.22	104.50	113.38
2	A	175	THR	N-CA-C	-7.21	105.32	112.97
2	C	42	ARG	N-CA-C	-7.20	95.53	108.48
2	C	234	VAL	N-CA-C	-7.20	98.09	108.17
3	F	252	LEU	N-CA-C	-7.19	98.14	109.07
3	E	42	PRO	N-CA-C	-7.18	107.22	114.68
3	E	43	GLN	N-CA-C	-7.12	103.91	112.59
2	B	93	THR	N-CA-C	-7.08	103.64	111.36
3	E	114	ARG	N-CA-C	-7.05	98.59	109.52
2	A	99	VAL	N-CA-C	-7.04	103.42	109.19
10	V	163	TYR	N-CA-C	-6.97	104.65	113.02
2	B	90	VAL	N-CA-C	-6.96	98.42	108.17
2	C	374	SER	N-CA-C	-6.95	95.78	107.80
10	V	55	PHE	N-CA-C	-6.93	104.44	113.17
5	H	61	GLU	N-CA-C	-6.93	96.98	108.34
2	A	42	ARG	N-CA-C	-6.92	97.14	108.41
2	A	78	PHE	N-CA-C	-6.89	105.02	113.50
3	D	317	LEU	N-CA-C	-6.89	104.91	113.38
1	6	10	ILE	CA-C-N	6.88	127.61	119.98
1	6	10	ILE	C-N-CA	6.88	127.61	119.98
2	B	363	ILE	N-CA-C	-6.84	96.41	107.28
3	F	207	ILE	N-CA-C	-6.83	97.78	107.75
7	O	192	GLU	N-CA-C	-6.78	104.90	113.72
8	T	77	ILE	N-CA-C	-6.66	106.52	112.12
9	U	143	LYS	CA-C-N	6.66	128.95	120.56
9	U	143	LYS	C-N-CA	6.66	128.95	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	224	GLU	CA-C-N	6.64	124.51	119.66
3	F	224	GLU	C-N-CA	6.64	124.51	119.66
3	F	163	LYS	N-CA-C	-6.63	103.98	111.07
3	D	225	PRO	CA-C-O	-6.61	116.14	120.90
8	T	54	ILE	N-CA-C	-6.61	106.80	113.47
5	H	13	GLN	N-CA-C	-6.60	96.39	107.80
3	E	207	ILE	N-CA-C	-6.59	98.24	107.80
2	C	130	ARG	N-CA-C	-6.58	99.19	109.72
3	D	311	TYR	N-CA-C	-6.58	98.17	108.90
3	E	17	ILE	N-CA-C	-6.53	98.46	107.99
3	E	302	GLY	N-CA-C	-6.47	103.24	111.72
2	B	54	LEU	N-CA-C	-6.46	98.71	109.24
1	9	10	ILE	CA-C-N	6.46	127.15	119.98
1	9	10	ILE	C-N-CA	6.46	127.15	119.98
3	F	138	ILE	N-CA-C	-6.45	99.08	108.11
3	D	422	GLU	N-CA-C	-6.45	105.04	113.17
12	X	57	ASN	CA-C-N	6.44	133.56	121.97
12	X	57	ASN	C-N-CA	6.44	133.56	121.97
4	G	73	LEU	N-CA-C	-6.43	99.73	109.95
3	F	54	LEU	N-CA-C	-6.42	105.48	113.38
1	5	43	ILE	CA-C-N	6.41	129.74	120.38
1	5	43	ILE	C-N-CA	6.41	129.74	120.38
3	F	218	VAL	N-CA-C	-6.38	98.94	108.12
3	D	91	THR	N-CA-C	-6.36	105.56	113.38
11	W	5	ILE	CA-C-N	6.36	126.93	120.38
11	W	5	ILE	C-N-CA	6.36	126.93	120.38
2	A	296	TYR	N-CA-C	-6.35	101.32	110.40
3	D	256	ASP	N-CA-C	-6.32	99.46	109.07
2	A	232	ILE	N-CA-C	-6.30	99.13	108.45
2	C	169	ILE	N-CA-C	-6.29	98.80	107.99
3	E	181	PHE	N-CA-C	-6.29	99.99	108.86
5	H	45	HIS	N-CA-C	-6.29	99.75	109.24
3	D	214	LYS	N-CA-C	-6.29	105.55	112.72
11	W	39	ALA	CA-C-N	6.27	126.29	119.89
11	W	39	ALA	C-N-CA	6.27	126.29	119.89
10	V	81	VAL	N-CA-C	-6.27	96.71	107.24
2	B	289	ARG	N-CA-C	-6.26	101.76	109.65
3	D	206	VAL	N-CA-C	-6.26	104.40	110.72
3	D	224	GLU	CA-C-N	6.25	124.22	119.66
3	D	224	GLU	C-N-CA	6.25	124.22	119.66
1	4	43	ILE	CA-C-N	6.25	129.50	120.38
1	4	43	ILE	C-N-CA	6.25	129.50	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	420	VAL	N-CA-C	-6.23	105.55	113.22
8	T	210	PHE	CA-C-N	6.22	124.16	120.24
8	T	210	PHE	C-N-CA	6.22	124.16	120.24
7	O	176	VAL	N-CA-C	-6.21	99.19	108.12
4	G	112	ASP	N-CA-C	6.20	118.04	111.28
2	B	68	LEU	N-CA-C	-6.20	98.62	108.73
2	C	228	MET	N-CA-C	-6.20	106.40	112.97
1	1	42	SER	N-CA-C	6.19	120.30	112.87
3	D	208	ASN	N-CA-C	-6.19	97.98	108.26
2	A	193	ASN	CA-C-N	6.19	125.86	119.92
2	A	193	ASN	C-N-CA	6.19	125.86	119.92
3	D	58	THR	N-CA-C	-6.18	98.20	108.34
2	B	91	LYS	N-CA-C	-6.17	99.33	109.40
2	C	206	VAL	N-CA-C	-6.17	99.48	108.11
2	A	50	GLN	N-CA-C	-6.16	99.61	109.96
3	E	156	PHE	N-CA-C	-6.14	99.96	109.24
3	E	24	HIS	N-CA-C	-6.12	99.22	109.07
5	H	56	VAL	N-CA-C	-6.10	99.57	108.11
3	F	176	LYS	N-CA-C	-6.10	106.00	113.50
2	B	60	GLY	N-CA-C	-6.09	106.36	114.95
10	V	133	LEU	N-CA-C	-6.08	97.86	110.80
7	O	150	GLY	N-CA-C	-6.08	107.25	114.48
3	D	22	ASP	N-CA-C	-6.07	100.29	109.95
5	H	69	PHE	N-CA-C	-6.07	99.00	108.90
4	G	84	CYS	N-CA-C	-6.07	104.52	112.41
3	F	16	VAL	N-CA-C	-6.07	96.72	109.34
2	A	68	LEU	N-CA-C	-6.06	98.54	108.41
7	O	160	LYS	N-CA-C	-6.06	97.71	108.55
2	C	118	ASP	N-CA-C	-6.05	104.80	111.82
3	F	351	LEU	N-CA-C	-6.03	105.57	113.17
4	G	162	ILE	N-CA-C	-6.03	99.03	108.86
3	D	284	THR	N-CA-C	-6.03	105.10	112.88
2	C	355	GLU	CA-C-N	6.03	128.36	120.28
2	C	355	GLU	C-N-CA	6.03	128.36	120.28
3	E	254	PHE	N-CA-C	-6.03	100.74	110.32
3	F	426	GLY	N-CA-C	-6.01	106.94	115.30
11	W	31	TYR	N-CA-C	-6.00	104.67	112.23
2	B	175	THR	N-CA-C	-5.99	104.57	112.72
4	G	164	ILE	N-CA-C	-5.99	99.09	108.86
2	A	64	MET	N-CA-C	-5.99	100.30	109.41
1	6	54	GLY	CA-C-N	5.99	128.23	120.44
1	6	54	GLY	C-N-CA	5.99	128.23	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	180	LYS	N-CA-C	-5.99	102.74	108.07
2	B	7	PRO	N-CA-C	-5.98	106.87	114.35
3	E	22	ASP	N-CA-C	-5.97	99.97	109.59
3	F	156	PHE	N-CA-C	-5.96	101.37	109.54
3	E	304	VAL	N-CA-C	-5.96	103.55	110.05
2	B	262	ASN	N-CA-C	-5.96	104.72	112.23
1	7	20	LEU	CA-C-N	5.94	126.57	119.98
1	7	20	LEU	C-N-CA	5.94	126.57	119.98
2	A	352	ILE	N-CA-C	-5.93	99.58	108.12
1	8	17	ILE	CA-C-N	5.90	126.64	120.03
1	8	17	ILE	C-N-CA	5.90	126.64	120.03
1	8	10	ILE	CA-C-N	5.90	126.53	119.98
1	8	10	ILE	C-N-CA	5.90	126.53	119.98
4	G	166	TYR	N-CA-C	-5.89	99.57	107.88
11	W	61	ALA	N-CA-C	-5.89	105.41	112.59
8	T	205	THR	N-CA-C	-5.88	105.93	113.23
1	7	2	GLN	CA-C-N	5.88	128.16	120.28
1	7	2	GLN	C-N-CA	5.88	128.16	120.28
2	A	363	ILE	N-CA-C	-5.87	98.17	107.15
2	C	329	ILE	N-CA-C	-5.85	99.91	108.11
3	E	77	LEU	N-CA-C	-5.85	99.47	109.24
3	F	254	PHE	N-CA-C	-5.83	99.50	109.24
3	D	255	ILE	N-CA-C	-5.83	99.36	108.86
8	T	146	VAL	N-CA-C	-5.81	102.27	107.56
2	C	265	HIS	N-CA-C	-5.81	100.23	109.76
3	F	258	ILE	N-CA-C	-5.79	106.14	112.80
1	5	2	GLN	N-CA-C	-5.78	104.89	111.14
2	B	263	GLY	N-CA-C	-5.78	106.55	114.64
3	E	208	ASN	N-CA-C	-5.77	95.64	107.70
2	B	62	LYS	N-CA-C	-5.76	100.40	109.50
3	E	301	LYS	N-CA-C	-5.75	105.84	112.92
1	7	24	ILE	CA-C-N	5.73	126.30	119.94
1	7	24	ILE	C-N-CA	5.73	126.30	119.94
3	E	76	VAL	N-CA-C	-5.73	99.52	108.86
4	G	2	THR	N-CA-C	-5.71	104.97	111.14
3	F	63	ALA	N-CA-C	-5.71	99.22	108.52
1	8	43	ILE	CA-C-N	5.69	128.18	120.38
1	8	43	ILE	C-N-CA	5.69	128.18	120.38
3	E	54	LEU	N-CA-C	-5.68	106.20	113.02
7	O	154	LYS	N-CA-C	-5.68	97.90	108.02
2	C	479	ASN	N-CA-C	-5.67	106.19	113.23
3	D	89	ARG	N-CA-C	-5.67	106.13	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	40	GLY	N-CA-C	-5.66	101.56	111.46
7	O	84	TYR	N-CA-C	-5.64	104.75	111.69
3	F	53	HIS	N-CA-C	-5.63	100.00	109.07
3	D	53	HIS	N-CA-C	-5.63	100.22	109.40
3	E	317	LEU	CA-C-N	5.63	128.38	120.28
3	E	317	LEU	C-N-CA	5.63	128.38	120.28
3	F	22	ASP	N-CA-C	-5.63	99.84	109.24
3	F	336	SER	CA-C-N	5.62	128.38	120.28
3	F	336	SER	C-N-CA	5.62	128.38	120.28
2	A	350	GLY	N-CA-C	-5.61	106.62	111.95
1	2	20	LEU	CA-C-N	5.61	126.20	119.98
1	2	20	LEU	C-N-CA	5.61	126.20	119.98
4	G	75	VAL	N-CA-C	-5.61	99.72	108.86
9	U	144	VAL	CA-C-N	5.60	127.72	120.44
9	U	144	VAL	C-N-CA	5.60	127.72	120.44
2	A	201	LEU	N-CA-C	-5.60	100.06	108.96
4	G	165	PHE	N-CA-C	-5.59	100.66	109.50
3	E	424	PHE	N-CA-C	5.59	117.45	111.36
3	E	298	THR	N-CA-C	-5.58	100.08	108.96
1	7	43	ILE	CA-C-N	5.58	128.03	120.38
1	7	43	ILE	C-N-CA	5.58	128.03	120.38
1	6	43	ILE	CA-C-N	5.57	128.01	120.38
1	6	43	ILE	C-N-CA	5.57	128.01	120.38
7	O	147	VAL	N-CA-C	-5.55	98.44	106.88
3	D	138	ILE	N-CA-C	-5.55	99.65	107.75
5	H	66	LYS	N-CA-C	-5.54	99.99	109.24
3	E	204	THR	N-CA-C	-5.53	106.31	113.16
3	D	421	ALA	N-CA-C	-5.52	103.81	110.88
2	C	490	GLU	N-CA-C	-5.51	99.32	108.75
1	9	43	ILE	CA-C-N	5.51	127.66	120.28
1	9	43	ILE	C-N-CA	5.51	127.66	120.28
3	D	136	THR	N-CA-C	-5.51	106.61	113.55
8	T	207	VAL	N-CA-C	-5.51	99.81	108.23
10	V	83	ILE	CA-C-N	5.51	132.06	121.54
10	V	83	ILE	C-N-CA	5.51	132.06	121.54
2	C	133	VAL	N-CA-C	-5.50	101.08	108.35
2	A	128	ARG	N-CA-C	-5.50	99.93	108.90
2	C	109	VAL	N-CA-C	-5.49	100.54	108.71
3	F	395	GLU	N-CA-C	-5.48	106.59	113.28
3	E	65	ASP	CA-C-N	5.48	125.30	120.10
3	E	65	ASP	C-N-CA	5.48	125.30	120.10
2	B	176	GLY	N-CA-C	-5.48	103.21	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	61	THR	CA-C-N	5.47	126.06	119.98
1	1	61	THR	C-N-CA	5.47	126.06	119.98
1	2	43	ILE	CA-C-N	5.47	127.88	120.38
1	2	43	ILE	C-N-CA	5.47	127.88	120.38
4	G	163	SER	N-CA-C	-5.46	99.41	108.75
2	C	351	GLN	N-CA-C	-5.44	100.16	109.24
2	B	40	ILE	N-CA-C	-5.43	100.01	108.81
8	T	201	ILE	N-CA-C	-5.43	100.57	108.17
3	D	17	ILE	N-CA-C	-5.43	98.05	109.34
3	F	461	GLY	N-CA-C	-5.43	103.22	111.14
10	V	90	GLN	N-CA-C	-5.42	106.72	113.55
1	8	22	ALA	CA-C-N	5.42	125.95	119.94
1	8	22	ALA	C-N-CA	5.42	125.95	119.94
2	A	422	ARG	CA-C-N	5.42	125.99	119.98
2	A	422	ARG	C-N-CA	5.42	125.99	119.98
1	6	24	ILE	CA-C-N	5.40	125.94	119.94
1	6	24	ILE	C-N-CA	5.40	125.94	119.94
6	I	48	LYS	N-CA-C	-5.40	100.31	108.52
2	A	492	SER	N-CA-C	-5.40	102.76	110.59
2	B	128	ARG	N-CA-C	-5.40	100.97	109.50
3	F	81	GLY	CA-C-N	5.39	125.40	119.90
3	F	81	GLY	C-N-CA	5.39	125.40	119.90
2	C	287	LEU	N-CA-C	-5.39	105.34	112.94
1	1	15	SER	CA-C-N	5.39	128.04	120.28
1	1	15	SER	C-N-CA	5.39	128.04	120.28
1	7	44	LYS	N-CA-C	5.39	117.85	111.33
2	C	54	LEU	N-CA-C	-5.38	100.40	109.07
1	2	2	GLN	CA-C-N	5.38	127.49	120.28
1	2	2	GLN	C-N-CA	5.38	127.49	120.28
3	D	112	LYS	N-CA-C	-5.38	104.38	111.96
3	E	452	ILE	CA-C-N	5.38	125.37	119.89
3	E	452	ILE	C-N-CA	5.38	125.37	119.89
2	B	98	ASP	N-CA-C	-5.37	101.20	109.52
11	W	14	ASN	N-CA-C	-5.37	106.74	113.72
3	D	220	GLY	N-CA-C	-5.36	100.48	113.18
8	T	112	SER	N-CA-C	-5.35	106.59	113.23
1	2	10	ILE	CA-C-N	5.35	125.92	119.98
1	2	10	ILE	C-N-CA	5.35	125.92	119.98
2	C	296	TYR	CA-C-N	5.35	125.35	119.89
2	C	296	TYR	C-N-CA	5.35	125.35	119.89
3	D	21	VAL	N-CA-C	-5.35	100.36	108.17
2	C	60	GLY	N-CA-C	-5.35	107.53	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	150	GLY	CA-C-N	5.35	128.01	121.06
3	E	150	GLY	C-N-CA	5.35	128.01	121.06
3	D	162	GLY	N-CA-C	-5.34	105.62	114.48
2	C	193	ASN	N-CA-C	-5.33	105.55	111.36
3	E	351	LEU	N-CA-C	-5.33	106.55	113.16
2	B	22	SER	CA-C-N	5.33	127.42	120.28
2	B	22	SER	C-N-CA	5.33	127.42	120.28
1	9	61	THR	CA-C-N	5.32	125.89	119.98
1	9	61	THR	C-N-CA	5.32	125.89	119.98
2	B	296	TYR	CA-C-N	5.32	126.49	119.84
2	B	296	TYR	C-N-CA	5.32	126.49	119.84
5	H	41	VAL	N-CA-C	-5.32	100.46	108.12
2	B	355	GLU	CA-C-N	5.32	127.41	120.28
2	B	355	GLU	C-N-CA	5.32	127.41	120.28
8	T	46	LEU	CA-C-N	5.32	127.40	120.28
8	T	46	LEU	C-N-CA	5.32	127.40	120.28
3	D	392	GLY	N-CA-C	-5.31	106.91	111.95
8	T	74	LYS	N-CA-C	-5.30	105.55	112.23
2	A	375	ARG	N-CA-C	-5.29	106.05	112.88
3	F	317	LEU	N-CA-C	-5.29	106.33	112.89
2	B	148	VAL	N-CA-C	-5.29	100.70	108.11
3	E	25	PHE	N-CA-C	-5.29	101.49	109.85
2	B	389	ALA	N-CA-C	-5.29	103.99	110.65
3	D	211	GLY	N-CA-C	-5.28	104.94	112.55
8	T	76	GLN	N-CA-C	5.28	116.72	111.07
7	O	56	LEU	N-CA-C	-5.28	106.23	113.30
2	A	176	GLY	N-CA-C	-5.28	100.68	113.18
1	8	2	GLN	CA-C-N	5.27	127.34	120.28
1	8	2	GLN	C-N-CA	5.27	127.34	120.28
2	A	96	ILE	N-CA-C	-5.26	104.26	110.21
2	C	41	ALA	N-CA-C	-5.26	102.26	110.42
1	3	19	LEU	CA-C-N	5.26	127.58	120.38
1	3	19	LEU	C-N-CA	5.26	127.58	120.38
2	A	234	VAL	N-CA-C	-5.26	101.01	108.58
1	0	61	THR	CA-C-N	5.26	125.81	119.98
1	0	61	THR	C-N-CA	5.26	125.81	119.98
2	A	444	VAL	CA-C-O	-5.25	114.38	118.85
10	V	157	LYS	N-CA-C	-5.25	101.08	109.07
5	H	82	GLN	N-CA-C	-5.25	98.69	107.99
7	O	30	ASN	CA-C-N	5.25	129.58	122.07
7	O	30	ASN	C-N-CA	5.25	129.58	122.07
3	F	128	SER	N-CA-C	-5.24	99.97	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	61	THR	CA-C-N	5.24	125.80	119.98
1	4	61	THR	C-N-CA	5.24	125.80	119.98
2	C	129	SER	N-CA-C	-5.24	101.48	108.86
4	G	176	GLU	N-CA-C	-5.24	101.02	109.40
1	4	24	ILE	CA-C-N	5.23	125.75	119.94
1	4	24	ILE	C-N-CA	5.23	125.75	119.94
2	B	234	VAL	N-CA-C	-5.23	100.94	108.53
3	D	23	VAL	N-CA-C	-5.23	100.32	108.95
8	T	27	THR	CA-C-N	5.23	127.28	120.28
8	T	27	THR	C-N-CA	5.23	127.28	120.28
12	X	2	VAL	CA-C-N	5.22	127.14	120.56
12	X	2	VAL	C-N-CA	5.22	127.14	120.56
3	E	305	THR	N-CA-C	-5.22	101.14	109.23
3	F	23	VAL	N-CA-C	-5.21	100.87	108.99
3	F	452	ILE	CA-C-N	5.21	125.20	119.89
3	F	452	ILE	C-N-CA	5.21	125.20	119.89
3	E	185	THR	N-CA-C	-5.20	100.70	109.07
2	A	148	VAL	N-CA-C	-5.20	100.83	108.11
3	D	185	THR	N-CA-C	-5.19	100.00	108.76
8	T	200	LEU	N-CA-C	-5.18	106.64	113.17
3	F	104	ASP	N-CA-C	-5.18	107.00	113.38
5	H	47	PRO	N-CA-C	-5.18	101.80	112.47
2	C	193	ASN	CA-C-N	5.17	124.89	119.92
2	C	193	ASN	C-N-CA	5.17	124.89	119.92
2	C	443	GLN	N-CA-C	-5.17	107.52	113.88
3	D	10	THR	N-CA-C	-5.17	99.80	110.80
3	F	295	ARG	N-CA-C	-5.17	106.66	113.17
1	3	43	ILE	CA-C-N	5.17	127.92	120.38
1	3	43	ILE	C-N-CA	5.17	127.92	120.38
1	1	17	ILE	CA-C-N	5.16	126.64	120.13
1	1	17	ILE	C-N-CA	5.16	126.64	120.13
1	5	74	PHE	N-CA-C	-5.16	105.72	112.23
3	D	353	SER	N-CA-C	-5.16	100.11	108.52
1	8	5	LEU	CA-C-N	5.16	127.15	120.44
1	8	5	LEU	C-N-CA	5.16	127.15	120.44
3	E	464	GLU	CA-C-N	5.16	127.19	120.28
3	E	464	GLU	C-N-CA	5.16	127.19	120.28
1	6	6	ALA	CA-C-N	5.15	127.18	120.28
1	6	6	ALA	C-N-CA	5.15	127.18	120.28
2	C	85	LYS	N-CA-C	-5.15	99.94	108.75
3	F	60	ARG	N-CA-C	-5.15	100.06	108.76
1	4	18	GLY	CA-C-N	5.14	127.68	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	18	GLY	C-N-CA	5.14	127.68	120.28
3	D	179	GLY	N-CA-C	-5.13	108.30	114.66
2	B	386	LYS	N-CA-C	-5.13	106.71	113.12
1	9	24	ILE	CA-C-N	5.13	125.63	119.94
1	9	24	ILE	C-N-CA	5.13	125.63	119.94
3	D	81	GLY	CA-C-N	5.13	125.13	119.90
3	D	81	GLY	C-N-CA	5.13	125.13	119.90
3	F	88	GLY	N-CA-C	-5.11	104.29	111.09
4	G	101	ASP	N-CA-C	-5.11	106.73	113.17
2	C	176	GLY	N-CA-C	-5.11	108.20	115.30
12	X	58	VAL	N-CA-C	-5.10	98.72	109.34
3	F	299	THR	N-CA-C	-5.10	102.34	109.69
2	C	89	LEU	N-CA-C	-5.10	101.96	110.17
2	B	120	LYS	N-CA-C	-5.10	107.22	112.93
1	0	15	SER	CA-C-N	5.10	127.82	120.38
1	0	15	SER	C-N-CA	5.10	127.82	120.38
2	B	456	ASP	N-CA-C	-5.09	107.22	112.93
2	B	121	GLY	CA-C-N	5.09	126.21	119.84
2	B	121	GLY	C-N-CA	5.09	126.21	119.84
3	F	216	ALA	N-CA-C	-5.09	101.63	109.52
2	B	397	ALA	N-CA-C	-5.08	106.67	112.92
3	D	254	PHE	N-CA-C	-5.08	100.42	109.06
7	O	57	LEU	N-CA-C	-5.08	106.93	113.23
2	C	205	TYR	N-CA-C	-5.08	100.89	109.07
2	B	459	GLU	CA-C-N	5.07	127.08	120.28
2	B	459	GLU	C-N-CA	5.07	127.08	120.28
3	D	16	VAL	N-CA-C	-5.07	100.44	107.80
2	C	91	LYS	N-CA-C	-5.07	100.64	108.90
3	E	53	HIS	N-CA-C	-5.07	100.15	108.41
4	G	156	ALA	CA-C-N	5.07	126.47	120.14
4	G	156	ALA	C-N-CA	5.07	126.47	120.14
10	V	26	ALA	N-CA-C	-5.07	106.24	114.09
1	8	15	SER	CA-C-N	5.06	127.57	120.28
1	8	15	SER	C-N-CA	5.06	127.57	120.28
2	B	88	GLU	N-CA-C	-5.06	102.58	110.42
2	B	25	ALA	CA-C-N	5.06	127.02	120.44
2	B	25	ALA	C-N-CA	5.06	127.02	120.44
3	E	421	ALA	N-CA-C	-5.05	106.96	112.72
1	0	12	ALA	CA-C-N	5.05	125.55	119.94
1	0	12	ALA	C-N-CA	5.05	125.55	119.94
3	D	273	GLY	N-CA-C	-5.05	108.15	115.27
2	C	94	GLY	N-CA-C	-5.05	108.31	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	VAL	N-CA-C	-5.04	100.63	107.99
2	A	260	ARG	CA-C-N	5.04	127.44	120.29
2	A	260	ARG	C-N-CA	5.04	127.44	120.29
3	D	361	ALA	N-CA-C	-5.03	104.79	112.04
3	E	46	LEU	N-CA-C	-5.03	100.25	108.76
2	A	294	GLU	CA-C-N	5.02	129.46	122.08
2	A	294	GLU	C-N-CA	5.02	129.46	122.08
3	D	461	GLY	CA-C-N	5.02	131.25	121.41
3	D	461	GLY	C-N-CA	5.02	131.25	121.41
3	E	294	GLU	N-CA-C	-5.02	108.19	114.56
8	T	113	ALA	N-CA-C	-5.02	107.16	113.28
12	X	23	ASP	CA-C-N	5.01	127.00	120.28
12	X	23	ASP	C-N-CA	5.01	127.00	120.28

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	40	ASN	Peptide
1	3	40	ASN	Peptide
1	4	40	ASN	Peptide
1	5	40	ASN	Peptide
1	6	40	ASN	Peptide
1	7	40	ASN	Peptide
1	8	40	ASN	Peptide
1	9	40	ASN	Peptide
3	D	256	ASP	Peptide
3	F	345	TYR	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
2	B	2020	0	575	2	0
2	C	1992	0	572	1	0
3	D	1880	0	538	0	0
3	E	1872	0	537	1	0
3	F	1876	0	537	2	0
4	G	1060	0	277	0	0
5	H	479	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	20227	0	5731	7	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 (7) 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:160:GLY:C	3:F:162:GLY:H	2.24	0.45
2:A:174:GLN:C	2:A:176:GLY:H	2.24	0.44
2:B:102:GLY:HA3	2:B:126:ALA:H	1.82	0.44
3:F:278:ALA:C	3:F:280:GLY:H	2.26	0.43
2:C:227:ALA:C	2:C:229:LYS:H	2.27	0.42
2:B:24:GLU:C	2:B:26:ASN:H	2.28	0.41
3:E:41:THR:C	3:E:43:GLN:H	2.29	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%)	72 (99%)	1 (1%)	0	100	100
1	1	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	3	72/76 (95%)	69 (96%)	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%)	70 (97%)	1 (1%)	1 (1%)	9	40
2	A	495/510 (97%)	467 (94%)	21 (4%)	7 (1%)	9	40
2	B	501/510 (98%)	470 (94%)	26 (5%)	5 (1%)	12	48
2	C	496/510 (97%)	469 (95%)	22 (4%)	5 (1%)	12	48
3	D	468/478 (98%)	438 (94%)	21 (4%)	9 (2%)	6	32
3	E	466/478 (98%)	446 (96%)	15 (3%)	5 (1%)	11	46
3	F	467/478 (98%)	429 (92%)	30 (6%)	8 (2%)	7	36
4	G	261/278 (94%)	251 (96%)	7 (3%)	3 (1%)	11	46
5	H	110/138 (80%)	98 (89%)	9 (8%)	3 (3%)	4	25
6	I	42/61 (69%)	41 (98%)	1 (2%)	0	100	100
7	O	185/195 (95%)	165 (89%)	15 (8%)	5 (3%)	4	25
8	T	222/249 (89%)	213 (96%)	7 (3%)	2 (1%)	14	51
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	149 (88%)	11 (6%)	9 (5%)	1	14
11	W	83/95 (87%)	73 (88%)	6 (7%)	4 (5%)	2	16
12	X	60/92 (65%)	52 (87%)	5 (8%)	3 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Y	35/59 (59%)	34 (97%)	1 (3%)	0	100	100
14	Z	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
All	All	4984/5321 (94%)	4693 (94%)	214 (4%)	77 (2%)	11	40

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	41	PRO
1	3	41	PRO
1	4	41	PRO
1	5	41	PRO
1	6	41	PRO
1	7	41	PRO
1	8	41	PRO
1	9	41	PRO
2	A	229	LYS
2	A	311	ALA
2	C	35	ALA
2	C	165	GLN
2	C	379	ALA
3	D	395	GLU
3	D	451	ASN
3	D	462	GLY
3	F	159	ALA
3	F	279	VAL
3	F	451	ASN
5	H	80	ASP
7	O	81	LEU
7	O	82	ASP
8	T	50	ASN
10	V	65	THR
10	V	86	SER
10	V	89	LEU
11	W	47	ARG
12	X	58	VAL
2	A	22	SER
2	B	103	PRO
3	D	10	THR
3	D	131	ALA
3	E	34	LEU
3	E	279	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	E	359	ASP
5	H	33	PRO
7	O	165	GLY
8	T	202	ASN
10	V	82	LYS
10	V	84	ASP
10	V	130	PHE
10	V	133	LEU
11	W	42	ILE
2	A	25	ALA
2	A	319	GLY
2	A	406	ALA
2	B	29	GLU
2	C	49	ILE
3	D	34	LEU
3	F	68	GLU
7	O	10	VAL
10	V	170	LEU
11	W	11	SER
1	3	42	SER
2	A	49	ILE
2	B	143	SER
3	F	86	PRO
3	F	278	ALA
4	G	56	GLU
5	H	22	TYR
10	V	48	SER
11	W	59	ASP
12	X	38	ASN
2	B	145	HIS
2	B	189	LYS
2	C	380	ALA
3	D	249	GLN
3	E	16	VAL
3	E	31	PRO
3	F	131	ALA
7	O	149	GLN
3	D	30	LEU
3	F	282	GLN
3	D	86	PRO
4	G	123	PRO
4	G	181	PRO

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Mol	Chain	Res	Type
12	X	36	LYS

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

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

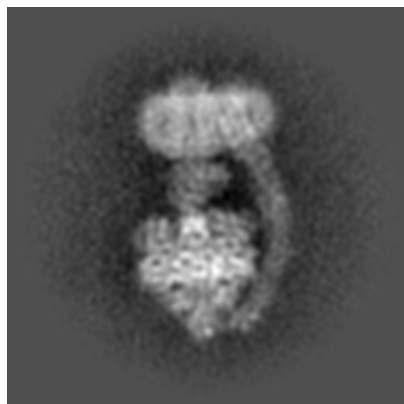
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25959. These allow visual inspection of the internal detail of the map and identification of artifacts.

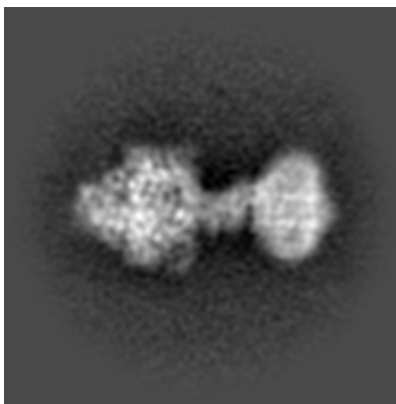
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

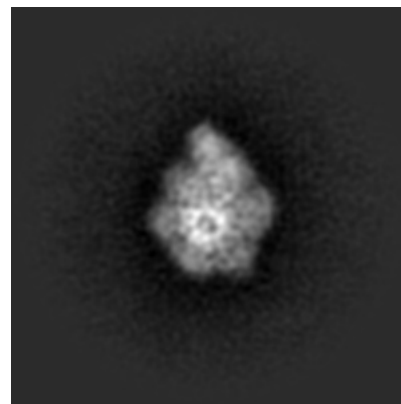
#### 6.1.1 Primary map



X

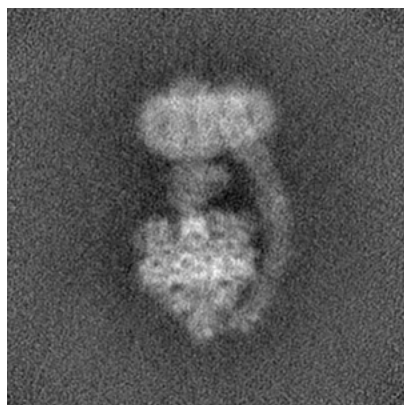


Y

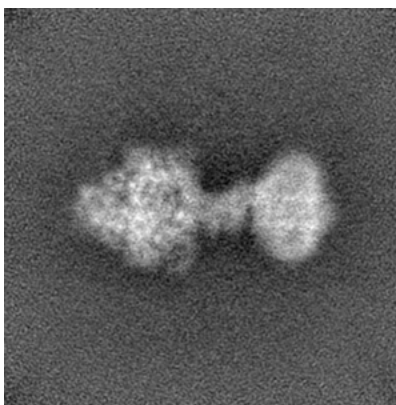


Z

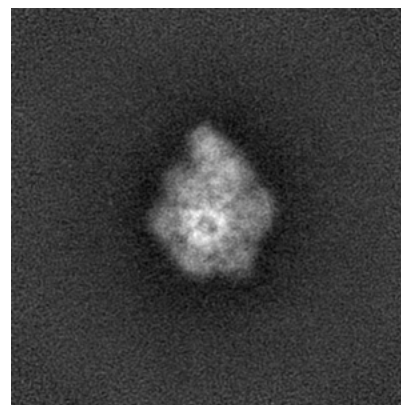
#### 6.1.2 Raw map



X



Y

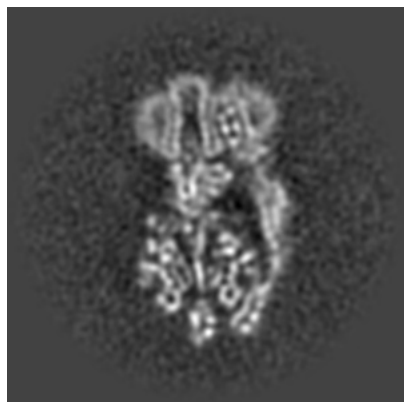


Z

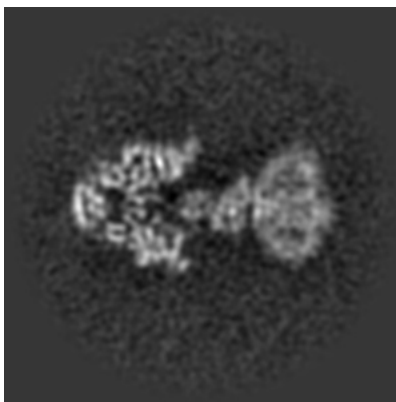
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

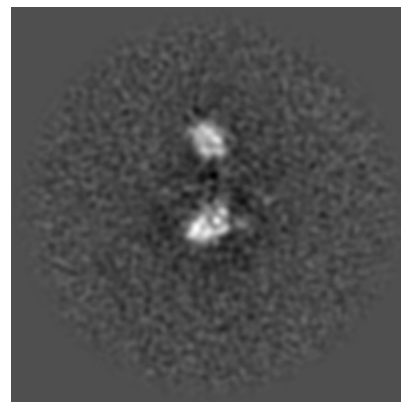
### 6.2.1 Primary map



X Index: 128

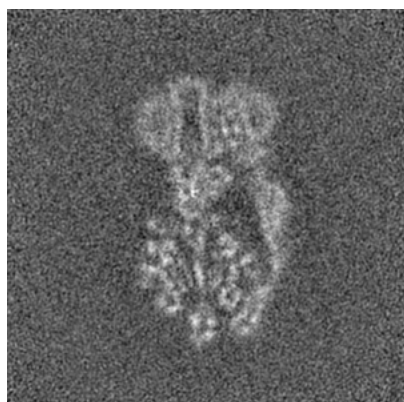


Y Index: 128

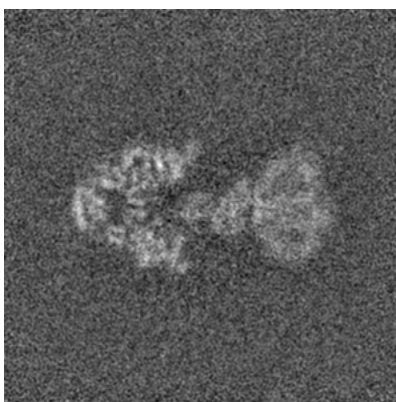


Z Index: 128

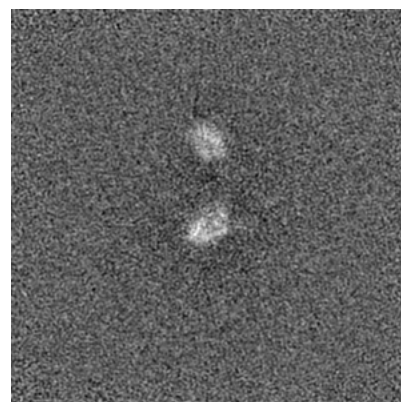
### 6.2.2 Raw map



X Index: 128



Y Index: 128

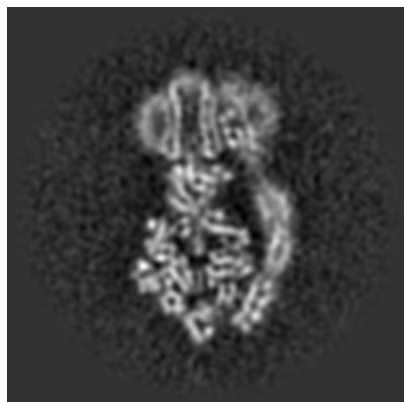


Z Index: 128

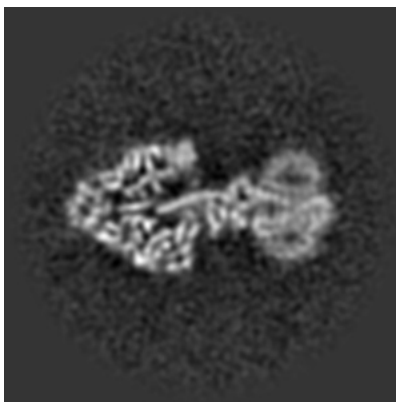
The images above show central slices of the map in three orthogonal directions.

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

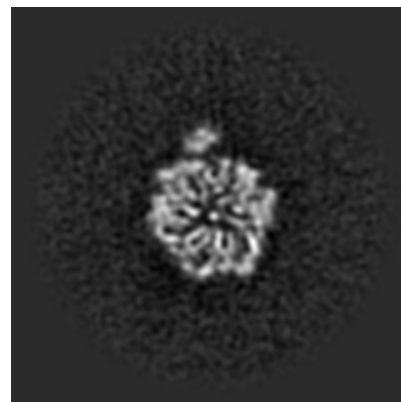
### 6.3.1 Primary map



X Index: 124

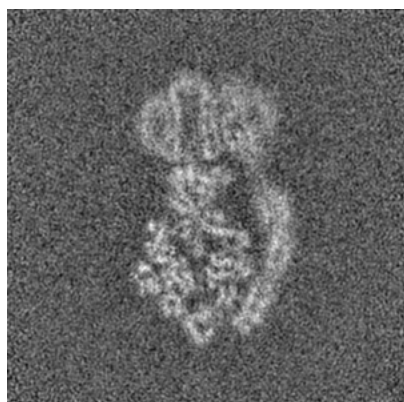


Y Index: 124

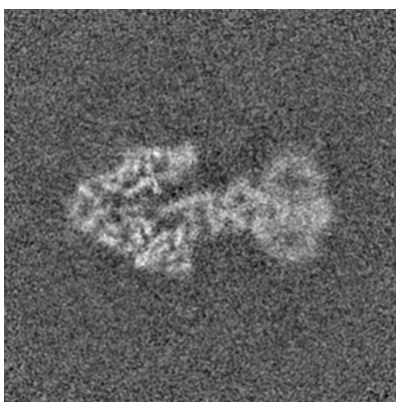


Z Index: 91

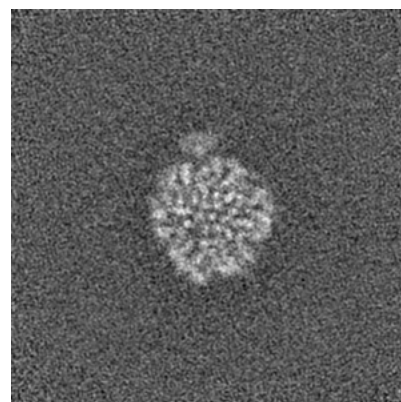
### 6.3.2 Raw map



X Index: 124



Y Index: 125

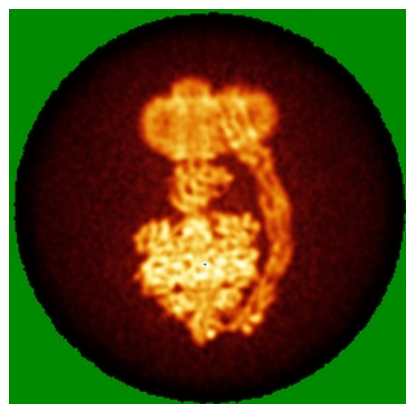


Z Index: 86

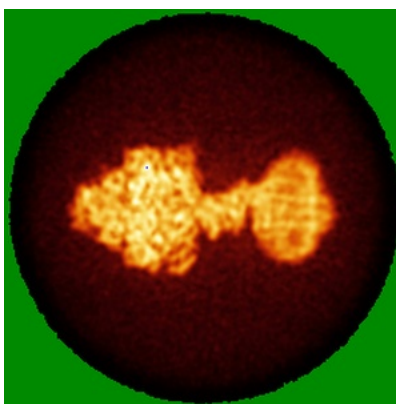
The images above show the largest variance slices of the map in three orthogonal directions.

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

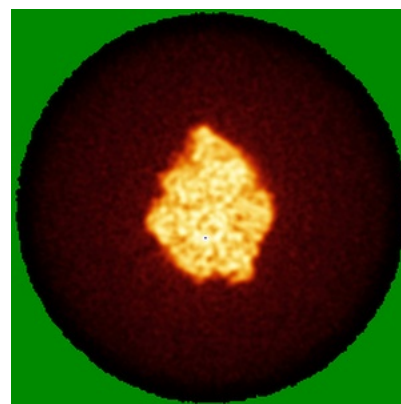
### 6.4.1 Primary map



X

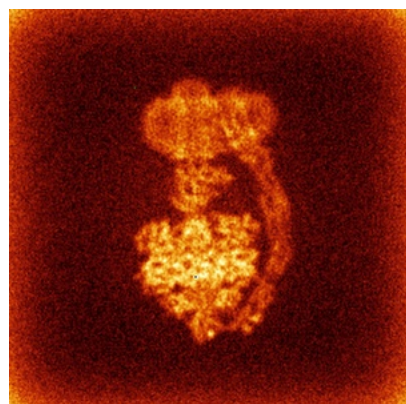


Y

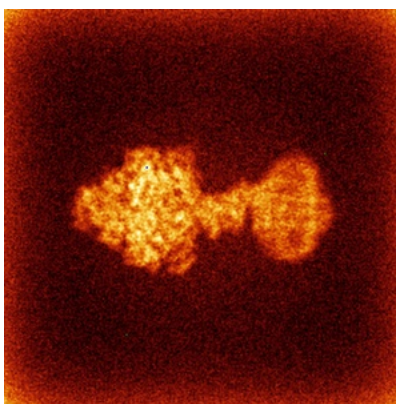


Z

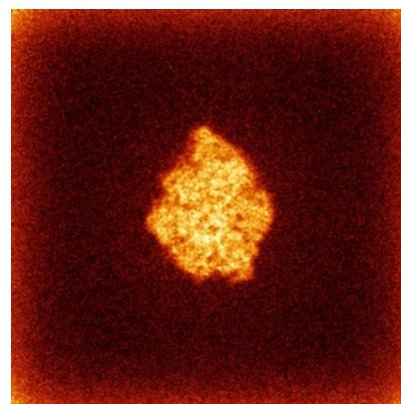
### 6.4.2 Raw map



X



Y

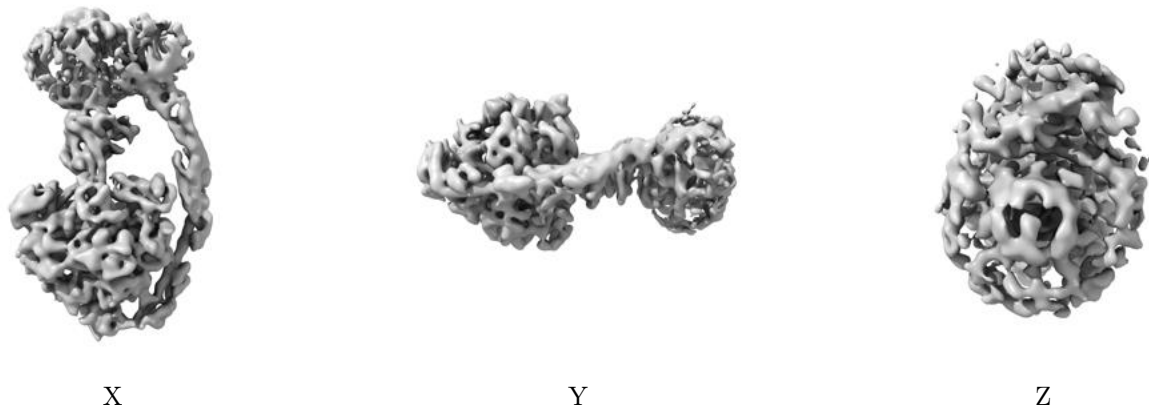


Z

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

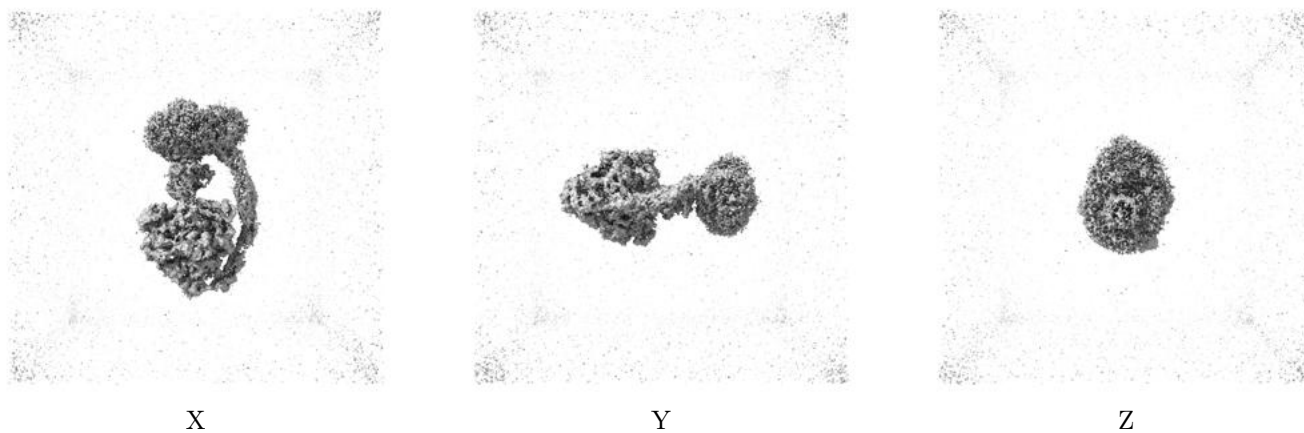
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

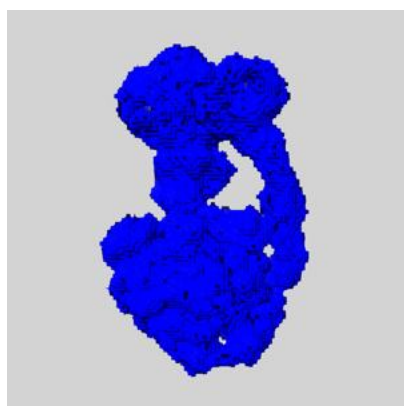
## 6.6 Mask visualisation [i](#)

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

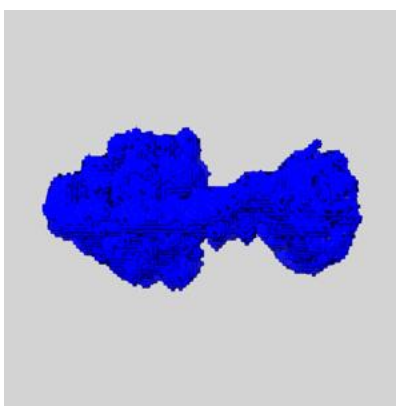
A mask typically either:

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

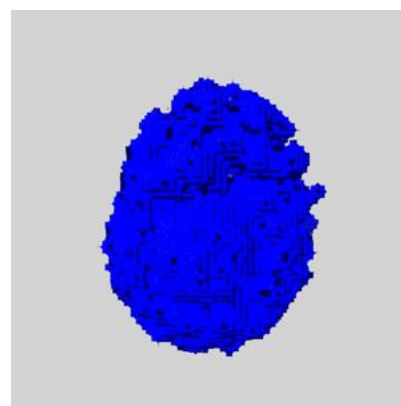
### 6.6.1 emd\_25959\_msk\_1.map [i](#)



X



Y

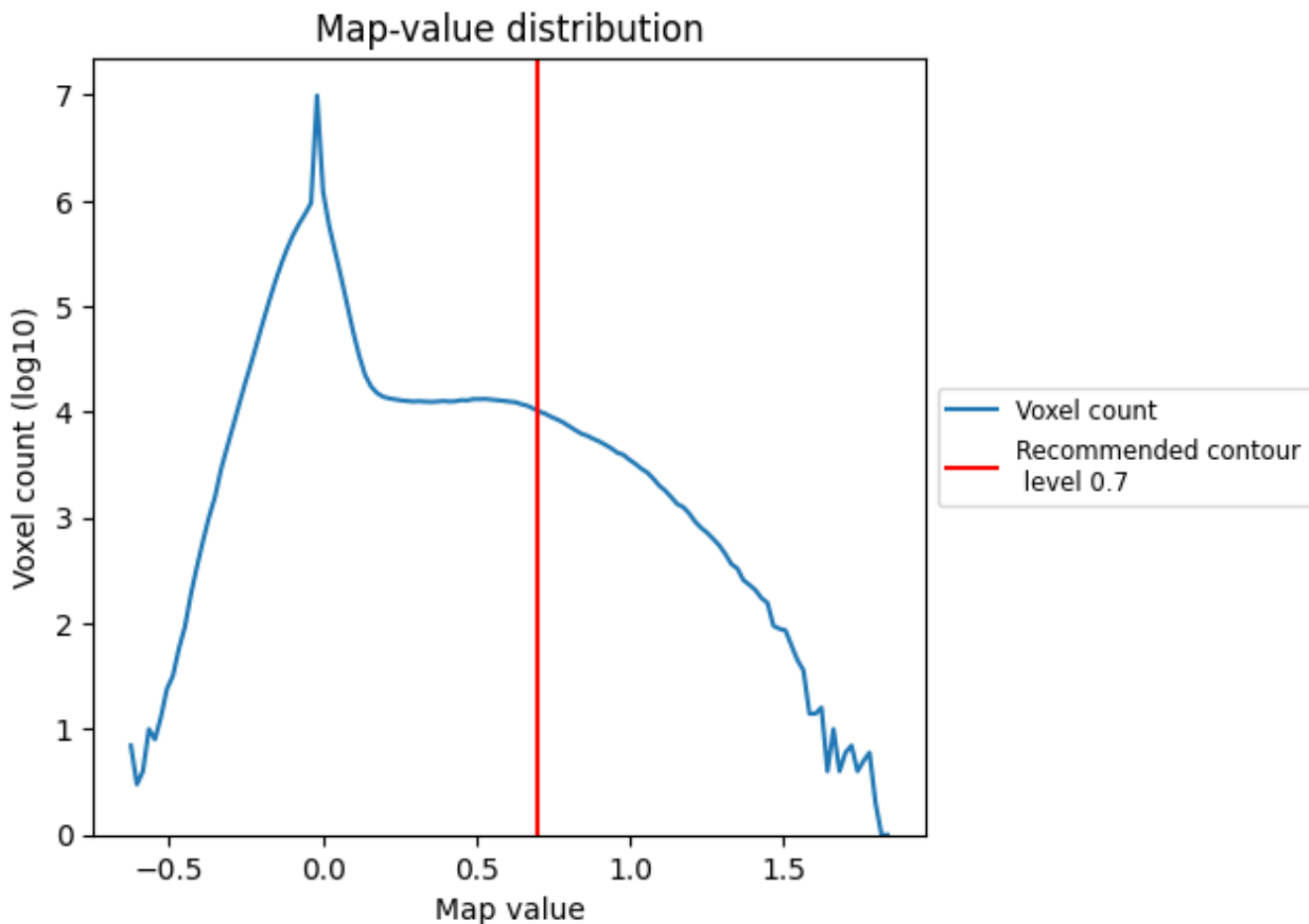


Z

## 7 Map analysis [i](#)

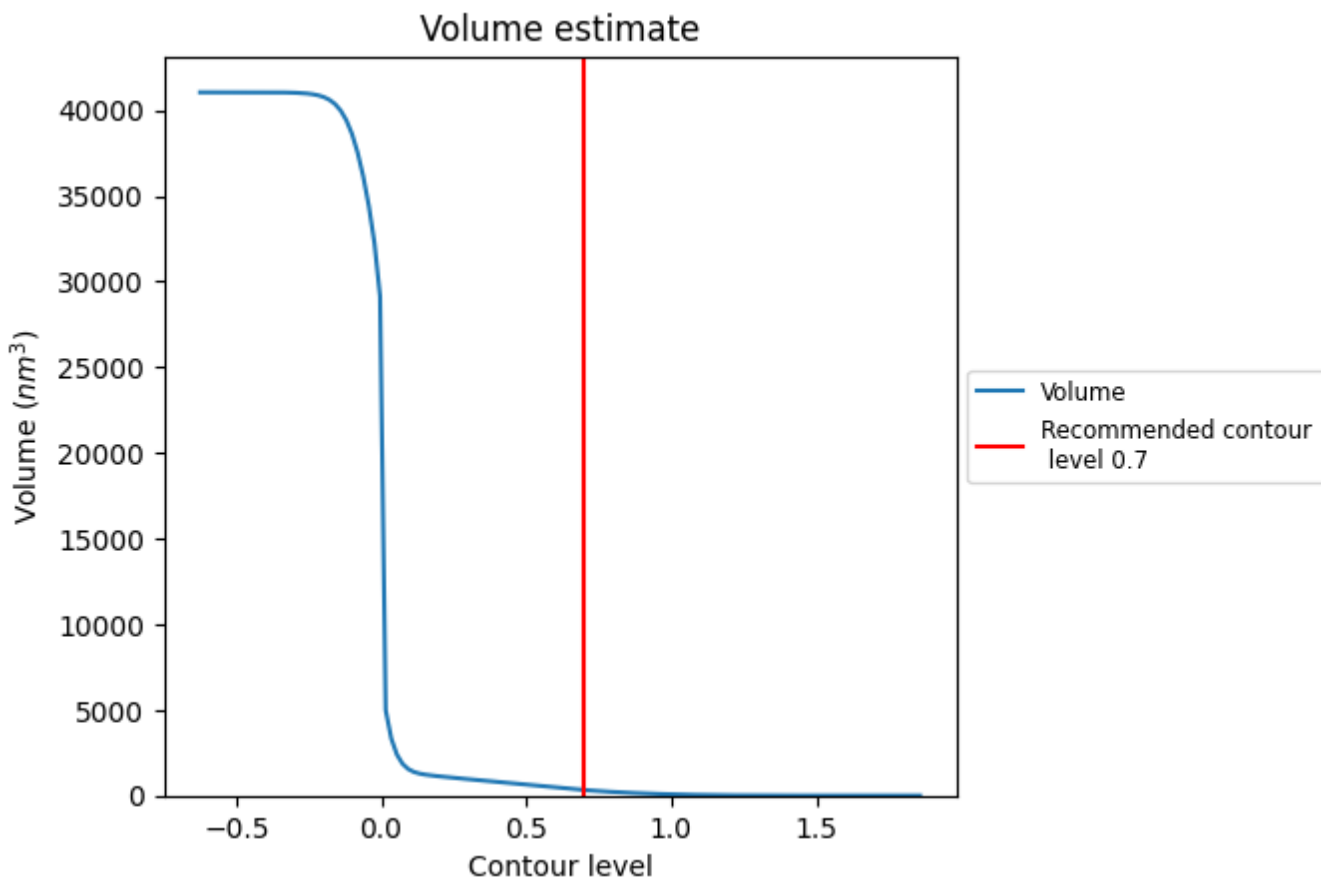
This section contains the results of statistical analysis of the map.

### 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.

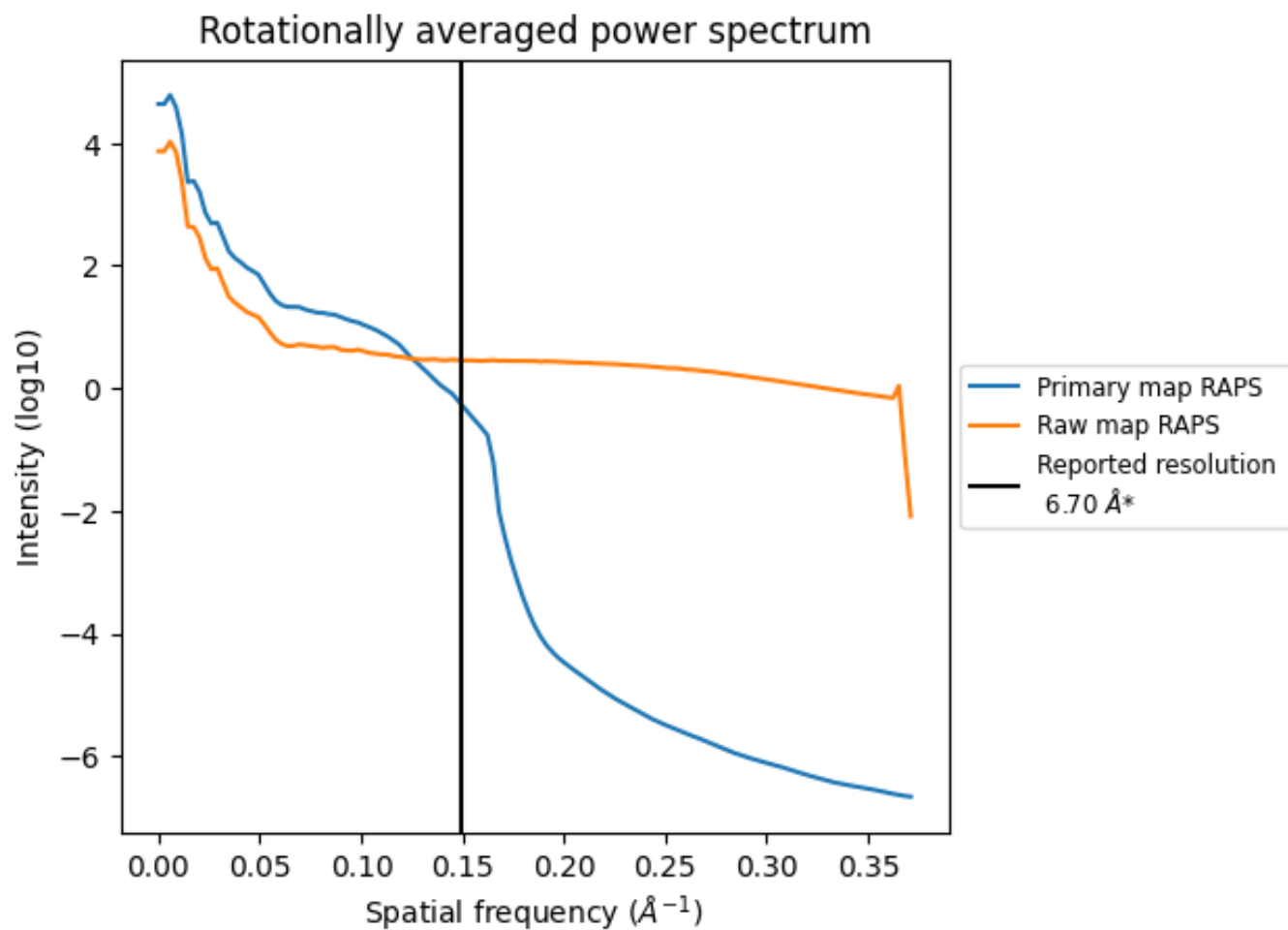
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 324 nm<sup>3</sup>; this corresponds to an approximate mass of 293 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

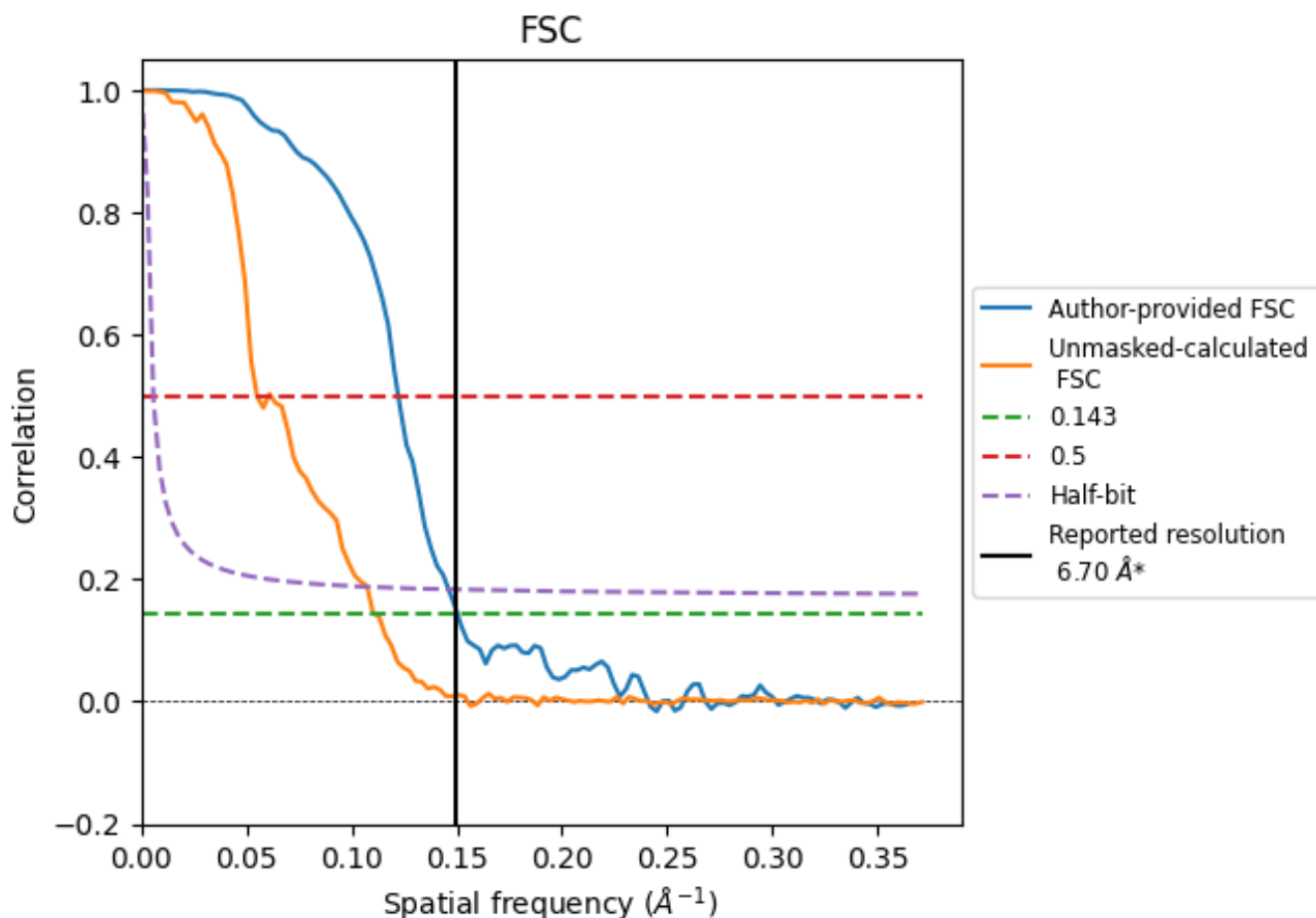


\*Reported resolution corresponds to spatial frequency of 0.149 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.149 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

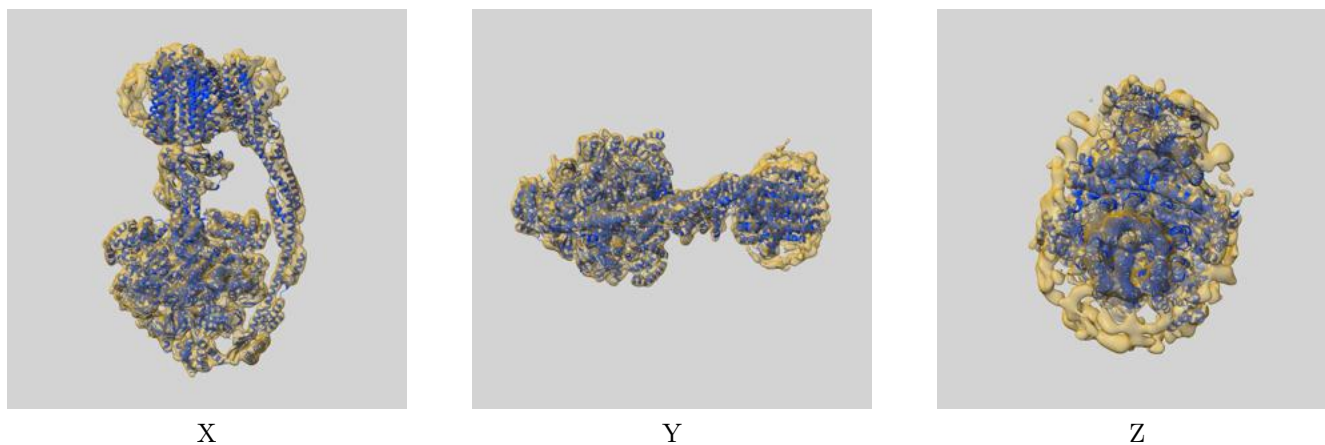
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.70	-	-
Author-provided FSC curve	6.65	8.18	6.84
Unmasked-calculated*	9.03	18.18	9.31

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.03 differs from the reported value 6.7 by more than 10 %

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

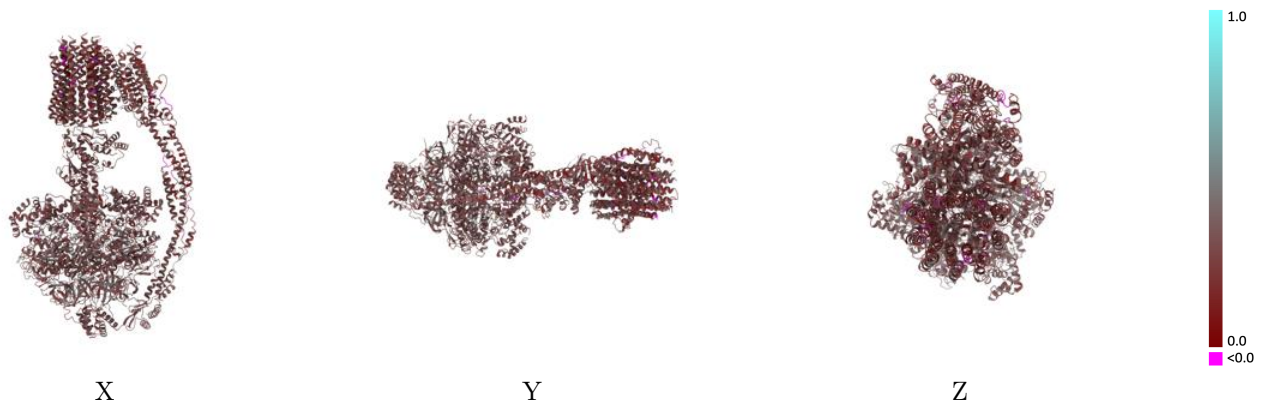
This section contains information regarding the fit between EMDB map EMD-25959 and PDB model 7TK7. Per-residue inclusion information can be found in section 3 on page 7.

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



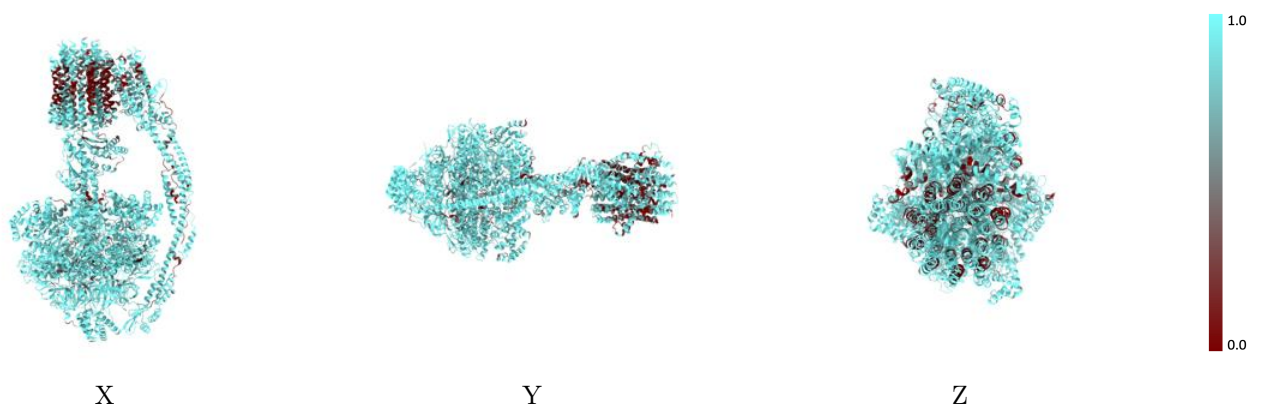
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



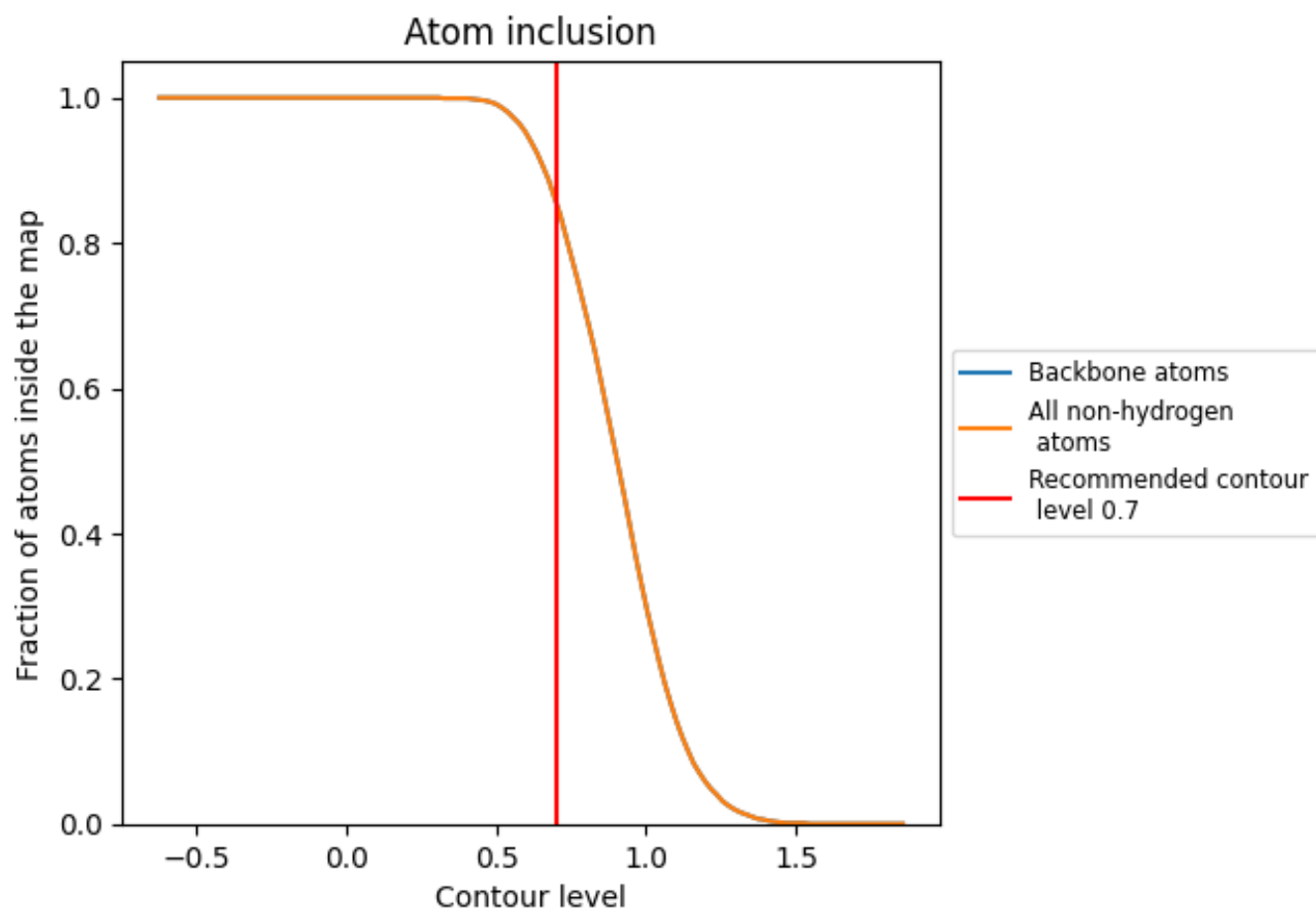
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8560	 0.2960
0	 0.5900	 0.2580
1	 0.4900	 0.2400
2	 0.5630	 0.2560
3	 0.5400	 0.2100
4	 0.5600	 0.2270
5	 0.5770	 0.2350
6	 0.7160	 0.2560
7	 0.6540	 0.2670
8	 0.6700	 0.2260
9	 0.7300	 0.2580
A	 0.9180	 0.3210
B	 0.9370	 0.3130
C	 0.9210	 0.3150
D	 0.9190	 0.3190
E	 0.9130	 0.3170
F	 0.9500	 0.3240
G	 0.9400	 0.2950
H	 0.8180	 0.2960
I	 0.9120	 0.3150
O	 0.9680	 0.3120
T	 0.7430	 0.2660
U	 0.9270	 0.2880
V	 0.8420	 0.2530
W	 0.6350	 0.1990
X	 0.5690	 0.2550
Y	 0.6890	 0.2580
Z	 0.8080	 0.2470

