



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:36 PM UTC

PDB ID : 7TKE / pdb_00007tke
EMDB ID : EMD-25966
Title : Yeast ATP synthase State 2binding(a) with 10 mM ATP backbone model
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2022-01-17
Resolution : 7.10 Å(reported)
Based on initial model : 2HLD

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

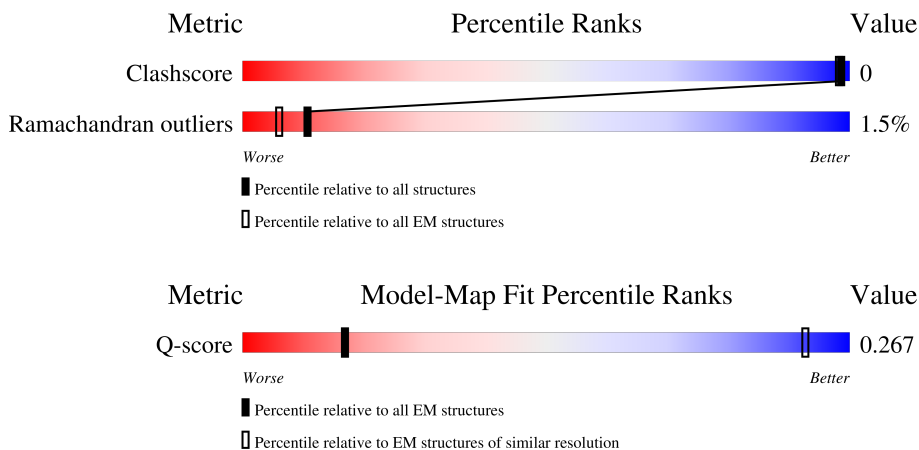
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	464 (6.60 - 7.60)

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

Mol	Chain	Length	Quality of chain
1	0	76	37% 88% 11% .
1	1	76	22% 96% . .
1	2	76	14% 96% . .
1	3	76	18% 92% 5% .
1	4	76	38% 91% 8% .

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

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	V	171	Total	C	N	O	0	0
			685	342	171	172		

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

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

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

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

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

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

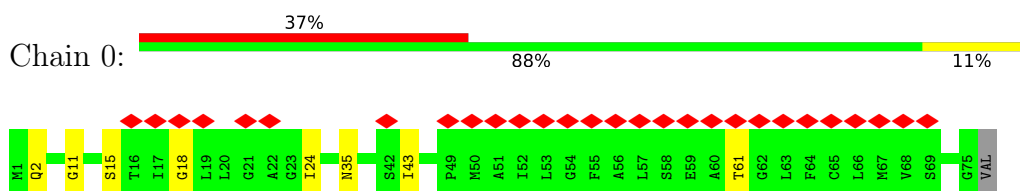
- Molecule 14 is a protein called ATP synthase protein 8.

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

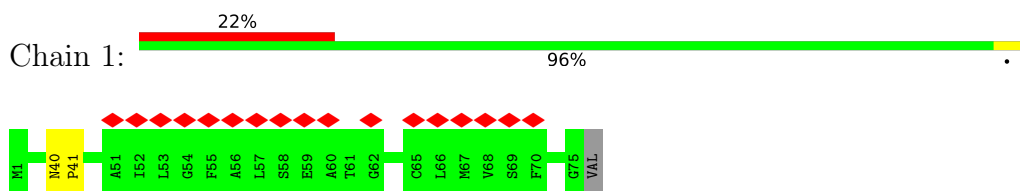
3 Residue-property plots [i](#)

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

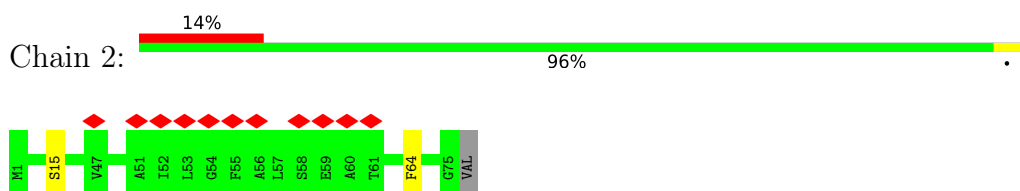
- Molecule 1: ATP synthase subunit 9



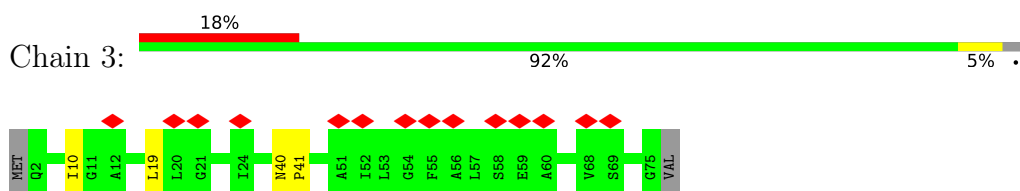
- Molecule 1: ATP synthase subunit 9



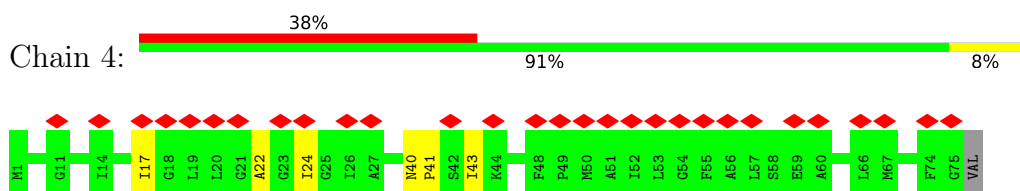
- Molecule 1: ATP synthase subunit 9



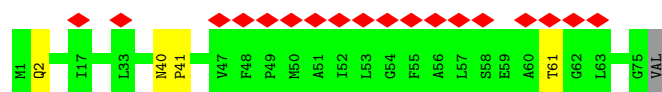
- Molecule 1: ATP synthase subunit 9



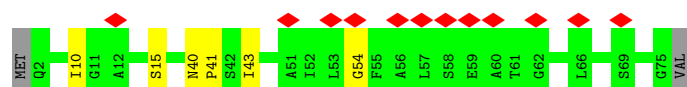
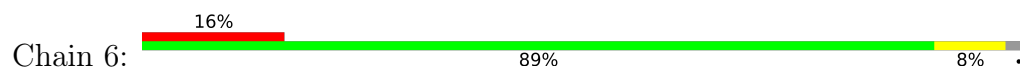
- Molecule 1: ATP synthase subunit 9



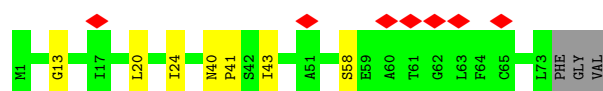
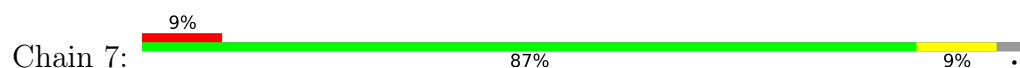
- Molecule 1: ATP synthase subunit 9



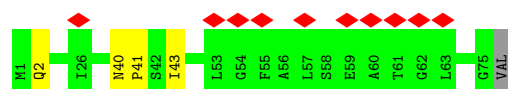
- Molecule 1: ATP synthase subunit 9



- Molecule 1: ATP synthase subunit 9



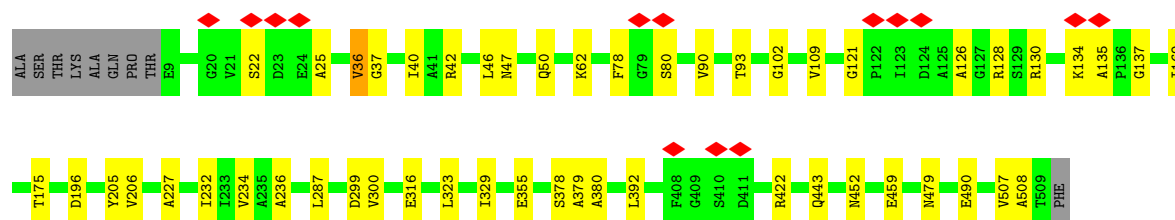
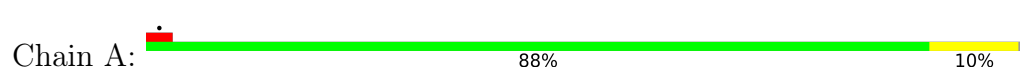
- Molecule 1: ATP synthase subunit 9



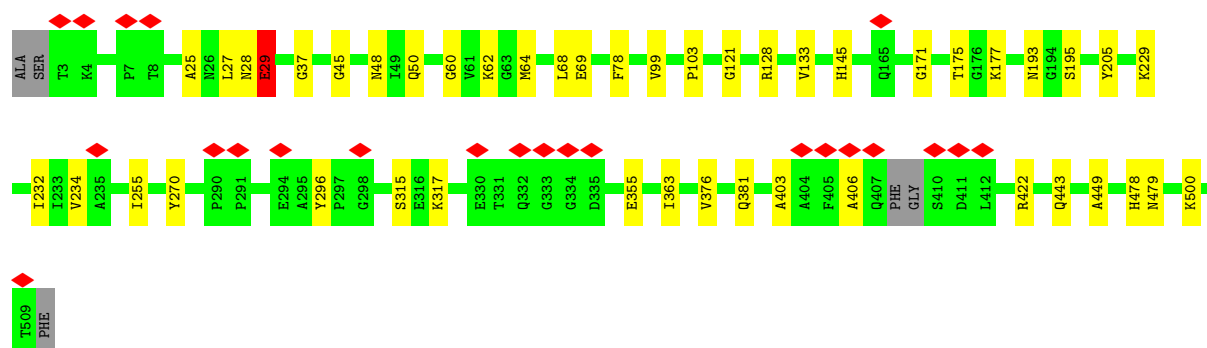
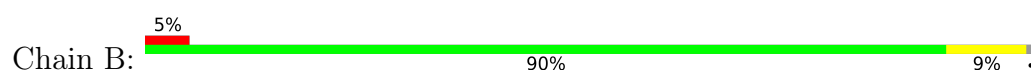
- Molecule 1: ATP synthase subunit 9



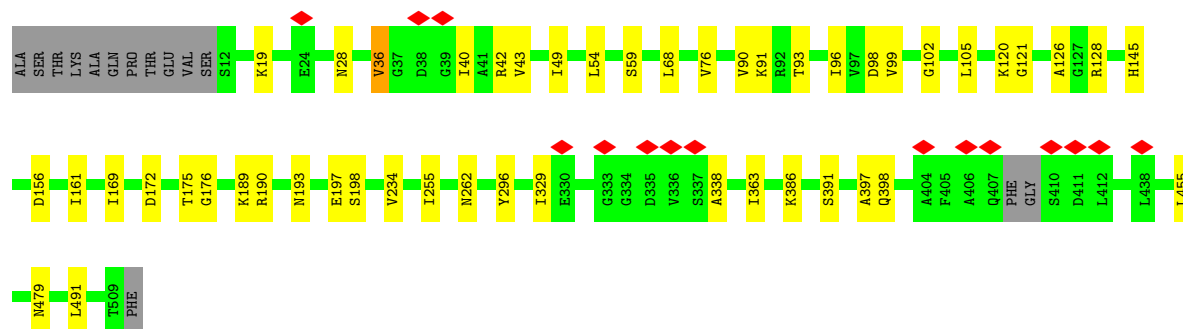
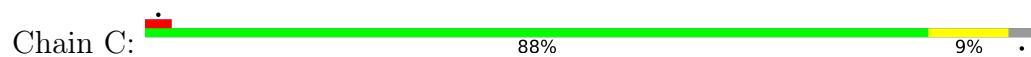
- Molecule 2: ATP synthase subunit alpha



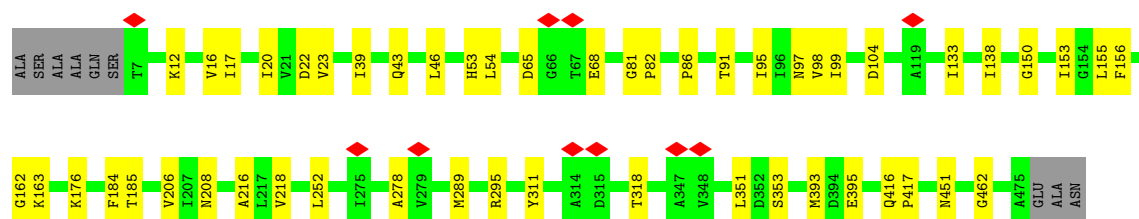
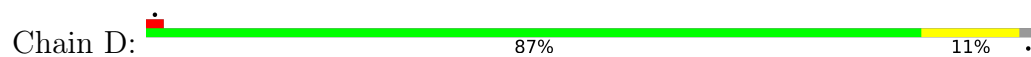
- Molecule 2: ATP synthase subunit alpha



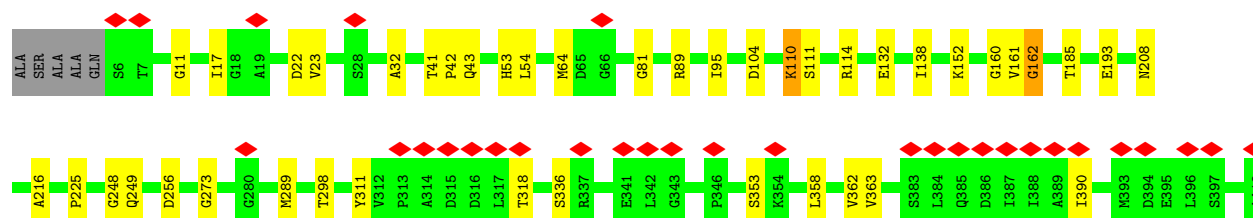
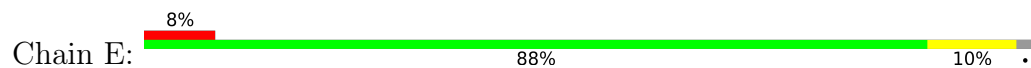
- Molecule 2: ATP synthase subunit alpha



- Molecule 3: ATP synthase subunit beta

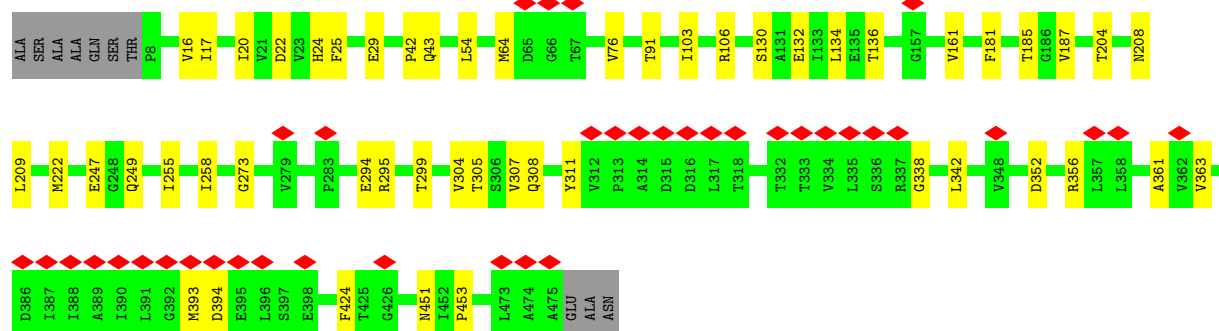
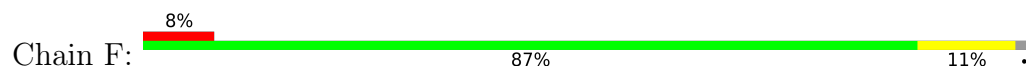


- Molecule 3: ATP synthase subunit beta

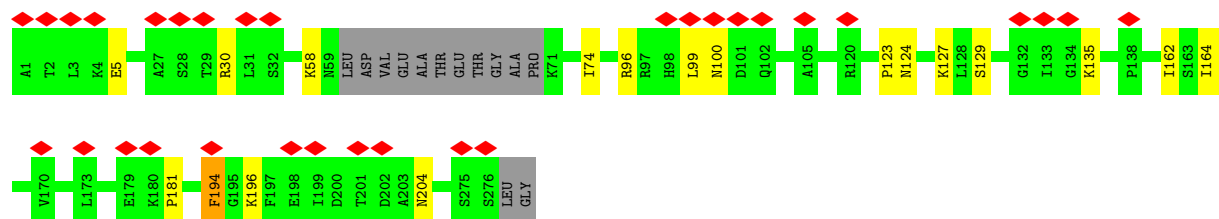
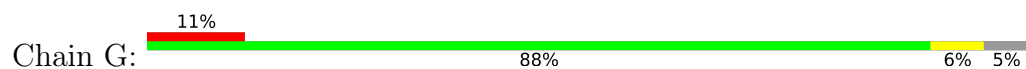




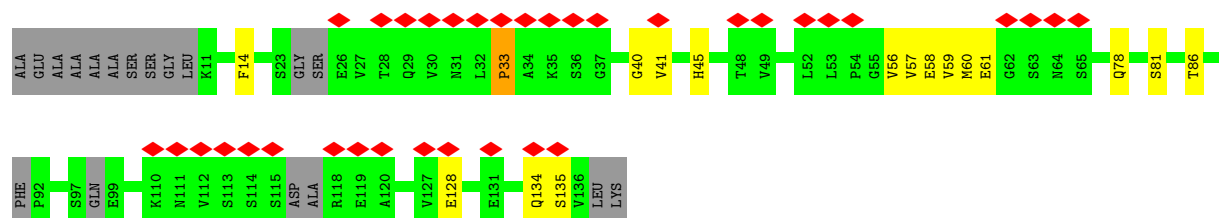
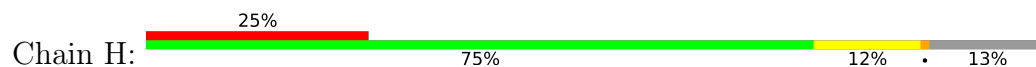
- Molecule 3: ATP synthase subunit beta



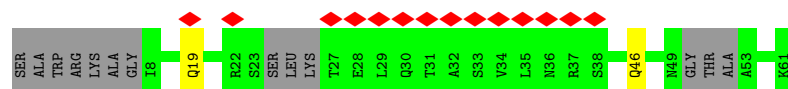
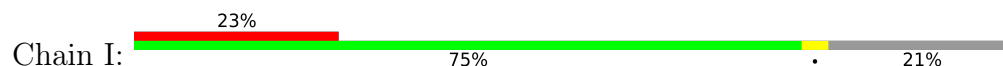
- Molecule 4: ATP synthase subunit gamma



- Molecule 5: ATP synthase subunit delta



- Molecule 6: ATP synthase subunit epsilon



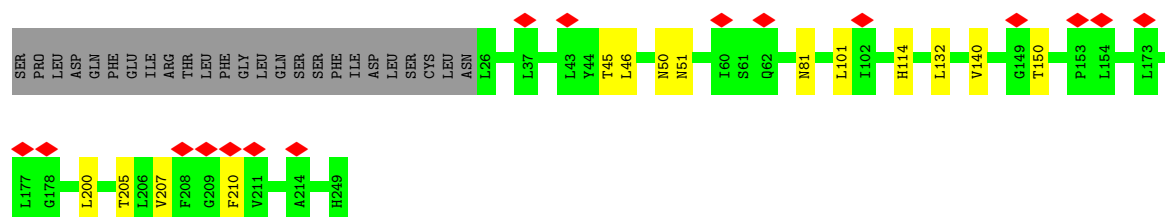
- Molecule 7: ATP synthase subunit 5

Chain O:  85% 11%



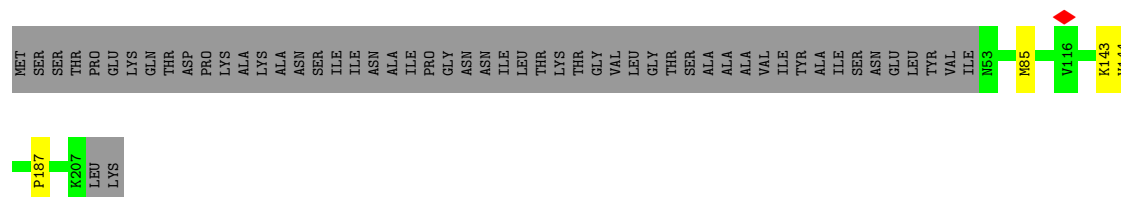
• Molecule 8: ATP synthase subunit a

Chain T:  6% 84% 6% 10%

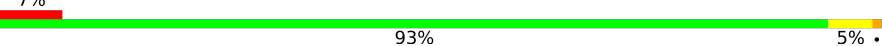


• Molecule 9: ATP synthase subunit 4

Chain U:  72% 26%



• Molecule 10: ATP synthase subunit d

Chain V:  7% 93% 5% ..



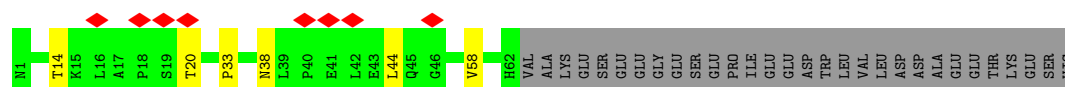
• Molecule 11: ATP synthase subunit f

Chain W:  11% 79% 11% 11%

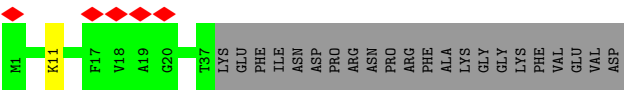


• Molecule 12: ATP synthase subunit H

Chain X:  9% 61% 7% 33%



● Molecule 13: ATP synthase subunit J



● Molecule 14: ATP synthase protein 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14051	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	1.569	Depositor
Minimum map value	-0.435	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	344.96, 344.96, 344.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3475, 1.3475, 1.3475	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	1.19	0/299	2.30	16/372 (4.3%)
1	1	1.21	0/299	2.09	0/372
1	2	1.20	0/299	2.11	4/372 (1.1%)
1	3	1.21	0/295	2.02	4/367 (1.1%)
1	4	1.22	0/299	2.18	8/372 (2.2%)
1	5	1.23	0/299	2.08	5/372 (1.3%)
1	6	1.23	0/295	2.24	8/367 (2.2%)
1	7	1.24	0/291	2.22	10/362 (2.8%)
1	8	1.21	0/299	2.24	4/372 (1.1%)
1	9	1.21	0/295	2.23	4/367 (1.1%)
2	A	1.58	0/2003	1.93	58/2502 (2.3%)
2	B	1.56	1/2018 (0.0%)	1.90	46/2519 (1.8%)
2	C	1.54	0/1982	1.92	51/2474 (2.1%)
3	D	1.61	0/1875	1.90	46/2342 (2.0%)
3	E	1.55	1/1879 (0.1%)	1.93	47/2347 (2.0%)
3	F	1.56	0/1871	1.98	53/2337 (2.3%)
4	G	1.43	0/1058	2.06	20/1319 (1.5%)
5	H	1.60	2/475 (0.4%)	1.99	18/585 (3.1%)
6	I	1.44	0/190	1.80	3/231 (1.3%)
7	O	1.53	0/747	1.94	16/932 (1.7%)
8	T	1.33	0/896	1.67	13/1117 (1.2%)
9	U	1.35	0/619	1.77	6/772 (0.8%)
10	V	1.45	0/684	1.78	6/852 (0.7%)
11	W	1.31	0/339	1.88	6/422 (1.4%)
12	X	1.42	0/247	2.16	8/307 (2.6%)
13	Y	1.28	0/147	1.58	1/182 (0.5%)
14	Z	1.35	0/192	1.50	0/237
All	All	1.48	4/20192 (0.0%)	1.95	461/25172 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	3	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
2	B	0	1
3	E	0	1
9	U	0	1
All	All	0	11

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	11	GLY	CA-C	-6.01	1.46	1.51
2	B	478	HIS	CA-C	-5.89	1.48	1.53
5	H	59	VAL	CA-C	-5.67	1.45	1.52
5	H	56	VAL	CA-C	-5.54	1.45	1.52

All (461) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	204	ASN	CA-C-N	11.87	127.72	120.24
4	G	204	ASN	C-N-CA	11.87	127.72	120.24
7	O	55	HIS	N-CA-C	-11.06	102.02	114.62
7	O	180	ILE	N-CA-C	-9.60	103.55	111.81
5	H	58	GLU	N-CA-C	-9.51	93.36	109.24
2	B	376	VAL	N-CA-C	-9.34	103.78	111.81
2	C	398	GLN	N-CA-C	-9.17	102.22	113.41
2	C	479	ASN	N-CA-C	-8.99	102.31	113.28
2	A	37	GLY	N-CA-C	-8.98	99.95	111.72
5	H	61	GLU	N-CA-C	-8.70	94.07	108.34
3	F	103	ILE	N-CA-C	-8.68	104.45	112.43
2	A	78	PHE	N-CA-C	-8.65	102.31	113.12
4	G	100	ASN	N-CA-C	-8.64	103.25	113.88
2	B	99	VAL	N-CA-C	-8.54	102.19	109.19
3	D	95	ILE	N-CA-C	-8.20	96.64	108.11
2	B	479	ASN	N-CA-C	-8.18	103.30	113.28
2	A	47	ASN	N-CA-C	-8.17	104.19	114.56
3	D	43	GLN	N-CA-C	-8.10	103.41	112.57
5	H	14	PHE	N-CA-C	-8.10	94.82	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	93	THR	N-CA-C	-8.00	102.64	111.36
2	C	96	ILE	N-CA-C	-7.96	101.21	110.21
7	O	176	VAL	N-CA-C	-7.92	96.71	108.12
10	V	87	LYS	N-CA-C	-7.90	103.66	113.38
2	C	190	ARG	N-CA-C	-7.74	102.63	112.93
3	F	305	THR	N-CA-C	-7.70	96.91	108.99
11	W	61	ALA	N-CA-C	-7.57	101.35	110.44
2	A	93	THR	N-CA-C	-7.56	103.04	111.28
11	W	6	PRO	N-CA-C	7.52	119.88	110.70
3	D	17	ILE	N-CA-C	-7.43	96.38	107.37
3	E	162	GLY	N-CA-C	-7.42	104.81	115.64
1	8	43	ILE	CA-C-N	7.37	130.48	120.38
1	8	43	ILE	C-N-CA	7.37	130.48	120.38
2	B	177	LYS	N-CA-C	-7.37	103.32	111.36
8	T	140	VAL	N-CA-C	-7.37	104.32	112.80
3	F	209	LEU	N-CA-C	-7.36	104.45	113.50
4	G	74	ILE	N-CA-C	-7.32	97.57	108.12
3	E	41	THR	N-CA-C	-7.29	101.58	108.07
3	F	29	GLU	N-CA-C	-7.25	99.61	109.54
2	B	422	ARG	CA-C-N	7.16	127.88	120.00
2	B	422	ARG	C-N-CA	7.16	127.88	120.00
3	D	99	ILE	N-CA-C	-7.14	105.76	112.83
5	H	45	HIS	N-CA-C	-7.14	97.78	108.99
1	6	10	ILE	CA-C-N	7.12	127.88	119.98
1	6	10	ILE	C-N-CA	7.12	127.88	119.98
3	F	43	GLN	N-CA-C	-7.10	104.63	112.72
3	F	352	ASP	N-CA-C	-7.09	105.55	114.56
2	B	78	PHE	N-CA-C	-7.07	103.64	112.90
3	F	308	GLN	N-CA-C	-7.03	98.62	109.52
3	F	161	VAL	N-CA-C	-7.02	104.72	112.80
2	C	175	THR	N-CA-C	-7.01	105.08	112.93
3	D	252	LEU	N-CA-C	-6.97	98.47	109.07
2	B	69	GLU	N-CA-C	-6.95	97.71	108.55
3	D	351	LEU	N-CA-C	-6.90	104.47	113.17
8	T	101	LEU	N-CA-C	-6.90	103.75	112.93
3	F	304	VAL	N-CA-C	-6.88	102.55	110.05
2	B	232	ILE	N-CA-C	-6.88	98.27	108.45
3	E	53	HIS	N-CA-C	-6.87	98.19	109.40
3	E	95	ILE	N-CA-C	-6.87	98.54	108.36
8	T	81	ASN	N-CA-C	-6.84	104.82	113.02
3	E	311	TYR	N-CA-C	-6.83	97.76	108.90
3	F	356	ARG	N-CA-C	-6.82	104.08	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	232	ILE	N-CA-C	-6.81	98.67	108.48
2	A	234	VAL	N-CA-C	-6.71	98.77	108.17
3	D	39	ILE	N-CA-C	-6.71	98.77	108.36
3	E	422	GLU	N-CA-C	-6.71	104.57	112.89
2	B	193	ASN	CA-C-N	6.70	126.36	119.92
2	B	193	ASN	C-N-CA	6.70	126.36	119.92
3	D	353	SER	N-CA-C	-6.66	98.92	109.23
2	A	206	VAL	N-CA-C	-6.64	98.92	108.48
3	E	104	ASP	N-CA-C	-6.64	105.21	113.38
3	F	185	THR	N-CA-C	-6.63	98.39	109.07
2	C	40	ILE	N-CA-C	-6.63	98.08	108.81
3	F	363	VAL	N-CA-C	-6.63	106.33	112.43
3	D	16	VAL	N-CA-C	-6.62	95.57	109.34
3	F	258	ILE	N-CA-C	-6.58	105.13	113.22
3	F	451	ASN	N-CA-C	-6.55	104.91	113.17
2	C	189	LYS	N-CA-C	-6.54	106.25	114.56
3	E	43	GLN	N-CA-C	-6.54	105.18	112.57
1	4	43	ILE	CA-C-N	6.48	129.26	120.38
1	4	43	ILE	C-N-CA	6.48	129.26	120.38
7	O	101	PHE	N-CA-C	-6.48	104.31	112.93
3	D	185	THR	N-CA-C	-6.47	97.72	108.34
5	H	59	VAL	N-CA-C	-6.45	98.84	108.12
7	O	125	SER	N-CA-C	-6.43	99.86	108.74
2	A	287	LEU	N-CA-C	-6.43	105.07	113.17
2	A	380	ALA	N-CA-C	-6.42	105.08	113.17
2	B	443	GLN	CA-C-N	6.42	124.28	120.24
2	B	443	GLN	C-N-CA	6.42	124.28	120.24
3	D	133	ILE	N-CA-C	-6.40	99.27	108.48
3	D	156	PHE	N-CA-C	-6.40	100.78	109.54
2	C	99	VAL	N-CA-C	-6.39	103.95	109.19
2	B	50	GLN	N-CA-C	-6.39	100.51	110.42
3	D	295	ARG	N-CA-C	-6.37	105.16	113.12
2	A	40	ILE	N-CA-C	-6.37	98.35	107.77
3	F	255	ILE	N-CA-C	-6.36	98.50	108.86
11	W	46	THR	N-CA-C	-6.34	104.10	113.61
3	F	181	PHE	N-CA-C	-6.33	99.93	108.86
2	C	128	ARG	N-CA-C	-6.33	99.50	109.50
3	E	89	ARG	N-CA-C	-6.32	104.83	113.30
4	G	127	LYS	N-CA-C	-6.32	105.47	113.43
2	A	236	ALA	N-CA-C	-6.31	96.90	107.32
3	F	24	HIS	N-CA-C	-6.31	98.91	109.07
3	F	17	ILE	N-CA-C	-6.31	98.78	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	128	ARG	N-CA-C	-6.30	99.75	109.52
1	9	10	ILE	CA-C-N	6.29	126.97	119.98
1	9	10	ILE	C-N-CA	6.29	126.97	119.98
2	C	172	ASP	CA-C-N	6.29	129.76	120.90
2	C	172	ASP	C-N-CA	6.29	129.76	120.90
1	6	43	ILE	CA-C-N	6.28	128.98	120.38
1	6	43	ILE	C-N-CA	6.28	128.98	120.38
3	D	53	HIS	N-CA-C	-6.28	98.97	109.07
2	C	156	ASP	N-CA-C	-6.27	105.11	114.64
2	A	42	ARG	N-CA-C	-6.26	97.20	108.48
3	E	421	ALA	N-CA-C	-6.26	102.86	110.88
7	O	140	ALA	CA-C-N	6.26	129.18	120.29
7	O	140	ALA	C-N-CA	6.26	129.18	120.29
2	C	455	LEU	N-CA-C	-6.25	105.69	113.38
2	A	379	ALA	N-CA-C	-6.25	105.24	112.92
1	7	43	ILE	CA-C-N	6.24	128.93	120.38
1	7	43	ILE	C-N-CA	6.24	128.93	120.38
2	A	175	THR	N-CA-C	-6.23	102.84	111.81
2	C	98	ASP	N-CA-C	-6.23	99.87	109.52
2	A	355	GLU	CA-C-N	6.22	128.62	120.28
2	A	355	GLU	C-N-CA	6.22	128.62	120.28
3	D	218	VAL	N-CA-C	-6.22	99.16	108.12
2	A	329	ILE	N-CA-C	-6.21	98.58	107.77
1	0	61	THR	CA-C-N	6.20	126.86	119.98
1	0	61	THR	C-N-CA	6.20	126.86	119.98
2	A	422	ARG	CA-C-N	6.18	126.84	119.98
2	A	422	ARG	C-N-CA	6.18	126.84	119.98
3	D	206	VAL	N-CA-C	-6.17	103.37	111.09
2	B	175	THR	N-CA-C	-6.17	106.44	112.97
2	C	262	ASN	N-CA-C	-6.13	105.55	113.16
3	F	132	GLU	CA-C-N	6.13	128.72	120.50
3	F	132	GLU	C-N-CA	6.13	128.72	120.50
3	F	394	ASP	N-CA-C	-6.13	105.84	113.38
3	F	453	PRO	CA-C-N	6.11	128.47	120.28
3	F	453	PRO	C-N-CA	6.11	128.47	120.28
3	F	295	ARG	N-CA-C	-6.11	105.66	113.23
3	D	54	LEU	N-CA-C	-6.08	105.51	113.17
10	V	51	THR	N-CA-C	-6.07	105.52	113.17
1	5	2	GLN	N-CA-C	-6.05	104.61	111.14
3	D	104	ASP	N-CA-C	-6.03	105.57	113.17
8	T	150	THR	N-CA-C	-6.02	101.22	108.14
2	C	363	ILE	N-CA-C	-5.99	97.75	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	289	MET	CA-C-N	5.99	126.63	119.98
3	E	289	MET	C-N-CA	5.99	126.63	119.98
7	O	192	GLU	N-CA-C	-5.97	105.30	113.30
5	H	40	GLY	N-CA-C	-5.96	101.02	111.46
2	A	137	GLY	CA-C-N	5.95	128.06	120.56
2	A	137	GLY	C-N-CA	5.95	128.06	120.56
2	A	169	ILE	N-CA-C	-5.94	99.32	107.99
2	C	28	ASN	N-CA-C	-5.94	99.51	108.96
4	G	162	ILE	N-CA-C	-5.94	99.66	108.45
2	C	90	VAL	N-CA-C	-5.93	99.87	108.17
2	C	42	ARG	N-CA-C	-5.92	98.76	108.76
1	0	43	ILE	CA-C-N	5.91	128.21	120.28
1	0	43	ILE	C-N-CA	5.91	128.21	120.28
3	D	176	LYS	N-CA-C	-5.91	105.38	113.30
5	H	60	MET	N-CA-C	-5.91	98.78	108.76
2	A	227	ALA	N-CA-C	-5.89	106.13	113.38
1	7	20	LEU	CA-C-N	5.89	126.52	119.98
1	7	20	LEU	C-N-CA	5.89	126.52	119.98
2	A	196	ASP	CA-C-N	5.87	128.63	120.29
2	A	196	ASP	C-N-CA	5.87	128.63	120.29
2	C	19	LYS	CA-C-N	5.87	126.50	119.98
2	C	19	LYS	C-N-CA	5.87	126.50	119.98
2	B	68	LEU	N-CA-C	-5.86	99.63	109.07
3	E	17	ILE	N-CA-C	-5.85	97.18	109.34
2	C	234	VAL	N-CA-C	-5.83	100.03	108.89
3	D	311	TYR	N-CA-C	-5.83	97.73	107.99
3	E	273	GLY	N-CA-C	-5.83	106.48	114.64
2	B	64	MET	N-CA-C	-5.83	100.56	109.41
13	Y	11	LYS	N-CA-C	-5.81	104.74	112.94
4	G	30	ARG	CA-C-N	5.81	128.07	120.28
4	G	30	ARG	C-N-CA	5.81	128.07	120.28
2	B	449	ALA	CA-C-N	5.79	126.38	120.00
2	B	449	ALA	C-N-CA	5.79	126.38	120.00
4	G	194	PHE	N-CA-C	-5.79	98.46	110.80
2	B	381	GLN	N-CA-C	-5.78	99.63	108.76
3	F	208	ASN	N-CA-C	-5.78	99.11	108.52
3	D	12	LYS	N-CA-C	-5.76	100.59	109.52
2	C	105	LEU	N-CA-C	-5.75	105.59	113.30
2	C	91	LYS	N-CA-C	-5.74	100.54	109.72
3	E	225	PRO	CA-C-N	5.74	125.59	119.28
3	E	225	PRO	C-N-CA	5.74	125.59	119.28
3	D	208	ASN	N-CA-C	-5.73	99.90	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	397	ALA	N-CA-C	-5.72	105.88	112.92
3	F	22	ASP	N-CA-C	-5.72	100.38	109.59
3	D	318	THR	N-CA-C	-5.71	106.32	113.28
8	T	210	PHE	CA-C-N	5.71	123.83	120.24
8	T	210	PHE	C-N-CA	5.71	123.83	120.24
3	E	193	GLU	CA-C-N	5.71	126.27	119.94
3	E	193	GLU	C-N-CA	5.71	126.27	119.94
3	F	361	ALA	N-CA-C	-5.70	105.34	112.93
2	B	62	LYS	N-CA-C	-5.70	100.85	109.85
2	C	169	ILE	N-CA-C	-5.70	99.43	107.75
5	H	57	VAL	N-CA-C	-5.70	99.57	108.86
1	0	18	GLY	CA-C-N	5.68	128.46	120.28
1	0	18	GLY	C-N-CA	5.68	128.46	120.28
3	E	23	VAL	N-CA-C	-5.66	99.61	108.95
3	D	20	ILE	N-CA-C	-5.65	97.58	109.34
3	D	155	LEU	N-CA-C	-5.65	99.80	109.24
3	E	363	VAL	N-CA-C	-5.65	106.27	113.22
2	A	507	VAL	N-CA-C	-5.64	104.85	111.00
3	E	64	MET	N-CA-C	-5.62	106.78	113.97
2	B	234	VAL	N-CA-C	-5.61	100.51	108.58
4	G	129	SER	N-CA-C	-5.59	100.57	109.07
1	5	61	THR	CA-C-N	5.58	126.14	119.94
1	5	61	THR	C-N-CA	5.58	126.14	119.94
3	D	91	THR	N-CA-C	-5.58	106.52	113.38
2	A	50	GLN	N-CA-C	-5.58	101.39	110.20
2	A	130	ARG	N-CA-C	-5.57	100.81	109.72
3	F	64	MET	N-CA-C	-5.56	106.54	113.38
3	F	342	LEU	N-CA-C	-5.55	106.36	113.02
7	O	169	VAL	N-CA-C	-5.54	100.46	108.71
2	A	109	VAL	N-CA-C	-5.54	100.46	108.71
1	4	22	ALA	CA-C-N	5.53	126.12	119.98
1	4	22	ALA	C-N-CA	5.53	126.12	119.98
1	9	43	ILE	CA-C-N	5.53	127.69	120.28
1	9	43	ILE	C-N-CA	5.53	127.69	120.28
2	C	161	ILE	CA-C-N	5.53	127.39	122.47
2	C	161	ILE	C-N-CA	5.53	127.39	122.47
3	E	450	ASP	N-CA-C	-5.53	106.21	113.17
7	O	57	LEU	N-CA-C	-5.52	106.22	113.17
3	E	54	LEU	N-CA-C	-5.52	105.76	112.88
3	F	311	TYR	N-CA-C	-5.52	98.23	107.99
7	O	152	SER	N-CA-C	-5.51	102.59	110.59
2	B	296	TYR	N-CA-C	-5.51	100.58	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	19	LEU	CA-C-N	5.51	127.93	120.38
1	3	19	LEU	C-N-CA	5.51	127.93	120.38
12	X	44	LEU	CA-C-N	5.50	129.58	120.94
12	X	44	LEU	C-N-CA	5.50	129.58	120.94
10	V	52	GLU	CA-C-N	5.50	129.03	120.34
10	V	52	GLU	C-N-CA	5.50	129.03	120.34
3	F	76	VAL	N-CA-C	-5.49	99.92	108.86
3	D	46	LEU	N-CA-C	-5.47	99.97	108.90
5	H	134	GLN	CA-C-N	5.47	128.16	120.28
5	H	134	GLN	C-N-CA	5.47	128.16	120.28
10	V	133	LEU	N-CA-C	-5.47	99.15	110.80
8	T	205	THR	N-CA-C	-5.47	106.45	113.23
2	A	479	ASN	N-CA-C	-5.46	106.46	113.23
3	F	42	PRO	N-CA-C	-5.46	107.52	114.35
3	E	22	ASP	N-CA-C	-5.45	101.28	109.95
3	F	273	GLY	N-CA-C	-5.45	107.84	114.92
3	E	114	ARG	N-CA-C	-5.45	101.08	109.52
3	F	91	THR	N-CA-C	-5.44	106.02	113.30
2	A	443	GLN	N-CA-C	-5.43	106.78	113.41
3	E	81	GLY	CA-C-N	5.43	125.44	119.90
3	E	81	GLY	C-N-CA	5.43	125.44	119.90
2	B	29	GLU	N-CA-C	-5.43	99.24	110.80
2	B	48	ASN	N-CA-C	-5.43	105.97	112.59
3	D	184	PHE	N-CA-C	-5.42	100.07	108.90
2	C	59	SER	N-CA-C	-5.42	106.44	113.16
5	H	78	GLN	N-CA-C	-5.42	101.96	110.14
1	5	2	GLN	CA-C-N	5.41	127.53	120.28
1	5	2	GLN	C-N-CA	5.41	127.53	120.28
5	H	86	THR	N-CA-C	-5.41	99.61	108.76
2	A	25	ALA	CA-C-N	5.41	128.39	120.71
2	A	25	ALA	C-N-CA	5.41	128.39	120.71
3	D	416	GLN	CA-C-N	5.41	126.60	119.84
3	D	416	GLN	C-N-CA	5.41	126.60	119.84
3	D	82	PRO	CA-C-N	5.40	127.86	120.35
3	D	82	PRO	C-N-CA	5.40	127.86	120.35
8	T	114	HIS	CA-C-N	5.40	128.51	120.31
8	T	114	HIS	C-N-CA	5.40	128.51	120.31
4	G	164	ILE	N-CA-C	-5.39	100.07	108.86
1	0	24	ILE	CA-C-N	5.39	125.92	119.94
1	0	24	ILE	C-N-CA	5.39	125.92	119.94
2	C	54	LEU	N-CA-C	-5.39	100.45	109.24
3	D	22	ASP	N-CA-C	-5.39	100.24	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	15	SER	CA-C-N	5.38	128.24	120.38
1	0	15	SER	C-N-CA	5.38	128.24	120.38
2	A	452	ASN	N-CA-C	-5.38	106.91	112.93
3	D	163	LYS	N-CA-C	-5.38	105.42	111.28
3	E	216	ALA	N-CA-C	-5.36	101.39	109.85
8	T	200	LEU	N-CA-C	-5.36	106.75	113.28
3	E	152	LYS	CA-C-N	5.35	127.79	120.35
3	E	152	LYS	C-N-CA	5.35	127.79	120.35
3	D	150	GLY	CA-C-N	5.35	126.27	120.44
3	D	150	GLY	C-N-CA	5.35	126.27	120.44
2	A	508	ALA	N-CA-C	-5.34	100.46	108.96
2	B	37	GLY	N-CA-C	-5.34	100.53	113.18
3	E	457	PHE	N-CA-C	-5.34	106.90	113.41
1	4	24	ILE	CA-C-N	5.33	125.86	119.94
1	4	24	ILE	C-N-CA	5.33	125.86	119.94
9	U	85	MET	CA-C-N	5.32	127.36	120.44
9	U	85	MET	C-N-CA	5.32	127.36	120.44
3	E	318	THR	N-CA-C	-5.32	106.56	113.16
2	A	62	LYS	N-CA-C	-5.31	100.74	109.40
2	A	316	GLU	CA-C-N	5.31	127.40	120.28
2	A	316	GLU	C-N-CA	5.31	127.40	120.28
2	B	270	TYR	N-CA-C	-5.31	100.08	108.73
1	6	15	SER	CA-C-N	5.31	127.92	120.28
1	6	15	SER	C-N-CA	5.31	127.92	120.28
3	E	390	ILE	N-CA-C	-5.31	106.49	111.48
2	C	120	LYS	N-CA-C	-5.29	106.69	112.72
3	E	362	VAL	N-CA-C	-5.29	105.15	112.50
4	G	5	GLU	CA-C-N	5.28	127.21	120.56
4	G	5	GLU	C-N-CA	5.28	127.21	120.56
2	A	323	LEU	N-CA-C	-5.28	100.70	109.46
2	C	76	VAL	N-CA-C	-5.28	100.72	108.11
4	G	99	LEU	N-CA-C	-5.28	106.70	112.72
7	O	50	ASN	N-CA-C	-5.28	101.35	109.79
2	C	198	SER	N-CA-C	-5.27	107.02	113.50
6	I	19	GLN	CA-C-N	5.27	127.34	120.28
6	I	19	GLN	C-N-CA	5.27	127.34	120.28
2	A	205	TYR	N-CA-C	-5.27	100.59	109.07
3	F	204	THR	N-CA-C	-5.27	106.63	113.16
4	G	165	PHE	N-CA-C	-5.27	101.18	109.50
3	F	299	THR	N-CA-C	-5.26	102.22	110.17
3	D	23	VAL	N-CA-C	-5.26	100.78	108.99
8	T	207	VAL	N-CA-C	-5.26	98.92	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	248	GLY	CA-C-N	5.26	131.59	121.54
3	E	248	GLY	C-N-CA	5.26	131.59	121.54
3	D	65	ASP	CA-C-N	5.25	126.17	120.44
3	D	65	ASP	C-N-CA	5.25	126.17	120.44
2	C	296	TYR	CA-C-N	5.25	126.41	119.84
2	C	296	TYR	C-N-CA	5.25	126.41	119.84
7	O	17	GLY	N-CA-C	-5.24	106.66	115.62
2	A	134	LYS	CA-C-N	5.24	127.77	120.65
2	A	134	LYS	C-N-CA	5.24	127.77	120.65
8	T	132	LEU	CA-C-N	5.23	125.75	120.00
8	T	132	LEU	C-N-CA	5.23	125.75	120.00
2	A	379	ALA	CA-C-N	5.23	131.17	122.54
2	A	379	ALA	C-N-CA	5.23	131.17	122.54
3	F	307	VAL	N-CA-C	-5.23	100.85	108.17
3	D	289	MET	CA-C-N	5.22	125.74	119.94
3	D	289	MET	C-N-CA	5.22	125.74	119.94
3	E	185	THR	N-CA-C	-5.22	100.38	108.90
1	0	35	ASN	CA-C-N	5.22	125.74	119.94
1	0	35	ASN	C-N-CA	5.22	125.74	119.94
2	C	176	GLY	N-CA-C	-5.22	100.81	113.18
5	H	41	VAL	N-CA-C	-5.21	100.69	108.46
1	2	15	SER	CA-C-N	5.21	127.78	120.28
1	2	15	SER	C-N-CA	5.21	127.78	120.28
6	I	46	GLN	N-CA-C	-5.21	103.51	110.55
2	A	36	VAL	N-CA-C	-5.21	98.50	109.34
3	D	153	ILE	N-CA-C	-5.21	100.97	108.89
3	F	187	VAL	N-CA-C	-5.21	100.88	108.17
2	C	329	ILE	N-CA-C	-5.19	100.90	108.17
3	D	216	ALA	N-CA-C	-5.19	101.47	109.52
3	D	138	ILE	N-CA-C	-5.19	100.65	108.12
3	F	424	PHE	N-CA-C	5.19	117.01	111.36
2	B	171	GLY	CA-C-N	5.19	128.07	120.71
2	B	171	GLY	C-N-CA	5.19	128.07	120.71
1	2	64	PHE	CA-C-N	5.18	127.22	120.28
1	2	64	PHE	C-N-CA	5.18	127.22	120.28
4	G	96	ARG	CA-C-N	5.18	127.22	120.28
4	G	96	ARG	C-N-CA	5.18	127.22	120.28
9	U	143	LYS	CA-C-N	5.18	127.09	120.56
9	U	143	LYS	C-N-CA	5.18	127.09	120.56
2	B	355	GLU	CA-C-N	5.18	127.22	120.28
2	B	355	GLU	C-N-CA	5.18	127.22	120.28
1	8	2	GLN	CA-C-N	5.17	127.21	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8	2	GLN	C-N-CA	5.17	127.21	120.28
2	A	490	GLU	N-CA-C	-5.17	99.17	108.48
2	C	255	ILE	CA-C-N	5.17	125.69	120.00
2	C	255	ILE	C-N-CA	5.17	125.69	120.00
2	C	491	LEU	N-CA-C	-5.16	98.86	107.99
12	X	38	ASN	CA-C-N	5.14	128.40	121.20
12	X	38	ASN	C-N-CA	5.14	128.40	121.20
3	F	393	MET	N-CA-C	-5.14	106.78	113.16
2	C	43	VAL	N-CA-C	-5.14	100.94	108.85
2	B	195	SER	N-CA-C	5.14	116.88	111.28
9	U	144	VAL	CA-C-N	5.14	127.12	120.44
9	U	144	VAL	C-N-CA	5.14	127.12	120.44
3	E	132	GLU	N-CA-C	-5.13	101.49	109.24
1	0	2	GLN	CA-C-N	5.13	127.11	120.44
1	0	2	GLN	C-N-CA	5.13	127.11	120.44
3	D	395	GLU	N-CA-C	-5.13	106.70	113.17
3	E	42	PRO	N-CA-C	-5.13	107.94	114.35
7	O	158	VAL	N-CA-C	-5.13	100.95	108.85
2	B	121	GLY	CA-C-N	5.13	126.25	119.84
2	B	121	GLY	C-N-CA	5.13	126.25	119.84
2	C	68	LEU	N-CA-C	-5.13	100.37	108.73
3	F	338	GLY	CA-C-N	5.13	127.70	120.42
3	F	338	GLY	C-N-CA	5.13	127.70	120.42
4	G	124	ASN	CA-C-N	5.13	127.15	120.28
4	G	124	ASN	C-N-CA	5.13	127.15	120.28
1	7	13	GLY	CA-C-N	5.13	127.48	120.46
1	7	13	GLY	C-N-CA	5.13	127.48	120.46
10	V	27	THR	N-CA-C	-5.12	105.61	111.14
2	C	479	ASN	CA-C-N	5.12	127.14	120.28
2	C	479	ASN	C-N-CA	5.12	127.14	120.28
3	F	222	MET	CA-C-N	5.12	127.14	120.28
3	F	222	MET	C-N-CA	5.12	127.14	120.28
1	7	24	ILE	CA-C-N	5.12	125.62	119.94
1	7	24	ILE	C-N-CA	5.12	125.62	119.94
2	B	255	ILE	CA-C-N	5.12	125.66	119.98
2	B	255	ILE	C-N-CA	5.12	125.66	119.98
7	O	30	ASN	N-CA-C	-5.11	107.09	113.38
11	W	84	PHE	N-CA-C	-5.10	105.14	112.13
2	B	28	ASN	N-CA-C	-5.10	105.96	113.61
5	H	128	GLU	CA-C-N	5.09	127.44	120.46
5	H	128	GLU	C-N-CA	5.09	127.44	120.46
3	E	111	SER	N-CA-C	-5.09	99.95	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	LYS	CA-C-N	5.09	127.10	120.28
2	B	500	LYS	C-N-CA	5.09	127.10	120.28
2	C	197	GLU	N-CA-C	-5.09	106.85	113.16
2	B	128	ARG	N-CA-C	-5.08	100.61	108.90
3	F	54	LEU	N-CA-C	-5.08	106.86	113.16
1	6	54	GLY	CA-C-N	5.08	127.05	120.44
1	6	54	GLY	C-N-CA	5.08	127.05	120.44
2	A	121	GLY	CA-C-N	5.08	126.19	119.84
2	A	121	GLY	C-N-CA	5.08	126.19	119.84
7	O	175	THR	N-CA-C	-5.08	101.57	109.24
2	B	403	ALA	N-CA-C	-5.08	106.68	112.92
3	F	134	LEU	N-CA-C	-5.07	100.15	108.41
12	X	20	THR	CA-C-N	5.07	127.49	120.29
12	X	20	THR	C-N-CA	5.07	127.49	120.29
3	D	393	MET	N-CA-C	-5.07	107.15	113.38
11	W	22	LYS	CA-C-N	5.07	127.03	120.44
11	W	22	LYS	C-N-CA	5.07	127.03	120.44
3	F	20	ILE	N-CA-C	-5.06	99.88	107.37
2	C	36	VAL	CA-C-N	5.06	124.91	120.10
2	C	36	VAL	C-N-CA	5.06	124.91	120.10
2	A	392	LEU	N-CA-C	-5.06	105.85	111.36
3	E	138	ILE	N-CA-C	-5.06	100.49	108.23
12	X	33	PRO	CA-C-N	5.06	125.33	119.92
12	X	33	PRO	C-N-CA	5.06	125.33	119.92
2	A	90	VAL	N-CA-C	-5.05	100.93	108.46
2	A	459	GLU	CA-C-N	5.05	127.05	120.28
2	A	459	GLU	C-N-CA	5.05	127.05	120.28
1	0	11	GLY	CA-C-N	5.05	127.00	120.44
1	0	11	GLY	C-N-CA	5.05	127.00	120.44
3	E	336	SER	CA-C-N	5.05	127.05	120.28
3	E	336	SER	C-N-CA	5.05	127.05	120.28
5	H	56	VAL	N-CA-C	-5.05	101.04	108.11
4	G	196	LYS	N-CA-C	-5.05	106.90	113.16
2	A	80	SER	CA-C-N	5.04	127.04	120.28
2	A	80	SER	C-N-CA	5.04	127.04	120.28
3	F	136	THR	CA-C-N	5.04	125.54	120.00
3	F	136	THR	C-N-CA	5.04	125.54	120.00
1	7	58	SER	CA-C-N	5.04	127.03	120.28
1	7	58	SER	C-N-CA	5.04	127.03	120.28
2	B	205	TYR	N-CA-C	-5.03	100.69	108.90
3	E	32	ALA	N-CA-C	-5.03	102.34	110.14
3	F	25	PHE	N-CA-C	-5.03	101.90	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	294	GLU	N-CA-C	-5.03	107.10	114.39
1	4	17	ILE	CA-C-N	5.03	126.42	120.14
1	4	17	ILE	C-N-CA	5.03	126.42	120.14
2	C	386	LYS	N-CA-C	-5.03	106.84	113.12
3	E	298	THR	N-CA-C	-5.02	99.61	108.20
2	B	60	GLY	CA-C-N	5.02	127.33	120.35
2	B	60	GLY	C-N-CA	5.02	127.33	120.35
1	3	10	ILE	CA-C-N	5.02	125.55	119.98
1	3	10	ILE	C-N-CA	5.02	125.55	119.98
3	E	110	LYS	N-CA-C	-5.02	100.11	110.80
3	F	247	GLU	N-CA-C	-5.02	105.97	113.89
2	A	135	ALA	CA-C-N	5.01	124.94	119.78
2	A	135	ALA	C-N-CA	5.01	124.94	119.78
3	E	208	ASN	N-CA-C	-5.01	101.58	109.25
2	B	363	ILE	N-CA-C	-5.01	99.29	106.55
2	C	121	GLY	CA-C-N	5.01	126.10	119.84
2	C	121	GLY	C-N-CA	5.01	126.10	119.84
3	F	106	ARG	N-CA-C	-5.01	106.48	112.59
5	H	135	SER	N-CA-C	5.01	117.47	111.71
2	A	300	VAL	N-CA-C	-5.00	104.84	111.09
2	B	133	VAL	N-CA-C	-5.00	100.87	108.17
5	H	33	PRO	N-CA-C	-5.00	102.17	112.47

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	40	ASN	Peptide
1	3	40	ASN	Peptide
1	4	40	ASN	Peptide
1	5	40	ASN	Peptide
1	6	40	ASN	Peptide
1	7	40	ASN	Peptide
1	8	40	ASN	Peptide
1	9	40	ASN	Peptide
2	B	29	GLU	Peptide
3	E	256	ASP	Peptide
9	U	187	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	2004	0	575	1	0
2	B	2020	0	575	1	0
2	C	1984	0	567	1	0
3	D	1876	0	537	0	0
3	E	1880	0	538	1	0
3	F	1872	0	537	0	0
4	G	1060	0	277	0	0
5	H	480	0	122	0	0
6	I	193	0	43	0	0
7	O	748	0	205	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	4	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (4) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:GLY:HA3	2:A:126:ALA:H	1.79	0.48
2:C:102:GLY:HA3	2:C:126:ALA:H	1.80	0.47
3:E:160:GLY:C	3:E:162:GLY:H	2.25	0.45
2:B:27:LEU:O	2:B:45:GLY:HA2	2.20	0.40

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%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	3	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	9	40
1	4	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	5	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	6	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	9	40
1	7	71/76 (93%)	69 (97%)	1 (1%)	1 (1%)	9	40
1	8	73/76 (96%)	71 (97%)	1 (1%)	1 (1%)	9	40
1	9	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	9	40
2	A	499/510 (98%)	472 (95%)	22 (4%)	5 (1%)	12	48
2	B	501/510 (98%)	469 (94%)	24 (5%)	8 (2%)	7	38
2	C	492/510 (96%)	467 (95%)	19 (4%)	6 (1%)	10	44
3	D	467/478 (98%)	428 (92%)	29 (6%)	10 (2%)	5	30
3	E	468/478 (98%)	433 (92%)	29 (6%)	6 (1%)	9	42
3	F	466/478 (98%)	443 (95%)	20 (4%)	3 (1%)	21	59
4	G	261/278 (94%)	250 (96%)	6 (2%)	5 (2%)	6	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	110/138 (80%)	103 (94%)	5 (4%)	2 (2%)	6	34
6	I	42/61 (69%)	38 (90%)	4 (10%)	0	100	100
7	O	185/195 (95%)	169 (91%)	10 (5%)	6 (3%)	3	21
8	T	222/249 (89%)	212 (96%)	6 (3%)	4 (2%)	6	34
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	151 (89%)	12 (7%)	6 (4%)	2	20
11	W	83/95 (87%)	67 (81%)	11 (13%)	5 (6%)	1	13
12	X	60/92 (65%)	53 (88%)	5 (8%)	2 (3%)	3	21
13	Y	35/59 (59%)	32 (91%)	3 (9%)	0	100	100
14	Z	46/48 (96%)	41 (89%)	4 (9%)	1 (2%)	5	29
All	All	4984/5321 (94%)	4684 (94%)	223 (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	299	ASP
2	B	25	ALA
2	B	29	GLU
2	B	229	LYS
2	B	315	SER
2	B	406	ALA
2	C	391	SER
3	D	451	ASN
3	E	110	LYS
3	E	353	SER
3	E	358	LEU
4	G	194	PHE
7	O	61	ALA
11	W	11	SER
11	W	42	ILE

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Mol	Chain	Res	Type
12	X	58	VAL
2	A	36	VAL
2	B	317	LYS
2	C	36	VAL
2	C	49	ILE
3	D	68	GLU
3	D	81	GLY
3	E	462	GLY
7	O	10	VAL
10	V	130	PHE
12	X	14	THR
2	A	22	SER
2	A	378	SER
2	B	145	HIS
2	C	193	ASN
2	C	338	ALA
3	D	86	PRO
3	D	162	GLY
3	F	130	SER
5	H	33	PRO
7	O	98	LEU
8	T	51	ASN
10	V	66	SER
10	V	133	LEU
11	W	31	TYR
11	W	38	PRO
2	C	145	HIS
3	E	249	GLN
4	G	123	PRO
4	G	135	LYS
8	T	45	THR
14	Z	4	LEU
2	B	103	PRO
3	D	97	ASN
3	D	98	VAL
3	D	278	ALA
3	D	417	PRO
3	F	16	VAL
3	F	249	GLN
5	H	81	SER
7	O	81	LEU
8	T	50	ASN

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Mol	Chain	Res	Type
10	V	50	PRO
10	V	128	ARG
10	V	166	ARG
2	A	46	LEU
4	G	58	LYS
4	G	181	PRO
7	O	82	ASP
8	T	46	LEU
11	W	39	ALA
3	E	161	VAL
7	O	9	PRO
3	D	462	GLY

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.

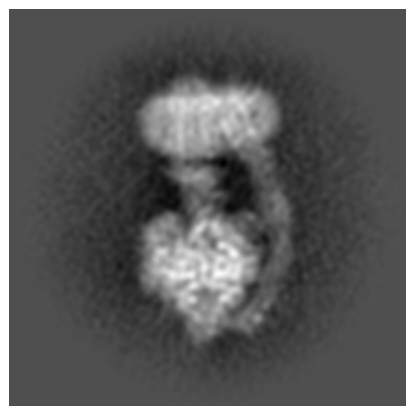
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25966. These allow visual inspection of the internal detail of the map and identification of artifacts.

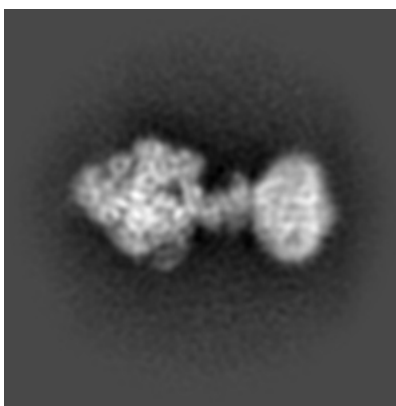
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

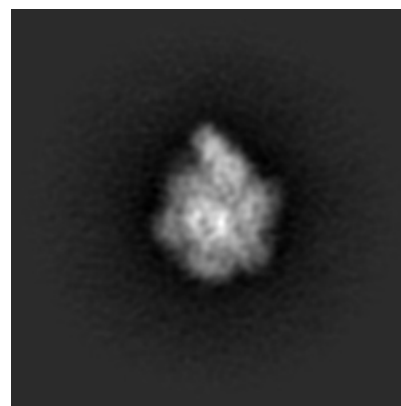
6.1.1 Primary map



X

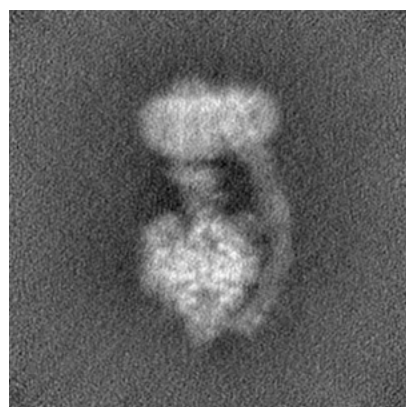


Y

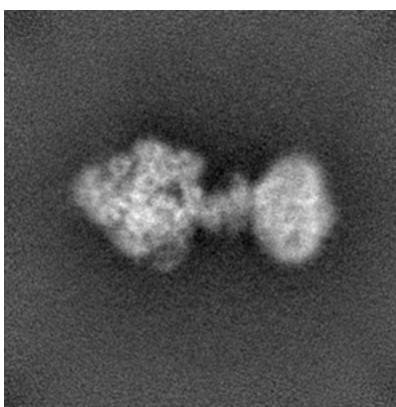


Z

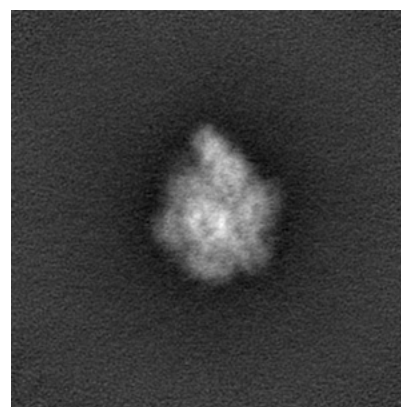
6.1.2 Raw map



X



Y

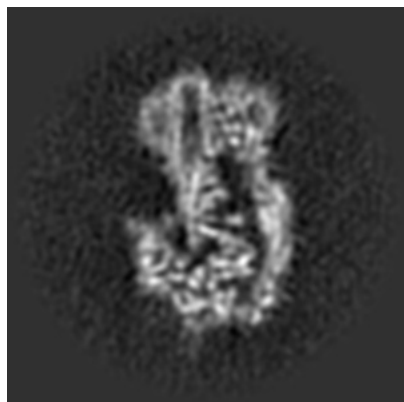


Z

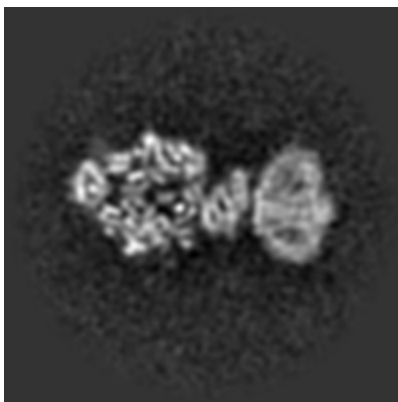
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

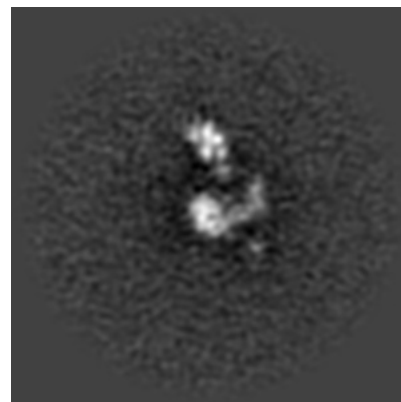
6.2.1 Primary map



X Index: 128

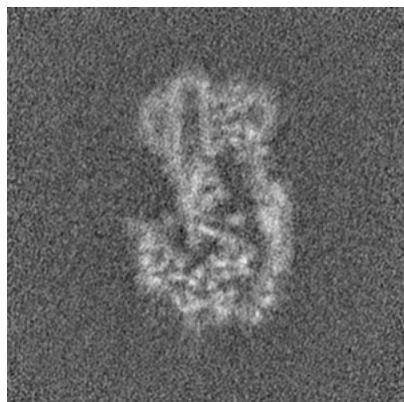


Y Index: 128

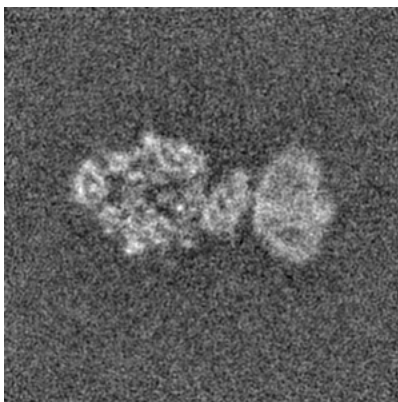


Z Index: 128

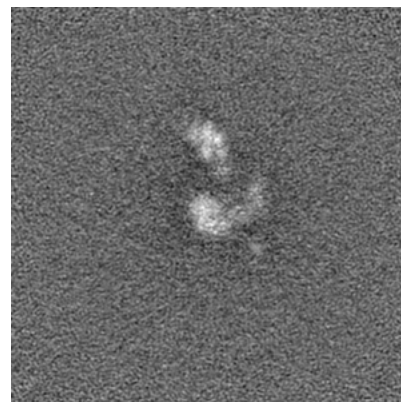
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

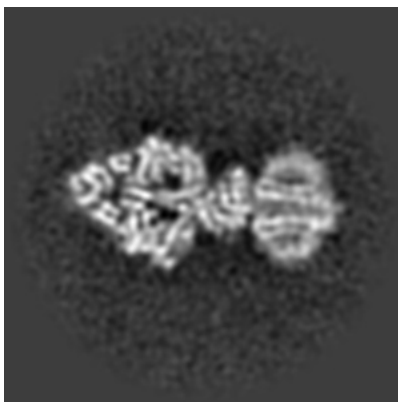
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

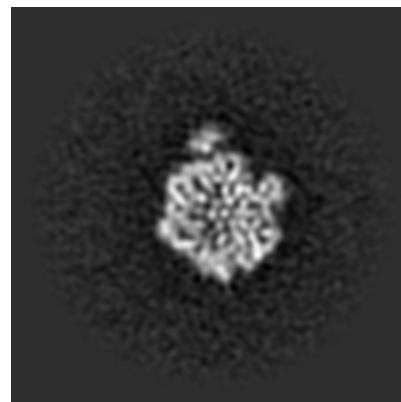
6.3.1 Primary map



X Index: 132

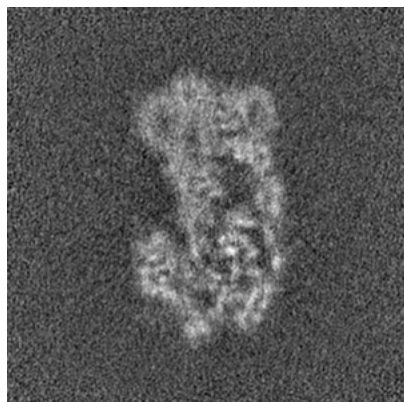


Y Index: 123

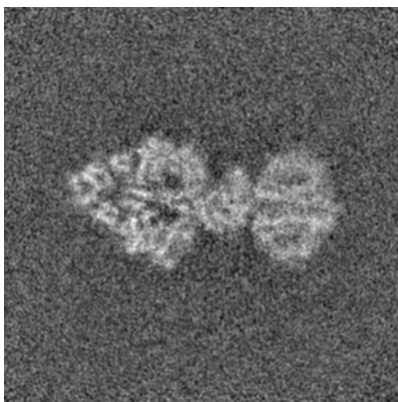


Z Index: 87

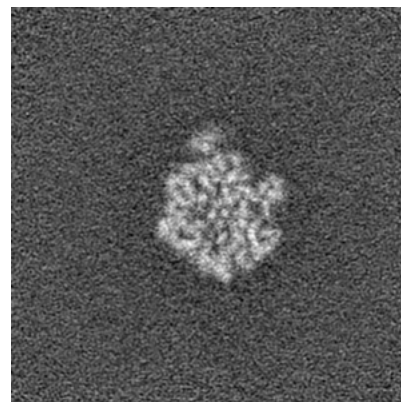
6.3.2 Raw map



X Index: 132



Y Index: 123

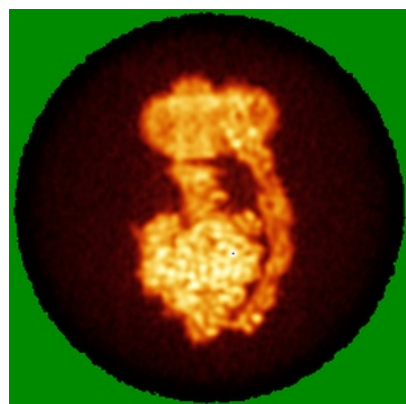


Z Index: 86

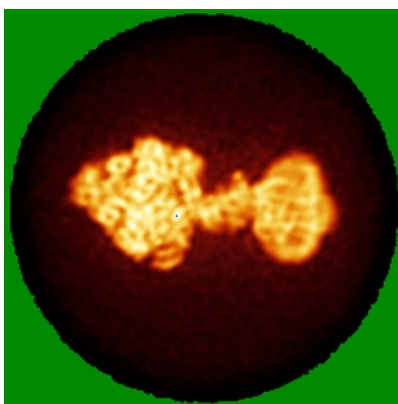
The images above show the largest variance slices of the map in three orthogonal directions.

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

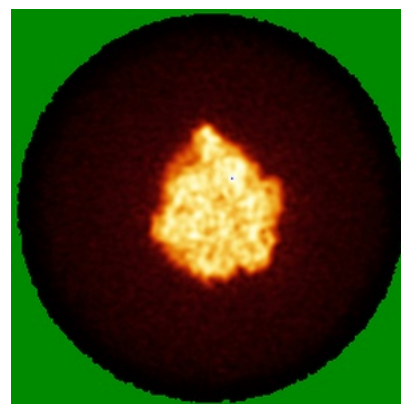
6.4.1 Primary map



X

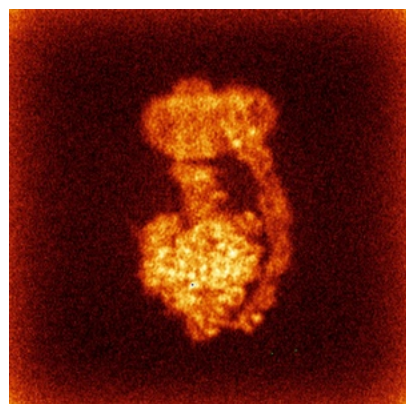


Y

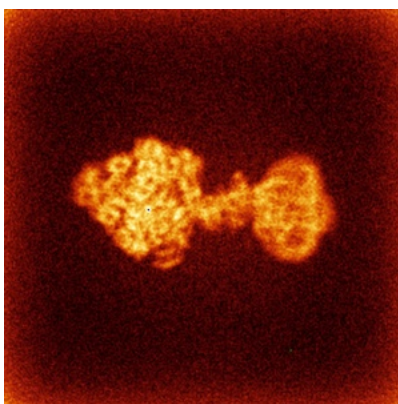


Z

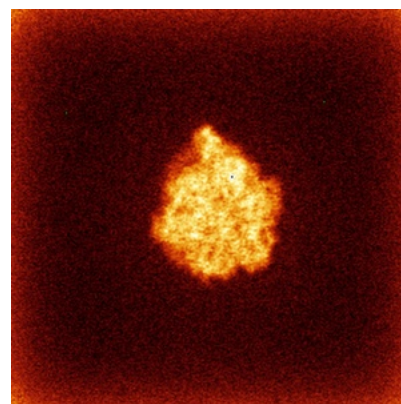
6.4.2 Raw map



X



Y

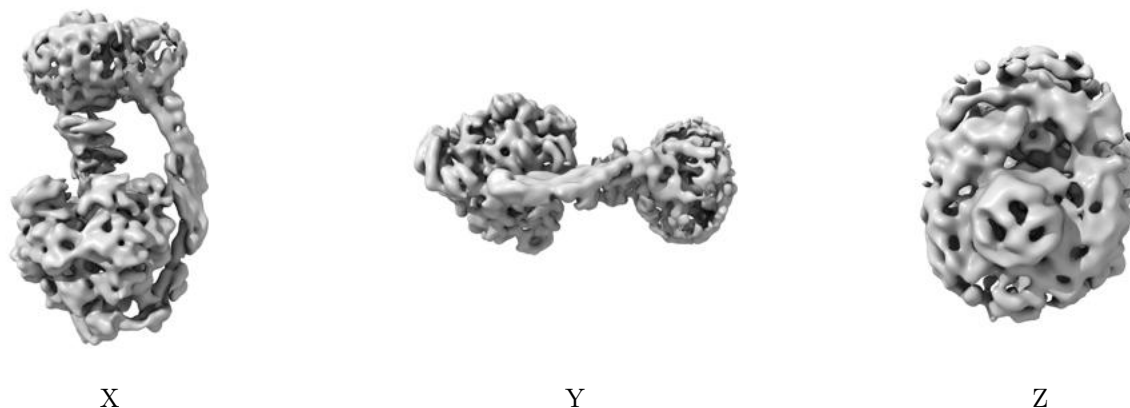


Z

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 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

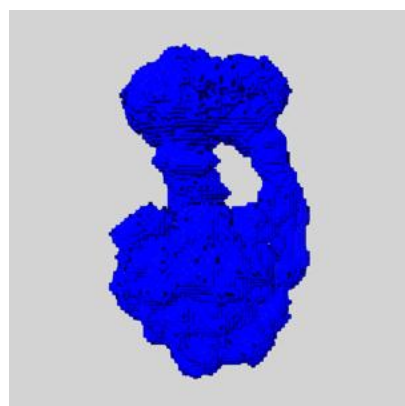
6.6 Mask visualisation [i](#)

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

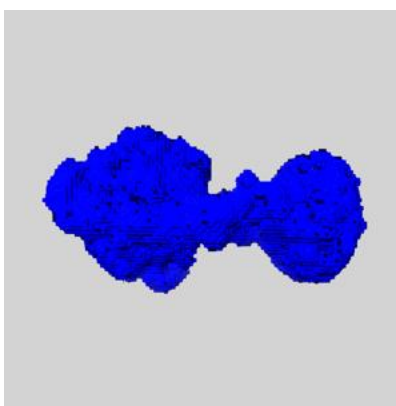
A mask typically either:

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

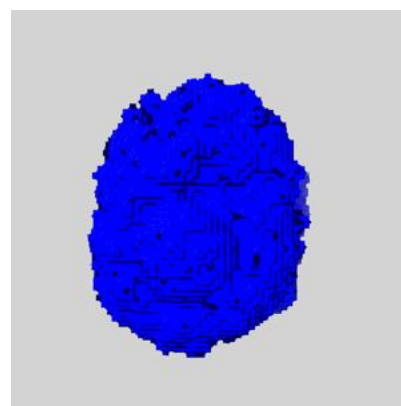
6.6.1 emd_25966_msk_1.map [i](#)



X



Y

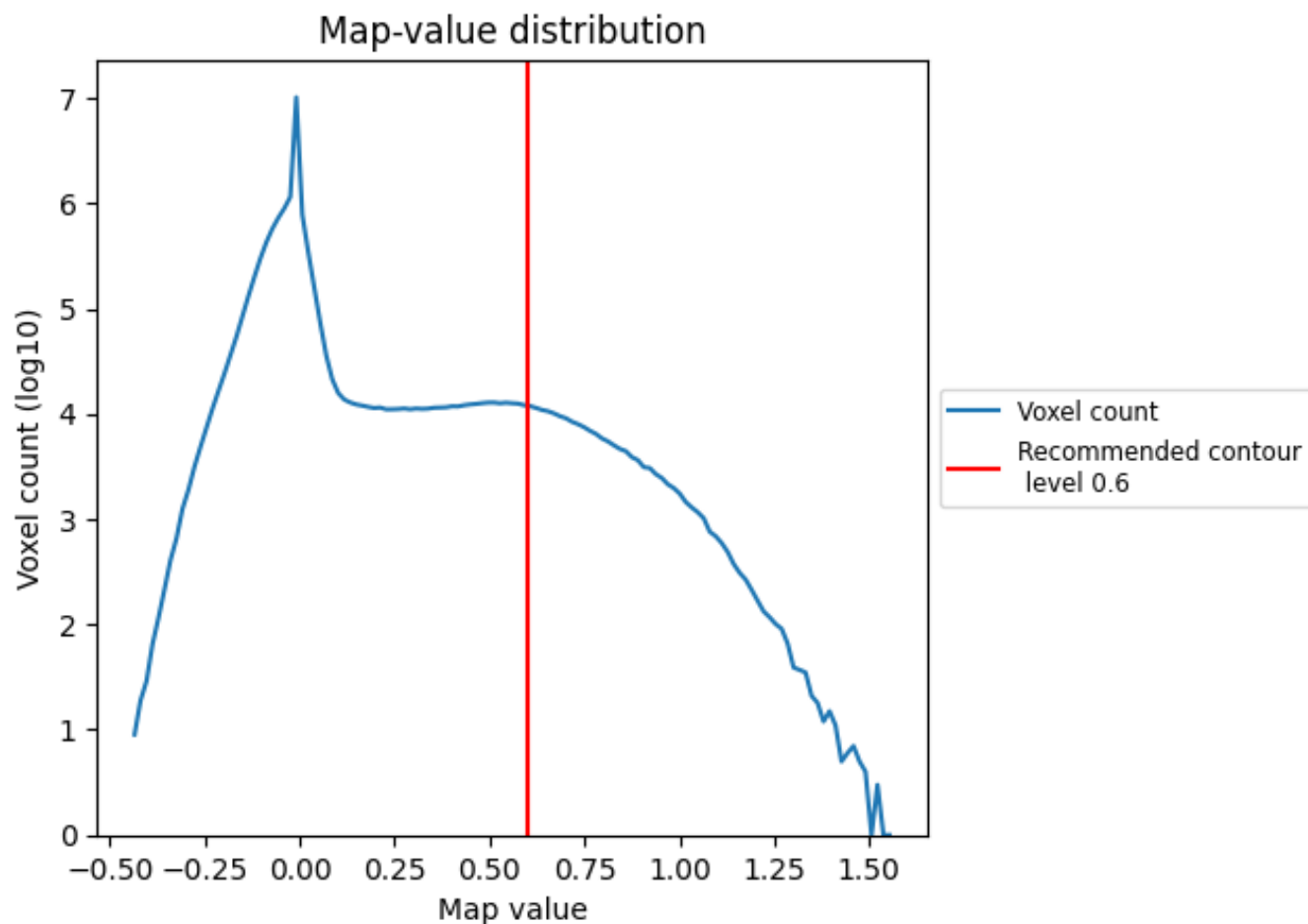


Z

7 Map analysis [i](#)

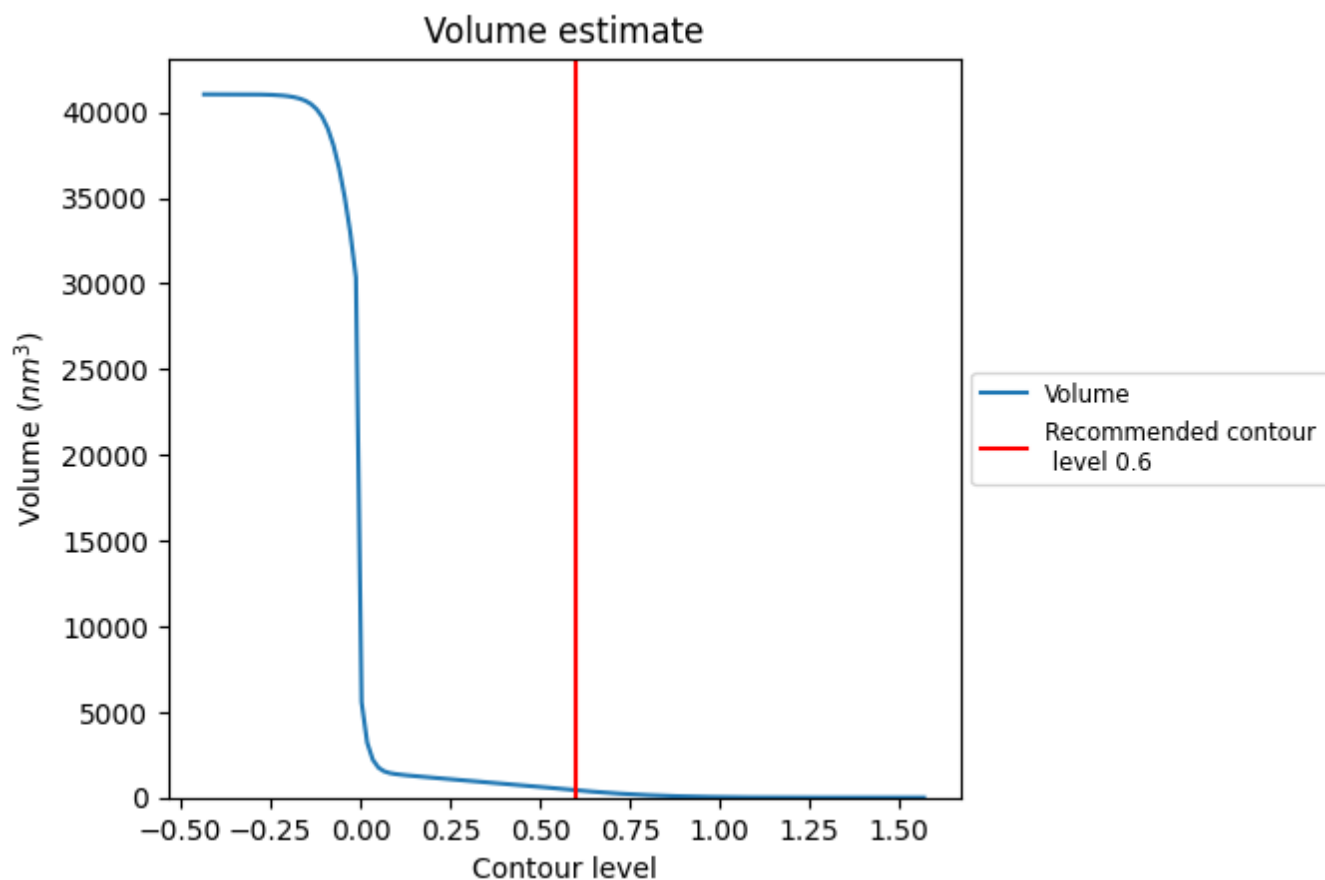
This section contains the results of statistical analysis of the map.

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.

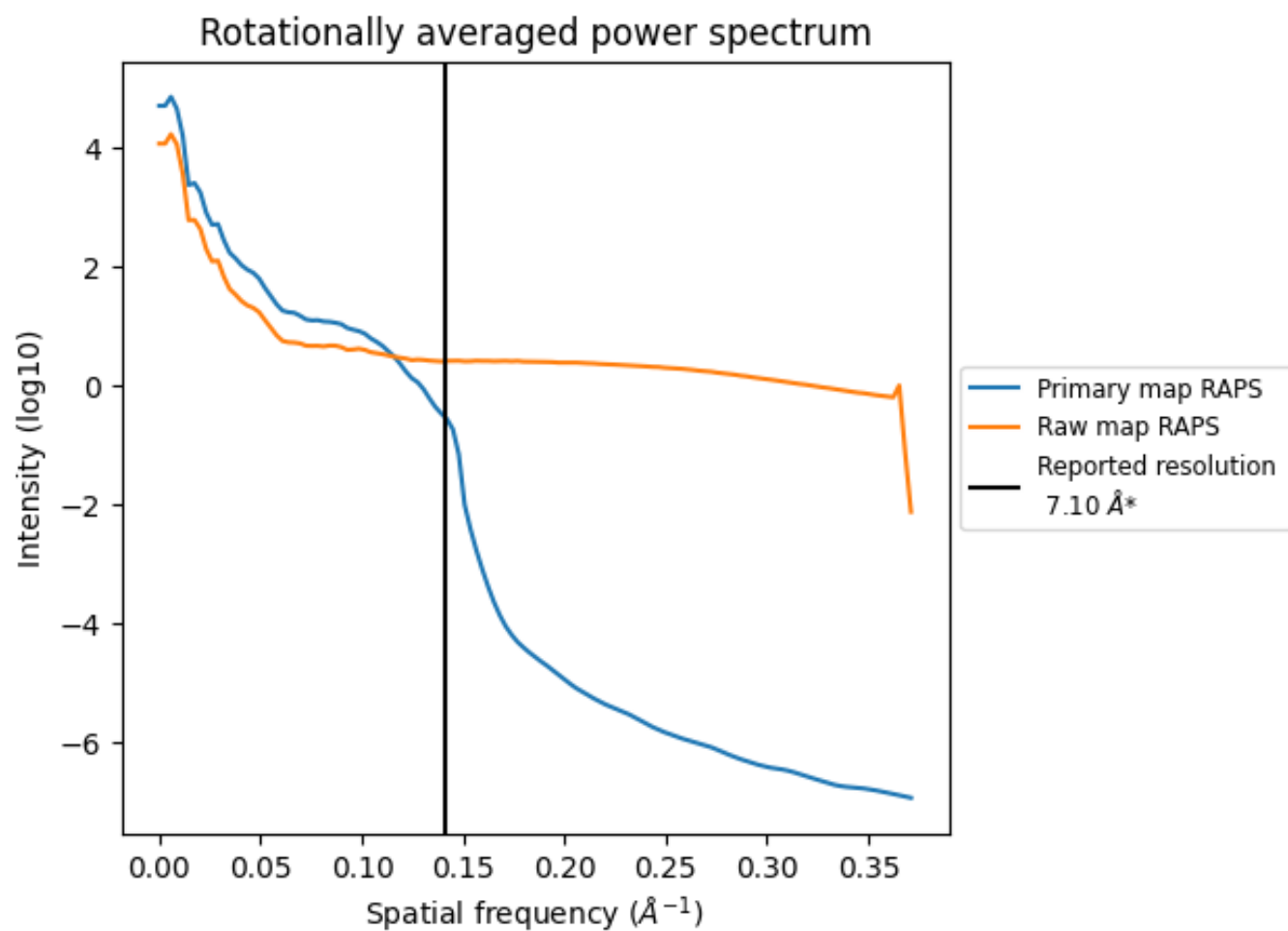
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 429 nm³; this corresponds to an approximate mass of 388 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

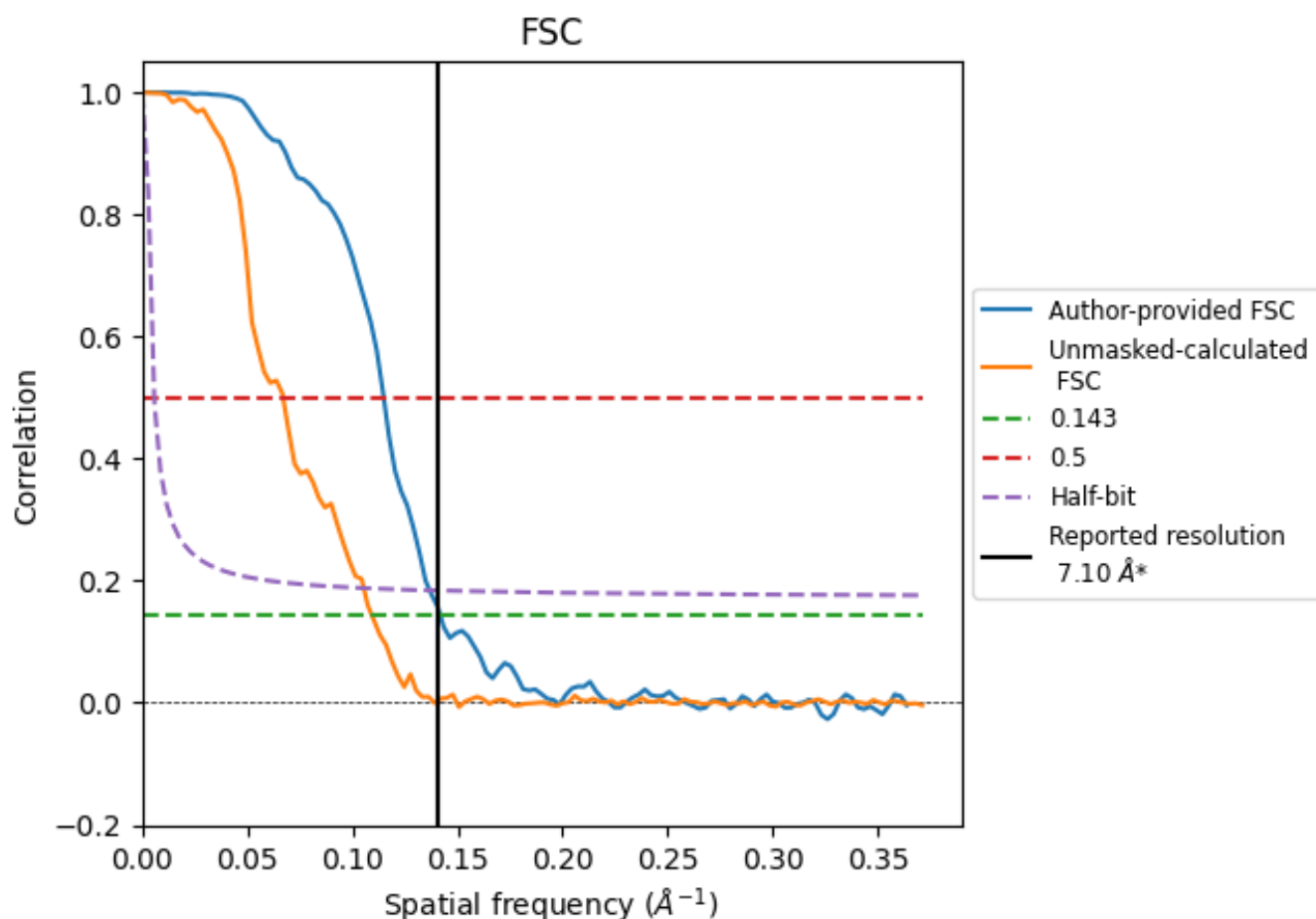


*Reported resolution corresponds to spatial frequency of 0.141 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.141 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

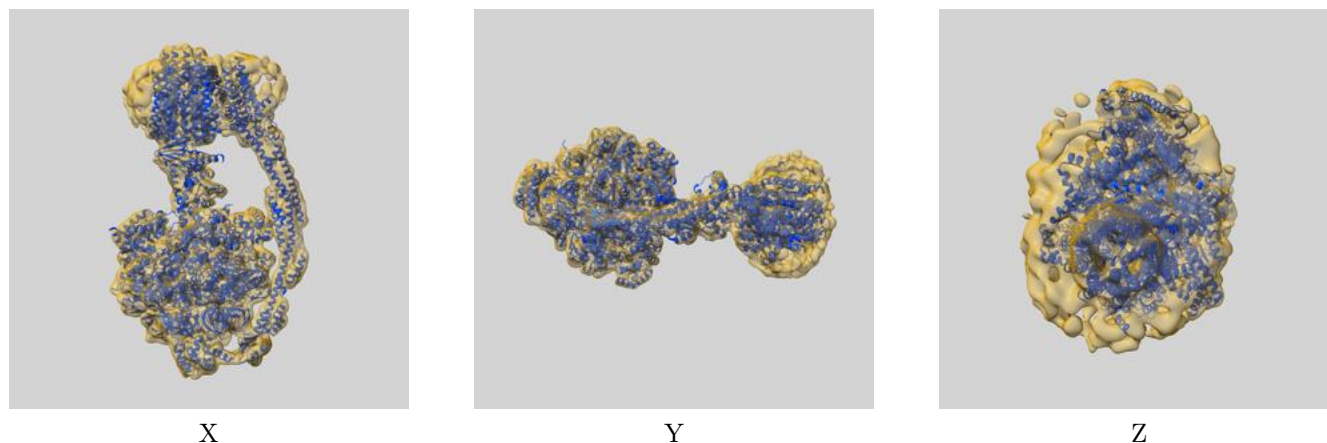
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.10	-	-
Author-provided FSC curve	7.05	8.70	7.31
Unmasked-calculated*	9.15	14.93	9.49

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

9 Map-model fit [i](#)

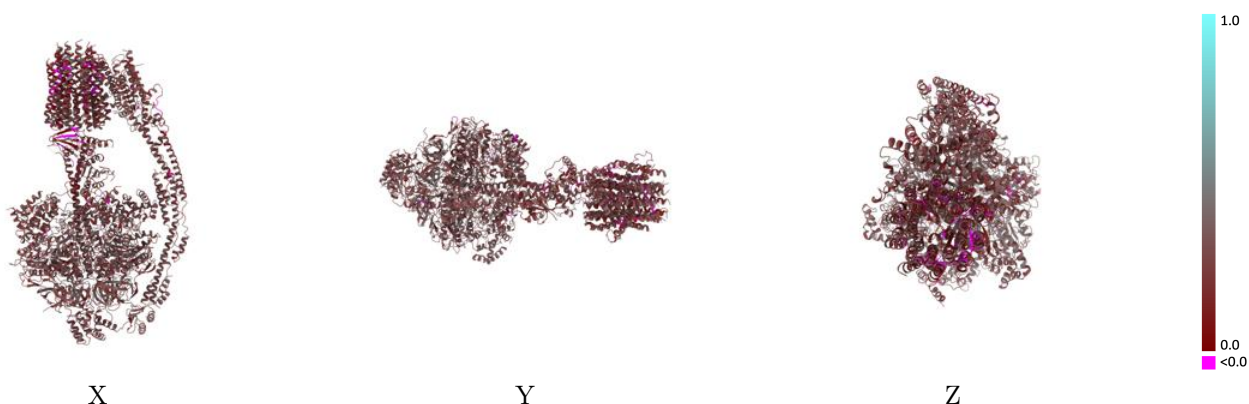
This section contains information regarding the fit between EMDB map EMD-25966 and PDB model 7TKE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



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

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

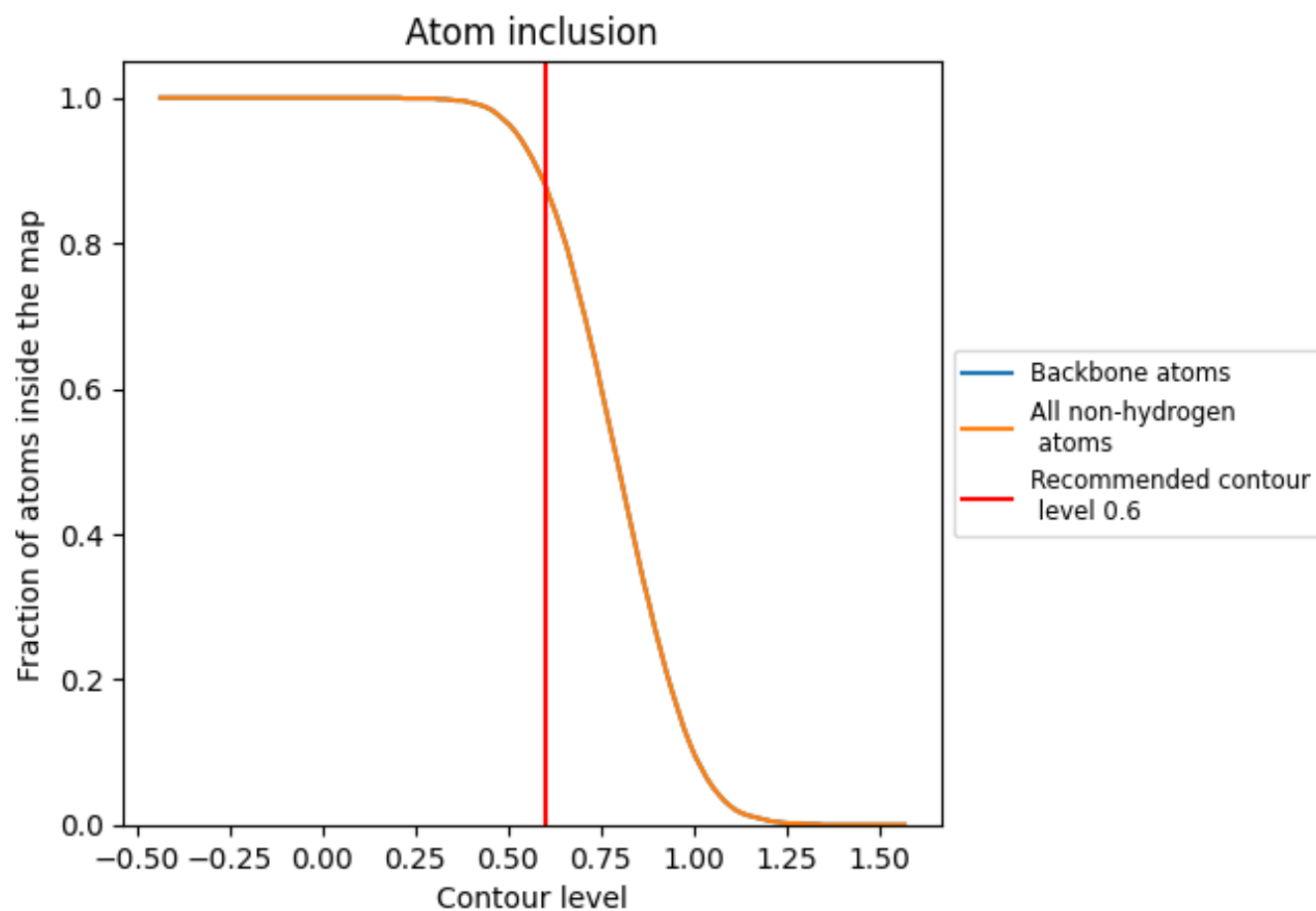


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.8820	 0.2670
0	 0.6130	 0.1800
1	 0.7430	 0.2090
2	 0.7970	 0.2210
3	 0.7260	 0.2190
4	 0.5730	 0.1890
5	 0.7070	 0.1940
6	 0.8070	 0.2220
7	 0.8250	 0.2260
8	 0.8170	 0.2200
9	 0.6690	 0.1540
A	 0.9530	 0.3010
B	 0.9300	 0.2910
C	 0.9450	 0.2940
D	 0.9630	 0.3030
E	 0.8910	 0.2770
F	 0.8820	 0.2720
G	 0.8400	 0.2390
H	 0.6650	 0.1640
I	 0.6630	 0.2310
O	 0.9670	 0.2900
T	 0.8660	 0.2580
U	 0.9920	 0.2930
V	 0.9110	 0.2740
W	 0.8470	 0.2160
X	 0.8150	 0.2450
Y	 0.8310	 0.2390
Z	 0.9740	 0.2670

