



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:34 PM UTC

PDB ID : 7TKB / pdb_00007tkb
EMDB ID : EMD-25963
Title : Yeast ATP synthase State 1catalytic(f) with 10 mM ATP backbone model
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2022-01-17
Resolution : 6.30 Å(reported)
Based on initial model : 2HLD

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

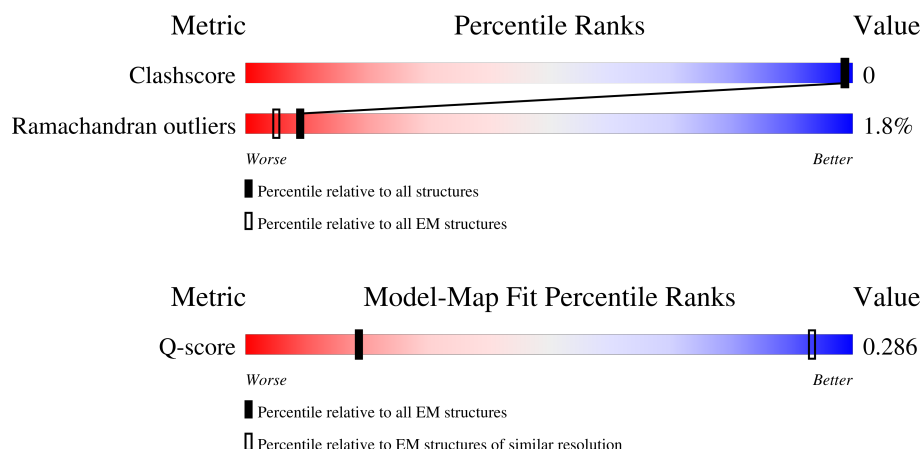
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	550 (5.80 - 6.80)

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

Mol	Chain	Length	Quality of chain
1	0	76	18% 91% 8%
1	1	76	25% 93% 5%
1	2	76	33% 92% 7%
1	3	76	36% 91% 7%
1	4	76	24% 93% 7%

Continued on next page...

Continued from previous page...

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 [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

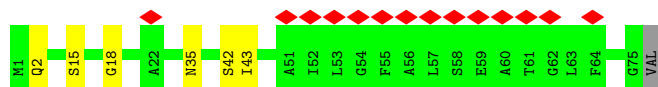
- Molecule 14 is a protein called ATP synthase protein 8.

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

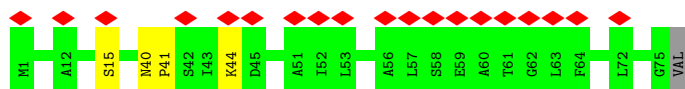
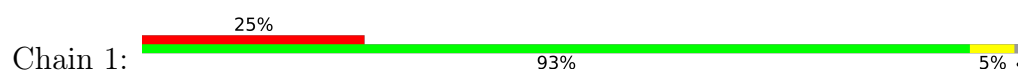
3 Residue-property plots [i](#)

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

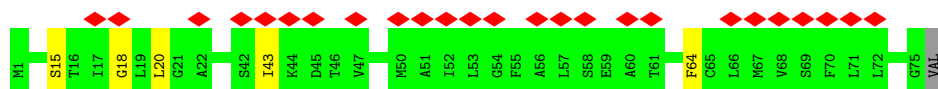
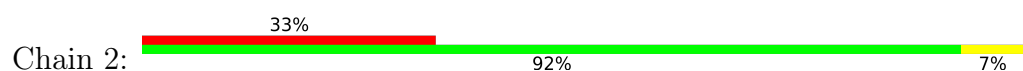
- Molecule 1: ATP synthase subunit 9, mitochondrial



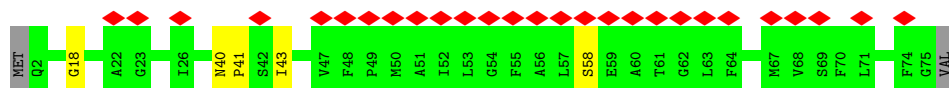
- Molecule 1: ATP synthase subunit 9, mitochondrial



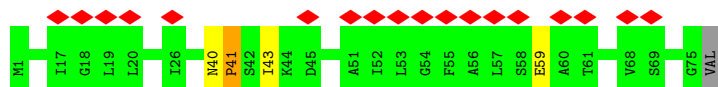
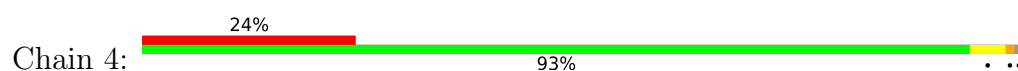
- Molecule 1: ATP synthase subunit 9, mitochondrial



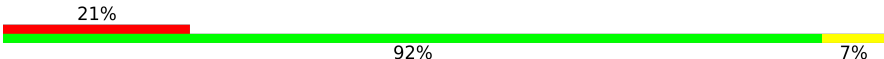
- Molecule 1: ATP synthase subunit 9, mitochondrial

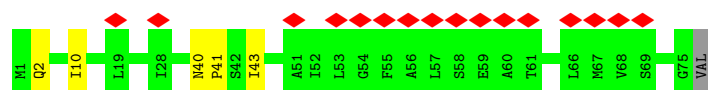


- Molecule 1: ATP synthase subunit 9, mitochondrial



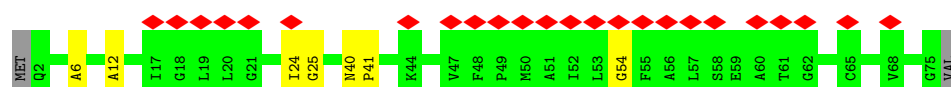
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 5: 



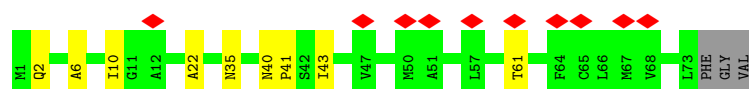
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 6: 

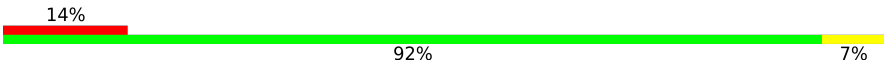


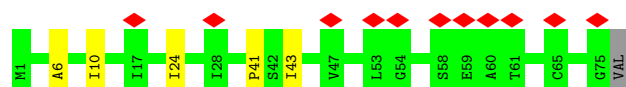
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 7: 



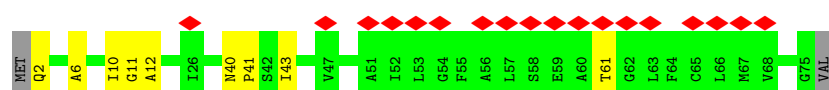
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 8: 

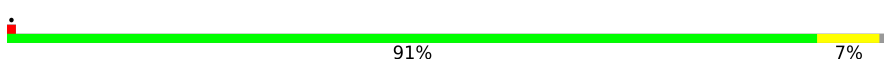


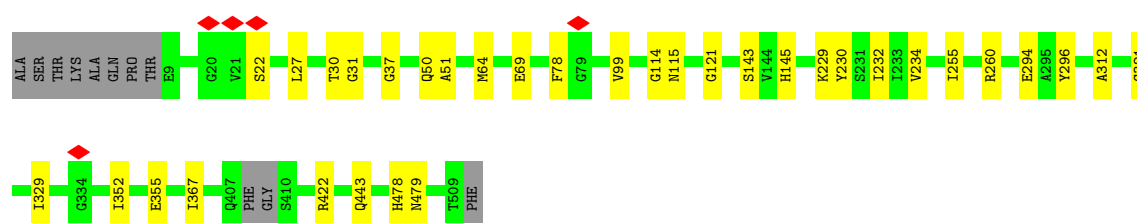
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 9: 

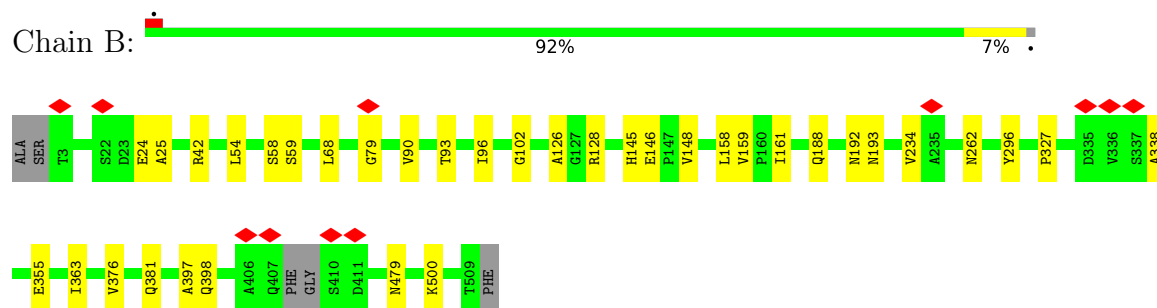


- Molecule 2: ATP synthase subunit alpha

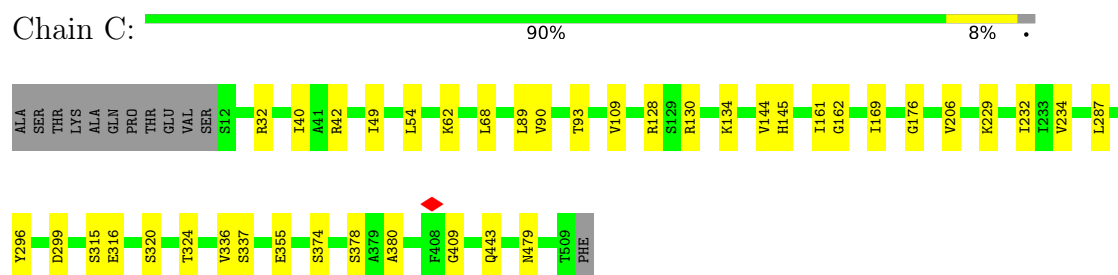
Chain A: 



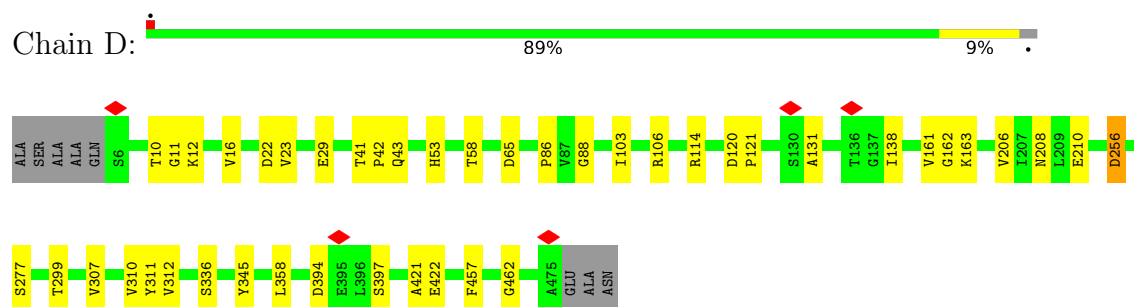
- Molecule 2: ATP synthase subunit alpha



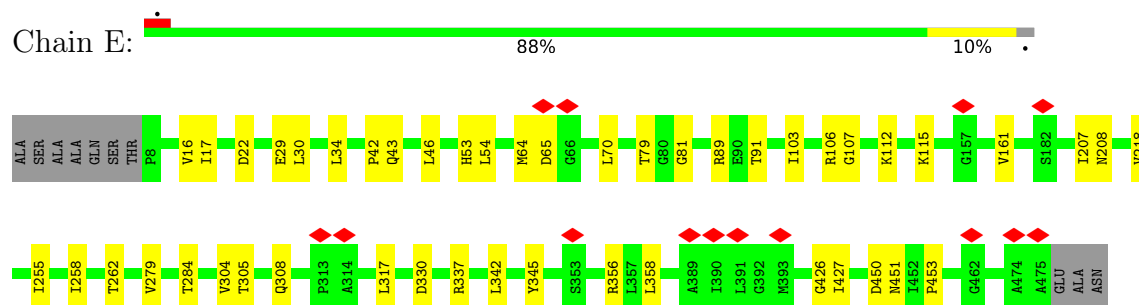
- Molecule 2: ATP synthase subunit alpha



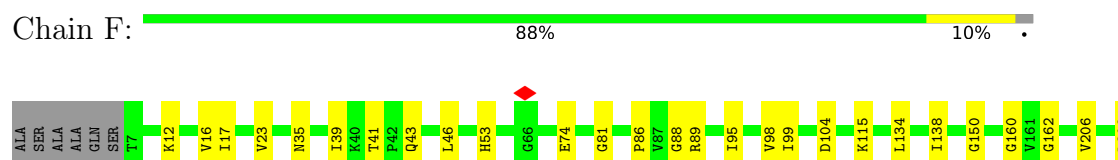
- Molecule 3: ATP synthase subunit beta



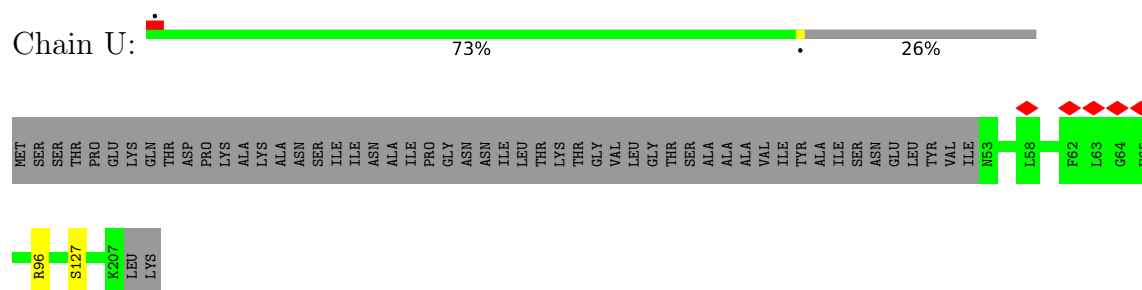
- Molecule 3: ATP synthase subunit beta



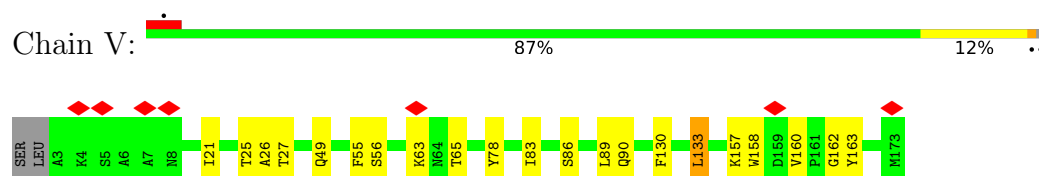
- Molecule 3: ATP synthase subunit beta



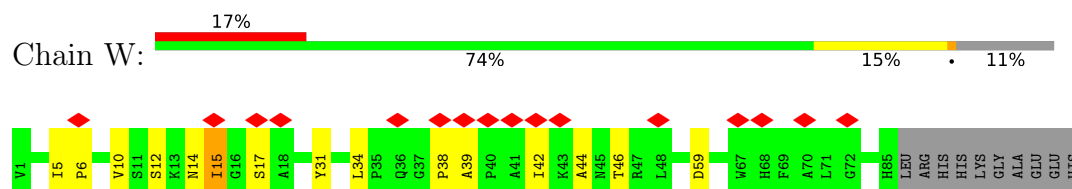
- Molecule 9: ATP synthase subunit 4



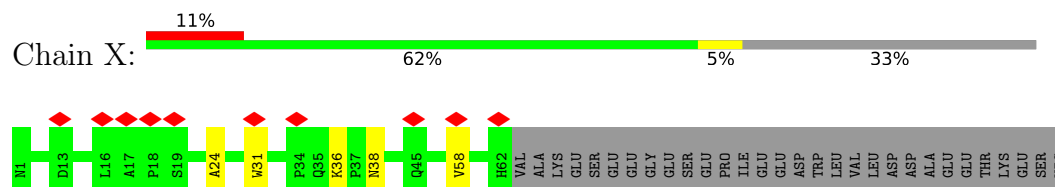
- Molecule 10: ATP synthase subunit d



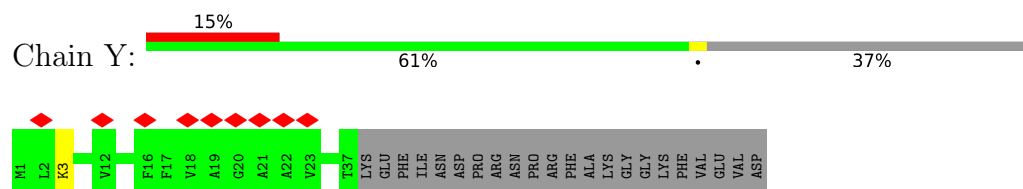
- Molecule 11: ATP synthase subunit f



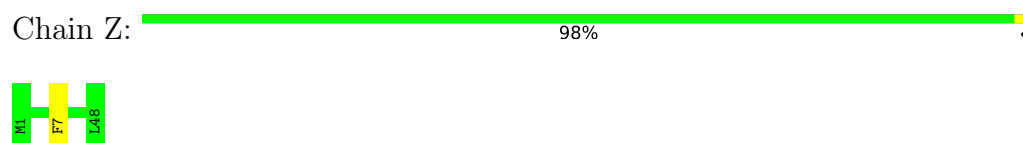
- Molecule 12: ATP synthase subunit H



- Molecule 13: ATP synthase subunit J



- Molecule 14: ATP synthase protein 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	103896	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.128	Depositor
Minimum map value	-0.763	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.119	Depositor
Recommended contour level	0.66	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	1.24	0/299	2.18	10/372 (2.7%)
1	1	1.20	0/299	2.01	3/372 (0.8%)
1	2	1.21	0/299	2.25	10/372 (2.7%)
1	3	1.22	0/295	2.07	6/367 (1.6%)
1	4	1.25	0/299	2.22	5/372 (1.3%)
1	5	1.24	0/299	2.17	6/372 (1.6%)
1	6	1.22	0/295	2.29	10/367 (2.7%)
1	7	1.21	0/291	2.35	14/362 (3.9%)
1	8	1.24	0/299	2.29	8/372 (2.2%)
1	9	1.20	0/295	2.23	14/367 (3.8%)
2	A	1.55	2/1994 (0.1%)	1.80	33/2489 (1.3%)
2	B	1.55	0/2018	1.84	39/2519 (1.5%)
2	C	1.57	0/1991	1.85	38/2487 (1.5%)
3	D	1.57	2/1879 (0.1%)	1.86	37/2347 (1.6%)
3	E	1.58	0/1871	1.90	49/2337 (2.1%)
3	F	1.58	1/1875 (0.1%)	1.84	42/2342 (1.8%)
4	G	1.47	0/1058	1.88	23/1319 (1.7%)
5	H	1.45	0/475	1.79	8/585 (1.4%)
6	I	1.32	0/190	1.86	2/231 (0.9%)
7	O	1.54	0/747	1.84	10/932 (1.1%)
8	T	1.28	0/896	1.78	14/1117 (1.3%)
9	U	1.33	0/619	1.88	4/772 (0.5%)
10	V	1.40	0/684	1.86	12/852 (1.4%)
11	W	1.27	0/339	2.00	11/422 (2.6%)
12	X	1.38	0/247	2.02	2/307 (0.7%)
13	Y	1.20	0/147	1.78	0/182
14	Z	1.29	0/192	1.84	1/237 (0.4%)
All	All	1.47	5/20192 (0.0%)	1.91	411/25172 (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	9	0	1
3	D	0	1
3	F	0	1
5	H	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	11	GLY	CA-C	-6.30	1.46	1.52
3	F	391	LEU	CA-C	-6.26	1.50	1.53
2	A	478	HIS	CA-C	-5.84	1.48	1.53
2	A	321	GLY	CA-C	-5.59	1.46	1.52
3	D	312	VAL	N-CA	-5.58	1.42	1.46

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	316	GLU	N-CA-C	-10.91	102.18	114.62
4	G	204	ASN	CA-C-N	10.65	126.95	120.24
4	G	204	ASN	C-N-CA	10.65	126.95	120.24
8	T	77	ILE	N-CA-C	-10.60	103.24	111.62
3	E	161	VAL	N-CA-C	-9.62	103.30	112.83
2	B	398	GLN	N-CA-C	-9.62	101.67	113.41
11	W	6	PRO	N-CA-C	9.22	121.95	110.70
10	V	90	GLN	N-CA-C	-9.00	102.81	113.88
3	F	225	PRO	CA-C-O	-8.73	114.61	120.90
5	H	61	GLU	N-CA-C	-8.12	95.03	108.34
2	A	479	ASN	N-CA-C	-7.92	103.62	113.28
3	F	99	ILE	N-CA-C	-7.90	104.88	111.91
3	E	103	ILE	N-CA-C	-7.88	105.18	112.43
3	E	64	MET	N-CA-C	-7.87	104.28	114.04
2	C	93	THR	N-CA-C	-7.86	102.80	111.36
2	B	262	ASN	N-CA-C	-7.75	103.40	113.17
2	B	192	ASN	N-CA-C	-7.71	104.02	113.50
3	E	17	ILE	N-CA-C	-7.66	96.81	107.99
3	F	43	GLN	N-CA-C	-7.66	103.25	112.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	208	ASN	N-CA-C	-7.54	94.75	107.80
2	B	93	THR	N-CA-C	-7.52	103.17	111.36
3	E	207	ILE	N-CA-C	-7.47	97.65	108.11
7	O	174	LYS	N-CA-C	-7.43	96.19	108.76
2	B	42	ARG	N-CA-C	-7.43	96.15	108.34
2	B	234	VAL	N-CA-C	-7.42	97.77	108.53
3	E	258	ILE	N-CA-C	-7.32	104.22	113.22
2	A	232	ILE	N-CA-C	-7.28	97.67	108.45
3	E	43	GLN	N-CA-C	-7.23	104.48	112.72
1	4	43	ILE	CA-C-N	7.21	130.91	120.38
1	4	43	ILE	C-N-CA	7.21	130.91	120.38
2	B	193	ASN	N-CA-C	-7.20	102.75	112.26
3	E	29	GLU	N-CA-C	-7.20	99.67	109.54
3	F	12	LYS	N-CA-C	-7.12	98.48	109.52
3	E	305	THR	N-CA-C	-7.10	98.22	109.23
1	1	44	LYS	N-CA-C	7.08	119.85	111.71
3	E	106	ARG	N-CA-C	-7.06	104.67	112.72
3	D	121	PRO	CA-C-O	-7.03	115.84	120.90
1	7	10	ILE	CA-C-N	6.97	127.72	119.98
1	7	10	ILE	C-N-CA	6.97	127.72	119.98
2	B	96	ILE	N-CA-C	-6.95	102.35	110.21
2	B	58	SER	N-CA-C	-6.94	101.90	110.65
2	A	30	THR	N-CA-C	-6.87	98.88	109.52
1	9	10	ILE	CA-C-N	6.83	127.57	119.98
1	9	10	ILE	C-N-CA	6.83	127.57	119.98
2	B	479	ASN	N-CA-C	-6.78	104.76	113.16
3	F	252	LEU	N-CA-C	-6.68	98.92	109.07
2	A	114	GLY	N-CA-C	-6.66	105.09	116.01
2	A	115	ASN	N-CA-C	-6.66	101.12	110.31
10	V	160	VAL	N-CA-C	-6.66	100.48	107.60
8	T	140	VAL	N-CA-C	-6.64	106.05	112.29
7	O	98	LEU	N-CA-C	-6.60	104.82	114.39
10	V	63	LYS	N-CA-C	-6.60	105.14	113.72
3	E	53	HIS	N-CA-C	-6.59	97.66	108.41
11	W	5	ILE	CA-C-N	6.59	127.17	120.38
11	W	5	ILE	C-N-CA	6.59	127.17	120.38
2	C	90	VAL	N-CA-C	-6.59	98.63	108.12
8	T	80	LYS	N-CA-C	-6.58	105.56	112.93
2	B	188	GLN	N-CA-C	-6.57	103.59	112.26
3	E	54	LEU	N-CA-C	-6.57	105.27	113.28
3	D	103	ILE	N-CA-C	-6.56	105.74	113.42
2	C	68	LEU	N-CA-C	-6.54	97.62	108.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	56	SER	N-CA-C	-6.53	102.82	111.24
1	3	43	ILE	CA-C-N	6.52	129.89	120.38
1	3	43	ILE	C-N-CA	6.52	129.89	120.38
3	D	312	VAL	N-CA-C	-6.52	101.10	107.55
4	G	2	THR	N-CA-C	-6.51	104.11	111.14
2	C	42	ARG	N-CA-C	-6.51	96.76	108.48
2	A	234	VAL	N-CA-C	-6.49	99.23	108.58
2	A	69	GLU	N-CA-C	-6.42	100.73	110.50
11	W	10	VAL	N-CA-C	-6.42	99.12	108.11
3	E	304	VAL	N-CA-C	-6.40	103.08	110.05
2	C	232	ILE	N-CA-C	-6.35	99.34	108.48
2	C	234	VAL	N-CA-C	-6.34	99.29	108.17
2	B	54	LEU	N-CA-C	-6.33	98.92	109.24
2	C	443	GLN	N-CA-C	-6.32	106.10	113.88
3	F	89	ARG	N-CA-C	-6.32	105.20	113.17
1	7	43	ILE	CA-C-N	6.32	129.04	120.38
1	7	43	ILE	C-N-CA	6.32	129.04	120.38
2	B	128	ARG	N-CA-C	-6.31	99.53	109.50
2	A	99	VAL	N-CA-C	-6.31	104.02	109.19
3	E	42	PRO	N-CA-C	-6.29	108.14	114.68
11	W	15	ILE	CA-C-N	6.28	126.07	120.10
11	W	15	ILE	C-N-CA	6.28	126.07	120.10
2	A	27	LEU	CA-C-N	6.27	128.68	120.28
2	A	27	LEU	C-N-CA	6.27	128.68	120.28
2	C	206	VAL	N-CA-C	-6.24	99.37	108.11
4	G	73	LEU	N-CA-C	-6.24	100.03	109.95
3	D	311	TYR	N-CA-C	-6.22	98.76	108.90
2	C	355	GLU	CA-C-N	6.21	128.60	120.28
2	C	355	GLU	C-N-CA	6.21	128.60	120.28
3	E	89	ARG	N-CA-C	-6.21	105.35	113.17
3	D	120	ASP	CA-C-N	6.21	124.19	119.66
3	D	120	ASP	C-N-CA	6.21	124.19	119.66
3	D	22	ASP	N-CA-C	-6.20	100.09	109.95
3	F	17	ILE	N-CA-C	-6.19	98.21	107.37
2	B	68	LEU	N-CA-C	-6.18	98.66	108.73
1	5	10	ILE	CA-C-N	6.17	126.83	119.98
1	5	10	ILE	C-N-CA	6.17	126.83	119.98
2	B	376	VAL	N-CA-C	-6.17	99.47	108.11
2	C	374	SER	CA-C-N	6.16	128.54	120.28
2	C	374	SER	C-N-CA	6.16	128.54	120.28
3	D	138	ILE	N-CA-C	-6.15	98.88	107.80
2	C	128	ARG	N-CA-C	-6.14	100.00	109.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	356	ARG	N-CA-C	-6.13	105.63	113.23
2	C	32	ARG	CA-C-N	6.13	128.87	120.35
2	C	32	ARG	C-N-CA	6.13	128.87	120.35
3	D	42	PRO	N-CA-C	-6.11	108.33	114.68
7	O	179	SER	N-CA-C	-6.11	99.75	109.76
1	8	43	ILE	CA-C-N	6.10	128.74	120.38
1	8	43	ILE	C-N-CA	6.10	128.74	120.38
7	O	176	VAL	N-CA-C	-6.10	98.74	107.77
3	E	450	ASP	N-CA-C	-6.08	104.37	112.94
2	C	296	TYR	CA-C-N	6.06	126.01	119.76
2	C	296	TYR	C-N-CA	6.06	126.01	119.76
2	B	25	ALA	CA-C-N	6.06	129.01	120.28
2	B	25	ALA	C-N-CA	6.06	129.01	120.28
3	F	138	ILE	N-CA-C	-6.06	99.02	107.80
5	H	56	VAL	N-CA-C	-6.06	99.63	108.11
2	C	169	ILE	N-CA-C	-6.04	99.17	107.99
3	F	224	GLU	CA-C-N	6.04	124.07	119.66
3	F	224	GLU	C-N-CA	6.04	124.07	119.66
3	E	22	ASP	N-CA-C	-6.03	99.87	109.76
2	B	363	ILE	N-CA-C	-6.03	98.95	107.75
7	O	101	PHE	N-CA-C	-6.01	104.93	112.93
10	V	78	TYR	N-CA-C	-6.00	105.88	112.72
3	D	106	ARG	N-CA-C	-6.00	105.80	112.57
3	F	134	LEU	N-CA-C	-5.99	98.08	108.69
2	A	294	GLU	CA-C-N	5.98	130.87	122.08
2	A	294	GLU	C-N-CA	5.98	130.87	122.08
11	W	39	ALA	CA-C-N	5.97	125.99	119.90
11	W	39	ALA	C-N-CA	5.97	125.99	119.90
1	9	43	ILE	CA-C-N	5.96	128.26	120.28
1	9	43	ILE	C-N-CA	5.96	128.26	120.28
3	E	427	ILE	CA-C-N	5.96	125.98	119.90
3	E	427	ILE	C-N-CA	5.96	125.98	119.90
3	F	53	HIS	N-CA-C	-5.96	99.48	109.07
3	F	395	GLU	N-CA-C	-5.94	105.61	112.92
4	G	171	SER	N-CA-C	-5.92	100.32	109.14
3	D	53	HIS	N-CA-C	-5.92	99.75	109.40
3	D	421	ALA	N-CA-C	-5.91	103.31	110.88
8	T	210	PHE	CA-C-N	5.91	123.97	120.24
8	T	210	PHE	C-N-CA	5.91	123.97	120.24
11	W	14	ASN	N-CA-C	-5.90	105.66	112.92
2	A	31	GLY	N-CA-C	-5.90	102.49	111.10
8	T	49	ASN	N-CA-C	-5.90	103.21	110.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	57	THR	N-CA-C	-5.89	99.74	108.99
4	G	162	ILE	N-CA-C	-5.89	100.00	108.42
7	O	50	ASN	N-CA-C	-5.89	101.25	110.14
3	F	336	SER	CA-C-N	5.88	128.16	120.28
3	F	336	SER	C-N-CA	5.88	128.16	120.28
3	E	112	LYS	N-CA-C	-5.87	105.20	112.72
1	6	24	ILE	CA-C-N	5.87	126.45	119.94
1	6	24	ILE	C-N-CA	5.87	126.45	119.94
2	B	90	VAL	N-CA-C	-5.84	100.00	108.17
2	C	287	LEU	N-CA-C	-5.83	105.83	113.17
3	E	46	LEU	N-CA-C	-5.82	99.41	108.90
3	D	23	VAL	N-CA-C	-5.82	99.37	108.86
3	F	255	ILE	N-CA-C	-5.80	99.70	108.17
4	G	75	VAL	N-CA-C	-5.80	99.41	108.86
2	A	329	ILE	N-CA-C	-5.79	99.83	108.46
3	E	79	THR	N-CA-C	-5.78	105.06	111.36
2	A	78	PHE	N-CA-C	-5.77	106.08	113.23
3	E	337	ARG	N-CA-C	-5.76	106.09	113.23
3	E	345	TYR	N-CA-C	-5.75	98.03	108.85
3	F	23	VAL	N-CA-C	-5.75	100.02	108.99
3	D	12	LYS	N-CA-C	-5.75	100.03	109.40
3	E	308	GLN	N-CA-C	-5.75	100.61	109.52
3	F	351	LEU	N-CA-C	-5.74	105.94	113.17
3	D	41	THR	N-CA-C	-5.73	102.97	108.07
3	E	81	GLY	CA-C-N	5.73	125.75	119.90
3	E	81	GLY	C-N-CA	5.73	125.75	119.90
1	6	25	GLY	CA-C-N	5.73	127.78	120.56
1	6	25	GLY	C-N-CA	5.73	127.78	120.56
12	X	24	ALA	CA-C-N	5.72	127.95	120.28
12	X	24	ALA	C-N-CA	5.72	127.95	120.28
3	D	43	GLN	N-CA-C	-5.72	104.71	112.26
1	2	43	ILE	CA-C-N	5.72	128.22	120.38
1	2	43	ILE	C-N-CA	5.72	128.22	120.38
3	F	39	ILE	N-CA-C	-5.72	100.18	108.36
1	6	54	GLY	CA-C-N	5.72	127.87	120.44
1	6	54	GLY	C-N-CA	5.72	127.87	120.44
2	C	54	LEU	N-CA-C	-5.71	99.88	109.07
2	B	296	TYR	N-CA-C	-5.68	101.39	109.62
3	F	104	ASP	N-CA-C	-5.68	106.40	113.38
3	D	114	ARG	N-CA-C	-5.68	100.72	109.52
3	D	422	GLU	N-CA-C	-5.67	105.47	112.90
3	D	162	GLY	N-CA-C	-5.67	106.35	115.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	300	LYS	N-CA-C	-5.66	106.14	113.16
5	H	79	PRO	N-CA-C	-5.64	108.81	114.68
3	F	218	VAL	N-CA-C	-5.64	100.00	108.12
2	A	422	ARG	CA-C-N	5.63	126.20	120.00
2	A	422	ARG	C-N-CA	5.63	126.20	120.00
3	F	95	ILE	N-CA-C	-5.63	100.29	108.17
1	7	61	THR	CA-C-N	5.62	126.22	119.98
1	7	61	THR	C-N-CA	5.62	126.22	119.98
4	G	100	ASN	N-CA-C	-5.62	106.47	113.38
2	C	409	GLY	N-CA-C	-5.61	107.04	114.95
2	C	336	VAL	N-CA-C	-5.61	107.28	112.83
1	3	58	SER	CA-C-N	5.60	127.79	120.28
1	3	58	SER	C-N-CA	5.60	127.79	120.28
2	C	62	LYS	N-CA-C	-5.60	100.76	109.72
5	H	20	THR	N-CA-C	-5.60	98.40	108.48
2	A	255	ILE	CA-C-N	5.60	126.19	119.98
2	A	255	ILE	C-N-CA	5.60	126.19	119.98
7	O	131	PRO	N-CA-C	-5.59	106.24	113.57
2	B	79	GLY	CA-C-N	5.59	129.19	120.75
2	B	79	GLY	C-N-CA	5.59	129.19	120.75
1	0	35	ASN	CA-C-N	5.59	126.14	119.94
1	0	35	ASN	C-N-CA	5.59	126.14	119.94
2	C	109	VAL	N-CA-C	-5.58	100.39	108.71
5	H	14	PHE	N-CA-C	-5.58	99.21	108.75
2	C	130	ARG	N-CA-C	-5.58	100.80	109.72
3	D	210	GLU	N-CA-C	-5.58	99.20	108.34
1	2	15	SER	CA-C-N	5.56	128.29	120.28
1	2	15	SER	C-N-CA	5.56	128.29	120.28
2	C	40	ILE	N-CA-C	-5.55	100.06	108.17
3	F	394	ASP	N-CA-C	-5.55	106.18	113.17
8	T	132	LEU	CA-C-N	5.55	126.11	120.00
8	T	132	LEU	C-N-CA	5.55	126.11	120.00
1	0	15	SER	CA-C-N	5.54	128.25	120.28
1	0	15	SER	C-N-CA	5.54	128.25	120.28
8	T	76	GLN	N-CA-C	5.53	116.99	111.07
1	0	2	GLN	CA-C-N	5.53	127.63	120.44
1	0	2	GLN	C-N-CA	5.53	127.63	120.44
4	G	123	PRO	CA-C-N	5.53	127.69	120.28
4	G	123	PRO	C-N-CA	5.53	127.69	120.28
8	T	101	LEU	N-CA-C	-5.52	106.47	113.43
10	V	26	ALA	N-CA-C	-5.52	105.17	113.89
3	E	426	GLY	N-CA-C	-5.51	107.06	115.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	13	GLN	N-CA-C	-5.51	99.92	108.90
3	F	213	SER	N-CA-C	-5.51	100.42	109.40
2	A	64	MET	N-CA-C	-5.50	101.04	109.41
3	D	310	VAL	N-CA-C	-5.49	100.32	108.45
3	D	345	TYR	N-CA-C	-5.48	97.43	109.11
1	0	18	GLY	CA-C-N	5.47	128.16	120.28
1	0	18	GLY	C-N-CA	5.47	128.16	120.28
2	B	148	VAL	N-CA-C	-5.46	99.69	107.77
1	0	43	ILE	CA-C-N	5.45	127.85	120.38
1	0	43	ILE	C-N-CA	5.45	127.85	120.38
3	F	115	LYS	CA-C-N	5.45	125.20	119.76
3	F	115	LYS	C-N-CA	5.45	125.20	119.76
2	A	121	GLY	CA-C-N	5.44	125.45	119.90
2	A	121	GLY	C-N-CA	5.44	125.45	119.90
2	B	59	SER	N-CA-C	-5.43	104.53	113.50
3	E	91	THR	N-CA-C	-5.43	106.33	113.17
10	V	162	GLY	N-CA-C	-5.42	108.02	114.48
1	8	6	ALA	CA-C-N	5.41	127.53	120.28
1	8	6	ALA	C-N-CA	5.41	127.53	120.28
2	A	296	TYR	N-CA-C	-5.41	102.67	110.40
2	A	352	ILE	N-CA-C	-5.41	100.33	108.12
9	U	96	ARG	CA-C-N	5.40	127.52	120.28
9	U	96	ARG	C-N-CA	5.40	127.52	120.28
3	D	457	PHE	N-CA-C	-5.40	106.82	113.41
1	7	2	GLN	CA-C-N	5.40	127.51	120.28
1	7	2	GLN	C-N-CA	5.40	127.51	120.28
4	G	159	TYR	N-CA-C	-5.39	101.44	109.42
2	C	337	SER	N-CA-C	-5.39	106.47	113.16
3	F	254	PHE	N-CA-C	-5.39	100.24	109.24
5	H	41	VAL	N-CA-C	-5.39	100.44	108.46
2	B	500	LYS	CA-C-N	5.38	127.43	120.44
2	B	500	LYS	C-N-CA	5.38	127.43	120.44
1	2	64	PHE	CA-C-N	5.38	127.49	120.28
1	2	64	PHE	C-N-CA	5.38	127.49	120.28
1	7	35	ASN	CA-C-N	5.37	125.90	119.94
1	7	35	ASN	C-N-CA	5.37	125.90	119.94
14	Z	7	PHE	N-CA-C	-5.37	105.02	113.02
3	F	343	GLY	N-CA-C	-5.37	107.62	115.72
2	C	144	VAL	N-CA-C	-5.37	100.60	108.11
2	A	145	HIS	N-CA-C	-5.36	106.78	113.38
1	9	61	THR	CA-C-N	5.36	125.93	119.98
1	9	61	THR	C-N-CA	5.36	125.93	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	V	27	THR	N-CA-C	-5.35	105.53	111.36
3	E	330	ASP	N-CA-C	-5.34	106.44	113.12
4	G	99	LEU	N-CA-C	-5.34	106.44	113.17
1	7	22	ALA	CA-C-N	5.34	125.86	119.94
1	7	22	ALA	C-N-CA	5.34	125.86	119.94
1	8	10	ILE	CA-C-N	5.34	125.90	119.98
1	8	10	ILE	C-N-CA	5.34	125.90	119.98
1	5	43	ILE	CA-C-N	5.33	128.17	120.38
1	5	43	ILE	C-N-CA	5.33	128.17	120.38
3	F	88	GLY	N-CA-C	-5.33	103.60	110.69
8	T	148	ALA	CA-C-N	5.32	125.03	119.92
8	T	148	ALA	C-N-CA	5.32	125.03	119.92
1	1	15	SER	CA-C-N	5.32	127.93	120.28
1	1	15	SER	C-N-CA	5.32	127.93	120.28
3	F	16	VAL	N-CA-C	-5.31	98.30	109.34
2	B	161	ILE	CA-C-N	5.30	126.89	122.17
2	B	161	ILE	C-N-CA	5.30	126.89	122.17
5	H	66	LYS	N-CA-C	-5.30	100.39	109.24
2	A	260	ARG	CA-C-N	5.29	127.80	120.29
2	A	260	ARG	C-N-CA	5.29	127.80	120.29
4	G	137	ALA	CA-C-N	5.29	126.45	119.84
4	G	137	ALA	C-N-CA	5.29	126.45	119.84
10	V	49	GLN	N-CA-C	-5.29	98.07	109.01
2	C	89	LEU	N-CA-C	-5.28	101.67	110.17
3	D	206	VAL	N-CA-C	-5.28	105.39	110.72
3	E	65	ASP	CA-C-N	5.28	126.19	120.44
3	E	65	ASP	C-N-CA	5.28	126.19	120.44
2	C	324	THR	N-CA-C	-5.28	101.56	109.95
1	5	2	GLN	CA-C-N	5.27	127.35	120.28
1	5	2	GLN	C-N-CA	5.27	127.35	120.28
3	D	163	LYS	N-CA-C	-5.27	105.62	111.36
1	6	12	ALA	CA-C-N	5.27	125.79	119.94
1	6	12	ALA	C-N-CA	5.27	125.79	119.94
4	G	176	GLU	N-CA-C	-5.26	100.98	109.40
3	D	208	ASN	N-CA-C	-5.26	100.33	108.90
3	D	336	SER	CA-C-N	5.26	127.33	120.28
3	D	336	SER	C-N-CA	5.26	127.33	120.28
7	O	150	GLY	N-CA-C	-5.26	107.28	114.64
3	D	65	ASP	CA-C-N	5.26	125.33	120.34
3	D	65	ASP	C-N-CA	5.26	125.33	120.34
2	A	50	GLN	N-CA-C	-5.25	101.97	110.32
3	E	107	GLY	CA-C-N	5.25	125.55	119.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	107	GLY	C-N-CA	5.25	125.55	119.93
2	A	355	GLU	CA-C-N	5.25	127.31	120.28
2	A	355	GLU	C-N-CA	5.25	127.31	120.28
3	E	218	VAL	N-CA-C	-5.24	100.01	107.77
3	E	451	ASN	N-CA-C	-5.24	106.75	112.72
10	V	163	TYR	N-CA-C	-5.24	105.63	112.23
3	E	317	LEU	N-CA-C	-5.24	106.57	113.17
3	E	453	PRO	CA-C-N	5.23	127.29	120.28
3	E	453	PRO	C-N-CA	5.23	127.29	120.28
2	B	479	ASN	CA-C-N	5.23	127.28	120.28
2	B	479	ASN	C-N-CA	5.23	127.28	120.28
2	B	381	GLN	CA-C-N	5.22	127.61	120.35
2	B	381	GLN	C-N-CA	5.22	127.61	120.35
3	F	216	ALA	N-CA-C	-5.22	101.42	109.52
2	C	162	GLY	N-CA-C	-5.22	103.14	111.18
3	F	41	THR	N-CA-C	-5.22	100.41	108.55
8	T	150	THR	N-CA-C	-5.22	103.52	108.22
3	F	335	LEU	N-CA-C	-5.22	100.40	108.90
3	D	10	THR	N-CA-C	-5.18	100.95	109.40
3	E	262	THR	CA-C-N	5.17	127.21	120.28
3	E	262	THR	C-N-CA	5.17	127.21	120.28
8	T	81	ASN	N-CA-C	-5.17	105.02	113.19
3	E	30	LEU	N-CA-C	-5.17	100.53	109.15
3	F	46	LEU	N-CA-C	-5.16	100.49	108.90
2	B	397	ALA	N-CA-C	-5.16	106.23	112.88
2	C	161	ILE	CA-C-N	5.15	126.01	121.58
2	C	161	ILE	C-N-CA	5.15	126.01	121.58
1	9	6	ALA	CA-C-N	5.15	127.18	120.28
1	9	6	ALA	C-N-CA	5.15	127.18	120.28
3	E	284	THR	N-CA-C	-5.15	105.72	112.41
2	A	443	GLN	CA-C-N	5.15	123.48	120.24
2	A	443	GLN	C-N-CA	5.15	123.48	120.24
10	V	133	LEU	N-CA-C	-5.14	99.84	110.80
1	2	20	LEU	CA-C-N	5.14	125.68	119.98
1	2	20	LEU	C-N-CA	5.14	125.68	119.98
3	E	342	LEU	N-CA-C	-5.12	106.87	113.02
4	G	168	ASP	N-CA-C	-5.12	103.19	109.65
1	3	18	GLY	CA-C-N	5.12	127.85	120.38
1	3	18	GLY	C-N-CA	5.12	127.85	120.38
1	2	18	GLY	CA-C-N	5.12	127.65	120.28
1	2	18	GLY	C-N-CA	5.12	127.65	120.28
2	B	158	LEU	CA-C-N	5.12	131.59	122.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	LEU	C-N-CA	5.12	131.59	122.13
2	A	37	GLY	N-CA-C	-5.11	101.06	113.18
4	G	166	TYR	N-CA-C	-5.11	100.68	107.88
4	G	137	ALA	N-CA-C	-5.09	103.26	110.29
7	O	151	LYS	N-CA-C	-5.08	100.06	108.75
2	B	146	GLU	CA-C-N	5.08	126.19	119.84
2	B	146	GLU	C-N-CA	5.08	126.19	119.84
1	9	2	GLN	CA-C-N	5.08	127.08	120.28
1	9	2	GLN	C-N-CA	5.08	127.08	120.28
3	E	115	LYS	CA-C-N	5.08	125.01	119.78
3	E	115	LYS	C-N-CA	5.08	125.01	119.78
3	F	206	VAL	N-CA-C	-5.08	105.59	110.72
3	F	209	LEU	N-CA-C	-5.08	105.40	112.45
1	9	12	ALA	CA-C-N	5.07	125.57	119.94
1	9	12	ALA	C-N-CA	5.07	125.57	119.94
4	G	156	ALA	CA-C-N	5.07	126.48	120.14
4	G	156	ALA	C-N-CA	5.07	126.48	120.14
4	G	164	ILE	N-CA-C	-5.07	100.60	108.86
3	F	262	THR	CA-C-N	5.07	127.07	120.28
3	F	262	THR	C-N-CA	5.07	127.07	120.28
11	W	46	THR	N-CA-C	-5.07	106.79	113.17
3	D	16	VAL	N-CA-C	-5.06	99.88	107.37
2	B	355	GLU	CA-C-N	5.06	127.06	120.28
2	B	355	GLU	C-N-CA	5.06	127.06	120.28
3	E	255	ILE	N-CA-C	-5.06	100.62	108.86
4	G	163	SER	N-CA-C	-5.06	100.10	108.75
1	6	6	ALA	CA-C-N	5.05	127.05	120.28
1	6	6	ALA	C-N-CA	5.05	127.05	120.28
3	D	299	THR	N-CA-C	-5.05	101.87	109.85
2	C	176	GLY	N-CA-C	-5.05	101.22	113.18
3	D	307	VAL	N-CA-C	-5.04	100.31	107.77
3	D	256	ASP	N-CA-C	-5.04	101.41	109.07
1	7	6	ALA	CA-C-N	5.04	127.03	120.28
1	7	6	ALA	C-N-CA	5.04	127.03	120.28
11	W	6	PRO	CA-C-O	-5.04	113.26	120.56
1	4	41	PRO	N-CA-C	5.03	122.84	112.47
7	O	180	ILE	N-CA-C	-5.03	105.26	112.35
10	V	157	LYS	N-CA-C	-5.03	100.09	110.80
1	8	24	ILE	CA-C-N	5.02	125.52	119.94
1	8	24	ILE	C-N-CA	5.02	125.52	119.94
3	F	35	ASN	N-CA-C	-5.02	104.05	110.53
6	I	59	ILE	CA-C-N	5.02	128.79	121.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	59	ILE	C-N-CA	5.02	128.79	121.31
3	F	150	GLY	CA-C-N	5.02	125.91	120.44
3	F	150	GLY	C-N-CA	5.02	125.91	120.44
1	9	11	GLY	CA-C-N	5.01	126.96	120.44
1	9	11	GLY	C-N-CA	5.01	126.96	120.44
2	C	479	ASN	N-CA-C	-5.01	107.01	113.23
3	D	58	THR	N-CA-C	-5.01	100.11	108.34
1	4	59	GLU	CA-C-N	5.01	126.99	120.28
1	4	59	GLU	C-N-CA	5.01	126.99	120.28
2	C	134	LYS	CA-C-N	5.01	127.35	120.39
2	C	134	LYS	C-N-CA	5.01	127.35	120.39
3	D	88	GLY	N-CA-C	-5.01	103.74	110.80
9	U	127	SER	CA-C-N	5.01	126.99	120.28
9	U	127	SER	C-N-CA	5.01	126.99	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	9	40	ASN	Peptide
3	D	256	ASP	Peptide
3	F	345	TYR	Peptide
5	H	54	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	300	0	95	0	0
1	1	300	0	95	0	0
1	2	300	0	95	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	296	0	91	0	0
1	4	300	0	95	0	0
1	5	300	0	95	0	0
1	6	296	0	91	0	0
1	7	292	0	91	0	0
1	8	300	0	95	0	0
1	9	296	0	91	0	0
2	A	1996	0	570	1	0
2	B	2020	0	575	1	0
2	C	1992	0	572	0	0
3	D	1880	0	538	0	0
3	E	1872	0	537	1	0
3	F	1876	0	537	1	0
4	G	1060	0	277	0	0
5	H	480	0	122	0	0
6	I	193	0	43	0	0
7	O	748	0	205	0	0
8	T	897	0	248	0	0
9	U	620	0	158	0	0
10	V	685	0	173	0	0
11	W	340	0	92	0	0
12	X	248	0	61	0	0
13	Y	148	0	40	0	0
14	Z	193	0	49	0	0
All	All	20228	0	5731	3	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 (3) 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:51:ALA:H	3:E:70:LEU:H	1.38	0.69
3:F:160:GLY:C	3:F:162:GLY:H	2.24	0.46
2:B:102:GLY:HA3	2:B:126:ALA:H	1.81	0.45

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
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%)	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%)	470 (95%)	19 (4%)	6 (1%)	10	43
2	B	501/510 (98%)	470 (94%)	26 (5%)	5 (1%)	12	48
2	C	496/510 (97%)	466 (94%)	22 (4%)	8 (2%)	7	37
3	D	468/478 (98%)	438 (94%)	21 (4%)	9 (2%)	6	32
3	E	466/478 (98%)	444 (95%)	18 (4%)	4 (1%)	14	50
3	F	467/478 (98%)	431 (92%)	31 (7%)	5 (1%)	11	46
4	G	261/278 (94%)	246 (94%)	11 (4%)	4 (2%)	8	39
5	H	110/138 (80%)	103 (94%)	4 (4%)	3 (3%)	4	25
6	I	42/61 (69%)	36 (86%)	4 (10%)	2 (5%)	2	16
7	O	185/195 (95%)	166 (90%)	14 (8%)	5 (3%)	4	25
8	T	222/249 (89%)	211 (95%)	7 (3%)	4 (2%)	6	34
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	147 (87%)	12 (7%)	10 (6%)	1	13
11	W	83/95 (87%)	67 (81%)	7 (8%)	9 (11%)	0	6
12	X	60/92 (65%)	55 (92%)	1 (2%)	4 (7%)	1	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Y	35/59 (59%)	32 (91%)	2 (6%)	1 (3%)	3	23
14	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
All	All	4984/5321 (94%)	4680 (94%)	216 (4%)	88 (2%)	9	34

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	41	PRO
1	3	41	PRO
1	4	41	PRO
1	5	41	PRO
1	6	41	PRO
1	7	41	PRO
1	8	41	PRO
1	9	41	PRO
2	A	229	LYS
2	B	24	GLU
2	B	159	VAL
2	C	49	ILE
2	C	299	ASP
2	C	380	ALA
3	D	358	LEU
8	T	110	ALA
10	V	65	THR
10	V	83	ILE
10	V	86	SER
10	V	89	LEU
10	V	133	LEU
11	W	17	SER
12	X	38	ASN
12	X	58	VAL
1	0	42	SER
2	B	338	ALA
2	C	145	HIS
2	C	315	SER
3	D	131	ALA
3	D	397	SER
3	F	74	GLU
3	F	98	VAL
4	G	79	SER
5	H	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	O	10	VAL
8	T	109	PHE
8	T	202	ASN
10	V	130	PHE
11	W	42	ILE
11	W	44	ALA
11	W	59	ASP
12	X	31	TRP
13	Y	3	LYS
2	B	145	HIS
2	C	320	SER
2	C	378	SER
3	D	29	GLU
3	D	277	SER
3	D	394	ASP
3	D	462	GLY
3	E	34	LEU
3	E	358	LEU
3	F	86	PRO
4	G	56	GLU
5	H	22	TYR
5	H	33	PRO
6	I	54	SER
10	V	158	TRP
2	A	143	SER
2	A	230	TYR
2	A	312	ALA
2	A	367	ILE
6	I	48	LYS
7	O	81	LEU
7	O	82	ASP
10	V	25	THR
11	W	12	SER
11	W	31	TYR
2	A	22	SER
2	C	229	LYS
3	E	16	VAL
4	G	123	PRO
7	O	171	LEU
8	T	51	ASN
10	V	55	PHE
12	X	36	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	327	PRO
3	F	278	ALA
3	F	81	GLY
4	G	181	PRO
11	W	38	PRO
3	D	86	PRO
7	O	14	GLY
11	W	34	LEU
3	D	161	VAL
3	E	279	VAL
10	V	21	ILE
11	W	15	ILE

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

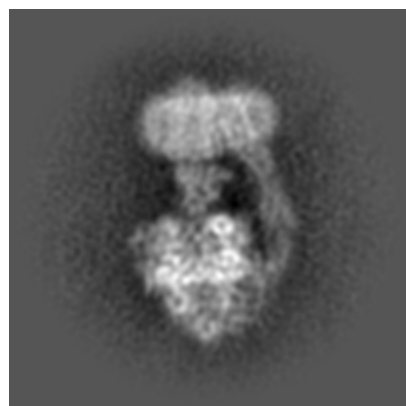
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25963. These allow visual inspection of the internal detail of the map and identification of artifacts.

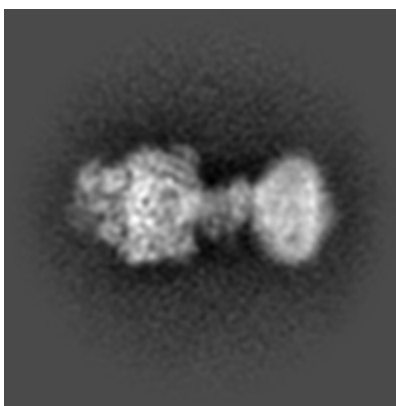
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

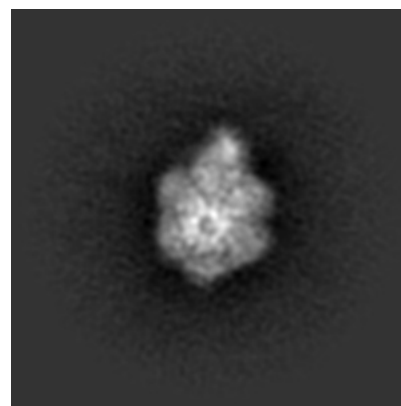
6.1.1 Primary map



X

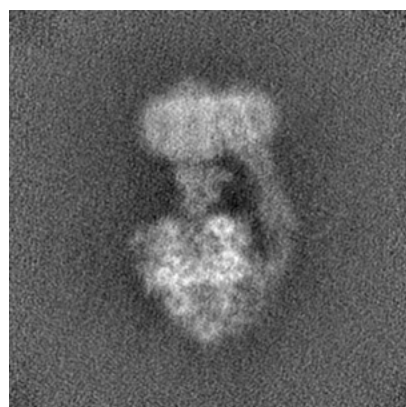


Y

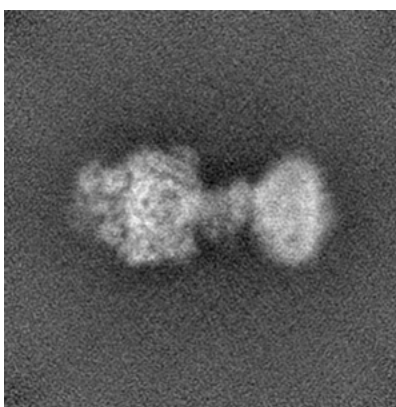


Z

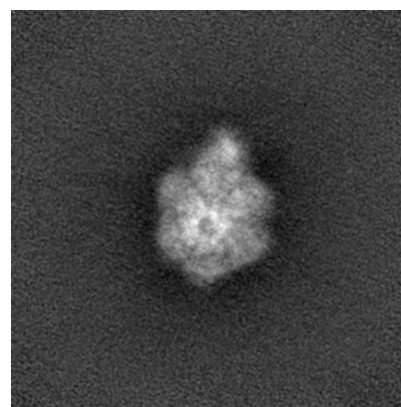
6.1.2 Raw map



X



Y

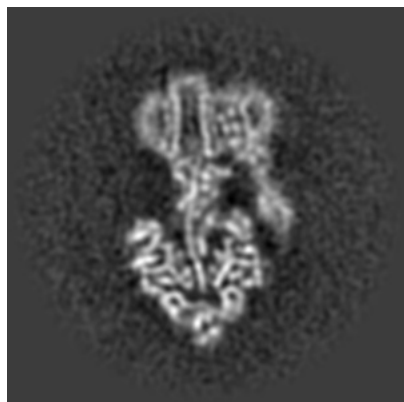


Z

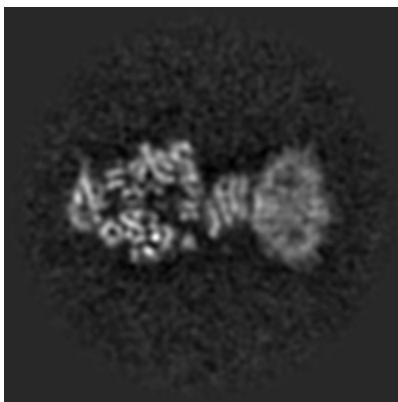
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

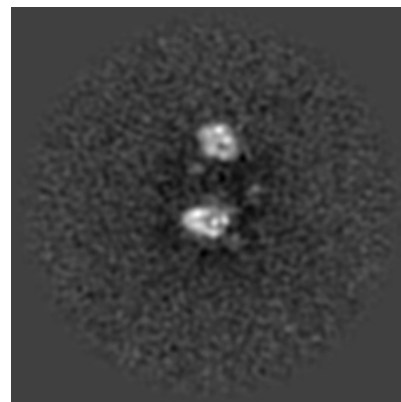
6.2.1 Primary map



X Index: 128



Y Index: 128

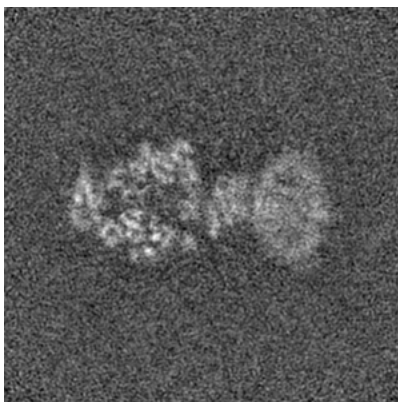


Z Index: 128

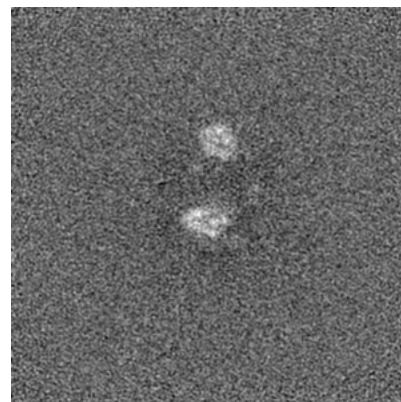
6.2.2 Raw map



X Index: 128



Y Index: 128

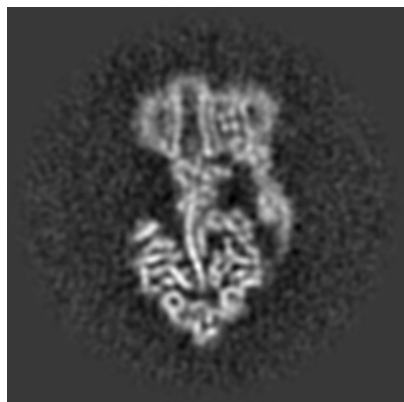


Z Index: 128

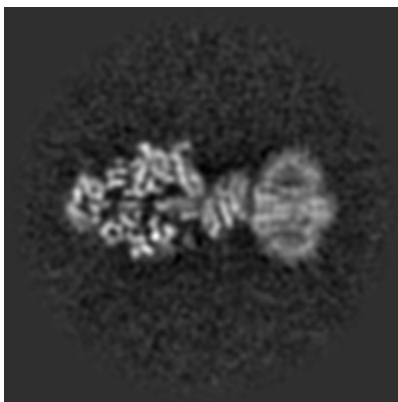
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

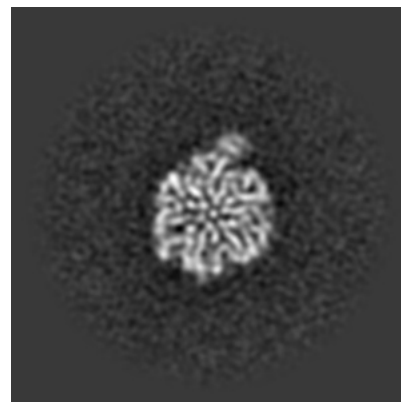
6.3.1 Primary map



X Index: 130



Y Index: 126

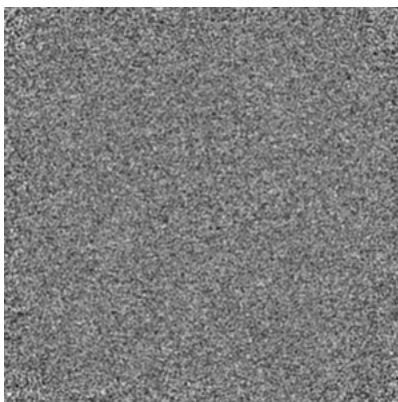


Z Index: 85

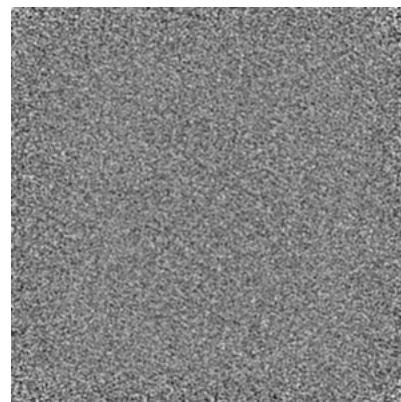
6.3.2 Raw map



X Index: 130



Y Index: 0

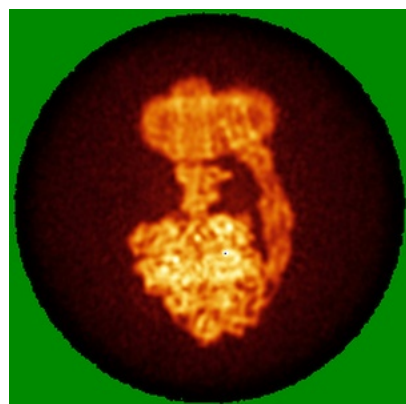


Z Index: 0

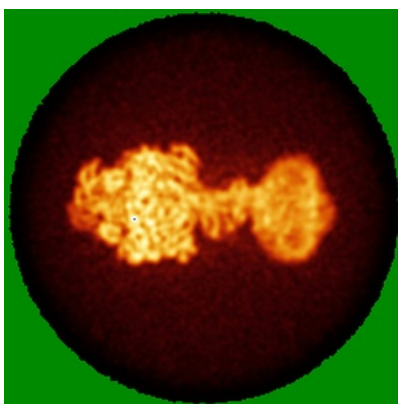
The images above show the largest variance slices of the map in three orthogonal directions.

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

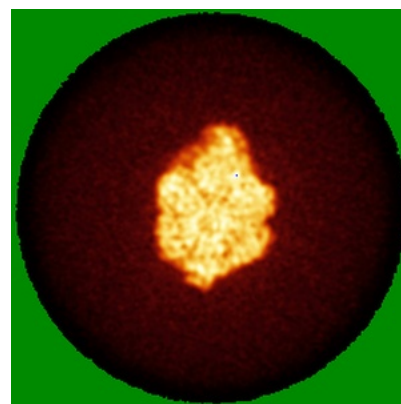
6.4.1 Primary map



X

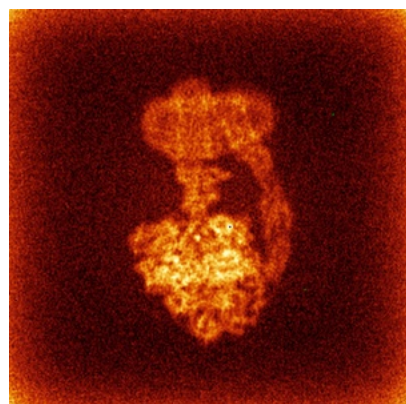


Y

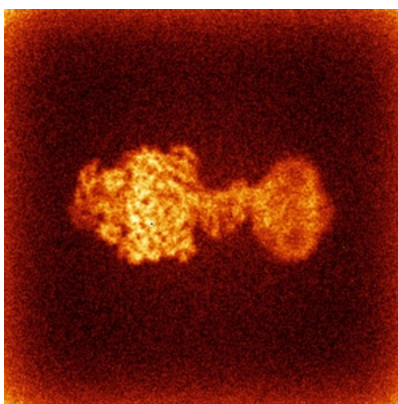


Z

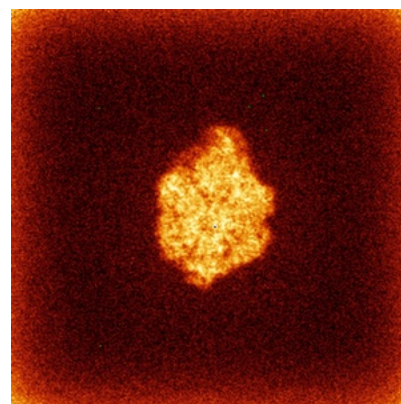
6.4.2 Raw map



X



Y

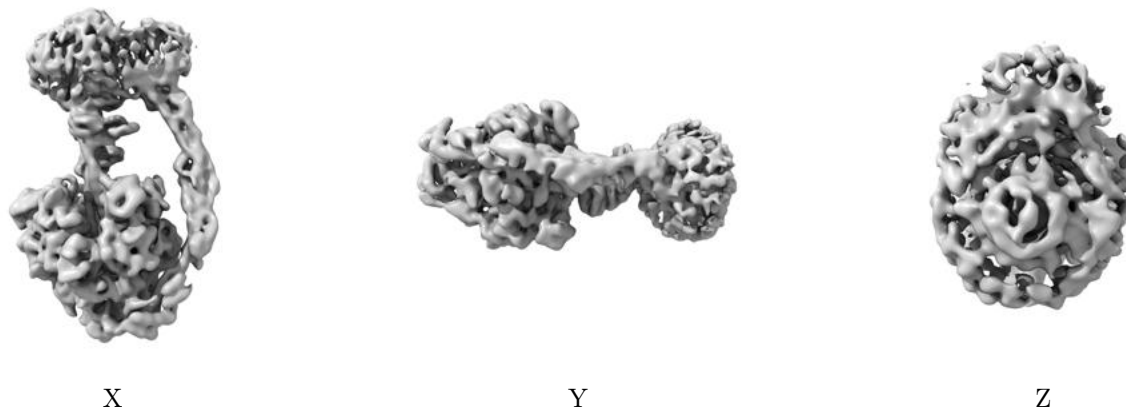


Z

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.

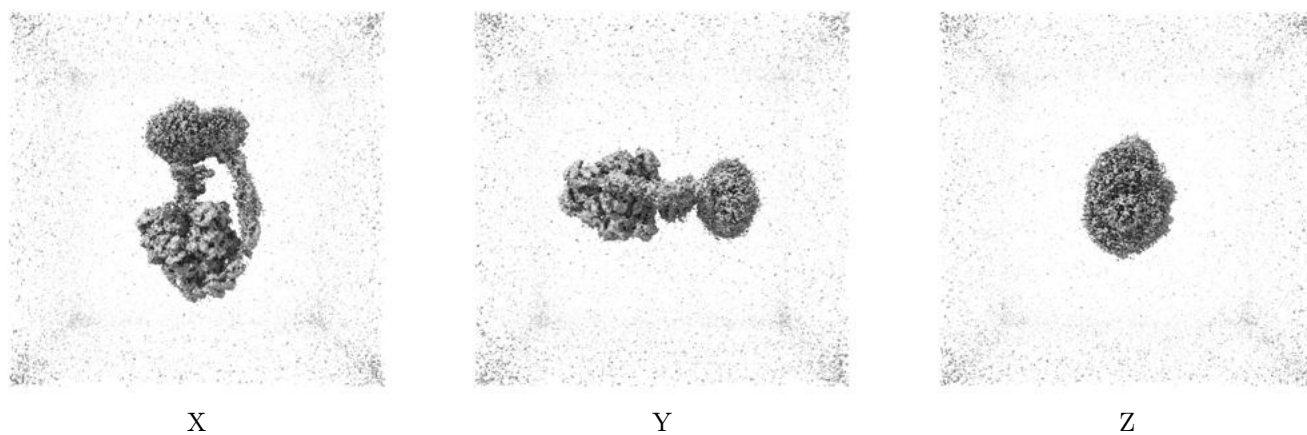
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.66. 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.

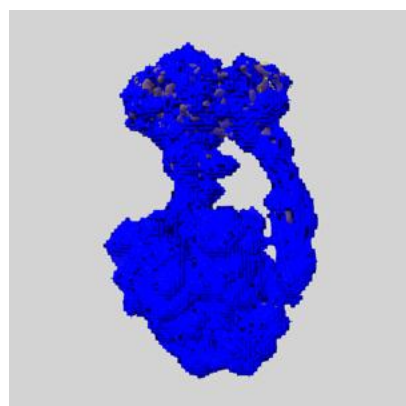
6.6 Mask visualisation [i](#)

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

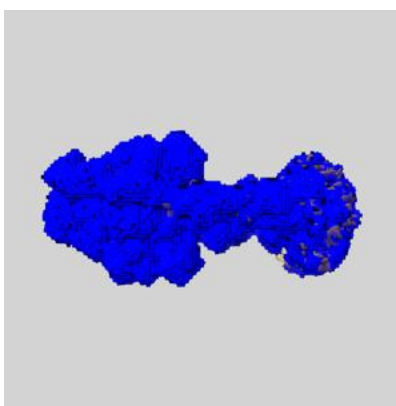
A mask typically either:

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

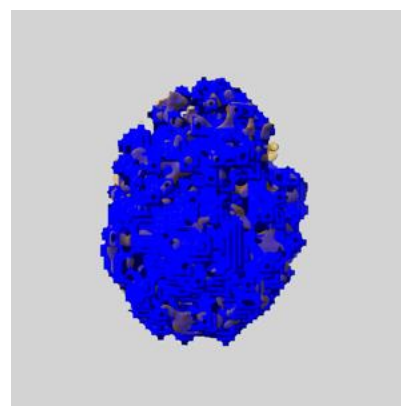
6.6.1 emd_25963_msk_1.map [i](#)



X



Y

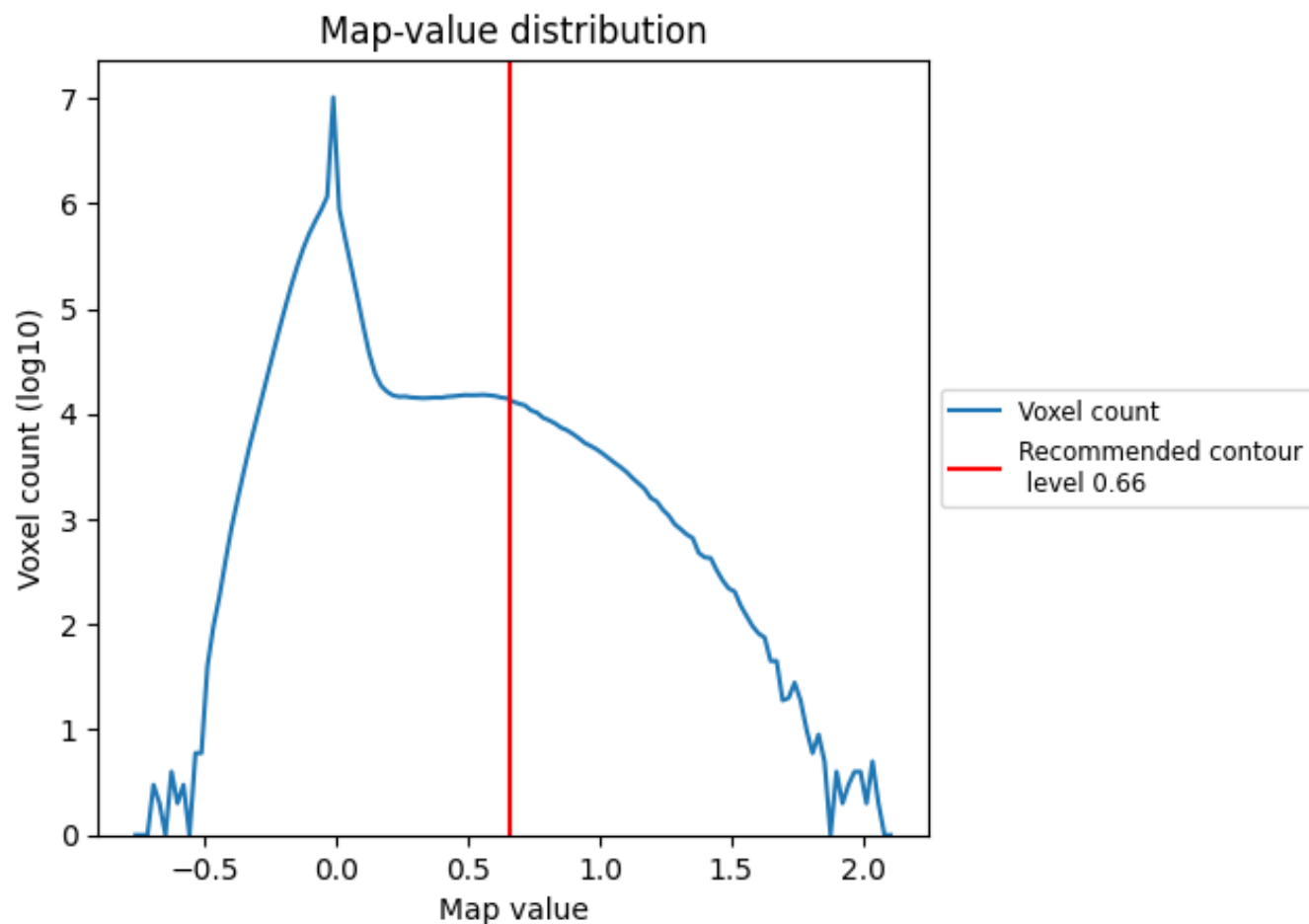


Z

7 Map analysis [i](#)

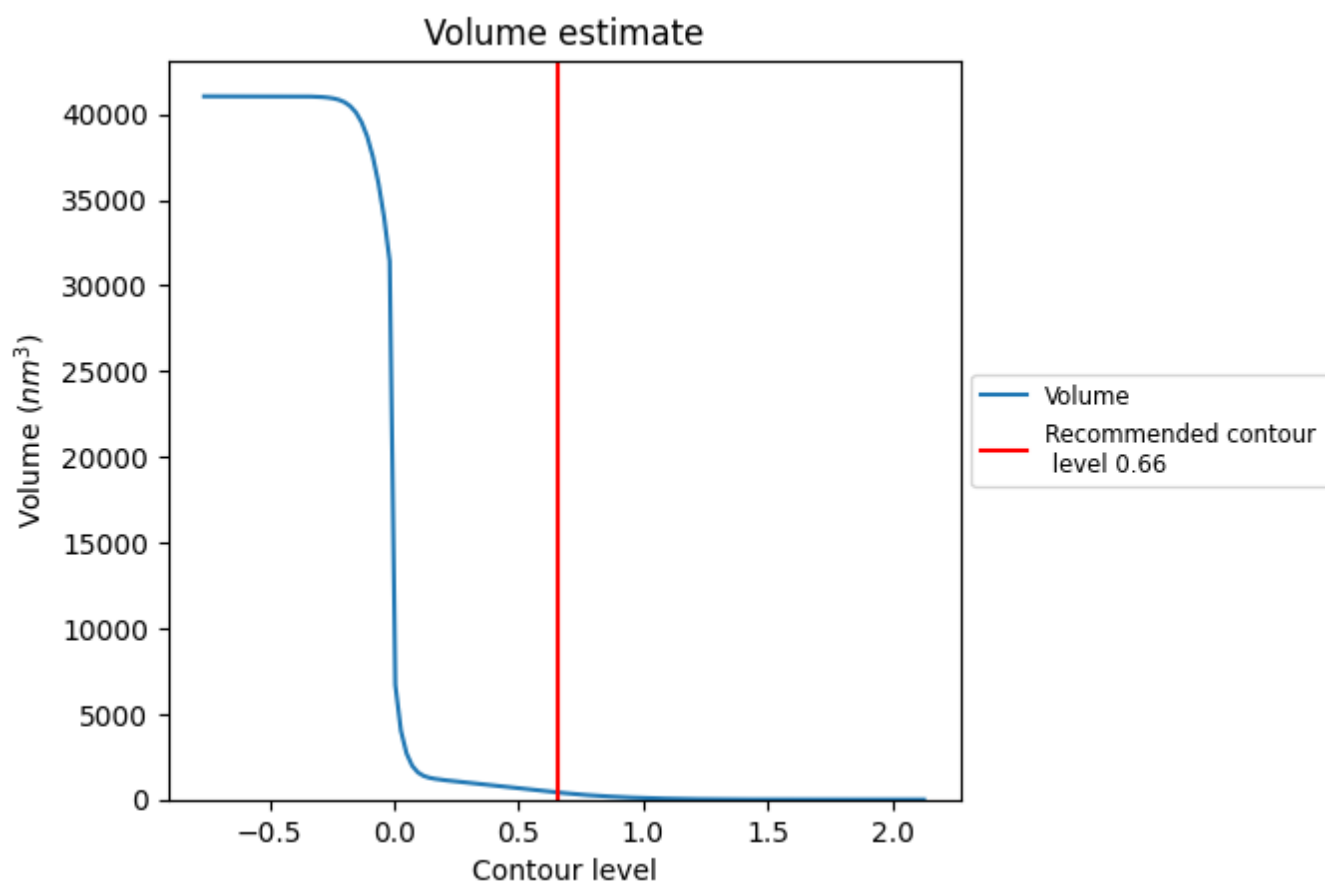
This section contains the results of statistical analysis of the map.

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.

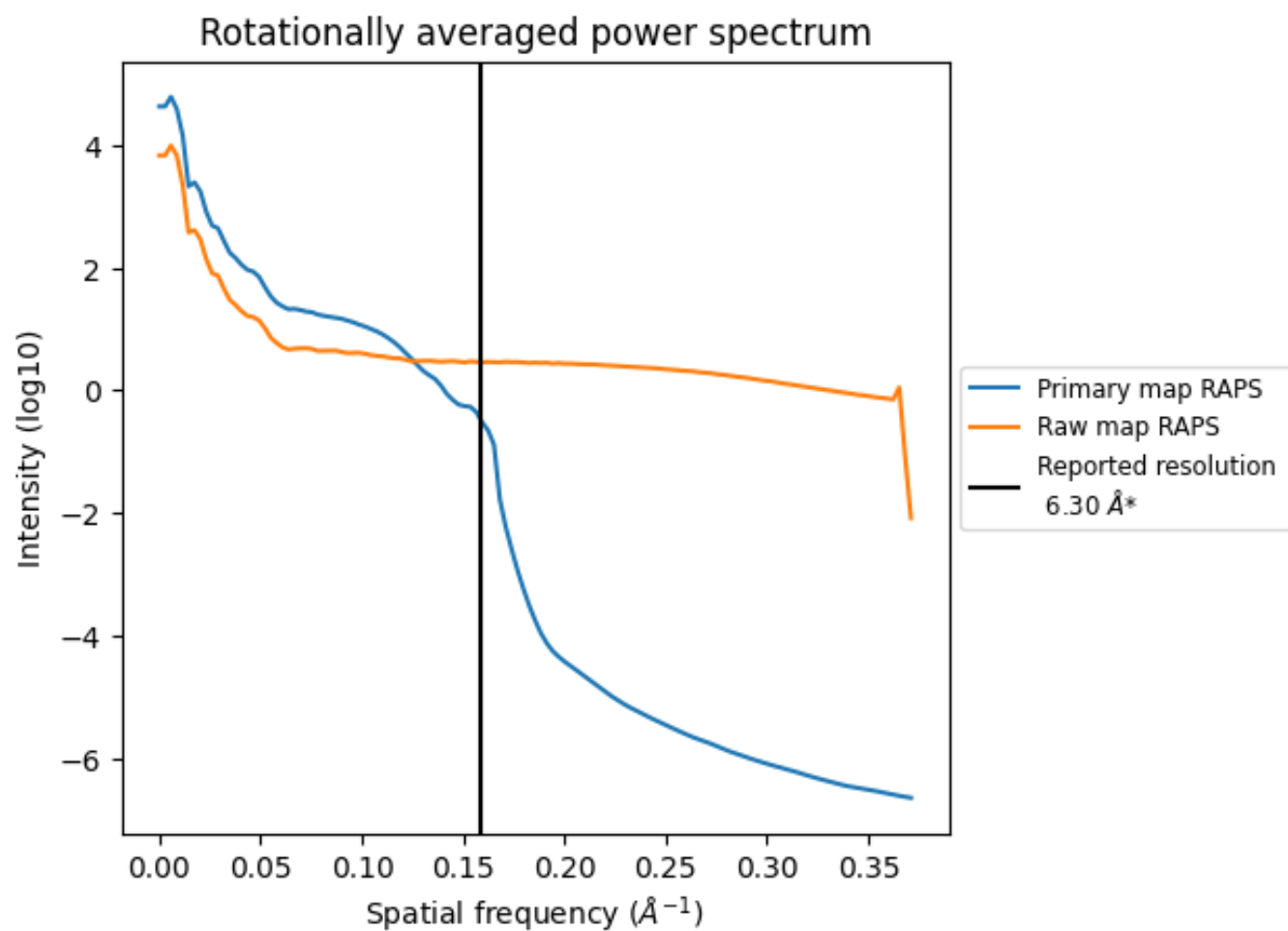
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 412 nm³; this corresponds to an approximate mass of 372 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 ⓘ

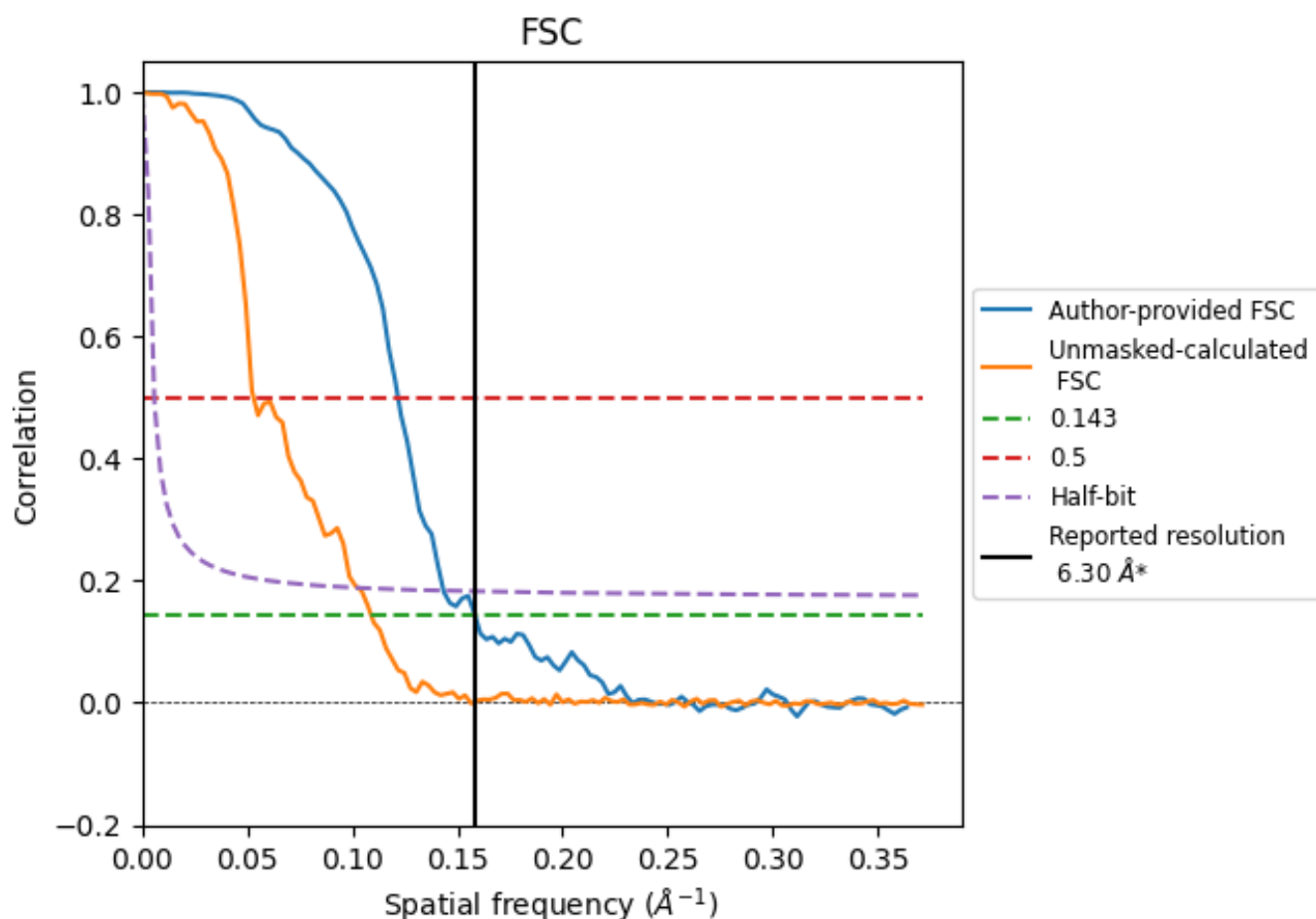


*Reported resolution corresponds to spatial frequency of 0.159 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

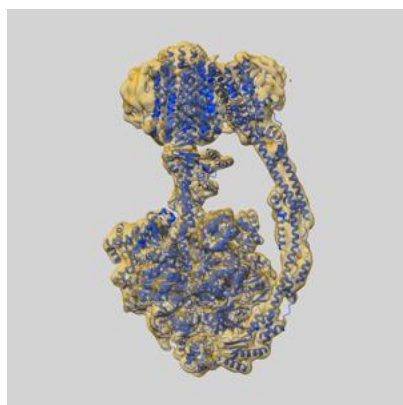
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.32	8.22	6.97
Unmasked-calculated*	9.18	18.87	9.76

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

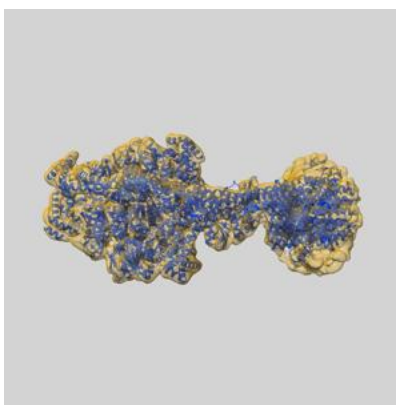
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25963 and PDB model 7TKB. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

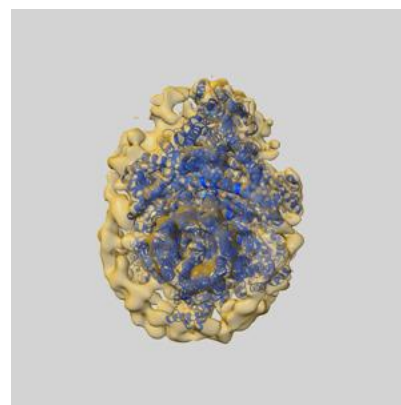
9.1 Map-model overlay [i](#)



X



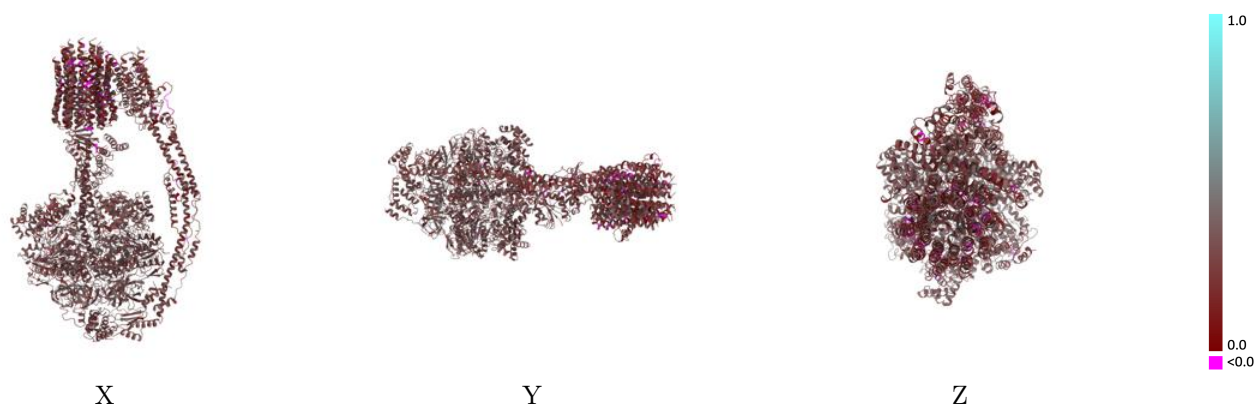
Y



Z

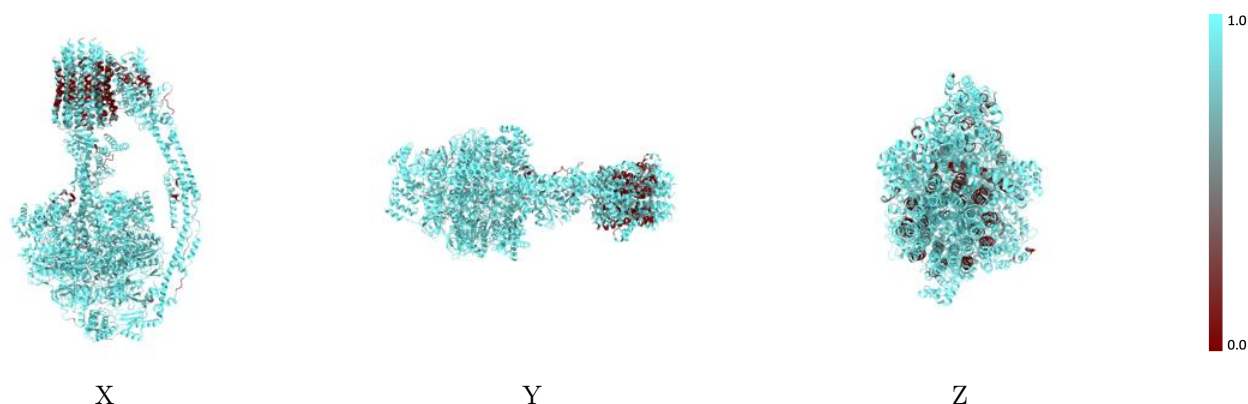
The images above show the 3D surface view of the map at the recommended contour level 0.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



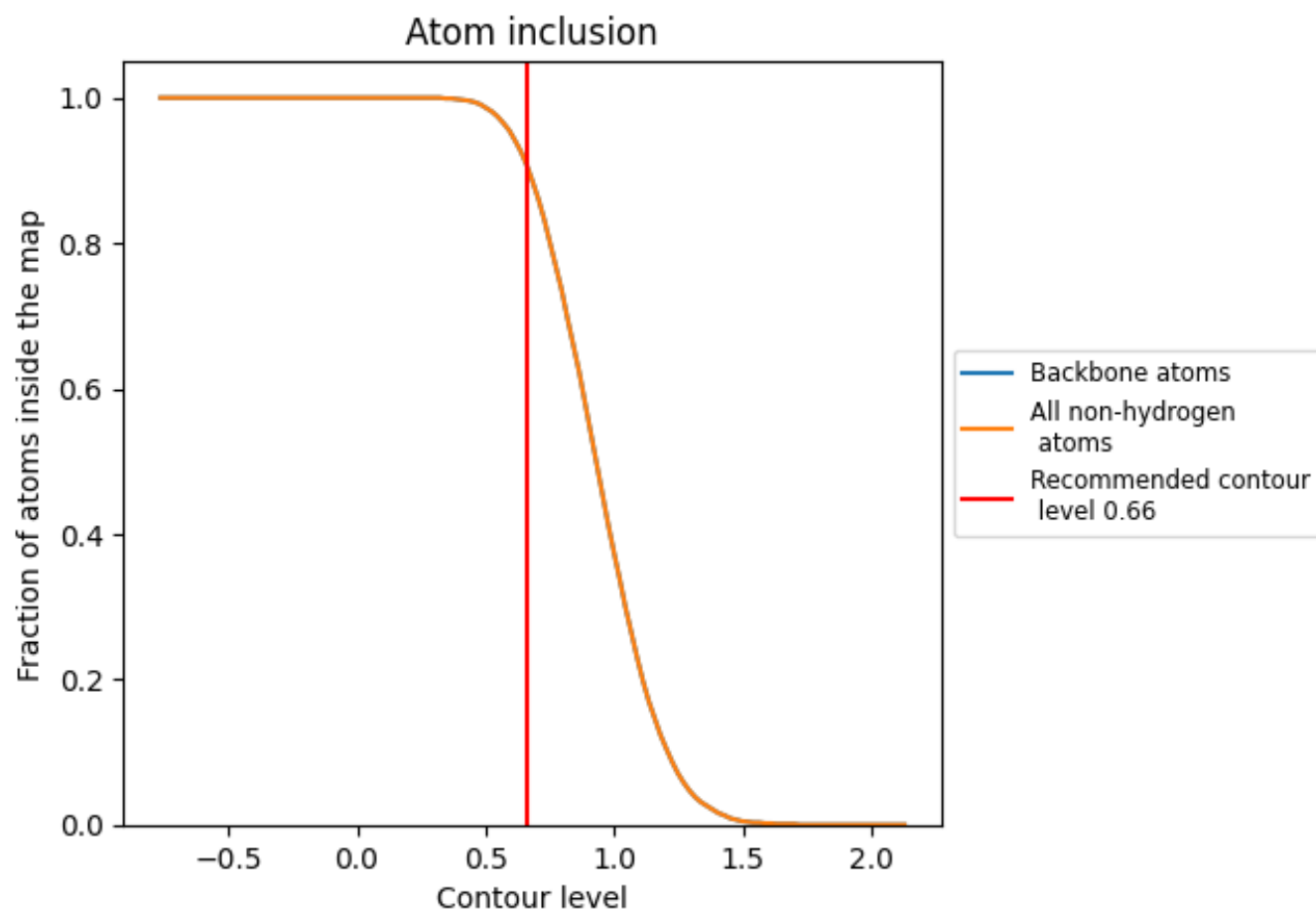
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.66).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.2860
0	 0.7530	 0.2360
1	 0.7100	 0.1980
2	 0.5870	 0.1930
3	 0.5570	 0.2080
4	 0.7200	 0.2130
5	 0.7230	 0.2140
6	 0.6250	 0.1950
7	 0.7670	 0.2220
8	 0.7970	 0.2230
9	 0.7130	 0.2210
A	 0.9760	 0.3190
B	 0.9660	 0.3150
C	 0.9760	 0.3180
D	 0.9660	 0.3160
E	 0.9440	 0.3080
F	 0.9780	 0.3200
G	 0.9570	 0.2900
H	 0.8960	 0.2660
I	 0.8710	 0.2770
O	 0.9910	 0.3010
T	 0.7770	 0.2410
U	 0.9520	 0.2800
V	 0.9150	 0.2460
W	 0.7620	 0.1880
X	 0.7980	 0.2570
Y	 0.6960	 0.1660
Z	 0.9380	 0.2490

