



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:03 PM UTC

PDB ID : 7TK4 / pdb_00007tk4
EMDB ID : EMD-25956
Title : Yeast ATP synthase State 1binding(c) with 10 mM ATP backbone model
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2022-01-17
Resolution : 7.00 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:

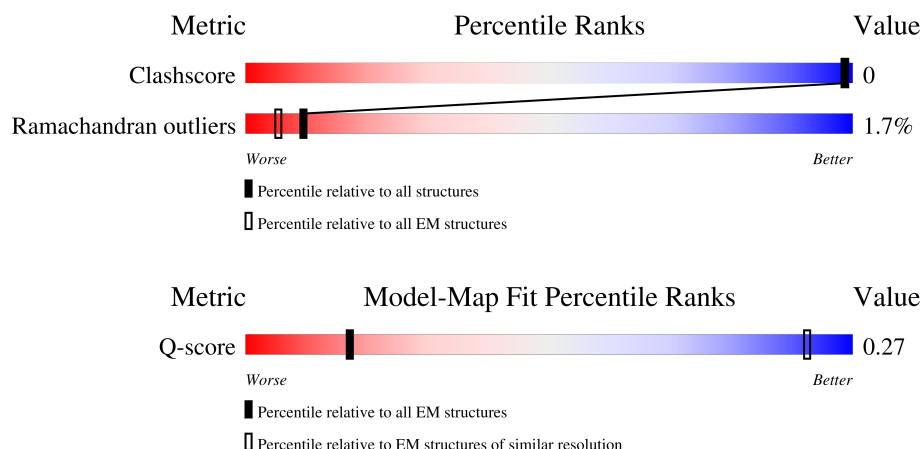
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 7.00 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	483 (6.50 - 7.50)

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	17% 92% 7%
1	1	76	12% 89% 9%
1	2	76	8% 92% 7%
1	3	76	91% 7%
1	4	76	11% 91% 7%

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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 20227 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	120	Total	C	N	O	0	0
			479	240	120	119		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
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		

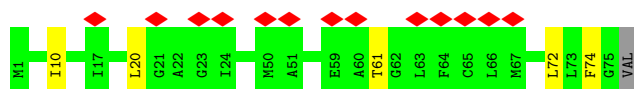
- Molecule 14 is a protein called ATP synthase protein 8.

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

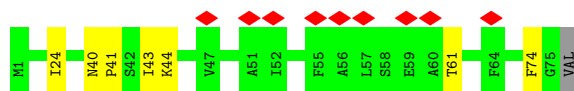
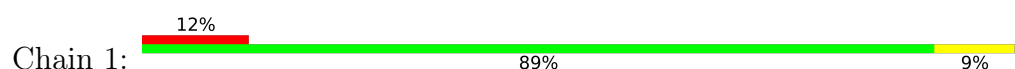
3 Residue-property plots [i](#)

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.

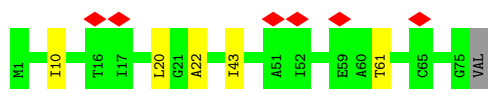
- Molecule 1: ATP synthase subunit 9, mitochondrial



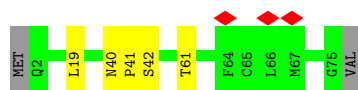
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial



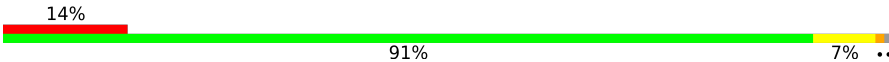
- Molecule 1: ATP synthase subunit 9, mitochondrial

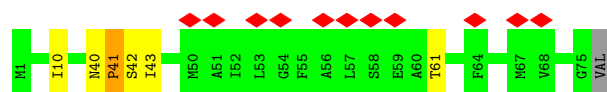


- Molecule 1: ATP synthase subunit 9, mitochondrial



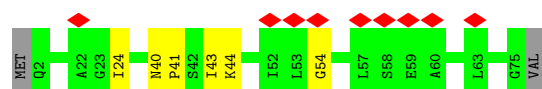
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 5: 



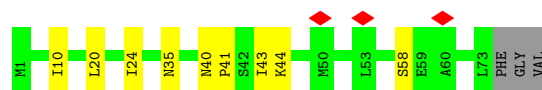
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 6: 

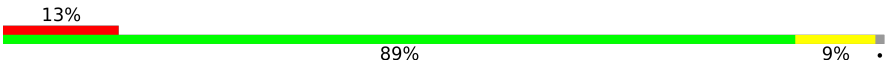


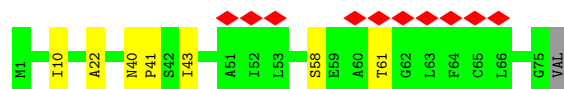
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 7: 



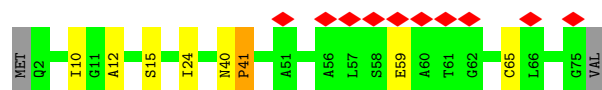
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 8: 

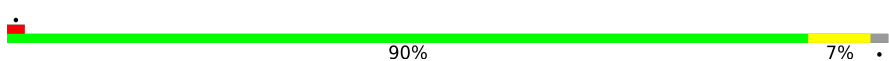


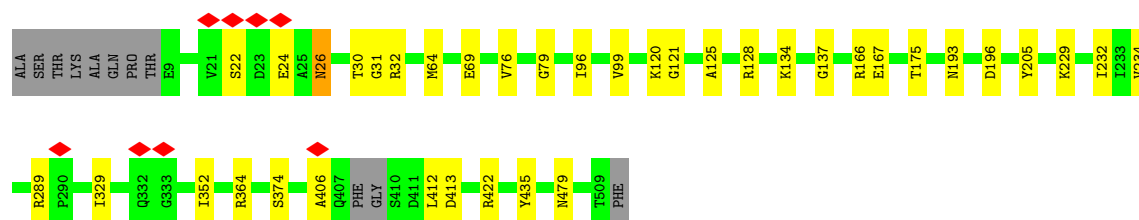
- Molecule 1: ATP synthase subunit 9, mitochondrial

Chain 9: 



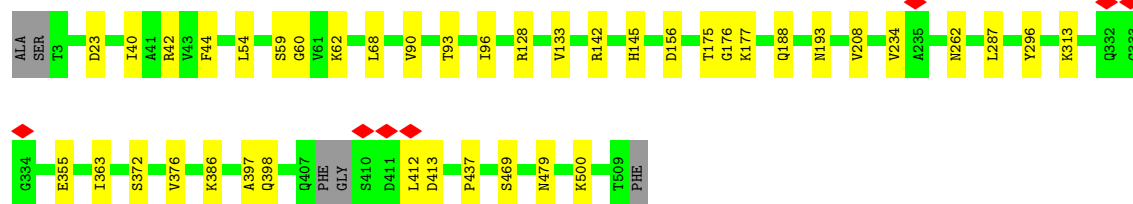
- Molecule 2: ATP synthase subunit alpha

Chain A: 



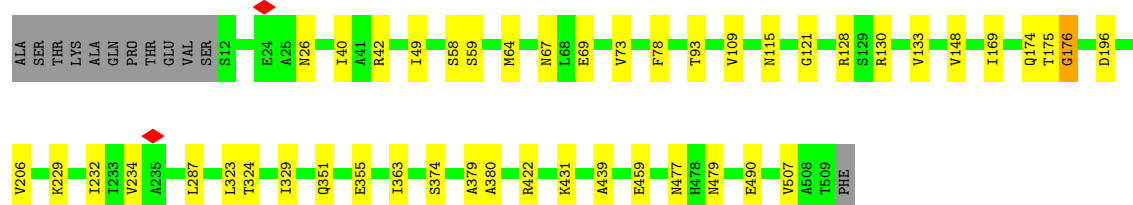
- Molecule 2: ATP synthase subunit alpha

Chain B:  91% 8%



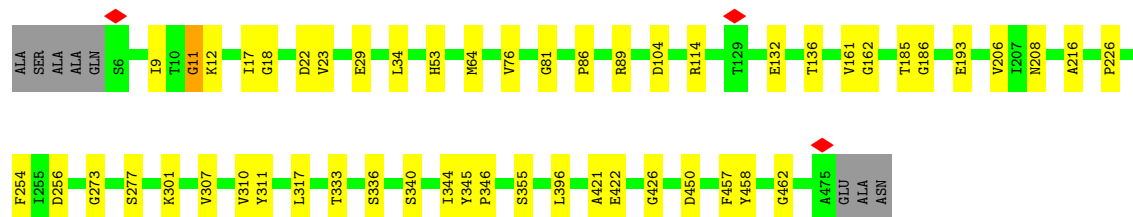
• Molecule 2: ATP synthase subunit alpha

Chain C:  89% 9%



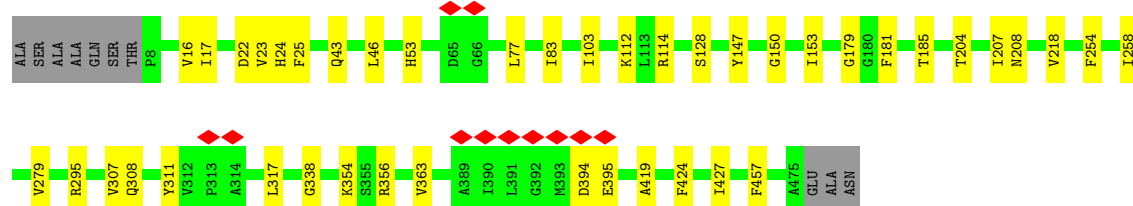
• Molecule 3: ATP synthase subunit beta

Chain D:  87% 11%



• Molecule 3: ATP synthase subunit beta

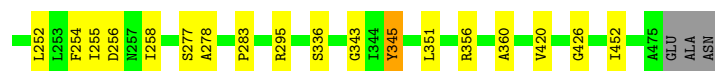
Chain E:  89% 9%



• Molecule 3: ATP synthase subunit beta

Chain F:  88% 10%





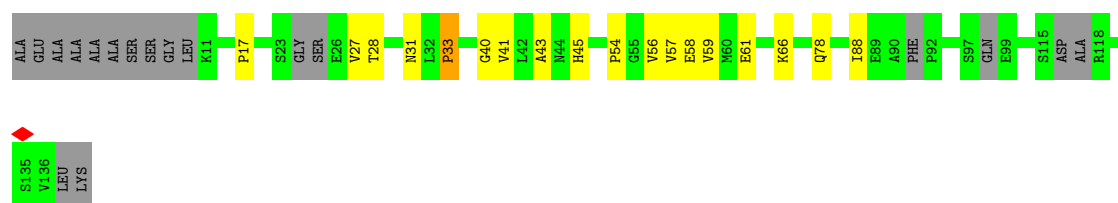
- Molecule 4: ATP synthase subunit gamma

Chain G: 88% 8% 5%



- Molecule 5: ATP synthase subunit delta

Chain H: 74% 12% 13%



- Molecule 6: ATP synthase subunit epsilon

Chain I: 75% 21%



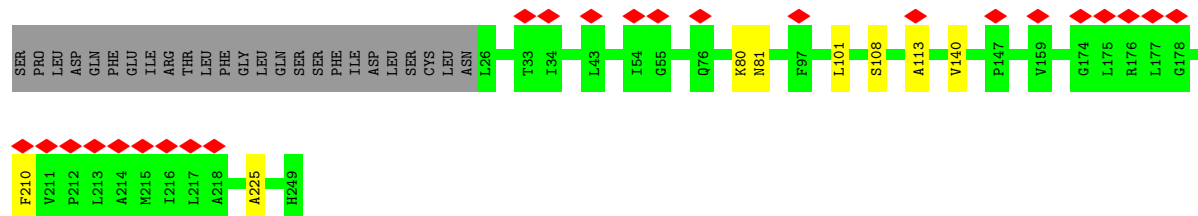
- Molecule 7: ATP synthase subunit 5

Chain O: 89% 7% 1%

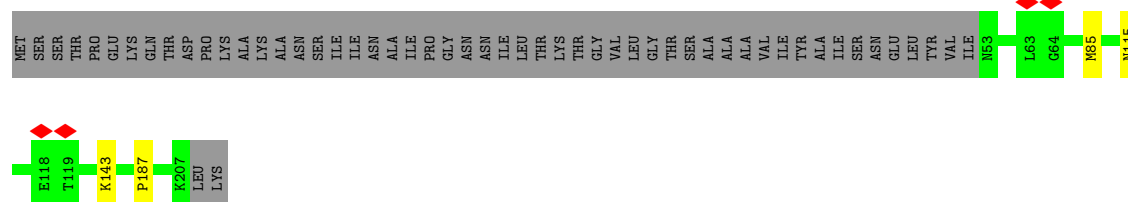


- Molecule 8: ATP synthase subunit a

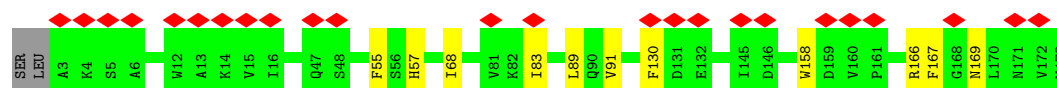
Chain T: 10% 87% 10%



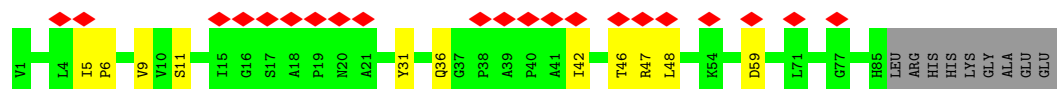
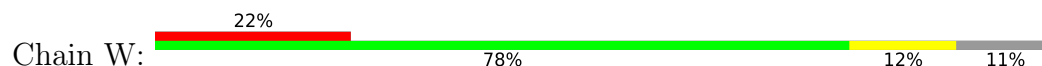
- Molecule 9: ATP synthase subunit 4



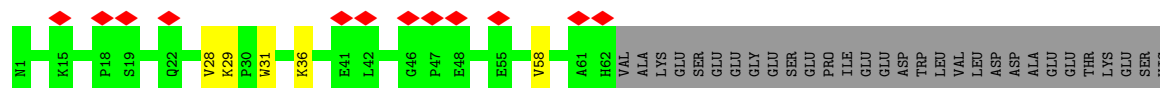
- Molecule 10: ATP synthase subunit d



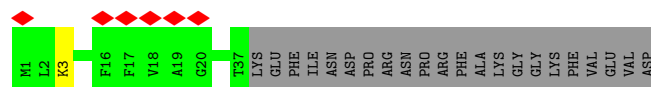
- Molecule 11: ATP synthase subunit f



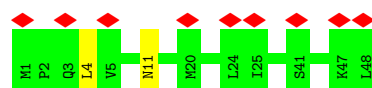
- Molecule 12: ATP synthase subunit H



- 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	6644	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	1.773	Depositor
Minimum map value	-0.573	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	344.96, 344.96, 344.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3475, 1.3475, 1.3475	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	1.23	0/299	2.14	9/372 (2.4%)
1	1	1.21	0/299	2.17	8/372 (2.2%)
1	2	1.18	0/299	2.12	10/372 (2.7%)
1	3	1.23	0/295	1.99	4/367 (1.1%)
1	4	1.24	0/299	2.25	9/372 (2.4%)
1	5	1.18	0/299	2.14	7/372 (1.9%)
1	6	1.17	0/295	2.25	7/367 (1.9%)
1	7	1.22	0/291	2.27	13/362 (3.6%)
1	8	1.23	0/299	2.24	10/372 (2.7%)
1	9	1.23	0/295	2.16	13/367 (3.5%)
2	A	1.58	0/1994	1.86	37/2489 (1.5%)
2	B	1.55	0/2018	1.86	44/2519 (1.7%)
2	C	1.58	1/1991 (0.1%)	1.87	44/2487 (1.8%)
3	D	1.60	1/1879 (0.1%)	1.92	47/2347 (2.0%)
3	E	1.59	1/1871 (0.1%)	1.94	40/2337 (1.7%)
3	F	1.60	0/1875	1.89	42/2342 (1.8%)
4	G	1.48	0/1058	1.98	24/1319 (1.8%)
5	H	1.41	1/474 (0.2%)	1.84	12/584 (2.1%)
6	I	1.39	0/190	1.85	1/231 (0.4%)
7	O	1.54	0/747	1.86	11/932 (1.2%)
8	T	1.29	0/896	1.73	7/1117 (0.6%)
9	U	1.31	0/619	1.87	7/772 (0.9%)
10	V	1.34	0/684	1.84	6/852 (0.7%)
11	W	1.22	0/339	2.01	4/422 (0.9%)
12	X	1.36	0/247	2.09	2/307 (0.7%)
13	Y	1.26	0/147	1.71	0/182
14	Z	1.26	0/192	1.83	4/237 (1.7%)
All	All	1.48	4/20191 (0.0%)	1.93	422/25171 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	3	0	1
1	4	0	1
1	5	0	1
1	6	0	1
1	7	0	1
1	8	0	1
1	9	0	1
3	D	0	1
3	F	0	2
5	H	0	1
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	11	GLY	CA-C	-6.67	1.46	1.51
2	C	477	ASN	CA-C	-5.19	1.48	1.52
3	E	153	ILE	C-N	5.09	1.36	1.33
5	H	40	GLY	CA-C	-5.02	1.48	1.52

All (422) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	204	ASN	CA-C-N	12.40	128.06	120.24
4	G	204	ASN	C-N-CA	12.40	128.06	120.24
2	C	507	VAL	N-CA-C	-9.94	102.99	112.83
8	T	140	VAL	N-CA-C	-9.56	103.30	112.29
7	O	101	PHE	N-CA-C	-9.46	100.61	112.72
3	E	207	ILE	N-CA-C	-8.85	95.78	108.17
2	A	99	VAL	N-CA-C	-8.60	102.14	109.19
2	B	479	ASN	N-CA-C	-8.18	103.01	113.16
3	E	356	ARG	N-CA-C	-8.08	101.49	113.61
3	F	95	ILE	N-CA-C	-8.08	96.86	108.17
2	C	176	GLY	N-CA-C	-8.07	101.84	115.08
3	D	345	TYR	N-CA-C	-8.05	95.53	108.82
3	F	252	LEU	N-CA-C	-8.01	96.89	109.07
3	D	11	GLY	N-CA-C	-7.99	98.35	111.38
11	W	6	PRO	N-CA-C	7.98	120.44	110.70
5	H	56	VAL	N-CA-C	-7.97	96.96	108.11
3	D	162	GLY	N-CA-C	-7.95	104.26	115.30
2	B	193	ASN	N-CA-C	-7.94	100.60	111.56
2	C	329	ILE	N-CA-C	-7.89	97.12	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	479	ASN	N-CA-C	-7.71	103.87	113.28
3	E	43	GLN	N-CA-C	-7.67	103.97	112.72
5	H	78	GLN	N-CA-C	-7.54	99.89	110.29
5	H	61	GLU	N-CA-C	-7.52	96.01	108.34
3	F	39	ILE	N-CA-C	-7.47	97.68	108.36
7	O	33	ILE	N-CA-C	-7.41	105.44	111.81
2	C	93	THR	N-CA-C	-7.37	103.32	111.36
3	E	208	ASN	N-CA-C	-7.32	95.31	108.48
11	W	46	THR	N-CA-C	-7.25	103.88	114.39
4	G	162	ILE	N-CA-C	-7.20	98.11	108.48
3	E	363	VAL	N-CA-C	-7.19	105.71	112.83
2	C	175	THR	N-CA-C	-7.19	105.35	112.97
3	E	103	ILE	N-CA-C	-7.17	106.14	113.10
1	4	43	ILE	CA-C-N	7.08	130.72	120.38
1	4	43	ILE	C-N-CA	7.08	130.72	120.38
3	D	114	ARG	N-CA-C	-7.06	98.58	109.52
4	G	75	VAL	N-CA-C	-6.98	97.48	108.86
10	V	83	ILE	N-CA-C	-6.97	106.34	113.10
2	C	73	VAL	N-CA-C	-6.97	98.55	108.58
2	B	372	SER	N-CA-C	-6.96	97.86	109.07
2	C	42	ARG	N-CA-C	-6.93	96.00	108.48
3	D	53	HIS	N-CA-C	-6.90	98.48	109.59
3	D	89	ARG	N-CA-C	-6.89	104.48	113.17
3	F	207	ILE	N-CA-C	-6.87	98.58	108.48
12	X	29	LYS	N-CA-C	-6.87	101.41	110.07
2	B	398	GLN	N-CA-C	-6.86	105.04	113.41
2	A	175	THR	N-CA-C	-6.84	105.26	112.93
2	B	175	THR	N-CA-C	-6.84	104.81	113.02
2	C	206	VAL	N-CA-C	-6.83	98.54	108.11
3	D	22	ASP	N-CA-C	-6.81	99.13	109.95
2	C	422	ARG	CA-C-N	6.78	127.51	119.98
2	C	422	ARG	C-N-CA	6.78	127.51	119.98
3	D	311	TYR	N-CA-C	-6.78	97.85	108.90
3	D	206	VAL	N-CA-C	-6.76	103.89	110.72
3	F	153	ILE	N-CA-C	-6.76	98.62	108.89
2	C	128	ARG	N-CA-C	-6.75	99.06	109.52
2	A	64	MET	N-CA-C	-6.73	99.18	109.41
3	F	255	ILE	N-CA-C	-6.69	98.41	108.17
3	E	22	ASP	N-CA-C	-6.68	98.83	109.59
3	F	54	LEU	N-CA-C	-6.68	104.76	113.17
2	B	93	THR	N-CA-C	-6.67	104.09	111.36
7	O	84	TYR	N-CA-C	-6.67	103.83	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	9	VAL	N-CA-C	-6.66	106.30	112.43
7	O	192	GLU	N-CA-C	-6.64	105.75	114.31
2	B	96	ILE	N-CA-C	-6.63	102.72	110.21
1	8	10	ILE	CA-C-N	6.59	127.29	119.98
1	8	10	ILE	C-N-CA	6.59	127.29	119.98
3	D	273	GLY	N-CA-C	-6.57	106.09	114.37
3	E	17	ILE	N-CA-C	-6.56	98.41	107.99
2	B	62	LYS	N-CA-C	-6.49	99.25	109.50
3	E	218	VAL	N-CA-C	-6.48	98.17	107.77
3	F	254	PHE	N-CA-C	-6.47	98.06	109.06
3	F	17	ILE	N-CA-C	-6.46	97.80	107.37
2	C	363	ILE	N-CA-C	-6.46	97.26	107.15
4	G	168	ASP	N-CA-C	-6.45	101.52	109.65
3	F	190	ARG	CA-C-N	6.41	128.87	120.28
3	F	190	ARG	C-N-CA	6.41	128.87	120.28
3	E	114	ARG	N-CA-C	-6.40	99.60	109.52
3	D	336	SER	CA-C-N	6.40	128.85	120.28
3	D	336	SER	C-N-CA	6.40	128.85	120.28
7	O	150	GLY	N-CA-C	-6.40	107.07	114.69
2	B	296	TYR	CA-C-N	6.39	127.83	119.84
2	B	296	TYR	C-N-CA	6.39	127.83	119.84
10	V	158	TRP	N-CA-C	-6.39	106.45	114.56
2	A	234	VAL	N-CA-C	-6.37	99.41	108.58
2	B	156	ASP	N-CA-C	-6.37	104.96	114.64
3	F	112	LYS	N-CA-C	-6.37	104.56	112.72
2	B	262	ASN	N-CA-C	-6.35	105.17	113.17
7	O	176	VAL	N-CA-C	-6.33	98.40	107.77
3	E	179	GLY	N-CA-C	-6.30	105.66	115.67
3	E	394	ASP	N-CA-C	-6.28	105.26	113.17
4	G	73	LEU	N-CA-C	-6.28	99.97	109.95
4	G	74	ILE	N-CA-C	-6.28	99.08	108.12
1	4	58	SER	CA-C-N	6.27	128.68	120.28
1	4	58	SER	C-N-CA	6.27	128.68	120.28
2	C	323	LEU	N-CA-C	-6.25	99.09	109.46
3	D	17	ILE	N-CA-C	-6.24	96.37	109.34
4	G	100	ASN	N-CA-C	-6.23	105.71	113.38
1	4	61	THR	CA-C-N	6.23	126.89	119.98
1	4	61	THR	C-N-CA	6.23	126.89	119.98
2	C	234	VAL	N-CA-C	-6.22	99.46	108.17
2	B	355	GLU	CA-C-N	6.22	128.62	120.28
2	B	355	GLU	C-N-CA	6.22	128.62	120.28
1	6	44	LYS	N-CA-C	6.21	118.84	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	351	LEU	N-CA-C	-6.21	105.35	113.17
3	F	420	VAL	N-CA-C	-6.16	104.34	113.39
1	8	43	ILE	CA-C-N	6.16	128.81	120.38
1	8	43	ILE	C-N-CA	6.16	128.81	120.38
3	F	216	ALA	N-CA-C	-6.16	99.98	109.52
7	O	180	ILE	N-CA-C	-6.12	105.09	111.58
3	F	336	SER	CA-C-N	6.12	128.48	120.28
3	F	336	SER	C-N-CA	6.12	128.48	120.28
3	E	150	GLY	CA-C-N	6.12	127.11	120.44
3	E	150	GLY	C-N-CA	6.12	127.11	120.44
3	F	218	VAL	N-CA-C	-6.11	99.32	108.12
2	C	479	ASN	N-CA-C	-6.11	105.66	113.23
2	A	289	ARG	N-CA-C	-6.10	100.12	109.64
3	E	181	PHE	N-CA-C	-6.10	100.26	108.86
1	4	22	ALA	CA-C-N	6.08	126.73	119.98
1	4	22	ALA	C-N-CA	6.08	126.73	119.98
3	E	53	HIS	N-CA-C	-6.08	98.50	108.41
1	0	74	PHE	N-CA-C	-6.06	104.06	112.30
3	E	424	PHE	N-CA-C	6.05	117.95	111.36
5	H	41	VAL	N-CA-C	-6.04	99.42	108.12
3	D	422	GLU	N-CA-C	-6.02	105.01	112.90
8	T	225	ALA	N-CA-C	6.02	117.51	111.07
1	5	61	THR	CA-C-N	6.02	126.66	119.98
1	5	61	THR	C-N-CA	6.02	126.66	119.98
1	7	20	LEU	CA-C-N	6.02	126.66	119.98
1	7	20	LEU	C-N-CA	6.02	126.66	119.98
2	A	31	GLY	N-CA-C	-6.01	102.33	111.10
2	C	26	ASN	N-CA-C	-6.00	105.61	113.17
2	B	68	LEU	N-CA-C	-5.99	98.96	108.73
3	F	126	GLU	N-CA-C	-5.99	106.01	113.38
1	7	35	ASN	CA-C-N	5.99	126.58	119.94
1	7	35	ASN	C-N-CA	5.99	126.58	119.94
3	E	354	LYS	N-CA-C	-5.98	99.59	108.99
3	D	307	VAL	N-CA-C	-5.98	97.77	107.28
2	C	287	LEU	N-CA-C	-5.98	105.57	112.92
5	H	45	HIS	N-CA-C	-5.97	100.22	109.24
4	G	161	LYS	N-CA-C	-5.95	100.02	109.59
2	A	30	THR	N-CA-C	-5.94	101.72	110.52
3	E	258	ILE	N-CA-C	-5.93	105.92	113.22
2	B	234	VAL	N-CA-C	-5.91	99.95	108.53
2	B	42	ARG	N-CA-C	-5.91	98.77	108.76
7	O	82	ASP	N-CA-C	-5.91	106.41	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	112	LYS	N-CA-C	-5.90	104.83	112.68
4	G	2	THR	N-CA-C	-5.90	104.77	111.14
3	D	310	VAL	N-CA-C	-5.88	99.74	108.45
2	C	69	GLU	N-CA-C	-5.85	98.75	108.23
3	F	16	VAL	N-CA-C	-5.84	97.19	109.34
2	A	128	ARG	N-CA-C	-5.84	98.89	108.41
1	5	43	ILE	CA-C-N	5.80	128.85	120.38
1	5	43	ILE	C-N-CA	5.80	128.85	120.38
2	B	177	LYS	CA-C-N	5.79	128.04	120.28
2	B	177	LYS	C-N-CA	5.79	128.04	120.28
3	F	356	ARG	N-CA-C	-5.78	106.00	113.16
3	E	317	LEU	N-CA-C	-5.77	106.40	113.50
4	G	199	ILE	CA-C-N	5.77	129.46	120.75
4	G	199	ILE	C-N-CA	5.77	129.46	120.75
8	T	80	LYS	N-CA-C	-5.76	103.39	110.65
3	F	426	GLY	N-CA-C	-5.75	107.16	115.27
2	A	134	LYS	CA-C-N	5.75	128.38	120.39
2	A	134	LYS	C-N-CA	5.75	128.38	120.39
2	A	137	GLY	CA-C-N	5.74	127.88	120.70
2	A	137	GLY	C-N-CA	5.74	127.88	120.70
1	6	43	ILE	CA-C-N	5.74	128.25	120.38
1	6	43	ILE	C-N-CA	5.74	128.25	120.38
3	D	355	SER	N-CA-C	-5.74	100.54	109.72
3	E	25	PHE	N-CA-C	-5.73	100.80	109.85
3	E	419	ALA	N-CA-C	5.71	117.51	111.28
2	C	169	ILE	N-CA-C	-5.71	99.66	107.99
2	A	193	ASN	CA-C-N	5.70	125.40	119.92
2	A	193	ASN	C-N-CA	5.70	125.40	119.92
3	E	427	ILE	CA-C-N	5.70	126.02	119.93
3	E	427	ILE	C-N-CA	5.70	126.02	119.93
3	F	208	ASN	N-CA-C	-5.70	99.38	109.06
3	F	65	ASP	CA-C-N	5.69	125.50	120.10
3	F	65	ASP	C-N-CA	5.69	125.50	120.10
2	B	128	ARG	N-CA-C	-5.68	100.53	109.50
2	A	422	ARG	CA-C-N	5.66	126.23	120.00
2	A	422	ARG	C-N-CA	5.66	126.23	120.00
2	C	133	VAL	N-CA-C	-5.66	100.88	108.35
1	7	44	LYS	N-CA-C	5.66	118.18	111.33
1	2	10	ILE	CA-C-N	5.65	126.25	119.98
1	2	10	ILE	C-N-CA	5.65	126.25	119.98
1	2	22	ALA	CA-C-N	5.65	126.25	119.98
1	2	22	ALA	C-N-CA	5.65	126.25	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	24	HIS	N-CA-C	-5.64	100.00	109.07
3	F	295	ARG	N-CA-C	-5.63	106.07	113.17
3	F	258	ILE	N-CA-C	-5.63	107.26	112.83
3	D	254	PHE	N-CA-C	-5.62	99.50	109.06
9	U	115	ASN	CA-C-N	5.62	127.64	120.56
9	U	115	ASN	C-N-CA	5.62	127.64	120.56
1	6	54	GLY	CA-C-N	5.61	127.74	120.44
1	6	54	GLY	C-N-CA	5.61	127.74	120.44
2	A	374	SER	N-CA-C	-5.61	99.28	108.76
3	F	206	VAL	N-CA-C	-5.61	104.70	112.50
5	H	57	VAL	N-CA-C	-5.59	99.75	108.86
1	6	24	ILE	CA-C-N	5.59	126.14	119.94
1	6	24	ILE	C-N-CA	5.59	126.14	119.94
3	D	12	LYS	N-CA-C	-5.59	99.79	108.90
3	D	136	THR	N-CA-C	-5.58	106.64	113.50
2	B	376	VAL	N-CA-C	-5.57	106.90	113.42
2	C	130	ARG	N-CA-C	-5.57	100.81	109.72
1	9	24	ILE	CA-C-N	5.56	126.11	119.94
1	9	24	ILE	C-N-CA	5.56	126.11	119.94
3	F	210	GLU	N-CA-C	-5.56	106.85	113.97
3	E	77	LEU	N-CA-C	-5.56	99.96	109.24
6	I	47	TYR	N-CA-C	-5.56	101.18	109.96
10	V	91	VAL	N-CA-C	-5.56	104.51	112.35
1	7	24	ILE	CA-C-N	5.55	126.10	119.94
1	7	24	ILE	C-N-CA	5.55	126.10	119.94
4	G	137	ALA	N-CA-C	-5.55	101.52	109.24
1	3	19	LEU	CA-C-N	5.54	127.97	120.38
1	3	19	LEU	C-N-CA	5.54	127.97	120.38
3	F	452	ILE	CA-C-N	5.53	125.53	119.89
3	F	452	ILE	C-N-CA	5.53	125.53	119.89
3	D	340	SER	CA-C-N	5.53	128.71	120.31
3	D	340	SER	C-N-CA	5.53	128.71	120.31
2	C	121	GLY	CA-C-N	5.51	125.82	119.92
2	C	121	GLY	C-N-CA	5.51	125.82	119.92
2	C	58	SER	N-CA-C	-5.50	106.42	113.02
3	D	216	ALA	N-CA-C	-5.50	101.16	109.85
2	C	490	GLU	N-CA-C	-5.49	100.39	108.79
3	D	333	THR	N-CA-C	-5.48	99.74	109.06
1	9	59	GLU	CA-C-N	5.48	127.62	120.28
1	9	59	GLU	C-N-CA	5.48	127.62	120.28
2	A	352	ILE	N-CA-C	-5.48	100.23	108.12
3	D	458	TYR	CA-C-N	5.47	130.17	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	458	TYR	C-N-CA	5.47	130.17	122.46
9	U	143	LYS	CA-C-N	5.46	127.44	120.56
9	U	143	LYS	C-N-CA	5.46	127.44	120.56
3	E	307	VAL	N-CA-C	-5.45	100.54	108.17
4	G	171	SER	N-CA-C	-5.45	100.84	108.96
2	A	120	LYS	CA-C-N	5.45	130.42	121.87
2	A	120	LYS	C-N-CA	5.45	130.42	121.87
2	C	40	ILE	N-CA-C	-5.45	99.71	107.77
8	T	210	PHE	CA-C-N	5.44	123.67	120.24
8	T	210	PHE	C-N-CA	5.44	123.67	120.24
2	A	26	ASN	N-CA-C	-5.44	99.21	110.80
2	C	78	PHE	N-CA-C	-5.44	106.14	112.89
3	D	226	PRO	CA-C-N	5.44	126.02	119.98
3	D	226	PRO	C-N-CA	5.44	126.02	119.98
2	B	479	ASN	CA-C-N	5.44	127.57	120.28
2	B	479	ASN	C-N-CA	5.44	127.57	120.28
1	9	12	ALA	CA-C-N	5.43	125.97	119.94
1	9	12	ALA	C-N-CA	5.43	125.97	119.94
3	F	283	PRO	N-CA-C	-5.43	107.07	113.86
4	G	99	LEU	N-CA-C	-5.43	106.33	113.17
2	B	176	GLY	N-CA-C	-5.42	100.33	113.18
2	B	208	VAL	N-CA-C	-5.42	100.68	108.48
1	2	20	LEU	CA-C-N	5.40	125.98	119.98
1	2	20	LEU	C-N-CA	5.40	125.98	119.98
3	D	23	VAL	N-CA-C	-5.40	100.06	108.86
2	A	412	LEU	CA-C-N	5.39	131.84	121.54
2	A	412	LEU	C-N-CA	5.39	131.84	121.54
4	G	5	GLU	CA-C-N	5.39	127.35	120.56
4	G	5	GLU	C-N-CA	5.39	127.35	120.56
3	E	308	GLN	N-CA-C	-5.39	101.17	109.52
3	F	247	GLU	N-CA-C	-5.39	106.71	113.72
10	V	68	ILE	N-CA-C	-5.39	104.22	111.44
1	2	43	ILE	CA-C-N	5.39	127.76	120.38
1	2	43	ILE	C-N-CA	5.39	127.76	120.38
2	A	232	ILE	N-CA-C	-5.39	100.44	108.46
2	C	115	ASN	N-CA-C	-5.38	102.01	110.14
3	D	421	ALA	N-CA-C	-5.38	104.00	110.88
3	E	254	PHE	N-CA-C	-5.37	101.78	110.32
1	9	41	PRO	N-CA-C	5.37	123.53	112.47
2	A	406	ALA	N-CA-C	-5.37	106.41	113.12
1	7	43	ILE	CA-C-N	5.37	127.73	120.38
1	7	43	ILE	C-N-CA	5.37	127.73	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	113	ALA	N-CA-C	-5.37	106.73	113.28
4	G	2	THR	CA-C-N	5.36	127.41	120.44
4	G	2	THR	C-N-CA	5.36	127.41	120.44
3	E	395	GLU	N-CA-C	-5.36	106.52	113.16
3	E	128	SER	N-CA-C	-5.35	100.46	108.96
2	B	40	ILE	N-CA-C	-5.34	100.15	108.81
1	0	10	ILE	CA-C-N	5.34	125.91	119.98
1	0	10	ILE	C-N-CA	5.34	125.91	119.98
1	2	61	THR	CA-C-N	5.34	125.88	120.00
1	2	61	THR	C-N-CA	5.34	125.88	120.00
2	C	109	VAL	N-CA-C	-5.34	100.76	108.71
3	D	185	THR	N-CA-C	-5.33	99.75	108.76
1	1	44	LYS	N-CA-C	5.33	118.57	111.75
7	O	98	LEU	N-CA-C	-5.33	106.79	113.72
2	C	64	MET	N-CA-C	-5.33	103.66	110.53
5	H	33	PRO	N-CA-C	-5.32	101.50	112.47
2	B	313	LYS	N-CA-C	-5.32	97.85	107.75
1	1	24	ILE	CA-C-N	5.32	125.88	119.98
1	1	24	ILE	C-N-CA	5.32	125.88	119.98
1	9	10	ILE	CA-C-N	5.32	125.88	119.98
1	9	10	ILE	C-N-CA	5.32	125.88	119.98
3	E	204	THR	N-CA-C	-5.32	106.57	113.16
2	C	324	THR	N-CA-C	-5.31	101.51	109.95
2	C	374	SER	CA-C-N	5.30	127.91	120.28
2	C	374	SER	C-N-CA	5.30	127.91	120.28
1	5	10	ILE	CA-C-N	5.30	125.86	119.98
1	5	10	ILE	C-N-CA	5.30	125.86	119.98
2	B	60	GLY	CA-C-N	5.30	127.72	120.35
2	B	60	GLY	C-N-CA	5.30	127.72	120.35
3	D	450	ASP	N-CA-C	-5.30	106.66	113.02
3	F	345	TYR	N-CA-C	-5.30	97.17	108.93
2	A	96	ILE	N-CA-C	-5.29	102.76	109.80
3	E	46	LEU	N-CA-C	-5.29	99.82	108.76
2	C	67	ASN	N-CA-C	-5.29	99.82	108.76
5	H	59	VAL	N-CA-C	-5.29	100.51	108.12
12	X	28	VAL	N-CA-C	-5.28	100.23	108.95
2	C	148	VAL	N-CA-C	-5.27	100.53	108.12
3	E	185	THR	N-CA-C	-5.25	100.62	109.07
2	B	142	ARG	N-CA-C	-5.25	100.34	108.90
3	F	53	HIS	N-CA-C	-5.25	100.62	109.07
2	A	32	ARG	N-CA-C	-5.25	99.40	108.69
3	D	18	GLY	CA-C-N	5.25	127.57	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	18	GLY	C-N-CA	5.25	127.57	120.38
3	D	104	ASP	N-CA-C	-5.24	106.27	113.30
1	1	43	ILE	CA-C-N	5.24	128.03	120.38
1	1	43	ILE	C-N-CA	5.24	128.03	120.38
2	C	196	ASP	CA-C-N	5.24	127.30	120.28
2	C	196	ASP	C-N-CA	5.24	127.30	120.28
3	D	317	LEU	N-CA-C	-5.23	106.74	113.23
3	E	23	VAL	N-CA-C	-5.22	100.68	108.46
2	C	351	GLN	N-CA-C	-5.22	100.52	109.24
1	7	10	ILE	CA-C-N	5.21	125.77	119.98
1	7	10	ILE	C-N-CA	5.21	125.77	119.98
2	B	287	LEU	N-CA-C	-5.21	106.60	113.17
3	F	76	VAL	N-CA-C	-5.21	100.35	108.95
3	E	295	ARG	N-CA-C	-5.20	105.68	112.23
2	C	459	GLU	CA-C-N	5.19	127.24	120.28
2	C	459	GLU	C-N-CA	5.19	127.24	120.28
1	8	22	ALA	CA-C-N	5.19	125.70	119.94
1	8	22	ALA	C-N-CA	5.19	125.70	119.94
5	H	31	ASN	N-CA-C	-5.19	99.99	108.76
10	V	167	PHE	N-CA-C	-5.19	101.65	109.85
2	C	355	GLU	CA-C-N	5.18	127.22	120.28
2	C	355	GLU	C-N-CA	5.18	127.22	120.28
1	8	58	SER	CA-C-N	5.18	127.22	120.28
1	8	58	SER	C-N-CA	5.18	127.22	120.28
3	D	344	ILE	CA-C-N	5.18	126.83	122.28
3	D	344	ILE	C-N-CA	5.18	126.83	122.28
1	5	41	PRO	N-CA-C	5.17	123.13	112.47
2	A	166	ARG	N-CA-C	-5.17	102.41	110.42
5	H	66	LYS	N-CA-C	-5.17	100.61	109.24
5	H	58	GLU	N-CA-C	-5.16	100.62	109.24
2	B	469	SER	CA-C-N	5.16	127.15	120.44
2	B	469	SER	C-N-CA	5.16	127.15	120.44
5	H	40	GLY	N-CA-C	-5.16	101.91	111.04
3	D	81	GLY	CA-C-N	5.14	126.27	119.84
3	D	81	GLY	C-N-CA	5.14	126.27	119.84
3	F	277	SER	CA-C-N	5.14	131.35	121.54
3	F	277	SER	C-N-CA	5.14	131.35	121.54
8	T	101	LEU	N-CA-C	-5.14	106.95	113.43
2	B	412	LEU	CA-C-N	5.14	131.35	121.54
2	B	412	LEU	C-N-CA	5.14	131.35	121.54
7	O	154	LYS	N-CA-C	-5.14	100.53	108.90
2	A	69	GLU	N-CA-C	-5.13	104.15	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	232	ILE	N-CA-C	-5.13	101.09	108.48
2	A	76	VAL	N-CA-C	-5.13	100.36	107.80
3	E	311	TYR	N-CA-C	-5.13	98.91	107.99
9	U	85	MET	CA-C-N	5.13	127.10	120.44
9	U	85	MET	C-N-CA	5.13	127.10	120.44
3	F	22	ASP	N-CA-C	-5.12	100.68	109.24
1	0	20	LEU	CA-C-N	5.12	125.67	119.98
1	0	20	LEU	C-N-CA	5.12	125.67	119.98
1	1	61	THR	CA-C-N	5.12	125.67	119.98
1	1	61	THR	C-N-CA	5.12	125.67	119.98
2	C	59	SER	N-CA-C	-5.12	106.29	112.54
3	D	186	GLY	N-CA-C	-5.12	101.04	113.18
2	A	329	ILE	N-CA-C	-5.12	100.84	108.46
1	0	61	THR	CA-C-N	5.11	125.62	120.00
1	0	61	THR	C-N-CA	5.11	125.62	120.00
3	E	457	PHE	N-CA-C	-5.11	107.10	113.38
4	G	156	ALA	CA-C-N	5.11	126.53	120.14
4	G	156	ALA	C-N-CA	5.11	126.53	120.14
1	3	61	THR	CA-C-N	5.11	125.65	119.98
1	3	61	THR	C-N-CA	5.11	125.65	119.98
1	7	58	SER	CA-C-N	5.10	127.11	120.28
1	7	58	SER	C-N-CA	5.10	127.11	120.28
2	B	54	LEU	N-CA-C	-5.10	100.93	109.24
11	W	48	LEU	N-CA-C	-5.09	106.90	114.64
4	G	204	ASN	N-CA-C	-5.09	106.66	112.92
2	B	44	PHE	N-CA-C	-5.09	100.88	109.07
14	Z	11	ASN	CA-C-N	5.09	127.41	120.54
14	Z	11	ASN	C-N-CA	5.09	127.41	120.54
3	D	193	GLU	CA-C-N	5.08	125.58	119.94
3	D	193	GLU	C-N-CA	5.08	125.58	119.94
3	E	338	GLY	N-CA-C	-5.08	106.64	112.73
3	D	64	MET	N-CA-C	-5.07	106.50	113.30
10	V	57	HIS	N-CA-C	-5.07	105.21	111.40
4	G	175	PHE	N-CA-C	-5.07	99.36	108.48
2	A	205	TYR	N-CA-C	-5.07	100.64	108.90
3	D	132	GLU	N-CA-C	-5.07	101.59	109.24
3	F	360	ALA	N-CA-C	-5.07	106.61	112.89
3	F	343	GLY	N-CA-C	-5.06	107.99	114.37
1	0	72	LEU	CA-C-N	5.06	127.48	120.29
1	0	72	LEU	C-N-CA	5.06	127.48	120.29
9	U	187	PRO	N-CA-C	-5.06	109.42	114.68
14	Z	4	LEU	CA-C-N	5.06	124.38	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Z	4	LEU	C-N-CA	5.06	124.38	120.33
3	F	90	GLU	N-CA-C	-5.06	106.70	112.92
2	A	22	SER	N-CA-C	-5.05	101.61	109.24
3	D	457	PHE	N-CA-C	-5.05	107.25	113.41
1	1	74	PHE	N-CA-C	-5.04	105.25	111.40
2	B	133	VAL	N-CA-C	-5.04	101.22	108.42
2	B	188	GLN	N-CA-C	-5.04	106.98	112.72
2	B	90	VAL	N-CA-C	-5.03	101.12	108.17
4	G	205	VAL	CA-C-O	-5.03	114.57	118.85
2	A	364	ARG	N-CA-C	-5.03	99.39	108.85
7	O	160	LYS	N-CA-C	-5.03	97.59	107.91
2	B	397	ALA	N-CA-C	-5.03	106.73	112.92
1	8	61	THR	CA-C-N	5.03	125.53	120.00
1	8	61	THR	C-N-CA	5.03	125.53	120.00
2	B	500	LYS	CA-C-N	5.02	126.97	120.44
2	B	500	LYS	C-N-CA	5.02	126.97	120.44
3	D	208	ASN	N-CA-C	-5.01	101.00	109.07
1	9	65	CYS	CA-C-N	5.01	127.00	120.28
1	9	65	CYS	C-N-CA	5.01	127.00	120.28
1	4	41	PRO	N-CA-C	5.01	122.79	112.47
2	A	79	GLY	CA-C-N	5.01	128.31	120.75
2	A	79	GLY	C-N-CA	5.01	128.31	120.75
2	B	386	LYS	N-CA-C	-5.01	106.86	113.12
1	9	15	SER	CA-C-N	5.00	127.48	120.28
1	9	15	SER	C-N-CA	5.00	127.48	120.28

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	40	ASN	Peptide
1	3	40	ASN	Peptide
1	4	40	ASN	Peptide
1	5	40	ASN	Peptide
1	6	40	ASN	Peptide
1	7	40	ASN	Peptide
1	8	40	ASN	Peptide
1	9	40	ASN	Peptide
3	D	256	ASP	Peptide
3	F	256	ASP	Peptide
3	F	345	TYR	Peptide
5	H	54	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	300	0	95	0	0
1	1	300	0	95	0	0
1	2	300	0	95	0	0
1	3	296	0	91	0	0
1	4	300	0	95	0	0
1	5	300	0	95	0	0
1	6	296	0	91	0	0
1	7	292	0	91	0	0
1	8	300	0	95	0	0
1	9	296	0	91	0	0
2	A	1996	0	570	0	0
2	B	2020	0	575	0	0
2	C	1992	0	572	1	0
3	D	1880	0	538	1	0
3	E	1872	0	537	0	0
3	F	1876	0	537	0	0
4	G	1060	0	277	0	0
5	H	479	0	122	1	0
6	I	193	0	43	0	0
7	O	748	0	205	0	0
8	T	897	0	248	0	0
9	U	620	0	158	0	0
10	V	685	0	173	0	0
11	W	340	0	92	0	0
12	X	248	0	61	0	0
13	Y	148	0	40	0	0
14	Z	193	0	49	0	0
All	All	20227	0	5731	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)
5:H:28:THR:CA	5:H:43:ALA:H	2.19	0.55
2:C:174:GLN:C	2:C:176:GLY:H	2.27	0.42
3:D:11:GLY:H	3:D:76:VAL:H	1.68	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	1	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	2	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
1	3	72/76 (95%)	69 (96%)	1 (1%)	2 (3%)	4	24
1	4	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	5	73/76 (96%)	70 (96%)	1 (1%)	2 (3%)	4	25
1	6	72/76 (95%)	70 (97%)	1 (1%)	1 (1%)	9	40
1	7	71/76 (93%)	69 (97%)	1 (1%)	1 (1%)	9	40
1	8	73/76 (96%)	70 (96%)	2 (3%)	1 (1%)	9	40
1	9	72/76 (95%)	69 (96%)	2 (3%)	1 (1%)	9	40
2	A	495/510 (97%)	468 (94%)	18 (4%)	9 (2%)	6	34
2	B	501/510 (98%)	470 (94%)	25 (5%)	6 (1%)	10	44
2	C	496/510 (97%)	471 (95%)	19 (4%)	6 (1%)	10	44
3	D	468/478 (98%)	432 (92%)	25 (5%)	11 (2%)	4	27
3	E	466/478 (98%)	444 (95%)	18 (4%)	4 (1%)	14	51
3	F	467/478 (98%)	417 (89%)	41 (9%)	9 (2%)	6	32
4	G	261/278 (94%)	251 (96%)	6 (2%)	4 (2%)	8	40
5	H	110/138 (80%)	102 (93%)	4 (4%)	4 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	I	42/61 (69%)	32 (76%)	9 (21%)	1 (2%)	4	27
7	O	185/195 (95%)	170 (92%)	13 (7%)	2 (1%)	11	46
8	T	222/249 (89%)	209 (94%)	11 (5%)	2 (1%)	14	51
9	U	153/209 (73%)	152 (99%)	1 (1%)	0	100	100
10	V	169/173 (98%)	155 (92%)	9 (5%)	5 (3%)	3	22
11	W	83/95 (87%)	69 (83%)	7 (8%)	7 (8%)	0	9
12	X	60/92 (65%)	54 (90%)	3 (5%)	3 (5%)	1	16
13	Y	35/59 (59%)	31 (89%)	3 (9%)	1 (3%)	3	23
14	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
All	All	4984/5321 (94%)	4672 (94%)	228 (5%)	84 (2%)	9	36

All (84) 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	26	ASN
2	A	229	LYS
2	B	59	SER
2	C	379	ALA
2	C	380	ALA
3	D	277	SER
3	F	159	ALA
3	F	278	ALA
5	H	27	VAL
7	O	61	ALA
8	T	81	ASN
11	W	31	TYR
11	W	42	ILE
2	A	24	GLU
2	A	413	ASP
2	C	49	ILE
3	D	29	GLU

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Mol	Chain	Res	Type
3	D	34	LEU
3	D	396	LEU
3	D	462	GLY
3	F	81	GLY
6	I	40	THR
10	V	130	PHE
11	W	11	SER
12	X	58	VAL
2	A	435	TYR
2	B	413	ASP
3	D	426	GLY
3	E	147	TYR
3	F	86	PRO
3	F	125	ALA
3	F	131	ALA
3	F	137	GLY
3	F	177	ALA
5	H	33	PRO
10	V	55	PHE
10	V	169	ASN
11	W	47	ARG
11	W	59	ASP
13	Y	3	LYS
1	3	42	SER
2	A	125	ALA
2	A	167	GLU
2	B	437	PRO
2	C	229	LYS
2	C	431	LYS
3	F	134	LEU
8	T	108	SER
10	V	166	ARG
12	X	31	TRP
1	5	42	SER
2	A	196	ASP
2	B	23	ASP
2	B	145	HIS
2	B	363	ILE
2	C	439	ALA
3	E	16	VAL
4	G	57	THR
4	G	58	LYS

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Mol	Chain	Res	Type
4	G	123	PRO
5	H	88	ILE
7	O	10	VAL
11	W	36	GLN
12	X	36	LYS
3	D	301	LYS
10	V	89	LEU
11	W	5	ILE
3	E	83	ILE
4	G	181	PRO
2	A	121	GLY
3	D	161	VAL
3	D	9	ILE
3	E	279	VAL
5	H	17	PRO
3	D	86	PRO
3	D	346	PRO

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

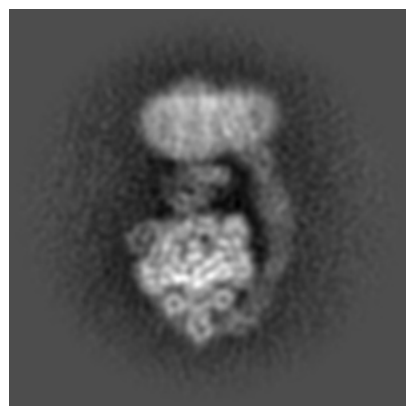
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25956. These allow visual inspection of the internal detail of the map and identification of artifacts.

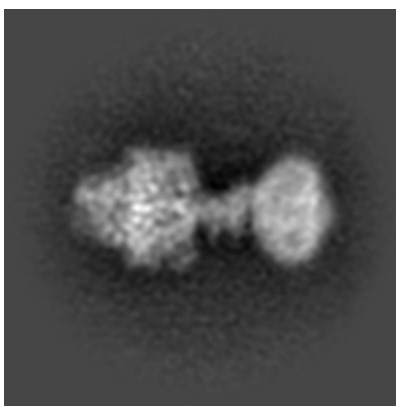
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

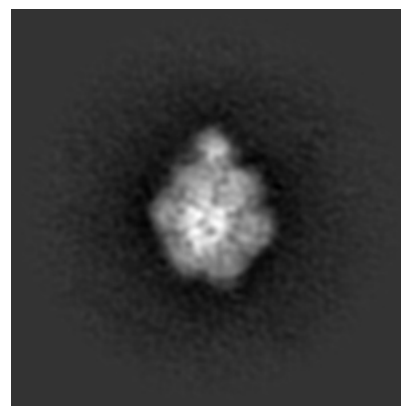
6.1.1 Primary map



X

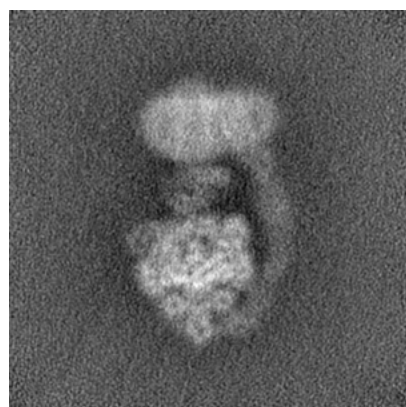


Y

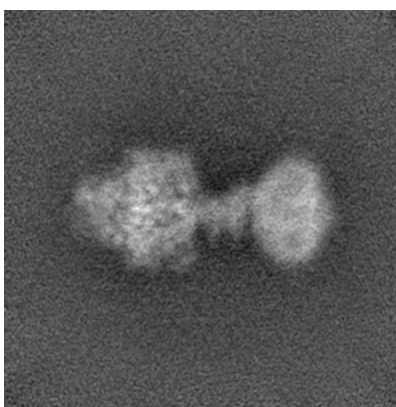


Z

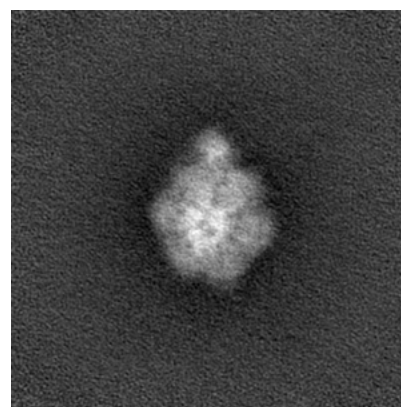
6.1.2 Raw map



X



Y

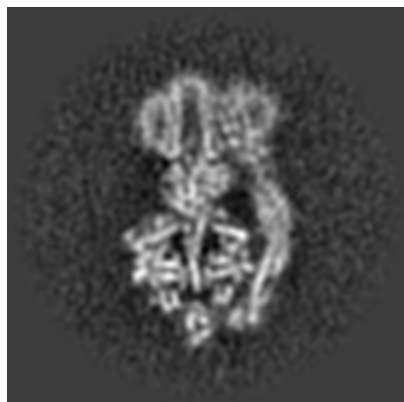


Z

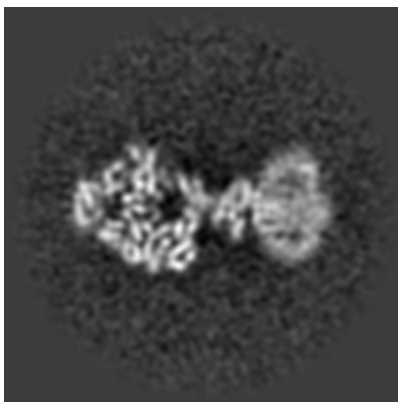
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

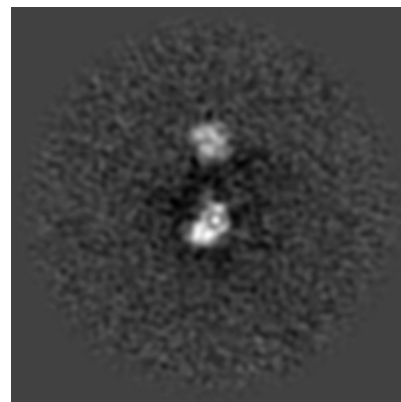
6.2.1 Primary map



X Index: 128

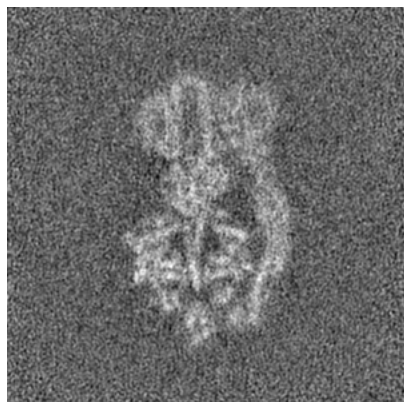


Y Index: 128

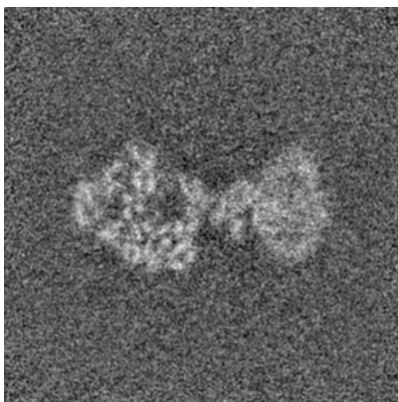


Z Index: 128

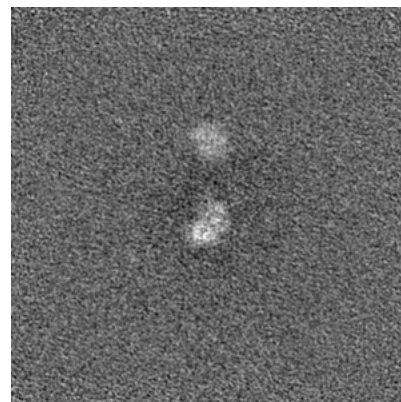
6.2.2 Raw map



X Index: 128



Y Index: 128



Z Index: 128

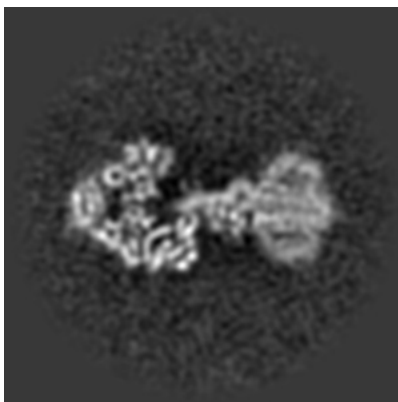
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

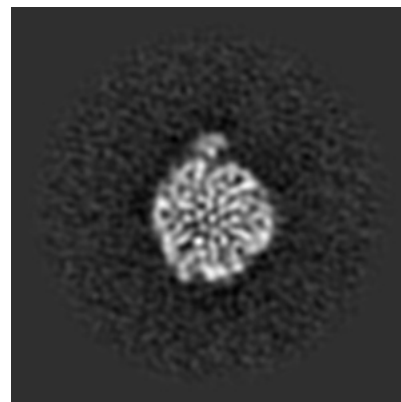
6.3.1 Primary map



X Index: 134

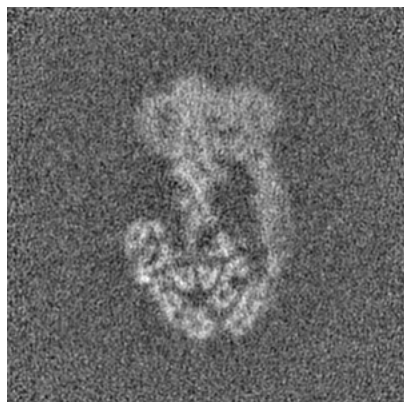


Y Index: 125

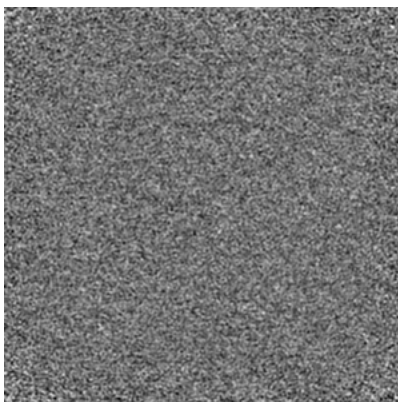


Z Index: 85

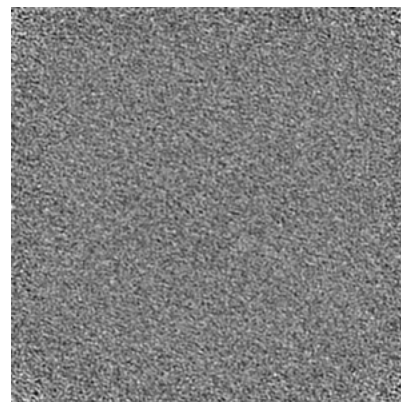
6.3.2 Raw map



X Index: 134



Y Index: 0

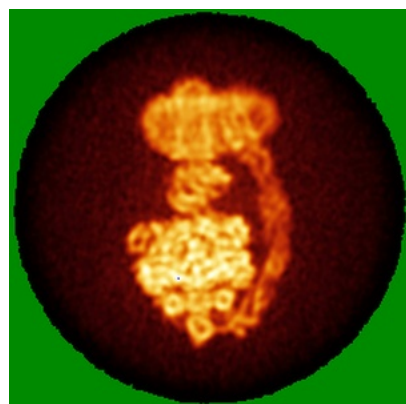


Z Index: 0

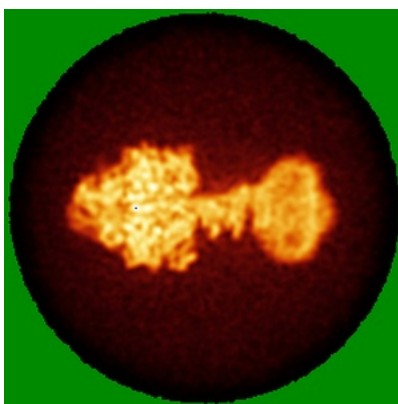
The images above show the largest variance slices of the map in three orthogonal directions.

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

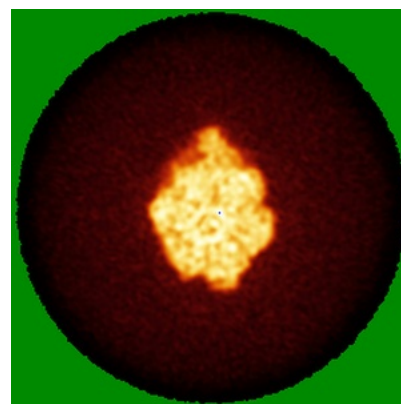
6.4.1 Primary map



X

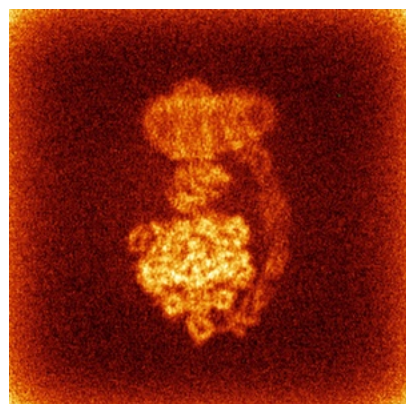


Y

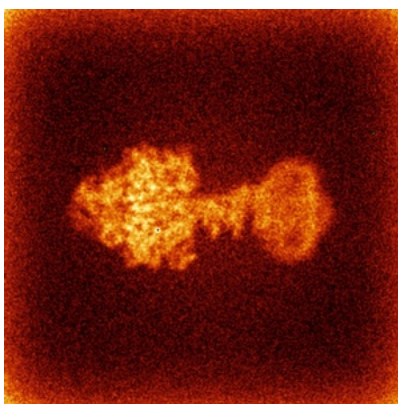


Z

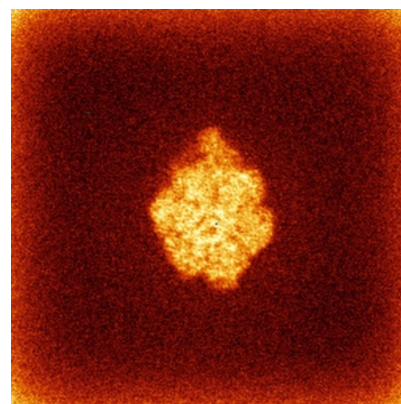
6.4.2 Raw map



X



Y

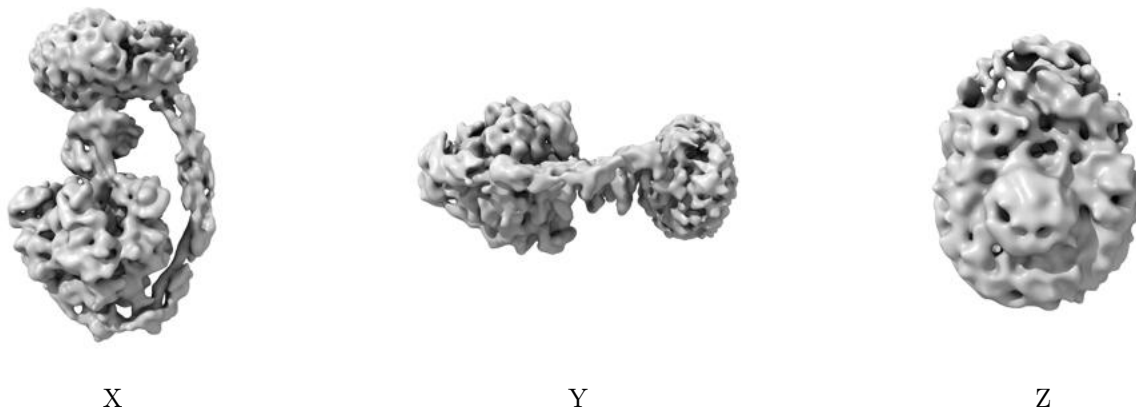


Z

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.

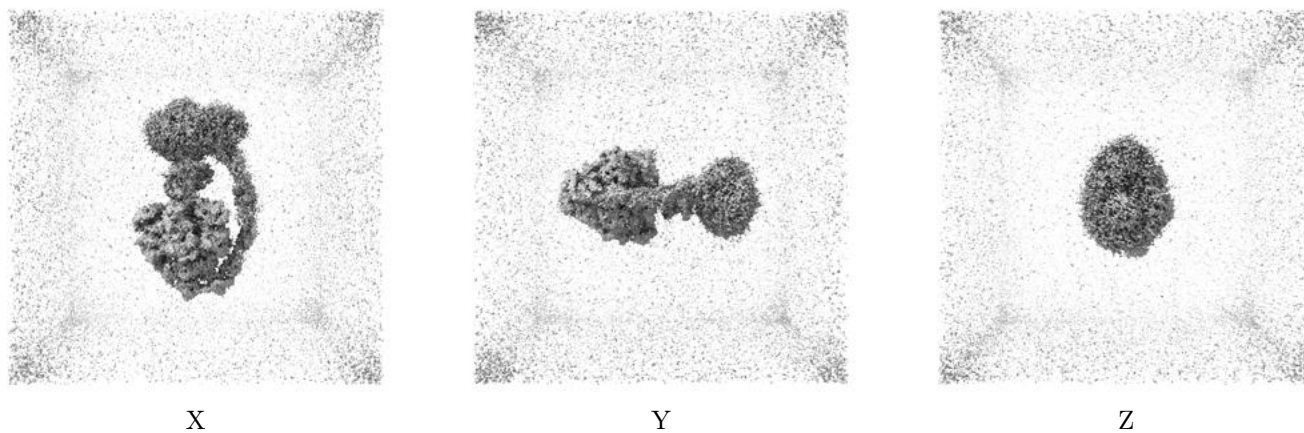
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. 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.

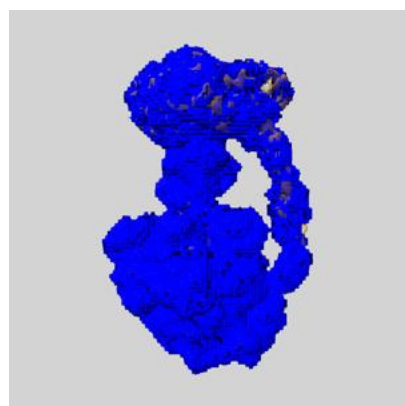
6.6 Mask visualisation [i](#)

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

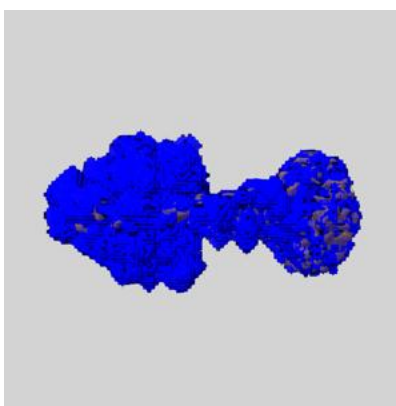
A mask typically either:

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

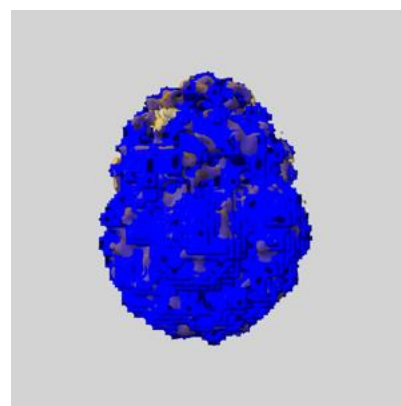
6.6.1 emd_25956_msk_1.map [i](#)



X



Y

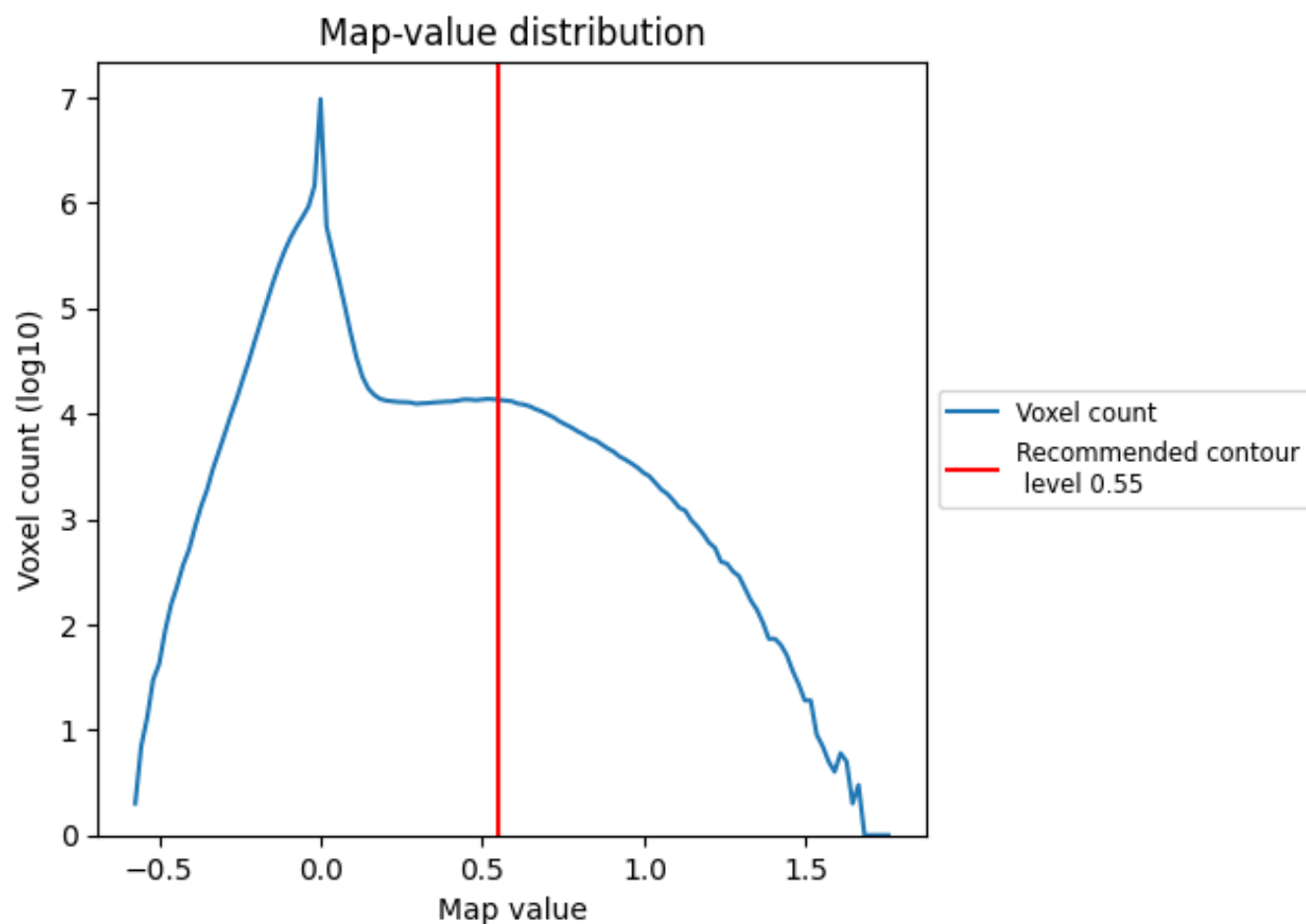


Z

7 Map analysis [i](#)

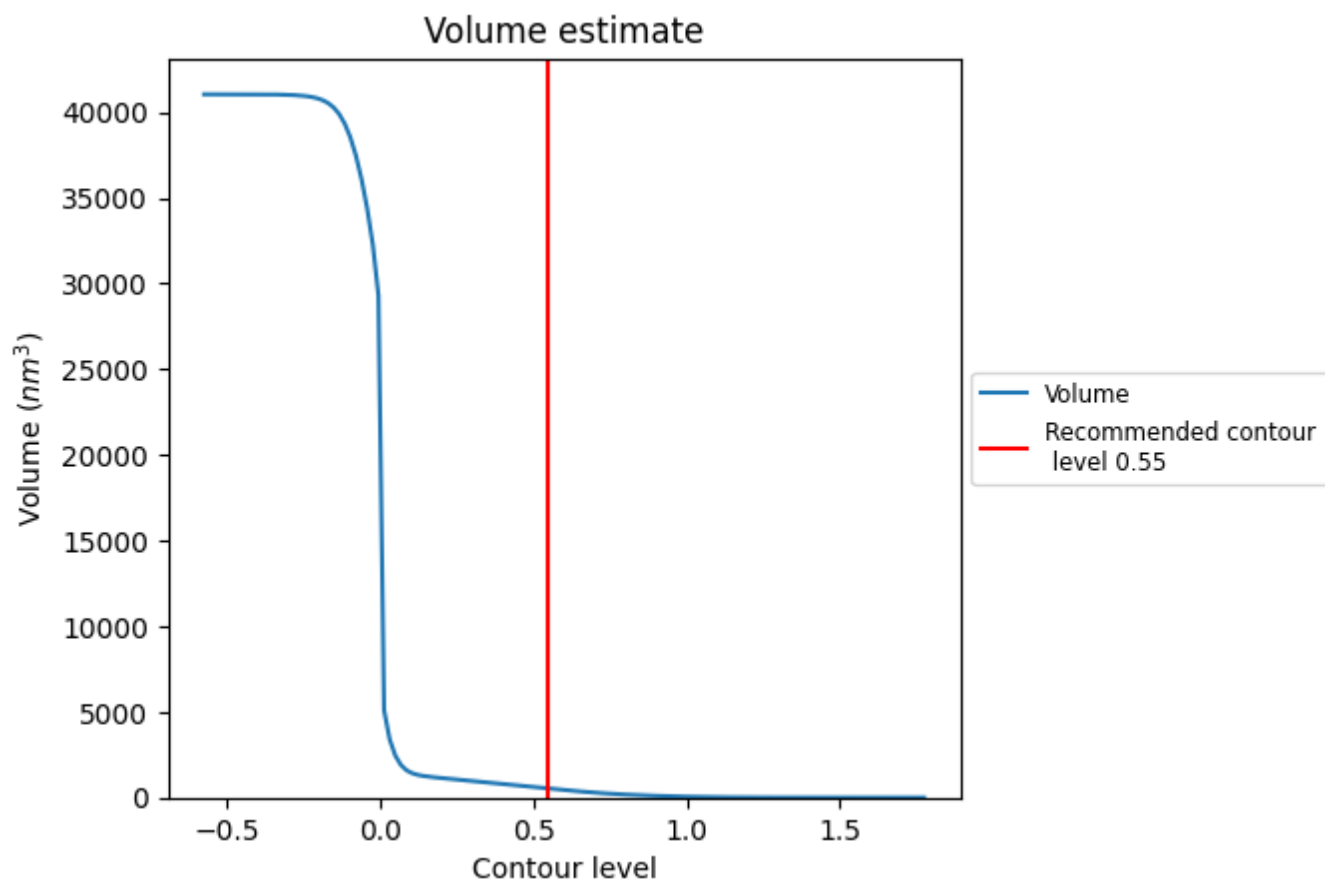
This section contains the results of statistical analysis of the map.

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.

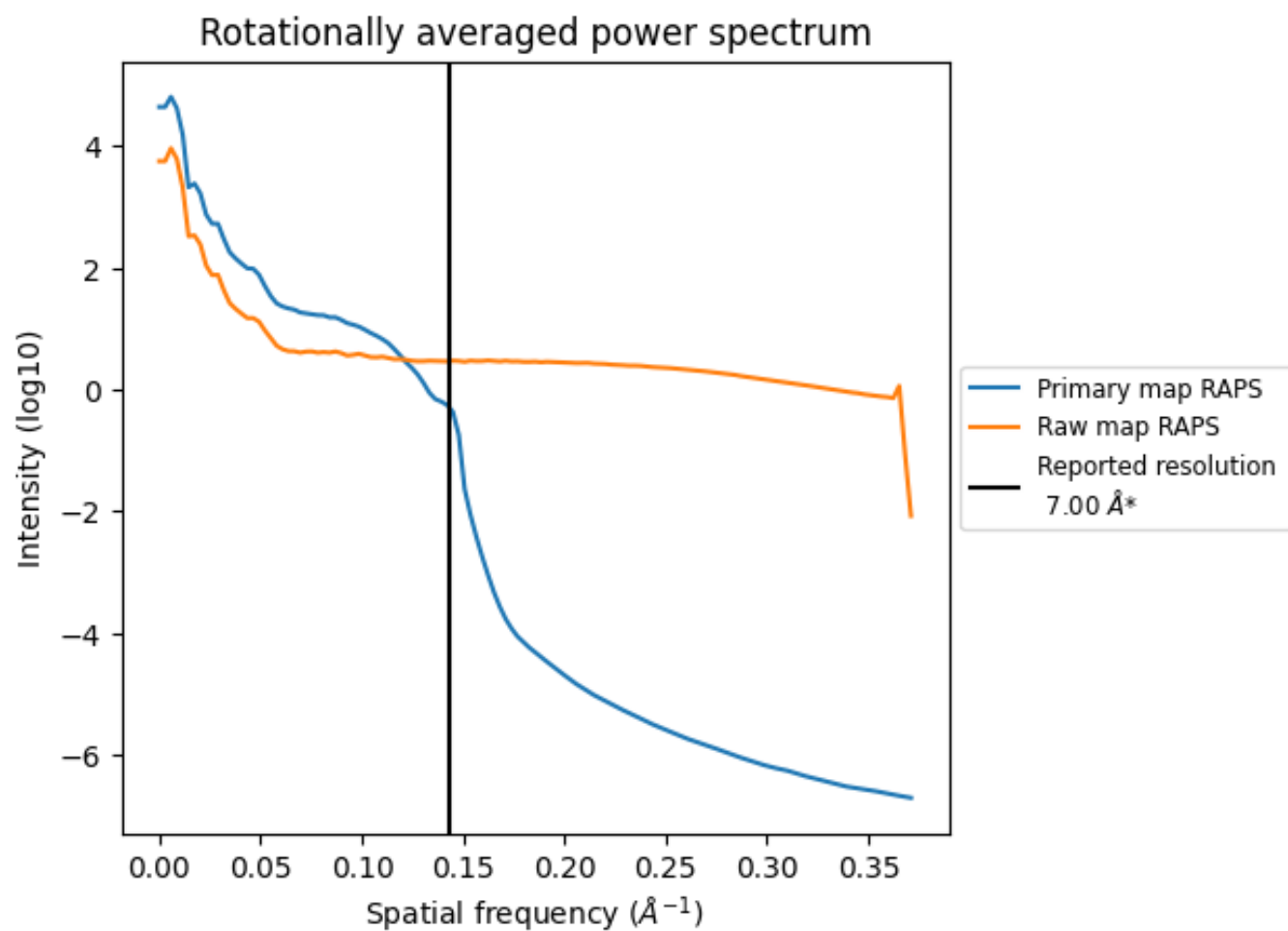
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 532 nm³; this corresponds to an approximate mass of 480 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 ⓘ

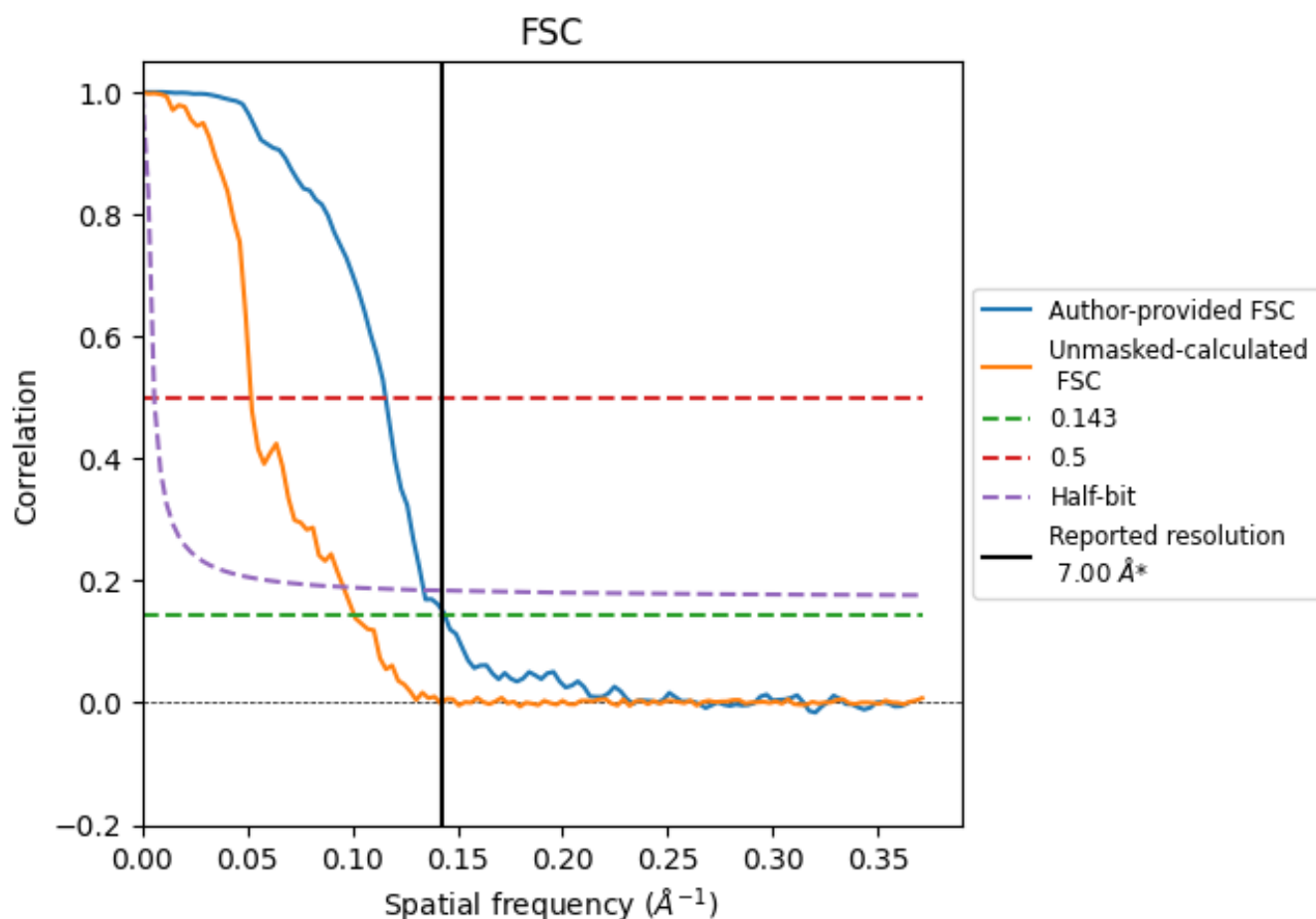


*Reported resolution corresponds to spatial frequency of 0.143 Å⁻¹

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 0.143 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

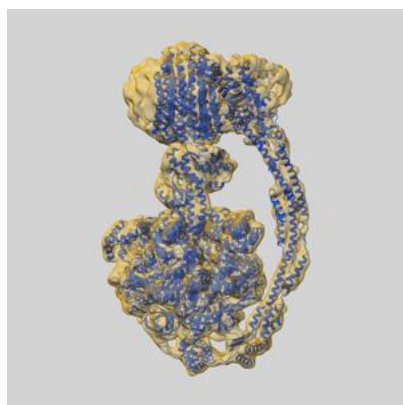
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.00	-	-
Author-provided FSC curve	6.94	8.64	7.46
Unmasked-calculated*	9.91	19.31	10.45

*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 9.91 differs from the reported value 7.0 by more than 10 %

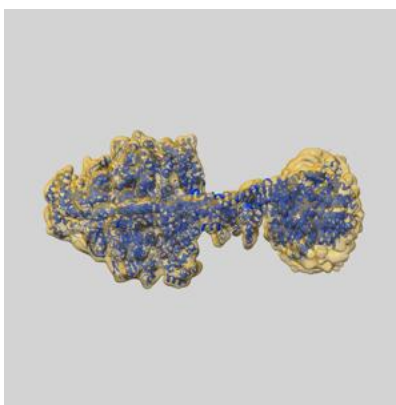
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25956 and PDB model 7TK4. Per-residue inclusion information can be found in section [3](#) on page [7](#).

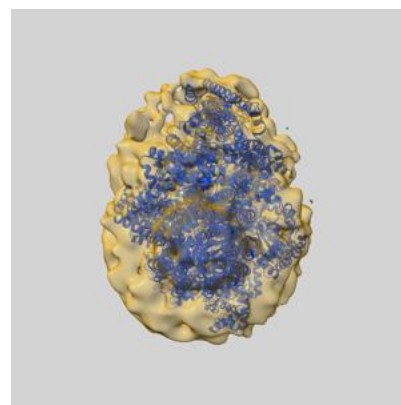
9.1 Map-model overlay [i](#)



X



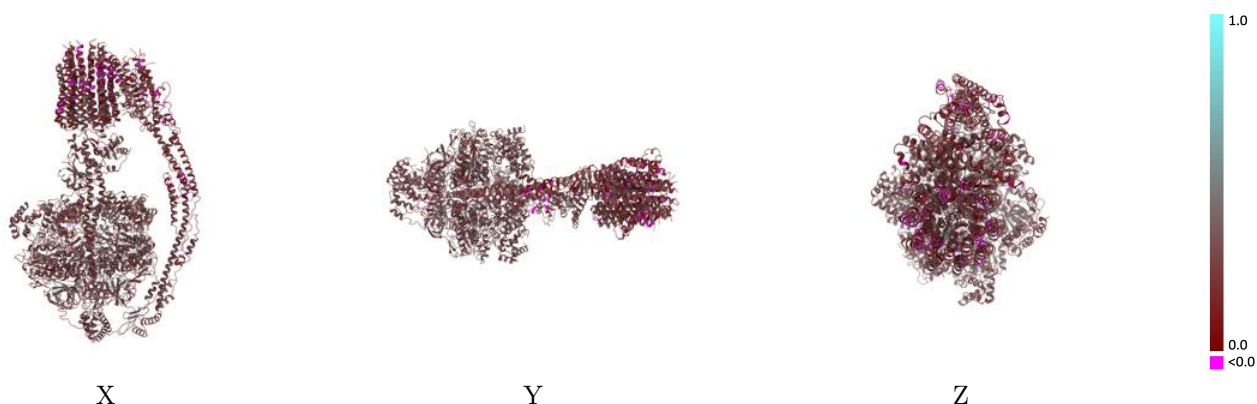
Y



Z

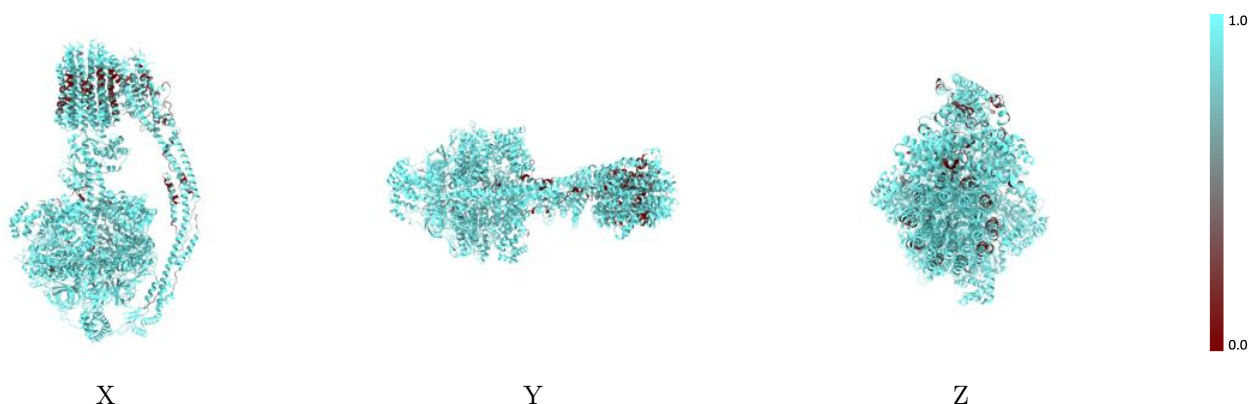
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



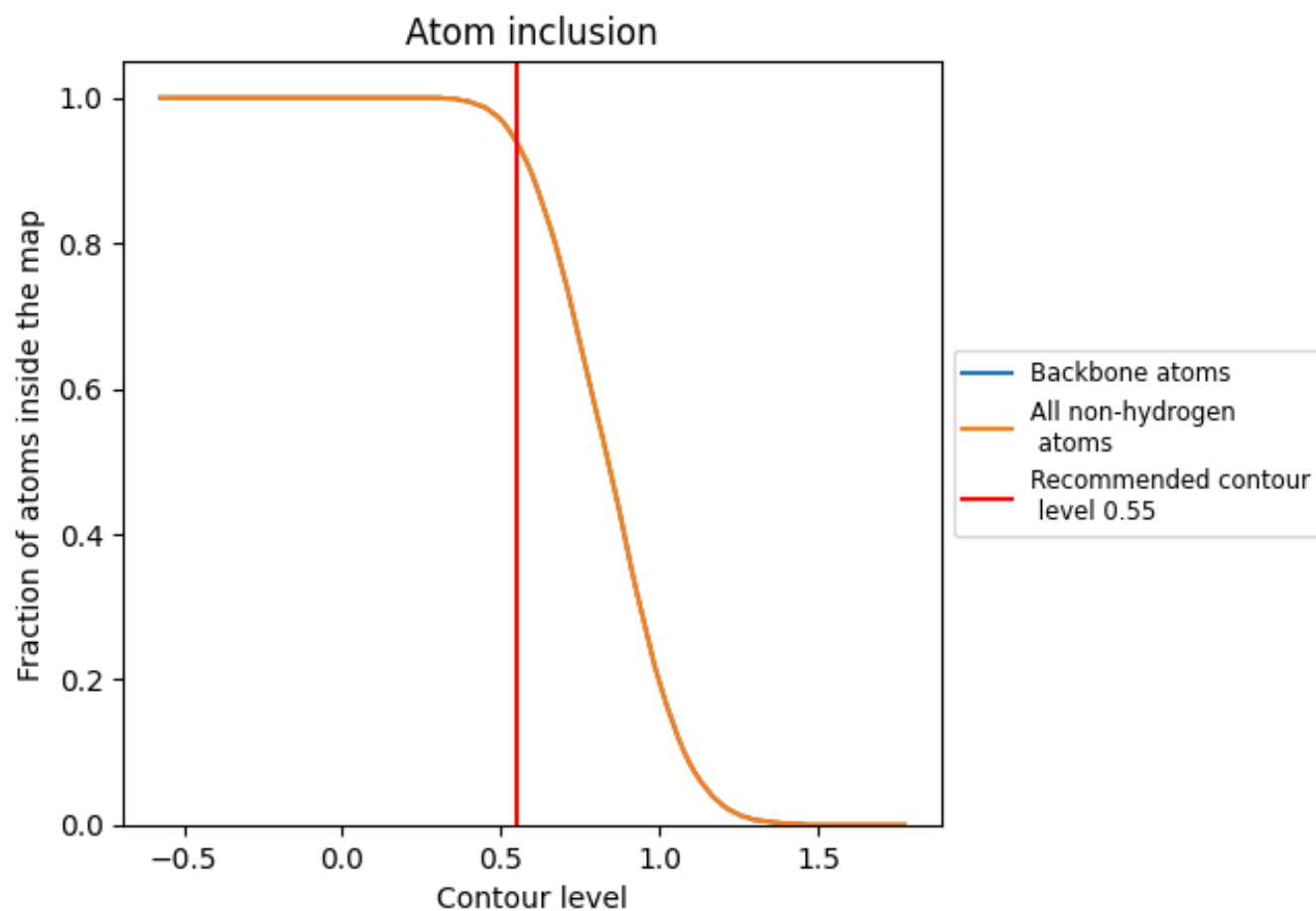
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.2700
0	 0.8070	 0.1910
1	 0.8200	 0.1760
2	 0.8670	 0.1740
3	 0.9460	 0.2320
4	 0.8670	 0.1850
5	 0.8330	 0.1870
6	 0.8480	 0.2000
7	 0.9040	 0.2110
8	 0.8370	 0.2040
9	 0.8550	 0.1860
A	 0.9730	 0.3020
B	 0.9800	 0.3010
C	 0.9900	 0.3030
D	 0.9800	 0.2910
E	 0.9740	 0.2940
F	 0.9880	 0.2990
G	 0.9720	 0.2840
H	 0.9880	 0.2570
I	 0.9740	 0.2990
O	 0.9880	 0.2990
T	 0.8570	 0.2340
U	 0.9530	 0.2600
V	 0.7880	 0.2110
W	 0.6970	 0.1700
X	 0.7500	 0.2230
Y	 0.8180	 0.1900
Z	 0.7720	 0.2160

