



wwPDB EM Validation Summary Report ⓘ

Jul 31, 2023 – 10:57 pm BST

PDB ID : 8OW1
EMDB ID : EMD-17227
Title : Cryo-EM structure of the yeast Inner kinetochore bound to a CENP-A nucleosome.
Authors : Dendooven, T.D.; Zhang, Z.; Yang, J.; McLaughlin, S.; Schwabb, J.; Scheres, S.; Yatskevich, S.; Barford, D.
Deposited on : 2023-04-26
Resolution : 3.70 Å(reported)

This is a wwPDB EM Validation Summary 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:

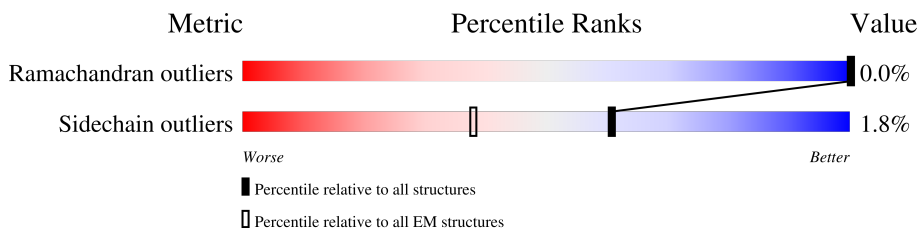
EMDB validation analysis : 0.0.1.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

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 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	351	31% 69%
1	B	351	32% 67%
2	I	733	89% 10%
2	II	733	96%
3	K	239	91% 8%
3	KK	239	10% 94% 5%
4	H	181	94% 6%
4	HH	181	97%
5	L	245	88% 10%



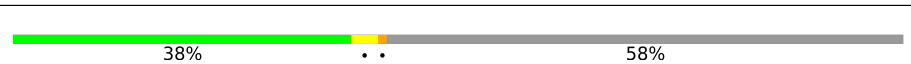



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Mol	Chain	Length	Quality of chain
5	LL	245	88% 10% ..
6	N	458	84% 16%
6	NN	458	84% 16%
7	CT	478	81% 18%
8	CE	608	5% 91% 8%
8	ce	608	86% 14%
9	SK	194	77% . 22%
10	P	369	69% 31%
10	PP	369	68% . 31%
11	Q	406	64% 36%
11	QQ	406	60% . 39%
12	O	368	67% 33%
12	OO	368	65% . 35%
13	T	361	25% 75%
13	TT	361	17% 25% 75%
14	U	324	56% . 43%
14	UU	324	55% 45%
15	W	89	78% 22%
15	WW	89	61% 78% 22%
16	Y	238	84% 9% . 6%
16	YY	238	84% 9% . 6%
17	Z	153	97% ..
17	ZZ	153	97% ..
18	D	153	. 99% .
19	E	153	. 99% .

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Mol	Chain	Length	Quality of chain
20	b	103	 77% 23%
20	f	103	 76% 23%
21	d	131	 72% 27%
21	h	131	 74% 26%
22	a	229	 38% 58%
22	e	229	 38% 58%
23	c	132	 73% 27%
23	g	132	 73% 26%

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 78671 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 Centromere-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	110	Total 898	C 554	N 162	O 179	S 3	0	0
1	B	116	Total 957	C 592	N 174	O 188	S 3	0	0

- Molecule 2 is a protein called Inner kinetochore subunit CTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	659	Total 5337	C 3459	N 890	O 958	S 30	0	0
2	II	704	Total 5705	C 3692	N 954	O 1028	S 31	0	0

- Molecule 3 is a protein called Inner kinetochore subunit MCM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	219	Total 1762	C 1113	N 304	O 340	S 5	0	0
3	KK	227	Total 1805	C 1143	N 307	O 349	S 6	0	0

- Molecule 4 is a protein called Inner kinetochore subunit MCM16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	171	Total 1412	C 890	N 247	O 273	S 2	0	0
4	HH	176	Total 1449	C 912	N 252	O 283	S 2	0	0

- Molecule 5 is a protein called Inner kinetochore subunit IML3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LL	241	Total	C	N	O	S	0	0
			1941	1244	320	366	11		
5	L	241	Total	C	N	O	S	0	0
			1941	1244	320	366	11		

- Molecule 6 is a protein called Inner kinetochore subunit CHL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	NN	385	Total	C	N	O	S	0	0
			3121	2021	530	557	13		
6	N	386	Total	C	N	O	S	0	0
			3129	2027	531	558	13		

- Molecule 7 is a protein called Centromere DNA-binding protein complex CBF3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CT	391	Total	C	N	O	S	0	0
			3298	2154	556	576	12		

- Molecule 8 is a protein called Centromere DNA-binding protein complex CBF3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	ce	524	Total	C	N	O	S	0	0
			4352	2834	700	797	21		
8	CE	557	Total	C	N	O	S	0	0
			4608	2980	758	841	29		

- Molecule 9 is a protein called Suppressor of kinetochore protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SK	151	Total	C	N	O	S	0	0
			1230	769	214	243	4		

- Molecule 10 is a protein called Inner kinetochore subunit CTF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	255	Total	C	N	O	S	0	0
			2098	1348	362	374	14		
10	PP	254	Total	C	N	O	S	0	0
			2094	1346	360	374	14		

- Molecule 11 is a protein called Inner kinetochore subunit OKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	261	Total	C	N	O	S	0	0
			2193	1384	388	412	9		
11	QQ	247	Total	C	N	O	S	0	0
			2060	1296	364	391	9		

- Molecule 12 is a protein called Inner kinetochore subunit MCM21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	OO	240	Total	C	N	O	S	0	0
			1967	1272	323	368	4		
12	O	245	Total	C	N	O	S	0	0
			2015	1302	333	375	5		

- Molecule 13 is a protein called Inner kinetochore subunit CNN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	92	Total	C	N	O	S	0	0
			761	488	125	144	4		
13	TT	92	Total	C	N	O	S	0	0
			761	488	125	144	4		

- Molecule 14 is a protein called Inner kinetochore subunit AME1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	184	Total	C	N	O	S	0	0
			1485	928	255	299	3		
14	UU	179	Total	C	N	O	S	0	0
			1445	904	249	289	3		

- Molecule 15 is a protein called Inner kinetochore subunit WIP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	69	Total	C	N	O	S	0	0
			551	348	96	105	2		
15	WW	69	Total	C	N	O	S	0	0
			550	348	96	104	2		

- Molecule 16 is a protein called Inner kinetochore subunit NKP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	223	Total	C	N	O	S	0	0
			1663	1027	281	349	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
16	YY	223	Total	C	N	O	S	0	0
			1663	1027	281	349	6		

- Molecule 17 is a protein called Inner kinetochore subunit NKP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	151	Total	C	N	O	S	0	0
			1180	740	204	235	1		
17	ZZ	151	Total	C	N	O	S	0	0
			1180	740	204	235	1		

- Molecule 18 is a DNA chain called C0N3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D	153	Total	C	N	O	P	0	0
			3139	1499	574	913	153		

- Molecule 19 is a DNA chain called C0N3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	E	153	Total	C	N	O	P	0	0
			3134	1499	559	923	153		

- Molecule 20 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	b	79	Total	C	N	O	0	0
			625	393	120	112		
20	f	79	Total	C	N	O	0	0
			627	395	120	112		

- Molecule 21 is a protein called Histone H2B.1.

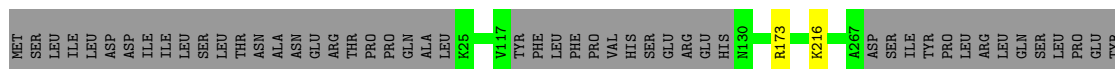
Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	95	Total	C	N	O	S	0	0
			735	461	129	144	1		
21	h	97	Total	C	N	O	S	0	0
			745	467	129	148	1		

- Molecule 22 is a protein called Histone H3-like centromeric protein CSE4.

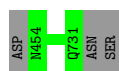
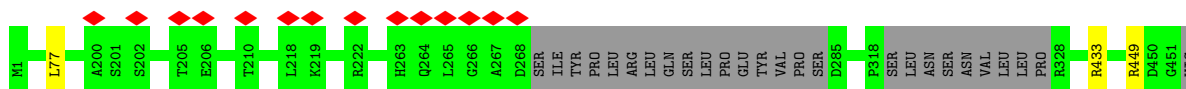
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	e	97	781	498	139	140	4	0	0
22	a	97	781	498	139	140	4	0	0

- Molecule 23 is a protein called Histone H2A.1.

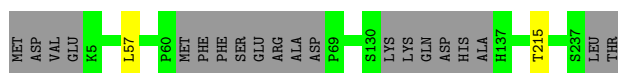
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	g	98	751	470	147	134	0	0
23	c	97	742	464	146	132	0	0



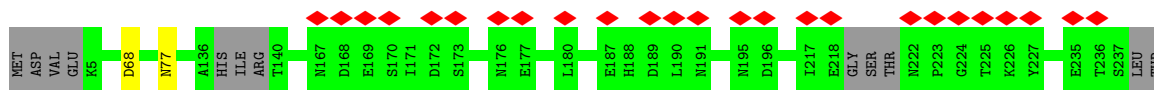
- Molecule 2: Inner kinetochore subunit CTF3



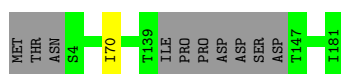
- Molecule 3: Inner kinetochore subunit MCM22



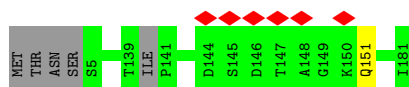
- Molecule 3: Inner kinetochore subunit MCM22



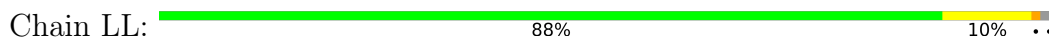
- Molecule 4: Inner kinetochore subunit MCM16



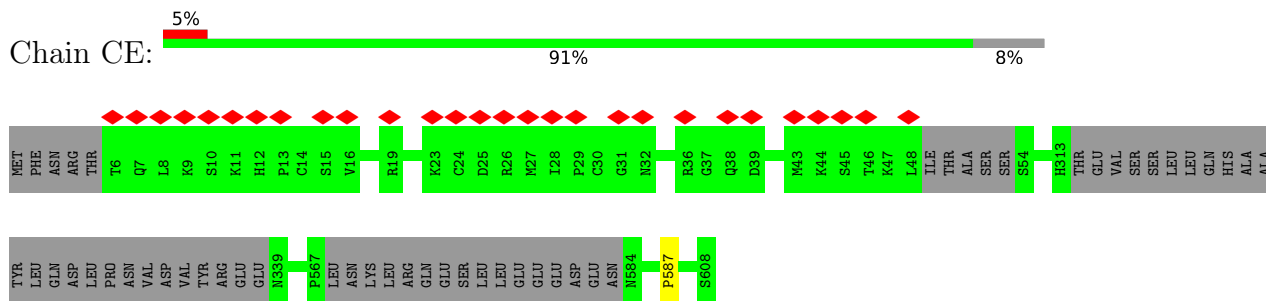
- Molecule 4: Inner kinetochore subunit MCM16



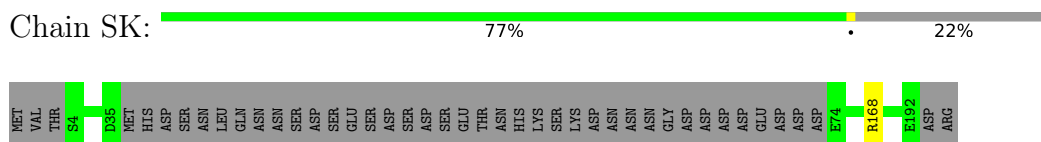
- Molecule 5: Inner kinetochore subunit IML3



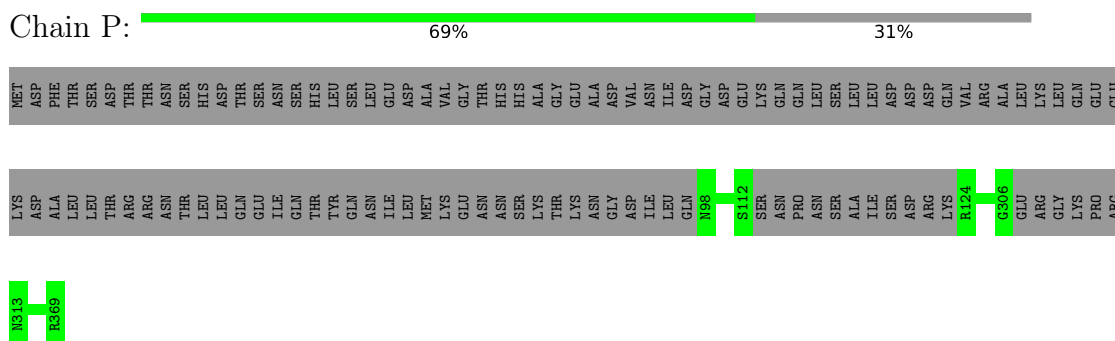
• Molecule 8: Centromere DNA-binding protein complex CBF3 subunit B



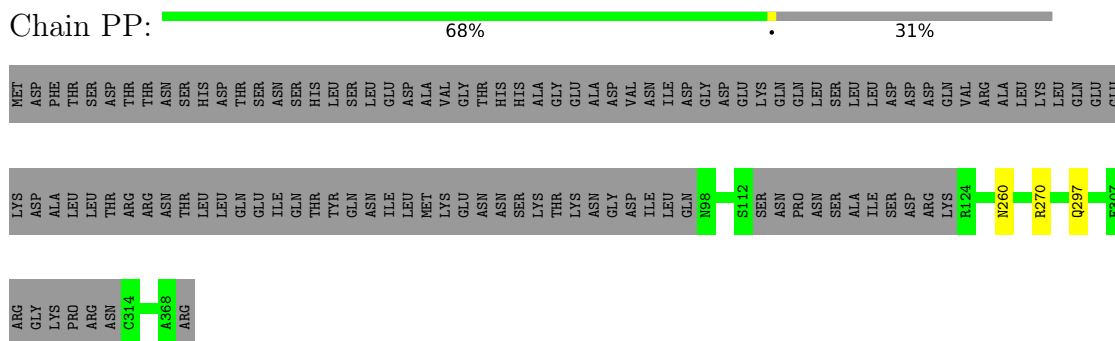
• Molecule 9: Suppressor of kinetochore protein 1



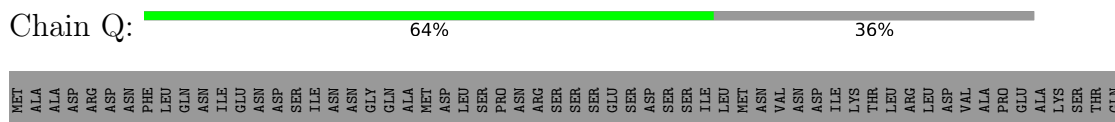
• Molecule 10: Inner kinetochore subunit CTF19

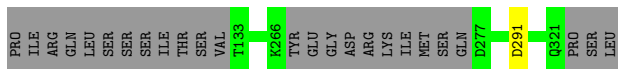


• Molecule 10: Inner kinetochore subunit CTF19

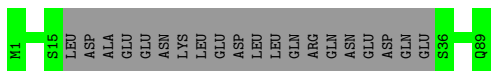
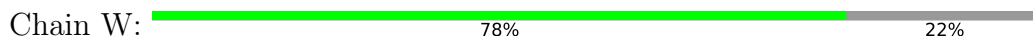


• Molecule 11: Inner kinetochore subunit OKP1

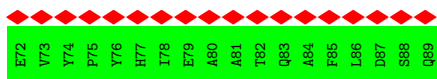
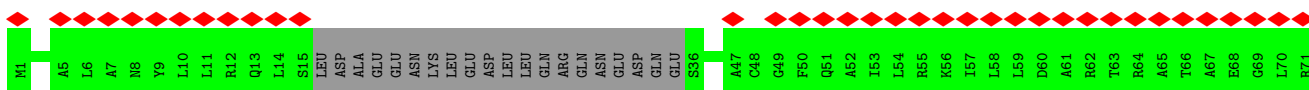
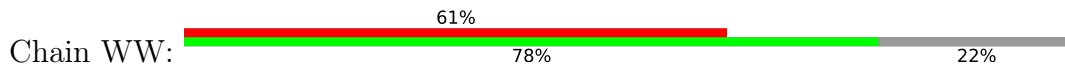




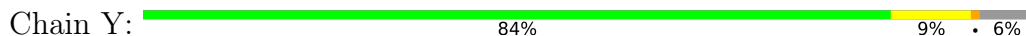
- Molecule 15: Inner kinetochore subunit WIP1



- Molecule 15: Inner kinetochore subunit WIP1



- Molecule 16: Inner kinetochore subunit NKP1



- Molecule 16: Inner kinetochore subunit NKP1



- Molecule 17: Inner kinetochore subunit NKP2



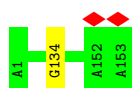
- Molecule 17: Inner kinetochore subunit NKP2

Chain ZZ:  97%



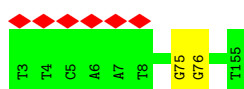
● Molecule 18: C0N3

Chain D:  99%




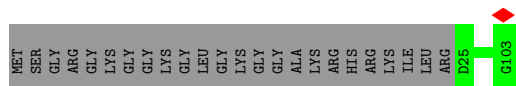
● Molecule 19: C0N3

Chain E:  99%



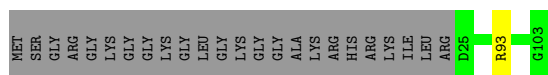
● Molecule 20: Histone H4

Chain b:  77% 23%



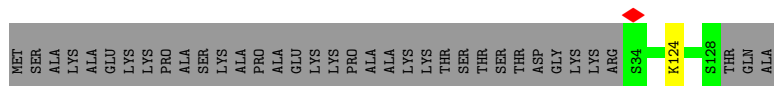
● Molecule 20: Histone H4

Chain f:  76% 23%



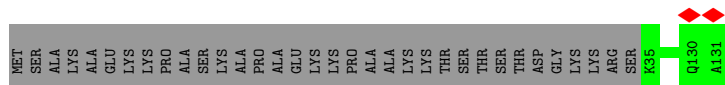
● Molecule 21: Histone H2B.1

Chain d:  72% 27%



● Molecule 21: Histone H2B.1

Chain h:  74% 26%



● Molecule 22: Histone H3-like centromeric protein CSE4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108672	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)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00271	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	A	0.25	0/905	0.39	0/1210
1	B	0.25	0/968	0.44	0/1296
2	I	0.25	0/5458	0.42	0/7402
2	II	0.24	0/5837	0.40	1/7921 (0.0%)
3	K	0.24	0/1784	0.44	1/2404 (0.0%)
3	KK	0.24	0/1828	0.42	0/2466
4	H	0.26	0/1429	0.48	0/1923
4	HH	0.24	0/1468	0.44	0/1979
5	L	0.27	0/1981	0.58	3/2684 (0.1%)
5	LL	0.27	0/1981	0.58	3/2684 (0.1%)
6	N	0.25	0/3201	0.42	0/4322
6	NN	0.24	0/3193	0.40	0/4311
7	CT	0.24	0/3369	0.41	0/4544
8	CE	0.24	0/4716	0.39	0/6375
8	ce	0.24	0/4458	0.37	0/6038
9	SK	0.23	0/1251	0.43	0/1692
10	P	0.25	0/2131	0.41	0/2866
10	PP	0.24	0/2127	0.42	0/2860
11	Q	0.27	0/2228	0.42	0/2983
11	QQ	0.24	0/2087	0.40	0/2791
12	O	0.25	0/2054	0.41	0/2761
12	OO	0.25	0/2004	0.41	0/2695
13	T	0.24	0/772	0.39	0/1040
13	TT	0.49	1/772 (0.1%)	0.72	3/1040 (0.3%)
14	U	0.25	0/1499	0.48	1/2018 (0.0%)
14	UU	0.23	0/1458	0.45	1/1963 (0.1%)
15	W	0.24	0/557	0.38	0/748
15	WW	0.23	0/556	0.35	0/748
16	Y	0.31	0/1672	0.63	3/2252 (0.1%)
16	YY	0.31	0/1672	0.63	3/2252 (0.1%)
17	Z	0.26	0/1195	0.53	1/1616 (0.1%)
17	ZZ	0.24	0/1195	0.41	1/1616 (0.1%)
18	D	0.50	1/3523 (0.0%)	0.93	0/5435
19	E	0.51	2/3513 (0.1%)	0.93	0/5420

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	b	0.28	0/632	0.46	0/845
20	f	0.25	0/634	0.44	0/848
21	d	0.26	0/745	0.44	0/1003
21	h	0.24	0/755	0.42	0/1017
22	a	0.32	0/792	0.90	10/1066 (0.9%)
22	e	0.32	0/792	0.90	10/1066 (0.9%)
23	c	0.25	0/751	0.46	0/1015
23	g	0.25	0/760	0.41	0/1027
All	All	0.29	4/80703 (0.0%)	0.52	41/110242 (0.0%)

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
2	I	0	4
3	K	0	1
3	KK	0	1
4	H	0	1
7	CT	0	2
11	Q	0	1
16	Y	0	1
16	YY	0	1
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	TT	272	PRO	CG-CD	-11.67	1.12	1.50
19	E	75	DG	C1'-N9	-5.57	1.39	1.47
19	E	76	DG	C1'-N9	-5.55	1.39	1.47
18	D	134	DG	C1'-N9	-5.24	1.40	1.47

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	TT	272	PRO	N-CD-CG	-14.38	81.62	103.20
13	TT	272	PRO	CA-N-CD	-9.20	98.62	111.50
22	e	225	ARG	NE-CZ-NH1	9.09	124.84	120.30
22	e	225	ARG	CG-CD-NE	9.01	130.71	111.80
22	a	225	ARG	CG-CD-NE	9.01	130.71	111.80

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	425	LYS	Mainchain
2	I	456	CYS	Peptide
2	I	534	TYR	Peptide
2	I	612	LYS	Peptide
3	K	215	THR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	A	108/351 (31%)	108 (100%)	0	0	100	100
1	B	114/351 (32%)	113 (99%)	1 (1%)	0	100	100
2	I	649/733 (88%)	624 (96%)	25 (4%)	0	100	100
2	II	696/733 (95%)	676 (97%)	20 (3%)	0	100	100
3	K	213/239 (89%)	207 (97%)	6 (3%)	0	100	100
3	KK	221/239 (92%)	209 (95%)	12 (5%)	0	100	100
4	H	167/181 (92%)	159 (95%)	8 (5%)	0	100	100
4	HH	172/181 (95%)	168 (98%)	4 (2%)	0	100	100
5	L	239/245 (98%)	228 (95%)	11 (5%)	0	100	100
5	LL	239/245 (98%)	228 (95%)	11 (5%)	0	100	100
6	N	378/458 (82%)	365 (97%)	13 (3%)	0	100	100
6	NN	377/458 (82%)	369 (98%)	8 (2%)	0	100	100
7	CT	383/478 (80%)	362 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CE	549/608 (90%)	532 (97%)	16 (3%)	1 (0%)	47	78
8	ce	518/608 (85%)	506 (98%)	12 (2%)	0	100	100
9	SK	147/194 (76%)	142 (97%)	5 (3%)	0	100	100
10	P	249/369 (68%)	246 (99%)	3 (1%)	0	100	100
10	PP	248/369 (67%)	241 (97%)	7 (3%)	0	100	100
11	Q	257/406 (63%)	253 (98%)	4 (2%)	0	100	100
11	QQ	241/406 (59%)	233 (97%)	8 (3%)	0	100	100
12	O	241/368 (66%)	230 (95%)	11 (5%)	0	100	100
12	OO	236/368 (64%)	228 (97%)	8 (3%)	0	100	100
13	T	90/361 (25%)	87 (97%)	3 (3%)	0	100	100
13	TT	90/361 (25%)	87 (97%)	3 (3%)	0	100	100
14	U	180/324 (56%)	177 (98%)	3 (2%)	0	100	100
14	UU	175/324 (54%)	172 (98%)	3 (2%)	0	100	100
15	W	65/89 (73%)	65 (100%)	0	0	100	100
15	WW	65/89 (73%)	65 (100%)	0	0	100	100
16	Y	217/238 (91%)	208 (96%)	9 (4%)	0	100	100
16	YY	217/238 (91%)	208 (96%)	9 (4%)	0	100	100
17	Z	149/153 (97%)	146 (98%)	3 (2%)	0	100	100
17	ZZ	149/153 (97%)	148 (99%)	1 (1%)	0	100	100
20	b	77/103 (75%)	74 (96%)	3 (4%)	0	100	100
20	f	77/103 (75%)	73 (95%)	4 (5%)	0	100	100
21	d	93/131 (71%)	90 (97%)	3 (3%)	0	100	100
21	h	95/131 (72%)	93 (98%)	2 (2%)	0	100	100
22	a	95/229 (42%)	94 (99%)	1 (1%)	0	100	100
22	e	95/229 (42%)	94 (99%)	1 (1%)	0	100	100
23	c	95/132 (72%)	92 (97%)	3 (3%)	0	100	100
23	g	96/132 (73%)	96 (100%)	0	0	100	100
All	All	8762/12108 (72%)	8496 (97%)	265 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	CE	587	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/305 (32%)	97 (100%)	0	100	100
1	B	103/305 (34%)	101 (98%)	2 (2%)	57	76
2	I	612/683 (90%)	607 (99%)	5 (1%)	81	89
2	II	654/683 (96%)	652 (100%)	2 (0%)	92	96
3	K	202/223 (91%)	202 (100%)	0	100	100
3	KK	202/223 (91%)	201 (100%)	1 (0%)	88	94
4	H	162/172 (94%)	162 (100%)	0	100	100
4	HH	167/172 (97%)	166 (99%)	1 (1%)	86	93
5	L	217/221 (98%)	191 (88%)	26 (12%)	5	25
5	LL	217/221 (98%)	191 (88%)	26 (12%)	5	25
6	N	350/416 (84%)	350 (100%)	0	100	100
6	NN	349/416 (84%)	348 (100%)	1 (0%)	92	96
7	CT	368/449 (82%)	368 (100%)	0	100	100
8	CE	521/569 (92%)	521 (100%)	0	100	100
8	ce	488/569 (86%)	488 (100%)	0	100	100
9	SK	137/179 (76%)	136 (99%)	1 (1%)	84	91
10	P	240/344 (70%)	240 (100%)	0	100	100
10	PP	240/344 (70%)	237 (99%)	3 (1%)	69	83
11	Q	250/378 (66%)	249 (100%)	1 (0%)	91	95
11	QQ	234/378 (62%)	231 (99%)	3 (1%)	69	83
12	O	230/347 (66%)	230 (100%)	0	100	100
12	OO	225/347 (65%)	223 (99%)	2 (1%)	78	88
13	T	89/339 (26%)	89 (100%)	0	100	100
13	TT	89/339 (26%)	89 (100%)	0	100	100
14	U	168/308 (54%)	166 (99%)	2 (1%)	71	84
14	UU	164/308 (53%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	W	57/76 (75%)	57 (100%)	0	100	100
15	WW	57/76 (75%)	57 (100%)	0	100	100
16	Y	175/219 (80%)	154 (88%)	21 (12%)	5	25
16	YY	175/219 (80%)	154 (88%)	21 (12%)	5	25
17	Z	121/143 (85%)	120 (99%)	1 (1%)	81	89
17	ZZ	121/143 (85%)	120 (99%)	1 (1%)	81	89
20	b	65/81 (80%)	65 (100%)	0	100	100
20	f	66/81 (82%)	65 (98%)	1 (2%)	65	81
21	d	81/109 (74%)	80 (99%)	1 (1%)	71	84
21	h	81/109 (74%)	81 (100%)	0	100	100
22	a	82/207 (40%)	71 (87%)	11 (13%)	4	21
22	e	82/207 (40%)	71 (87%)	11 (13%)	4	21
23	c	75/99 (76%)	74 (99%)	1 (1%)	69	83
23	g	77/99 (78%)	76 (99%)	1 (1%)	69	83
All	All	8090/11106 (73%)	7944 (98%)	146 (2%)	61	77

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	KK	77	ASN
22	a	209	LYS
11	QQ	365	LYS
22	e	222	ARG
5	L	115	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
11	QQ	187	GLN
21	h	51	GLN
15	W	51	GLN
16	Y	79	GLN
17	Z	8	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

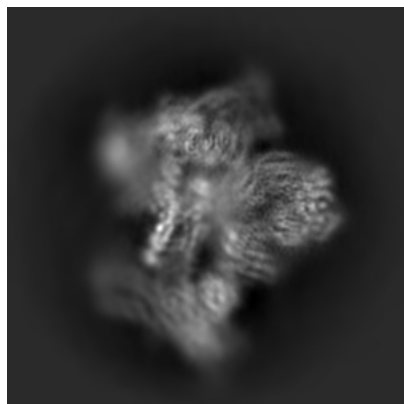
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17227. These allow visual inspection of the internal detail of the map and identification of artifacts.

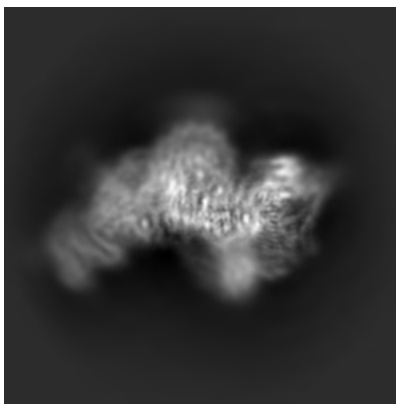
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

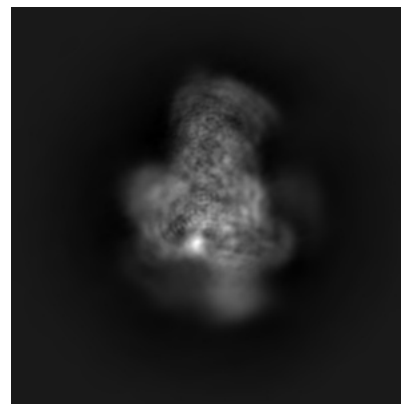
6.1.1 Primary map



X

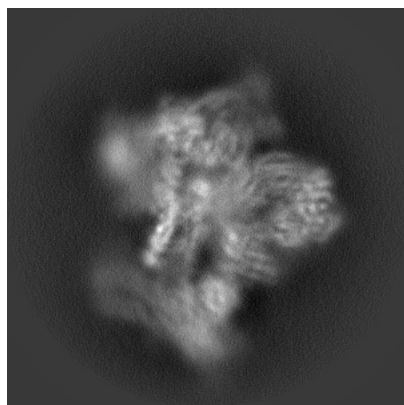


Y

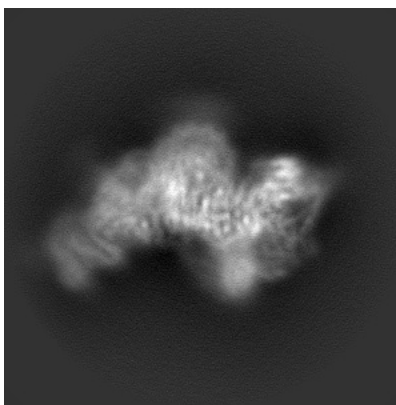


Z

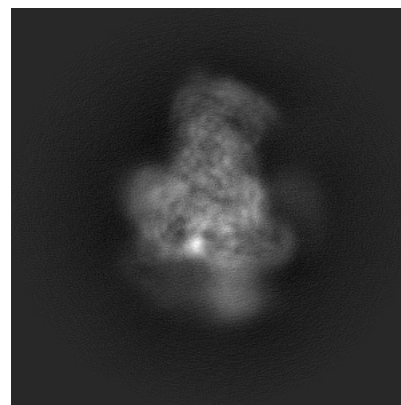
6.1.2 Raw map



X



Y

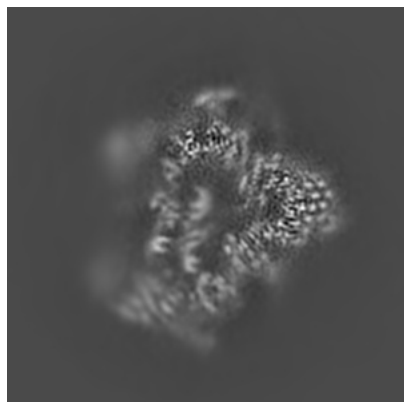


Z

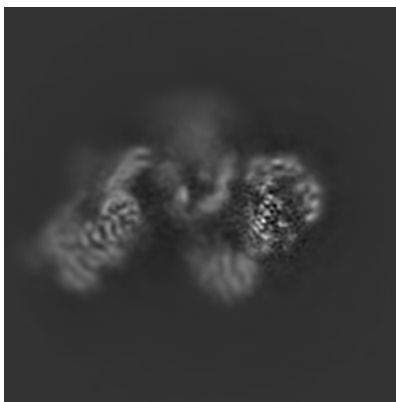
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

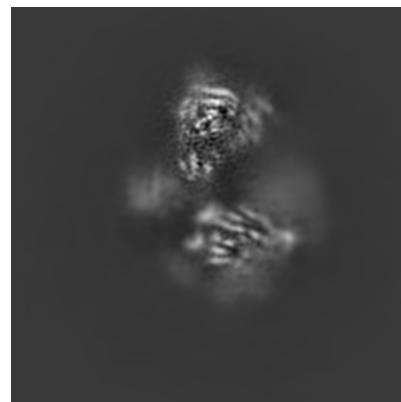
6.2.1 Primary map



X Index: 176

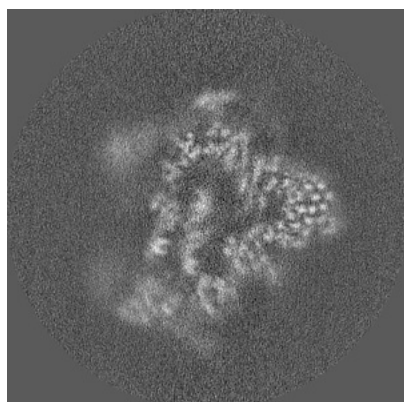


Y Index: 176

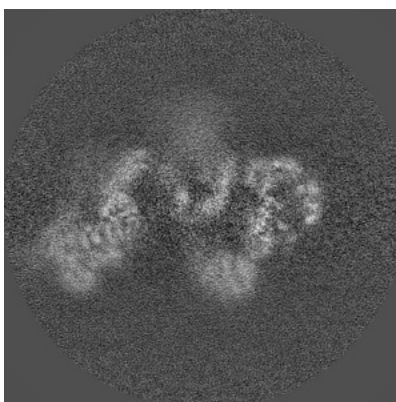


Z Index: 176

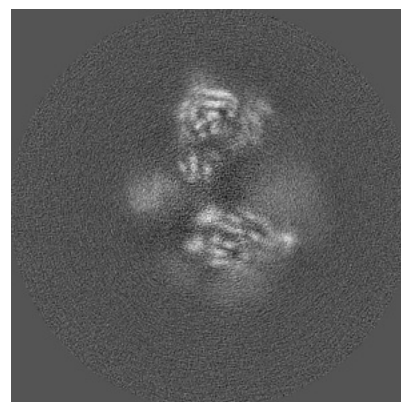
6.2.2 Raw map



X Index: 176



Y Index: 176

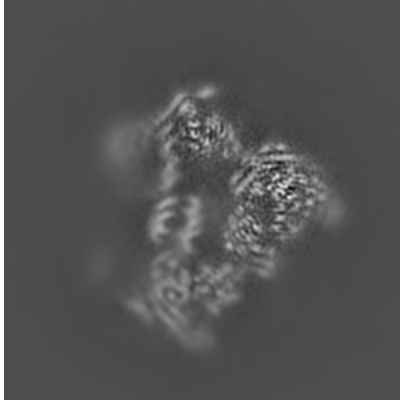


Z Index: 176

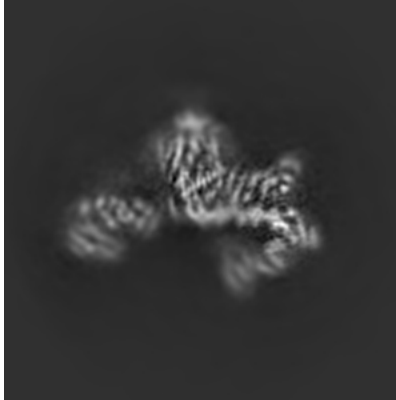
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

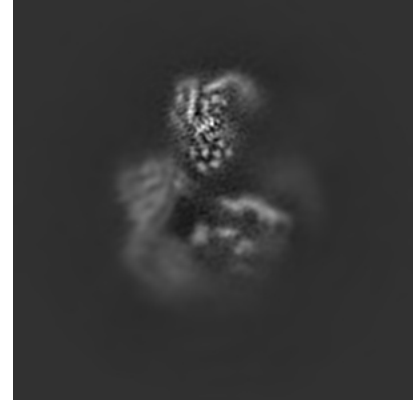
6.3.1 Primary map



X Index: 167

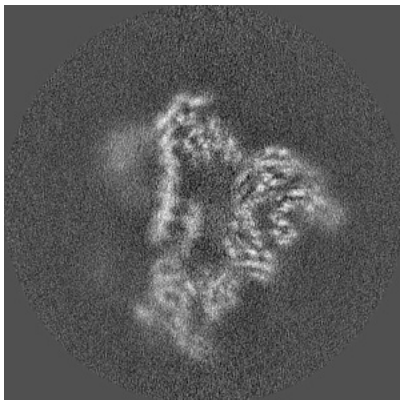


Y Index: 143

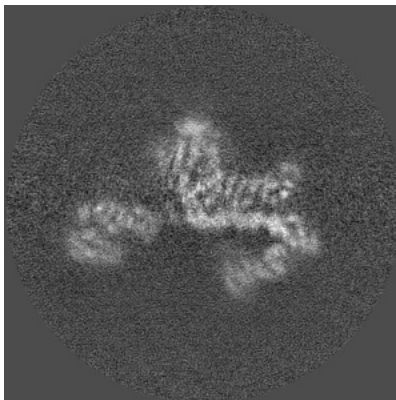


Z Index: 196

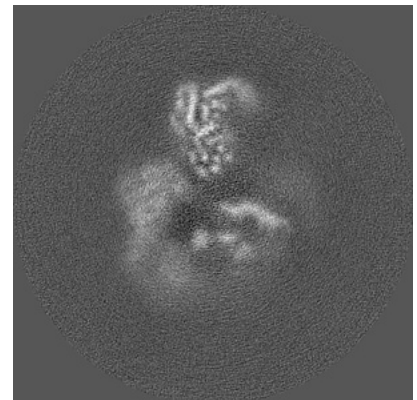
6.3.2 Raw map



X Index: 163



Y Index: 144

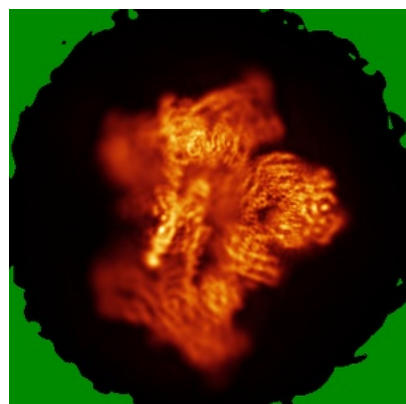


Z Index: 196

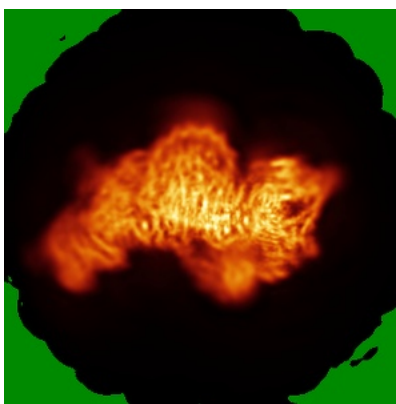
The images above show the largest variance slices of the map in three orthogonal directions.

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

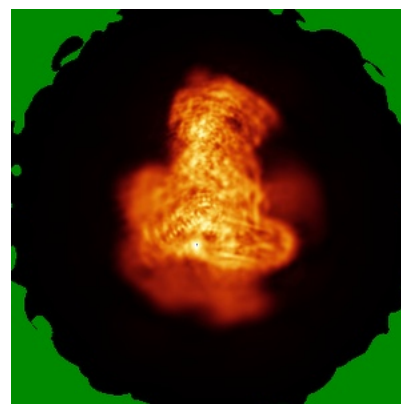
6.4.1 Primary map



X

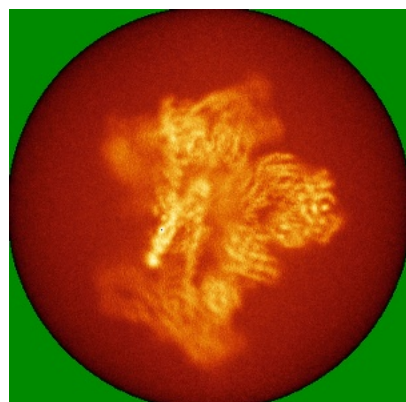


Y

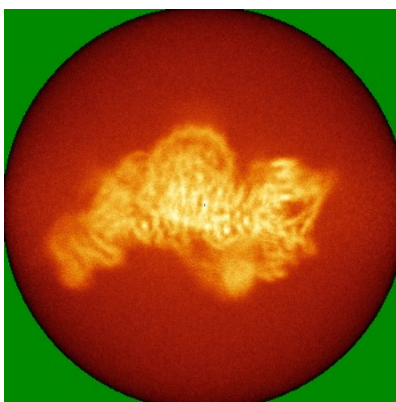


Z

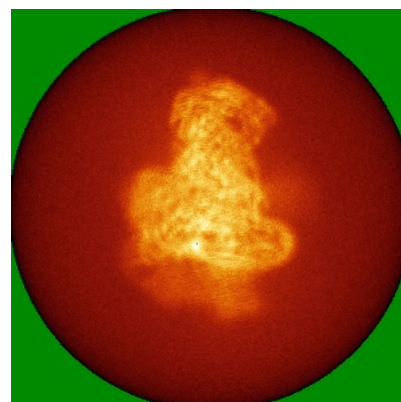
6.4.2 Raw map



X



Y

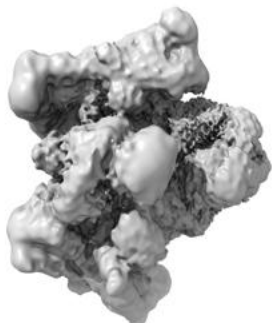


Z

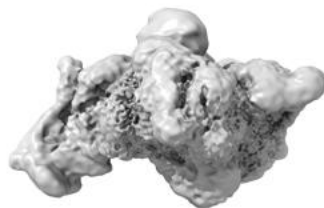
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



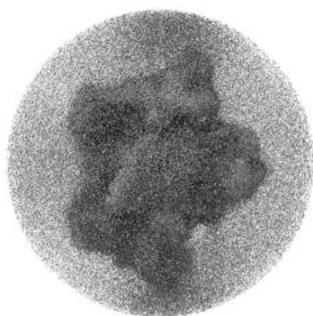
Y



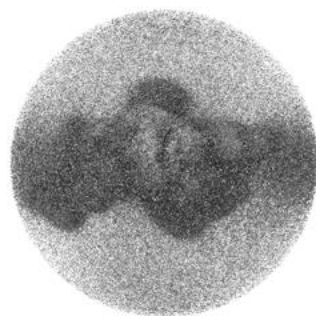
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00271. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

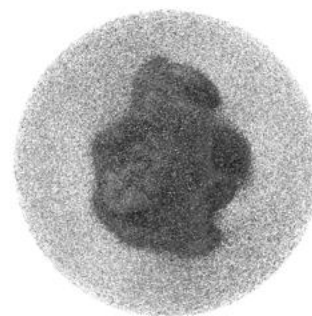
6.5.2 Raw map



X



Y



Z

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.

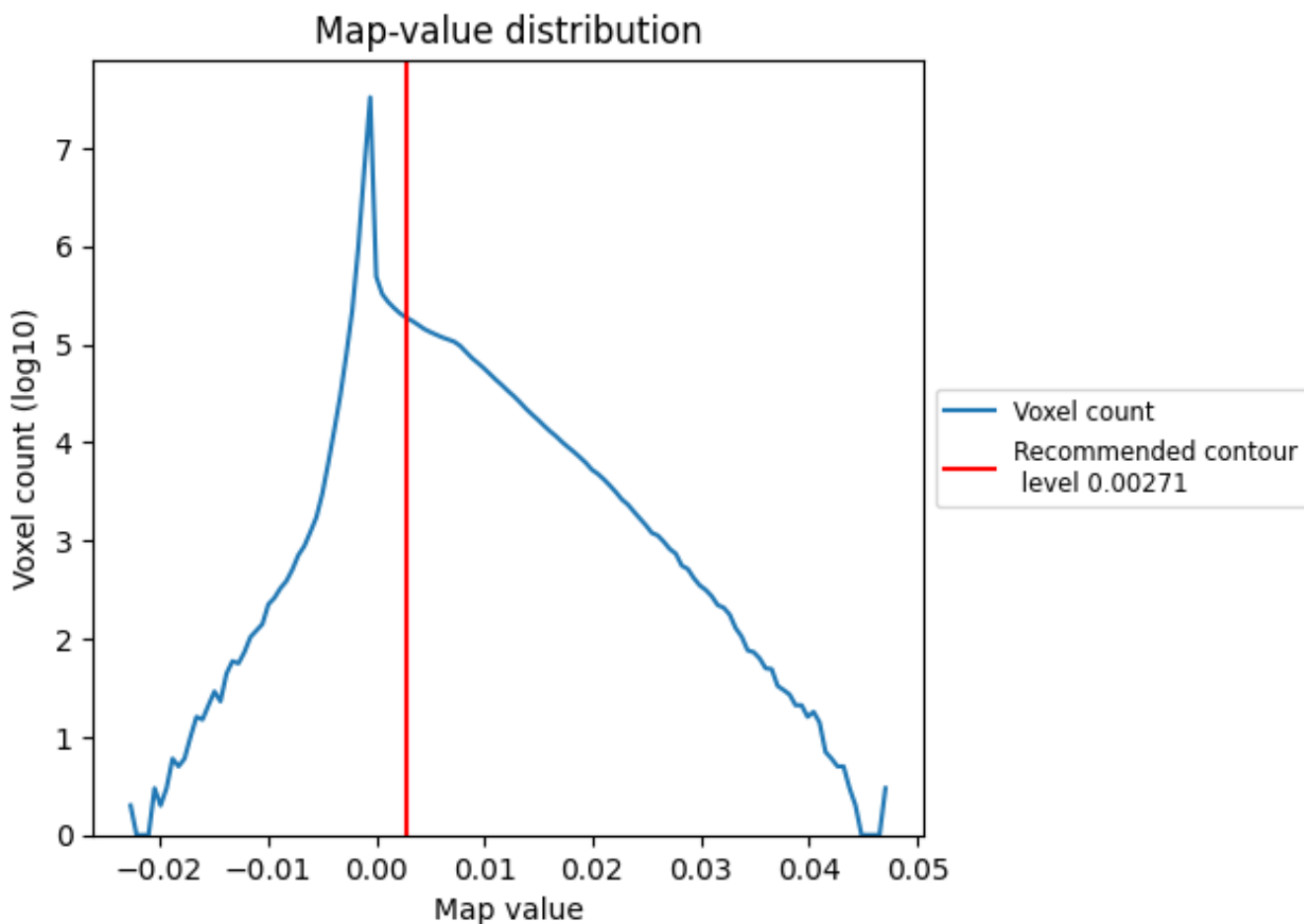
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

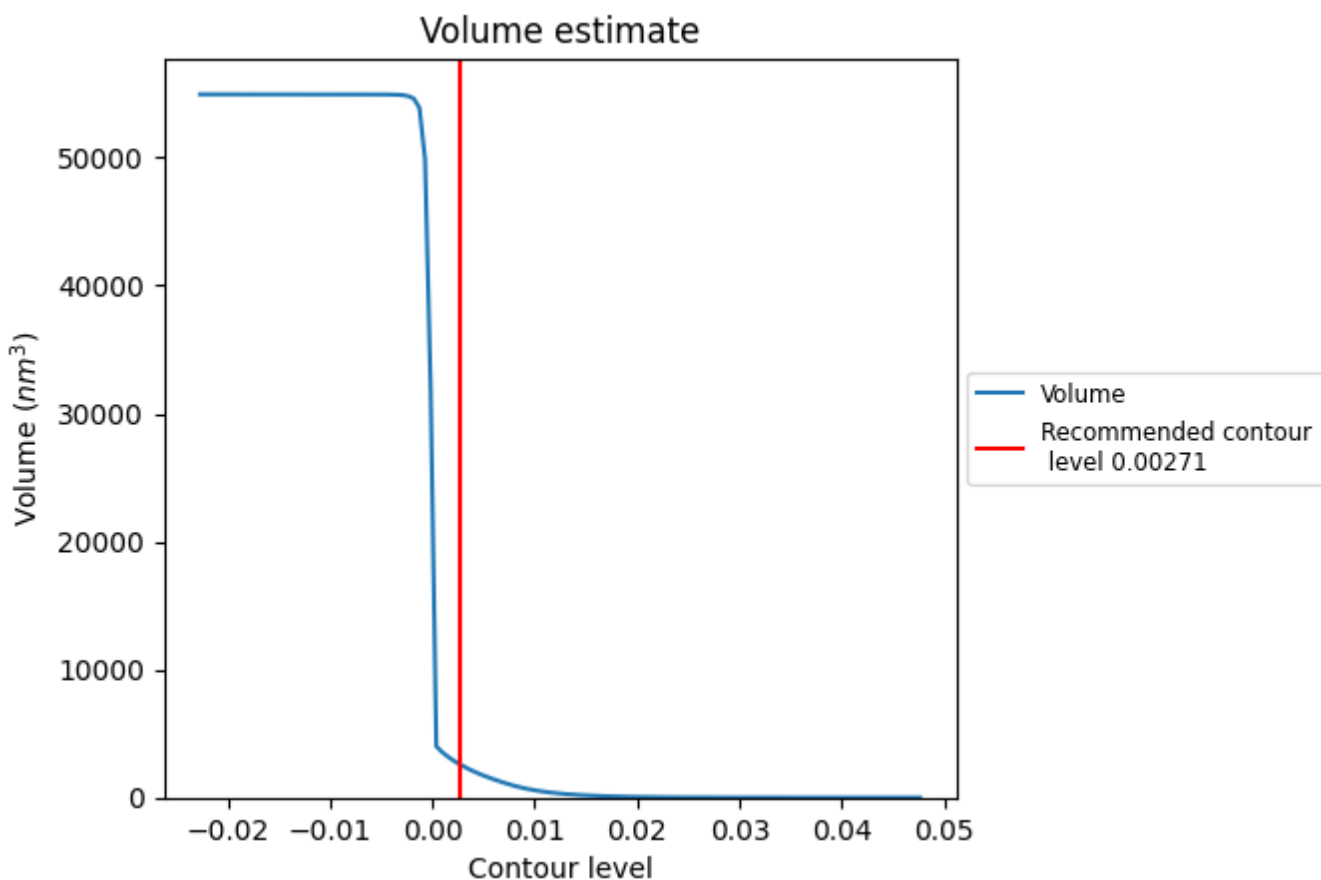
This section contains the results of statistical analysis of the map.

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.

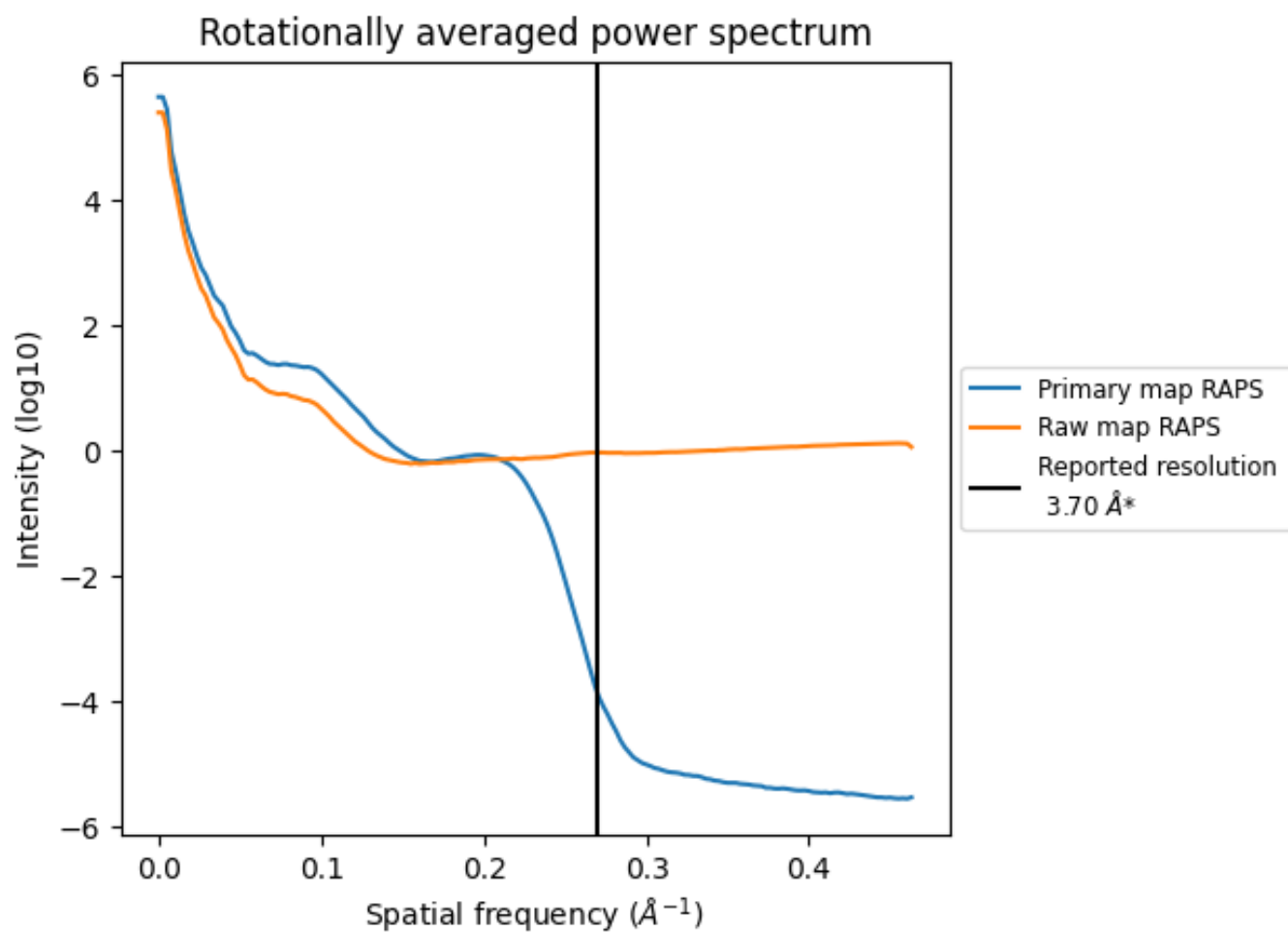
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2581 nm³; this corresponds to an approximate mass of 2331 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

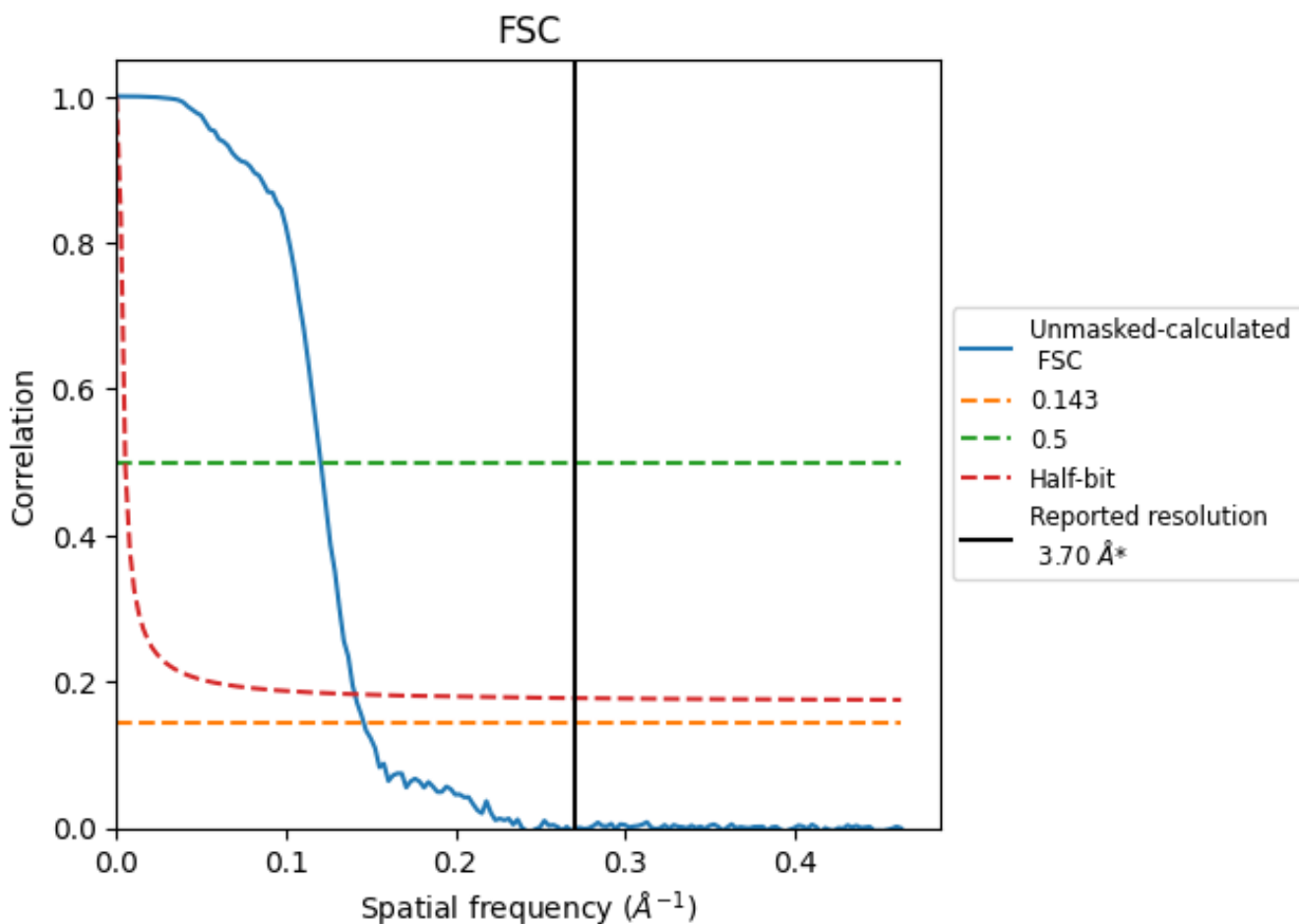


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

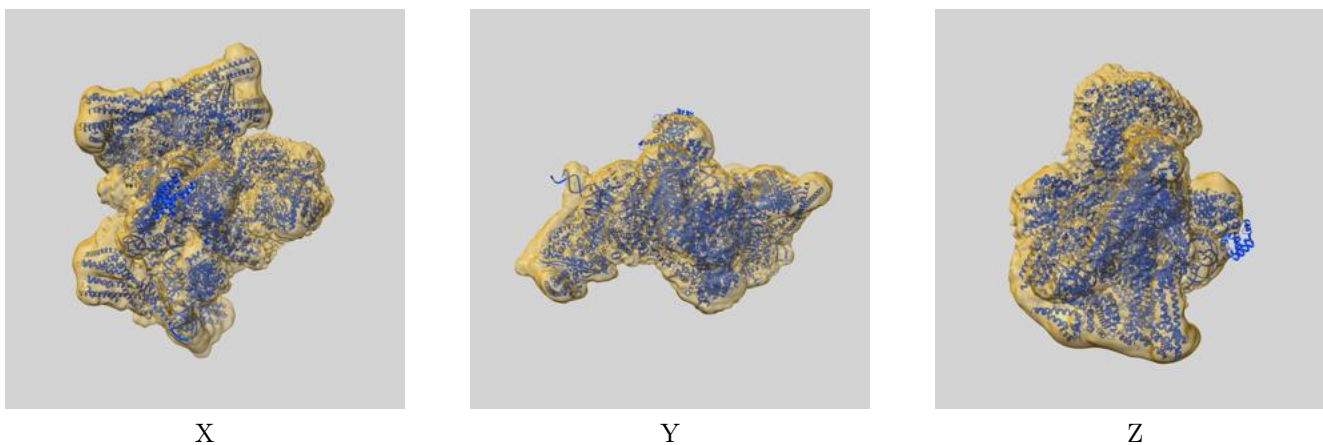
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.85	8.29	7.11

*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 6.85 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

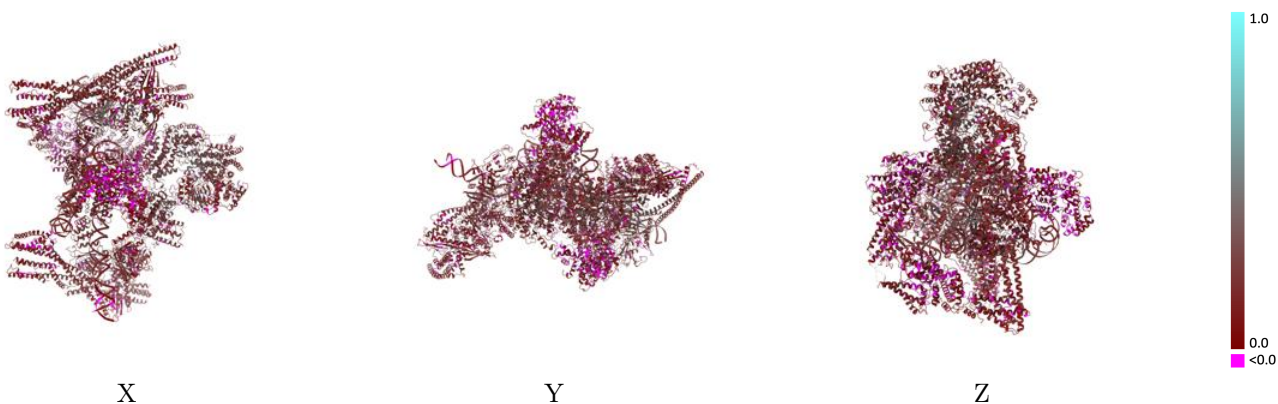
This section contains information regarding the fit between EMDB map EMD-17227 and PDB model 8OW1. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



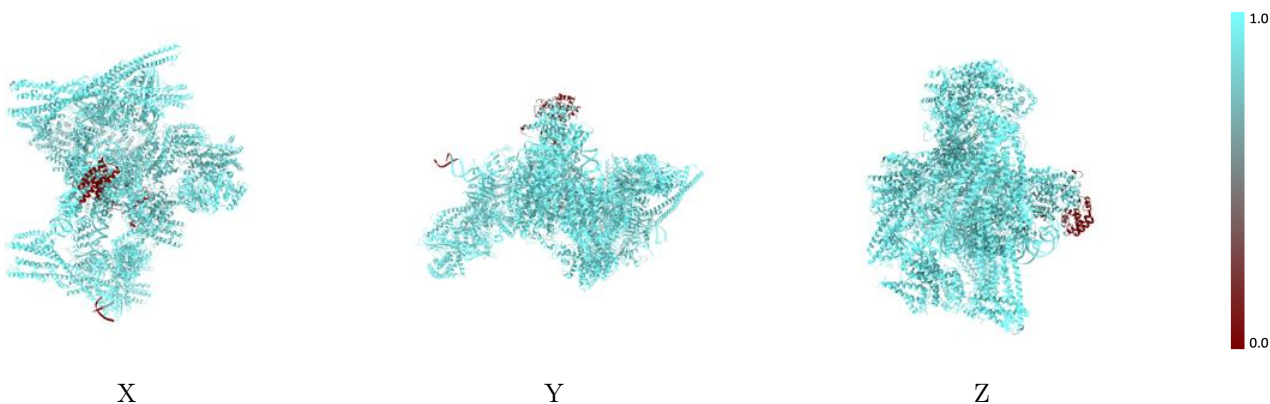
The images above show the 3D surface view of the map at the recommended contour level 0.00271 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



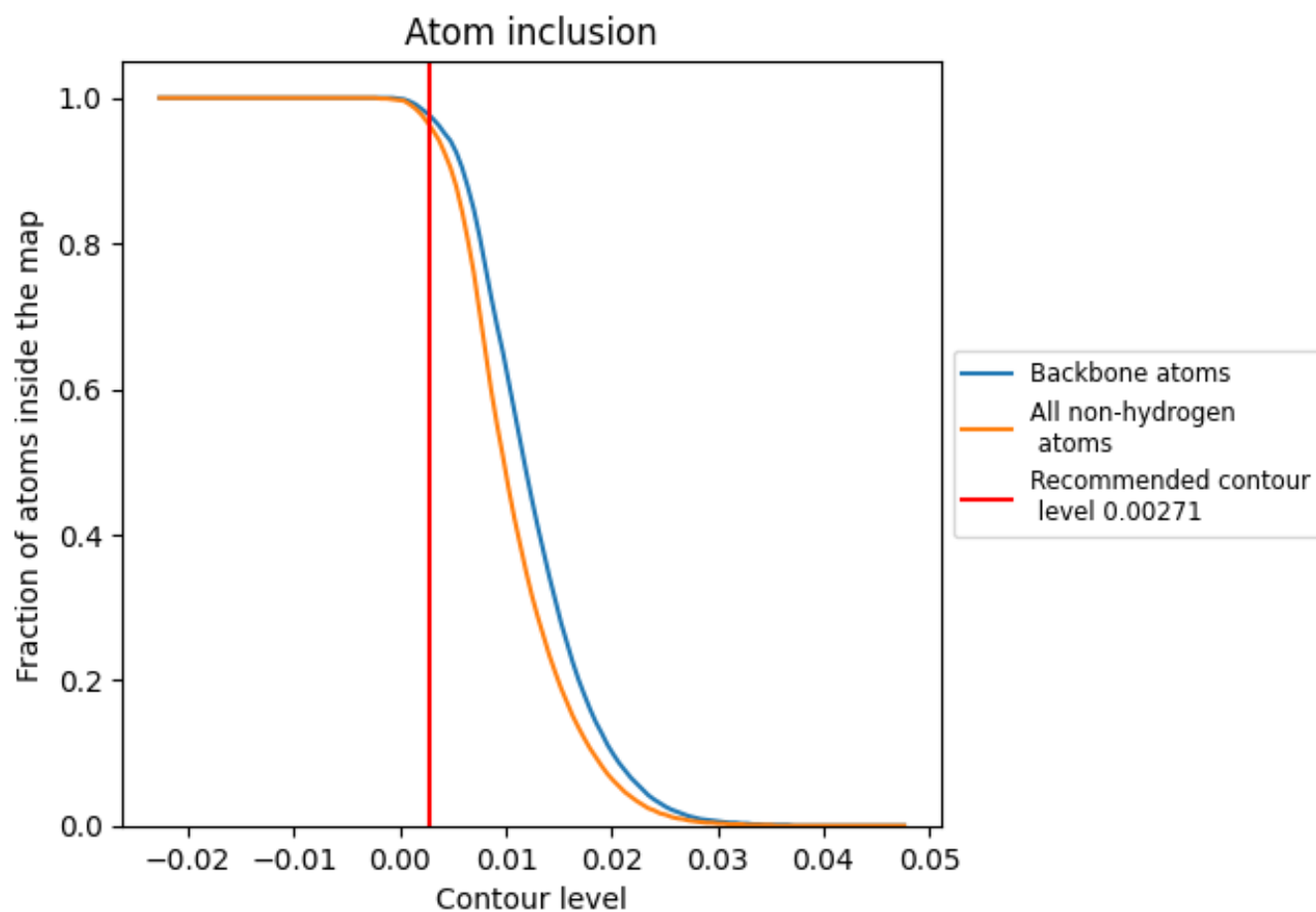
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00271).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.00271) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.1650
A	 0.9900	 0.1660
B	 0.9880	 0.2000
CE	 0.9230	 0.2300
CT	 0.9840	 0.2070
D	 0.9780	 0.1910
E	 0.9630	 0.1940
H	 0.9990	 0.0860
HH	 0.9440	 0.1480
I	 0.9990	 0.0650
II	 0.9650	 0.1480
K	 0.9970	 0.0900
KK	 0.8670	 0.1080
L	 0.9850	 0.1950
LL	 0.9900	 0.1570
N	 0.9600	 0.2510
NN	 0.9910	 0.1860
O	 0.9690	 0.2320
OO	 0.9840	 0.1560
P	 0.9880	 0.1810
PP	 0.9960	 0.1480
Q	 0.9960	 0.1390
QQ	 1.0000	 0.1290
SK	 0.9930	 0.1920
T	 0.9970	 0.0560
TT	 0.3070	 -0.0000
U	 0.9970	 0.1460
UU	 0.9980	 0.1240
W	 1.0000	 0.0940
WW	 0.2070	 0.0250
Y	 0.9950	 0.1540
YY	 0.9950	 0.1510
Z	 0.9830	 0.1560
ZZ	 0.9970	 0.1470
a	 0.9750	 0.1650



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Chain	Atom inclusion	Q-score
b	 0.9670	 0.2090
c	 0.9610	 0.2250
ce	 0.9750	 0.2360
d	 0.9570	 0.2170
e	 0.9650	 0.1700
f	 0.9670	 0.1920
g	 0.9780	 0.1810
h	 0.9600	 0.1950