



## wwPDB EM Validation Summary Report ⓘ

Jan 15, 2023 – 10:18 PM JST

PDB ID : 7XHN  
EMDB ID : EMD-33196  
Title : Structure of human inner kinetochore CCAN-DNA complex  
Authors : Sun, L.F.; Tian, T.; Wang, C.L.; Yang, Z.S.; Zang, J.Y.  
Deposited on : 2022-04-09  
Resolution : 3.71 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

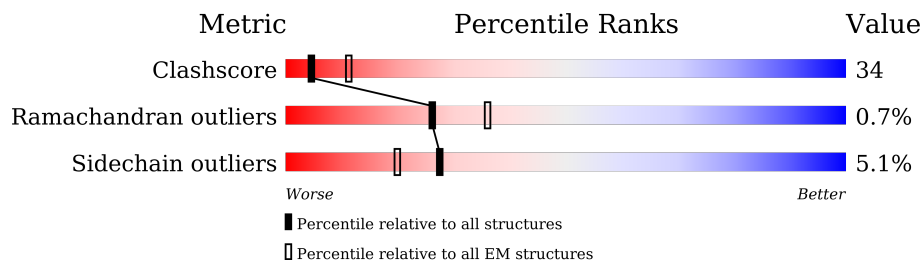
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.71 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.





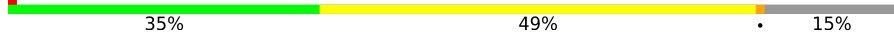
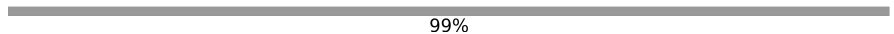
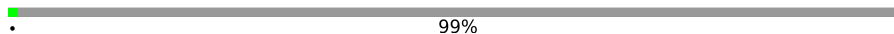
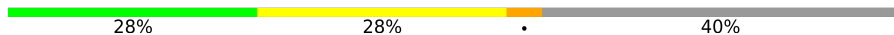

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	O	300	29% 37% 31%
1	o	300	96%
2	H	253	34% 40% 23%
3	I	756	31% 35% 32%
4	K	269	39% 38% 7% 14%
5	L	344	51% 35% 12%
6	M	180	43% 46% 7%
7	N	345	48% 37% 12%

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Mol	Chain	Length	Quality of chain
8	P	288	
9	S	138	
10	T	561	
11	W	88	
12	X	81	
13	G	25	
14	J	25	
15	C	943	
15	c	943	
16	Q	274	
17	U	418	
18	R	177	

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 23364 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 protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	o	12	Total	C	N	O		0	0
			95	59	18	18			
1	O	206	Total	C	N	O	S	0	0
			1588	1017	269	294	8		

- Molecule 2 is a protein called Centromere protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	195	Total	C	N	O	S	0	0
			1560	980	273	299	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	248	HIS	-	expression tag	UNP Q9H3R5
H	249	HIS	-	expression tag	UNP Q9H3R5
H	250	HIS	-	expression tag	UNP Q9H3R5
H	251	HIS	-	expression tag	UNP Q9H3R5
H	252	HIS	-	expression tag	UNP Q9H3R5
H	253	HIS	-	expression tag	UNP Q9H3R5

- Molecule 3 is a protein called Centromere protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	517	Total	C	N	O	S	0	0
			4111	2700	661	724	26		

- Molecule 4 is a protein called Centromere protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	230	Total	C	N	O	S	0	0
			1869	1183	312	364	10		

- Molecule 5 is a protein called Centromere protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	302	2422	1576	396	436	14	0	0

- Molecule 6 is a protein called Centromere protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	168	1298	825	232	234	7	0	0

- Molecule 7 is a protein called Centromere protein N.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	305	2493	1601	434	448	10	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	340	HIS	-	expression tag	UNP Q96H22
N	341	HIS	-	expression tag	UNP Q96H22
N	342	HIS	-	expression tag	UNP Q96H22
N	343	HIS	-	expression tag	UNP Q96H22
N	344	HIS	-	expression tag	UNP Q96H22
N	345	HIS	-	expression tag	UNP Q96H22

- Molecule 8 is a protein called Centromere protein P.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	224	1808	1144	311	344	9	0	0

- Molecule 9 is a protein called Centromere protein S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	97	790	494	141	150	5	0	0

- Molecule 10 is a protein called Centromere protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	T	99	Total	C	N	O	S	0	0
			804	516	139	142	7		

- Molecule 11 is a protein called CENP-W.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	W	75	Total	C	N	O	S	0	0
			584	367	119	95	3		

- Molecule 12 is a protein called Centromere protein X.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	74	Total	C	N	O	S	0	0
			590	378	104	107	1		

- Molecule 13 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	25	Total	C	N	O	P	0	0
			513	241	98	149	25		

- Molecule 14 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	25	Total	C	N	O	P	0	0
			512	241	95	151	25		

- Molecule 15 is a protein called Centromere protein C.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	C	5	Total	C	N	O	0	0
			40	28	5	7		
15	c	13	Total	C	N	O	0	0
			105	69	17	19		

- Molecule 16 is a protein called Centromere protein Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	164	Total	C	N	O	S	0	0
			1175	718	207	242	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	269	HIS	-	expression tag	UNP Q7L2Z9
Q	270	HIS	-	expression tag	UNP Q7L2Z9
Q	271	HIS	-	expression tag	UNP Q7L2Z9
Q	272	HIS	-	expression tag	UNP Q7L2Z9
Q	273	HIS	-	expression tag	UNP Q7L2Z9
Q	274	HIS	-	expression tag	UNP Q7L2Z9

- Molecule 17 is a protein called Centromere protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	U	140	699	419	140	140	0	0

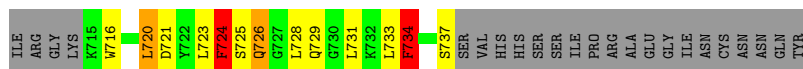
- Molecule 18 is a protein called Centromere protein R.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	R	62	308	184	62	62	0	0

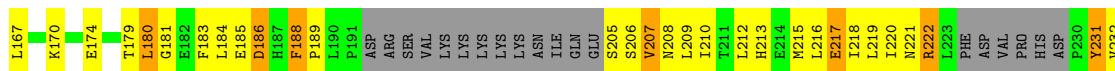
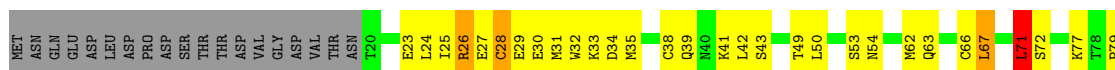




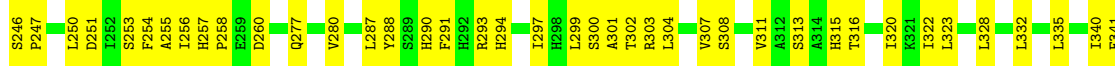
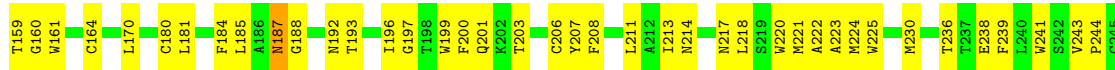
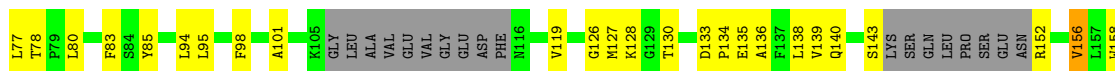




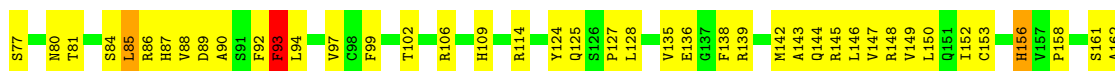
• Molecule 4: Centromere protein K



• Molecule 5: Centromere protein L

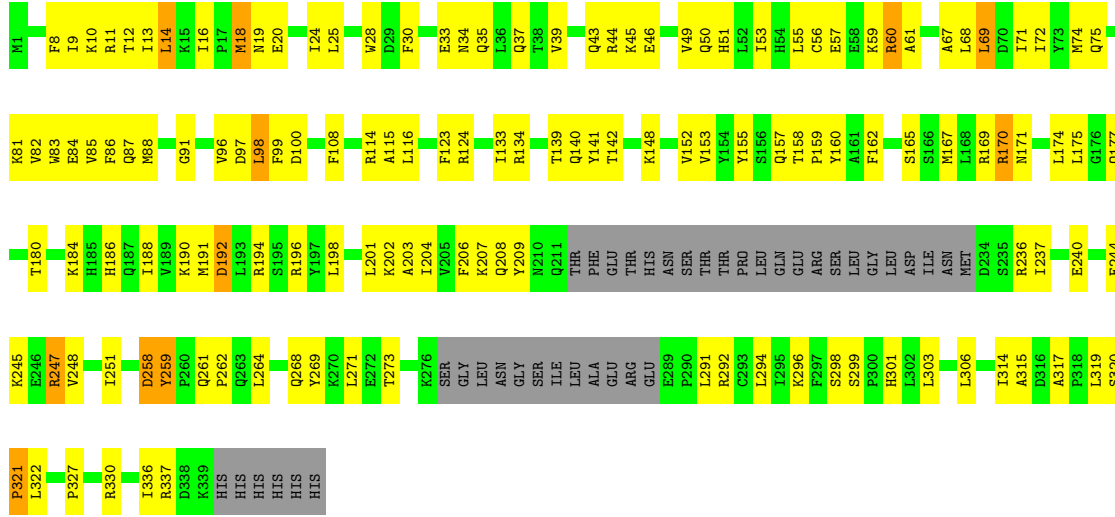


• Molecule 6: Centromere protein M

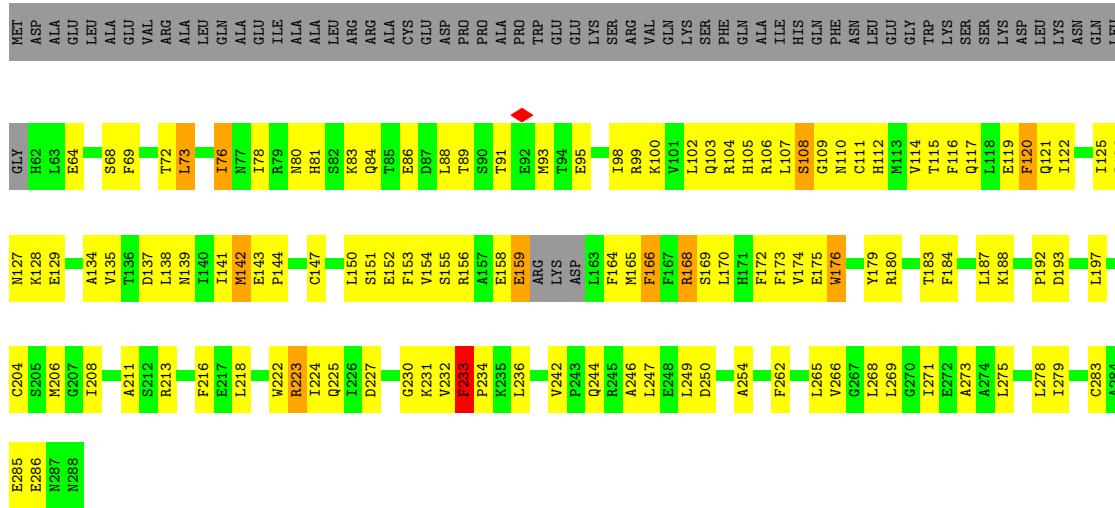
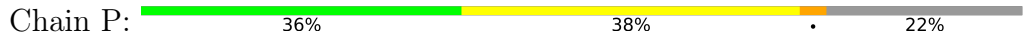




• Molecule 7: Centromere protein N



• Molecule 8: Centromere protein P











MET	ASN	SER
PRO	GLU	ARG
VAL	LYS	HIS
LYS	ARG	LEU
ARG	LYS	ASP
SER	LYS	SER
LEU	LEU	TYR
LYS	ASN	GLU
LEU	HIS	PHE
LEU	PRO	LEU
ASP	SER	LYS
GLY	LEU	ALA
LEU	THR	ILE
LEU	GLU	LEU
GLU	SER	LEU
GLU	LYS	ASN
ASN	LYS	ASN
SER	GLU	D84
PHE	SER	L89
ASP	THR	V93
PRO	THR	L96
SER	LYS	S97
LYS	ASP	S116
ASN	ASN	R117
THR	D84	
ARG	L89	
LYS	V93	
LYS	L96	
VAL	S97	
ILE	S116	
THR	R117	
TYR		
SER		
PRO		
THR		
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LYS		
LYS		
HIS		
ARG		
ASN		
GLY		
LEU		
SER		
LYS		
ALA		



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79777	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.924	Depositor
Minimum map value	-2.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.2	Depositor
Map size ( $\text{\AA}$ )	380.64, 380.64, 380.64	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.22, 1.22, 1.22	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	O	0.82	6/1624 (0.4%)	1.14	8/2208 (0.4%)
1	o	0.31	0/95	0.62	0/127
2	H	0.35	0/1566	0.64	0/2093
3	I	0.51	7/4210 (0.2%)	0.63	5/5704 (0.1%)
4	K	0.38	2/1897 (0.1%)	0.66	5/2558 (0.2%)
5	L	0.40	1/2487 (0.0%)	0.56	1/3379 (0.0%)
6	M	0.60	4/1320 (0.3%)	0.75	3/1791 (0.2%)
7	N	0.32	0/2547	0.58	3/3440 (0.1%)
8	P	0.58	7/1839 (0.4%)	0.68	2/2474 (0.1%)
9	S	0.39	1/799 (0.1%)	0.74	2/1070 (0.2%)
10	T	0.71	3/821 (0.4%)	0.74	1/1105 (0.1%)
11	W	0.34	0/590	0.69	0/785
12	X	0.38	0/596	0.72	1/801 (0.1%)
13	G	0.53	0/575	0.83	0/885
14	J	0.55	0/573	0.89	0/882
15	C	0.24	0/40	0.67	0/53
15	c	0.24	0/106	0.55	0/141
16	Q	0.39	1/1175 (0.1%)	0.65	1/1580 (0.1%)
17	U	0.25	0/697	0.39	1/972 (0.1%)
18	R	0.22	0/306	0.36	0/424
All	All	0.49	32/23863 (0.1%)	0.70	33/32472 (0.1%)

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	H	0	1
8	P	0	1
All	All	0	2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	208	PRO	CB-CG	18.91	2.44	1.50
1	O	208	PRO	CG-CD	-14.15	1.03	1.50
3	I	724	PHE	CE1-CZ	-12.82	1.12	1.37
6	M	52	LEU	CG-CD2	-11.77	1.08	1.51
8	P	159	GLU	CD-OE2	-11.29	1.13	1.25

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	208	PRO	CB-CG-CD	-27.30	0.05	106.50
1	O	208	PRO	CA-N-CD	-21.06	82.02	111.50
1	O	207	GLY	C-N-CD	17.51	165.16	128.40
6	M	53	PRO	CA-N-CD	-12.48	94.02	111.50
1	O	208	PRO	N-CD-CG	-12.45	84.53	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	47	ARG	Sidechain
8	P	168	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1588	0	1540	135	0
1	o	95	0	96	0	0
2	H	1560	0	1633	158	0
3	I	4111	0	4032	308	0
4	K	1869	0	1857	147	0
5	L	2422	0	2398	120	0
6	M	1298	0	1349	117	0
7	N	2493	0	2511	136	0
8	P	1808	0	1810	147	0
9	S	790	0	798	77	0
10	T	804	0	814	87	0
11	W	584	0	631	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X	590	0	620	75	0
13	G	513	0	279	19	0
14	J	512	0	280	23	0
15	C	40	0	36	3	0
15	c	105	0	106	0	0
16	Q	1175	0	1058	144	0
17	U	699	0	303	46	0
18	R	308	0	127	4	0
All	All	23364	0	22278	1545	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 34.

The worst 5 of 1545 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)
16:Q:145:ARG:HH12	17:U:308:LYS:CB	1.13	1.56
8:P:165:MET:CE	8:P:168:ARG:HD2	1.10	1.54
8:P:165:MET:CE	8:P:168:ARG:CD	1.93	1.45
8:P:165:MET:HE2	8:P:168:ARG:CD	1.47	1.38
16:Q:145:ARG:NH1	17:U:308:LYS:CB	1.93	1.30

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	O	204/300 (68%)	176 (86%)	25 (12%)	3 (2%)	10	44
1	o	10/300 (3%)	10 (100%)	0	0	100	100
2	H	191/253 (76%)	179 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	503/756 (66%)	447 (89%)	53 (10%)	3 (1%)	25	61
4	K	224/269 (83%)	202 (90%)	19 (8%)	3 (1%)	12	47
5	L	296/344 (86%)	261 (88%)	32 (11%)	3 (1%)	15	51
6	M	166/180 (92%)	146 (88%)	20 (12%)	0	100	100
7	N	299/345 (87%)	262 (88%)	36 (12%)	1 (0%)	41	74
8	P	220/288 (76%)	195 (89%)	22 (10%)	3 (1%)	11	45
9	S	95/138 (69%)	94 (99%)	1 (1%)	0	100	100
10	T	97/561 (17%)	93 (96%)	4 (4%)	0	100	100
11	W	73/88 (83%)	72 (99%)	1 (1%)	0	100	100
12	X	72/81 (89%)	71 (99%)	1 (1%)	0	100	100
15	C	3/943 (0%)	1 (33%)	1 (33%)	1 (33%)	0	0
15	c	11/943 (1%)	6 (54%)	4 (36%)	1 (9%)	1	10
16	Q	156/274 (57%)	151 (97%)	4 (3%)	1 (1%)	25	61
17	U	136/418 (32%)	131 (96%)	5 (4%)	0	100	100
18	R	58/177 (33%)	56 (97%)	2 (3%)	0	100	100
All	All	2814/6658 (42%)	2553 (91%)	242 (9%)	19 (1%)	26	59

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	44	PRO
1	O	156	PRO
15	C	304	ILE
16	Q	100	ILE
4	K	207	VAL

### 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	O	170/263 (65%)	159 (94%)	11 (6%)	17	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	10/263 (4%)	9 (90%)	1 (10%)	7	32
2	H	174/230 (76%)	165 (95%)	9 (5%)	23	54
3	I	440/691 (64%)	422 (96%)	18 (4%)	30	59
4	K	211/260 (81%)	195 (92%)	16 (8%)	13	43
5	L	268/306 (88%)	264 (98%)	4 (2%)	65	81
6	M	147/158 (93%)	142 (97%)	5 (3%)	37	63
7	N	273/317 (86%)	258 (94%)	15 (6%)	21	53
8	P	204/259 (79%)	194 (95%)	10 (5%)	25	55
9	S	86/121 (71%)	80 (93%)	6 (7%)	15	46
10	T	88/461 (19%)	84 (96%)	4 (4%)	27	57
11	W	61/77 (79%)	55 (90%)	6 (10%)	8	33
12	X	65/67 (97%)	62 (95%)	3 (5%)	27	56
15	C	4/875 (0%)	4 (100%)	0	100	100
15	c	12/875 (1%)	11 (92%)	1 (8%)	11	40
16	Q	109/254 (43%)	99 (91%)	10 (9%)	9	36
All	All	2322/5477 (42%)	2203 (95%)	119 (5%)	27	55

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	N	69	LEU
16	Q	101	LYS
1	O	170	GLN
16	Q	83	HIS
16	Q	184	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	185	ASN
16	Q	85	GLN
1	O	193	GLN
8	P	121	GLN
4	K	132	GLN

### 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.

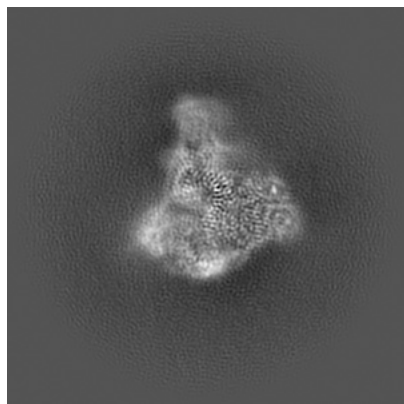
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33196. These allow visual inspection of the internal detail of the map and identification of artifacts.

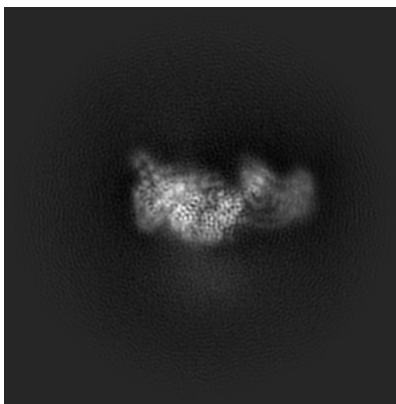
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

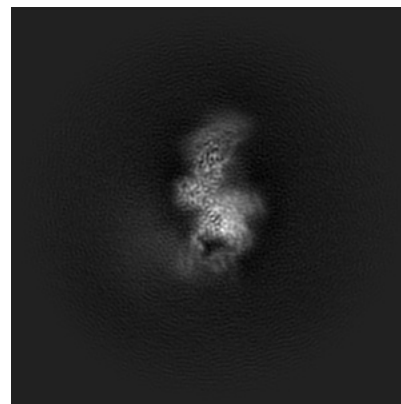
#### 6.1.1 Primary map



X

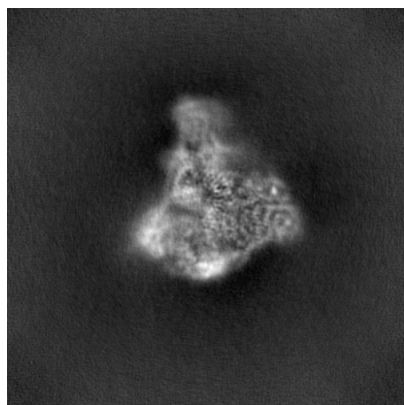


Y

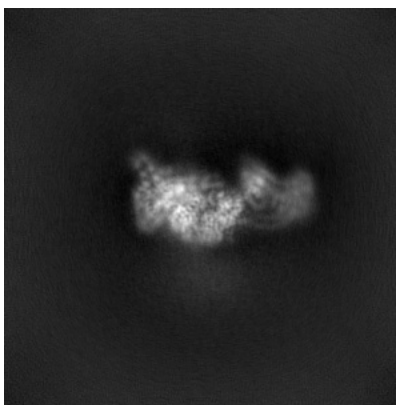


Z

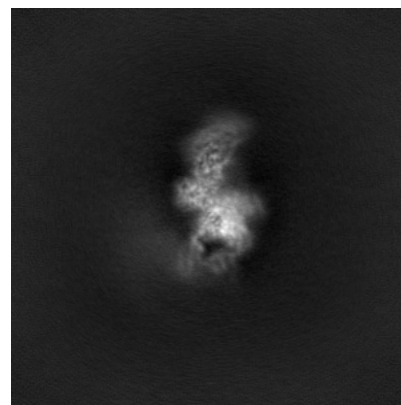
#### 6.1.2 Raw map



X



Y



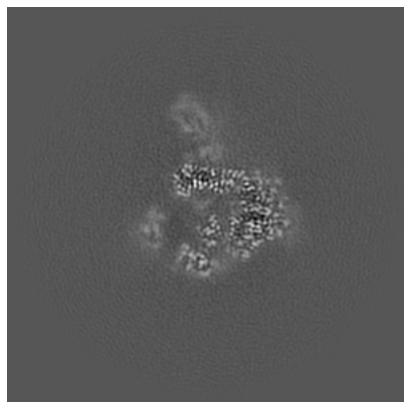
Z

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

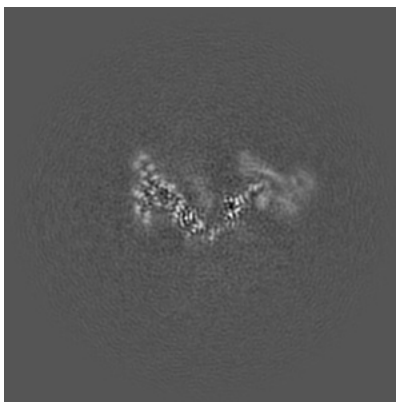


## 6.2 Central slices [i](#)

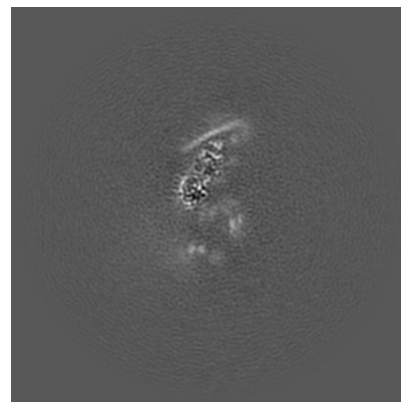
### 6.2.1 Primary map



X Index: 156

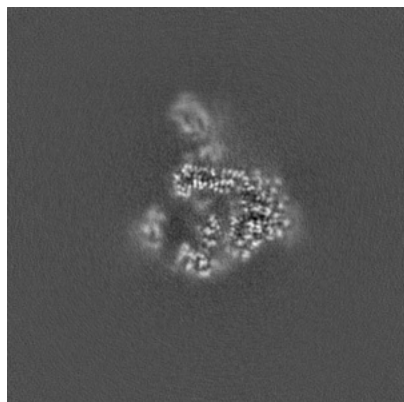


Y Index: 156

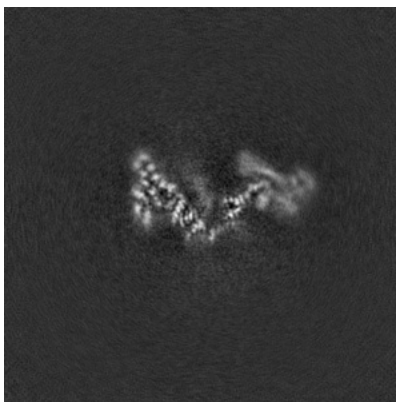


Z Index: 156

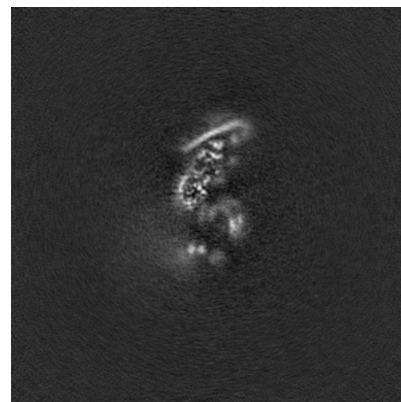
### 6.2.2 Raw map



X Index: 156



Y Index: 156

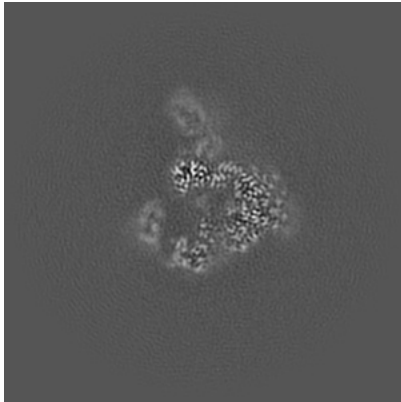


Z Index: 156

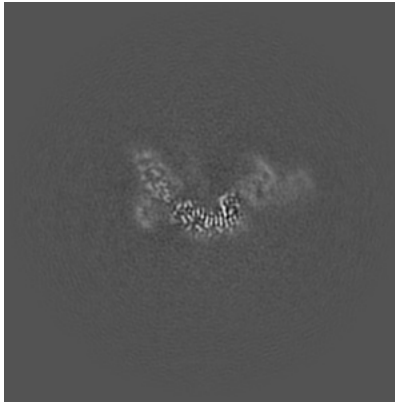
The images above show central slices of the map in three orthogonal directions.

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

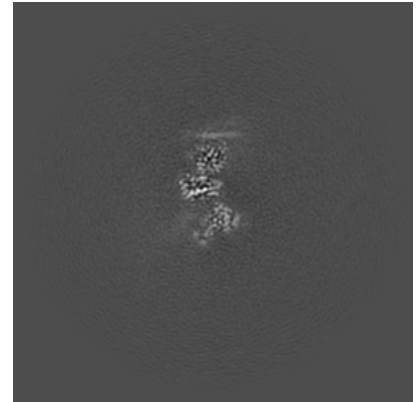
### 6.3.1 Primary map



X Index: 158

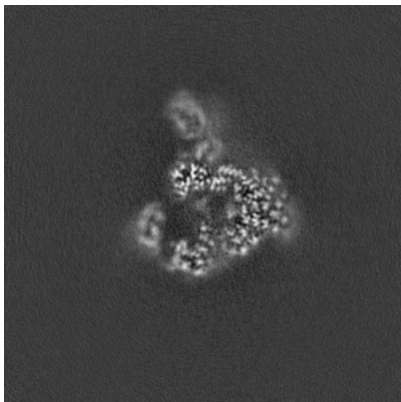


Y Index: 162

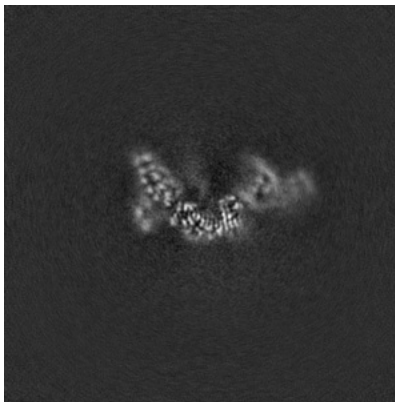


Z Index: 169

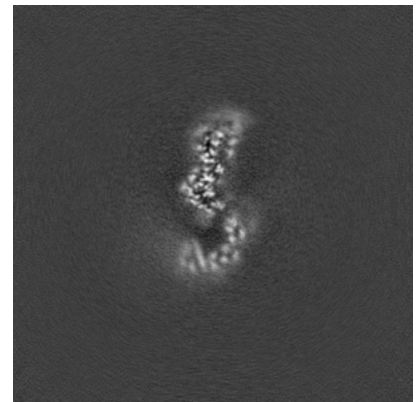
### 6.3.2 Raw map



X Index: 158



Y Index: 161



Z Index: 139

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

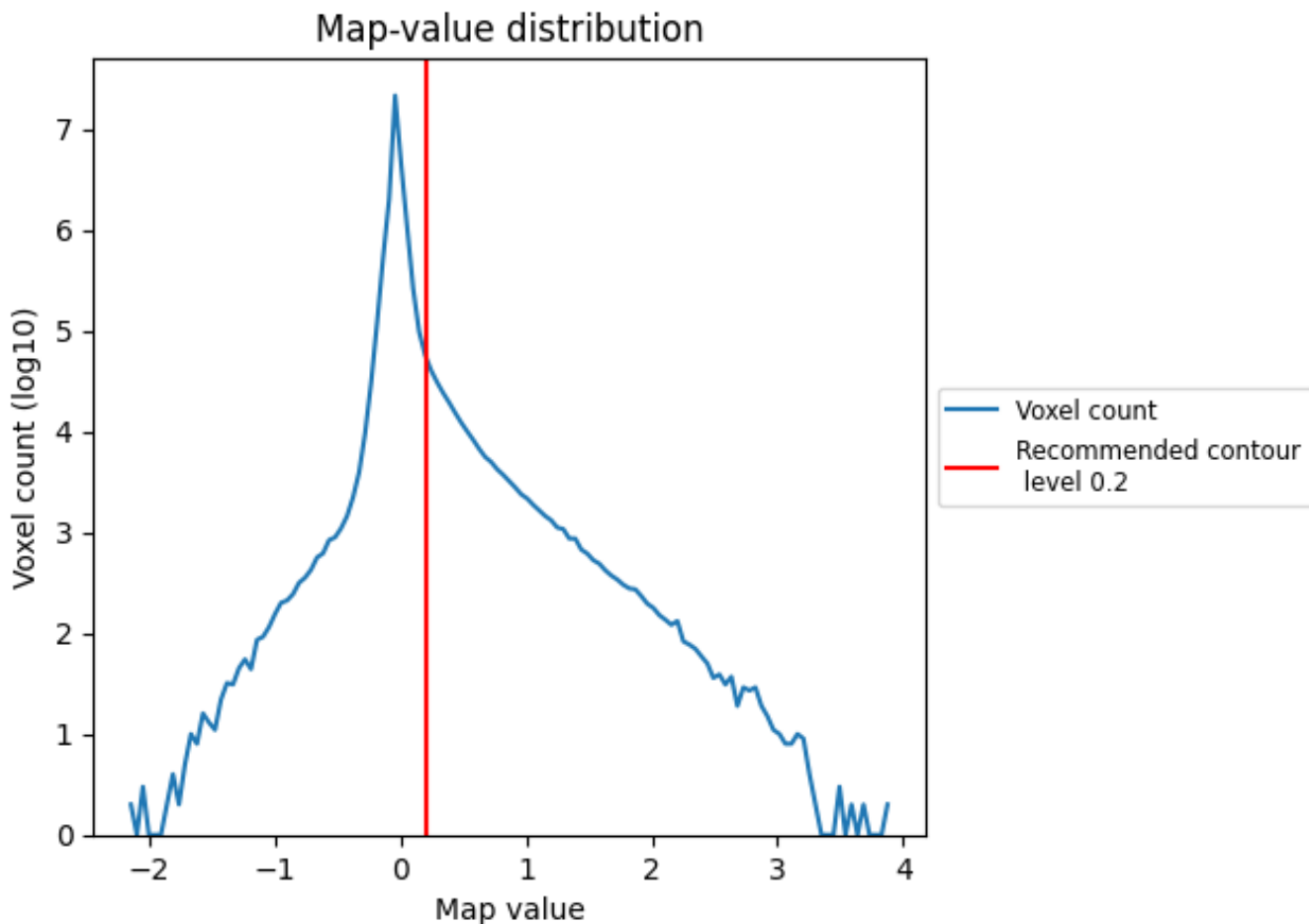
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

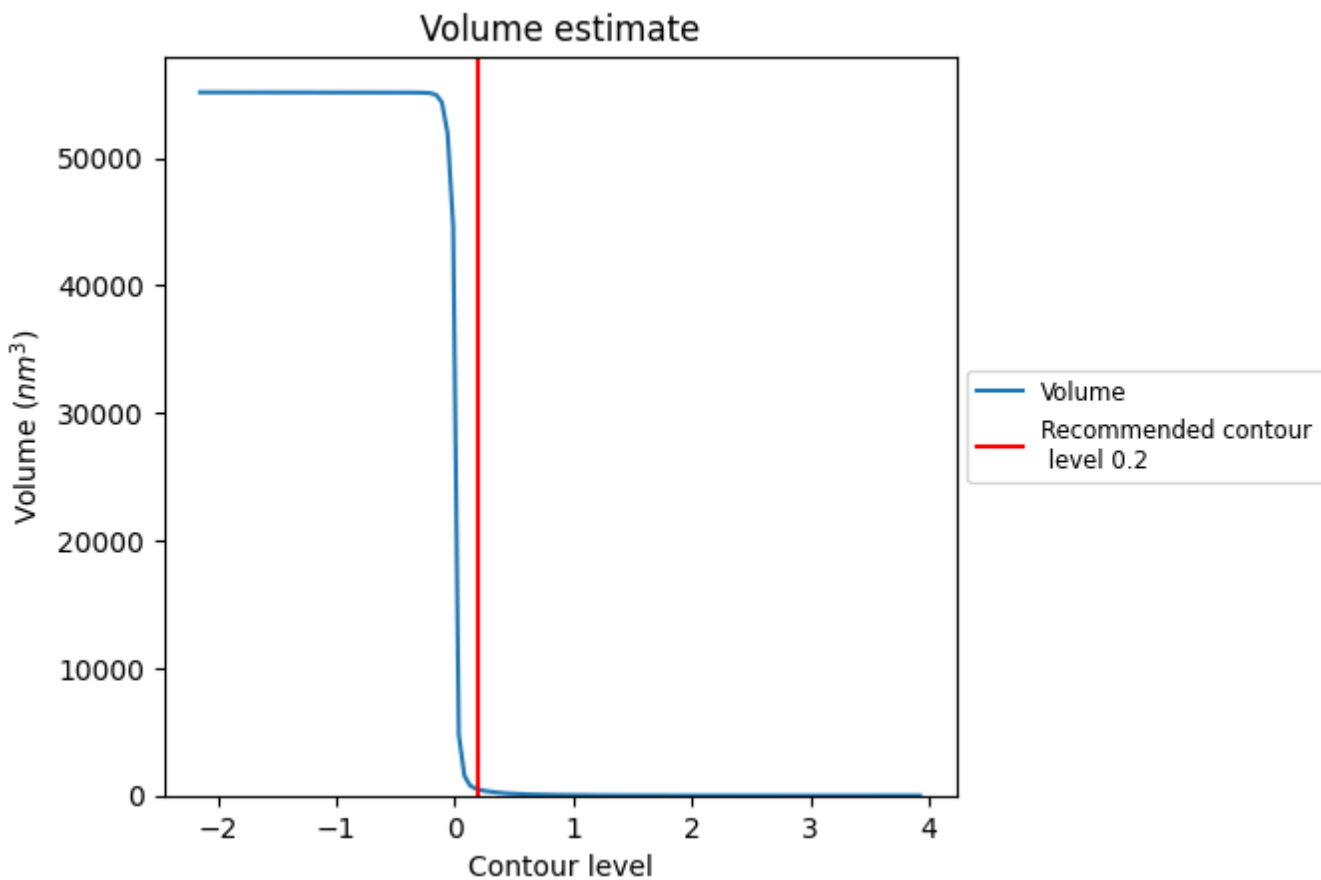
This section contains the results of statistical analysis of the map.

### 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.

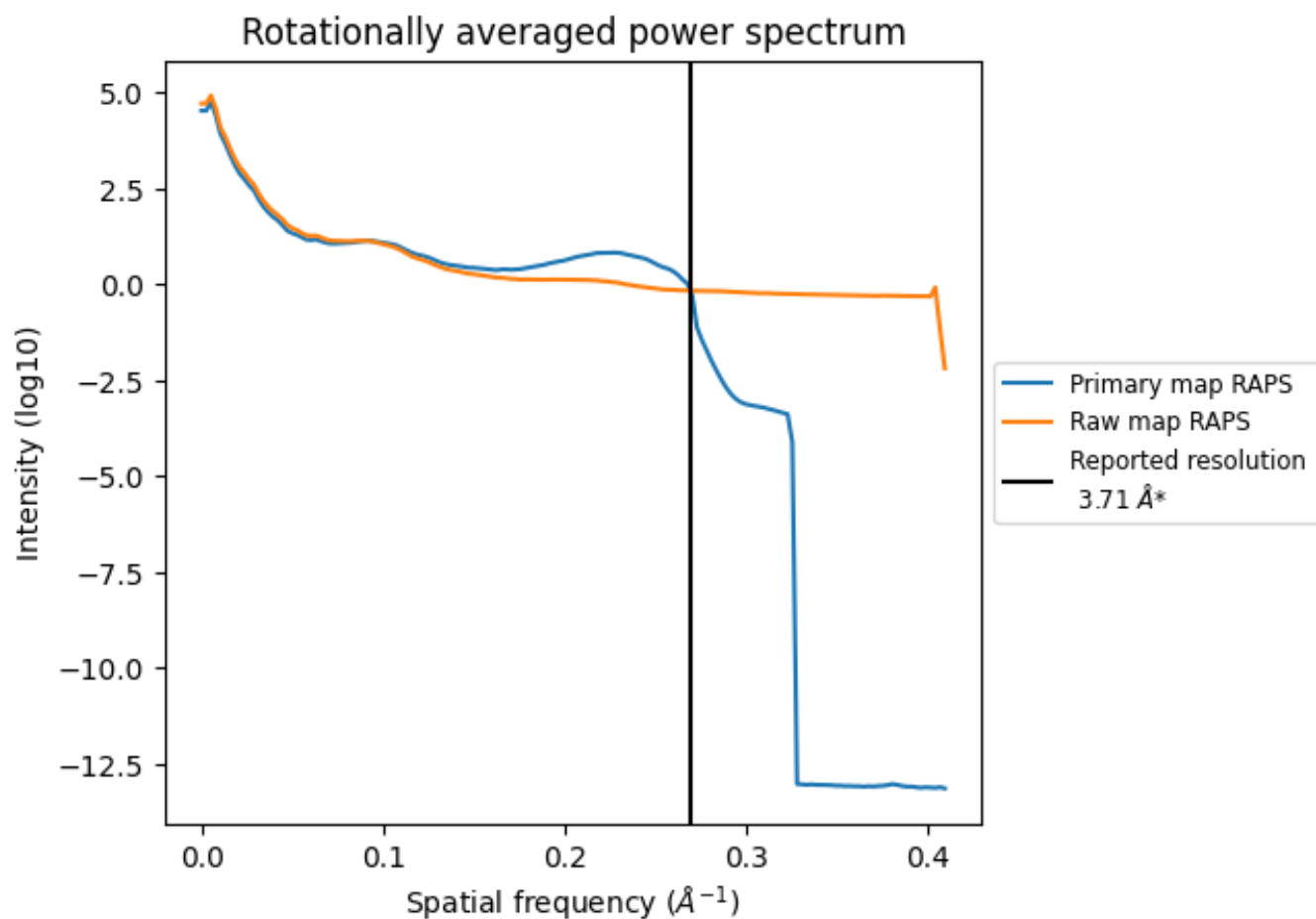
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 482 nm<sup>3</sup>; this corresponds to an approximate mass of 435 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

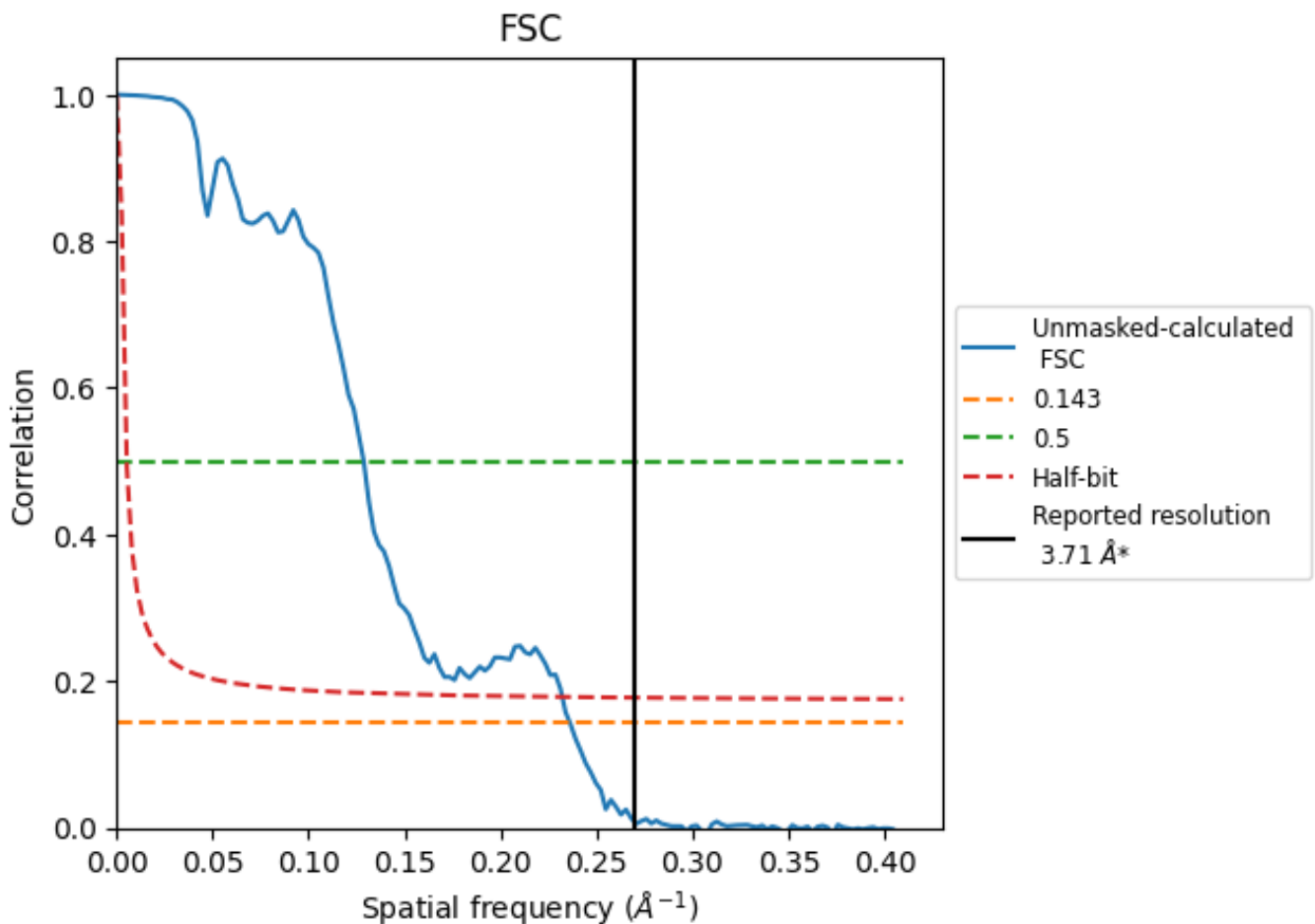


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.77	4.31

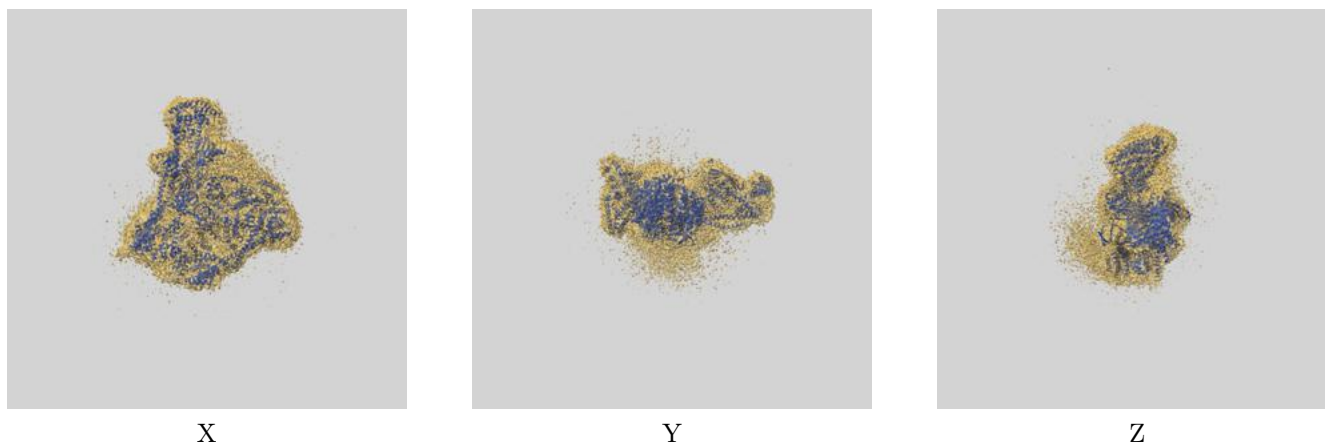
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.71 by more than 10 %



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

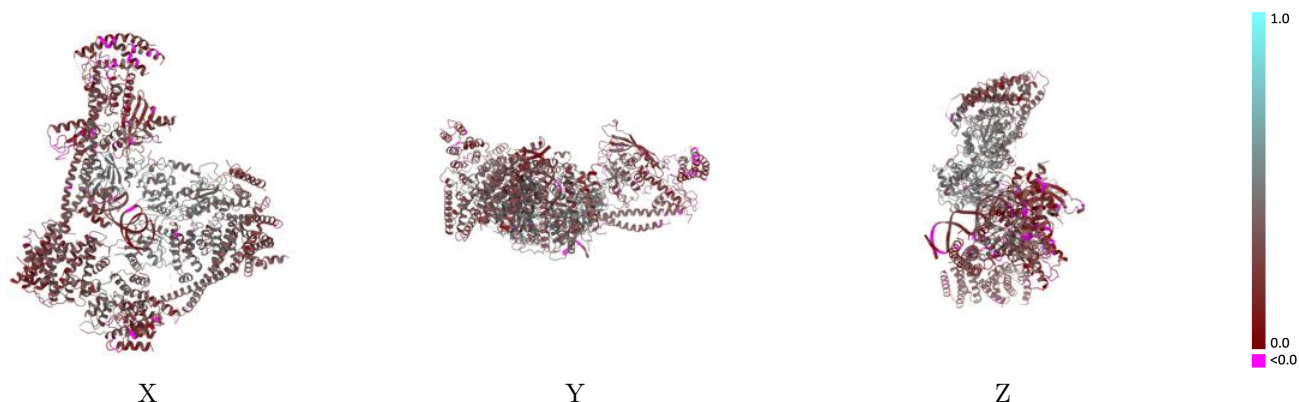
This section contains information regarding the fit between EMDB map EMD-33196 and PDB model 7XHN. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



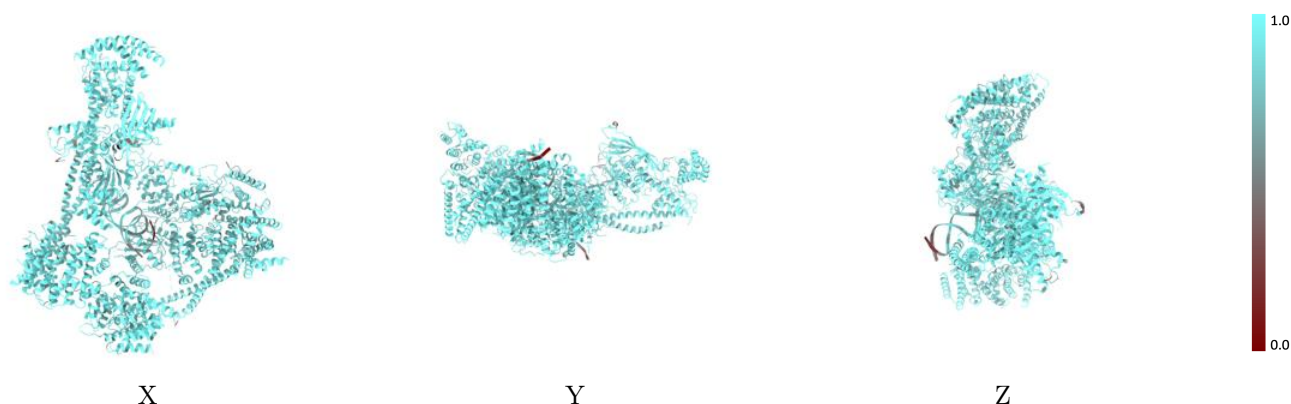
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



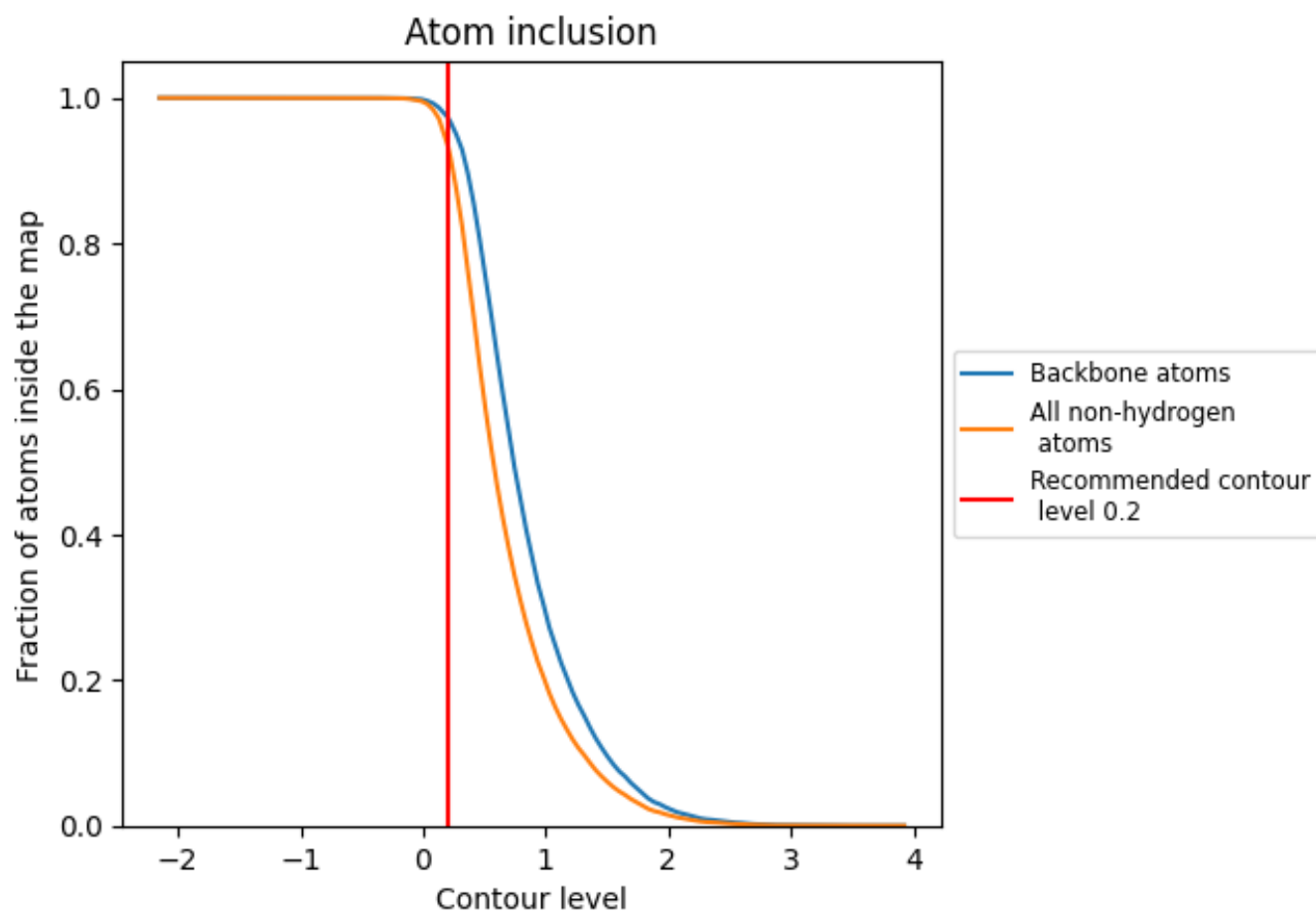
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9351	 0.3210
C	 0.8750	 0.1220
G	 0.6745	 0.1440
H	 0.9279	 0.3090
I	 0.9459	 0.3450
J	 0.6445	 0.1300
K	 0.9251	 0.3320
L	 0.9589	 0.4510
M	 0.9459	 0.4530
N	 0.9611	 0.4220
O	 0.9271	 0.2580
P	 0.9600	 0.1920
Q	 0.9536	 0.2150
R	 0.9545	 0.1730
S	 0.9651	 0.2430
T	 0.9720	 0.3410
U	 0.9986	 0.2840
W	 0.9648	 0.3230
X	 0.9155	 0.2020
c	 0.7379	 0.1720
o	 0.8817	 0.3490

