



Full wwPDB EM Validation Report ⓘ

Oct 7, 2026 – 04:24 PM EDT

PDB ID : 9ZU0 / pdb_00009zu0
EMDB ID : EMD-74785
Title : Nucleosome with an SSB at SHL +5.3 in complex with human PARP2, Class 10
Authors : Gregory-Lott, E.; Jayathilake, C.; Virk, R.K.; Kim, T.H.; Khurana, A.; Me-whinney, C.; Yang, J.; Cho, E.
Deposited on : 2025-12-23
Resolution : 2.33 Å(reported)

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.dev133
MolProbity : 4-5-2 with Phenix2.2
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) : 2.51

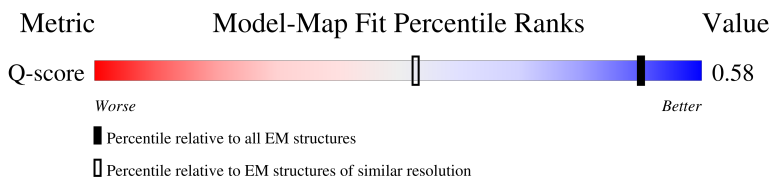
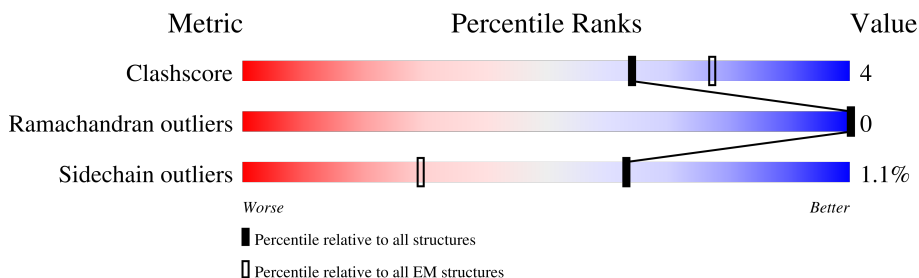
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.33 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	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4434 (1.83 - 2.83)

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	124	
1	B	124	
2	C	125	
2	D	125	

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Mol	Chain	Length	Quality of chain
3	E	136	
3	F	136	
4	G	104	
4	H	104	
5	I	274	
5	J	274	
6	K	130	
7	L	23	
8	M	153	
9	P	494	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 31296 atoms, of which 14348 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 Histone H2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	107	Total	C	H	N	O	S	0	0
			1701	518	880	160	142	1		
1	B	107	Total	C	H	N	O	S	0	0
			1701	518	880	160	142	1		

- Molecule 2 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	97	Total	C	H	N	O	S	0	0
			1584	486	813	141	142	2		
2	D	97	Total	C	H	N	O	S	0	0
			1583	486	812	141	142	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P02283
C	1	MET	-	expression tag	UNP P02283
C	2	ILE	-	expression tag	UNP P02283
D	0	GLY	-	expression tag	UNP P02283
D	1	MET	-	expression tag	UNP P02283
D	2	ILE	-	expression tag	UNP P02283

- Molecule 3 is a protein called Histone H3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	99	Total	C	H	N	O	S	0	0
			1673	514	857	158	142	2		
3	F	99	Total	C	H	N	O	S	0	0
			1673	514	857	158	142	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	111	SER	CYS	engineered mutation	UNP P02299
F	111	SER	CYS	engineered mutation	UNP P02299

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	G	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		
4	H	83	Total	C	H	N	O	S	0	0
			1372	418	710	129	114	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP P84040
G	2	ILE	-	expression tag	UNP P84040
H	1	MET	-	initiating methionine	UNP P84040
H	2	ILE	-	expression tag	UNP P84040

- Molecule 5 is a protein called mAb PL2-6 antibody.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	I	230	Total	C	H	N	O	S	0	0
			3543	1132	1743	296	363	9		
5	J	230	Total	C	H	N	O	S	0	0
			3542	1132	1742	296	363	9		

- Molecule 6 is a DNA chain called DNA (130-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	130	Total	C	H	N	O	P	0	0
			4103	1255	1458	479	781	130		

- Molecule 7 is a DNA chain called DNA (23-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	L	23	Total	C	H	N	O	P	0	0
			734	226	262	83	140	23		

- Molecule 8 is a DNA chain called DNA (153-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	M	153	Total	C	H	N	O	P	0	0
			4874	1494	1717	594	916	153		

- Molecule 9 is a protein called Poly [ADP-ribose] polymerase 2.

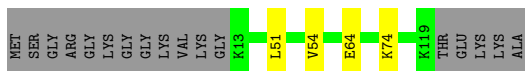
Mol	Chain	Residues	Atoms						AltConf	Trace
9	P	113	Total	C	H	N	O	S	0	0
			1841	590	907	163	173	8		

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: Histone H2A

Chain A:  83% 14%



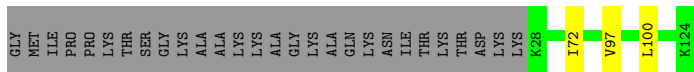
- Molecule 1: Histone H2A

Chain B:  84% 14%



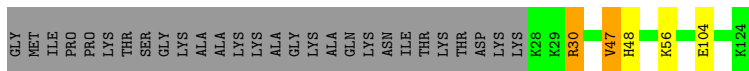
- Molecule 2: Histone H2B

Chain C:  75% 22%



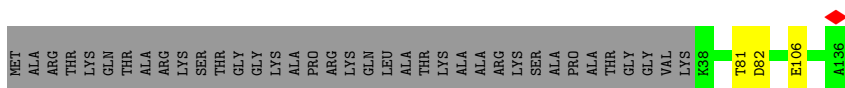
- Molecule 2: Histone H2B

Chain D:  74% 22%



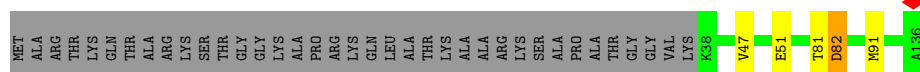
- Molecule 3: Histone H3

Chain E:  71% 27%



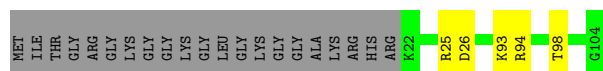
- Molecule 3: Histone H3

Chain F:  69% 27%



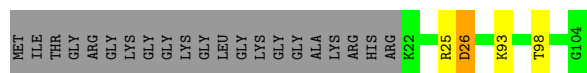
- Molecule 4: Histone H4

Chain G:  75% 5% 20%



- Molecule 4: Histone H4

Chain H:  76% 20%



- Molecule 5: mAb PL2-6 antibody

Chain I:  73% 11% 16%



- Molecule 5: mAb PL2-6 antibody

Chain J:  72% 12% 16%



- Molecule 6: DNA (130-MER)

Chain K:  72% 28%



- Molecule 7: DNA (23-MER)

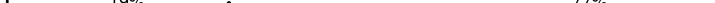
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graph LR
    G1[G1] --- C13_A14[C13  
A14]
    C13_A14 --- G19_T20[G19  
T20]
    G19_T20 --- T23[T23]

```

- Chain M: 80% 20%

A1	T2	C3	A4		T14	A15	T16		T20	G21		G33	T34		T53	T54		T60	T61		A76	G77		C84	G85		C88	G89	T90	T91	T92		G98	T99		G114	G115		T131	C132		G145	T146		T153	
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- Chain P:  19% . 77%

ser	ala	leu	ile	lys	leu	gly
ser	asp	phe	lys	ile	lys	leu
ala	met	glu	leu	glu	ser	ala
his	ser	val	val	asp	pro	pro
phe	ser	glu	lys	cys	leu	val
val	lys	lys	thr	ile	lys	asp
thr	ser	asp	thr	arg	pro	pro
leu	ala	gly	leu	ala	glu	glu
asn	asn	glu	glu	glu	ser	ser
gly	tyr	lys	ser	glu	glu	k101
ser	cys	glu	pro	his	leu	k101
thr	phe	ala	glu	gly	asp	e110
val	ala	phe	his	arg	leu	e110
pro	pro	ser	pro	ala	arg	m118
leu	arg	glu	leu	leu	val	l119
gly	leu	asp	asp	met	glu	l119
pro	lys	leu	glu	glu	glu	t122
ala	asn	his	his	ala	leu	t122
asn	asn	thr	tyr	cys	leu	m128
asp	gly	arg	asn	asn	lys	m128
thr	leu	met	asn	glu	leu	y132
leu	leu	leu	phe	ile	ile	l133
ile	leu	leu	his	tyr	cys	l133
leu	leu	trp	cys	thr	asn	l137
asn	ser	his	ala	arg	val	l137
pro	glu	gly	leu	ile	glu	y147
asp	val	ser	arg	pro	ala	w148
gly	ala	arg	pro	his	met	m149
tyr	leu	met	leu	asp	glu	r150
thr	gly	ser	asp	phe	glu	r150
leu	asn	asn	asn	gly	met	l162
asn	asn	trp	glu	leu	met	l162
asn	glu	val	tyr	arg	met	l169
glu	glu	gly	tyr	thr	glu	l169
tyr	leu	ile	glu	pro	met	k178
trp	leu	leu	phe	lys	tyr	k178
ile	glu	ser	lys	leu	tyr	l181
val	ala	his	val	ile	asn	d182
tyr	asn	gly	ile	arg	thr	d182
asn	pro	leu	ser	thr	lys	d190
pro	lys	arg	thr	glu	lys	d190
asn	ala	ile	tyr	glu	lys	l204
glu	glu	ala	glu	glu	pro	l204
val	glu	pro	glu	leu	leu	q205
arg	leu	pro	asn	ser	gly	q205
met	leu	glu	thr	glu	lys	m206
arg	glu	ala	his	thr	lys	m206
tyr	gly	pro	ala	ile	leu	a209
leu	lys	ile	pro	glu	thr	a209
leu	his	thr	thr	asn	thr	thr
val	ser	thr	asn	glu	val	thr
thr	glu	thr	lys	leu	ala	glu
val	thr	tyr	his	leu	glu	asp
glu	met	met	asp	glu	ile	glu
phe	gly	met	asp	ala	lys	glu
asn	leu	gly	thr	leu	ala	glu
phe	lys	tyr	met	glu	gly	thr
leu	lys	tyr	thr	asn	tyr	lys
glu	met	ile	ile	glu	lys	glu
leu	ala	tyr	leu	ile	leu	glu

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	156495	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.398	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.828, 0.828, 0.828	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	0.18	0/831	0.31	0/1119
1	B	0.19	0/831	0.30	0/1119
2	C	0.18	0/782	0.29	0/1046
2	D	0.18	0/782	0.29	0/1046
3	E	0.19	0/828	0.30	0/1109
3	F	0.19	0/828	0.30	0/1109
4	G	0.18	0/669	0.30	0/894
4	H	0.20	0/669	0.34	0/894
5	I	0.16	0/1842	0.38	0/2493
5	J	0.17	0/1842	0.38	0/2493
6	K	0.78	0/2962	0.87	0/4564
7	L	0.74	0/528	0.94	0/811
8	M	0.75	0/3546	0.86	0/5476
9	P	0.15	0/953	0.38	0/1278
All	All	0.50	0/17893	0.62	0/25451

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	821	880	879	3	0
1	B	821	880	879	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	771	813	811	3	0
2	D	771	812	811	2	0
3	E	816	857	856	2	0
3	F	816	857	856	4	0
4	G	662	710	709	2	0
4	H	662	710	709	2	0
5	I	1800	1743	1740	23	0
5	J	1800	1742	1740	26	0
6	K	2645	1458	1458	23	0
7	L	472	262	262	2	0
8	M	3157	1717	1717	18	0
9	P	934	907	906	20	0
All	All	16948	14348	14333	127	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 4.

All (127) 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:I:35:MET:HE1	5:I:44:THR:O	1.95	0.66
9:P:118:MET:HE3	9:P:204:LEU:HD21	1.79	0.64
5:I:61:GLN:HB2	5:I:71:LEU:HD21	1.80	0.64
6:K:107:DT:H2'	6:K:108:DT:H71	1.80	0.64
9:P:169:LEU:HD13	9:P:169:LEU:O	2.01	0.61
9:P:133:LEU:HD21	9:P:150:ARG:HH11	1.67	0.60
5:J:72:ILE:HG22	5:J:74:TYR:O	2.02	0.59
6:K:14:DC:H2'	6:K:15:DC:C6	2.39	0.58
5:I:190:TRP:CE3	5:I:235:MET:HE2	2.39	0.57
5:J:164:GLU:N	5:J:164:GLU:OE1	2.37	0.57
9:P:148:TRP:HE3	9:P:162:LEU:HD13	1.69	0.57
5:I:261:LEU:HD22	5:I:261:LEU:H	1.70	0.56
8:M:53:DT:H2'	8:M:54:DT:H71	1.87	0.56
5:I:32:PRO:HG3	5:I:35:MET:HE3	1.87	0.55
9:P:147:VAL:O	9:P:162:LEU:HD12	2.07	0.54
5:I:57:LEU:HD11	5:I:112:CYS:SG	2.48	0.54
6:K:1:DA:H2''	6:K:2:DT:H71	1.89	0.54
5:I:266:GLN:HA	5:I:266:GLN:OE1	2.07	0.53
5:J:167:GLU:OE2	5:J:167:GLU:N	2.42	0.53
2:D:30:ARG:HD3	2:D:30:ARG:H	1.74	0.53
9:P:118:MET:CE	9:P:204:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:200:GLU:HA	5:J:200:GLU:OE1	2.08	0.52
5:I:61:GLN:CB	5:I:71:LEU:HD21	2.40	0.52
3:F:91:MET:HA	3:F:91:MET:HE3	1.92	0.52
3:E:81:THR:C	3:E:82:ASP:OD1	2.53	0.52
9:P:190:ASP:OD1	9:P:190:ASP:C	2.53	0.52
5:J:58:SER:HB3	5:J:260:THR:HG21	1.91	0.51
4:G:93:LYS:HG3	4:G:98:THR:HG22	1.93	0.51
5:J:117:GLU:N	5:J:117:GLU:OE2	2.43	0.51
3:F:81:THR:C	3:F:82:ASP:OD2	2.54	0.51
5:J:243:GLU:OE2	5:J:243:GLU:C	2.54	0.51
5:J:129:GLU:C	5:J:129:GLU:OE1	2.54	0.51
5:I:94:ASP:OD2	5:I:94:ASP:C	2.53	0.50
9:P:204:LEU:N	9:P:204:LEU:HD23	2.26	0.50
6:K:73:DC:H2''	6:K:74:DG:C8	2.45	0.50
9:P:181:LEU:O	9:P:181:LEU:HD13	2.10	0.50
5:J:128:LEU:C	5:J:128:LEU:HD13	2.36	0.49
8:M:90:DT:H4'	8:M:91:DT:OP1	2.13	0.49
3:F:81:THR:O	3:F:82:ASP:OD2	2.31	0.49
5:I:219:LYS:C	5:I:219:LYS:HD3	2.38	0.49
5:J:266:GLN:HA	5:J:266:GLN:OE1	2.13	0.49
5:J:107:THR:HG23	5:J:107:THR:O	2.12	0.49
6:K:106:DA:H4'	6:K:107:DT:OP1	2.13	0.49
5:J:105:ASP:OD2	5:J:105:ASP:C	2.56	0.48
6:K:20:DC:H2''	6:K:21:DC:C6	2.47	0.48
8:M:84:DC:H2''	8:M:85:DG:C8	2.49	0.48
1:B:64:GLU:HG2	5:J:257:LEU:CD1	2.44	0.48
5:J:41:GLU:HA	5:J:41:GLU:OE1	2.13	0.48
4:H:25:ARG:O	4:H:26:ASP:OD1	2.32	0.48
5:J:24:MET:N	5:J:24:MET:HE3	2.29	0.48
5:I:194:THR:HG22	5:I:196:ARG:H	1.79	0.47
6:K:108:DT:H4'	6:K:109:DA:OP1	2.15	0.47
8:M:76:DA:H2''	8:M:77:DG:H5'	1.96	0.47
8:M:114:DC:H2''	8:M:115:DG:C8	2.50	0.46
1:A:64:GLU:HG2	5:I:257:LEU:CD1	2.46	0.46
6:K:4:DC:C2'	6:K:5:DT:H71	2.45	0.46
5:I:57:LEU:HD12	5:I:113:LEU:O	2.15	0.46
8:M:14:DT:C2	8:M:15:DA:C8	3.04	0.46
5:J:166:VAL:HG12	5:J:167:GLU:H	1.80	0.46
5:J:202:ILE:HG21	5:J:235:MET:HE1	1.97	0.46
5:I:103:GLU:OE1	5:I:103:GLU:HA	2.16	0.46
5:J:241:THR:HG22	5:J:242:SER:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:196:ARG:HB3	5:I:196:ARG:CZ	2.46	0.46
9:P:147:VAL:HG22	9:P:149:MET:HE2	1.98	0.46
5:J:225:THR:HG22	5:J:226:SER:N	2.31	0.46
6:K:114:DC:C2'	6:K:115:DT:H72	2.46	0.46
5:I:190:TRP:CD2	5:I:235:MET:HE2	2.52	0.45
1:A:54:VAL:HG21	2:C:97:VAL:HG21	1.99	0.45
5:I:162:GLY:O	5:I:268:THR:HG23	2.16	0.45
7:L:13:DC:H2''	7:L:14:DA:C8	2.52	0.45
6:K:50:DC:H2''	6:K:51:DT:H71	1.98	0.45
8:M:98:DG:H2'	8:M:99:DT:H71	1.99	0.45
8:M:91:DT:H2'	8:M:92:DT:H72	1.99	0.45
5:I:57:LEU:HD22	5:I:95:PHE:CG	2.52	0.44
4:G:25:ARG:O	4:G:26:ASP:OD1	2.36	0.44
5:J:165:LEU:HD22	5:J:165:LEU:N	2.33	0.44
9:P:137:LEU:N	9:P:137:LEU:HD22	2.33	0.44
6:K:48:DC:H2'	6:K:49:DT:H72	1.99	0.44
9:P:110:GLU:O	9:P:110:GLU:CG	2.66	0.43
6:K:1:DA:H1'	6:K:2:DT:C5	2.54	0.43
2:C:72:ILE:HD13	2:C:100:LEU:HD12	2.01	0.43
5:I:225:THR:HG22	5:I:226:SER:N	2.32	0.43
6:K:81:DC:H2''	6:K:82:DC:C5	2.53	0.43
6:K:92:DT:H2''	6:K:93:DA:C8	2.53	0.43
9:P:110:GLU:O	9:P:110:GLU:CD	2.62	0.43
8:M:60:DT:H4'	8:M:61:DT:OP1	2.19	0.42
8:M:145:DC:C2'	8:M:146:DT:H71	2.49	0.42
5:J:166:VAL:HG12	5:J:167:GLU:N	2.35	0.42
6:K:112:DC:H2''	6:K:113:DC:C5	2.54	0.42
5:J:71:LEU:HA	5:J:82:VAL:HG21	2.01	0.42
9:P:181:LEU:HD13	9:P:181:LEU:C	2.45	0.42
3:F:47:VAL:O	3:F:51:GLU:HG3	2.20	0.42
8:M:20:DT:H1'	8:M:21:DG:C8	2.54	0.42
8:M:131:DT:H2''	8:M:132:DC:C5	2.54	0.42
6:K:2:DT:H2''	6:K:3:DC:C6	2.55	0.42
8:M:53:DT:C2'	8:M:54:DT:H71	2.49	0.42
9:P:122:THR:HA	9:P:128:ASN:O	2.20	0.42
3:E:81:THR:O	3:E:82:ASP:OD1	2.38	0.42
5:J:128:LEU:HD11	5:J:130:ILE:HD11	2.01	0.42
5:J:85:ARG:HG3	5:J:85:ARG:HH11	1.85	0.42
9:P:101:LYS:HD2	9:P:101:LYS:C	2.45	0.42
8:M:15:DA:H2'	8:M:16:DT:H72	2.02	0.42
9:P:178:LYS:O	9:P:182:ASP:OD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:93:LYS:HG3	4:H:98:THR:HG22	2.01	0.41
2:D:47:VAL:HG12	2:D:48:HIS:N	2.36	0.41
6:K:12:DT:H1'	6:K:13:DC:C6	2.55	0.41
8:M:145:DC:H2'	8:M:146:DT:H71	2.02	0.41
6:K:19:DG:H2''	6:K:20:DC:C6	2.55	0.41
7:L:19:DG:C8	7:L:20:DT:H72	2.56	0.41
6:K:41:DT:O3'	6:K:42:DA:C8	2.74	0.41
9:P:119:LEU:HD12	9:P:132:TYR:O	2.21	0.41
5:I:166:VAL:HG22	5:I:167:GLU:N	2.36	0.41
5:J:62:GLN:HB3	5:J:109:THR:HG23	2.02	0.41
6:K:112:DC:H2''	6:K:113:DC:C6	2.56	0.41
5:I:94:ASP:OD2	5:I:94:ASP:O	2.39	0.41
1:A:51:LEU:HD13	2:C:72:ILE:HG21	2.02	0.40
5:I:170:THR:O	5:I:240:LEU:HD12	2.21	0.40
6:K:30:DT:H2''	6:K:31:DC:C5	2.57	0.40
5:I:128:LEU:C	5:I:128:LEU:HD13	2.46	0.40
6:K:29:DC:H2''	6:K:30:DT:H71	2.04	0.40
6:K:39:DC:H2''	6:K:40:DG:C8	2.56	0.40
8:M:3:DC:H2''	8:M:4:DA:C8	2.57	0.40
8:M:88:DC:H2''	8:M:89:DG:C8	2.56	0.40
5:J:188:ILE:HG21	5:J:233:VAL:HG21	2.04	0.40
9:P:169:LEU:HD13	9:P:169:LEU:C	2.46	0.40
9:P:206:MET:O	9:P:206:MET:HE3	2.21	0.40
8:M:33:DG:H2'	8:M:34:DT:H71	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	105/124 (85%)	104 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	105/124 (85%)	104 (99%)	1 (1%)	0	100	100
2	C	95/125 (76%)	95 (100%)	0	0	100	100
2	D	95/125 (76%)	95 (100%)	0	0	100	100
3	E	97/136 (71%)	94 (97%)	3 (3%)	0	100	100
3	F	97/136 (71%)	96 (99%)	1 (1%)	0	100	100
4	G	81/104 (78%)	78 (96%)	3 (4%)	0	100	100
4	H	81/104 (78%)	79 (98%)	2 (2%)	0	100	100
5	I	226/274 (82%)	220 (97%)	6 (3%)	0	100	100
5	J	226/274 (82%)	220 (97%)	6 (3%)	0	100	100
9	P	111/494 (22%)	108 (97%)	3 (3%)	0	100	100
All	All	1319/2020 (65%)	1293 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	83/94 (88%)	82 (99%)	1 (1%)	63	75
1	B	83/94 (88%)	81 (98%)	2 (2%)	43	55
2	C	84/105 (80%)	84 (100%)	0	100	100
2	D	84/105 (80%)	80 (95%)	4 (5%)	23	29
3	E	86/111 (78%)	85 (99%)	1 (1%)	63	75
3	F	86/111 (78%)	85 (99%)	1 (1%)	63	75
4	G	68/80 (85%)	67 (98%)	1 (2%)	57	69
4	H	68/80 (85%)	67 (98%)	1 (2%)	57	69
5	I	202/226 (89%)	201 (100%)	1 (0%)	81	88
5	J	202/226 (89%)	202 (100%)	0	100	100
9	P	100/433 (23%)	99 (99%)	1 (1%)	68	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1146/1665 (69%)	1133 (99%)	13 (1%)	63 77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	B	73	ASN
1	B	101	THR
2	D	30	ARG
2	D	47	VAL
2	D	56	LYS
2	D	104	GLU
3	E	106	GLU
3	F	82	ASP
4	G	94	ARG
4	H	26	ASP
5	I	234	TYR
9	P	204	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	112	GLN
2	C	83	ASN
2	D	83	ASN
5	I	159	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

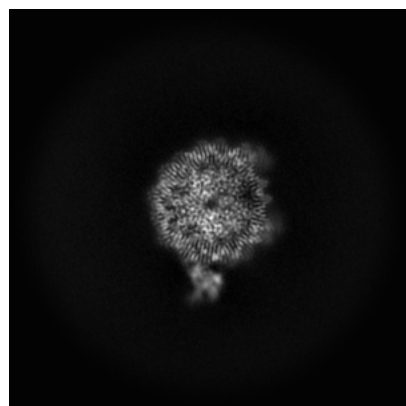
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74785. These allow visual inspection of the internal detail of the map and identification of artifacts.

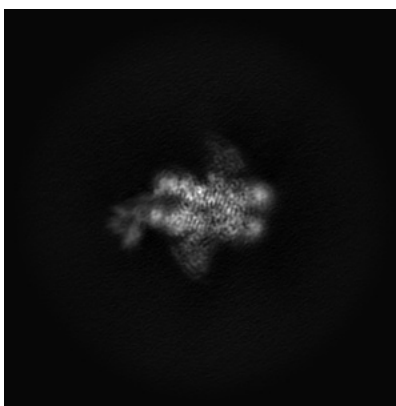
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

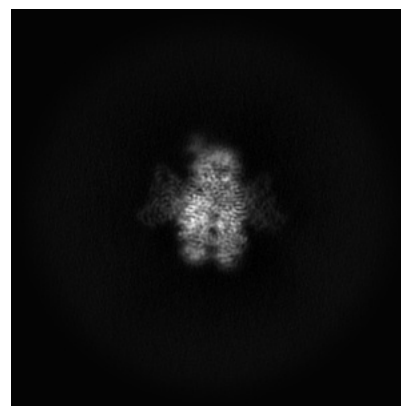
6.1.1 Primary map



X

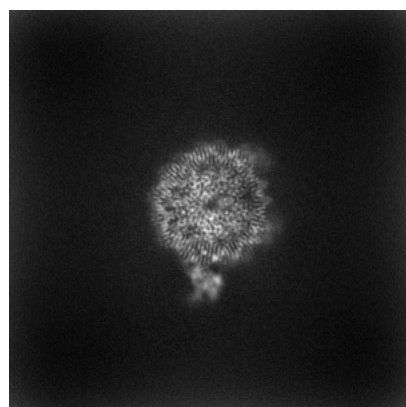


Y

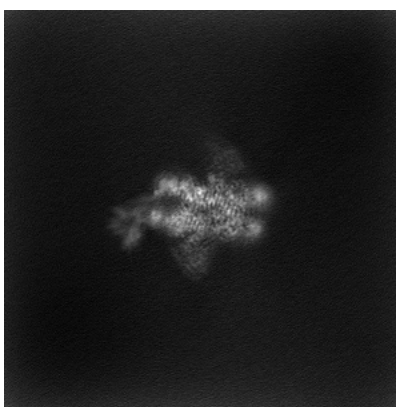


Z

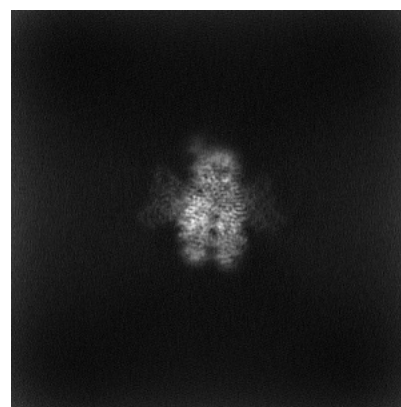
6.1.2 Raw map



X



Y

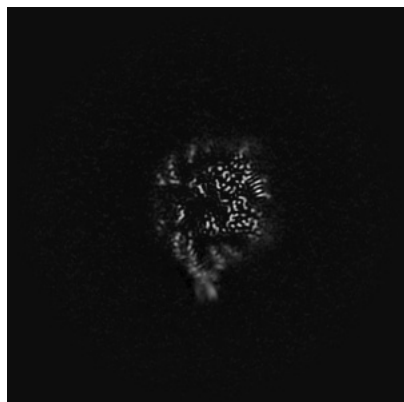


Z

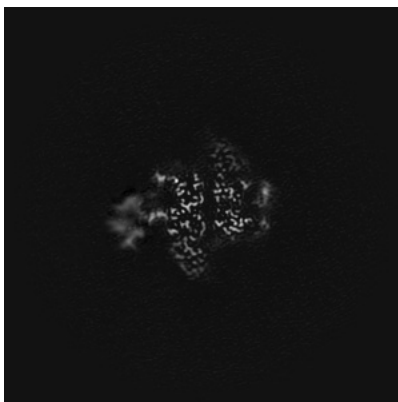
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

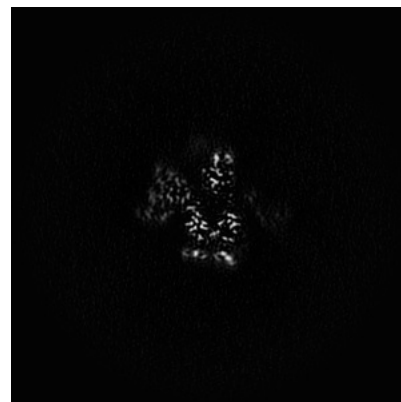
6.2.1 Primary map



X Index: 200

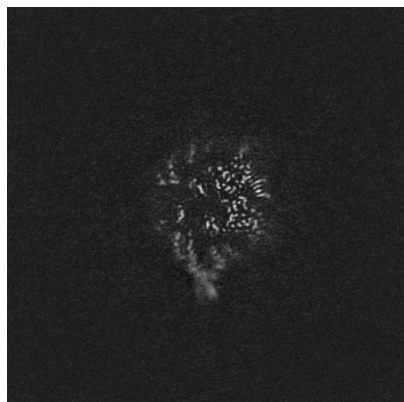


Y Index: 200

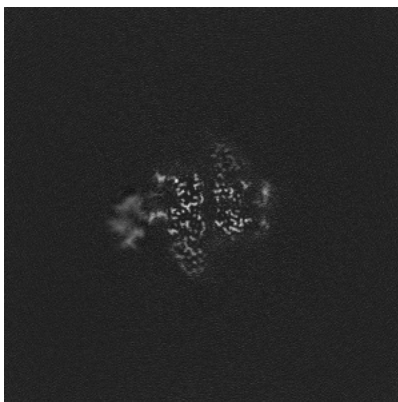


Z Index: 200

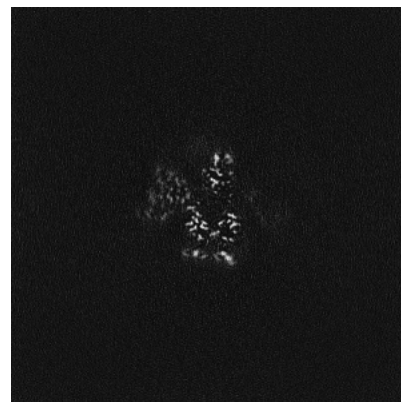
6.2.2 Raw map



X Index: 200



Y Index: 200

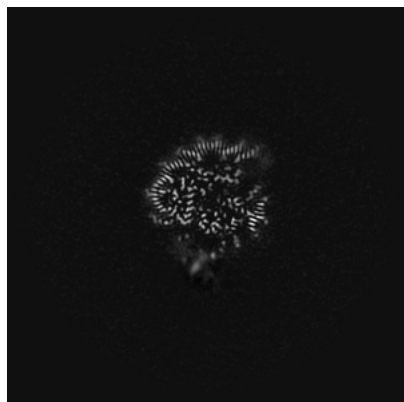


Z Index: 200

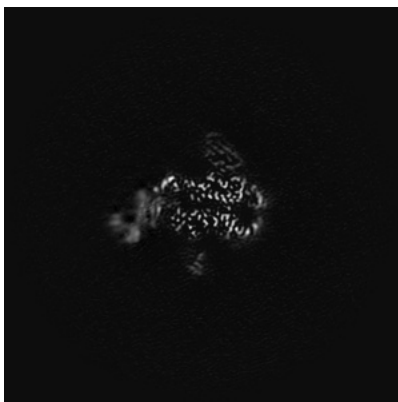
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

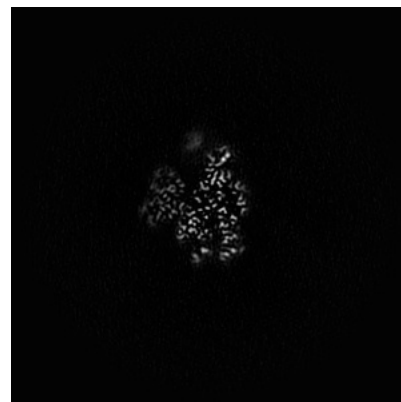
6.3.1 Primary map



X Index: 212

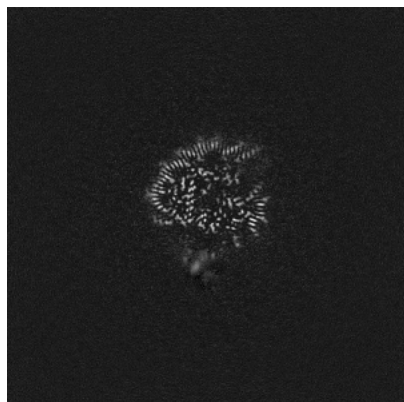


Y Index: 185

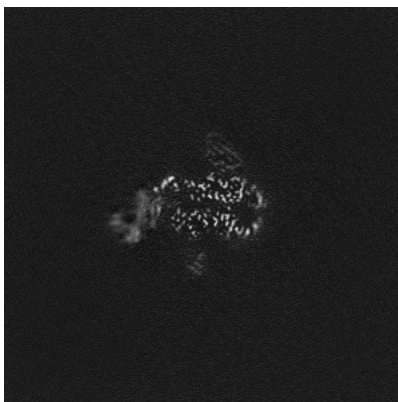


Z Index: 186

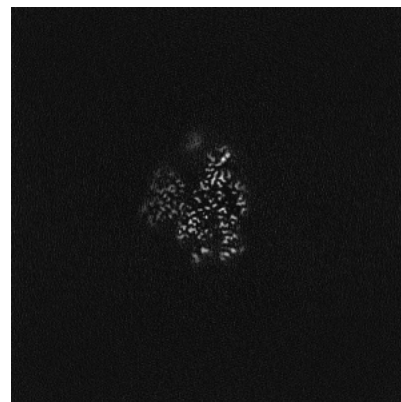
6.3.2 Raw map



X Index: 211



Y Index: 185

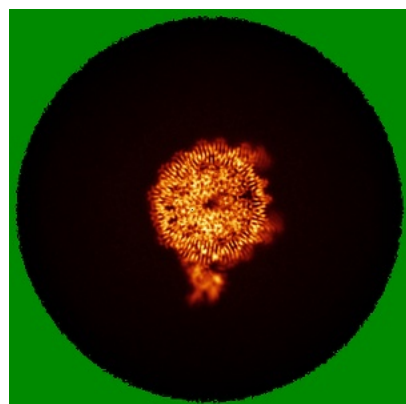


Z Index: 186

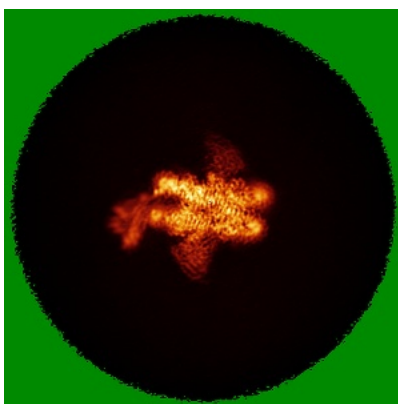
The images above show the largest variance slices of the map in three orthogonal directions.

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

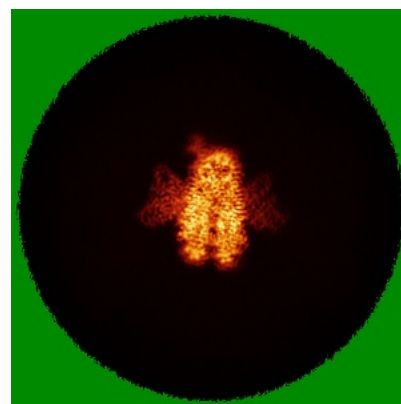
6.4.1 Primary map



X

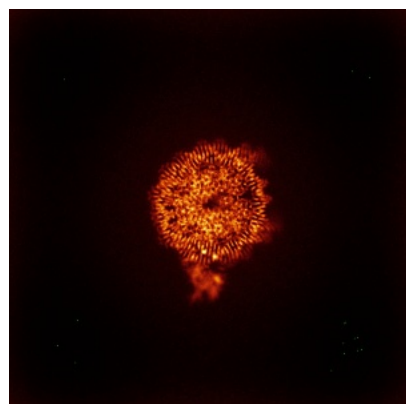


Y

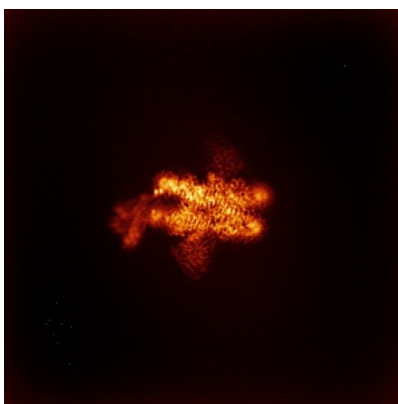


Z

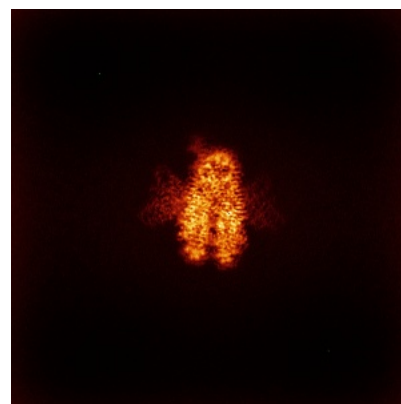
6.4.2 Raw map



X



Y

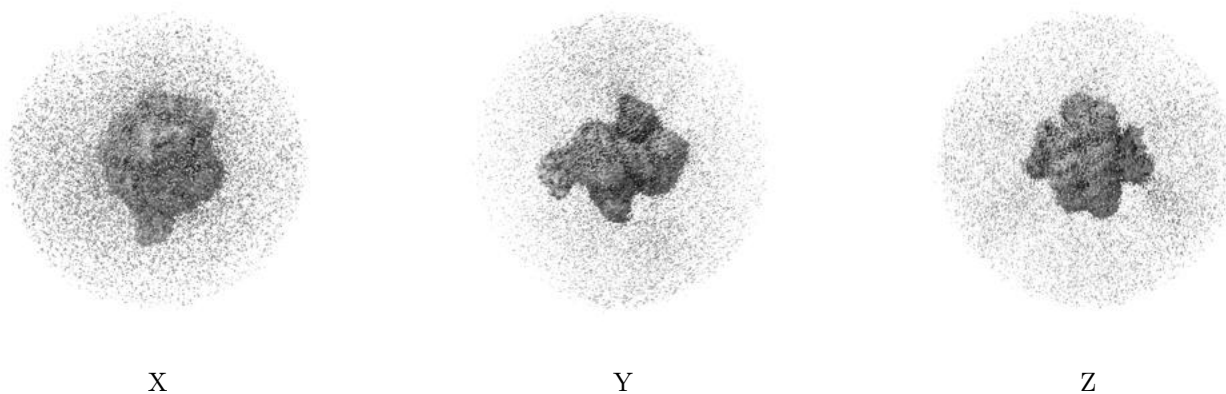


Z

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.

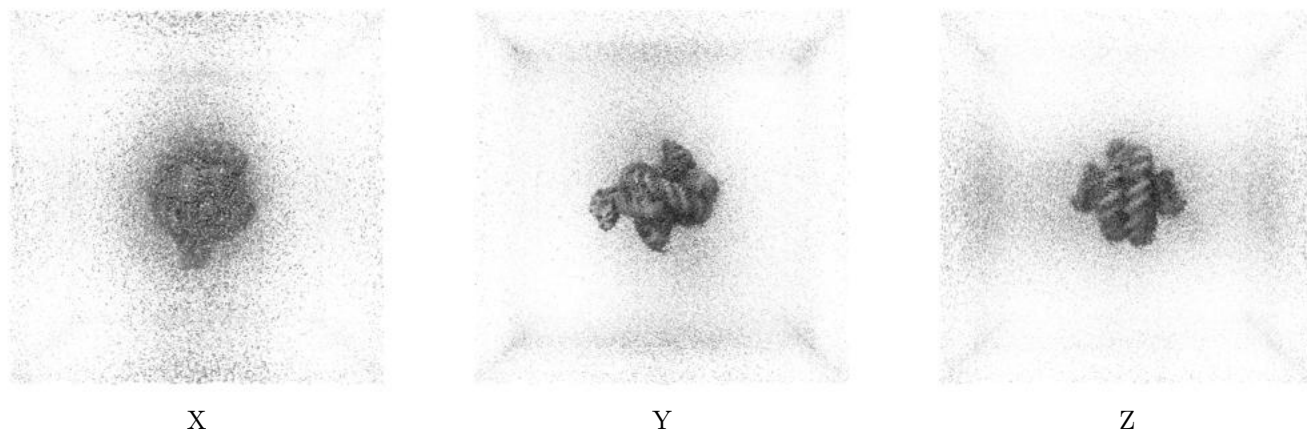
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

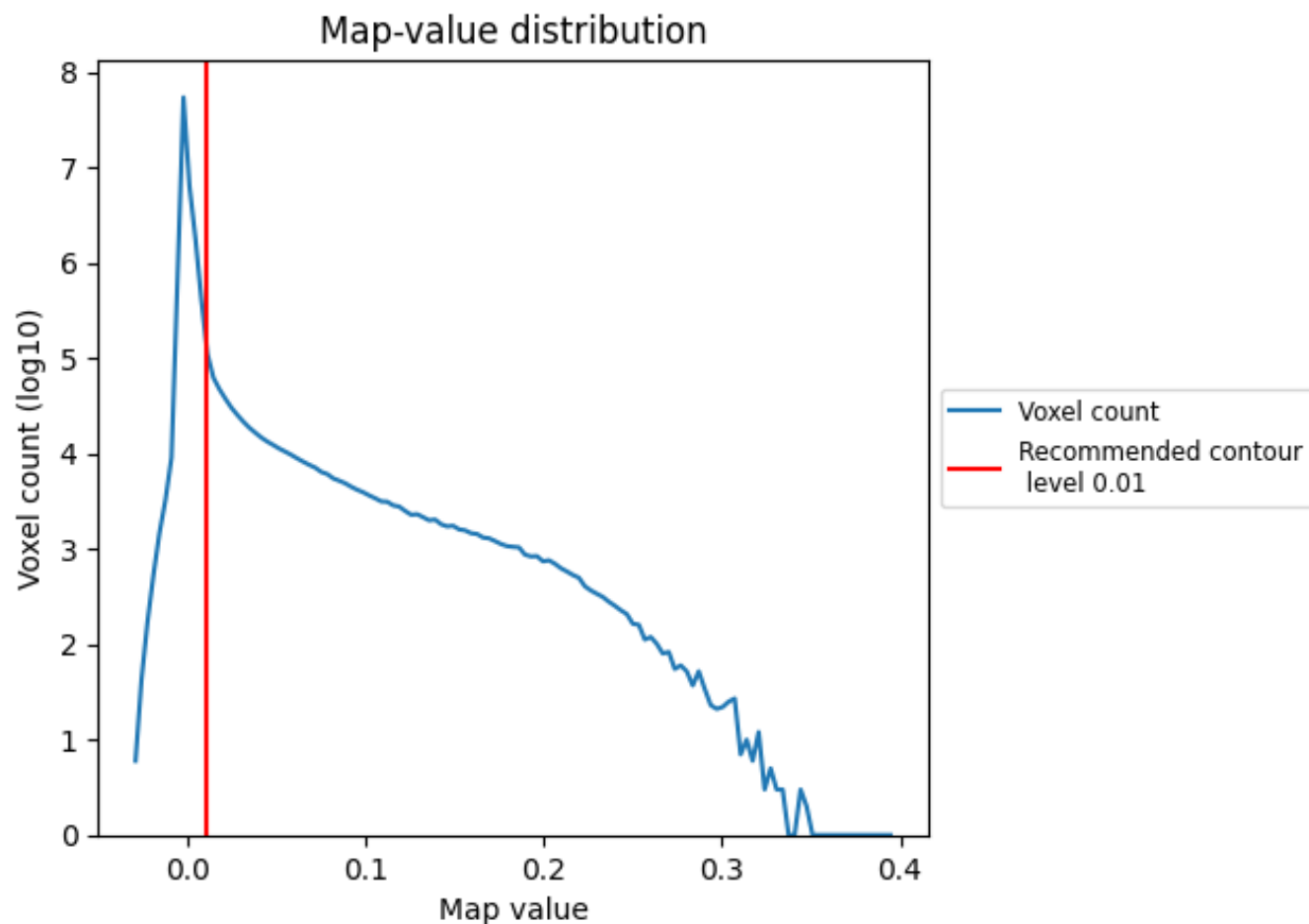
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

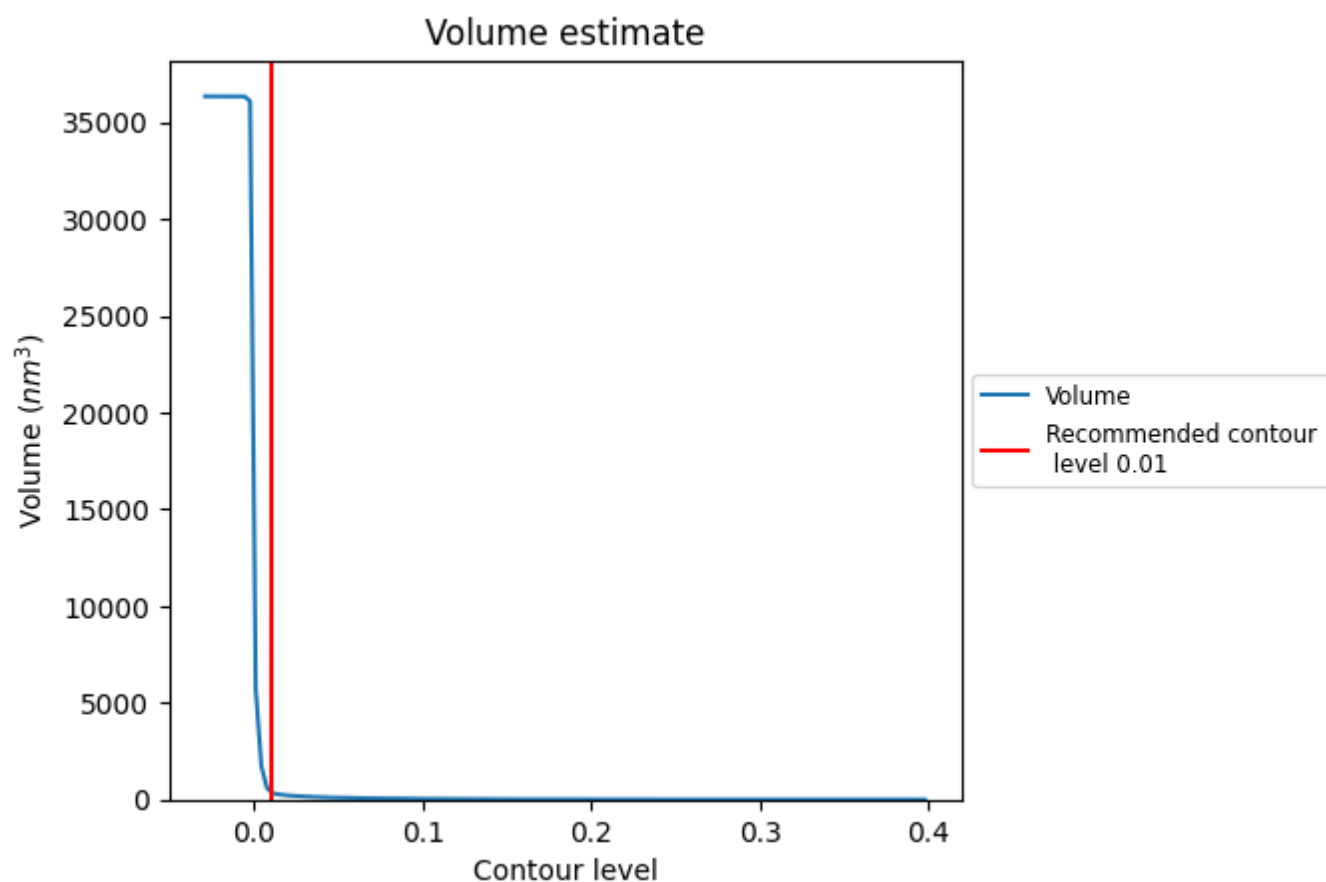
This section contains the results of statistical analysis of the map.

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.

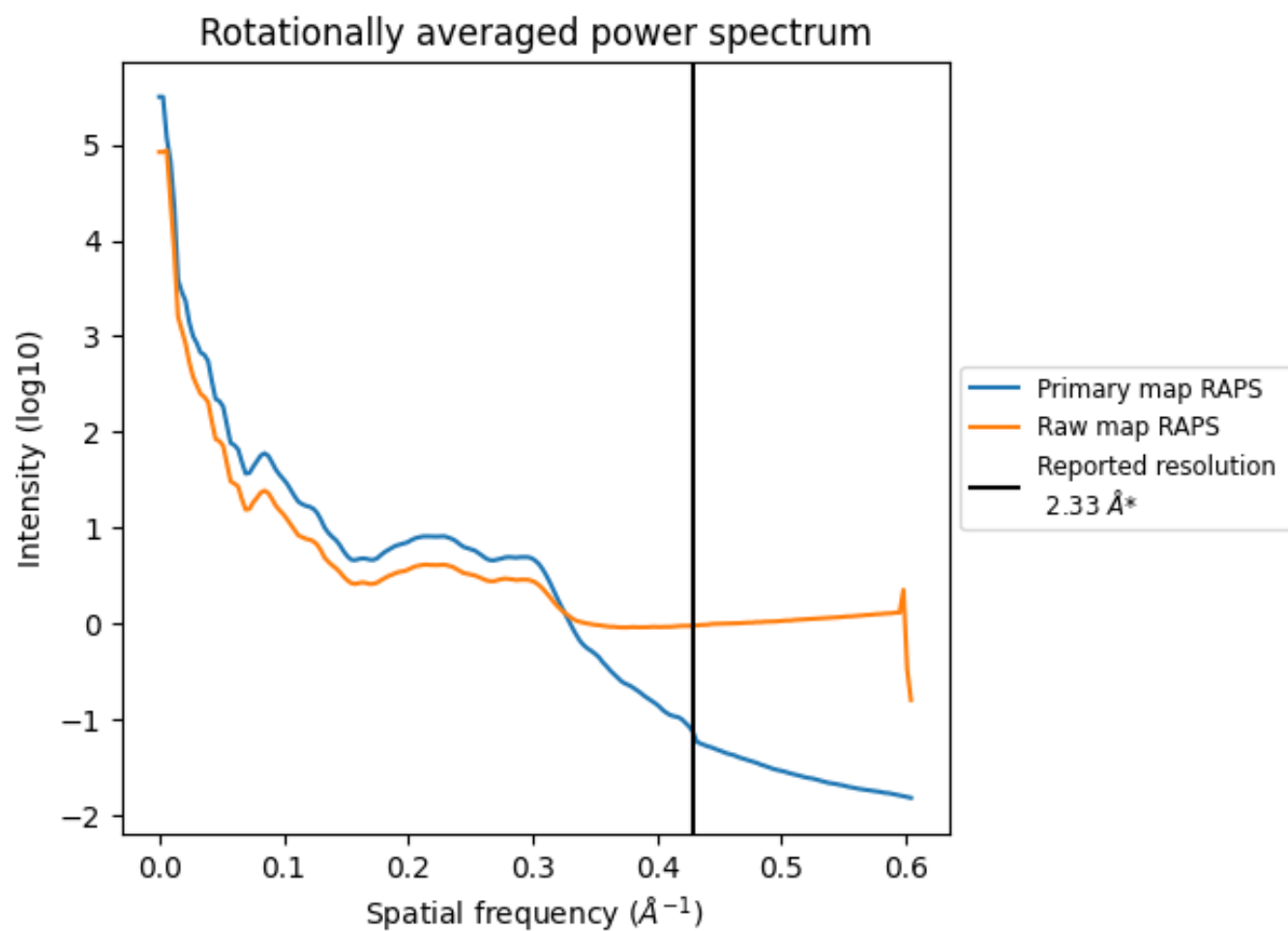
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 398 nm³; this corresponds to an approximate mass of 360 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 ⓘ

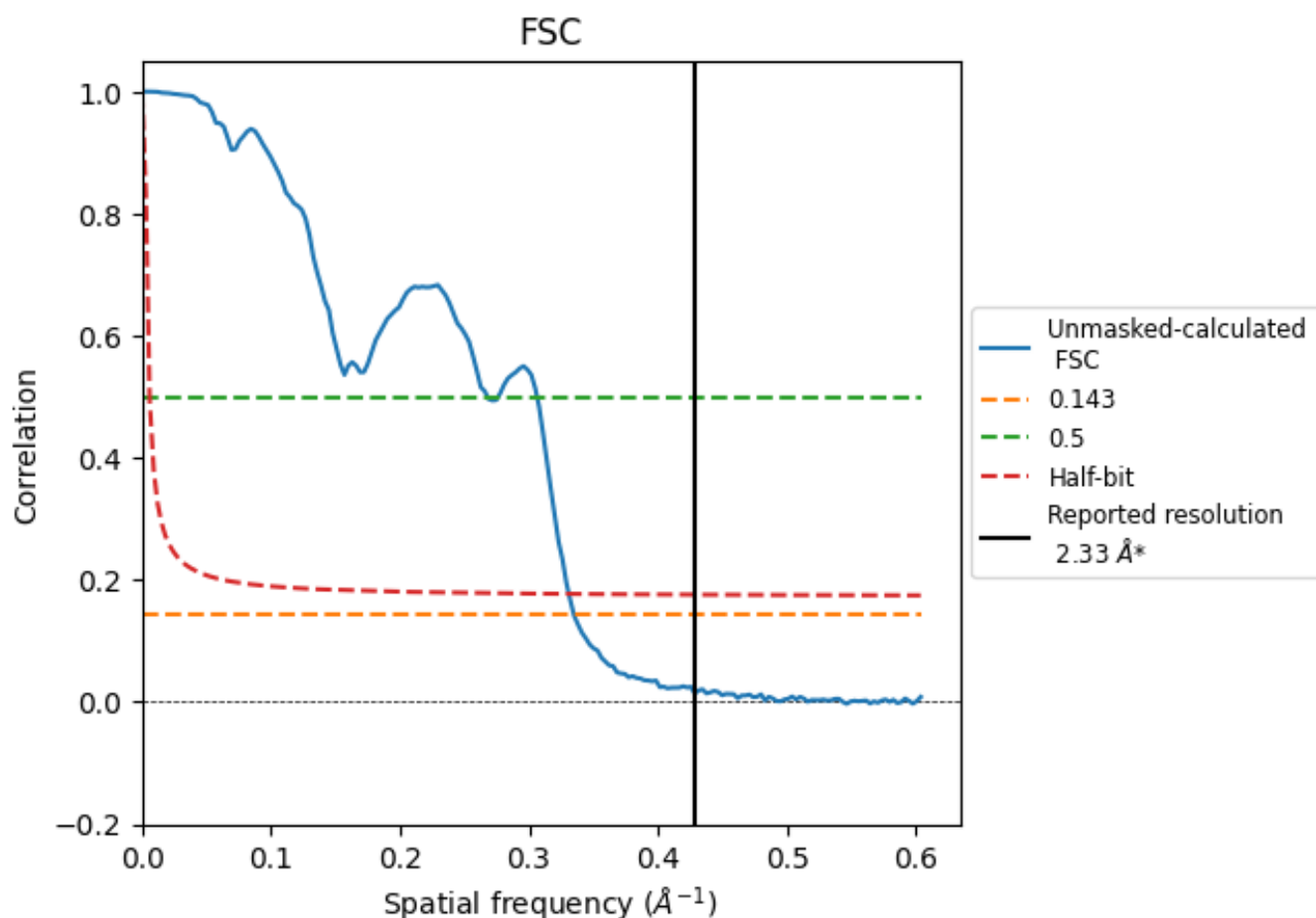


*Reported resolution corresponds to spatial frequency of 0.429 Å⁻¹

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 $0.429 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

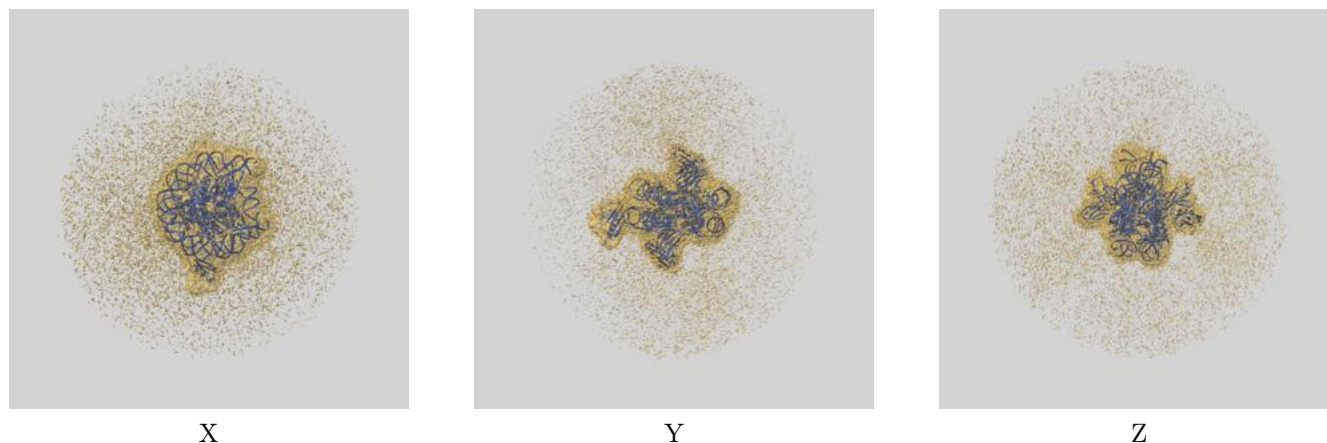
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.99	3.73	3.02

*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 2.99 differs from the reported value 2.33 by more than 10 %

9 Map-model fit [i](#)

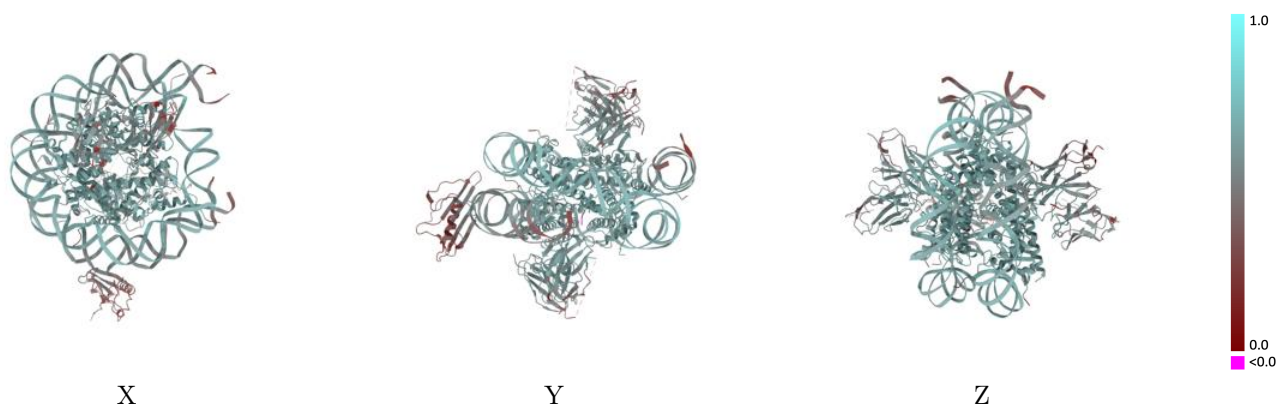
This section contains information regarding the fit between EMDB map EMD-74785 and PDB model 9ZU0. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



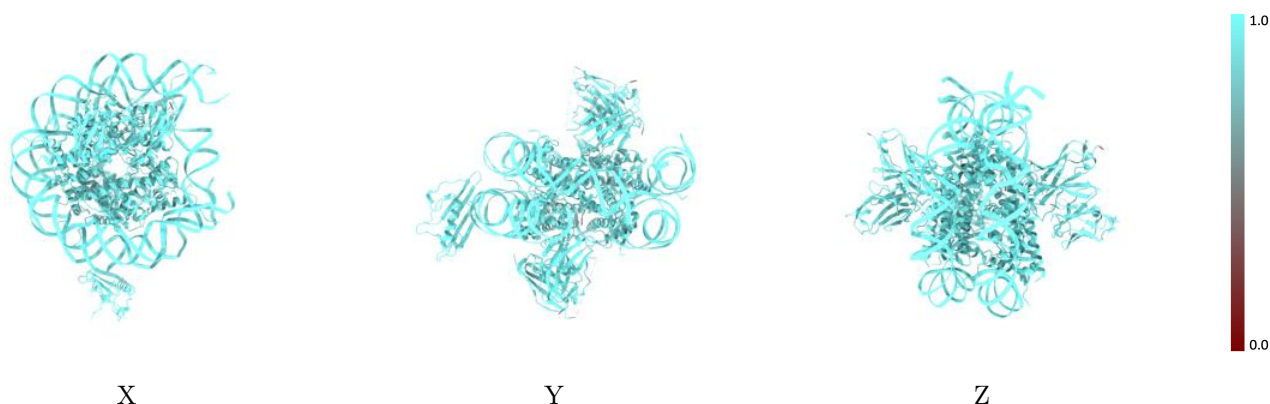
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



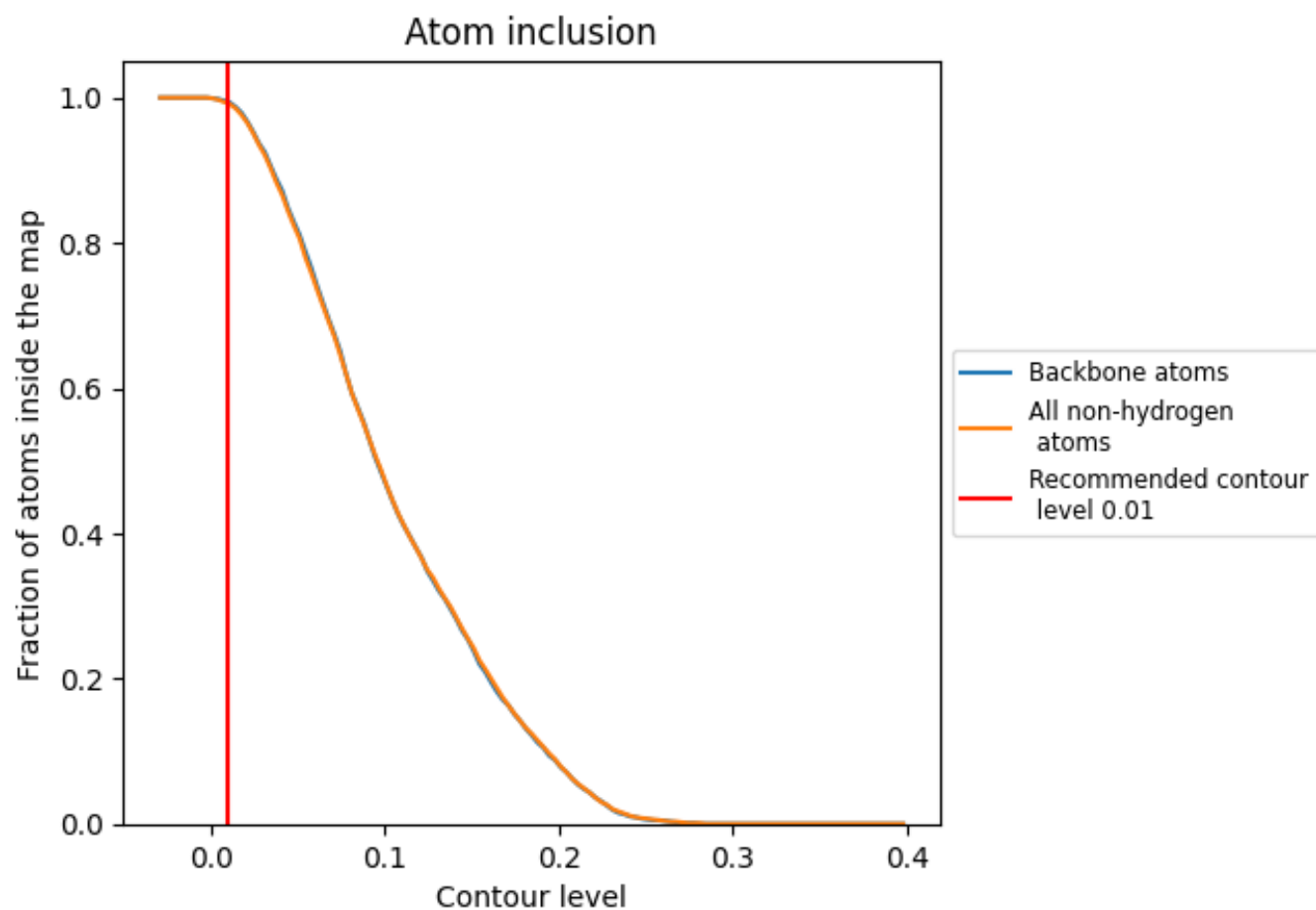
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9920	 0.5800
A	 0.9980	 0.6390
B	 0.9990	 0.6410
C	 0.9970	 0.6240
D	 0.9950	 0.6250
E	 0.9870	 0.6350
F	 0.9860	 0.6400
G	 0.9980	 0.6530
H	 0.9920	 0.6410
I	 0.9650	 0.5080
J	 0.9900	 0.5580
K	 1.0000	 0.6040
L	 1.0000	 0.5060
M	 0.9990	 0.5890
P	 0.9990	 0.3330

