wwPDB EM Validation Summary Report (i)

Sep 25, 2024 – 12:04 pm BST

PDB ID	:	9FPZ
EMDB ID	:	EMD-50641
Title	:	Human NatA-MAP2 80S ribosome complex
Authors	:	Klein, M.A.; Wild, K.; Sinning, I.
Deposited on	:	2024-06-14
Resolution	:	2.69 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 (i) 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 (i)) were used in the production of this report:

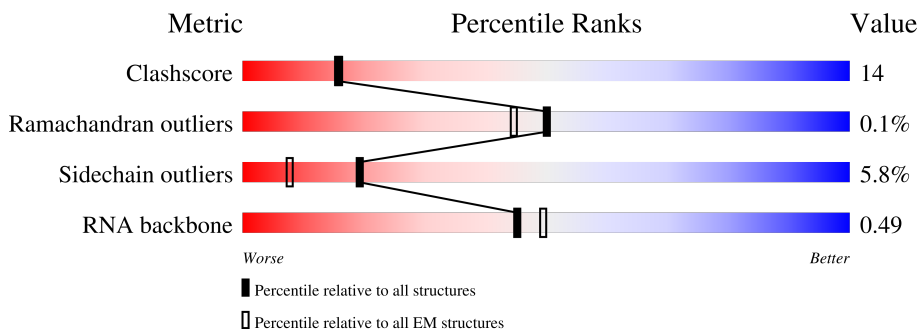|		
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.69 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.
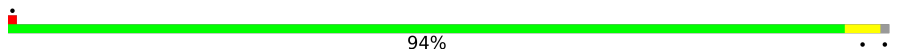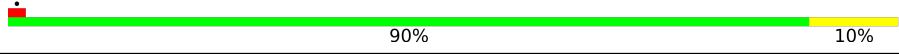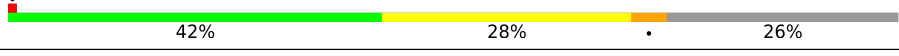
Metric	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		0.1%
Sidechain outliers		5.8%
RNA backbone		0.49

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	2	171	62% 42% 48% 8% ••
2	8	58	• 50% 43% 7%
3	A	484	• 52% 23% • 24%
4	B	840	60% 56% 40% ••
5	1	5070	• • • 94%
6	LC	427	• 72% 13% 15%
7	LE	288	56% 17% • 26%

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Mol	Chain	Length	Quality of chain
8	Lk	70	94%
9	LY	144	53% 35% 10%
10	Lh	122	90% 10%
11	LX	156	42% 28% 26%
12	LR	196	58% 18% 22%
13	Lr	137	88% 9%

2 Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 29394 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 N-alpha-acetyltransferase 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	169	Total 1388	C 869	N 253	O 256	S 10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	0	MET	-	initiating methionine	UNP P41227
2	1	GLY	-	expression tag	UNP P41227

- Molecule 2 is a RNA chain called 5.8S rRNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	8	58	Total 1237	C 554	N 224	O 401	P 58	0	0

- Molecule 3 is a protein called Methionine aminopeptidase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	370	Total 2901	C 1823	N 499	O 556	S 23	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P50579
A	-4	PRO	-	expression tag	UNP P50579
A	-3	GLY	-	expression tag	UNP P50579
A	-2	SER	-	expression tag	UNP P50579
A	-1	GLY	-	expression tag	UNP P50579
A	0	SER	-	expression tag	UNP P50579

- Molecule 4 is a protein called N-alpha-acetyltransferase 15, NatA auxiliary subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	834	Total	C	N	O	S	0	0
			6881	4379	1189	1272	41		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP Q9BXJ9

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1	300	Total	C	N	O	P	0	0
			6425	2859	1169	2097	300		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	365	Total	C	N	O	S	0	0
			2908	1829	580	486	13		

- Molecule 7 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LE	214	Total	C	N	O	S	0	0
			1724	1111	327	282	4		

- Molecule 8 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LY	129	Total	C	N	O	S	0	0
			1075	675	218	179	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LY	?	-	LYS	deletion	UNP P61254

- Molecule 10 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 11 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LX	116	Total	C	N	O	S	0	0
			950	606	178	165	1		

- Molecule 12 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LR	153	Total	C	N	O	S	0	0
			1281	799	276	197	9		

- Molecule 13 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 14 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		AltConf
14	A	2	Total	Co	0
			2	2	

- Molecule 15 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).

IHP

O46 OH
O26 O
P6
O41 O11 HO
HO P1 O O36
O21 O OH
O31
O12 C2
O42 HO P2 OH O32
P2 O
O22
O13 P3
HO
O43

O25 O
O35 HO P5 OH O45
P5
O O15
C6 C5 O34
C1 HO
C4 O24
C3 O P4
O14 OH
O44
O33
OH
O23
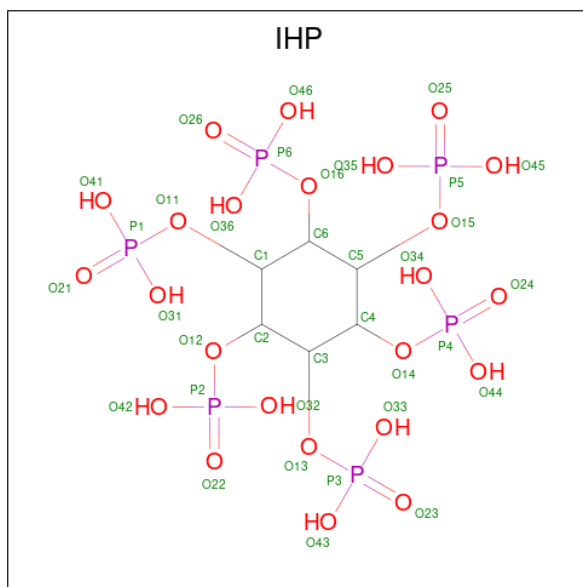
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
15	B	1	36	6	24	6	0

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3 Residue-property plots ⓘ

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: N-alpha-acetyltransferase 10

Chain 2:

- Molecule 2: 5.8S rRNA (58-MER)

Chain 8:

- Molecule 3: Methionine aminopeptidase 2

Chain A:

• Molecule 4: N-alpha-acetyltransferase 15, NatA auxiliary subunit

K646 L647 A648 K649 V650 E651 T652 P653 L654 E655 E656 A657 I658 K659 F660 L661 K665 N666 L667 V668 K669 N670 K671 I672 E673 T674 H675 L676 F677 A678 F679 E680 I681 Y682 F683 R684 K685 E686 K687 F688 L689 L690 M691 L692 Q693 S694 V695 K696 R697 A698 F699 A700 I701 D702 S703 S704 H705 P706 W707

L708 H709 E710 C711 M712 I713 R714 L715 F716 N717 T718 V719 C720 E721 S722 K723 D724 L725 S726 D727 T728 V729 R730 T731 V732 L733 K734 Q735 E736 M737 N738 R739 L740 F741 G742 A743 T744 N745 P746 K747 N748 F749 N750 E751 T752 F753 L754 K755 R756 D759 S760 H763 R764 L765 S766 A767 A768 K769

M770 Y773 L774 D775 P776 S777 S778 Q779 K780 R781 A782 I783 E784 L785 L789 D790 E791 S792 L793 T794 N795 R796 N797 L798 Q799 T800 C801 M802 E803 V804 L805 E806 A807 L808 Y809 D810 G811 S812 L813 G814 D815 C816 K817 E818 A819 A820 Y823 R824 A825 N826 C827 H828 K829 L830 F831 F832 Y833

A834 L835 A836 F837 P840

• Molecule 5: 28S rRNA

Chain 1: · · ·   94%

C G C G A C C U C A G A U C A G A C G U G G C G A C C C G G C U G A A U U D A A G C A U A U U A G U C A G C G G A G G A G

A A G A A A C U A A C C A G G A U U C C C U C A G U A A C G G C G A G U G A A C A G G G A A G A G C C C A G C G C C G A

A U C C C G C C C C C G C G G G G C G G G G C G C G G G A C A U G U G G C G U A C G G A A G A C C C G C U C C C C G G C

C G G U G G G G G C C G G U C U U C C C G G A G U C G G G U U G C U U G G G A A U G C A G C C C A A A G C G G G U G G

U A A A C U C C A U C U A A G G C U A A A U A C C G G C A C G A G A C C G A U A G U C A A C A A G U A C C G U A A G G G

A A A G U U G A A A A A G A A C U U U G A A G A G A G A G U U C A A G A G G G C G U G A A A C C G U U A A G A G G U A A

A C G G G U G G G G U C C G C G C A G U C C G C C C G G A G G A U U C A A C C C G G C G G C

G A U C C C G C C C C C G C G G G G C G G G G C G C G G G A C A U G U G G C G U A C G G A A G A C C C G C U C C C C G G C

U2371 A2376 C2377 G2378 U2385 G2386 G2387 A2388 A2389

U2519 C2520 G2521 G2522 G2523 U2524 U2525 C2526 A2527 G2528 A2529 U2530 C2531 C2532 C2533 A2537 U2538

C2690 U2691 U2692 G2693 G2694 A2695 A2696 G2700

U2701 G2705 G2706 U2707 U2708 C2709 C2710 C2711 G2712 C2713 G2714 G2715 C2716 C2717 U2718

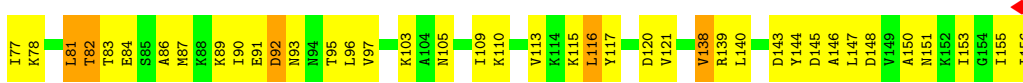A2894 A2895 G2896 G2897 G2898 C2899 U2900 G2901 G2902

U3595 A3596 G3597 G3598 A3599 G3600 C3601

A3604 C3605 U3606 U3607

• Molecule 6: 60S ribosomal protein L4

Chain LC:

72%   13%   15%

MET ALA CYS A4 L7 N21 P25 F28 D35 I36 Y52 E56 L57 H60 E65 S66 P77 R80 F92 M101 N116 Q119 K120 R121 M138 S139 K140 G141 H142 R143 I144 E145 E146 L150 P151 L152 D156 L170 L171 K175

A176 W177 N178 D179 R201 P207 C208 I209 N212 I218 K219 A220 F221 R222 N223 L229 L235 L240 H245 F249 C250 I251 S255 E262 R268 Y277 N278 I289 K294 E297 I298 Q299 R312 D352 A356 L361 Q362 A363 K364 S365

D366 E367 K368 ALA ALA VAL ALA GLY LYS LYS PRO VAL VAL GLY LYS LYS GLY LYS LYS ALA ALA VAL VAL LYS LYS GLN LYS LYS PRO LEU VAL GLY LYS LYS ALA ALA THR LYS LYS PRO ALA PRO GLU LYS LYS PRO ALA GLU LYS LYS PRO THR THR GLU GLU LYS LYS PRO

ALA ALA

- Molecule 7: Large ribosomal subunit protein eL6

Chain LE:

| 56% | 17% | • | 26% |

MET ALA GLY LYS GLU VAL GLU LYS PRO ASP THR LYS GLU LYS LYS PRO GLU ALA LYS LYS VAL ASP ALA GLY LYS LYS VAL LYS LYS GLY ASN LEU ALA LYS LYS PRO LYS LYS GLY LYS P42 H43 C44 N47 L50 M62 M68 Y73 SER ALA ALA LYS SER LYS

VAL GLU LYS LYS LYS LYS GLU LYS VAL L89 K94 P95 V96 D99 K100 N101 G102 G103 V107 R114 Y115 H128 L140 I144 T145 P146 L150 L153 T154 G155 R156 H157 R158 G159 K160 R161 F164 L165 K166 L174 V175 T176 G177 P178 L186 V194 I195

I203 K210 K220 LYS LEU ARG LYS PRO ARG HIS GLN GLU GLY GLU ILE PHE ASP THR GLU LYS GLU K239 Y240 E244 D254 I257 L258 K262 A263 I264 L267 Y270 S273 N279 G280 I281 L286 V287 F288

- Molecule 8: 60S ribosomal protein L38

Chain Lk:

| 94% | • | • |

MET P2 K18 D30 R40 K70

- Molecule 9: Large ribosomal subunit protein uL24

Chain LY:

| 53% | 35% | • | 10% |

M1 S9 D10 R11 S12 K13 R17 P22 S23 H24 I25 R26 I29 M30 S31 S32 P33 L34 E37 L38 R45 S46 M47 P48 I49 R50 K51 D52 D53 E54 K63 Q66 K69 V73 Y74 R75 K76 K77 I80 Y81 I82 E83 R84 V85 Q86 R87 E88 K89

H100 P101 S102 R108 L109 K110 K113 D114 R115 K116 K117 I118 L119 K124 S125 R126 Q127 V128 G129 GLU LYS GLY LYS TYR LYS GLU GLU THR ILE GLU LYS MET GLN GLU
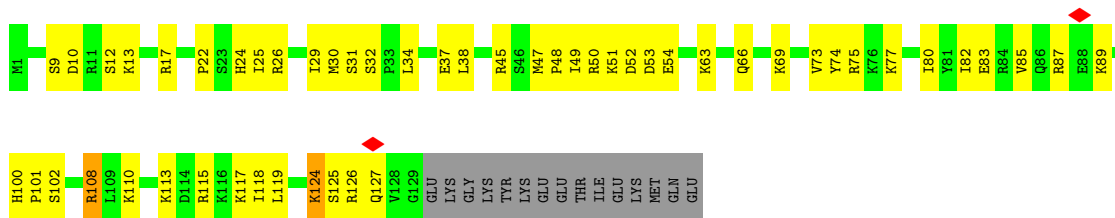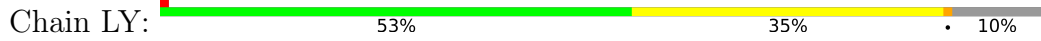
- Molecule 10: 60S ribosomal protein L35

Chain Lh:

| 90% | 10% |

A2 K14 Q20 S42 K43 L44 S45 Q65 N68 N96 E100 Q107 E111 K118 A123
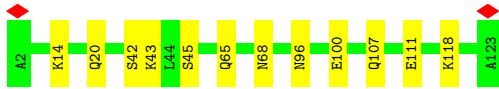
• Molecule 11: 60S ribosomal protein L23a

Chain LX:

42%   28%   •   26%

MET ALA PRO LYS ALA LYS LYS GLU ALA PRO ALA PRO PRO LYS ALA GLU ALA LYS LYS ALA LEU LYS ALA LYS LYS ALA VAL LEU LYS GLY VAL HIS SER HIS LYS LYS LYS LYS ILE R41 K50 T51 L52 R55 R56 Y60 P61 R62 R67 L71 D72 H73 I76

I77 K78 L81 T82 T83 E84 S85 A86 M87 K88 K89 I90 E91 D92 N93 N94 T95 L96 V97 K103 A104 N105 I109 K110 V113 K114 K115 L116 Y117 D120 V121 V138 R139 L140 D143 Y144 D145 A146 L147 D148 V149 A150 N151 K152 I153 G154 I155 I156

• Molecule 12: 60S ribosomal protein L19

Chain LR:

58%   18%   •   22%

MET S2 M3 R16 W23 P26 N27 E28 E31 I32 A33 N34 R38 R42 I45 K46 D47 I51 S59 C63 T67 R71 R74 I78 G79 M89 M96 R97 R98 M99 R100 I101 L102 R103 R104 R108 M119 N130 M139 E140

H141 I142 H143 K144 L145 K146 K149 K153 L154 LEU ALA ASP GLN ALA GLU ALA ARG ARG SER LYS THR LYS GLU ALA ARG LYS ARG ARG GLU GLU ARG LEU GLN ALA LYS LYS GLU GLU ILE ILE LYS THR LEU SER LYS GLU GLU GLU THR LYS LYS
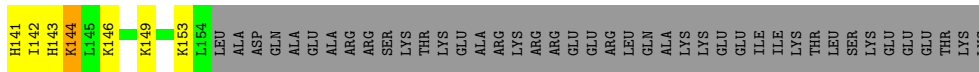
• Molecule 13: 60S ribosomal protein L28

Chain Lr:

88%   •   9%

MET S2 T24 K72 K101 R119 M125 V126 LYS ARG LYS ARG THR ARG PRO THR LYS SER SER
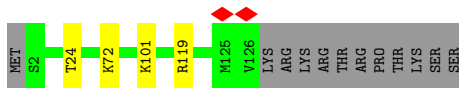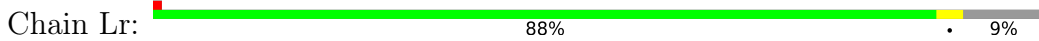
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	41.28	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.457	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	604.8, 604.8, 604.8	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CO, IHP

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	2	0.27	0/1418	0.64	1/1909 (0.1%)
2	8	0.23	0/1384	0.75	0/2154
3	A	0.27	0/2964	0.56	1/4014 (0.0%)
4	B	0.27	0/7019	0.55	4/9441 (0.0%)
5	1	0.22	0/7175	0.82	8/11173 (0.1%)
6	LC	0.25	0/2962	0.56	0/3977
7	LE	0.26	0/1758	0.59	0/2359
8	Lk	0.29	0/575	0.65	0/761
9	LY	0.29	0/1092	0.65	0/1454
10	Lh	0.28	0/1023	0.61	0/1351
11	LX	0.28	0/967	0.64	1/1301 (0.1%)
12	LR	0.26	0/1297	0.61	0/1716
13	Lr	0.25	0/1017	0.62	0/1364
All	All	0.26	0/30651	0.66	15/42974 (0.0%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	1	485	C	C2-N1-C1'	8.96	128.66	118.80
5	1	3598	C	C5-C6-N1	8.96	125.48	121.00
4	B	661	LEU	CA-CB-CG	8.01	133.72	115.30
5	1	3598	C	C6-N1-C2	-7.04	117.48	120.30
3	A	430	MET	CB-CG-SD	-6.97	91.49	112.40

There are no chirality outliers.

There are no planarity outliers.

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5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1388	0	1356	90	0
2	8	1237	0	625	18	0
3	A	2901	0	2848	75	0
4	B	6881	0	6924	303	0
5	1	6425	0	3260	122	0
6	LC	2908	0	3082	33	0
7	LE	1724	0	1874	30	0
8	Lk	569	0	637	0	0
9	LY	1075	0	1157	45	0
10	Lh	1015	0	1148	0	0
11	LX	950	0	1016	45	0
12	LR	1281	0	1418	30	0
13	Lr	1002	0	1068	0	0
14	A	2	0	0	0	0
15	B	36	0	6	1	0
All	All	29394	0	26419	733	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 14.

The worst 5 of 733 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)
4:B:93:ASP:HB2	4:B:95:LYS:HE2	1.52	0.89
4:B:166:MET:HB2	4:B:169:LYS:HE3	1.51	0.89
5:1:3597:G:HO2'	5:1:3598:C:H6	0.96	0.88
5:1:196:C:O2'	9:LY:126:ARG:NH2	2.07	0.86
4:B:496:LYS:HD2	4:B:560:ILE:HG23	1.58	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	167/171 (98%)	161 (96%)	5 (3%)	1 (1%)	22	45
3	A	368/484 (76%)	356 (97%)	12 (3%)	0	100	100
4	B	832/840 (99%)	808 (97%)	23 (3%)	1 (0%)	48	73
6	LC	363/427 (85%)	345 (95%)	18 (5%)	0	100	100
7	LE	208/288 (72%)	195 (94%)	13 (6%)	0	100	100
8	Lk	67/70 (96%)	67 (100%)	0	0	100	100
9	LY	127/144 (88%)	124 (98%)	3 (2%)	0	100	100
10	Lh	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
11	LX	114/156 (73%)	113 (99%)	1 (1%)	0	100	100
12	LR	151/196 (77%)	151 (100%)	0	0	100	100
13	Lr	123/137 (90%)	115 (94%)	8 (6%)	0	100	100
All	All	2640/3035 (87%)	2554 (97%)	84 (3%)	2 (0%)	50	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	292	VAL
1	2	8	PRO

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	2	148/149 (99%)	127 (86%)	21 (14%)	2	7
3	A	318/402 (79%)	306 (96%)	12 (4%)	28	56
4	B	744/749 (99%)	700 (94%)	44 (6%)	16	38
6	LC	304/348 (87%)	298 (98%)	6 (2%)	50	78
7	LE	190/252 (75%)	179 (94%)	11 (6%)	17	39
8	Lk	64/65 (98%)	61 (95%)	3 (5%)	22	49
9	LY	120/134 (90%)	116 (97%)	4 (3%)	33	62
10	Lh	109/109 (100%)	97 (89%)	12 (11%)	5	12
11	LX	104/133 (78%)	96 (92%)	8 (8%)	10	26
12	LR	137/175 (78%)	125 (91%)	12 (9%)	8	20
13	Lr	109/121 (90%)	105 (96%)	4 (4%)	29	58
All	All	2347/2637 (89%)	2210 (94%)	137 (6%)	19	39

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	LX	67	ARG
11	LX	116	LEU
12	LR	139	MET
4	B	262	LYS
4	B	232	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	624	GLN
6	LC	299	GLN
12	LR	34	ASN
11	LX	93	ASN
4	B	620	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	8	57/58 (98%)	12 (21%)	0
5	1	291/5070 (5%)	76 (26%)	1 (0%)
All	All	348/5128 (6%)	88 (25%)	1 (0%)

5 of 88 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	8	52	A
2	8	59	A
2	8	62	A
2	8	63	U
2	8	80	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	1	685	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
15	IHP	B	901	-	36,36,36	0.76	0	54,60,60	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	IHP	B	901	-	-	11/30/54/54	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	901	IHP	C4-C5-O15-P5
15	B	901	IHP	C6-C5-O15-P5
15	B	901	IHP	C5-O15-P5-O35
15	B	901	IHP	C4-C3-O13-P3
15	B	901	IHP	C3-O13-P3-O23

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	901	IHP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IHP B 901

Bond lengths

Bond angles

Torsions

Rings
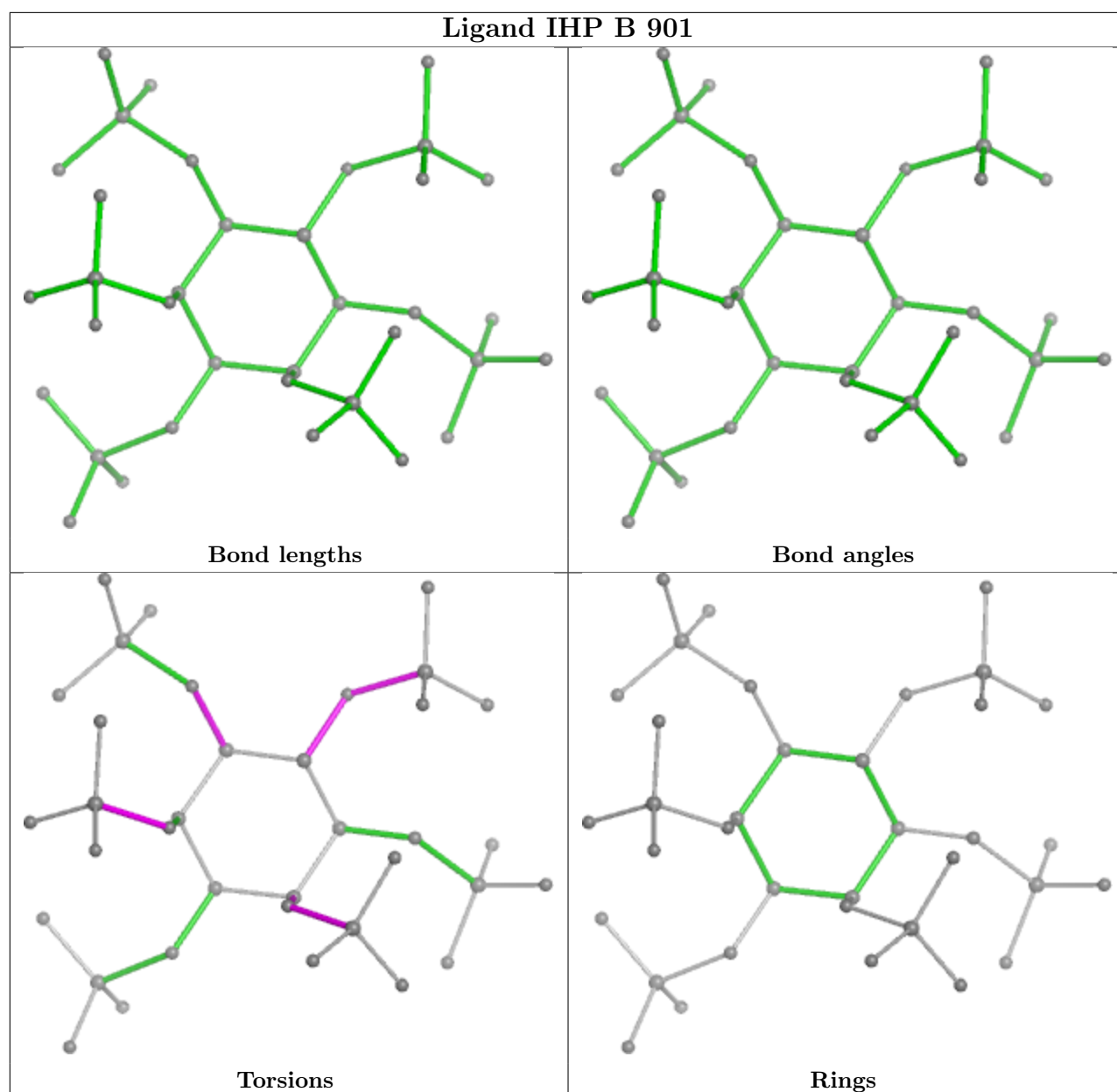
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-50641. 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 ⓘ
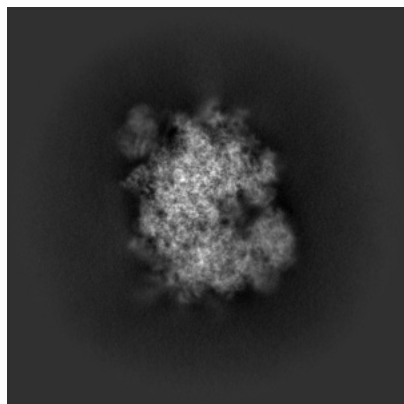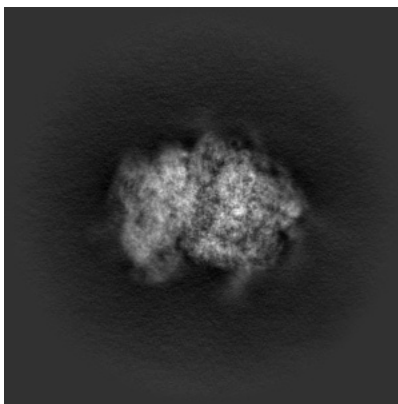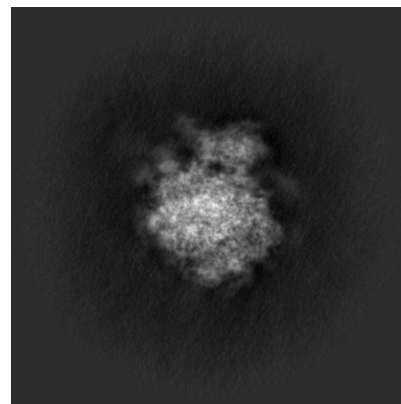
6.1.1 Primary map

X	Y	Z

6.1.2 Raw map

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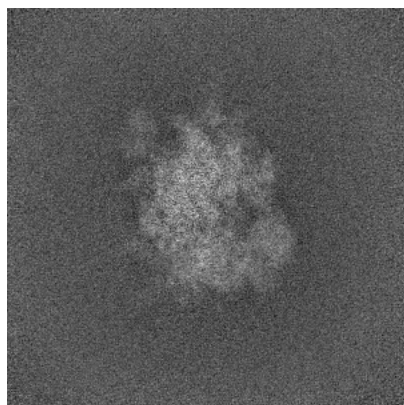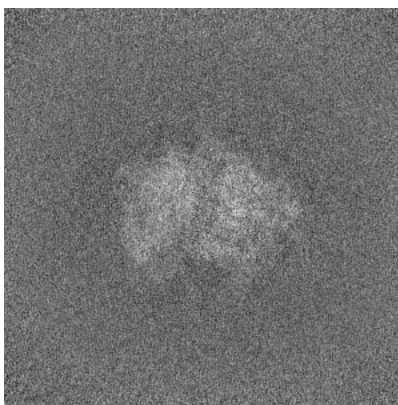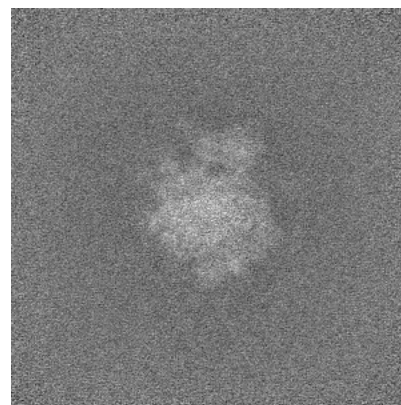
The images above show the map projected in three orthogonal directions.

6.2　Central slices ⓘ
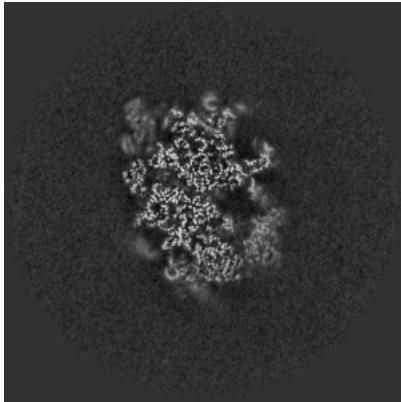
6.2.1　Primary map
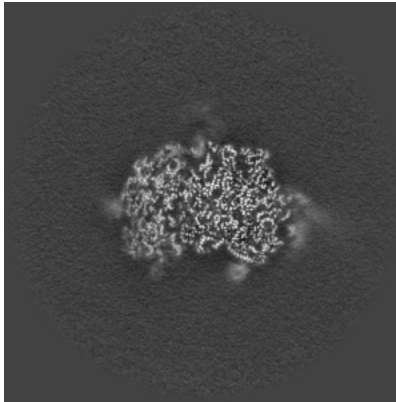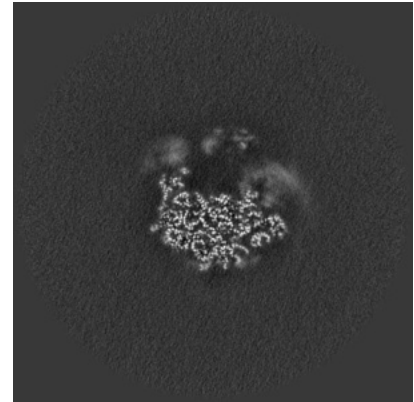
| X Index: 360 | Y Index: 360 | Z Index: 360 |

6.2.2　Raw map
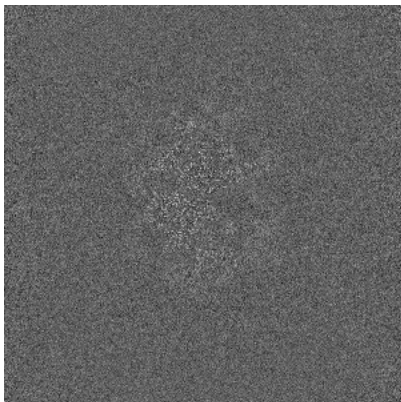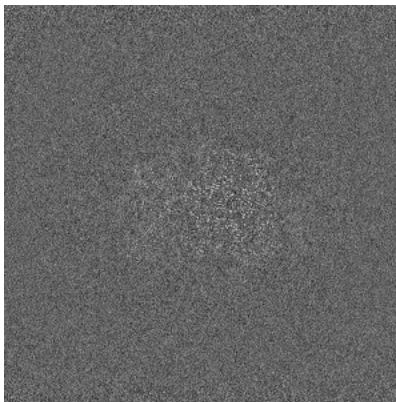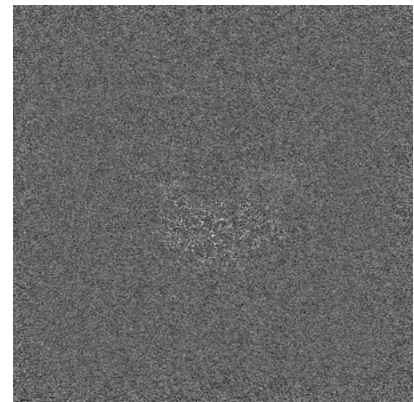
| X Index: 360 | Y Index: 360 | Z Index: 360 |

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

6.3   Largest variance slices ⓘ
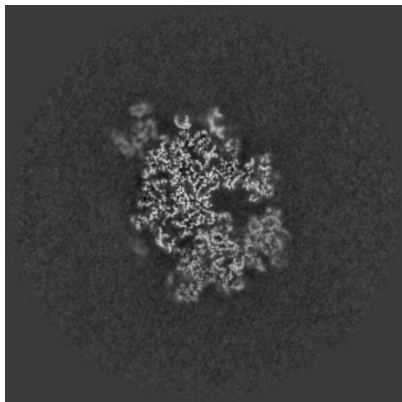
6.3.1   Primary map
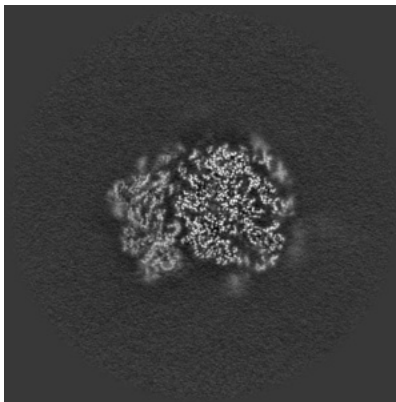
| X Index: 383 | Y Index: 343 | Z Index: 409 |
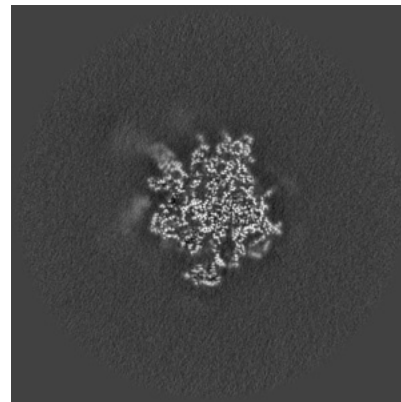
6.3.2   Raw map
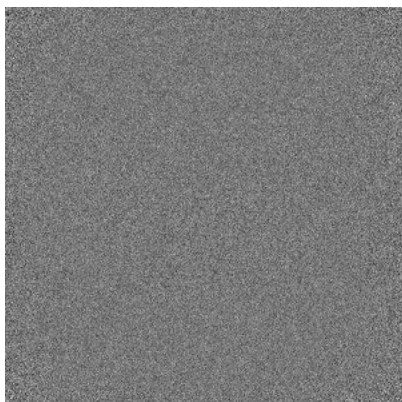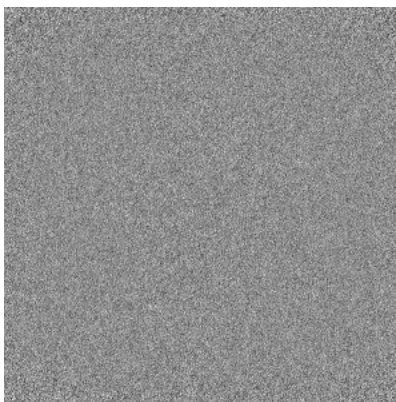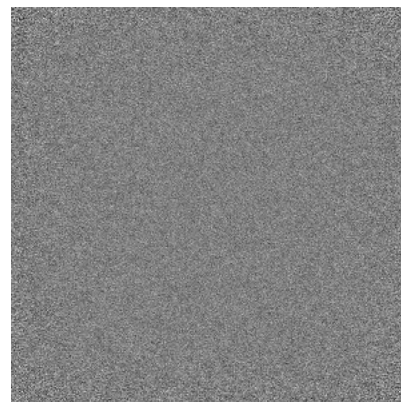
| X Index: 0 | Y Index: 0 | Z Index: 0 |

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

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map

<center>X   Y   Z</center>

6.4.2 Raw map

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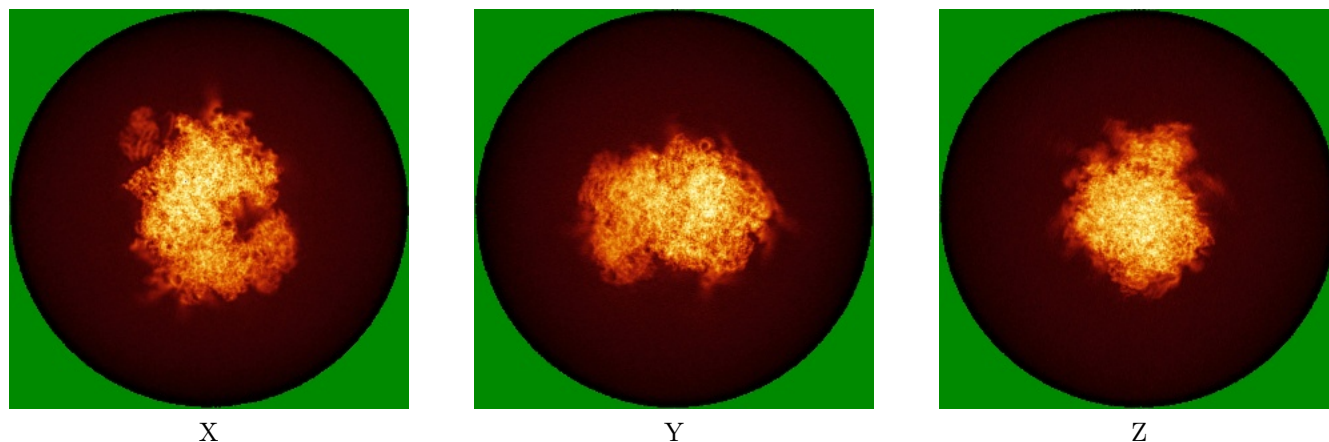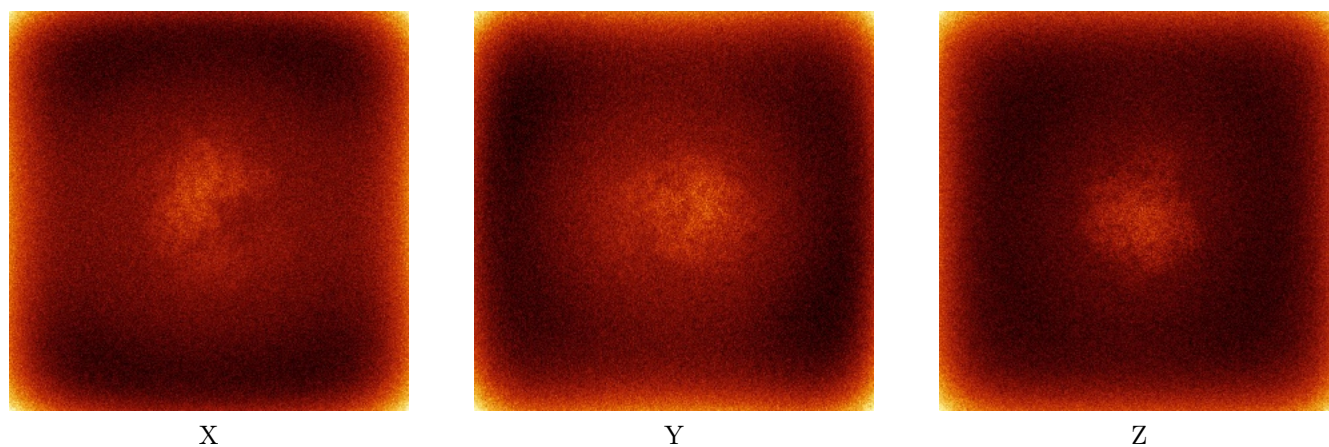
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
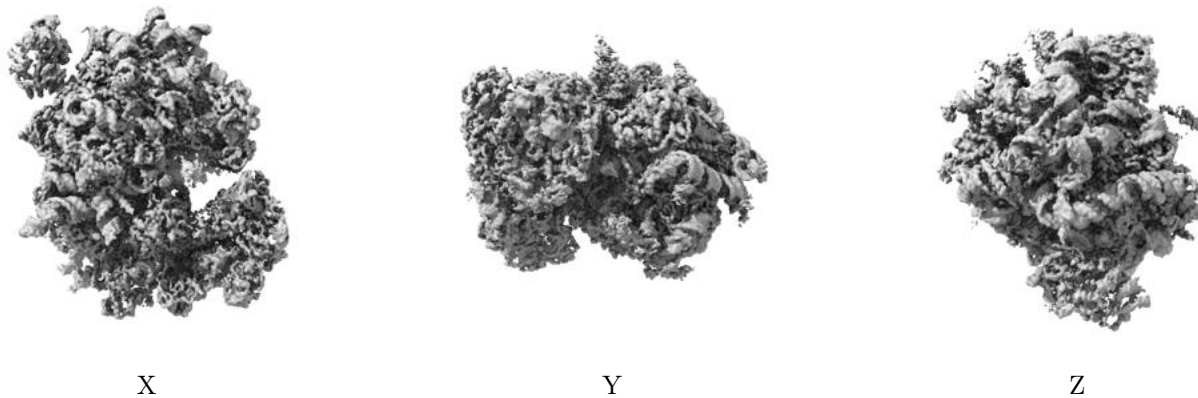
The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

| X | Y | Z |
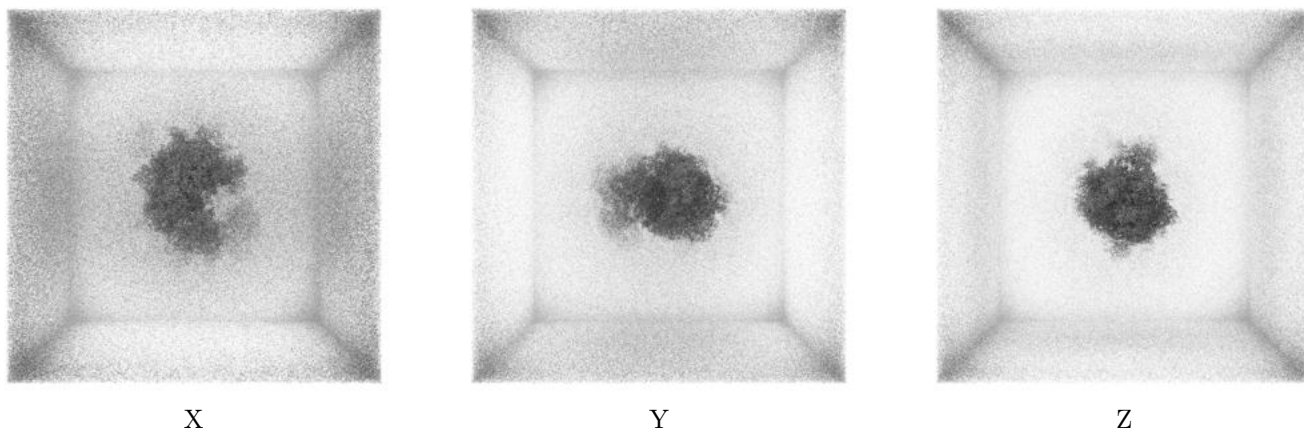
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation ⓘ

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

7　Map analysis ⓘ

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

7.1　Map-value distribution ⓘ
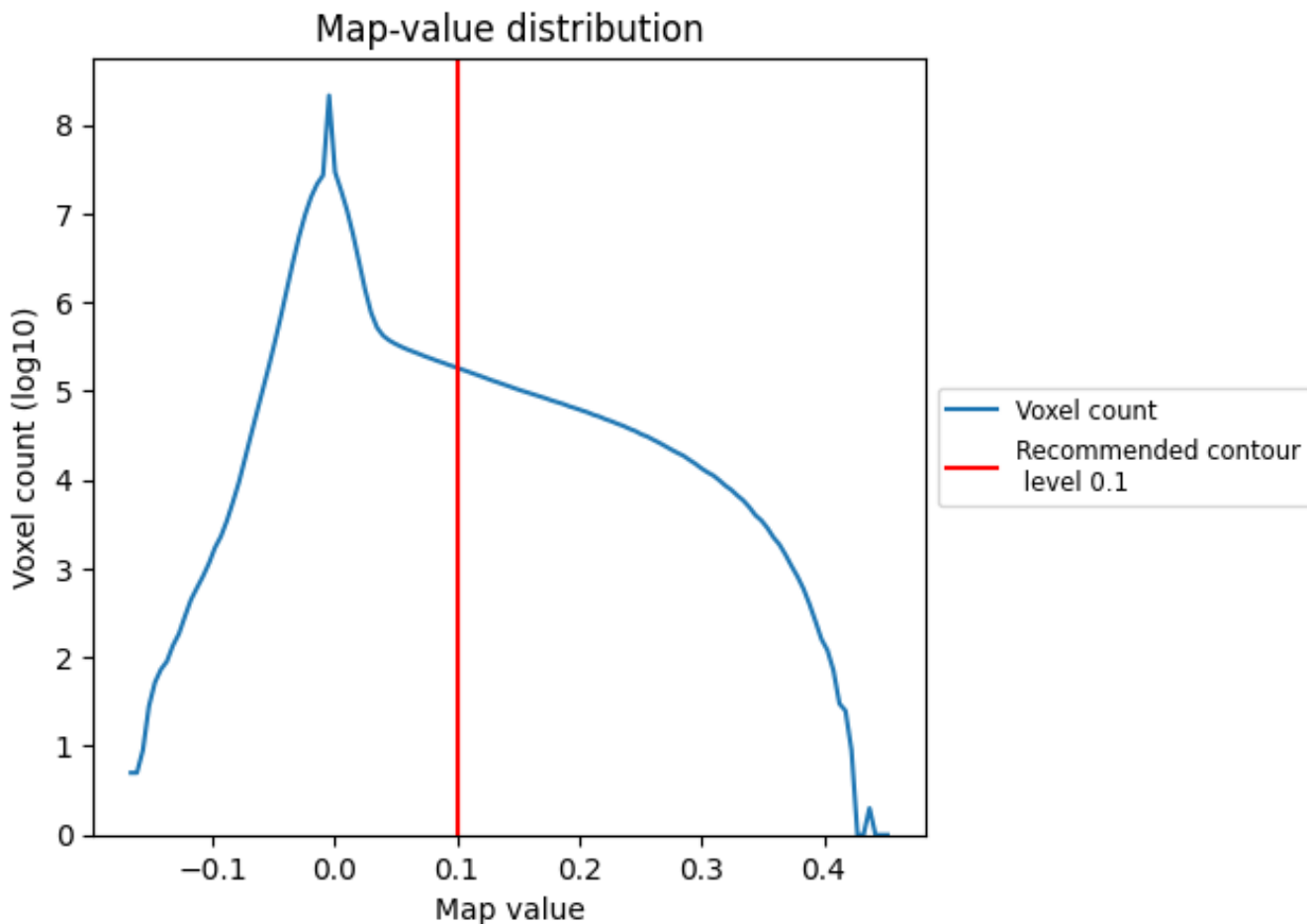
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate (i)
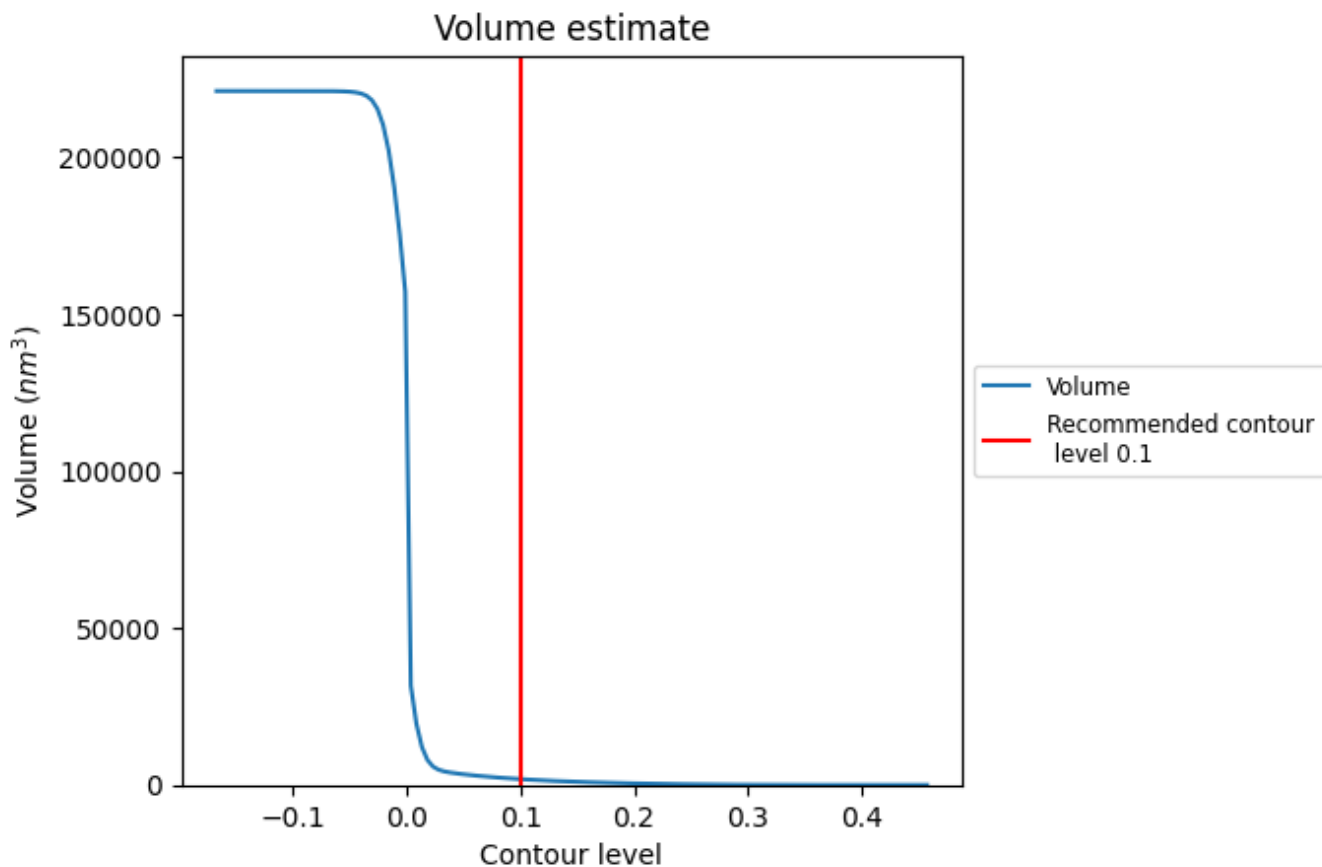
The volume at the recommended contour level is 1862 nm³; this corresponds to an approximate mass of 1682 kDa.

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 ⓘ
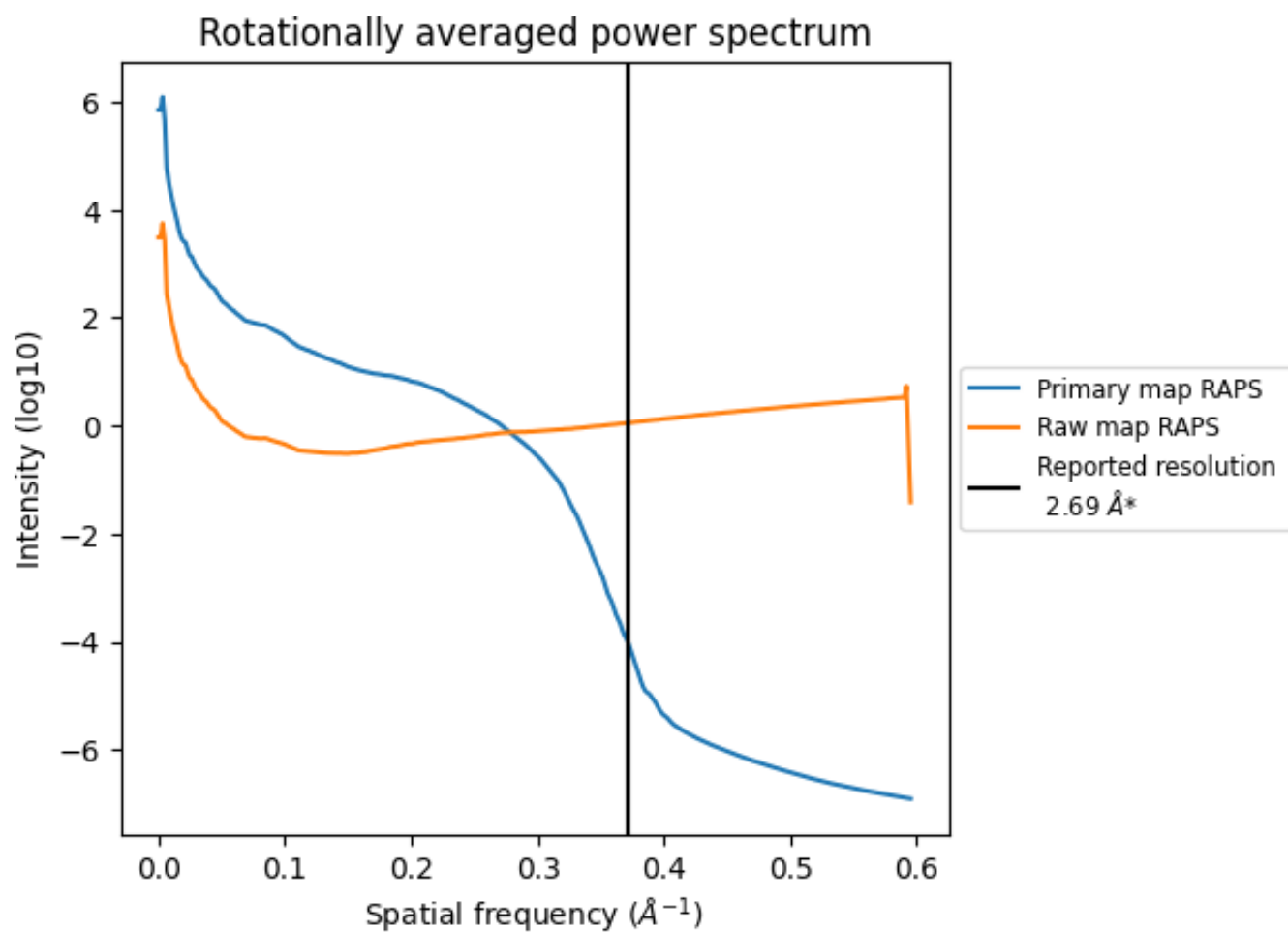
*Reported resolution corresponds to spatial frequency of 0.372 Å^{-1}

8   Fourier-Shell correlation ⓘ

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 ⓘ
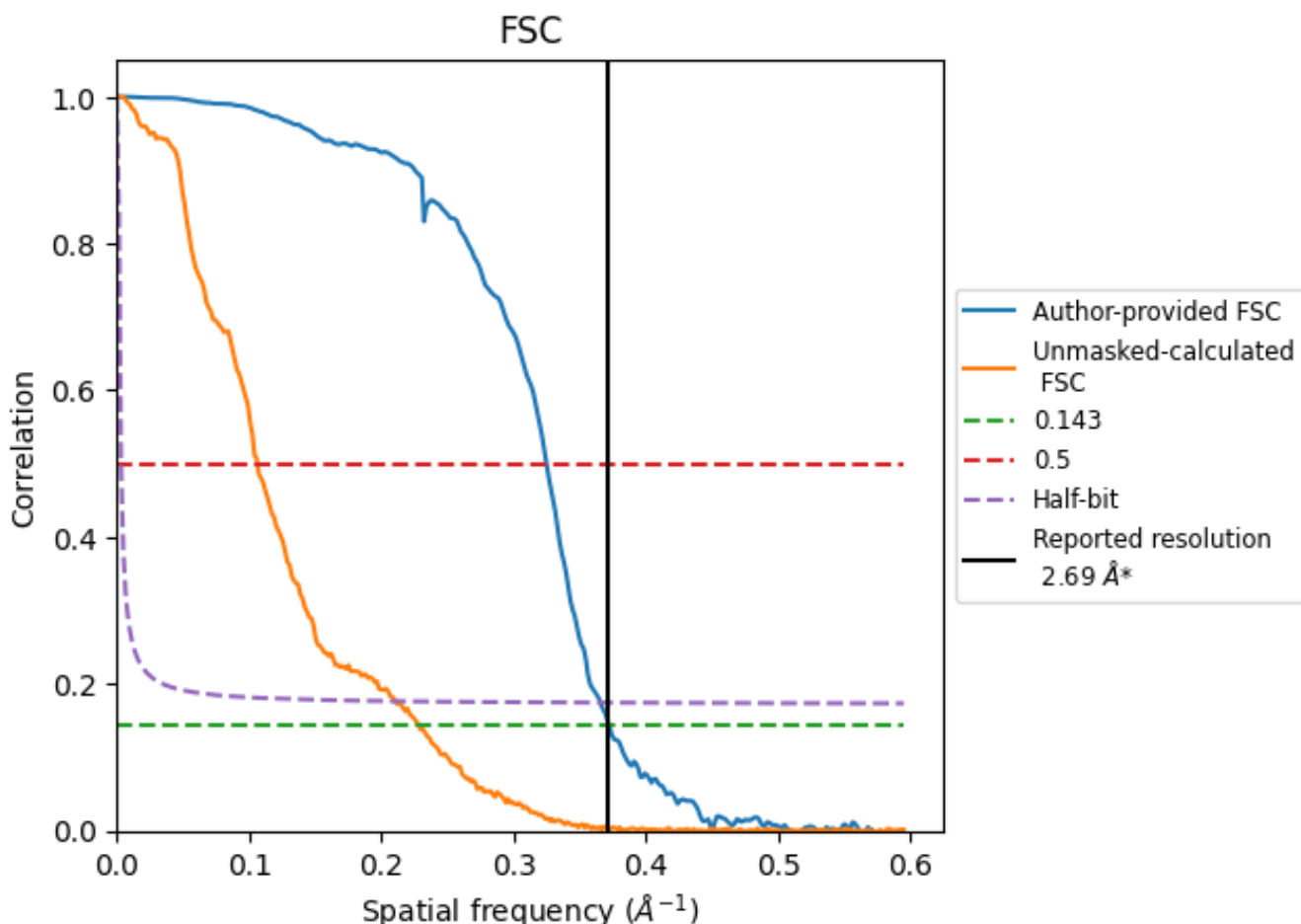
*Reported resolution corresponds to spatial frequency of 0.372 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.69	3.08	2.73
Unmasked-calculated*	4.38	9.40	4.75

*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 4.38 differs from the reported value 2.69 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-50641 and PDB model 9FPZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay ⓘ

| X | Y | Z |
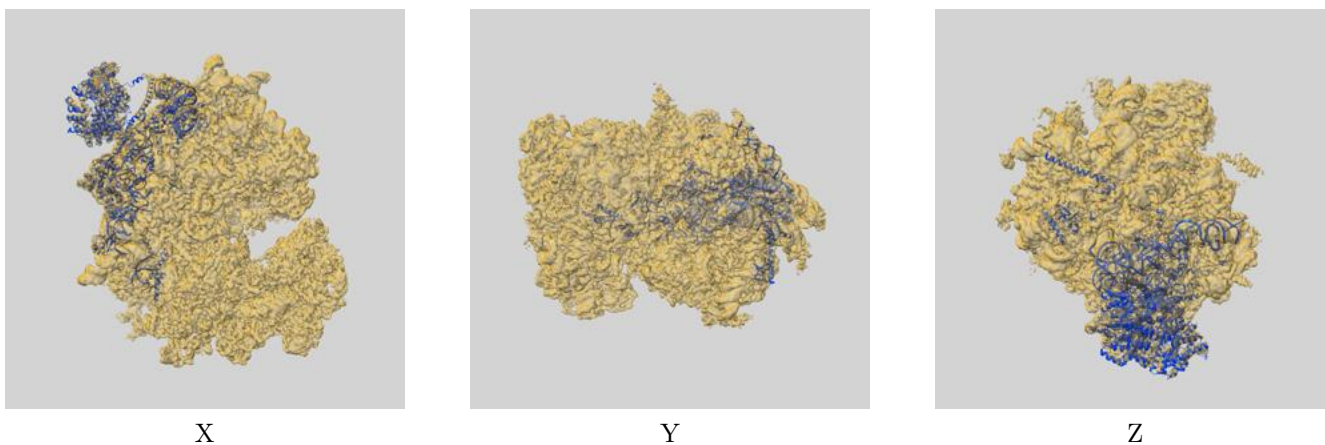
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ

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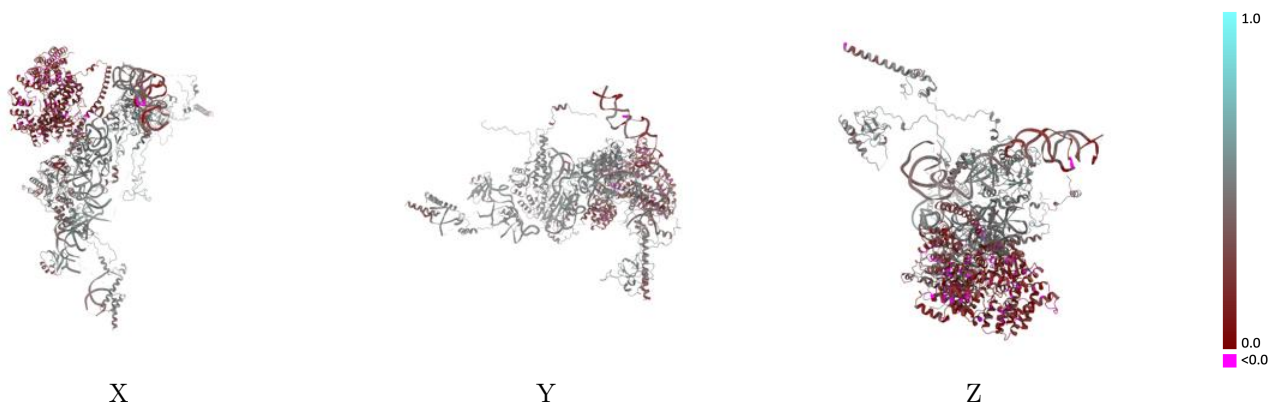
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
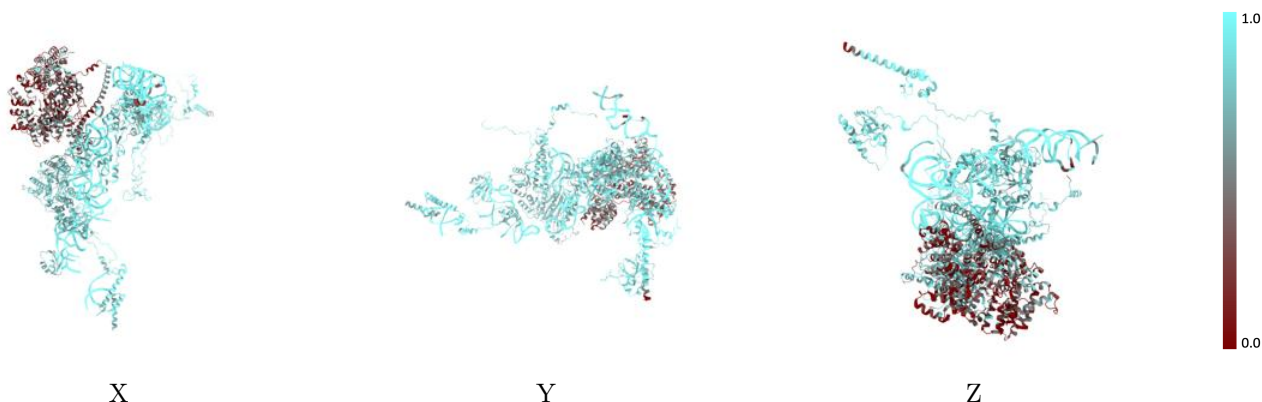
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4   Atom inclusion (i)
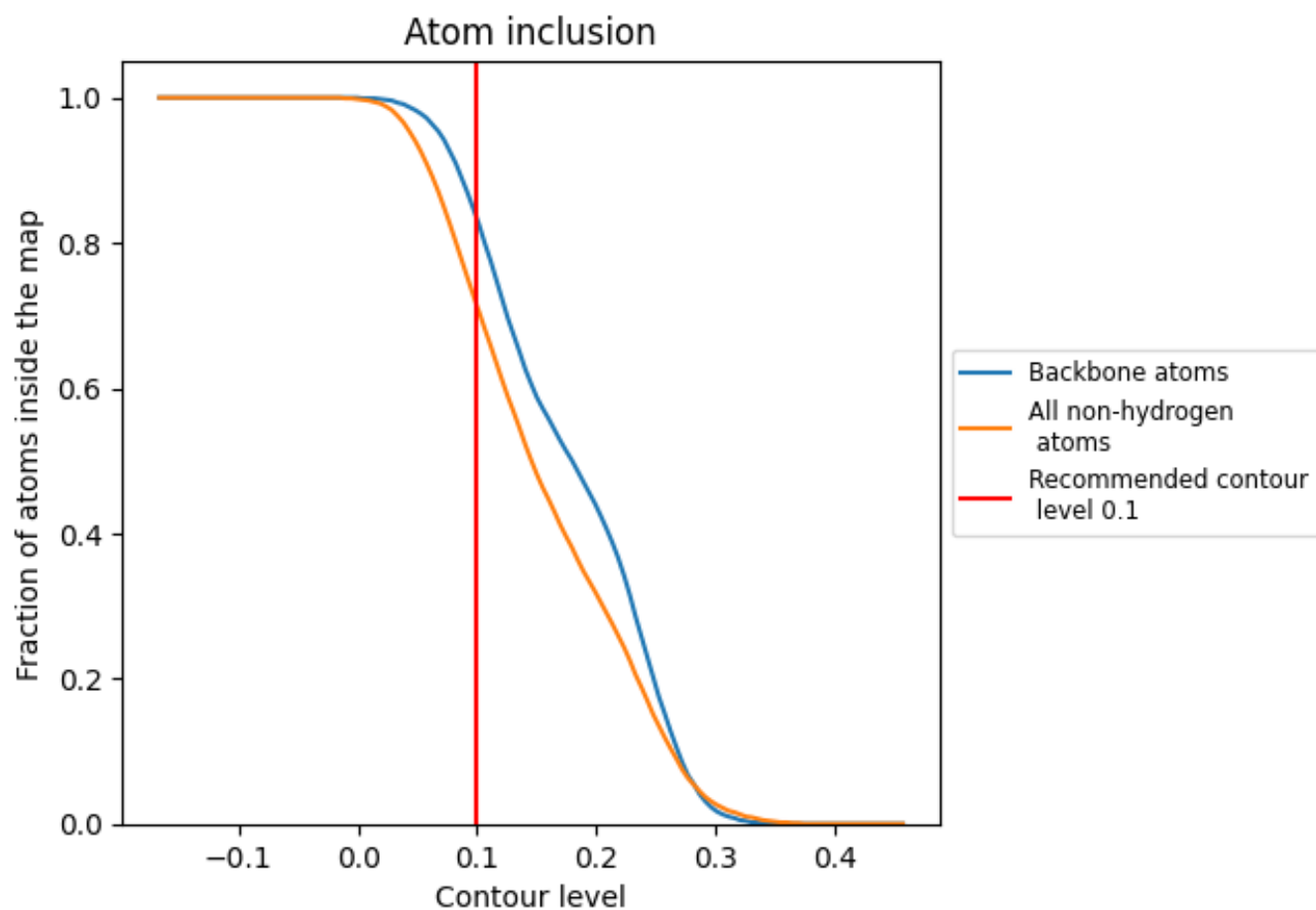
At the recommended contour level, 83% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7120	0.3740
1	0.9420	0.4200
2	0.3260	0.1820
8	0.9600	0.4630
A	0.7950	0.4330
B	0.3280	0.1690
LC	0.8240	0.4960
LE	0.8550	0.4700
LR	0.8320	0.4790
LX	0.8030	0.4750
LY	0.8110	0.4800
Lh	0.7950	0.4510
Lk	0.7470	0.4380
Lr	0.8410	0.4970

1.0

0.0
<0.0